



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:25 PM GMT

PDB ID : 4RKU
Title : Crystal structure of plant Photosystem I at 3 Angstrom resolution
Authors : Mazor, Y.; Borovikova, A.; Greenberg, I.; Nelson, N.
Deposited on : 2014-10-14
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

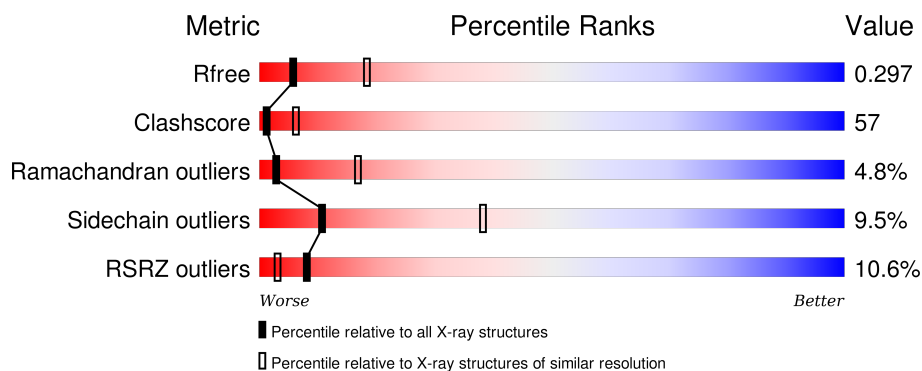
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	721	<div> <div>6%</div> <div>64%</div> <div>34%</div> <div>•</div> </div>
2	B	731	<div> <div>5%</div> <div>71%</div> <div>29%</div> <div>•</div> </div>
3	C	80	<div> <div>3%</div> <div>60%</div> <div>34%</div> <div>6%</div> </div>
4	D	137	<div> <div>14%</div> <div>43%</div> <div>44%</div> <div>11%</div> <div>•</div> </div>
5	E	63	<div> <div>19%</div> <div>44%</div> <div>41%</div> <div>13%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	152	
7	G	84	
8	H	82	
9	I	26	
10	J	40	
11	K	72	
12	L	163	
13	N	85	
14	1	182	
15	2	199	
16	3	275	
17	4	196	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	BCR	A	6002	-	-	-	X
19	BCR	A	6003	-	-	-	X
19	BCR	A	6007	-	-	-	X
19	BCR	B	6004	-	-	-	X
19	BCR	I	6020	-	-	-	X
19	BCR	J	6012	-	-	-	X
19	BCR	J	6013	-	-	-	X
20	LHG	1	1801	-	-	X	X
20	LHG	2	2801	-	-	X	-
20	LHG	B	7004	-	-	-	X
21	CLA	1	1001	X	-	X	-
21	CLA	1	1002	X	-	X	-
21	CLA	1	1003	X	-	X	-
21	CLA	1	1004	X	-	X	-
21	CLA	1	1005	X	-	-	-
21	CLA	1	1006	X	-	X	X
21	CLA	1	1007	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	1008	X	-	X	X
21	CLA	1	1009	X	-	X	X
21	CLA	1	1010	X	-	X	X
21	CLA	1	1011	X	-	-	-
21	CLA	1	1012	X	-	X	-
21	CLA	1	1013	X	-	X	X
21	CLA	1	1014	X	-	X	-
21	CLA	2	2001	X	-	-	-
21	CLA	2	2002	X	-	X	-
21	CLA	2	2003	X	-	X	-
21	CLA	2	2004	X	-	X	-
21	CLA	2	2005	X	-	X	X
21	CLA	2	2006	X	-	X	-
21	CLA	2	2007	X	-	-	-
21	CLA	2	2008	X	-	X	X
21	CLA	2	2009	X	-	X	-
21	CLA	2	2010	X	-	-	-
21	CLA	2	2011	X	-	X	-
21	CLA	2	2012	X	-	X	-
21	CLA	2	2013	X	-	X	-
21	CLA	2	2014	X	-	-	-
21	CLA	3	3001	X	-	X	-
21	CLA	3	3002	X	-	-	-
21	CLA	3	3003	X	-	-	X
21	CLA	3	3004	X	-	-	X
21	CLA	3	3005	X	-	-	-
21	CLA	3	3006	X	-	-	X
21	CLA	3	3008	X	-	-	-
21	CLA	3	3009	X	-	X	-
21	CLA	3	3010	X	-	-	-
21	CLA	3	3011	X	-	X	-
21	CLA	3	3012	X	-	X	-
21	CLA	3	3013	X	-	-	-
21	CLA	3	3014	X	-	-	X
21	CLA	3	3015	X	-	-	-
21	CLA	3	3016	X	-	-	-
21	CLA	3	3017	X	-	-	X
21	CLA	4	4001	X	-	X	X
21	CLA	4	4002	X	-	X	-
21	CLA	4	4003	X	-	X	-
21	CLA	4	4004	X	-	X	-
21	CLA	4	4005	X	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	4	4006	X	-	-	-
21	CLA	4	4007	X	-	-	X
21	CLA	4	4008	X	-	X	-
21	CLA	4	4009	X	-	-	-
21	CLA	4	4010	X	-	-	-
21	CLA	4	4011	X	-	X	-
21	CLA	4	4012	X	-	X	-
21	CLA	4	4013	X	-	-	-
21	CLA	4	4014	X	-	X	-
21	CLA	4	4015	X	-	-	-
21	CLA	A	1101	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	X
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	-	-
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1125	X	-	-	-
21	CLA	A	1126	X	-	-	X
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1129	X	-	X	-
21	CLA	A	1130	X	-	-	-
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1135	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1141	X	-	-	-
21	CLA	A	1142	X	-	-	-
21	CLA	A	1143	X	-	-	-
21	CLA	A	9012	X	-	-	-
21	CLA	A	9013	X	-	-	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	X
21	CLA	B	1207	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1209	X	-	-	-
21	CLA	B	1210	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	X
21	CLA	B	1213	X	-	X	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	X
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1219	X	-	-	-
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1227	X	-	X	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	1230	X	-	-	-
21	CLA	B	1231	X	-	-	-
21	CLA	B	1234	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	X	X
21	CLA	B	9010	X	-	X	-
21	CLA	B	9022	X	-	-	-
21	CLA	B	9023	X	-	-	-
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	X
21	CLA	F	1303	X	-	X	-
21	CLA	G	1001	X	-	-	-
21	CLA	G	1002	X	-	X	-
21	CLA	H	1000	X	-	-	-
21	CLA	J	1302	X	-	-	X
21	CLA	J	6014	X	-	-	-
21	CLA	J	6015	X	-	-	-
21	CLA	L	1501	X	-	X	-
21	CLA	L	1502	X	-	-	-
21	CLA	L	1503	X	-	-	-
23	CL0	A	9011	X	-	-	-
26	LUT	1	1501	X	-	X	-
26	LUT	1	1502	X	-	X	X
26	LUT	2	2501	X	-	X	X
26	LUT	2	2502	X	-	X	-
26	LUT	4	4501	X	-	X	X
26	LUT	4	4502	X	-	X	-
27	NEX	4	4503	-	-	X	X

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 34540 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	721	Total	C	N	O	S	0	0	0
			5675	3717	968	972	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	ARG	GLY	CONFLICT	UNP P05310
A	627	SER	THR	CONFLICT	UNP P05310
A	639	GLY	ALA	CONFLICT	UNP P05310

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5834	3833	989	998	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	LEU	ILE	CONFLICT	UNP P05311
B	273	MET	VAL	CONFLICT	UNP P05311
B	471	SER	THR	CONFLICT	UNP P05311
B	476	VAL	ILE	CONFLICT	UNP P05311
B	477	LEU	PRO	CONFLICT	UNP P05311
B	483	SER	GLY	CONFLICT	UNP P05311
B	491	SER	ASN	CONFLICT	UNP P05311
B	603	GLN	ARG	CONFLICT	UNP P05311
B	635	TYR	ILE	CONFLICT	UNP P05311

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	137	Total	C	N	O	S	0	0	0
			1070	685	187	195	3			

- Molecule 5 is a protein called Photosystem I reaction center subunit IV B, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	63	Total	C	N	O	0	0	0
			507	321	89	97			

- Molecule 6 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	152	Total	C	N	O	S	0	0	0
			1196	776	206	212	2			

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	0	0	0
			639	414	107	118			

- Molecule 8 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	H	82	Total	C	N	O	0	0	0
			628	415	95	118			

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	26	Total	C	N	O	S	0	0	0
			197	137	29	30	1			

- Molecule 10 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	40	Total	C	N	O	0	0	0
			316	214	49	53			

- Molecule 11 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	66	Total	C	N	O	S	0	0	0
			459	291	78	87	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	52	SER	PRO	CONFLICT	UNP E1C9L3
K	55	VAL	LEU	CONFLICT	UNP E1C9L3
K	59	ALA	THR	CONFLICT	UNP E1C9L3
K	62	THR	SER	CONFLICT	UNP E1C9L3
K	88	ALA	VAL	CONFLICT	UNP E1C9L3
K	111	THR	VAL	CONFLICT	UNP E1C9L3

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	163	Total	C	N	O	S	0	0	0
			1214	800	195	218	1			

- Molecule 13 is a protein called Photosystem I-N subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	85	Total	C	N	O	S	0	0	0
			684	438	114	128	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	86	SER	GLY	CONFLICT	UNP E1C9K7
N	88	PHE	ILE	CONFLICT	UNP E1C9K7
N	89	ASP	GLU	CONFLICT	UNP E1C9K7
N	90	ALA	GLU	CONFLICT	UNP E1C9K7
N	97	ALA	THR	CONFLICT	UNP E1C9K7
N	110	SER	THR	CONFLICT	UNP E1C9K7
N	121	GLN	GLU	CONFLICT	UNP E1C9K7
N	124	THR	SER	CONFLICT	UNP E1C9K7

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Chain	Residue	Modelled	Actual	Comment	Reference
N	146	ILE	LEU	CONFLICT	UNP E1C9K7
N	148	GLU	ASP	CONFLICT	UNP E1C9K7
N	151	GLU	ASP	CONFLICT	UNP E1C9K7
N	160	PHE	TYR	CONFLICT	UNP E1C9K7

- Molecule 14 is a protein called Chlorophyll a-b binding protein 6A, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	171	Total	C	N	O	S	0	0	0
			1271	823	218	226	4			

- Molecule 15 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	146	Total	C	N	O	S	0	0	0
			1116	726	189	198	3			

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	151	Total	C	N	O	S	0	0	0
			1118	730	184	199	5			

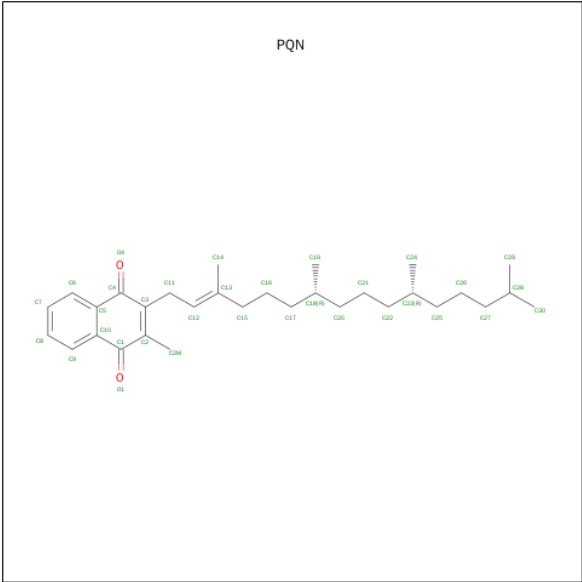
- Molecule 17 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	4	196	Total	C	N	O	S	0	0	0
			1439	934	242	260	3			

There are 2 discrepancies between the modelled and reference sequences:

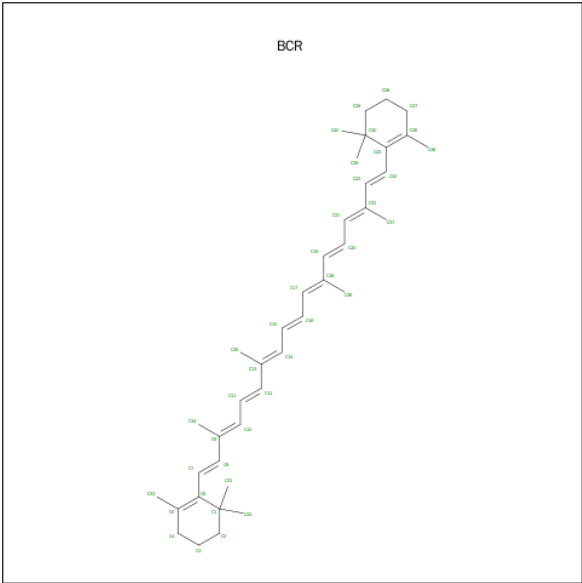
Chain	Residue	Modelled	Actual	Comment	Reference
4	129	ASP	ALA	CONFLICT	UNP Q9SQL2
4	151	PHE	SER	CONFLICT	UNP Q9SQL2

- Molecule 18 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			33	31	2	

- Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



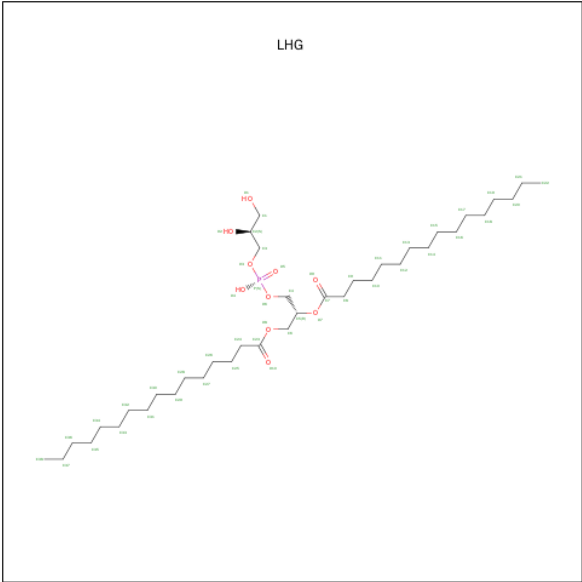
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C		0
			40	40		
19	A	1	Total	C		0
			40	40		

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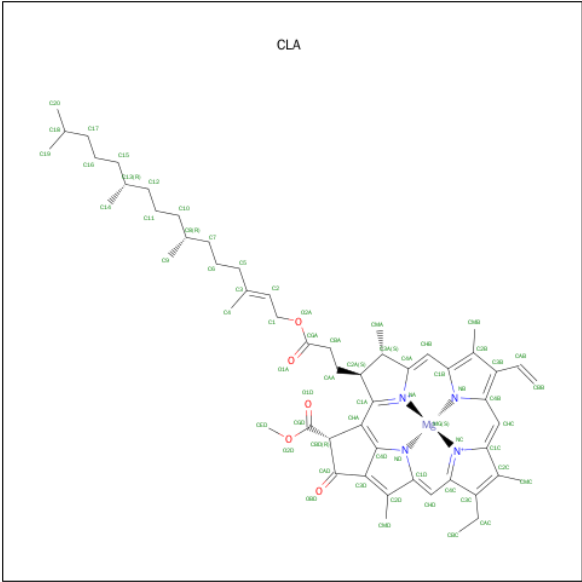
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	A	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 40 40	0	0
19	B	1	Total C 25 25	0	0
19	F	1	Total C 40 40	0	0
19	F	1	Total C 40 40	0	0
19	G	1	Total C 40 40	0	0
19	I	1	Total C 40 40	0	0
19	I	1	Total C 40 40	0	0
19	J	1	Total C 40 40	0	0
19	J	1	Total C 40 40	0	0
19	L	1	Total C 40 40	0	0
19	L	1	Total C 40 40	0	0

- Molecule 20 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			49	38	10	1		
20	A	1	Total	C	O	P	0	0
			49	38	10	1		
20	B	1	Total	C	O	P	0	0
			49	38	10	1		
20	1	1	Total	C	O	P	0	0
			49	38	10	1		
20	2	1	Total	C	O	P	0	0
			36	25	10	1		

- Molecule 21 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			44	34	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			54	44	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			58	48	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	F	1	Total 45	C 35	Mg 1	N 4	O 5	0	0
21	F	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	F	1	Total 64	C 55	Mg 1	N 4	O 4	0	0
21	G	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	G	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	H	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
21	J	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
21	J	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	L	1	Total 46	C 36	Mg 1	N 4	O 5	0	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
21	1	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
21	1	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	1	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	2	1	Total	C	Mg	N		0	0
			27	22	1	4			
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			59	50	1	4	4		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	2	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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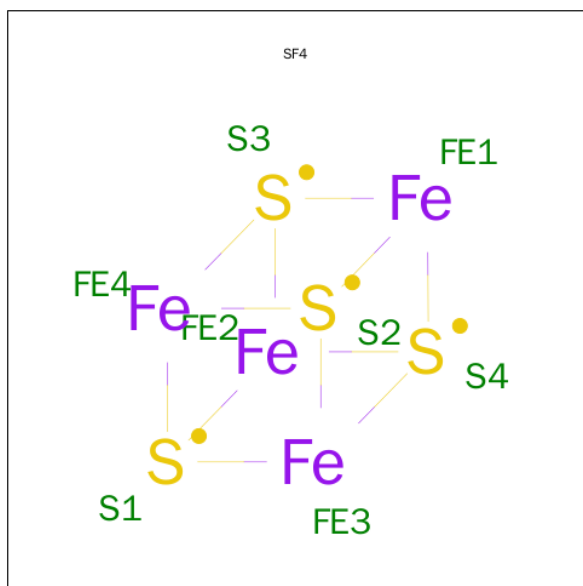
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			52	42	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	3	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
21	4	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



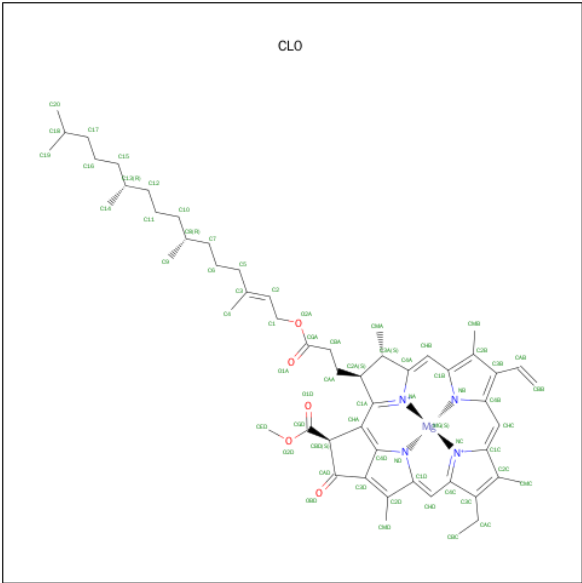
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	Fe	S	0	0
			8	4	4		
22	C	1	Total	Fe	S	0	0
			8	4	4		

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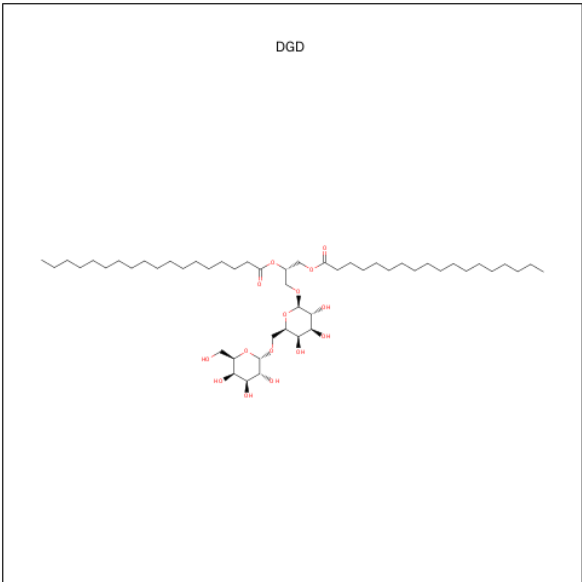
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 23 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



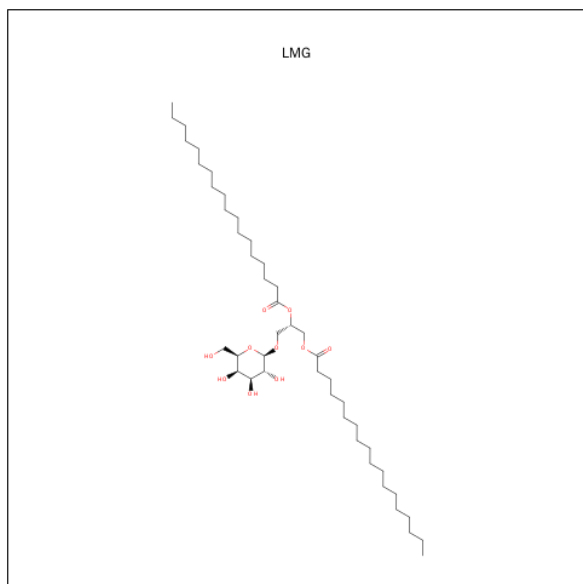
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



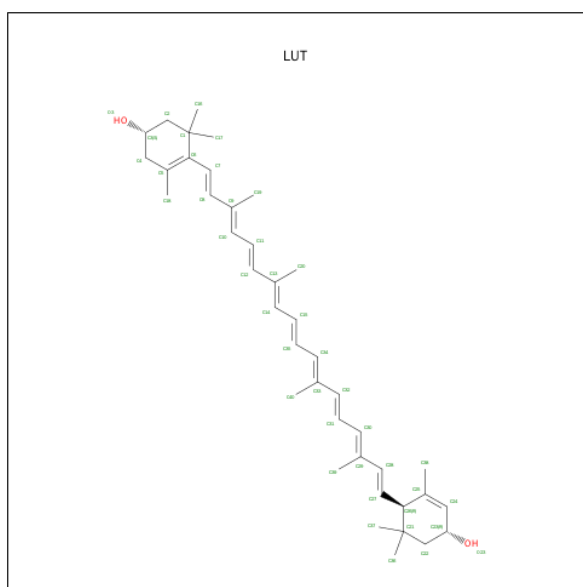
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			61	46	15		

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



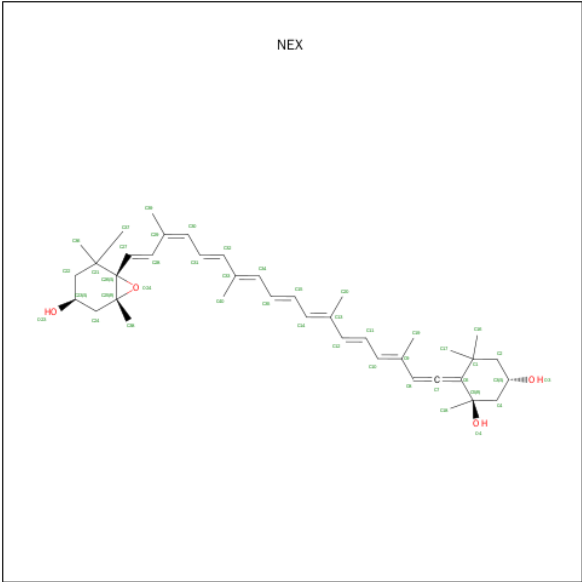
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	G	1	Total	C	O	0	0
			23	13	10		
25	J	1	Total	C	O	0	0
			35	25	10		

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



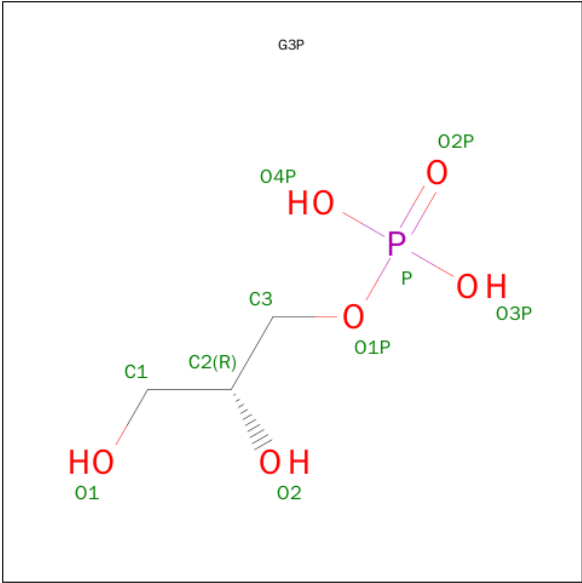
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	1	1	Total	C	O	0	0
			42	40	2		
26	1	1	Total	C	O	0	0
			42	40	2		
26	2	1	Total	C	O	0	0
			42	40	2		
26	2	1	Total	C	O	0	0
			42	40	2		
26	4	1	Total	C	O	0	0
			42	40	2		
26	4	1	Total	C	O	0	0
			42	40	2		

- Molecule 27 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	4	1	Total	C	O	0	0
			44	40	4		

- Molecule 28 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: C₃H₉O₆P).

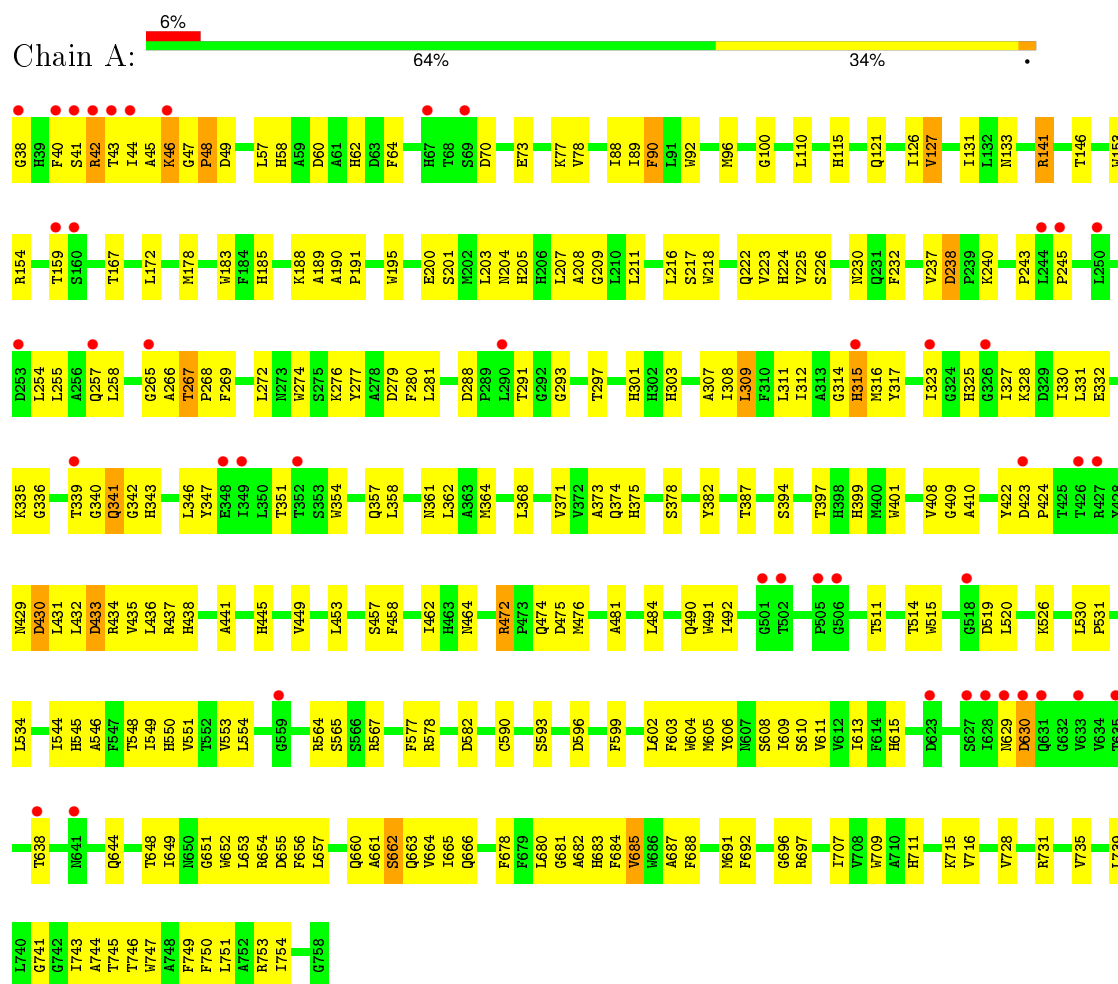


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	4	1	Total	C	O	P	0	0
			10	3	6	1		

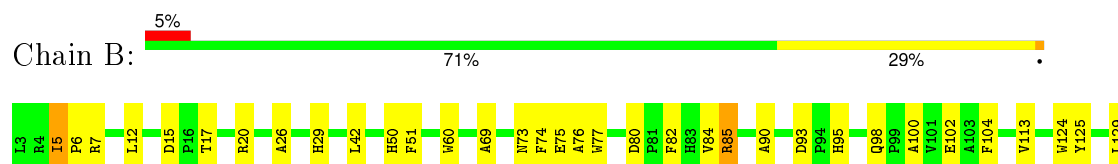
3 Residue-property plots

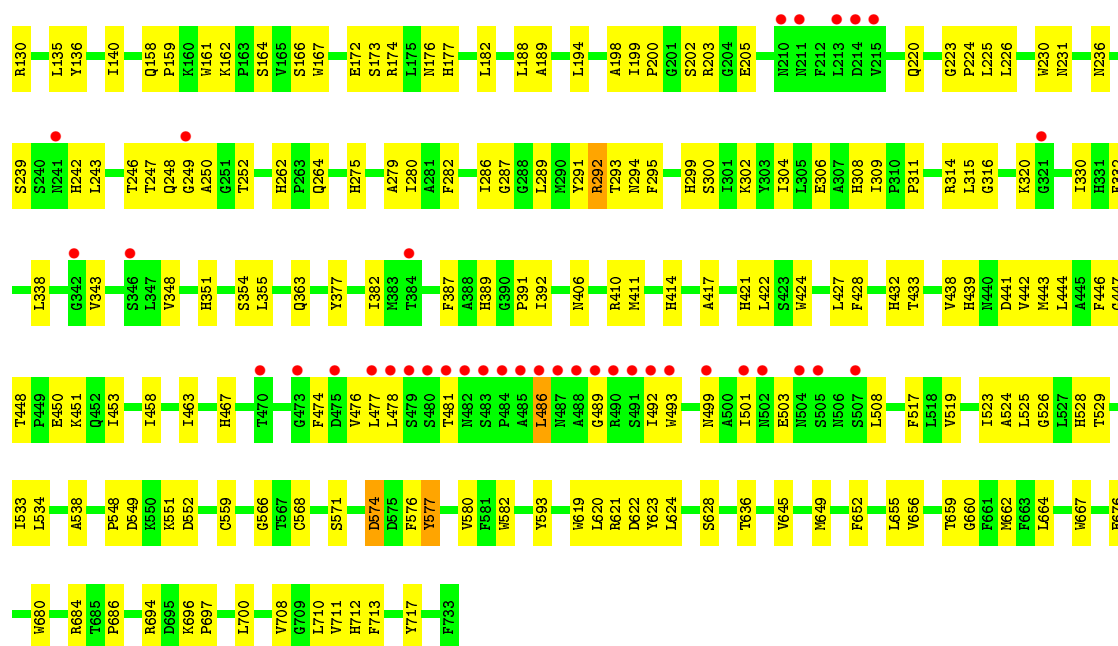
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

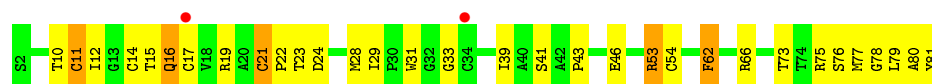


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

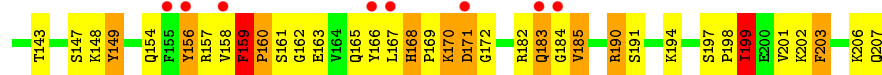
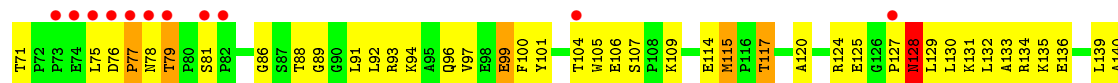
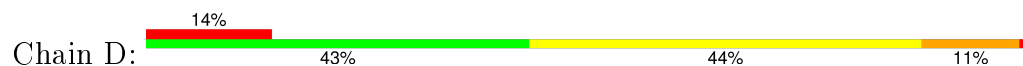




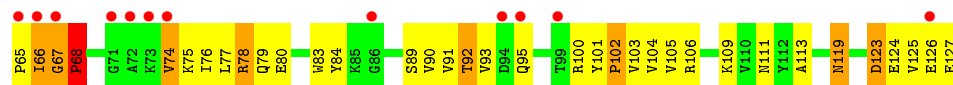
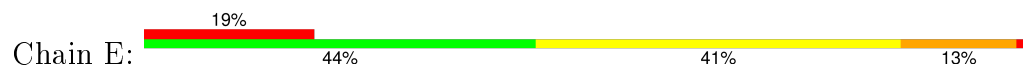
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



- Molecule 5: Photosystem I reaction center subunit IV B, chloroplastic

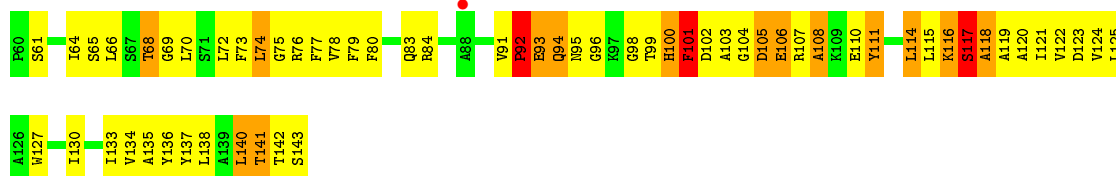


- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

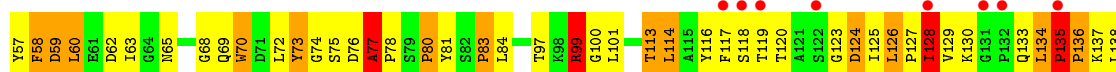
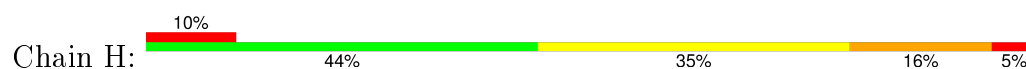




- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction center subunit VI, chloroplastic



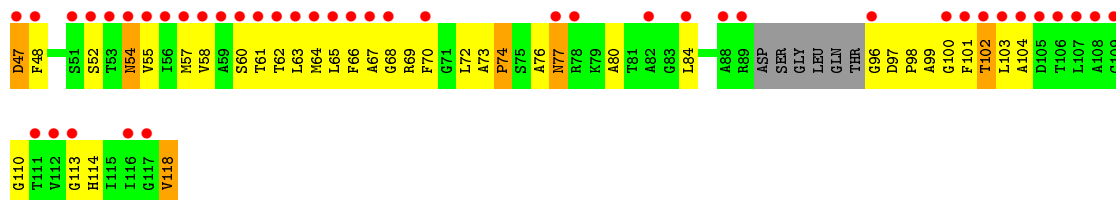
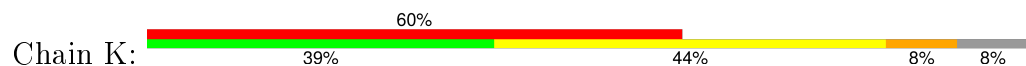
- Molecule 9: Photosystem I reaction center subunit VIII



- Molecule 10: Photosystem I reaction center subunit IX

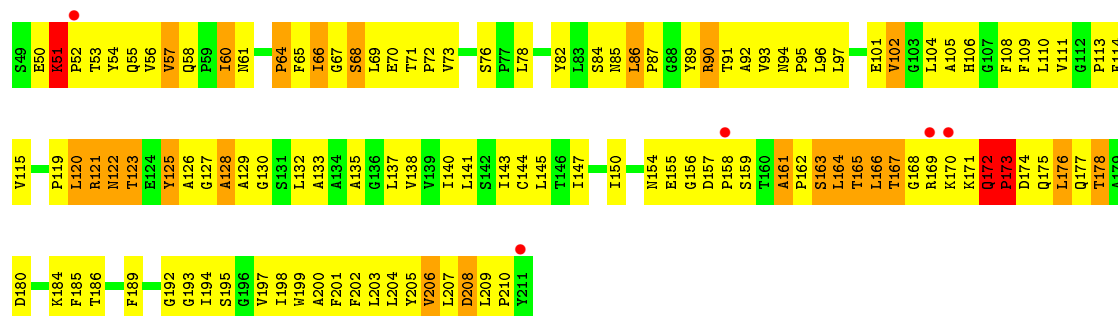


- Molecule 11: Photosystem I reaction center subunit X psaK

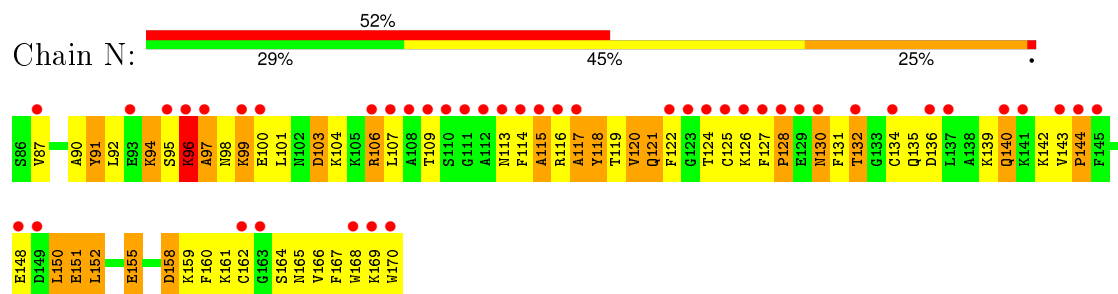


- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

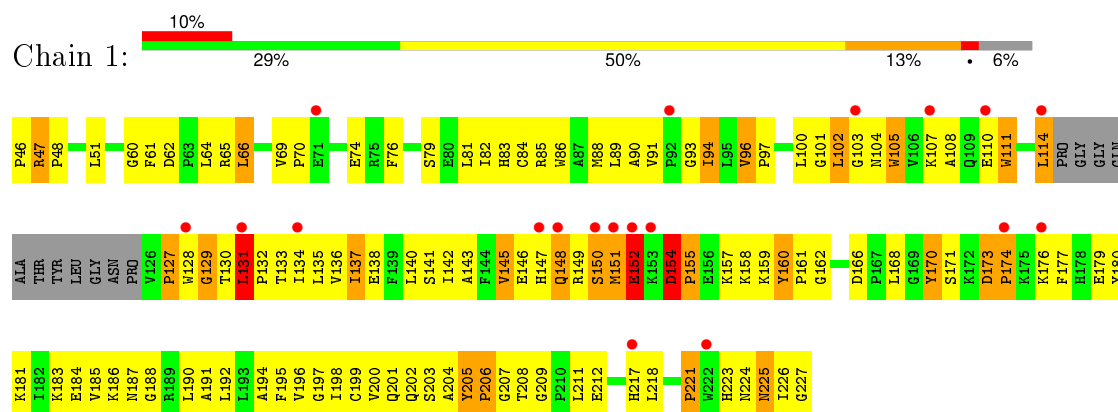




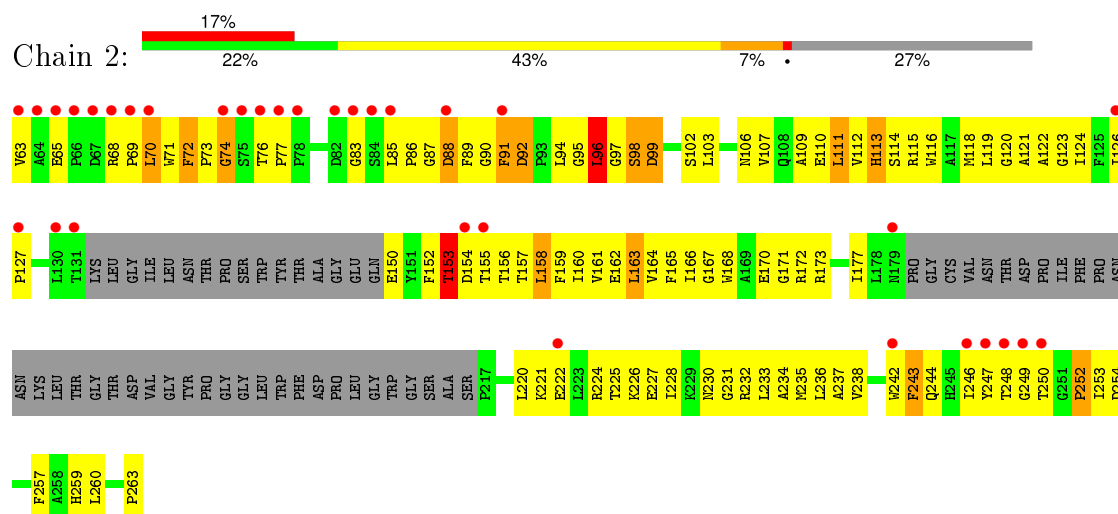
• Molecule 13: Photosystem I-N subunit



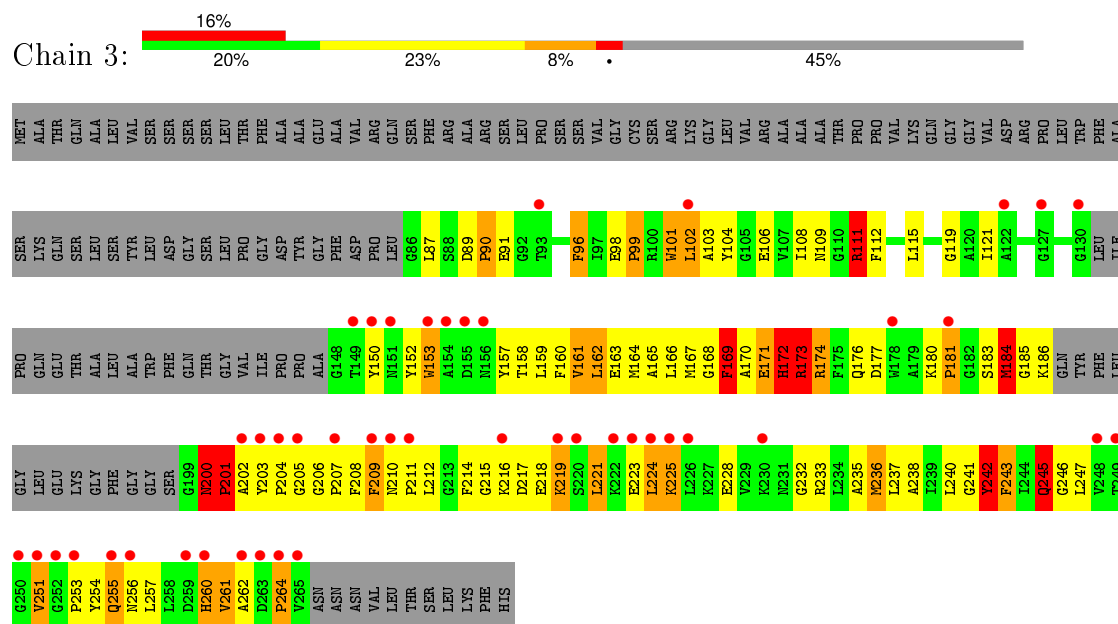
• Molecule 14: Chlorophyll a-b binding protein 6A, chloroplastic



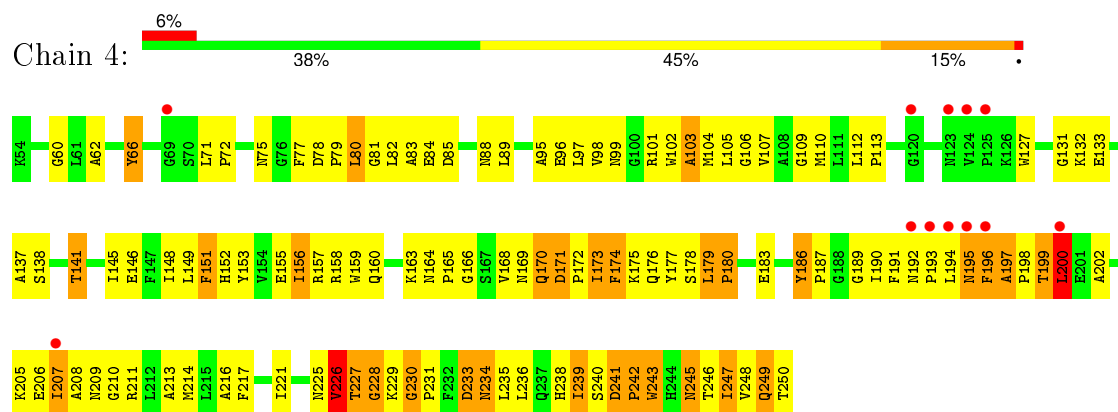
• Molecule 15: Type II chlorophyll a/b binding protein from photosystem I



• Molecule 16: Chlorophyll a-b binding protein 3, chloroplastic



• Molecule 17: Chlorophyll a-b binding protein P4, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.63Å 189.17Å 129.67Å 90.00° 91.11° 90.00°	Depositor
Resolution (Å)	39.69 – 3.00 48.59 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.69-3.00) 91.2 (48.59-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.258 , 0.293 0.266 , 0.297	Depositor DCC
R_{free} test set	5774 reflections (5.74%)	DCC
Wilson B-factor (Å ²)	66.1	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 77.5	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 115991 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	34540	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, G3P, LUT, DGD, SF4, CLA, PQN, NEX, CL0, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/5867	0.48	2/8006 (0.0%)
2	B	0.39	0/6045	0.44	0/8259
3	C	0.32	0/625	0.49	1/846 (0.1%)
4	D	0.64	0/1097	0.84	3/1483 (0.2%)
5	E	0.62	0/518	0.75	2/704 (0.3%)
6	F	0.56	0/1223	0.61	2/1652 (0.1%)
7	G	0.77	0/653	0.93	2/885 (0.2%)
8	H	0.64	0/648	0.98	7/883 (0.8%)
9	I	0.26	0/203	0.62	0/276
10	J	0.60	0/325	0.66	1/445 (0.2%)
11	K	0.30	0/464	0.64	0/627
12	L	0.89	0/1250	0.97	6/1711 (0.4%)
13	N	0.37	0/699	0.77	1/935 (0.1%)
14	1	0.92	3/1308 (0.2%)	1.01	4/1783 (0.2%)
15	2	0.68	0/1153	0.77	1/1577 (0.1%)
16	3	0.54	0/1150	0.78	1/1562 (0.1%)
17	4	0.80	0/1483	0.82	2/2031 (0.1%)
All	All	0.58	3/24711 (0.0%)	0.67	35/33665 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
5	E	0	1
8	H	0	1
11	K	0	1
13	N	0	2
16	3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	1	152	GLU	C-N	8.00	1.52	1.34
14	1	151	MET	C-N	-5.52	1.21	1.34
14	1	150	SER	C-N	5.16	1.46	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	67	GLY	N-CA-C	7.16	131.00	113.10
6	F	200	VAL	N-CA-C	-6.80	92.64	111.00
8	H	135	PRO	C-N-CD	6.56	142.17	128.40
8	H	134	LEU	CA-CB-CG	-6.49	100.37	115.30
8	H	136	PRO	CA-N-CD	-6.49	102.41	111.50
7	G	92	PRO	CA-N-CD	-6.36	102.60	111.50
7	G	101	PHE	N-CA-C	-6.35	93.86	111.00
14	1	160	TYR	C-N-CD	6.10	141.21	128.40
12	L	121	ARG	N-CA-C	6.04	127.30	111.00
12	L	157	ASP	N-CA-C	-5.92	95.00	111.00
4	D	76	ASP	C-N-CD	5.70	140.37	128.40
14	1	154	ASP	O-C-N	5.65	131.84	121.10
8	H	135	PRO	CA-N-CD	-5.64	103.61	111.50
5	E	67	GLY	C-N-CD	5.57	140.09	128.40
14	1	131	LEU	C-N-CD	5.50	139.95	128.40
12	L	166	LEU	N-CA-C	-5.39	96.44	111.00
14	1	96	VAL	C-N-CD	5.32	139.56	128.40
16	3	201	PRO	CA-N-CD	-5.30	104.08	111.50
13	N	152	LEU	CA-CB-CG	5.29	127.46	115.30
4	D	159	PHE	C-N-CD	5.27	139.46	128.40
12	L	161	ALA	C-N-CD	5.27	139.46	128.40
1	A	47	GLY	C-N-CD	5.22	139.37	128.40
8	H	80	PRO	CA-N-CD	-5.22	104.19	111.50
4	D	71	THR	C-N-CD	5.22	139.35	128.40
8	H	80	PRO	N-CA-C	5.21	125.65	112.10
6	F	200	VAL	C-N-CD	5.20	139.32	128.40
15	2	85	LEU	C-N-CD	5.20	139.32	128.40
3	C	21	CYS	C-N-CD	5.16	139.23	128.40
12	L	173	PRO	CA-N-CD	-5.13	104.32	111.50
10	J	11	ALA	C-N-CD	5.13	139.16	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	233	ASP	N-CA-C	-5.12	97.17	111.00
1	A	423	ASP	C-N-CD	5.08	139.06	128.40
8	H	77	ALA	C-N-CD	5.06	139.02	128.40
17	4	197	ALA	C-N-CD	5.02	138.94	128.40
12	L	51	LYS	C-N-CD	5.01	138.93	128.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	3	111	ARG	Sidechain
2	B	684	ARG	Sidechain
5	E	100	ARG	Sidechain
8	H	128	ILE	Peptide
11	K	97	ASP	Peptide
13	N	143	VAL	Peptide
13	N	144	PRO	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5675	0	5527	290	0
2	B	5834	0	5615	225	0
3	C	612	0	598	35	0
4	D	1070	0	1073	108	0
5	E	507	0	501	33	0
6	F	1196	0	1228	60	0
7	G	639	0	631	205	0
8	H	628	0	616	58	0
9	I	197	0	213	16	0
10	J	316	0	326	32	0
11	K	459	0	465	31	0
12	L	1214	0	1212	226	0
13	N	684	0	670	72	0
14	1	1271	0	1204	302	0
15	2	1116	0	1036	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	3	1118	0	1046	228	0
17	4	1439	0	1303	323	0
18	A	33	0	46	4	0
18	B	33	0	46	6	0
19	A	240	0	292	30	0
19	B	225	0	269	25	0
19	F	80	0	98	14	0
19	G	40	0	48	14	0
19	I	80	0	97	13	0
19	J	80	0	96	7	0
19	L	80	0	98	35	0
20	1	49	0	74	41	0
20	2	36	0	42	23	0
20	A	98	0	148	26	0
20	B	49	0	74	16	0
21	1	819	0	811	499	0
21	2	799	0	780	321	0
21	3	819	0	703	186	0
21	4	846	0	808	385	0
21	A	2538	0	2415	267	0
21	B	2467	0	2510	279	0
21	F	155	0	138	27	0
21	G	101	0	82	60	0
21	H	46	0	33	5	0
21	J	177	0	171	15	0
21	L	161	0	144	51	0
22	A	8	0	0	0	0
22	C	16	0	0	0	0
23	A	65	0	72	15	0
24	B	61	0	83	4	0
25	G	23	0	16	12	0
25	J	35	0	40	3	0
26	1	84	0	110	112	0
26	2	84	0	110	89	0
26	4	84	0	110	95	0
27	4	44	0	54	43	0
28	4	10	0	7	0	0
All	All	34540	0	33889	3868	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (3868) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:CB	1:A:46:LYS:HE3	1.47	1.45
1:A:43:THR:HB	1:A:46:LYS:CE	1.61	1.29
21:4:4011:CLA:HMB1	21:4:4011:CLA:HBB1	1.19	1.19
1:A:43:THR:CA	1:A:46:LYS:HE3	1.74	1.17
17:4:199:THR:HA	17:4:200:LEU:HD22	1.25	1.17
10:J:2:ARG:HA	21:J:6015:CLA:HAB	1.23	1.16
21:2:2003:CLA:H71	21:2:2003:CLA:H41	1.17	1.16
14:1:47:ARG:NH2	14:1:51:LEU:O	1.79	1.15
1:A:38:GLY:HA3	1:A:44:ILE:HG22	1.21	1.15
21:3:3012:CLA:HED3	21:3:3012:CLA:H2A	1.25	1.15
21:2:2002:CLA:HMB2	26:2:2501:LUT:H11	1.17	1.14
21:2:2002:CLA:HHB	26:2:2501:LUT:H202	1.24	1.14
14:1:102:LEU:HG	21:1:1006:CLA:CED	1.77	1.13
21:G:1002:CLA:HBA2	21:G:1002:CLA:HBD	1.22	1.13
21:B:1213:CLA:HBA1	21:B:1213:CLA:HBD	1.23	1.12
21:1:1009:CLA:H2	21:4:4005:CLA:HMD2	1.15	1.12
21:2:2003:CLA:H72	21:2:2003:CLA:H143	1.30	1.12
21:3:3013:CLA:HBB1	21:3:3013:CLA:HHC	1.21	1.12
1:A:43:THR:O	1:A:46:LYS:HG3	1.47	1.12
14:1:111:TRP:HE1	21:1:1013:CLA:HBA1	1.11	1.11
15:2:226:LYS:CB	21:2:2007:CLA:HED3	1.81	1.11
21:4:4004:CLA:HBC2	21:4:4009:CLA:HBB2	1.32	1.11
21:1:1005:CLA:HHC	21:1:1005:CLA:HBB1	1.32	1.11
14:1:168:LEU:HB2	14:1:170:TYR:HE1	1.12	1.11
20:A:7001:LHG:H252	21:A:1128:CLA:H42	1.29	1.11
21:4:4004:CLA:H41	21:4:4004:CLA:H72	1.31	1.11
7:G:73:PHE:CD1	7:G:77:PHE:HD2	1.69	1.11
21:A:1125:CLA:HBB1	21:A:1133:CLA:HMA2	1.31	1.10
21:1:1004:CLA:HMB1	21:1:1004:CLA:HBB1	1.27	1.10
21:1:1007:CLA:H71	21:1:1007:CLA:H41	1.21	1.10
21:1:1011:CLA:H111	21:1:1011:CLA:H62	1.18	1.10
15:2:155:THR:HA	15:2:158:LEU:HD11	1.28	1.10
26:1:1502:LUT:H173	21:1:1004:CLA:H62	1.28	1.09
12:L:204:LEU:HA	12:L:207:LEU:HG	1.26	1.09
21:L:1503:CLA:HHC	21:L:1503:CLA:HBB1	1.34	1.08
21:4:4004:CLA:H42	26:4:4502:LUT:H162	1.09	1.08
20:2:2801:LHG:H131	20:2:2801:LHG:HC81	1.08	1.08
15:2:68:ARG:NH2	15:2:88:ASP:OD1	1.85	1.08
21:3:3009:CLA:HBB1	21:3:3009:CLA:HHC	1.25	1.08
12:L:201:PHE:CE1	12:L:205:TYR:HD2	1.70	1.08
8:H:135:PRO:HD2	8:H:136:PRO:HD2	1.30	1.08
21:L:1501:CLA:HHC	21:L:1501:CLA:HBB1	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:4005:CLA:H2A	21:4:4005:CLA:HED2	1.35	1.07
7:G:93:GLU:O	7:G:94:GLN:NE2	1.87	1.07
21:2:2005:CLA:HBB1	21:2:2012:CLA:H171	1.37	1.07
21:4:4004:CLA:HMB1	21:4:4004:CLA:HBB1	1.23	1.07
12:L:104:LEU:HD22	21:L:1501:CLA:HMA2	1.09	1.07
12:L:171:LYS:O	12:L:172:GLN:NE2	1.88	1.07
15:2:173:ARG:NH2	21:2:2012:CLA:O1D	1.87	1.07
21:2:2013:CLA:HMC1	21:2:2013:CLA:HBC2	1.29	1.07
17:4:158:ARG:NH2	21:4:4012:CLA:O1D	1.87	1.07
21:3:3009:CLA:HBA2	21:3:3009:CLA:HBD	1.30	1.06
21:2:2008:CLA:HHD	21:2:2008:CLA:HBC3	1.37	1.06
17:4:101:ARG:NH1	21:4:4011:CLA:OBD	1.87	1.06
7:G:84:ARG:NH2	7:G:123:ASP:OD2	1.87	1.06
15:2:259:HIS:HB3	21:2:2003:CLA:HBC3	1.38	1.06
15:2:73:PRO:O	16:3:176:GLN:NE2	1.87	1.06
21:1:1013:CLA:HBC2	21:1:1013:CLA:HHD	1.35	1.06
21:A:1129:CLA:HHC	21:A:1129:CLA:HBB1	1.33	1.06
15:2:110:GLU:OE2	15:2:232:ARG:NH1	1.88	1.05
26:1:1502:LUT:H392	21:1:1010:CLA:HMA2	1.10	1.05
21:1:1005:CLA:H52	21:1:1005:CLA:H92	1.34	1.05
4:D:134:ARG:NH2	4:D:136:GLU:OE2	1.88	1.05
1:A:358:LEU:HD11	21:A:1128:CLA:HBB1	1.37	1.05
4:D:199:ILE:HD13	4:D:201:VAL:HG22	1.38	1.05
21:4:4014:CLA:HBB1	21:4:4014:CLA:HHC	1.38	1.05
21:4:4001:CLA:H2	26:4:4501:LUT:H373	1.11	1.05
7:G:93:GLU:HB3	7:G:99:THR:HB	1.35	1.05
21:G:1002:CLA:HBC2	21:G:1002:CLA:HHD	1.37	1.04
7:G:105:ASP:HA	7:G:106:GLU:HB3	1.33	1.04
3:C:24:ASP:OD2	4:D:168:HIS:ND1	1.89	1.04
16:3:157:TYR:CD1	21:3:3010:CLA:HBC1	1.92	1.04
26:4:4501:LUT:H181	26:4:4501:LUT:H8	1.37	1.04
21:B:1228:CLA:HBC3	21:B:1228:CLA:HHD	1.36	1.04
15:2:235:MET:HE3	21:2:2004:CLA:HMC3	1.36	1.04
21:3:3011:CLA:HBC2	21:3:3011:CLA:HHD	1.33	1.04
17:4:169:ASN:HD22	27:4:4503:NEX:H173	1.20	1.04
21:1:1013:CLA:HHC	21:1:1013:CLA:HBB1	1.38	1.03
21:4:4012:CLA:HHC	21:4:4012:CLA:HBB1	1.39	1.03
12:L:145:LEU:HD21	19:L:6019:BCR:H392	1.07	1.03
14:1:107:LYS:NZ	14:1:110:GLU:OE1	1.89	1.03
12:L:120:LEU:HD12	12:L:126:ALA:HB2	1.37	1.03
21:4:4012:CLA:H152	21:4:4012:CLA:H192	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:99:THR:O	7:G:101:PHE:N	1.91	1.03
14:1:46:PRO:HD3	21:4:4005:CLA:HBA1	1.35	1.03
21:4:4001:CLA:HMB1	21:4:4001:CLA:HBB1	1.37	1.03
21:2:2009:CLA:CBB	20:2:2801:LHG:HC82	1.89	1.03
16:3:108:ILE:HG12	21:3:3011:CLA:HBB2	1.07	1.03
17:4:227:THR:O	17:4:229:LYS:N	1.91	1.03
13:N:161:LYS:HG3	13:N:167:PHE:CD2	1.92	1.03
21:3:3012:CLA:HHD	21:3:3012:CLA:HBC2	1.39	1.03
21:4:4001:CLA:H41	21:4:4002:CLA:HBA1	1.40	1.02
23:A:9011:CL0:H2	23:A:9011:CL0:H15	1.41	1.02
21:2:2002:CLA:H3A	26:2:2501:LUT:H201	1.41	1.02
21:2:2013:CLA:HBB1	26:2:2502:LUT:H382	1.41	1.02
26:1:1501:LUT:H35	21:1:1002:CLA:CAD	1.88	1.02
21:4:4001:CLA:H62	26:4:4501:LUT:C37	1.89	1.02
12:L:64:PRO:HG2	12:L:65:PHE:CE1	1.93	1.02
1:A:43:THR:O	1:A:46:LYS:CG	2.05	1.02
14:1:186:LYS:HZ3	21:1:1007:CLA:HED1	1.25	1.02
21:2:2002:CLA:HBC2	21:2:2002:CLA:HMC1	1.39	1.02
21:1:1010:CLA:HHD	21:1:1010:CLA:HBC2	1.38	1.02
21:A:1129:CLA:HBB2	21:A:1137:CLA:CBB	1.90	1.02
14:1:66:LEU:CD2	21:1:1004:CLA:H42	1.90	1.02
14:1:46:PRO:CD	21:4:4005:CLA:HBA1	1.90	1.02
4:D:171:ASP:OD2	4:D:182:ARG:NE	1.93	1.02
21:4:4014:CLA:HBC2	21:4:4014:CLA:HMC1	1.40	1.01
14:1:194:ALA:CB	26:1:1501:LUT:H193	1.90	1.01
17:4:77:PHE:CE2	26:4:4502:LUT:H173	1.95	1.01
7:G:116:LYS:HA	21:G:1002:CLA:HMA3	1.41	1.01
12:L:193:GLY:O	12:L:197:VAL:HG23	1.60	1.01
21:B:9010:CLA:HBC3	21:B:9010:CLA:HHD	1.40	1.01
12:L:145:LEU:HD21	19:L:6019:BCR:C39	1.90	1.01
12:L:50:GLU:OE2	12:L:50:GLU:N	1.93	1.01
1:A:648:THR:HG23	1:A:651:GLY:H	1.22	1.01
10:J:2:ARG:HA	21:J:6015:CLA:CAB	1.90	1.01
7:G:116:LYS:CA	21:G:1002:CLA:HMA3	1.90	1.01
14:1:160:TYR:HB3	21:1:1001:CLA:HED2	1.37	1.01
21:3:3010:CLA:HBC2	21:3:3010:CLA:HHD	1.40	1.01
1:A:665:ILE:HD12	2:B:621:ARG:HG3	1.40	1.01
21:1:1002:CLA:HED3	21:1:1002:CLA:C6	1.90	1.01
14:1:146:GLU:OE1	14:1:149:ARG:NH1	1.94	1.00
21:3:3008:CLA:CED	21:3:3008:CLA:H2A	1.89	1.00
8:H:116:TYR:O	8:H:120:THR:HG23	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1008:CLA:HHC	21:1:1008:CLA:HBB1	1.38	1.00
21:4:4011:CLA:HBC2	21:4:4011:CLA:HHD	1.40	1.00
21:1:1003:CLA:HBA1	21:1:1003:CLA:HBD	1.41	1.00
15:2:166:ILE:HD11	21:2:2013:CLA:HMB3	1.40	1.00
15:2:166:ILE:CD1	21:2:2013:CLA:HMB3	1.91	1.00
15:2:155:THR:HG22	15:2:156:THR:H	1.26	1.00
21:2:2005:CLA:CBB	21:2:2012:CLA:H171	1.90	1.00
21:2:2006:CLA:HMC2	26:2:2502:LUT:C22	1.92	1.00
14:1:94:ILE:HD13	26:1:1502:LUT:H382	1.42	1.00
21:2:2013:CLA:HHC	21:2:2013:CLA:HBB1	1.40	1.00
12:L:104:LEU:CD2	21:L:1501:CLA:HMA2	1.92	1.00
21:1:1002:CLA:H42	21:1:1007:CLA:C10	1.92	0.99
21:4:4007:CLA:HHD	21:4:4007:CLA:HBC2	1.44	0.99
16:3:200:ASN:H	16:3:201:PRO:HD2	1.27	0.99
1:A:38:GLY:HA3	1:A:44:ILE:CG2	1.92	0.99
21:1:1002:CLA:HAB	21:1:1007:CLA:HBD	1.40	0.99
20:1:1801:LHG:H383	20:1:1801:LHG:C20	1.93	0.99
17:4:169:ASN:HA	17:4:178:SER:HB2	1.41	0.99
14:1:102:LEU:HG	21:1:1006:CLA:HED2	1.41	0.99
14:1:142:ILE:HD11	21:1:1013:CLA:HMC2	1.43	0.99
21:1:1009:CLA:C2	21:4:4005:CLA:HMD2	1.93	0.99
14:1:94:ILE:HG22	14:1:105:TRP:HB3	1.40	0.99
2:B:173:SER:OG	21:B:1209:CLA:HED1	1.60	0.99
21:2:2008:CLA:HMD2	16:3:162:LEU:CD1	1.92	0.98
21:4:4006:CLA:CMC	26:4:4502:LUT:H222	1.92	0.98
1:A:433:ASP:OD2	1:A:437:ARG:NH1	1.95	0.98
8:H:58:PHE:CE1	8:H:60:LEU:HD11	1.98	0.98
21:4:4001:CLA:H41	21:4:4002:CLA:CGA	1.93	0.98
15:2:109:ALA:HA	21:2:2012:CLA:HED3	1.43	0.98
21:2:2009:CLA:HBC1	21:3:3009:CLA:CGA	1.92	0.98
17:4:246:THR:CG2	17:4:248:VAL:HG23	1.94	0.98
21:F:1303:CLA:CED	21:F:1303:CLA:HBA2	1.93	0.98
8:H:133:GLN:HB3	8:H:135:PRO:HB3	1.44	0.98
21:3:3013:CLA:HMC1	21:3:3013:CLA:HBC3	1.46	0.98
2:B:292:ARG:NH1	7:G:107:ARG:HH21	1.61	0.98
26:1:1502:LUT:H222	21:1:1006:CLA:HAB	1.46	0.98
21:1:1008:CLA:HMC2	21:1:1008:CLA:H152	1.44	0.97
21:1:1009:CLA:H52	21:4:4005:CLA:C3D	1.93	0.97
21:2:2012:CLA:HBC2	21:2:2012:CLA:HHD	1.43	0.97
21:1:1009:CLA:H52	21:4:4005:CLA:C2D	1.94	0.97
21:1:1009:CLA:H93	21:1:1009:CLA:H122	1.43	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:113:HIS:ND1	21:2:2004:CLA:HBB2	1.78	0.97
14:1:194:ALA:HB1	26:1:1501:LUT:H193	1.42	0.97
2:B:292:ARG:CZ	7:G:107:ARG:HH21	1.77	0.97
21:4:4004:CLA:C4	26:4:4502:LUT:H162	1.94	0.97
15:2:259:HIS:HE2	21:2:2003:CLA:HMD2	1.29	0.97
21:4:4001:CLA:H41	21:4:4002:CLA:CBA	1.93	0.97
16:3:204:PRO:HG3	16:3:211:PRO:HD2	1.42	0.97
21:G:1002:CLA:HBA2	21:G:1002:CLA:CBD	1.95	0.96
1:A:43:THR:C	1:A:46:LYS:HG3	1.86	0.96
21:1:1013:CLA:H72	21:1:1014:CLA:HBB2	1.44	0.96
21:3:3009:CLA:HED2	21:3:3009:CLA:C1A	1.95	0.96
21:G:1001:CLA:H42	19:G:2011:BCR:H343	1.44	0.96
21:1:1002:CLA:HMC1	21:1:1002:CLA:HBC3	1.47	0.96
15:2:95:GLY:O	15:2:97:GLY:N	1.98	0.96
2:B:85:ARG:HG3	2:B:85:ARG:HH11	1.29	0.96
21:2:2003:CLA:H143	21:2:2003:CLA:C7	1.96	0.96
15:2:235:MET:CE	21:2:2004:CLA:HMC3	1.95	0.96
21:2:2013:CLA:CBB	26:2:2502:LUT:H382	1.94	0.96
20:2:2801:LHG:C8	20:2:2801:LHG:H131	1.95	0.96
2:B:292:ARG:NE	7:G:91:VAL:HG11	1.80	0.95
21:1:1008:CLA:CMC	21:1:1008:CLA:H152	1.95	0.95
21:4:4006:CLA:HMC2	26:4:4502:LUT:H222	1.48	0.95
21:1:1010:CLA:HMB3	21:1:1013:CLA:HMB2	1.47	0.95
14:1:91:VAL:HG11	26:1:1501:LUT:C19	1.96	0.95
13:N:160:PHE:CE2	13:N:166:VAL:HG11	2.01	0.95
12:L:64:PRO:HG2	12:L:65:PHE:CD1	2.02	0.95
8:H:72:LEU:HG	8:H:76:ASP:HB3	1.47	0.95
21:1:1004:CLA:H92	21:1:1005:CLA:HMA1	1.44	0.95
7:G:74:LEU:HA	7:G:78:VAL:HG12	1.49	0.95
16:3:160:PHE:CE1	16:3:164:MET:HG3	2.00	0.95
17:4:247:ILE:HD13	21:4:4003:CLA:HMD1	1.49	0.95
2:B:292:ARG:NH2	7:G:91:VAL:HG21	1.81	0.95
16:3:108:ILE:HA	16:3:111:ARG:HD2	1.48	0.94
21:3:3010:CLA:HBA1	21:3:3010:CLA:HBD	1.49	0.94
21:A:1131:CLA:H93	21:A:1131:CLA:H52	1.47	0.94
20:B:7004:LHG:H242	21:B:1227:CLA:H71	1.47	0.94
21:B:1213:CLA:H11	7:G:140:LEU:HD11	1.46	0.94
7:G:114:LEU:HD12	21:G:1002:CLA:HED2	1.48	0.94
16:3:108:ILE:HG12	21:3:3011:CLA:CBB	1.96	0.94
14:1:160:TYR:CB	21:1:1001:CLA:HED2	1.97	0.94
21:2:2009:CLA:C1A	21:2:2009:CLA:HED2	1.98	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1213:CLA:H12	21:B:1213:CLA:ND	1.82	0.94
12:L:121:ARG:N	12:L:122:ASN:HB2	1.83	0.94
1:A:342:GLY:HA2	1:A:431:LEU:HD21	1.48	0.94
12:L:201:PHE:CE1	12:L:205:TYR:CD2	2.55	0.94
21:3:3008:CLA:HHC	21:3:3008:CLA:HBB1	1.46	0.94
21:2:2005:CLA:HBC1	21:2:2012:CLA:HBC1	1.48	0.94
17:4:246:THR:HG23	21:4:4008:CLA:HED3	1.49	0.94
21:4:4004:CLA:H42	26:4:4502:LUT:C16	1.99	0.93
17:4:199:THR:HA	17:4:200:LEU:CD2	1.97	0.93
20:2:2801:LHG:H122	20:2:2801:LHG:C23	1.98	0.93
17:4:192:ASN:OD1	26:4:4501:LUT:O23	1.85	0.93
7:G:137:TYR:O	7:G:141:THR:OG1	1.85	0.93
7:G:73:PHE:CD1	7:G:77:PHE:CD2	2.55	0.93
14:1:168:LEU:HB2	14:1:170:TYR:CE1	2.04	0.93
21:A:1132:CLA:CBC	21:B:1206:CLA:HBB2	1.97	0.93
21:B:1239:CLA:HBC2	21:B:1239:CLA:HMC1	1.50	0.93
26:1:1502:LUT:H392	21:1:1010:CLA:CMA	1.98	0.93
21:2:2005:CLA:HMD2	21:2:2012:CLA:C1D	1.99	0.93
21:2:2010:CLA:H171	21:2:2010:CLA:H143	1.51	0.93
20:2:2801:LHG:O1	20:2:2801:LHG:O5	1.84	0.93
16:3:204:PRO:CB	16:3:209:PHE:HA	1.99	0.93
7:G:141:THR:CG2	25:G:2021:LMG:HC72	1.98	0.93
1:A:43:THR:HB	1:A:46:LYS:HE3	0.93	0.93
21:1:1011:CLA:H111	21:1:1011:CLA:C6	1.98	0.93
21:1:1004:CLA:C9	21:1:1005:CLA:HHB	1.99	0.93
21:G:1001:CLA:HMC1	21:G:1001:CLA:HBC2	1.51	0.93
26:1:1502:LUT:H203	21:1:1004:CLA:HAB	1.51	0.93
15:2:244:GLN:O	15:2:248:THR:OG1	1.85	0.93
17:4:246:THR:HG22	17:4:248:VAL:H	1.34	0.93
21:1:1014:CLA:HMC1	21:1:1014:CLA:HBC2	1.50	0.92
1:A:434:ARG:O	1:A:438:HIS:ND1	2.02	0.92
21:2:2001:CLA:C2B	21:2:2014:CLA:H2A	1.98	0.92
17:4:217:PHE:CD1	26:4:4502:LUT:H402	2.05	0.92
21:2:2008:CLA:H172	21:2:2008:CLA:H143	1.51	0.92
21:A:1117:CLA:H143	21:A:1125:CLA:C10	2.00	0.92
14:1:91:VAL:HG11	26:1:1501:LUT:H191	1.51	0.92
21:B:1213:CLA:H12	21:B:1213:CLA:C4D	1.99	0.92
26:1:1501:LUT:H382	21:1:1001:CLA:HBA1	1.48	0.92
20:B:7004:LHG:H181	20:B:7004:LHG:H321	1.51	0.92
12:L:87:PRO:HD2	21:L:1502:CLA:HED2	1.50	0.92
12:L:109:PHE:CE1	21:L:1503:CLA:C2C	2.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1009:CLA:CBB	17:4:156:ILE:HG12	1.99	0.92
21:A:1125:CLA:CBB	21:A:1133:CLA:HMA2	2.00	0.92
12:L:104:LEU:HD21	19:L:6020:BCR:C12	2.00	0.92
1:A:648:THR:HG23	1:A:651:GLY:N	1.85	0.92
14:1:142:ILE:CD1	21:1:1013:CLA:HMC2	2.00	0.92
21:3:3008:CLA:HED2	21:3:3008:CLA:H2A	1.52	0.92
2:B:246:THR:HG22	2:B:248:GLN:HG2	1.50	0.91
20:B:7004:LHG:H201	20:B:7004:LHG:H342	1.52	0.91
7:G:94:GLN:HE21	7:G:94:GLN:HA	1.33	0.91
26:1:1501:LUT:C11	21:1:1002:CLA:HBA1	1.99	0.91
21:3:3012:CLA:HED3	21:3:3012:CLA:C2A	2.00	0.91
20:B:7004:LHG:H181	20:B:7004:LHG:C34	2.01	0.91
21:1:1006:CLA:HBA1	21:1:1014:CLA:C4C	2.01	0.91
21:2:2001:CLA:CHB	21:2:2014:CLA:HMA2	2.00	0.91
7:G:73:PHE:HD1	7:G:77:PHE:HD2	1.18	0.91
21:1:1002:CLA:C7	21:1:1002:CLA:HED3	2.00	0.91
16:3:171:GLU:HA	16:3:174:ARG:CD	2.01	0.91
21:B:1213:CLA:CBD	21:B:1213:CLA:HBA1	2.01	0.91
7:G:92:PRO:HD2	7:G:93:GLU:H	1.34	0.91
15:2:259:HIS:CB	21:2:2003:CLA:HBC3	1.99	0.90
21:4:4001:CLA:H72	21:4:4002:CLA:H43	1.51	0.90
16:3:206:GLY:HA2	16:3:209:PHE:CZ	2.04	0.90
21:J:6015:CLA:HHC	21:J:6015:CLA:HBB1	1.51	0.90
17:4:171:ASP:HB3	27:4:4503:NEX:C12	2.01	0.90
21:4:4001:CLA:H2	26:4:4501:LUT:C37	2.00	0.90
21:4:4008:CLA:HMC1	21:4:4008:CLA:HBC2	1.53	0.90
21:2:2002:CLA:HMB2	26:2:2501:LUT:C11	2.01	0.90
7:G:141:THR:HB	25:G:2021:LMG:HC72	1.51	0.90
16:3:167:MET:HA	16:3:167:MET:CE	2.01	0.90
16:3:204:PRO:HB2	16:3:209:PHE:HA	1.54	0.90
21:3:3011:CLA:HBA2	21:3:3011:CLA:HBD	1.50	0.90
8:H:116:TYR:O	8:H:120:THR:CG2	2.19	0.90
19:G:2011:BCR:H403	19:G:2011:BCR:H23C	1.54	0.90
1:A:281:LEU:HD11	21:A:1115:CLA:HMA3	1.52	0.90
19:L:6020:BCR:H372	21:L:1503:CLA:HBC1	1.52	0.90
21:1:1013:CLA:H71	21:1:1013:CLA:C4	1.99	0.90
14:1:211:LEU:HG	21:1:1003:CLA:HED3	1.52	0.90
26:1:1502:LUT:C39	21:1:1010:CLA:HMA2	2.01	0.90
21:4:4001:CLA:C7	21:4:4002:CLA:H43	2.02	0.90
21:2:2006:CLA:H2A	21:2:2006:CLA:HED2	1.53	0.90
21:1:1010:CLA:HED2	21:1:1010:CLA:C4D	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:111:LEU:O	15:2:114:SER:OG	1.88	0.89
17:4:95:ALA:HB2	21:4:4012:CLA:CED	2.03	0.89
21:1:1010:CLA:C3	21:1:1010:CLA:H92	2.01	0.89
17:4:214:MET:HE3	21:4:4004:CLA:HHC	1.52	0.89
21:A:1125:CLA:HBB1	21:A:1133:CLA:CMA	2.02	0.89
12:L:108:PHE:CD1	12:L:200:ALA:HB2	2.07	0.89
21:1:1009:CLA:HMC1	21:1:1009:CLA:HBC3	1.55	0.89
4:D:166:TYR:HE1	4:D:170:LYS:HA	1.35	0.89
21:G:1002:CLA:HHC	21:G:1002:CLA:HBB1	1.52	0.89
12:L:102:VAL:HG23	21:L:1502:CLA:O1D	1.73	0.89
7:G:65:SER:HA	7:G:68:THR:CG2	2.03	0.89
21:4:4008:CLA:C1	21:4:4008:CLA:H3A	2.03	0.89
12:L:119:PRO:C	12:L:120:LEU:HD23	1.93	0.89
17:4:246:THR:HG21	17:4:248:VAL:HG23	1.52	0.88
1:A:38:GLY:CA	1:A:44:ILE:HG22	2.02	0.88
21:A:1104:CLA:HBB1	21:A:1127:CLA:HBB1	1.56	0.88
7:G:114:LEU:HG	7:G:116:LYS:H	1.38	0.88
21:1:1005:CLA:HMD2	21:1:1012:CLA:C1D	2.03	0.88
21:2:2006:CLA:HMC2	26:2:2502:LUT:C23	2.04	0.88
14:1:102:LEU:HG	21:1:1006:CLA:HED3	1.54	0.88
15:2:118:MET:SD	21:2:2001:CLA:HHD	2.14	0.88
7:G:116:LYS:HD3	7:G:117:SER:N	1.88	0.88
15:2:155:THR:HA	15:2:158:LEU:CD1	2.03	0.88
21:4:4002:CLA:HBB1	21:4:4002:CLA:HHC	1.55	0.88
16:3:264:PRO:HB3	21:3:3008:CLA:HMA3	1.51	0.88
21:1:1010:CLA:C3D	21:1:1010:CLA:HED2	2.03	0.88
17:4:104:MET:CE	21:4:4001:CLA:HMC3	2.03	0.88
1:A:546:ALA:O	1:A:550:HIS:ND1	2.07	0.88
12:L:201:PHE:CZ	12:L:205:TYR:CD2	2.62	0.88
1:A:544:ILE:O	1:A:548:THR:HG23	1.74	0.88
1:A:741:GLY:O	1:A:745:THR:OG1	1.90	0.88
21:1:1009:CLA:C2D	27:4:4503:NEX:H202	2.03	0.87
12:L:121:ARG:CA	12:L:122:ASN:HB2	2.03	0.87
2:B:621:ARG:NH2	2:B:622:ASP:OD2	2.07	0.87
15:2:158:LEU:HD12	15:2:159:PHE:N	1.87	0.87
1:A:474:GLN:N	1:A:474:GLN:OE1	2.08	0.87
21:2:2002:CLA:CHB	26:2:2501:LUT:H202	2.04	0.87
21:4:4001:CLA:H62	26:4:4501:LUT:H371	1.57	0.87
21:1:1009:CLA:HBB2	17:4:156:ILE:HG12	1.55	0.87
14:1:111:TRP:NE1	21:1:1013:CLA:HBA1	1.90	0.87
15:2:162:GLU:HG3	15:2:166:ILE:HD12	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:4012:CLA:C12	21:4:4012:CLA:H192	2.04	0.87
21:1:1005:CLA:OBD	21:1:1012:CLA:HBA2	1.75	0.87
21:2:2004:CLA:H42	21:2:2004:CLA:HMB2	1.57	0.87
15:2:259:HIS:CG	21:2:2003:CLA:HBC3	2.10	0.87
17:4:246:THR:CG2	21:4:4008:CLA:HED3	2.04	0.87
12:L:85:ASN:HD22	21:L:1501:CLA:HAC1	1.40	0.87
2:B:292:ARG:CZ	7:G:91:VAL:HG21	2.03	0.87
14:1:226:ILE:N	14:1:227:GLY:HA2	1.87	0.87
1:A:335:LYS:O	21:A:1141:CLA:HBC2	1.74	0.87
20:A:7003:LHG:C9	21:A:1129:CLA:HBA1	2.04	0.87
12:L:106:HIS:O	12:L:110:LEU:HD23	1.74	0.87
1:A:654:ARG:NE	1:A:655:ASP:OD1	2.07	0.87
16:3:171:GLU:HA	16:3:174:ARG:HD2	1.55	0.86
17:4:227:THR:HG21	17:4:234:ASN:CG	1.96	0.86
12:L:159:SER:H	12:L:178:THR:HG22	1.39	0.86
7:G:114:LEU:CD1	21:G:1002:CLA:HED2	2.05	0.86
6:F:170:ILE:O	6:F:174:ILE:HG13	1.74	0.86
26:1:1501:LUT:H171	21:1:1003:CLA:HBB1	1.56	0.86
21:1:1009:CLA:HHD	27:4:4503:NEX:C12	2.04	0.86
20:2:2801:LHG:C13	20:2:2801:LHG:HC81	2.00	0.86
21:1:1002:CLA:HBA2	21:1:1002:CLA:CGD	2.06	0.86
21:2:2013:CLA:HMC2	26:2:2502:LUT:H383	1.56	0.86
21:3:3009:CLA:CBA	21:3:3009:CLA:HBD	2.06	0.86
17:4:170:GLN:HG2	17:4:173:ILE:CG2	2.04	0.86
21:1:1007:CLA:C7	21:1:1007:CLA:H41	2.01	0.86
21:4:4010:CLA:HMC3	21:4:4013:CLA:HAB	1.57	0.86
21:2:2003:CLA:HBC2	21:2:2003:CLA:HHD	1.55	0.86
16:3:204:PRO:CG	16:3:211:PRO:HD2	2.05	0.86
2:B:246:THR:CG2	2:B:248:GLN:HG2	2.06	0.86
7:G:74:LEU:CA	7:G:78:VAL:HG12	2.06	0.86
21:1:1001:CLA:H61	21:1:1002:CLA:HAC2	1.57	0.86
21:1:1002:CLA:HED3	21:1:1002:CLA:H72	1.54	0.86
16:3:109:ASN:HB3	21:3:3012:CLA:O2D	1.76	0.86
26:1:1502:LUT:H171	21:1:1004:CLA:H101	1.58	0.86
15:2:83:GLY:N	15:2:88:ASP:OD2	2.08	0.86
21:1:1009:CLA:CMD	27:4:4503:NEX:H11	2.06	0.85
14:1:202:GLN:HE22	14:1:208:THR:N	1.74	0.85
14:1:66:LEU:HD23	21:1:1004:CLA:H42	1.57	0.85
4:D:198:PRO:HA	4:D:199:ILE:HG13	1.55	0.85
21:2:2009:CLA:HMB1	21:2:2009:CLA:HBB1	1.56	0.85
7:G:141:THR:CB	25:G:2021:LMG:HC72	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:150:SER:O	14:1:152:GLU:N	2.09	0.85
21:2:2002:CLA:HHB	26:2:2501:LUT:C20	2.06	0.85
8:H:135:PRO:CD	8:H:136:PRO:HD2	2.05	0.85
21:1:1001:CLA:C6	21:1:1002:CLA:HAC2	2.05	0.85
12:L:145:LEU:CD2	19:L:6019:BCR:H392	2.01	0.85
21:2:2002:CLA:HMA2	21:2:2002:CLA:CGA	2.07	0.85
12:L:90:ARG:HH21	21:L:1501:CLA:HAC2	1.42	0.85
12:L:86:LEU:HD11	21:L:1501:CLA:HMC3	1.58	0.85
7:G:73:PHE:CE1	7:G:77:PHE:CD2	2.64	0.85
7:G:94:GLN:NE2	7:G:98:GLY:H	1.75	0.85
15:2:118:MET:HB2	26:2:2501:LUT:H35	1.58	0.85
17:4:199:THR:CA	17:4:200:LEU:HD22	2.06	0.85
7:G:73:PHE:CE1	7:G:77:PHE:HD2	1.94	0.85
4:D:130:LEU:HD23	4:D:131:LYS:N	1.91	0.85
26:1:1501:LUT:H393	21:1:1001:CLA:H43	1.58	0.85
1:A:342:GLY:CA	1:A:431:LEU:HD21	2.07	0.85
15:2:112:VAL:HG21	15:2:173:ARG:NH1	1.92	0.85
7:G:103:ALA:O	7:G:105:ASP:N	2.10	0.85
8:H:58:PHE:HE1	8:H:60:LEU:HD11	1.41	0.85
21:1:1009:CLA:C1D	21:4:4005:CLA:HAC1	2.06	0.85
17:4:169:ASN:HB3	27:4:4503:NEX:C17	2.07	0.85
14:1:131:LEU:HG	14:1:135:LEU:HD11	1.59	0.84
26:1:1501:LUT:H403	21:1:1001:CLA:CAB	2.07	0.84
17:4:169:ASN:ND2	27:4:4503:NEX:H173	1.90	0.84
17:4:190:ILE:N	21:4:4014:CLA:O2A	2.10	0.84
16:3:183:SER:H	16:3:184:MET:CE	1.90	0.84
1:A:342:GLY:HA2	1:A:431:LEU:CD2	2.06	0.84
14:1:177:PHE:O	14:1:181:LYS:HG3	1.78	0.84
15:2:222:GLU:OE2	21:2:2007:CLA:H43	1.77	0.84
21:3:3012:CLA:HBD	21:3:3012:CLA:CGA	2.06	0.84
21:1:1004:CLA:H92	21:1:1005:CLA:HHB	1.56	0.84
14:1:198:ILE:O	14:1:202:GLN:HG2	1.77	0.84
2:B:292:ARG:CZ	7:G:107:ARG:NH2	2.40	0.84
16:3:214:PHE:CZ	21:3:3001:CLA:C3D	2.60	0.84
1:A:434:ARG:HA	1:A:437:ARG:HB2	1.58	0.84
21:1:1006:CLA:HMB2	21:1:1013:CLA:H2	1.58	0.84
26:1:1501:LUT:C38	21:1:1001:CLA:HBA1	2.08	0.84
17:4:170:GLN:HG2	17:4:173:ILE:HB	1.60	0.84
6:F:202:LEU:HD12	6:F:205:ARG:HA	1.58	0.84
13:N:159:LYS:NZ	13:N:162:CYS:SG	2.51	0.84
16:3:160:PHE:HE1	16:3:164:MET:HE3	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:4001:CLA:H52	21:4:4002:CLA:O1A	1.77	0.84
21:4:4003:CLA:CBB	26:4:4501:LUT:H182	2.08	0.84
1:A:323:ILE:HG12	21:A:1121:CLA:HMD1	1.60	0.84
4:D:198:PRO:HA	4:D:199:ILE:CG1	2.07	0.84
26:1:1501:LUT:H24	21:1:1001:CLA:HBA2	1.58	0.83
21:1:1006:CLA:CMB	21:1:1013:CLA:HMA3	2.07	0.83
21:4:4005:CLA:CED	21:4:4005:CLA:H2A	2.07	0.83
14:1:101:GLY:O	14:1:102:LEU:HD23	1.76	0.83
1:A:429:ASN:HD21	1:A:431:LEU:HB2	1.42	0.83
15:2:234:ALA:O	15:2:238:VAL:HG23	1.78	0.83
14:1:211:LEU:HD21	21:1:1003:CLA:CGD	2.08	0.83
17:4:103:ALA:O	17:4:107:VAL:HG12	1.77	0.83
21:4:4004:CLA:H171	21:4:4004:CLA:H141	1.60	0.83
14:1:146:GLU:CD	14:1:149:ARG:HH11	1.80	0.83
15:2:152:PHE:HB3	17:4:243:TRP:CZ3	2.13	0.83
7:G:93:GLU:OE1	7:G:99:THR:OG1	1.94	0.83
15:2:259:HIS:HB3	21:2:2003:CLA:CBC	2.08	0.83
21:B:1226:CLA:H122	21:B:1226:CLA:H91	1.60	0.83
12:L:111:VAL:O	12:L:115:VAL:HG23	1.78	0.83
1:A:43:THR:HA	1:A:46:LYS:HE3	1.60	0.83
21:1:1013:CLA:O1A	21:1:1013:CLA:HMA2	1.79	0.83
15:2:121:ALA:O	15:2:124:ILE:HG22	1.78	0.83
16:3:210:ASN:OD1	16:3:211:PRO:HD3	1.78	0.83
21:4:4003:CLA:O1A	21:4:4008:CLA:HED2	1.78	0.83
21:4:4002:CLA:HMB2	26:4:4501:LUT:C15	2.09	0.83
12:L:85:ASN:HD22	21:L:1501:CLA:CAC	1.91	0.83
13:N:168:TRP:CD1	16:3:262:ALA:HB2	2.14	0.83
15:2:113:HIS:CD2	21:2:2012:CLA:HMD1	2.14	0.83
21:4:4001:CLA:H52	21:4:4002:CLA:CGA	2.09	0.83
26:1:1501:LUT:H173	21:1:1003:CLA:C2B	2.08	0.83
12:L:176:LEU:HD12	12:L:176:LEU:O	1.78	0.83
20:1:1801:LHG:H201	20:1:1801:LHG:H383	1.61	0.83
5:E:68:PRO:HG2	5:E:93:VAL:HG21	1.60	0.83
21:1:1003:CLA:C6	20:1:1801:LHG:H191	2.08	0.82
15:2:87:GLY:C	21:2:2004:CLA:HED1	1.99	0.82
23:A:9011:CL0:H13	21:A:9012:CLA:OBD	1.78	0.82
7:G:91:VAL:HB	7:G:92:PRO:HB3	1.61	0.82
21:A:1132:CLA:HBC2	21:B:1206:CLA:HBB2	1.59	0.82
7:G:114:LEU:HD22	7:G:119:ALA:C	2.00	0.82
14:1:218:LEU:O	14:1:221:PRO:HD2	1.79	0.82
14:1:211:LEU:CD2	21:1:1003:CLA:HED3	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:1303:CLA:CED	21:F:1303:CLA:H12	2.09	0.82
26:1:1501:LUT:H393	21:1:1001:CLA:C4	2.08	0.82
15:2:171:GLY:C	21:4:4009:CLA:HED1	1.98	0.82
21:4:4006:CLA:HBC3	21:4:4006:CLA:CHD	2.07	0.82
17:4:151:PHE:CD2	21:4:4012:CLA:HMC3	2.15	0.82
14:1:211:LEU:CG	21:1:1003:CLA:HED3	2.09	0.82
17:4:190:ILE:O	17:4:193:PRO:HD3	1.80	0.82
17:4:247:ILE:CD1	21:4:4003:CLA:HMD1	2.09	0.82
21:1:1005:CLA:HMD2	21:1:1012:CLA:ND	1.94	0.82
21:1:1014:CLA:HMC1	21:1:1014:CLA:CBC	2.10	0.82
21:4:4006:CLA:HBC3	21:4:4006:CLA:HHD	1.59	0.82
12:L:86:LEU:CD1	21:L:1501:CLA:HMC3	2.09	0.82
21:2:2011:CLA:HMC1	21:2:2011:CLA:HBC2	1.58	0.82
1:A:441:ALA:HB1	21:A:1130:CLA:HED1	1.62	0.82
6:F:181:TYR:OH	6:F:198:ILE:HG22	1.80	0.82
21:2:2008:CLA:HMD2	16:3:162:LEU:HD13	1.61	0.82
17:4:110:MET:HB3	26:4:4502:LUT:C38	2.10	0.82
1:A:401:TRP:CD1	21:A:1126:CLA:HAB	2.15	0.82
12:L:82:TYR:OH	21:L:1501:CLA:HBB2	1.79	0.82
21:1:1001:CLA:H61	21:1:1002:CLA:HHD	1.60	0.82
14:1:197:GLY:O	14:1:201:GLN:HG3	1.80	0.82
21:3:3010:CLA:HBC2	21:3:3010:CLA:CHD	2.10	0.82
7:G:130:ILE:O	7:G:134:VAL:HG23	1.79	0.82
7:G:120:ALA:HB3	7:G:123:ASP:OD1	1.78	0.82
21:2:2001:CLA:CHD	26:2:2501:LUT:H393	2.09	0.82
21:4:4002:CLA:HAC2	21:4:4007:CLA:HBB	1.61	0.82
21:4:4011:CLA:H122	21:4:4011:CLA:C7	2.09	0.82
4:D:104:THR:HG22	4:D:129:LEU:HD23	1.59	0.82
21:1:1013:CLA:H72	21:1:1014:CLA:CBB	2.09	0.81
1:A:457:SER:HB3	1:A:544:ILE:HD13	1.61	0.81
15:2:155:THR:H	15:2:158:LEU:HD21	1.44	0.81
21:3:3009:CLA:CHC	21:3:3009:CLA:HBB1	2.07	0.81
20:A:7003:LHG:H252	21:A:1129:CLA:C5	2.11	0.81
5:E:103:VAL:HG11	5:E:124:GLU:OE2	1.80	0.81
14:1:85:ARG:NH2	14:1:184:GLU:OE2	2.13	0.81
21:4:4011:CLA:HAA1	21:4:4011:CLA:HBD	1.63	0.81
21:F:1303:CLA:HMD2	21:4:4012:CLA:C1D	2.11	0.81
26:4:4501:LUT:H201	26:4:4501:LUT:C35	2.08	0.81
21:B:1223:CLA:HED1	21:B:1231:CLA:HAB	1.62	0.81
14:1:133:THR:O	14:1:137:ILE:HG23	1.81	0.81
21:A:1129:CLA:O1D	12:L:57:VAL:HG11	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:64:ILE:O	7:G:68:THR:HG22	1.79	0.81
21:1:1009:CLA:HMB1	21:4:4015:CLA:CAD	2.11	0.81
21:2:2003:CLA:C4	21:2:2003:CLA:H71	2.04	0.81
20:2:2801:LHG:O10	20:2:2801:LHG:H141	1.80	0.81
21:1:1009:CLA:C1D	27:4:4503:NEX:H202	2.10	0.81
15:2:161:VAL:HG12	15:2:165:PHE:CE2	2.15	0.81
15:2:115:ARG:NH1	21:2:2011:CLA:OBD	2.13	0.81
12:L:120:LEU:HD12	12:L:126:ALA:CB	2.09	0.81
21:1:1006:CLA:HBA1	21:1:1014:CLA:C3C	2.10	0.81
8:H:65:ASN:HA	8:H:70:TRP:HD1	1.46	0.81
14:1:186:LYS:HZ3	21:1:1007:CLA:CED	1.93	0.81
21:3:3012:CLA:CHD	21:3:3012:CLA:HBC2	2.10	0.81
21:4:4012:CLA:HBB1	21:4:4012:CLA:CHC	2.10	0.81
17:4:190:ILE:H	21:4:4014:CLA:CBA	1.93	0.81
1:A:328:LYS:O	1:A:332:GLU:HG3	1.79	0.81
4:D:197:SER:O	4:D:199:ILE:HG23	1.81	0.81
20:1:1801:LHG:H383	20:1:1801:LHG:H202	1.59	0.81
15:2:118:MET:CE	21:2:2001:CLA:HHD	2.11	0.81
21:4:4001:CLA:C6	21:4:4002:CLA:H12	2.10	0.81
13:N:161:LYS:HE3	13:N:168:TRP:CZ3	2.15	0.81
16:3:264:PRO:HB3	21:3:3008:CLA:CMA	2.11	0.81
21:1:1001:CLA:H42	21:1:1002:CLA:HBC2	1.63	0.80
21:1:1013:CLA:H111	21:1:1013:CLA:H162	1.61	0.80
21:2:2001:CLA:C1D	26:2:2501:LUT:H393	2.11	0.80
21:4:4012:CLA:H122	21:4:4012:CLA:H192	1.61	0.80
21:4:4001:CLA:H61	21:4:4002:CLA:C4	2.10	0.80
2:B:77:TRP:HA	2:B:84:VAL:HG11	1.63	0.80
21:4:4012:CLA:H192	21:4:4012:CLA:C15	2.12	0.80
21:B:1226:CLA:H142	21:B:1226:CLA:H101	1.61	0.80
21:G:1002:CLA:HBC2	21:G:1002:CLA:CHD	2.11	0.80
16:3:171:GLU:HA	16:3:174:ARG:CG	2.10	0.80
7:G:76:ARG:HH12	21:G:1002:CLA:CHC	1.94	0.80
4:D:199:ILE:HD13	4:D:201:VAL:CG2	2.09	0.80
12:L:121:ARG:HH11	12:L:121:ARG:HG3	1.47	0.80
11:K:67:ALA:HA	11:K:70:PHE:HB2	1.63	0.80
21:4:4011:CLA:H122	21:4:4011:CLA:H71	1.64	0.80
2:B:292:ARG:NH2	7:G:107:ARG:NH2	2.30	0.80
1:A:43:THR:CA	1:A:46:LYS:CE	2.57	0.80
21:4:4011:CLA:H202	21:4:4011:CLA:H143	1.62	0.80
7:G:114:LEU:HD12	21:G:1002:CLA:CED	2.10	0.80
21:G:1001:CLA:HMC1	21:G:1001:CLA:CBC	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:170:GLN:CG	17:4:173:ILE:HB	2.12	0.80
21:J:6014:CLA:H2	21:J:6014:CLA:HBA2	1.64	0.80
21:4:4012:CLA:HMC1	21:4:4012:CLA:HBC2	1.63	0.80
21:H:1000:CLA:HMB2	21:L:1501:CLA:HAA1	1.62	0.80
17:4:199:THR:OG1	17:4:200:LEU:HB2	1.82	0.80
21:4:4001:CLA:H52	21:4:4002:CLA:H12	1.64	0.80
14:1:46:PRO:HD3	21:4:4005:CLA:CBA	2.11	0.80
21:F:1303:CLA:O2D	21:F:1303:CLA:H12	1.81	0.80
21:B:1226:CLA:H122	21:B:1226:CLA:C9	2.12	0.80
15:2:110:GLU:HB2	21:2:2004:CLA:C1B	2.12	0.79
21:2:2008:CLA:HBC3	21:2:2008:CLA:CHD	2.12	0.79
1:A:434:ARG:H	1:A:437:ARG:HG3	1.46	0.79
1:A:429:ASN:ND2	1:A:431:LEU:HB2	1.96	0.79
21:1:1001:CLA:C5	21:1:1002:CLA:HAC2	2.12	0.79
7:G:114:LEU:HD12	21:G:1002:CLA:CGD	2.12	0.79
15:2:153:THR:HG21	17:4:243:TRP:O	1.82	0.79
7:G:73:PHE:HD1	7:G:77:PHE:CD2	1.96	0.79
26:1:1502:LUT:C17	21:1:1004:CLA:H62	2.10	0.79
15:2:161:VAL:HG12	15:2:165:PHE:CD2	2.16	0.79
16:3:157:TYR:CE1	21:3:3010:CLA:HBC1	2.16	0.79
16:3:161:VAL:O	16:3:165:ALA:HB2	1.82	0.79
14:1:100:LEU:HD21	21:1:1014:CLA:HAA1	1.63	0.79
14:1:131:LEU:HD23	14:1:132:PRO:N	1.98	0.79
21:B:9010:CLA:HMB3	21:B:9022:CLA:OBD	1.81	0.79
7:G:127:TRP:O	7:G:130:ILE:HG22	1.81	0.79
20:1:1801:LHG:H172	20:1:1801:LHG:H212	1.65	0.79
21:2:2002:CLA:CMB	26:2:2501:LUT:H191	2.13	0.79
17:4:190:ILE:H	21:4:4014:CLA:CGA	1.95	0.79
21:A:9012:CLA:O1D	21:B:9010:CLA:H52	1.83	0.79
21:1:1010:CLA:HBA1	21:1:1010:CLA:H2	1.65	0.79
15:2:118:MET:HB2	26:2:2501:LUT:C35	2.12	0.79
1:A:43:THR:HA	1:A:46:LYS:CE	2.12	0.79
14:1:223:HIS:NE2	21:1:1003:CLA:HBD	1.98	0.79
21:1:1011:CLA:H71	21:1:1011:CLA:H2	1.63	0.79
21:2:2004:CLA:HMC2	26:2:2502:LUT:C11	2.13	0.79
17:4:110:MET:HB3	26:4:4502:LUT:H382	1.63	0.79
21:1:1006:CLA:HMB1	21:1:1013:CLA:HMA3	1.64	0.78
14:1:111:TRP:HE1	21:1:1013:CLA:CBA	1.94	0.78
17:4:110:MET:HE1	17:4:217:PHE:CE1	2.17	0.78
21:2:2009:CLA:C2A	21:2:2009:CLA:HED2	2.13	0.78
19:B:6004:BCR:HC7	21:B:1218:CLA:HMD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:4002:CLA:HMB2	26:4:4501:LUT:H15	1.65	0.78
2:B:29:HIS:HB2	21:B:1226:CLA:O1A	1.84	0.78
3:C:22:PRO:O	4:D:139:LEU:HD23	1.84	0.78
21:2:2003:CLA:C14	21:2:2003:CLA:H72	2.10	0.78
14:1:140:LEU:O	14:1:140:LEU:HD12	1.83	0.78
16:3:164:MET:SD	21:3:3012:CLA:HAC1	2.23	0.78
1:A:43:THR:CA	1:A:46:LYS:HG3	2.13	0.78
14:1:149:ARG:HG3	21:1:1011:CLA:CHD	2.13	0.78
15:2:157:THR:O	15:2:161:VAL:HG23	1.83	0.78
21:2:2003:CLA:HMC2	26:2:2501:LUT:O3	1.82	0.78
20:2:2801:LHG:C23	20:2:2801:LHG:H141	2.14	0.78
21:4:4002:CLA:C4C	21:4:4007:CLA:HMB2	2.13	0.78
19:L:6019:BCR:C8	19:L:6019:BCR:H331	2.12	0.78
21:2:2001:CLA:C1B	21:2:2014:CLA:HMA2	2.12	0.78
21:4:4002:CLA:C3C	21:4:4007:CLA:HMB2	2.13	0.78
21:4:4002:CLA:CHD	21:4:4007:CLA:HMB2	2.14	0.78
21:4:4002:CLA:H11	26:4:4501:LUT:H392	1.66	0.78
21:A:1132:CLA:HBC1	21:B:1206:CLA:HBB2	1.64	0.78
17:4:199:THR:CB	17:4:200:LEU:HB2	2.13	0.78
21:1:1006:CLA:HMB2	21:1:1013:CLA:C2	2.13	0.78
15:2:92:ASP:OD1	15:2:95:GLY:N	2.16	0.78
21:4:4004:CLA:C7	21:4:4004:CLA:H41	2.06	0.78
21:B:1228:CLA:HBC3	21:B:1228:CLA:CHD	2.13	0.78
1:A:222:GLN:HA	1:A:226:SER:HB2	1.63	0.78
21:2:2003:CLA:C9	21:2:2003:CLA:H52	2.13	0.78
21:2:2012:CLA:HBC2	21:2:2012:CLA:CHD	2.14	0.78
21:2:2014:CLA:CGA	21:2:2014:CLA:H3A	2.13	0.78
17:4:238:HIS:O	17:4:242:PRO:HG3	1.84	0.78
20:A:7003:LHG:HC92	21:A:1129:CLA:HBA1	1.66	0.78
21:L:1503:CLA:HBB1	21:L:1503:CLA:CHC	2.13	0.78
2:B:292:ARG:NH1	7:G:107:ARG:NH2	2.31	0.78
13:N:160:PHE:CD1	13:N:161:LYS:HA	2.19	0.78
21:J:1302:CLA:H52	21:J:6014:CLA:HMA3	1.65	0.78
1:A:204:ASN:HD21	1:A:317:TYR:HB2	1.49	0.78
12:L:164:LEU:N	12:L:164:LEU:HD23	1.99	0.78
4:D:100:PHE:CZ	4:D:158:VAL:HG11	2.18	0.78
21:1:1009:CLA:HMD2	27:4:4503:NEX:H11	1.66	0.78
21:4:4001:CLA:H61	21:4:4002:CLA:H12	1.66	0.78
21:4:4004:CLA:CMB	21:4:4004:CLA:HBB1	2.06	0.78
6:F:202:LEU:CD1	6:F:205:ARG:HA	2.14	0.78
12:L:109:PHE:HE1	21:L:1503:CLA:C1C	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:4002:CLA:HHC	21:4:4002:CLA:CBB	2.13	0.77
1:A:378:SER:OG	21:A:1125:CLA:HMC1	1.83	0.77
7:G:105:ASP:CA	7:G:106:GLU:HB3	2.13	0.77
21:4:4011:CLA:HBC2	21:4:4011:CLA:CHD	2.09	0.77
21:B:1227:CLA:HBA2	21:B:1240:CLA:H42	1.65	0.77
13:N:161:LYS:HG3	13:N:167:PHE:HD2	1.45	0.77
26:4:4501:LUT:H181	26:4:4501:LUT:C8	2.06	0.77
7:G:107:ARG:HA	7:G:108:ALA:HB3	1.66	0.77
15:2:83:GLY:HA2	15:2:88:ASP:CB	2.15	0.77
15:2:259:HIS:NE2	21:2:2003:CLA:HMD2	2.00	0.77
5:E:66:ILE:HG22	5:E:67:GLY:H	1.49	0.77
1:A:43:THR:O	1:A:46:LYS:CD	2.32	0.77
14:1:88:MET:CE	21:1:1001:CLA:HHC	2.15	0.77
21:1:1013:CLA:H71	21:1:1013:CLA:H41	1.65	0.77
16:3:214:PHE:HZ	21:3:3001:CLA:C3D	1.97	0.77
17:4:246:THR:HG22	17:4:248:VAL:HG23	1.66	0.77
21:A:1117:CLA:H203	21:A:1125:CLA:HBA2	1.66	0.77
14:1:82:ILE:HD13	21:1:1012:CLA:C3D	2.14	0.77
21:4:4001:CLA:C2	26:4:4501:LUT:H373	2.06	0.77
8:H:63:ILE:HD12	12:L:170:LYS:HE3	1.66	0.77
26:1:1501:LUT:H382	21:1:1001:CLA:CBA	2.13	0.77
17:4:104:MET:HE2	21:4:4001:CLA:HMC3	1.67	0.77
23:A:9011:CL0:H13	21:A:9012:CLA:CAD	2.14	0.77
21:1:1006:CLA:HBA1	21:1:1014:CLA:C1C	2.15	0.77
21:1:1010:CLA:CHD	21:1:1010:CLA:HBC2	2.11	0.77
26:2:2501:LUT:H391	26:2:2501:LUT:C32	2.15	0.77
21:4:4011:CLA:CMB	21:4:4011:CLA:HBB1	2.04	0.77
21:1:1009:CLA:HBD	21:1:1009:CLA:HAA1	1.66	0.76
14:1:130:THR:O	14:1:134:ILE:HG13	1.85	0.76
15:2:150:GLU:CB	21:2:2006:CLA:HMB1	2.14	0.76
16:3:163:GLU:OE2	21:3:3013:CLA:HMC3	1.85	0.76
26:1:1501:LUT:H403	21:1:1001:CLA:HAB	1.66	0.76
21:4:4001:CLA:C4	21:4:4002:CLA:HBA1	2.14	0.76
21:4:4001:CLA:H61	21:4:4002:CLA:H43	1.67	0.76
21:A:1129:CLA:H3A	21:A:1129:CLA:O1A	1.85	0.76
1:A:739:LEU:O	1:A:743:ILE:HG13	1.85	0.76
21:L:1503:CLA:CHA	21:L:1503:CLA:HBA1	2.15	0.76
7:G:124:VAL:HG22	21:G:1002:CLA:HMD3	1.66	0.76
21:3:3010:CLA:HMA3	21:3:3014:CLA:O1D	1.84	0.76
17:4:82:LEU:HD12	21:4:4004:CLA:H43	1.67	0.76
21:J:6015:CLA:HHC	21:J:6015:CLA:CBB	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:91:TYR:HB2	13:N:94:LYS:HA	1.66	0.76
15:2:160:ILE:O	15:2:164:VAL:HG23	1.85	0.76
21:1:1002:CLA:HED2	21:1:1002:CLA:OBD	1.84	0.76
21:1:1013:CLA:HBC2	21:1:1013:CLA:CHD	2.15	0.76
21:2:2008:CLA:HMD2	16:3:162:LEU:HD12	1.68	0.76
21:4:4006:CLA:HAC2	21:4:4013:CLA:C2C	2.15	0.76
4:D:104:THR:HG22	4:D:129:LEU:CD2	2.15	0.76
8:H:58:PHE:CD1	8:H:60:LEU:HD11	2.21	0.76
17:4:238:HIS:NE2	21:4:4003:CLA:O1D	2.18	0.76
19:A:6008:BCR:C35	21:A:1125:CLA:HED1	2.16	0.76
21:A:9012:CLA:O1D	21:B:9010:CLA:H71	1.86	0.76
21:1:1002:CLA:C5	21:1:1002:CLA:HED3	2.16	0.76
15:2:83:GLY:HA2	15:2:88:ASP:HB3	1.66	0.76
17:4:146:GLU:O	17:4:151:PHE:HB2	1.85	0.76
20:A:7001:LHG:H252	21:A:1128:CLA:C4	2.13	0.76
7:G:91:VAL:HB	7:G:92:PRO:CA	2.16	0.76
21:1:1013:CLA:C3D	21:1:1013:CLA:H91	2.15	0.75
21:2:2003:CLA:H52	21:2:2003:CLA:H92	1.66	0.75
20:1:1801:LHG:H211	17:4:148:ILE:HG12	1.67	0.75
23:A:9011:CL0:H15	23:A:9011:CL0:CHC	2.16	0.75
1:A:343:HIS:H	1:A:431:LEU:CD2	1.99	0.75
14:1:211:LEU:HD11	21:1:1003:CLA:O1D	1.86	0.75
15:2:152:PHE:O	15:2:153:THR:HG23	1.86	0.75
17:4:95:ALA:HA	21:4:4012:CLA:HED3	1.66	0.75
21:B:1220:CLA:HAB	21:B:1227:CLA:HMD2	1.67	0.75
20:B:7004:LHG:H242	21:B:1227:CLA:C7	2.16	0.75
21:F:1303:CLA:HHD	21:F:1303:CLA:HBC2	1.67	0.75
21:L:1501:CLA:HBB1	21:L:1501:CLA:CHC	2.16	0.75
12:L:120:LEU:HB2	12:L:126:ALA:CB	2.16	0.75
21:4:4002:CLA:O2D	21:4:4002:CLA:HBA2	1.87	0.75
21:A:9012:CLA:HMD3	21:B:9010:CLA:O1A	1.85	0.75
14:1:173:ASP:OD1	14:1:173:ASP:N	2.19	0.75
21:2:2003:CLA:CBC	21:2:2003:CLA:HHD	2.16	0.75
21:3:3011:CLA:CBD	21:3:3011:CLA:HBA2	2.14	0.75
21:3:3011:CLA:HMB1	21:3:3011:CLA:HBB1	1.66	0.75
17:4:243:TRP:CD1	21:4:4008:CLA:HMA1	2.22	0.75
1:A:343:HIS:H	1:A:431:LEU:HD23	1.52	0.75
14:1:94:ILE:HG22	14:1:105:TRP:CB	2.15	0.75
21:2:2002:CLA:HBA1	26:2:2501:LUT:H15	1.68	0.75
21:B:1226:CLA:C14	21:B:1226:CLA:H101	2.16	0.75
12:L:203:LEU:O	12:L:207:LEU:N	2.20	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:205:TYR:O	12:L:206:VAL:HG23	1.87	0.75
13:N:162:CYS:O	13:N:167:PHE:HB2	1.87	0.75
14:1:74:GLU:OE1	14:1:159:LYS:NZ	2.20	0.75
15:2:228:ILE:O	15:2:232:ARG:HG3	1.87	0.75
16:3:159:LEU:HD13	21:3:3013:CLA:C1D	2.17	0.75
21:2:2011:CLA:CBC	21:2:2011:CLA:HMC1	2.16	0.75
1:A:200:GLU:O	1:A:204:ASN:ND2	2.19	0.75
14:1:133:THR:O	14:1:136:VAL:HG22	1.86	0.75
3:C:78:GLY:HA2	4:D:134:ARG:NH1	2.02	0.75
14:1:60:GLY:O	21:1:1009:CLA:H43	1.87	0.74
21:A:1119:CLA:HMB2	21:A:1123:CLA:HMA3	1.67	0.74
10:J:2:ARG:NH2	21:2:2005:CLA:H43	2.03	0.74
21:4:4002:CLA:CGA	21:4:4002:CLA:HMA2	2.17	0.74
21:B:1227:CLA:H193	21:B:1236:CLA:H52	1.67	0.74
21:B:1227:CLA:H8	21:B:1240:CLA:H11	1.69	0.74
21:2:2013:CLA:CHC	21:2:2013:CLA:HBB1	2.12	0.74
7:G:105:ASP:HA	7:G:106:GLU:CB	2.14	0.74
17:4:170:GLN:HG2	17:4:173:ILE:HG21	1.69	0.74
12:L:145:LEU:HB3	12:L:186:THR:HG22	1.69	0.74
13:N:117:ALA:O	13:N:119:THR:N	2.18	0.74
21:2:2005:CLA:O1D	21:2:2012:CLA:H61	1.87	0.74
12:L:144:CYS:HB3	19:L:6019:BCR:H19C	1.69	0.74
2:B:621:ARG:HH21	2:B:622:ASP:CG	1.90	0.74
5:E:76:ILE:C	5:E:77:LEU:HD12	2.07	0.74
16:3:160:PHE:HE1	16:3:164:MET:CE	1.98	0.74
12:L:119:PRO:O	12:L:120:LEU:HD23	1.87	0.74
21:1:1002:CLA:O1A	21:1:1002:CLA:HMA2	1.88	0.74
15:2:168:TRP:HE1	21:2:2011:CLA:CBB	2.01	0.74
15:2:235:MET:HE3	21:2:2004:CLA:CMC	2.17	0.74
17:4:179:LEU:N	21:4:4014:CLA:HMA1	2.03	0.74
4:D:166:TYR:CE1	4:D:170:LYS:HA	2.22	0.74
15:2:74:GLY:O	16:3:176:GLN:NE2	2.21	0.74
17:4:217:PHE:CG	26:4:4502:LUT:H402	2.23	0.74
21:4:4001:CLA:H101	21:4:4002:CLA:C4	2.18	0.74
21:4:4012:CLA:C19	21:4:4012:CLA:H122	2.18	0.74
17:4:170:GLN:HE22	21:4:4014:CLA:C1C	2.00	0.74
21:4:4004:CLA:HAB	26:4:4502:LUT:H203	1.70	0.74
8:H:135:PRO:HG2	8:H:136:PRO:CD	2.18	0.74
3:C:23:THR:O	4:D:135:LYS:HE2	1.87	0.74
21:1:1009:CLA:H93	21:1:1009:CLA:C12	2.16	0.74
21:3:3008:CLA:HHC	21:3:3008:CLA:CBB	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:109:ALA:CA	21:2:2012:CLA:HED3	2.17	0.73
21:2:2002:CLA:C3A	26:2:2501:LUT:H201	2.16	0.73
20:B:7004:LHG:H321	20:B:7004:LHG:C18	2.18	0.73
21:2:2008:CLA:C17	21:2:2008:CLA:H143	2.18	0.73
7:G:91:VAL:HB	7:G:92:PRO:CB	2.18	0.73
15:2:124:ILE:HD11	26:2:2501:LUT:H172	1.71	0.73
21:4:4011:CLA:H101	27:4:4503:NEX:H382	1.71	0.73
4:D:167:LEU:HD12	4:D:167:LEU:O	1.89	0.73
21:2:2003:CLA:H143	21:2:2003:CLA:C10	2.18	0.73
21:3:3009:CLA:O1A	21:3:3009:CLA:H2A	1.88	0.73
20:B:7004:LHG:H181	20:B:7004:LHG:H341	1.69	0.73
7:G:94:GLN:HE21	7:G:94:GLN:CA	2.01	0.73
7:G:61:SER:HB2	21:G:1001:CLA:OBD	1.88	0.73
21:3:3011:CLA:HBC2	21:3:3011:CLA:CHD	2.17	0.73
17:4:170:GLN:HG2	17:4:173:ILE:CB	2.19	0.73
21:4:4001:CLA:C5	21:4:4002:CLA:H12	2.19	0.73
21:4:4001:CLA:C6	21:4:4002:CLA:H43	2.18	0.73
21:A:1126:CLA:H192	21:A:9012:CLA:H161	1.70	0.73
21:F:1303:CLA:HMD2	21:4:4012:CLA:CHD	2.18	0.73
12:L:109:PHE:HE1	21:L:1503:CLA:C2C	1.97	0.73
13:N:115:ALA:HB1	13:N:122:PHE:HB2	1.71	0.73
12:L:91:THR:HG21	12:L:174:ASP:OD1	1.88	0.73
21:1:1009:CLA:HMD1	20:1:1801:LHG:HC12	1.69	0.73
21:2:2002:CLA:H71	26:2:2501:LUT:H362	1.70	0.73
21:3:3010:CLA:HBA1	21:3:3010:CLA:CBD	2.19	0.73
21:A:1129:CLA:HMB2	21:A:1130:CLA:C2D	2.19	0.73
12:L:90:ARG:NH2	21:L:1501:CLA:HAC2	2.03	0.73
21:1:1001:CLA:C4	21:1:1002:CLA:HAC2	2.19	0.73
21:1:1002:CLA:CED	21:1:1002:CLA:H72	2.17	0.73
15:2:257:PHE:CE1	21:2:2008:CLA:H42	2.24	0.73
17:4:149:LEU:HB3	27:4:4503:NEX:H361	1.71	0.73
2:B:166:SER:CB	7:G:102:ASP:HB2	2.19	0.73
12:L:120:LEU:HB2	12:L:126:ALA:HB3	1.69	0.73
21:2:2006:CLA:HMC2	26:2:2502:LUT:H222	1.68	0.73
21:4:4001:CLA:H61	21:4:4002:CLA:C1	2.19	0.73
7:G:116:LYS:N	21:G:1002:CLA:HMA3	2.03	0.73
26:2:2502:LUT:H28	26:2:2502:LUT:H371	1.70	0.73
21:3:3010:CLA:HMA3	21:3:3014:CLA:CGD	2.19	0.73
21:4:4004:CLA:CHC	26:4:4502:LUT:H193	2.19	0.73
21:A:1129:CLA:HMA2	12:L:71:THR:HG21	1.70	0.73
26:1:1501:LUT:H382	21:1:1001:CLA:CGA	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:202:GLN:HE22	14:1:208:THR:CA	2.02	0.72
21:F:1301:CLA:HHC	21:F:1301:CLA:HBB1	1.70	0.72
17:4:169:ASN:HB3	27:4:4503:NEX:H173	1.71	0.72
1:A:209:GLY:HA2	21:A:1118:CLA:HBC1	1.70	0.72
1:A:232:PHE:HB3	1:A:237:VAL:HG11	1.70	0.72
21:1:1013:CLA:C11	21:1:1013:CLA:H162	2.20	0.72
15:2:152:PHE:HE2	21:2:2006:CLA:H62	1.52	0.72
15:2:155:THR:HG22	15:2:156:THR:N	2.04	0.72
16:3:173:ARG:HB3	21:3:3011:CLA:HBC3	1.70	0.72
21:3:3008:CLA:CHC	21:3:3008:CLA:HBB1	2.18	0.72
16:3:176:GLN:HA	16:3:176:GLN:OE1	1.88	0.72
6:F:207:VAL:HG23	6:F:208:PHE:H	1.54	0.72
7:G:99:THR:HG23	7:G:100:HIS:N	2.04	0.72
21:G:1001:CLA:HBB1	21:G:1001:CLA:HHC	1.71	0.72
17:4:227:THR:HG21	17:4:234:ASN:OD1	1.88	0.72
21:4:4003:CLA:H72	21:4:4003:CLA:H41	1.71	0.72
21:4:4015:CLA:HBC2	21:4:4015:CLA:HMC1	1.70	0.72
14:1:196:VAL:O	14:1:200:VAL:HG23	1.89	0.72
14:1:46:PRO:N	21:4:4005:CLA:HBA1	2.03	0.72
16:3:200:ASN:H	16:3:201:PRO:CD	2.02	0.72
21:3:3013:CLA:HMC1	21:3:3013:CLA:CBC	2.17	0.72
17:4:95:ALA:CA	21:4:4012:CLA:HED3	2.18	0.72
1:A:126:ILE:HD11	10:J:31:ARG:HG2	1.72	0.72
12:L:121:ARG:HG3	12:L:121:ARG:NH1	2.00	0.72
21:A:1122:CLA:HHC	21:A:1122:CLA:HBB1	1.71	0.72
26:1:1501:LUT:H35	21:1:1002:CLA:OBD	1.89	0.72
15:2:162:GLU:HG3	15:2:166:ILE:CD1	2.19	0.72
1:A:362:LEU:HD21	21:A:1128:CLA:CBB	2.19	0.72
21:B:1213:CLA:O2A	7:G:140:LEU:HD21	1.90	0.72
12:L:201:PHE:HE1	12:L:205:TYR:HD2	1.28	0.72
4:D:198:PRO:CA	4:D:199:ILE:HG13	2.19	0.72
14:1:225:ASN:C	14:1:227:GLY:HA2	2.10	0.72
17:4:246:THR:HG23	21:4:4008:CLA:CED	2.19	0.72
21:4:4014:CLA:HBC2	21:4:4014:CLA:CMC	2.16	0.72
21:A:1106:CLA:HMC3	21:A:1107:CLA:HMD2	1.72	0.72
21:B:1234:CLA:HMB2	21:B:1236:CLA:HED1	1.72	0.72
21:1:1001:CLA:H3A	21:1:1001:CLA:O1A	1.89	0.72
21:4:4008:CLA:H3A	21:4:4008:CLA:CGA	2.20	0.72
8:H:135:PRO:HD2	8:H:136:PRO:CD	2.14	0.72
21:1:1003:CLA:H62	20:1:1801:LHG:H191	1.72	0.71
21:4:4006:CLA:HMC1	26:4:4502:LUT:H222	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:6020:BCR:C19	21:L:1501:CLA:HMB2	2.20	0.71
26:1:1501:LUT:C39	21:1:1001:CLA:H62	2.20	0.71
15:2:152:PHE:CE2	21:2:2006:CLA:H62	2.24	0.71
21:2:2002:CLA:C7	26:2:2501:LUT:H362	2.20	0.71
21:1:1009:CLA:ND	21:4:4005:CLA:HAC1	2.05	0.71
21:4:4004:CLA:CBC	21:4:4009:CLA:HBB2	2.15	0.71
21:A:1129:CLA:HBB2	21:A:1137:CLA:HBB2	1.71	0.71
21:B:1213:CLA:C1	7:G:140:LEU:HD21	2.19	0.71
21:2:2004:CLA:C4	21:2:2004:CLA:HMB2	2.20	0.71
21:3:3011:CLA:CBC	21:3:3011:CLA:HHD	2.18	0.71
21:B:1216:CLA:HMB2	21:B:1221:CLA:HMA3	1.72	0.71
21:1:1003:CLA:H41	20:1:1801:LHG:C19	2.20	0.71
15:2:259:HIS:HE2	21:2:2003:CLA:CMD	2.02	0.71
21:2:2004:CLA:H13	26:2:2502:LUT:H193	1.72	0.71
17:4:169:ASN:HD22	27:4:4503:NEX:C17	2.01	0.71
17:4:238:HIS:ND1	21:4:4003:CLA:HMA2	2.06	0.71
21:4:4003:CLA:C2B	26:4:4501:LUT:H42	2.19	0.71
7:G:114:LEU:HD12	21:G:1002:CLA:O1D	1.89	0.71
7:G:74:LEU:HD12	7:G:78:VAL:HG11	1.70	0.71
7:G:78:VAL:HG13	7:G:79:PHE:CD2	2.25	0.71
21:1:1002:CLA:H61	21:1:1002:CLA:HED3	1.72	0.71
26:1:1501:LUT:C10	21:1:1002:CLA:HBA1	2.20	0.71
14:1:160:TYR:HB3	21:1:1001:CLA:CED	2.15	0.71
26:2:2502:LUT:H181	26:2:2502:LUT:C8	2.20	0.71
7:G:141:THR:HB	25:G:2021:LMG:C7	2.20	0.71
1:A:43:THR:CB	1:A:46:LYS:CE	2.37	0.71
21:2:2002:CLA:HBC2	21:2:2002:CLA:CMC	2.16	0.71
17:4:160:GLN:CB	21:4:4005:CLA:HMA3	2.20	0.71
21:G:1002:CLA:CBA	21:G:1002:CLA:HBD	2.13	0.71
2:B:292:ARG:CZ	7:G:91:VAL:HG11	2.20	0.71
1:A:474:GLN:O	1:A:481:ALA:HB1	1.91	0.71
26:1:1502:LUT:H222	21:1:1006:CLA:CAB	2.19	0.71
21:1:1013:CLA:HED3	21:1:1014:CLA:CMC	2.21	0.71
14:1:81:LEU:O	14:1:85:ARG:N	2.20	0.71
21:1:1011:CLA:H141	21:1:1011:CLA:H171	1.72	0.71
15:2:110:GLU:O	15:2:110:GLU:HG2	1.88	0.71
14:1:46:PRO:HA	21:4:4005:CLA:O1A	1.90	0.71
21:4:4009:CLA:HHC	21:4:4009:CLA:HBB1	1.72	0.71
5:E:79:GLN:HA	5:E:84:TYR:CD1	2.26	0.71
12:L:155:GLU:HB2	12:L:156:GLY:HA2	1.72	0.71
21:A:1137:CLA:HHC	21:A:1137:CLA:HBB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:659:THR:HA	21:B:9023:CLA:HAB	1.72	0.71
7:G:65:SER:OG	21:G:1001:CLA:HBA1	1.91	0.71
16:3:221:LEU:C	16:3:223:GLU:HA	2.11	0.71
1:A:43:THR:HB	1:A:46:LYS:NZ	2.06	0.71
21:1:1006:CLA:HBB1	21:1:1006:CLA:HHC	1.72	0.71
15:2:113:HIS:CG	21:2:2004:CLA:HBB2	2.26	0.71
16:3:108:ILE:CG1	21:3:3011:CLA:HBB2	2.03	0.71
17:4:243:TRP:NE1	21:4:4008:CLA:O1A	2.23	0.71
21:B:1227:CLA:CBA	21:B:1240:CLA:H42	2.21	0.71
21:2:2009:CLA:CED	21:2:2009:CLA:H2A	2.20	0.70
21:4:4012:CLA:CBB	21:4:4012:CLA:HHC	2.18	0.70
12:L:120:LEU:CD1	12:L:126:ALA:HB2	2.17	0.70
2:B:203:ARG:HG2	2:B:250:ALA:HB1	1.72	0.70
14:1:128:TRP:O	14:1:130:THR:N	2.22	0.70
7:G:107:ARG:HA	7:G:108:ALA:CB	2.20	0.70
7:G:93:GLU:CB	7:G:99:THR:HB	2.17	0.70
8:H:65:ASN:HA	8:H:70:TRP:CD1	2.25	0.70
26:1:1502:LUT:H173	21:1:1004:CLA:C6	2.16	0.70
21:B:1222:CLA:H191	21:B:1227:CLA:C20	2.22	0.70
21:1:1005:CLA:CHC	21:1:1005:CLA:HBB1	2.14	0.70
21:2:2002:CLA:HMB1	26:2:2501:LUT:C19	2.21	0.70
7:G:140:LEU:HD23	7:G:141:THR:HA	1.72	0.70
21:1:1009:CLA:H203	21:4:4015:CLA:OBD	1.90	0.70
21:A:1130:CLA:HED3	2:B:680:TRP:HH2	1.56	0.70
21:1:1012:CLA:HBC2	21:1:1013:CLA:HAB	1.74	0.70
15:2:110:GLU:HB2	21:2:2004:CLA:CHB	2.22	0.70
15:2:170:GLU:OE1	15:2:173:ARG:NH2	2.21	0.70
15:2:99:ASP:O	15:2:102:SER:HB2	1.91	0.70
21:4:4015:CLA:HHC	21:4:4015:CLA:HBB1	1.73	0.70
21:1:1002:CLA:H52	21:1:1002:CLA:CED	2.21	0.70
21:1:1001:CLA:C6	21:1:1002:CLA:HHD	2.20	0.70
15:2:167:GLY:HA2	21:2:2012:CLA:CAB	2.22	0.70
6:F:111:ALA:O	6:F:112:ASP:HB3	1.92	0.70
26:2:2501:LUT:H32	26:2:2501:LUT:H391	1.73	0.70
2:B:85:ARG:HG3	2:B:85:ARG:NH1	1.97	0.70
14:1:61:PHE:CE2	26:1:1502:LUT:H42	2.26	0.70
21:2:2003:CLA:HBB2	26:2:2501:LUT:C4	2.22	0.70
15:2:232:ARG:HH22	21:2:2004:CLA:HED2	1.56	0.70
17:4:104:MET:HE3	21:4:4001:CLA:HMC3	1.73	0.70
17:4:225:ASN:HD21	21:4:4010:CLA:C5	2.05	0.70
20:A:7003:LHG:O4	20:A:7003:LHG:O2	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:207:VAL:HG23	6:F:208:PHE:N	2.06	0.70
12:L:51:LYS:N	12:L:52:PRO:HD3	2.07	0.70
13:N:99:LYS:HE2	13:N:100:GLU:HB3	1.72	0.70
14:1:142:ILE:HD11	21:1:1013:CLA:CMC	2.20	0.70
16:3:208:PHE:HB3	21:3:3001:CLA:O2D	1.90	0.70
21:B:1205:CLA:H2	21:B:1205:CLA:H101	1.73	0.70
21:B:9010:CLA:CBC	21:B:9010:CLA:HHD	2.20	0.70
7:G:138:LEU:HD22	25:G:2021:LMG:O10	1.92	0.70
10:J:2:ARG:HG2	10:J:2:ARG:O	1.91	0.70
1:A:331:LEU:HD12	21:A:1122:CLA:CED	2.21	0.70
7:G:75:GLY:O	7:G:80:PHE:HB2	1.91	0.70
21:1:1004:CLA:HMB1	21:1:1004:CLA:CBB	2.15	0.69
17:4:217:PHE:HE1	26:4:4502:LUT:H392	1.57	0.69
20:A:7001:LHG:C25	21:A:1128:CLA:H42	2.15	0.69
21:A:1132:CLA:H141	21:A:1132:CLA:H172	1.74	0.69
12:L:85:ASN:ND2	21:L:1501:CLA:HAC1	2.07	0.69
14:1:108:ALA:HB1	21:1:1006:CLA:HMA1	1.72	0.69
16:3:109:ASN:HB3	21:3:3012:CLA:CGD	2.21	0.69
21:4:4007:CLA:CHD	21:4:4007:CLA:HBC2	2.21	0.69
21:F:1303:CLA:C2B	26:4:4502:LUT:H202	2.22	0.69
7:G:74:LEU:O	7:G:78:VAL:HG12	1.92	0.69
12:L:135:ALA:O	12:L:138:VAL:HG22	1.91	0.69
21:1:1009:CLA:CBB	21:1:1009:CLA:HHC	2.21	0.69
21:1:1010:CLA:CBA	21:1:1010:CLA:H2	2.22	0.69
21:2:2010:CLA:CAD	21:2:2010:CLA:HED2	2.22	0.69
17:4:160:GLN:HB3	21:4:4005:CLA:HMA3	1.72	0.69
21:4:4002:CLA:CAC	21:4:4007:CLA:HMB2	2.22	0.69
1:A:43:THR:HA	1:A:46:LYS:CG	2.22	0.69
21:1:1001:CLA:C3	21:1:1002:CLA:HAC2	2.22	0.69
26:1:1501:LUT:C12	21:1:1002:CLA:HBA1	2.21	0.69
16:3:172:HIS:HA	21:3:3012:CLA:HBB2	1.73	0.69
16:3:173:ARG:O	16:3:176:GLN:HB2	1.92	0.69
21:1:1013:CLA:HED3	21:1:1014:CLA:HMC2	1.75	0.69
16:3:108:ILE:HG23	21:3:3011:CLA:HBB1	1.74	0.69
17:4:169:ASN:CB	27:4:4503:NEX:H173	2.22	0.69
1:A:609:ILE:HD12	1:A:609:ILE:N	2.08	0.69
21:B:9023:CLA:H3A	21:B:9023:CLA:CGA	2.23	0.69
17:4:199:THR:CA	17:4:200:LEU:HB2	2.23	0.69
7:G:116:LYS:HA	21:G:1002:CLA:CMA	2.18	0.69
17:4:235:LEU:O	17:4:235:LEU:HD12	1.92	0.69
21:4:4001:CLA:CGA	21:4:4001:CLA:H3A	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:160:PHE:CE1	16:3:164:MET:HE3	2.27	0.69
17:4:171:ASP:HB3	27:4:4503:NEX:C10	2.23	0.69
17:4:247:ILE:HD12	17:4:247:ILE:O	1.93	0.69
19:G:2011:BCR:H403	19:G:2011:BCR:C23	2.15	0.69
11:K:98:PRO:HA	11:K:101:PHE:H	1.58	0.69
1:A:42:ARG:C	1:A:42:ARG:HD2	2.12	0.69
21:1:1006:CLA:HBA1	21:1:1014:CLA:C2C	2.21	0.69
14:1:168:LEU:CB	14:1:170:TYR:HE1	1.97	0.69
12:L:104:LEU:HA	12:L:192:GLY:O	1.93	0.69
17:4:104:MET:CE	21:4:4001:CLA:HHC	2.23	0.69
4:D:133:ALA:O	4:D:134:ARG:HB2	1.92	0.69
12:L:54:TYR:HE1	12:L:55:GLN:HE21	1.39	0.69
12:L:129:ALA:O	12:L:132:LEU:HB2	1.92	0.69
21:1:1008:CLA:H92	21:1:1008:CLA:H51	1.73	0.69
17:4:151:PHE:HB3	21:4:4012:CLA:CBB	2.23	0.69
8:H:65:ASN:O	8:H:70:TRP:HB2	1.92	0.69
21:3:3009:CLA:HED2	21:3:3009:CLA:C2A	2.21	0.69
17:4:214:MET:CE	21:4:4004:CLA:HMC3	2.23	0.69
21:G:1001:CLA:O1A	19:G:2011:BCR:H352	1.93	0.69
11:K:96:GLY:O	11:K:99:ALA:HB3	1.92	0.69
21:2:2003:CLA:H102	21:2:2003:CLA:H143	1.73	0.68
17:4:149:LEU:CB	27:4:4503:NEX:H361	2.23	0.68
21:4:4011:CLA:HMB3	27:4:4503:NEX:O24	1.93	0.68
21:B:1220:CLA:HMA1	21:B:1240:CLA:CED	2.23	0.68
12:L:87:PRO:CD	21:L:1502:CLA:HED2	2.21	0.68
4:D:79:THR:CG2	4:D:129:LEU:HB2	2.23	0.68
15:2:221:LYS:O	15:2:225:THR:HG23	1.94	0.68
14:1:88:MET:HE3	21:1:1001:CLA:HHC	1.75	0.68
16:3:233:ARG:HA	16:3:236:MET:HB2	1.75	0.68
4:D:77:PRO:CG	4:D:78:ASN:H	2.05	0.68
4:D:198:PRO:HA	4:D:199:ILE:HG23	1.75	0.68
21:A:1114:CLA:HBB1	21:A:1114:CLA:HMB1	1.75	0.68
2:B:98:GLN:NE2	8:H:126:LEU:O	2.25	0.68
14:1:86:TRP:CE2	21:1:1011:CLA:HED3	2.28	0.68
14:1:91:VAL:HG11	26:1:1501:LUT:H192	1.73	0.68
15:2:109:ALA:HB2	21:2:2012:CLA:HED1	1.74	0.68
21:2:2002:CLA:H8	21:2:2002:CLA:H41	1.75	0.68
17:4:163:LYS:HE2	21:4:4005:CLA:CED	2.23	0.68
2:B:230:TRP:CE3	7:G:140:LEU:HD12	2.29	0.68
12:L:109:PHE:CE1	21:L:1503:CLA:C1C	2.76	0.68
12:L:199:TRP:O	12:L:203:LEU:HD13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:89:TYR:O	12:L:90:ARG:HB2	1.93	0.68
21:1:1003:CLA:C4	20:1:1801:LHG:H192	2.22	0.68
15:2:118:MET:HG3	15:2:119:LEU:HD12	1.75	0.68
16:3:112:PHE:HA	16:3:115:LEU:HG	1.75	0.68
16:3:207:PRO:HB2	16:3:208:PHE:CD1	2.28	0.68
17:4:243:TRP:HD1	21:4:4008:CLA:HMA1	1.57	0.68
7:G:95:ASN:CB	7:G:96:GLY:HA3	2.23	0.68
21:1:1002:CLA:CBB	21:1:1002:CLA:HHC	2.24	0.68
21:1:1002:CLA:H52	21:1:1002:CLA:O2D	1.93	0.68
21:B:1239:CLA:HMC1	21:B:1239:CLA:CBC	2.24	0.68
20:B:7004:LHG:H181	20:B:7004:LHG:C32	2.22	0.68
15:2:113:HIS:CE1	21:2:2004:CLA:HBB2	2.29	0.68
21:2:2006:CLA:C12	21:2:2006:CLA:H52	2.24	0.68
21:2:2013:CLA:HHC	21:2:2013:CLA:CBB	2.18	0.68
21:B:1231:CLA:HBB2	21:B:1234:CLA:HBA1	1.75	0.68
1:A:654:ARG:HH21	1:A:655:ASP:CG	1.96	0.68
15:2:234:ALA:O	15:2:238:VAL:N	2.20	0.68
14:1:160:TYR:HB3	21:1:1001:CLA:O1D	1.94	0.68
19:A:6008:BCR:H353	21:A:1137:CLA:H43	1.76	0.68
7:G:116:LYS:HB2	21:G:1002:CLA:C1A	2.24	0.68
5:E:78:ARG:O	5:E:79:GLN:HB2	1.93	0.68
12:L:96:LEU:C	12:L:96:LEU:HD23	2.13	0.68
21:1:1009:CLA:O1D	20:1:1801:LHG:HC62	1.94	0.68
20:A:7003:LHG:HC91	21:A:1129:CLA:HBA1	1.75	0.68
13:N:151:GLU:HA	13:N:165:ASN:OD1	1.94	0.68
21:1:1013:CLA:HBA2	21:1:1013:CLA:O2D	1.93	0.68
15:2:155:THR:O	15:2:158:LEU:HG	1.93	0.68
16:3:209:PHE:CE1	21:3:3011:CLA:HMC3	2.29	0.68
21:4:4004:CLA:HBC2	21:4:4009:CLA:CBB	2.19	0.68
4:D:104:THR:CG2	4:D:129:LEU:HD23	2.23	0.68
15:2:155:THR:H	15:2:158:LEU:CD2	2.07	0.67
21:2:2002:CLA:HMB1	26:2:2501:LUT:H191	1.75	0.67
2:B:422:LEU:HG	21:B:1236:CLA:HAB	1.74	0.67
21:J:6015:CLA:CHC	21:J:6015:CLA:HBB1	2.21	0.67
16:3:256:ASN:HB3	21:3:3003:CLA:HMC1	1.74	0.67
1:A:43:THR:HA	1:A:46:LYS:HG3	1.76	0.67
21:1:1003:CLA:H41	20:1:1801:LHG:H192	1.76	0.67
21:1:1005:CLA:C5	21:1:1005:CLA:H92	2.15	0.67
21:4:4005:CLA:CBD	21:4:4005:CLA:HAA1	2.22	0.67
21:4:4010:CLA:HMC3	21:4:4013:CLA:CAB	2.24	0.67
19:B:6005:BCR:H311	21:B:1209:CLA:HBC3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:74:LEU:CD1	7:G:78:VAL:HG11	2.24	0.67
11:K:57:MET:HA	11:K:60:SER:HB2	1.76	0.67
14:1:94:ILE:CG2	14:1:105:TRP:HB3	2.19	0.67
20:A:7001:LHG:H211	21:A:1109:CLA:H202	1.76	0.67
21:L:1503:CLA:CBB	21:L:1503:CLA:HHC	2.19	0.67
5:E:79:GLN:HG2	5:E:84:TYR:CZ	2.30	0.67
10:J:11:ALA:HB1	10:J:12:PRO:CD	2.25	0.67
20:1:1801:LHG:C21	20:1:1801:LHG:H172	2.20	0.67
1:A:323:ILE:HG23	21:A:1118:CLA:HED2	1.77	0.67
2:B:311:PRO:HD2	20:B:7004:LHG:O1	1.95	0.67
21:B:9022:CLA:O1A	21:B:9022:CLA:H3A	1.95	0.67
7:G:107:ARG:CA	7:G:108:ALA:HB3	2.25	0.67
7:G:94:GLN:HE22	7:G:98:GLY:H	1.42	0.67
21:1:1006:CLA:C4B	21:1:1013:CLA:H43	2.25	0.67
21:2:2013:CLA:CMC	21:2:2013:CLA:HBC2	2.12	0.67
17:4:99:ASN:HD22	21:4:4004:CLA:CBB	2.07	0.67
21:4:4011:CLA:HAA1	21:4:4011:CLA:CBD	2.21	0.67
7:G:92:PRO:HD2	7:G:93:GLU:N	2.08	0.67
4:D:198:PRO:HA	4:D:199:ILE:CB	2.23	0.67
21:1:1012:CLA:HMC1	21:1:1012:CLA:HBC2	1.76	0.67
21:4:4002:CLA:HBB1	21:4:4002:CLA:CHC	2.24	0.67
21:A:1131:CLA:H93	21:A:1131:CLA:C5	2.24	0.67
23:A:9011:CL0:H2	23:A:9011:CL0:CBB	2.23	0.67
15:2:94:LEU:HB3	15:2:96:LEU:HD21	1.76	0.67
21:1:1002:CLA:HBA2	21:1:1002:CLA:O1D	1.94	0.67
15:2:97:GLY:HA2	15:2:102:SER:HB3	1.76	0.67
21:4:4001:CLA:HMD2	21:4:4011:CLA:O2A	1.95	0.67
13:N:168:TRP:HD1	16:3:262:ALA:HB2	1.58	0.67
21:3:3008:CLA:HBA1	21:3:3008:CLA:CHA	2.25	0.67
10:J:11:ALA:HB1	10:J:12:PRO:HD2	1.76	0.67
15:2:113:HIS:HD2	21:2:2012:CLA:HMD1	1.57	0.67
15:2:110:GLU:HB2	21:2:2004:CLA:C2B	2.25	0.67
21:2:2009:CLA:HED2	21:2:2009:CLA:H2A	1.76	0.67
17:4:190:ILE:H	21:4:4014:CLA:HBA1	1.59	0.67
21:4:4004:CLA:C4	21:4:4004:CLA:H72	2.18	0.67
7:G:105:ASP:CA	7:G:106:GLU:CB	2.72	0.67
1:A:615:HIS:HD2	21:A:1135:CLA:CMC	2.08	0.67
2:B:443:MET:HG2	2:B:451:LYS:HB2	1.76	0.67
21:1:1009:CLA:HBB2	17:4:156:ILE:HG21	1.76	0.67
1:A:457:SER:HB3	1:A:544:ILE:CD1	2.25	0.67
21:1:1008:CLA:HBD	21:1:1008:CLA:HAA1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:100:LEU:CD2	21:1:1014:CLA:HAA1	2.25	0.66
21:4:4008:CLA:H3A	21:4:4008:CLA:H12	1.76	0.66
21:A:1130:CLA:O1A	2:B:686:PRO:CD	2.44	0.66
2:B:292:ARG:NH2	7:G:107:ARG:HH22	1.90	0.66
13:N:168:TRP:HD1	16:3:262:ALA:CB	2.08	0.66
13:N:116:ARG:HG2	13:N:117:ALA:O	1.95	0.66
21:2:2011:CLA:H2A	21:2:2011:CLA:O2D	1.94	0.66
21:1:1009:CLA:HMC2	17:4:156:ILE:HD11	1.77	0.66
17:4:171:ASP:HB2	17:4:172:PRO:CD	2.25	0.66
21:A:1132:CLA:HBC1	21:B:1206:CLA:CBB	2.25	0.66
21:B:1213:CLA:HHH	21:B:1213:CLA:HBC3	1.77	0.66
1:A:615:HIS:CD2	21:A:1135:CLA:CMC	2.79	0.66
14:1:200:VAL:HG21	21:1:1003:CLA:HAC2	1.77	0.66
21:2:2013:CLA:CBC	21:2:2013:CLA:HMC1	2.18	0.66
1:A:609:ILE:H	1:A:609:ILE:HD12	1.60	0.66
7:G:140:LEU:C	7:G:140:LEU:HD23	2.16	0.66
12:L:110:LEU:O	12:L:113:PRO:HD2	1.95	0.66
13:N:165:ASN:O	13:N:166:VAL:HG12	1.95	0.66
1:A:683:HIS:CE1	1:A:745:THR:HG21	2.31	0.66
21:2:2008:CLA:HBB2	26:2:2501:LUT:H183	1.77	0.66
17:4:110:MET:HE1	17:4:217:PHE:CD1	2.30	0.66
21:4:4003:CLA:HMB1	26:4:4501:LUT:H183	1.77	0.66
21:A:1106:CLA:HMB1	21:A:1106:CLA:HBB1	1.77	0.66
7:G:93:GLU:HB3	7:G:99:THR:CB	2.21	0.66
16:3:206:GLY:HA2	16:3:209:PHE:HZ	1.58	0.66
6:F:169:TYR:HA	6:F:213:TRP:CZ3	2.31	0.66
21:A:1115:CLA:H8	11:K:110:GLY:HA2	1.77	0.66
14:1:94:ILE:HG23	26:1:1502:LUT:H383	1.78	0.66
21:2:2011:CLA:HAA1	21:2:2011:CLA:HBD	1.76	0.66
17:4:170:GLN:HE22	21:4:4014:CLA:CHC	2.08	0.66
1:A:126:ILE:HG23	1:A:127:VAL:HG22	1.78	0.66
4:D:162:GLY:O	4:D:163:GLU:HB2	1.94	0.66
14:1:131:LEU:HD23	14:1:131:LEU:C	2.15	0.66
15:2:158:LEU:CD1	21:2:2010:CLA:HBC1	2.25	0.66
21:2:2003:CLA:C8	21:2:2003:CLA:H143	2.25	0.66
16:3:167:MET:HA	16:3:167:MET:HE1	1.77	0.66
8:H:134:LEU:HB3	8:H:138:LEU:HA	1.77	0.66
21:2:2002:CLA:HHC	21:2:2002:CLA:HBB1	1.77	0.66
21:2:2006:CLA:O2A	21:2:2006:CLA:HMA2	1.95	0.66
17:4:238:HIS:CE1	21:4:4003:CLA:H2A	2.31	0.66
1:A:62:HIS:HB2	21:A:1128:CLA:O1A	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:124:VAL:CG2	21:G:1002:CLA:HMD3	2.25	0.66
3:C:78:GLY:HA2	4:D:134:ARG:HH12	1.59	0.66
21:1:1012:CLA:CBC	21:1:1013:CLA:HAB	2.26	0.66
14:1:137:ILE:HD12	14:1:137:ILE:C	2.15	0.66
15:2:159:PHE:CD1	21:2:2010:CLA:HBC3	2.31	0.66
16:3:183:SER:H	16:3:184:MET:HE1	1.60	0.66
21:3:3012:CLA:O2A	21:3:3012:CLA:HBD	1.95	0.66
17:4:197:ALA:O	17:4:199:THR:N	2.29	0.66
21:3:3011:CLA:HBA2	21:3:3011:CLA:CGD	2.25	0.66
17:4:77:PHE:HE2	26:4:4502:LUT:H173	1.60	0.66
9:I:14:LEU:HD11	19:I:6018:BCR:H351	1.77	0.66
17:4:163:LYS:HE2	21:4:4005:CLA:HED3	1.78	0.65
21:4:4003:CLA:CMB	26:4:4501:LUT:H183	2.26	0.65
1:A:735:VAL:O	1:A:739:LEU:HG	1.96	0.65
25:G:2021:LMG:HC71	25:G:2021:LMG:O2	1.94	0.65
12:L:109:PHE:CZ	21:L:1503:CLA:HMC3	2.31	0.65
7:G:115:LEU:HD12	21:G:1002:CLA:C1	2.25	0.65
2:B:85:ARG:CG	2:B:85:ARG:HH11	2.07	0.65
12:L:121:ARG:HB2	12:L:122:ASN:ND2	2.11	0.65
17:4:225:ASN:C	17:4:226:VAL:HG13	2.17	0.65
7:G:83:GLN:OE1	7:G:84:ARG:N	2.30	0.65
13:N:160:PHE:CZ	13:N:166:VAL:HG11	2.31	0.65
7:G:74:LEU:CG	7:G:78:VAL:HG11	2.25	0.65
7:G:74:LEU:HG	7:G:78:VAL:HG11	1.78	0.65
12:L:143:ILE:O	12:L:147:ILE:HG12	1.95	0.65
21:1:1003:CLA:C19	21:1:1003:CLA:H152	2.25	0.65
21:1:1008:CLA:H152	21:1:1008:CLA:HMC1	1.76	0.65
15:2:168:TRP:N	21:4:4009:CLA:O1A	2.29	0.65
21:2:2005:CLA:HED1	21:2:2005:CLA:O1A	1.96	0.65
21:2:2011:CLA:HBB1	21:2:2011:CLA:HHC	1.78	0.65
21:2:2013:CLA:O1D	21:2:2013:CLA:HBA1	1.95	0.65
26:4:4501:LUT:H401	26:4:4501:LUT:C15	2.26	0.65
2:B:50:HIS:ND1	21:B:1210:CLA:OBD	2.25	0.65
21:1:1006:CLA:CBB	21:1:1006:CLA:HHC	2.25	0.65
21:4:4001:CLA:H52	21:4:4002:CLA:C1	2.27	0.65
17:4:95:ALA:CB	21:4:4012:CLA:CED	2.75	0.65
21:B:9010:CLA:HMB1	21:B:9010:CLA:HBB1	1.77	0.65
15:2:109:ALA:HB2	21:2:2012:CLA:CED	2.27	0.65
20:2:2801:LHG:HC62	20:2:2801:LHG:C14	2.27	0.65
16:3:183:SER:O	16:3:184:MET:HB2	1.96	0.65
17:4:156:ILE:O	17:4:159:TRP:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:162:GLY:N	21:1:1001:CLA:O2D	2.30	0.65
21:1:1006:CLA:HMB2	21:1:1013:CLA:HMA3	1.78	0.65
2:B:656:VAL:HG22	21:B:1239:CLA:HMB3	1.78	0.65
1:A:255:LEU:HD23	21:A:1113:CLA:HED1	1.78	0.65
1:A:530:LEU:HD12	1:A:531:PRO:HD2	1.78	0.65
21:1:1007:CLA:C4C	20:1:1801:LHG:HC42	2.26	0.65
21:1:1008:CLA:H91	21:1:1008:CLA:H121	1.79	0.65
7:G:65:SER:HA	7:G:68:THR:HG22	1.77	0.65
5:E:123:ASP:N	5:E:123:ASP:OD1	2.30	0.65
21:1:1003:CLA:HBA1	21:1:1003:CLA:CBD	2.23	0.65
21:2:2003:CLA:HBB2	26:2:2501:LUT:H41	1.78	0.65
16:3:211:PRO:O	16:3:212:LEU:HB3	1.96	0.65
16:3:214:PHE:HZ	21:3:3001:CLA:C2D	2.10	0.65
21:3:3009:CLA:CBD	21:3:3009:CLA:HBA2	2.19	0.65
21:A:1125:CLA:H52	21:A:1125:CLA:C10	2.27	0.65
21:G:1002:CLA:O1D	21:G:1002:CLA:H2A	1.97	0.65
4:D:168:HIS:HA	4:D:169:PRO:C	2.15	0.65
5:E:93:VAL:HG22	5:E:103:VAL:HA	1.79	0.65
17:4:194:LEU:O	17:4:195:ASN:HB2	1.96	0.65
16:3:171:GLU:HA	16:3:174:ARG:HG3	1.79	0.64
17:4:105:LEU:HG	21:4:4006:CLA:HBB2	1.77	0.64
21:4:4001:CLA:H101	21:4:4002:CLA:H41	1.79	0.64
17:4:199:THR:HA	17:4:200:LEU:CG	2.27	0.64
26:1:1501:LUT:H24	21:1:1001:CLA:CBA	2.27	0.64
21:1:1008:CLA:O1D	21:1:1008:CLA:H2A	1.97	0.64
17:4:207:ILE:O	17:4:210:GLY:N	2.30	0.64
17:4:99:ASN:ND2	21:4:4004:CLA:HBB2	2.12	0.64
1:A:602:LEU:HG	1:A:739:LEU:HD11	1.79	0.64
24:B:7101:DGD:HBG2	21:B:1224:CLA:HBC3	1.79	0.64
7:G:73:PHE:HE1	7:G:77:PHE:CD2	2.14	0.64
13:N:160:PHE:HA	13:N:161:LYS:C	2.15	0.64
12:L:169:ARG:O	12:L:170:LYS:HB2	1.98	0.64
14:1:142:ILE:C	21:1:1012:CLA:HBB1	2.17	0.64
21:1:1006:CLA:HMB1	21:1:1013:CLA:CMA	2.26	0.64
21:A:1117:CLA:C14	21:A:1125:CLA:C10	2.73	0.64
7:G:140:LEU:HD23	7:G:141:THR:N	2.11	0.64
6:F:198:ILE:O	10:J:10:VAL:HG11	1.98	0.64
13:N:130:ASN:OD1	13:N:131:PHE:N	2.29	0.64
15:2:220:LEU:O	15:2:224:ARG:HG3	1.97	0.64
16:3:164:MET:CE	21:3:3012:CLA:HBC1	2.27	0.64
21:A:1130:CLA:CAD	12:L:73:VAL:HG11	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1140:CLA:H192	10:J:22:LEU:HD23	1.77	0.64
4:D:139:LEU:HD12	4:D:139:LEU:O	1.98	0.64
21:A:1140:CLA:CMC	21:A:9013:CLA:H71	2.27	0.64
4:D:129:LEU:C	4:D:129:LEU:HD13	2.17	0.64
21:1:1001:CLA:H42	21:1:1002:CLA:CBC	2.27	0.64
17:4:214:MET:HE2	21:4:4004:CLA:HMC3	1.78	0.64
3:C:28:MET:HE3	3:C:39:ILE:O	1.98	0.64
21:1:1002:CLA:H52	21:1:1002:CLA:HED3	1.79	0.64
21:1:1006:CLA:CMB	21:1:1013:CLA:CMA	2.74	0.64
14:1:155:PRO:O	14:1:159:LYS:N	2.31	0.64
14:1:105:TRP:HE1	14:1:202:GLN:HG3	1.63	0.64
21:2:2004:CLA:H2A	21:2:2004:CLA:O1D	1.97	0.64
1:A:205:HIS:O	1:A:209:GLY:N	2.31	0.64
1:A:608:SER:O	1:A:611:VAL:HG12	1.98	0.64
1:A:744:ALA:HA	19:A:6011:BCR:H391	1.78	0.64
16:3:160:PHE:HA	16:3:163:GLU:HB3	1.80	0.64
17:4:225:ASN:O	17:4:226:VAL:HG22	1.98	0.64
7:G:133:ILE:HA	19:G:2011:BCR:H401	1.78	0.64
26:1:1502:LUT:C20	21:1:1004:CLA:HAB	2.25	0.64
21:1:1009:CLA:HMA3	20:1:1801:LHG:H282	1.79	0.64
21:1:1006:CLA:C1B	21:1:1013:CLA:H43	2.28	0.64
15:2:173:ARG:O	15:2:177:ILE:HG12	1.97	0.64
21:2:2003:CLA:H102	21:2:2003:CLA:C14	2.27	0.64
21:2:2010:CLA:H171	21:2:2010:CLA:C14	2.24	0.64
15:2:243:PHE:HA	15:2:246:ILE:HG12	1.78	0.64
2:B:458:ILE:HG21	6:F:151:SER:HB3	1.79	0.64
14:1:134:ILE:O	14:1:137:ILE:HG13	1.97	0.64
17:4:106:GLY:O	17:4:109:GLY:N	2.30	0.64
21:1:1003:CLA:H62	20:1:1801:LHG:C19	2.28	0.63
14:1:128:TRP:CB	14:1:133:THR:HG21	2.28	0.63
21:4:4003:CLA:HBD	21:4:4003:CLA:HAA1	1.80	0.63
2:B:628:SER:CB	21:B:9010:CLA:HBC1	2.27	0.63
21:B:9023:CLA:HBC2	21:B:9023:CLA:HHB	1.80	0.63
21:F:1303:CLA:O2D	21:F:1303:CLA:HBA2	1.98	0.63
12:L:177:GLN:C	12:L:178:THR:HG23	2.18	0.63
14:1:66:LEU:CG	21:1:1004:CLA:H42	2.28	0.63
21:1:1006:CLA:HBA1	21:1:1014:CLA:NC	2.13	0.63
14:1:170:TYR:HD2	14:1:180:TYR:HE2	1.46	0.63
19:A:6017:BCR:H362	21:B:9023:CLA:H112	1.81	0.63
2:B:50:HIS:HB3	21:B:1210:CLA:HED3	1.78	0.63
12:L:104:LEU:HD21	19:L:6020:BCR:C11	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:132:THR:HA	13:N:134:CYS:N	2.13	0.63
21:2:2002:CLA:H62	26:2:2501:LUT:H362	1.80	0.63
16:3:173:ARG:NH1	16:3:183:SER:OG	2.31	0.63
17:4:225:ASN:O	17:4:226:VAL:HG13	1.98	0.63
17:4:214:MET:CE	21:4:4004:CLA:HHC	2.26	0.63
21:G:1002:CLA:HBA2	21:G:1002:CLA:CGD	2.28	0.63
16:3:257:LEU:HD22	21:3:3003:CLA:HAB	1.79	0.63
17:4:127:TRP:HE1	17:4:231:PRO:HD3	1.63	0.63
21:1:1008:CLA:C15	21:1:1008:CLA:HMC2	2.26	0.63
21:A:1102:CLA:HMA2	21:A:1109:CLA:HMD2	1.79	0.63
21:A:1138:CLA:H12	21:B:1229:CLA:HAA2	1.80	0.63
1:A:308:ILE:HA	1:A:311:LEU:HB2	1.80	0.63
10:J:6:THR:O	10:J:10:VAL:HG23	1.99	0.63
12:L:174:ASP:O	12:L:175:GLN:HB2	1.99	0.63
16:3:204:PRO:HB2	16:3:209:PHE:CA	2.27	0.63
21:3:3010:CLA:H12	21:3:3010:CLA:C4D	2.28	0.63
21:4:4005:CLA:HAA1	21:4:4005:CLA:HBD	1.81	0.63
12:L:159:SER:N	12:L:178:THR:HG22	2.12	0.63
6:F:198:ILE:C	6:F:200:VAL:H	2.01	0.63
15:2:167:GLY:O	15:2:171:GLY:N	2.31	0.63
21:A:1129:CLA:HMB2	21:A:1130:CLA:C1D	2.29	0.63
6:F:169:TYR:HA	6:F:213:TRP:HZ3	1.61	0.63
2:B:166:SER:HB3	7:G:102:ASP:HB2	1.81	0.63
21:3:3008:CLA:O2D	21:3:3008:CLA:H2A	1.97	0.63
4:D:158:VAL:O	4:D:159:PHE:HB2	1.97	0.63
2:B:315:LEU:CA	2:B:410:ARG:HH21	2.12	0.63
17:4:104:MET:HE1	21:4:4001:CLA:HHC	1.80	0.63
17:4:155:GLU:OE1	17:4:158:ARG:NH1	2.31	0.63
21:4:4014:CLA:CGA	21:4:4014:CLA:H3A	2.29	0.63
4:D:156:TYR:CE2	4:D:166:TYR:HD2	2.16	0.63
21:A:1115:CLA:H51	11:K:113:GLY:HA3	1.81	0.63
13:N:132:THR:HB	13:N:135:GLN:HG3	1.80	0.63
17:4:202:ALA:O	17:4:206:GLU:N	2.28	0.63
14:1:94:ILE:HD13	26:1:1502:LUT:C38	2.26	0.63
1:A:746:THR:O	1:A:749:PHE:HB3	1.98	0.63
21:2:2002:CLA:HMA1	26:2:2501:LUT:C20	2.29	0.63
21:B:1228:CLA:HBB1	21:B:1229:CLA:H202	1.81	0.63
21:B:1229:CLA:HAB	21:B:1230:CLA:HMB2	1.80	0.63
21:G:1002:CLA:CHC	21:G:1002:CLA:HBB1	2.26	0.63
7:G:116:LYS:O	7:G:118:ALA:N	2.32	0.63
12:L:158:PRO:HA	12:L:178:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:102:LEU:CG	21:1:1006:CLA:HED2	2.22	0.62
21:F:1303:CLA:HED1	21:F:1303:CLA:H12	1.81	0.62
21:F:1303:CLA:HED1	21:F:1303:CLA:C1	2.28	0.62
1:A:648:THR:CG2	1:A:651:GLY:HA3	2.29	0.62
21:1:1002:CLA:HMB2	21:1:1007:CLA:C3D	2.30	0.62
21:A:1140:CLA:HMC3	21:A:9013:CLA:H71	1.81	0.62
21:B:1213:CLA:C1	7:G:140:LEU:HD11	2.23	0.62
8:H:117:PHE:CG	9:I:11:LEU:HD21	2.34	0.62
10:J:10:VAL:O	10:J:10:VAL:HG12	1.98	0.62
3:C:15:THR:OG1	3:C:19:ARG:NH1	2.32	0.62
6:F:113:SER:O	6:F:116:ALA:HB3	1.99	0.62
21:1:1013:CLA:CBC	21:1:1013:CLA:HHD	2.22	0.62
21:1:1013:CLA:C7	21:1:1014:CLA:HBB2	2.25	0.62
21:2:2004:CLA:HAB	26:2:2502:LUT:H12	1.81	0.62
19:A:6011:BCR:H333	21:A:9013:CLA:C14	2.29	0.62
21:B:1230:CLA:H12	25:J:5001:LMG:H111	1.79	0.62
4:D:100:PHE:CE1	4:D:158:VAL:HG21	2.34	0.62
13:N:106:ARG:HG3	13:N:113:ASN:HB2	1.79	0.62
17:4:202:ALA:O	17:4:205:LYS:N	2.32	0.62
1:A:653:LEU:O	1:A:653:LEU:HG	1.99	0.62
12:L:61:ASN:ND2	12:L:166:LEU:HG	2.13	0.62
21:1:1004:CLA:H91	21:1:1005:CLA:HMB3	1.81	0.62
21:1:1009:CLA:C4D	21:4:4005:CLA:HAC1	2.28	0.62
15:2:118:MET:O	15:2:121:ALA:HB3	1.99	0.62
17:4:189:GLY:O	17:4:192:ASN:N	2.21	0.62
2:B:166:SER:OG	7:G:103:ALA:N	2.33	0.62
4:D:198:PRO:HA	4:D:199:ILE:CG2	2.30	0.62
1:A:648:THR:HG23	1:A:651:GLY:CA	2.29	0.62
19:B:6004:BCR:H382	19:B:6004:BCR:H23C	1.80	0.62
16:3:163:GLU:O	16:3:167:MET:HB2	1.99	0.62
21:4:4008:CLA:H3A	21:4:4008:CLA:C2	2.29	0.62
12:L:172:GLN:CA	12:L:172:GLN:HE21	2.12	0.62
21:1:1003:CLA:H192	21:1:1003:CLA:H152	1.82	0.62
14:1:223:HIS:NE2	21:1:1003:CLA:HBA1	2.15	0.62
17:4:168:VAL:O	21:4:4014:CLA:HMB3	1.99	0.62
1:A:394:SER:HB2	21:A:1126:CLA:HMA1	1.82	0.62
21:B:1210:CLA:HBB1	21:B:1210:CLA:HMB1	1.82	0.62
19:F:6016:BCR:HC7	21:F:1302:CLA:HMB2	1.81	0.62
1:A:751:LEU:HA	1:A:754:ILE:HD11	1.81	0.62
12:L:125:TYR:HD1	12:L:125:TYR:O	1.82	0.62
14:1:195:PHE:CE1	26:1:1502:LUT:H402	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1003:CLA:H92	20:1:1801:LHG:H182	1.81	0.62
21:2:2005:CLA:HBC1	21:2:2012:CLA:CBC	2.27	0.62
12:L:155:GLU:N	12:L:156:GLY:HA2	2.15	0.62
5:E:91:VAL:HG22	5:E:106:ARG:HG3	1.81	0.62
16:3:224:LEU:O	16:3:228:GLU:N	2.31	0.62
15:2:115:ARG:O	15:2:118:MET:HG2	2.00	0.62
21:3:3009:CLA:CBB	21:3:3009:CLA:HHC	2.14	0.62
17:4:110:MET:CG	26:4:4502:LUT:H383	2.30	0.62
17:4:148:ILE:O	17:4:152:HIS:HB3	2.00	0.62
15:2:152:PHE:HB3	17:4:243:TRP:CH2	2.35	0.62
17:4:104:MET:HE1	21:4:4001:CLA:CHC	2.29	0.62
21:B:1222:CLA:H191	21:B:1227:CLA:H201	1.82	0.62
8:H:72:LEU:CG	8:H:76:ASP:HB3	2.27	0.62
7:G:70:LEU:HD22	14:1:140:LEU:HD22	1.82	0.62
26:2:2501:LUT:H171	26:2:2501:LUT:H8	1.82	0.62
17:4:211:ARG:HD2	21:4:4004:CLA:C4C	2.30	0.62
21:4:4006:CLA:HBC1	21:4:4013:CLA:C3C	2.29	0.62
1:A:546:ALA:HB1	21:A:1136:CLA:HMB3	1.82	0.62
21:B:1204:CLA:HED2	9:I:6:SER:HB2	1.81	0.62
1:A:281:LEU:HB2	1:A:301:HIS:HB2	1.79	0.62
12:L:60:ILE:HA	12:L:70:GLU:HG3	1.81	0.62
12:L:78:LEU:HD12	12:L:78:LEU:O	1.98	0.62
21:1:1002:CLA:H52	21:1:1002:CLA:CGD	2.29	0.62
21:2:2010:CLA:HMC3	21:2:2013:CLA:CHC	2.30	0.62
21:A:1130:CLA:CBB	21:A:1136:CLA:H192	2.30	0.62
15:2:96:LEU:H	15:2:96:LEU:HD23	1.65	0.62
2:B:315:LEU:C	2:B:410:ARG:HH21	2.03	0.62
1:A:269:PHE:HD1	1:A:274:TRP:HE1	1.47	0.62
14:1:134:ILE:HD13	21:1:1013:CLA:HAA2	1.80	0.61
21:A:1129:CLA:CHC	21:A:1129:CLA:HBB1	2.15	0.61
21:B:1207:CLA:HAB	9:I:14:LEU:HG	1.81	0.61
21:H:1000:CLA:HHB	21:L:1501:CLA:HBA2	1.82	0.61
21:G:1002:CLA:CBB	21:G:1002:CLA:HHC	2.28	0.61
3:C:28:MET:HA	3:C:28:MET:HE3	1.81	0.61
17:4:239:ILE:O	17:4:241:ASP:N	2.33	0.61
14:1:224:ASN:O	14:1:225:ASN:HB2	1.98	0.61
21:2:2009:CLA:CBC	21:3:3009:CLA:HBA1	2.30	0.61
21:3:3010:CLA:H2A	21:3:3010:CLA:O1D	1.99	0.61
7:G:94:GLN:HA	7:G:94:GLN:NE2	2.12	0.61
21:B:1217:CLA:HAB	19:G:2011:BCR:C37	2.31	0.61
21:2:2005:CLA:HMD2	21:2:2012:CLA:ND	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:2:2801:LHG:HC62	20:2:2801:LHG:H141	1.83	0.61
17:4:171:ASP:CA	27:4:4503:NEX:H10	2.30	0.61
21:4:4006:CLA:HAC2	21:4:4013:CLA:C3C	2.30	0.61
21:4:4007:CLA:HED2	21:4:4007:CLA:OBD	2.00	0.61
1:A:401:TRP:NE1	21:A:1126:CLA:HAB	2.15	0.61
21:B:1221:CLA:HMB1	21:B:1221:CLA:HBB1	1.81	0.61
19:B:6006:BCR:H353	21:B:1211:CLA:H2	1.82	0.61
12:L:166:LEU:O	12:L:167:THR:HG22	1.99	0.61
17:4:233:ASP:O	17:4:236:LEU:N	2.33	0.61
21:1:1001:CLA:H61	21:1:1002:CLA:CAC	2.30	0.61
14:1:190:LEU:HD23	21:1:1002:CLA:HAA1	1.83	0.61
14:1:102:LEU:CD1	21:1:1006:CLA:H2A	2.29	0.61
21:2:2013:CLA:H2A	21:2:2013:CLA:O1D	2.01	0.61
21:3:3011:CLA:HMB1	21:3:3011:CLA:CBB	2.31	0.61
26:4:4501:LUT:H201	26:4:4501:LUT:H35	1.82	0.61
21:A:1131:CLA:C9	21:A:1131:CLA:H52	2.28	0.61
1:A:434:ARG:CA	1:A:437:ARG:HB2	2.28	0.61
21:1:1008:CLA:HHC	21:1:1008:CLA:CBB	2.24	0.61
26:1:1502:LUT:H192	21:1:1004:CLA:H61	1.83	0.61
15:2:118:MET:HB2	26:2:2501:LUT:C34	2.30	0.61
12:L:56:VAL:O	12:L:57:VAL:HG22	2.01	0.61
19:L:6019:BCR:HC8	19:L:6019:BCR:H331	1.81	0.61
13:N:161:LYS:HG3	13:N:167:PHE:CE2	2.34	0.61
17:4:175:LYS:O	17:4:176:GLN:HG2	2.00	0.61
21:1:1002:CLA:H2A	21:1:1002:CLA:O1D	2.00	0.61
21:2:2002:CLA:H41	21:2:2002:CLA:C8	2.31	0.61
19:L:6019:BCR:C38	19:L:6019:BCR:H23C	2.30	0.61
7:G:74:LEU:HA	7:G:78:VAL:CG1	2.25	0.61
21:1:1007:CLA:C4	21:1:1007:CLA:H71	2.14	0.61
16:3:157:TYR:O	16:3:160:PHE:HB3	2.00	0.61
16:3:200:ASN:HD22	16:3:201:PRO:N	1.98	0.61
21:3:3013:CLA:CBB	21:3:3013:CLA:HHC	2.11	0.61
1:A:549:ILE:O	1:A:553:VAL:HG23	2.00	0.61
12:L:56:VAL:O	12:L:57:VAL:HG13	2.01	0.61
21:G:1001:CLA:HMB2	19:G:2011:BCR:C14	2.31	0.61
1:A:331:LEU:HD12	21:A:1122:CLA:HED1	1.82	0.61
1:A:43:THR:O	1:A:46:LYS:HD2	2.00	0.61
20:1:1801:LHG:C35	21:4:4015:CLA:HBA1	2.31	0.61
21:2:2006:CLA:HMC2	26:2:2502:LUT:H23	1.82	0.61
17:4:104:MET:HB3	26:4:4501:LUT:H35	1.83	0.61
17:4:171:ASP:HB3	27:4:4503:NEX:C11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:F:1303:CLA:HMB3	21:4:4004:CLA:H101	1.82	0.61
21:A:1129:CLA:CGD	12:L:57:VAL:HG11	2.30	0.61
2:B:292:ARG:NH1	7:G:92:PRO:HB3	2.16	0.61
4:D:147:SER:O	4:D:149:TYR:N	2.33	0.61
20:1:1801:LHG:H211	17:4:148:ILE:CG1	2.30	0.61
7:G:76:ARG:O	7:G:76:ARG:HD2	2.00	0.61
4:D:130:LEU:HD23	4:D:131:LYS:H	1.65	0.61
12:L:163:SER:C	12:L:164:LEU:HD23	2.20	0.61
5:E:74:VAL:HG12	5:E:125:VAL:O	2.00	0.61
1:A:605:MET:O	1:A:609:ILE:HD13	2.00	0.61
2:B:655:LEU:HD22	21:B:9022:CLA:H2	1.83	0.61
16:3:256:ASN:ND2	21:3:3017:CLA:HMD2	2.16	0.61
19:G:2011:BCR:H331	19:G:2011:BCR:C8	2.30	0.61
21:A:1141:CLA:HHC	21:A:1141:CLA:HBB1	1.82	0.61
12:L:58:GLN:O	12:L:70:GLU:HB2	2.01	0.61
4:D:92:LEU:HD12	4:D:92:LEU:O	2.01	0.61
14:1:195:PHE:CE2	26:1:1502:LUT:H393	2.36	0.60
17:4:226:VAL:C	17:4:228:GLY:H	2.05	0.60
14:1:66:LEU:HD22	26:1:1502:LUT:H22	1.82	0.60
16:3:201:PRO:O	16:3:212:LEU:HD23	2.00	0.60
16:3:207:PRO:HB2	16:3:208:PHE:HD1	1.65	0.60
1:A:434:ARG:HD3	21:A:1129:CLA:OBD	2.01	0.60
7:G:76:ARG:NH1	7:G:116:LYS:HZ1	1.99	0.60
21:3:3008:CLA:H101	21:3:3008:CLA:H171	1.83	0.60
14:1:173:ASP:HB2	14:1:176:LYS:HB2	1.83	0.60
1:A:327:ILE:HA	1:A:330:ILE:CG2	2.32	0.60
21:2:2002:CLA:HBA1	26:2:2501:LUT:C34	2.31	0.60
21:B:1240:CLA:HHD	21:B:1240:CLA:HBC3	1.82	0.60
2:B:60:TRP:HB2	21:B:1205:CLA:H202	1.82	0.60
14:1:131:LEU:CG	14:1:135:LEU:HD11	2.30	0.60
17:4:227:THR:HG21	17:4:234:ASN:ND2	2.16	0.60
21:A:1130:CLA:CED	2:B:680:TRP:HH2	2.14	0.60
4:D:134:ARG:O	4:D:135:LYS:HB3	2.00	0.60
4:D:199:ILE:CD1	4:D:201:VAL:HG22	2.25	0.60
5:E:65:PRO:C	5:E:66:ILE:HG13	2.21	0.60
14:1:88:MET:HE1	21:1:1001:CLA:CHC	2.31	0.60
16:3:173:ARG:CG	16:3:173:ARG:HH11	2.15	0.60
17:4:242:PRO:HA	17:4:245:ASN:OD1	2.01	0.60
21:A:9012:CLA:CED	2:B:620:LEU:HD13	2.32	0.60
12:L:109:PHE:CE1	21:L:1503:CLA:HMC3	2.37	0.60
1:A:474:GLN:H	1:A:474:GLN:CD	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1001:CLA:H41	21:1:1002:CLA:HAC2	1.84	0.60
14:1:192:LEU:HD22	26:1:1502:LUT:H35	1.84	0.60
15:2:89:PHE:CD2	21:2:2009:CLA:CBB	2.85	0.60
16:3:208:PHE:HB3	21:3:3001:CLA:CGD	2.31	0.60
17:4:227:THR:HB	17:4:234:ASN:HD21	1.67	0.60
1:A:201:SER:O	1:A:205:HIS:ND1	2.26	0.60
21:B:1227:CLA:HBB1	21:B:1240:CLA:H142	1.84	0.60
21:F:1303:CLA:HBA2	21:F:1303:CLA:HED2	1.78	0.60
12:L:203:LEU:HD12	12:L:203:LEU:N	2.16	0.60
21:G:1002:CLA:O1A	21:G:1002:CLA:H2A	2.01	0.60
12:L:171:LYS:C	12:L:172:GLN:HE21	2.04	0.60
21:B:1217:CLA:HAB	19:G:2011:BCR:H373	1.84	0.60
20:2:2801:LHG:H122	20:2:2801:LHG:C25	2.30	0.60
1:A:361:ASN:ND2	21:A:1103:CLA:OBD	2.33	0.60
19:A:6011:BCR:H312	21:B:1229:CLA:HMB3	1.83	0.60
7:G:114:LEU:HD21	7:G:116:LYS:HB3	1.84	0.60
13:N:160:PHE:CG	13:N:161:LYS:HA	2.35	0.60
13:N:166:VAL:HG13	13:N:166:VAL:O	2.01	0.60
21:G:1001:CLA:HHC	21:G:1001:CLA:CBB	2.32	0.60
2:B:73:ASN:O	2:B:75:GLU:N	2.33	0.60
21:1:1009:CLA:H122	21:1:1009:CLA:C9	2.16	0.60
14:1:134:ILE:HD13	21:1:1013:CLA:HBD	1.84	0.60
14:1:170:TYR:CD2	14:1:180:TYR:HE2	2.19	0.60
21:2:2009:CLA:HED1	16:3:169:PHE:HZ	1.66	0.60
16:3:173:ARG:NH1	16:3:173:ARG:HG2	2.15	0.60
17:4:217:PHE:CE1	26:4:4502:LUT:C39	2.85	0.60
21:A:1128:CLA:CED	21:A:1128:CLA:H2A	2.32	0.60
15:2:94:LEU:HB3	15:2:96:LEU:CD2	2.31	0.60
1:A:746:THR:O	1:A:749:PHE:N	2.35	0.60
12:L:60:ILE:O	12:L:60:ILE:HG23	2.02	0.60
12:L:194:ILE:O	12:L:198:ILE:HG13	2.02	0.60
8:H:114:LEU:HD13	9:I:8:PHE:CD1	2.36	0.60
14:1:154:ASP:O	14:1:157:LYS:N	2.35	0.60
17:4:227:THR:O	17:4:227:THR:HG22	2.01	0.60
21:4:4004:CLA:H11	26:4:4502:LUT:H162	1.83	0.60
7:G:114:LEU:HG	7:G:116:LYS:N	2.15	0.60
12:L:122:ASN:O	12:L:123:THR:HG23	2.00	0.60
15:2:161:VAL:CG1	15:2:165:PHE:CE2	2.84	0.60
15:2:87:GLY:O	21:2:2004:CLA:HED1	2.00	0.60
2:B:377:TYR:CD2	21:B:1224:CLA:HAB	2.36	0.60
6:F:202:LEU:HD12	6:F:205:ARG:CA	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:195:PHE:CD1	26:1:1502:LUT:C40	2.85	0.59
15:2:91:PHE:O	15:2:92:ASP:HB2	2.02	0.59
17:4:169:ASN:HB3	27:4:4503:NEX:H171	1.84	0.59
17:4:217:PHE:CG	26:4:4502:LUT:C40	2.85	0.59
1:A:609:ILE:H	1:A:609:ILE:CD1	2.15	0.59
1:A:90:PHE:HE2	1:A:178:MET:HE2	1.66	0.59
21:1:1009:CLA:HHD	27:4:4503:NEX:C11	2.32	0.59
14:1:105:TRP:NE1	14:1:202:GLN:HG3	2.17	0.59
21:4:4004:CLA:O2A	26:4:4502:LUT:H163	2.02	0.59
16:3:256:ASN:ND2	21:3:3003:CLA:HAC1	2.17	0.59
14:1:94:ILE:HG23	26:1:1502:LUT:C38	2.31	0.59
1:A:441:ALA:CB	21:A:1130:CLA:HED1	2.32	0.59
21:B:1206:CLA:CMA	21:B:1207:CLA:HBB1	2.33	0.59
2:B:173:SER:CB	21:B:1209:CLA:HED1	2.32	0.59
2:B:173:SER:OG	21:B:1209:CLA:CED	2.45	0.59
21:L:1503:CLA:CBA	21:L:1503:CLA:HBD	2.32	0.59
12:L:109:PHE:CE1	21:L:1503:CLA:CMC	2.85	0.59
14:1:85:ARG:HE	21:1:1001:CLA:C4C	2.15	0.59
16:3:157:TYR:CE1	21:3:3010:CLA:CBC	2.86	0.59
21:4:4014:CLA:HBB1	21:4:4014:CLA:CHC	2.17	0.59
19:A:6011:BCR:H333	21:A:9013:CLA:H142	1.83	0.59
7:G:114:LEU:HD11	7:G:116:LYS:HB3	1.85	0.59
7:G:99:THR:HG23	7:G:100:HIS:H	1.65	0.59
4:D:199:ILE:C	4:D:199:ILE:HD12	2.23	0.59
12:L:120:LEU:CB	12:L:126:ALA:HB3	2.32	0.59
2:B:295:PHE:CD2	21:B:1217:CLA:HBD	2.37	0.59
21:1:1006:CLA:CHB	21:1:1013:CLA:C2	2.80	0.59
12:L:204:LEU:CA	12:L:207:LEU:HG	2.17	0.59
7:G:74:LEU:HD12	7:G:78:VAL:CG1	2.32	0.59
20:2:2801:LHG:H141	20:2:2801:LHG:C6	2.33	0.59
21:A:1132:CLA:HBC2	21:A:1132:CLA:HHD	1.83	0.59
2:B:292:ARG:HH22	7:G:107:ARG:HH22	1.49	0.59
1:A:266:ALA:HB2	21:3:3017:CLA:H3A	1.84	0.59
2:B:236:ASN:HB3	2:B:252:THR:OG1	2.03	0.59
15:2:103:LEU:O	15:2:107:VAL:HG23	2.02	0.59
2:B:524:ALA:O	2:B:528:HIS:ND1	2.35	0.59
1:A:42:ARG:HD2	1:A:43:THR:N	2.16	0.59
14:1:82:ILE:HD13	21:1:1012:CLA:CAD	2.33	0.59
21:4:4004:CLA:HMB1	21:4:4004:CLA:CBB	2.15	0.59
18:B:5002:PQN:H162	21:B:1238:CLA:HAB	1.85	0.59
21:A:1118:CLA:HMB3	11:K:102:THR:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HB3	1:A:44:ILE:CG1	2.32	0.59
12:L:121:ARG:H	12:L:122:ASN:HB2	1.63	0.59
13:N:161:LYS:CD	13:N:168:TRP:HZ3	2.15	0.59
6:F:185:ILE:HD12	6:F:194:LYS:HG2	1.83	0.59
14:1:102:LEU:HD12	21:1:1006:CLA:H2A	1.85	0.59
14:1:187:ASN:O	14:1:190:LEU:HB3	2.03	0.59
16:3:210:ASN:HB3	21:3:3001:CLA:HBD	1.83	0.59
17:4:156:ILE:HG13	17:4:157:ARG:N	2.18	0.59
17:4:238:HIS:CD2	21:4:4003:CLA:CED	2.85	0.59
21:4:4004:CLA:CGA	21:4:4004:CLA:H3A	2.32	0.59
19:A:6008:BCR:H352	21:A:1125:CLA:HED1	1.84	0.59
15:2:65:GLU:HG3	15:2:68:ARG:HG3	1.83	0.59
4:D:130:LEU:HD22	4:D:132:LEU:HG	1.84	0.59
13:N:161:LYS:CE	13:N:168:TRP:CZ3	2.86	0.59
12:L:155:GLU:HB2	12:L:156:GLY:CA	2.33	0.59
4:D:107:SER:OG	4:D:109:LYS:O	2.20	0.59
14:1:149:ARG:HD3	21:1:1011:CLA:C1D	2.33	0.59
14:1:195:PHE:CE2	26:1:1502:LUT:C39	2.85	0.59
15:2:155:THR:CA	15:2:158:LEU:HG	2.33	0.59
16:3:210:ASN:O	16:3:214:PHE:HD2	1.86	0.59
21:4:4001:CLA:H61	21:4:4002:CLA:H42	1.84	0.59
21:A:1131:CLA:H71	18:B:5002:PQN:H202	1.84	0.59
21:L:1503:CLA:CBD	21:L:1503:CLA:HBA1	2.33	0.59
5:E:92:THR:OG1	5:E:93:VAL:N	2.36	0.59
6:F:200:VAL:O	6:F:200:VAL:HG23	2.02	0.59
21:1:1006:CLA:CHB	21:1:1013:CLA:C3	2.80	0.59
21:1:1009:CLA:CBD	21:1:1009:CLA:HAA1	2.26	0.59
21:1:1006:CLA:C1B	21:1:1013:CLA:C3	2.81	0.59
15:2:118:MET:HG2	15:2:119:LEU:H	1.68	0.59
21:2:2009:CLA:HBC1	21:3:3009:CLA:CBA	2.33	0.59
15:2:153:THR:OG1	17:4:243:TRP:CZ3	2.48	0.59
1:A:687:ALA:O	21:A:9013:CLA:HAB	2.03	0.59
21:A:1120:CLA:HAB	21:A:1141:CLA:HBB1	1.85	0.59
6:F:198:ILE:C	10:J:10:VAL:HG11	2.22	0.59
10:J:11:ALA:CB	10:J:12:PRO:HD2	2.33	0.59
12:L:154:ASN:N	12:L:154:ASN:OD1	2.30	0.59
26:1:1501:LUT:H393	21:1:1001:CLA:C3	2.32	0.58
14:1:82:ILE:HG23	14:1:83:HIS:N	2.18	0.58
16:3:201:PRO:HB2	16:3:212:LEU:HD22	1.83	0.58
21:4:4004:CLA:C14	21:4:4004:CLA:H171	2.33	0.58
1:A:57:LEU:HD11	21:A:1101:CLA:HBC2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:195:PHE:CD2	26:1:1502:LUT:H403	2.38	0.58
16:3:214:PHE:CE2	21:3:3001:CLA:CAD	2.86	0.58
17:4:151:PHE:CE2	21:4:4012:CLA:HMC3	2.38	0.58
17:4:243:TRP:CD1	21:4:4008:CLA:CMA	2.85	0.58
21:A:1125:CLA:HBB1	21:A:1133:CLA:C3A	2.33	0.58
2:B:12:LEU:HD13	24:B:7101:DGD:HE1	1.83	0.58
1:A:683:HIS:CE1	1:A:745:THR:CG2	2.86	0.58
21:A:1120:CLA:HAB	21:A:1141:CLA:CBB	2.33	0.58
5:E:103:VAL:O	5:E:103:VAL:HG12	2.03	0.58
1:A:131:ILE:HG21	2:B:446:PHE:HA	1.83	0.58
21:1:1009:CLA:C4D	21:4:4005:CLA:CAC	2.81	0.58
17:4:110:MET:CE	17:4:217:PHE:CD1	2.85	0.58
21:4:4003:CLA:NC	21:4:4003:CLA:H42	2.18	0.58
17:4:163:LYS:NZ	21:4:4005:CLA:O1D	2.29	0.58
8:H:119:THR:O	8:H:120:THR:HG23	2.03	0.58
21:G:1001:CLA:HMB2	19:G:2011:BCR:C15	2.33	0.58
12:L:130:GLY:O	12:L:133:ALA:N	2.36	0.58
11:K:73:ALA:N	11:K:74:PRO:HD3	2.18	0.58
1:A:341:GLN:N	1:A:341:GLN:OE1	2.36	0.58
14:1:79:SER:HA	21:1:1012:CLA:HED2	1.85	0.58
14:1:105:TRP:HB2	26:1:1502:LUT:H24	1.84	0.58
15:2:89:PHE:CE2	21:2:2009:CLA:CBB	2.85	0.58
16:3:170:ALA:O	16:3:172:HIS:N	2.37	0.58
17:4:110:MET:HB3	26:4:4502:LUT:H383	1.83	0.58
19:B:6004:BCR:H372	19:G:2011:BCR:H272	1.83	0.58
1:A:347:TYR:O	1:A:351:THR:OG1	2.17	0.58
4:D:100:PHE:CZ	4:D:158:VAL:CG1	2.86	0.58
21:1:1008:CLA:O1D	17:4:145:ILE:HD11	2.03	0.58
26:1:1502:LUT:C17	21:1:1004:CLA:H71	2.33	0.58
15:2:152:PHE:HB3	17:4:243:TRP:HZ3	1.67	0.58
21:2:2009:CLA:HBC3	21:3:3009:CLA:HBA1	1.83	0.58
16:3:214:PHE:CZ	21:3:3001:CLA:C4D	2.86	0.58
16:3:164:MET:HE1	21:3:3012:CLA:CBC	2.33	0.58
12:L:121:ARG:CB	12:L:122:ASN:HB2	2.32	0.58
13:N:160:PHE:CD1	13:N:161:LYS:CA	2.86	0.58
13:N:96:LYS:O	13:N:98:ASN:N	2.37	0.58
13:N:139:LYS:HE2	13:N:140:GLN:HB2	1.85	0.58
21:1:1004:CLA:C9	21:1:1005:CLA:HMA1	2.27	0.58
16:3:160:PHE:CZ	16:3:164:MET:HG3	2.36	0.58
17:4:103:ALA:HA	26:4:4502:LUT:H403	1.85	0.58
17:4:95:ALA:HB2	21:4:4012:CLA:HED1	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:199:THR:HA	17:4:200:LEU:CB	2.33	0.58
4:D:77:PRO:CD	4:D:78:ASN:H	2.16	0.58
21:1:1005:CLA:C9	21:1:1005:CLA:H52	2.21	0.58
21:1:1006:CLA:O1A	21:1:1014:CLA:HBC2	2.02	0.58
21:1:1008:CLA:CHC	21:1:1008:CLA:HBB1	2.17	0.58
15:2:232:ARG:NH2	21:2:2004:CLA:HED2	2.16	0.58
21:4:4014:CLA:HBD	21:4:4014:CLA:HAA1	1.85	0.58
1:A:205:HIS:CG	21:A:1111:CLA:HMC2	2.39	0.58
21:B:1203:CLA:H13	21:B:1225:CLA:HBB2	1.84	0.58
12:L:120:LEU:HD23	12:L:120:LEU:N	2.18	0.58
12:L:176:LEU:HD12	12:L:176:LEU:C	2.23	0.58
1:A:331:LEU:CD1	21:A:1122:CLA:HED1	2.33	0.58
2:B:501:ILE:HA	2:B:508:LEU:HD22	1.86	0.58
16:3:242:TYR:H	16:3:242:TYR:HD1	1.51	0.58
8:H:73:TYR:O	8:H:75:SER:N	2.36	0.58
21:1:1004:CLA:H92	21:1:1005:CLA:CMA	2.27	0.58
15:2:124:ILE:CD1	26:2:2501:LUT:H172	2.33	0.58
15:2:257:PHE:CE1	21:2:2008:CLA:C4	2.86	0.58
17:4:172:PRO:HG2	17:4:173:ILE:N	2.18	0.58
4:D:166:TYR:HE1	4:D:170:LYS:CA	2.13	0.58
12:L:155:GLU:CB	12:L:156:GLY:HA2	2.31	0.58
26:1:1502:LUT:C22	21:1:1006:CLA:HAB	2.27	0.58
21:3:3011:CLA:CMB	21:3:3011:CLA:HBB1	2.34	0.58
2:B:15:ASP:HB3	2:B:20:ARG:HB3	1.85	0.58
21:1:1013:CLA:CGA	21:1:1013:CLA:HMA2	2.34	0.58
14:1:131:LEU:O	14:1:135:LEU:HG	2.03	0.58
21:3:3001:CLA:HBB1	21:3:3001:CLA:HHC	1.85	0.58
21:4:4003:CLA:H72	21:4:4003:CLA:C4	2.33	0.58
17:4:83:ALA:HB1	17:4:89:LEU:HG	1.86	0.58
7:G:140:LEU:HD23	7:G:141:THR:CA	2.34	0.58
25:G:2021:LMG:HC91	25:G:2021:LMG:O2	2.04	0.58
12:L:114:PHE:HZ	12:L:137:LEU:HD22	1.69	0.58
19:L:6019:BCR:H402	21:L:1502:CLA:HAC2	1.86	0.58
5:E:74:VAL:CG2	5:E:90:VAL:HG13	2.34	0.58
17:4:60:GLY:O	17:4:62:ALA:N	2.31	0.58
1:A:662:SER:O	1:A:666:GLN:HG3	2.04	0.58
21:1:1009:CLA:H52	21:4:4005:CLA:CMD	2.34	0.57
21:4:4011:CLA:H72	21:4:4011:CLA:H122	1.86	0.57
4:D:129:LEU:HD13	4:D:130:LEU:N	2.18	0.57
13:N:161:LYS:HE3	13:N:168:TRP:HZ3	1.67	0.57
21:G:1001:CLA:C4	19:G:2011:BCR:H343	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:GLN:NE2	8:H:127:PRO:O	2.37	0.57
1:A:660:GLN:HG2	1:A:753:ARG:CZ	2.33	0.57
21:1:1006:CLA:NB	21:1:1013:CLA:H43	2.19	0.57
26:1:1502:LUT:H8	26:1:1502:LUT:H181	1.85	0.57
21:4:4001:CLA:O1A	21:4:4001:CLA:H3A	2.04	0.57
17:4:95:ALA:HB2	21:4:4012:CLA:HED2	1.85	0.57
17:4:110:MET:HG2	26:4:4502:LUT:H383	1.86	0.57
2:B:355:LEU:HD13	21:B:1214:CLA:HAA2	1.86	0.57
1:A:281:LEU:HD13	1:A:301:HIS:CG	2.39	0.57
12:L:165:THR:OG1	12:L:166:LEU:N	2.37	0.57
1:A:288:ASP:HB3	1:A:291:THR:HG22	1.86	0.57
17:4:78:ASP:OD2	17:4:81:GLY:HA2	2.04	0.57
12:L:121:ARG:HH11	12:L:121:ARG:CG	2.15	0.57
1:A:750:PHE:O	1:A:754:ILE:HG13	2.03	0.57
16:3:119:GLY:HA3	21:3:3006:CLA:HBB1	1.86	0.57
14:1:142:ILE:O	21:1:1012:CLA:HBB1	2.05	0.57
21:2:2011:CLA:HAA1	21:2:2011:CLA:CBD	2.34	0.57
17:4:217:PHE:CD1	26:4:4502:LUT:C40	2.86	0.57
21:1:1006:CLA:HBB1	21:1:1006:CLA:CHC	2.33	0.57
17:4:186:TYR:N	17:4:186:TYR:CD1	2.73	0.57
1:A:608:SER:OG	1:A:609:ILE:HD12	2.04	0.57
21:B:1213:CLA:HBC2	21:B:1214:CLA:HMC2	1.86	0.57
2:B:700:LEU:HD21	18:B:5002:PQN:H151	1.85	0.57
21:B:9010:CLA:HMB3	21:B:9022:CLA:CAD	2.35	0.57
1:A:696:GLY:HA3	2:B:568:CYS:HB2	1.87	0.57
21:1:1001:CLA:HMB1	21:1:1001:CLA:HBB1	1.87	0.57
14:1:143:ALA:HA	21:1:1012:CLA:HBB1	1.85	0.57
14:1:158:LYS:C	14:1:159:LYS:HG3	2.25	0.57
15:2:259:HIS:CD2	21:2:2003:CLA:HBC3	2.40	0.57
12:L:121:ARG:HB2	12:L:122:ASN:HB2	1.87	0.57
17:4:213:ALA:O	17:4:216:ALA:HB3	2.04	0.57
21:1:1002:CLA:CMC	21:1:1002:CLA:HBC3	2.27	0.57
21:1:1003:CLA:O2A	21:1:1008:CLA:HED1	2.04	0.57
20:1:1801:LHG:HC61	20:1:1801:LHG:O9	2.03	0.57
21:4:4010:CLA:H3A	21:4:4010:CLA:O1A	2.05	0.57
17:4:197:ALA:HB1	17:4:199:THR:HG22	1.86	0.57
7:G:98:GLY:O	7:G:99:THR:HG22	2.04	0.57
21:1:1003:CLA:C5	20:1:1801:LHG:H191	2.35	0.57
21:2:2010:CLA:HMC3	21:2:2013:CLA:HHC	1.86	0.57
15:2:99:ASP:OD1	15:2:102:SER:OG	2.21	0.57
16:3:204:PRO:HG2	16:3:209:PHE:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:3:3013:CLA:HBB1	21:3:3013:CLA:CHC	2.08	0.57
17:4:190:ILE:CB	21:4:4014:CLA:CGA	2.83	0.57
17:4:217:PHE:HE1	26:4:4502:LUT:C39	2.17	0.57
21:A:1102:CLA:HBA2	21:A:1109:CLA:H71	1.87	0.57
23:A:9011:CL0:H3	23:A:9011:CL0:H24	1.87	0.57
2:B:411:MET:HE3	21:B:1227:CLA:CHD	2.34	0.57
19:A:6017:BCR:C14	21:B:9023:CLA:H203	2.35	0.57
7:G:101:PHE:CD1	7:G:101:PHE:N	2.72	0.57
4:D:198:PRO:CB	4:D:199:ILE:HG13	2.35	0.57
4:D:198:PRO:HB2	4:D:199:ILE:O	2.04	0.57
4:D:198:PRO:CA	4:D:199:ILE:HG23	2.35	0.57
12:L:159:SER:H	12:L:178:THR:CG2	2.13	0.57
14:1:170:TYR:N	14:1:170:TYR:CD1	2.73	0.57
21:2:2002:CLA:HMC2	21:2:2007:CLA:C4C	2.34	0.57
15:2:226:LYS:CB	21:2:2007:CLA:CED	2.71	0.57
17:4:210:GLY:O	17:4:214:MET:HG3	2.05	0.57
21:4:4008:CLA:C3A	21:4:4008:CLA:H12	2.33	0.57
19:B:6004:BCR:HC31	21:B:1218:CLA:O2A	2.04	0.57
5:E:75:LYS:HB3	5:E:125:VAL:HG23	1.86	0.57
14:1:209:GLY:O	14:1:212:GLU:N	2.38	0.57
4:D:97:VAL:HG12	4:D:97:VAL:O	2.04	0.57
14:1:143:ALA:CA	21:1:1012:CLA:CBB	2.82	0.57
16:3:171:GLU:O	16:3:174:ARG:HG3	2.05	0.57
17:4:110:MET:SD	26:4:4502:LUT:C38	2.93	0.57
17:4:169:ASN:CA	17:4:178:SER:HB2	2.26	0.57
1:A:515:TRP:CH2	21:A:1125:CLA:HMC3	2.40	0.57
7:G:117:SER:O	7:G:118:ALA:HB2	2.04	0.57
7:G:74:LEU:C	7:G:78:VAL:HG12	2.24	0.57
16:3:164:MET:SD	21:3:3012:CLA:CBC	2.93	0.56
21:A:9012:CLA:H61	2:B:438:VAL:HG13	1.87	0.56
7:G:141:THR:HG21	25:G:2021:LMG:HC72	1.82	0.56
4:D:199:ILE:HD12	4:D:199:ILE:O	2.04	0.56
21:1:1002:CLA:HMB2	21:1:1007:CLA:C4D	2.35	0.56
14:1:143:ALA:HA	21:1:1012:CLA:CBB	2.36	0.56
21:1:1013:CLA:O1D	21:1:1013:CLA:H92	2.04	0.56
21:2:2002:CLA:CBA	26:2:2501:LUT:C34	2.83	0.56
16:3:184:MET:HE1	16:3:184:MET:N	2.20	0.56
21:B:1226:CLA:C12	21:B:1226:CLA:H91	2.30	0.56
21:B:9010:CLA:CAB	21:B:9022:CLA:HED2	2.35	0.56
14:1:218:LEU:HB2	14:1:221:PRO:HD3	1.87	0.56
8:H:84:LEU:HD12	8:H:84:LEU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1004:CLA:CMB	21:1:1004:CLA:HBB1	2.11	0.56
21:1:1009:CLA:HBB1	21:1:1009:CLA:HHC	1.86	0.56
21:1:1009:CLA:HMC1	21:1:1009:CLA:CBC	2.30	0.56
21:1:1006:CLA:CMB	21:1:1013:CLA:H2	2.32	0.56
21:2:2003:CLA:CBB	26:2:2501:LUT:H42	2.35	0.56
20:2:2801:LHG:O10	20:2:2801:LHG:H161	2.05	0.56
21:A:1132:CLA:CBC	21:B:1206:CLA:CBB	2.78	0.56
20:B:7004:LHG:O2	14:1:66:LEU:HD12	2.05	0.56
21:L:1503:CLA:HBA1	21:L:1503:CLA:HBD	1.86	0.56
16:3:160:PHE:CE1	16:3:164:MET:CE	2.85	0.56
21:1:1008:CLA:H2A	17:4:145:ILE:HD11	1.87	0.56
21:B:1220:CLA:HMA1	21:B:1240:CLA:O2D	2.05	0.56
21:F:1303:CLA:HMB2	26:4:4502:LUT:H202	1.88	0.56
4:D:79:THR:HG21	4:D:129:LEU:HB2	1.86	0.56
13:N:151:GLU:O	13:N:152:LEU:HG	2.05	0.56
12:L:54:TYR:CE1	12:L:55:GLN:NE2	2.73	0.56
12:L:130:GLY:O	12:L:133:ALA:HB3	2.05	0.56
2:B:80:ASP:O	2:B:84:VAL:HG12	2.05	0.56
12:L:61:ASN:CG	12:L:166:LEU:HD11	2.26	0.56
1:A:458:PHE:CZ	1:A:462:ILE:HD11	2.40	0.56
4:D:105:TRP:O	4:D:128:ASN:HB2	2.06	0.56
26:1:1502:LUT:C12	21:1:1004:CLA:HMC2	2.35	0.56
14:1:142:ILE:HD13	21:1:1013:CLA:HMC2	1.86	0.56
14:1:105:TRP:CH2	21:1:1010:CLA:O2D	2.59	0.56
21:2:2005:CLA:CBC	21:2:2012:CLA:HBC1	2.28	0.56
21:2:2002:CLA:HMB2	26:2:2501:LUT:H191	1.87	0.56
17:4:160:GLN:HG2	21:4:4005:CLA:CED	2.35	0.56
21:1:1009:CLA:CMB	21:4:4015:CLA:CAD	2.83	0.56
19:B:6010:BCR:H19C	21:B:1223:CLA:H71	1.85	0.56
13:N:164:SER:O	13:N:165:ASN:ND2	2.38	0.56
6:F:109:TYR:O	6:F:110:ALA:HB3	2.05	0.56
14:1:145:VAL:O	14:1:146:GLU:HB2	2.05	0.56
14:1:195:PHE:CG	26:1:1502:LUT:H403	2.40	0.56
21:2:2014:CLA:C3A	21:2:2014:CLA:CGA	2.84	0.56
16:3:173:ARG:HB3	21:3:3011:CLA:CBC	2.36	0.56
17:4:171:ASP:CB	27:4:4503:NEX:C10	2.83	0.56
21:4:4001:CLA:H62	26:4:4501:LUT:H373	1.84	0.56
21:4:4011:CLA:CBB	21:4:4011:CLA:HMB1	2.11	0.56
16:3:253:PRO:HA	21:3:3003:CLA:HMC2	1.88	0.56
7:G:95:ASN:HB3	7:G:96:GLY:HA3	1.87	0.56
16:3:206:GLY:HA2	16:3:209:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:160:GLN:HG2	21:4:4005:CLA:HED1	1.87	0.56
21:4:4015:CLA:HHC	21:4:4015:CLA:CBB	2.36	0.56
17:4:110:MET:HE2	26:4:4502:LUT:H393	1.87	0.56
12:L:108:PHE:HD1	12:L:200:ALA:HB2	1.69	0.56
2:B:262:HIS:HE1	2:B:264:GLN:HB3	1.70	0.56
2:B:194:LEU:HA	2:B:198:ALA:HB3	1.88	0.56
21:2:2002:CLA:H62	26:2:2501:LUT:C28	2.36	0.56
16:3:112:PHE:HZ	21:3:3012:CLA:CGD	2.18	0.56
17:4:186:TYR:HB3	21:4:4001:CLA:O2D	2.06	0.56
21:A:1128:CLA:HED2	21:A:1128:CLA:H2A	1.87	0.56
21:A:1131:CLA:HMA1	19:I:6018:BCR:HC32	1.87	0.56
7:G:101:PHE:N	7:G:101:PHE:HD1	2.04	0.56
4:D:77:PRO:HG2	4:D:78:ASN:H	1.69	0.56
12:L:120:LEU:HB3	12:L:123:THR:OG1	2.06	0.56
14:1:217:HIS:C	14:1:218:LEU:HG	2.25	0.56
15:2:96:LEU:N	15:2:96:LEU:HD23	2.19	0.56
26:1:1502:LUT:C28	26:1:1502:LUT:H361	2.36	0.56
21:2:2010:CLA:H2A	21:2:2010:CLA:O1D	2.04	0.56
16:3:206:GLY:CA	16:3:209:PHE:CZ	2.86	0.56
2:B:523:ILE:HD13	21:B:1234:CLA:HAB	1.88	0.56
12:L:109:PHE:CE2	21:L:1502:CLA:HMB3	2.41	0.56
21:H:1000:CLA:HMB2	21:L:1501:CLA:CAA	2.32	0.56
12:L:85:ASN:O	12:L:86:LEU:HB2	2.06	0.56
17:4:199:THR:CA	17:4:200:LEU:CB	2.84	0.56
17:4:149:LEU:HB2	27:4:4503:NEX:C36	2.36	0.56
17:4:110:MET:HE1	26:4:4502:LUT:C39	2.36	0.56
2:B:167:TRP:CZ2	21:B:1208:CLA:HMA1	2.41	0.56
2:B:351:HIS:ND1	21:B:1214:CLA:OBD	2.31	0.56
21:B:1222:CLA:H191	21:B:1227:CLA:H203	1.86	0.56
7:G:116:LYS:HG2	21:G:1002:CLA:CHB	2.36	0.56
7:G:91:VAL:HB	7:G:92:PRO:HA	1.87	0.56
12:L:51:LYS:O	12:L:51:LYS:HG3	2.06	0.56
21:2:2006:CLA:CBA	21:2:2013:CLA:CAD	2.84	0.56
15:2:230:ASN:OD1	15:2:231:GLY:N	2.39	0.56
17:4:104:MET:HE3	21:4:4001:CLA:CMC	2.36	0.56
17:4:110:MET:CB	26:4:4502:LUT:H383	2.35	0.56
21:A:9012:CLA:HAB	2:B:582:TRP:CH2	2.40	0.56
7:G:107:ARG:CA	7:G:108:ALA:CB	2.83	0.56
1:A:514:THR:HA	1:A:531:PRO:HA	1.88	0.56
12:L:61:ASN:OD1	12:L:166:LEU:HD21	2.05	0.56
15:2:252:PRO:HD2	15:2:253:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:88:MET:HE1	21:1:1001:CLA:HHC	1.86	0.55
21:1:1013:CLA:O2D	21:1:1013:CLA:H12	2.06	0.55
14:1:88:MET:CE	21:1:1001:CLA:HMC3	2.36	0.55
21:2:2002:CLA:O1A	21:2:2002:CLA:HMA2	2.05	0.55
21:2:2011:CLA:CBB	21:2:2011:CLA:HHC	2.35	0.55
15:2:172:ARG:HD3	21:2:2011:CLA:HMC3	1.88	0.55
21:3:3010:CLA:H12	21:3:3010:CLA:C3D	2.36	0.55
21:3:3013:CLA:H11	21:3:3013:CLA:O2D	2.06	0.55
11:K:62:THR:HB	11:K:104:ALA:HB1	1.87	0.55
21:1:1013:CLA:CHC	21:1:1013:CLA:HBB1	2.20	0.55
20:1:1801:LHG:H352	21:4:4015:CLA:CBA	2.36	0.55
21:2:2002:CLA:H62	26:2:2501:LUT:C36	2.36	0.55
26:2:2502:LUT:C37	26:2:2502:LUT:H28	2.34	0.55
21:4:4001:CLA:H101	21:4:4002:CLA:H43	1.89	0.55
17:4:247:ILE:HB	21:4:4003:CLA:CAD	2.36	0.55
1:A:685:VAL:HG21	19:A:6011:BCR:H362	1.86	0.55
21:B:9010:CLA:CHD	21:B:9010:CLA:HBC3	2.23	0.55
12:L:144:CYS:HB3	19:L:6019:BCR:C19	2.36	0.55
5:E:119:ASN:N	5:E:119:ASN:OD1	2.39	0.55
21:1:1009:CLA:H71	21:1:1009:CLA:H122	1.89	0.55
21:2:2002:CLA:C6	26:2:2501:LUT:H362	2.35	0.55
21:4:4015:CLA:HBB1	21:4:4015:CLA:CHC	2.37	0.55
21:A:1102:CLA:H2	21:A:1109:CLA:H43	1.87	0.55
1:A:408:VAL:HG11	1:A:602:LEU:HD13	1.87	0.55
7:G:114:LEU:CG	7:G:116:LYS:HB3	2.35	0.55
7:G:65:SER:CA	7:G:68:THR:HG22	2.37	0.55
26:1:1501:LUT:C17	21:1:1003:CLA:C2B	2.84	0.55
21:2:2010:CLA:C1C	21:2:2013:CLA:HMC3	2.36	0.55
16:3:237:LEU:HA	16:3:240:LEU:HB3	1.87	0.55
16:3:108:ILE:CG2	21:3:3011:CLA:HBB1	2.36	0.55
21:B:1210:CLA:H151	21:B:1225:CLA:HMD2	1.89	0.55
7:G:114:LEU:HD13	7:G:119:ALA:O	2.07	0.55
21:1:1009:CLA:O1A	21:4:4005:CLA:HAC2	2.06	0.55
26:1:1502:LUT:H28	26:1:1502:LUT:H361	1.87	0.55
15:2:118:MET:HG2	15:2:119:LEU:HD13	1.89	0.55
17:4:110:MET:CG	26:4:4502:LUT:C38	2.85	0.55
21:4:4006:CLA:CBC	21:4:4013:CLA:C4C	2.85	0.55
19:G:2011:BCR:C40	19:G:2011:BCR:C23	2.85	0.55
13:N:113:ASN:O	13:N:115:ALA:N	2.38	0.55
15:2:119:LEU:O	15:2:122:ALA:N	2.40	0.55
15:2:155:THR:N	15:2:158:LEU:HD21	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:2010:CLA:HAA2	21:2:2010:CLA:H12	1.89	0.55
26:2:2501:LUT:H171	26:2:2501:LUT:C8	2.37	0.55
21:2:2009:CLA:HED1	16:3:169:PHE:CZ	2.41	0.55
21:4:4005:CLA:C2A	21:4:4005:CLA:CGD	2.84	0.55
21:4:4013:CLA:HBC2	21:4:4013:CLA:HMC1	1.87	0.55
13:N:161:LYS:CD	13:N:168:TRP:CZ3	2.90	0.55
14:1:94:ILE:CG2	26:1:1502:LUT:C24	2.84	0.55
21:2:2005:CLA:CBC	21:2:2012:CLA:CBC	2.85	0.55
20:2:2801:LHG:H122	20:2:2801:LHG:H252	1.88	0.55
17:4:149:LEU:CB	27:4:4503:NEX:C36	2.85	0.55
17:4:238:HIS:CD2	21:4:4003:CLA:HED3	2.42	0.55
21:4:4001:CLA:HAB	26:4:4501:LUT:C40	2.37	0.55
21:4:4003:CLA:C7	21:4:4003:CLA:C4	2.85	0.55
21:4:4014:CLA:C3A	21:4:4014:CLA:CGA	2.85	0.55
21:1:1001:CLA:C4	21:1:1002:CLA:CAC	2.85	0.55
15:2:172:ARG:CD	21:2:2011:CLA:HMC3	2.36	0.55
21:2:2002:CLA:O1A	21:2:2002:CLA:H2A	2.07	0.55
21:3:3001:CLA:CBC	21:3:3011:CLA:HMA1	2.36	0.55
21:4:4006:CLA:CBC	21:4:4013:CLA:C3C	2.84	0.55
17:4:170:GLN:NE2	21:4:4014:CLA:C4B	2.69	0.55
21:A:1130:CLA:O1A	2:B:686:PRO:CG	2.54	0.55
10:J:2:ARG:HH22	21:2:2005:CLA:H43	1.71	0.55
1:A:48:PRO:HG2	6:F:192:THR:HB	1.89	0.55
2:B:619:TRP:O	2:B:623:TYR:HB3	2.06	0.55
21:1:1001:CLA:C3	21:1:1002:CLA:CBC	2.85	0.55
17:4:151:PHE:N	27:4:4503:NEX:H372	2.22	0.55
1:A:441:ALA:O	1:A:445:HIS:ND1	2.33	0.55
7:G:95:ASN:CB	7:G:96:GLY:CA	2.85	0.55
1:A:615:HIS:CD2	21:A:1135:CLA:C2C	2.89	0.55
26:1:1501:LUT:C12	21:1:1002:CLA:CAA	2.85	0.55
21:1:1003:CLA:CGA	21:1:1003:CLA:C1A	2.84	0.55
14:1:66:LEU:HG	21:1:1004:CLA:H42	1.89	0.55
21:1:1010:CLA:CED	21:1:1010:CLA:CHA	2.86	0.55
15:2:118:MET:CG	15:2:119:LEU:CD1	2.85	0.55
15:2:166:ILE:HD11	21:2:2013:CLA:CMB	2.26	0.55
21:2:2004:CLA:CMB	21:2:2004:CLA:C4	2.85	0.55
21:2:2002:CLA:C7	26:2:2501:LUT:C36	2.85	0.55
21:3:3012:CLA:C1A	21:3:3012:CLA:CED	2.85	0.55
17:4:160:GLN:HA	21:4:4005:CLA:HED1	1.89	0.55
21:4:4007:CLA:CGA	21:4:4007:CLA:C1A	2.85	0.55
8:H:135:PRO:CG	8:H:136:PRO:CD	2.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:ARG:HE	4:D:157:ARG:NH1	2.05	0.55
7:G:68:THR:HG23	7:G:69:GLY:N	2.22	0.55
21:1:1001:CLA:C4	21:1:1002:CLA:CB	2.85	0.54
21:1:1002:CLA:HMB2	21:1:1007:CLA:C2D	2.38	0.54
21:1:1013:CLA:O1D	21:1:1013:CLA:H62	2.07	0.54
21:2:2001:CLA:C1B	21:2:2014:CLA:CMA	2.83	0.54
21:2:2008:CLA:C17	21:2:2008:CLA:C14	2.85	0.54
21:2:2010:CLA:CED	21:2:2010:CLA:CAD	2.85	0.54
21:3:3009:CLA:CGA	21:3:3009:CLA:CGD	2.85	0.54
17:4:104:MET:HB3	26:4:4501:LUT:C35	2.36	0.54
17:4:217:PHE:CE1	26:4:4502:LUT:H391	2.41	0.54
17:4:110:MET:CB	26:4:4502:LUT:C38	2.84	0.54
1:A:657:LEU:HD22	23:A:9011:CL0:H26	1.90	0.54
1:A:684:PHE:HB2	21:A:9012:CLA:O1A	2.07	0.54
21:B:1210:CLA:H52	21:B:1215:CLA:HBC3	1.87	0.54
19:I:6018:BCR:HC31	19:I:6020:BCR:H353	1.88	0.54
10:J:2:ARG:HA	21:J:6015:CLA:CBB	2.36	0.54
7:G:124:VAL:CG2	21:G:1002:CLA:CMD	2.85	0.54
2:B:166:SER:CB	7:G:102:ASP:CB	2.85	0.54
16:3:256:ASN:HD21	21:3:3017:CLA:HMD2	1.73	0.54
12:L:91:THR:O	12:L:92:ALA:HB3	2.06	0.54
13:N:169:LYS:O	13:N:170:TRP:HB2	2.07	0.54
1:A:387:THR:HG23	1:A:526:LYS:HB2	1.89	0.54
21:1:1009:CLA:H71	21:1:1009:CLA:H13	1.89	0.54
21:1:1013:CLA:C9	21:1:1013:CLA:C3D	2.85	0.54
15:2:155:THR:CA	15:2:158:LEU:CG	2.85	0.54
21:2:2004:CLA:C2B	21:2:2004:CLA:C4	2.85	0.54
15:2:110:GLU:N	21:2:2004:CLA:HMB3	2.22	0.54
15:2:73:PRO:HG3	21:2:2009:CLA:HBD	1.89	0.54
16:3:159:LEU:CD1	21:3:3013:CLA:C2D	2.85	0.54
16:3:164:MET:SD	21:3:3012:CLA:CAC	2.94	0.54
17:4:163:LYS:CE	21:4:4005:CLA:CED	2.85	0.54
17:4:246:THR:HG22	17:4:247:ILE:N	2.23	0.54
17:4:110:MET:CE	26:4:4502:LUT:C39	2.85	0.54
17:4:149:LEU:HB2	27:4:4503:NEX:H363	1.89	0.54
19:L:6019:BCR:C38	19:L:6019:BCR:C23	2.85	0.54
12:L:60:ILE:HD12	12:L:68:SER:HB3	1.89	0.54
21:1:1008:CLA:C9	21:1:1008:CLA:C5	2.85	0.54
15:2:158:LEU:HD11	21:2:2010:CLA:HBC1	1.88	0.54
16:3:108:ILE:CG2	21:3:3011:CLA:CBB	2.86	0.54
7:G:138:LEU:CD2	25:G:2021:LMG:C28	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ARG:CA	21:J:6015:CLA:HAB	2.17	0.54
7:G:65:SER:HA	7:G:68:THR:HG21	1.84	0.54
12:L:67:GLY:O	12:L:68:SER:HB2	2.07	0.54
11:K:73:ALA:HB1	11:K:77:ASN:N	2.22	0.54
15:2:70:LEU:HG	15:2:76:THR:HB	1.88	0.54
21:1:1010:CLA:H92	21:1:1010:CLA:C4	2.37	0.54
21:2:2008:CLA:CBC	21:2:2008:CLA:CHD	2.85	0.54
16:3:159:LEU:CD1	21:3:3013:CLA:C1D	2.85	0.54
21:4:4001:CLA:CGA	21:4:4001:CLA:C3A	2.85	0.54
21:4:4006:CLA:HBC1	21:4:4013:CLA:C4C	2.38	0.54
21:4:4006:CLA:HBC1	21:4:4013:CLA:CAC	2.38	0.54
21:4:4008:CLA:HMA1	21:4:4008:CLA:H12	1.88	0.54
21:4:4001:CLA:HAB	26:4:4501:LUT:H403	1.89	0.54
1:A:608:SER:OG	1:A:609:ILE:N	2.41	0.54
2:B:620:LEU:HG	2:B:620:LEU:O	2.05	0.54
7:G:116:LYS:C	7:G:116:LYS:HD3	2.26	0.54
2:B:417:ALA:O	2:B:421:HIS:ND1	2.41	0.54
14:1:183:LYS:NZ	21:1:1002:CLA:HMC2	2.22	0.54
21:2:2003:CLA:C14	21:2:2003:CLA:C10	2.85	0.54
21:2:2003:CLA:CBB	26:2:2501:LUT:C4	2.85	0.54
21:A:1126:CLA:H172	21:A:9012:CLA:H112	1.90	0.54
12:L:54:TYR:CD1	12:L:55:GLN:HG3	2.42	0.54
21:2:2002:CLA:HAC2	21:2:2007:CLA:ND	2.23	0.54
26:2:2502:LUT:C18	26:2:2502:LUT:C8	2.85	0.54
20:2:2801:LHG:C14	20:2:2801:LHG:C6	2.85	0.54
16:3:217:ASP:HB3	16:3:219:LYS:HE3	1.90	0.54
17:4:152:HIS:O	17:4:156:ILE:HG23	2.07	0.54
21:4:4006:CLA:CAC	21:4:4013:CLA:C3C	2.86	0.54
7:G:92:PRO:CD	7:G:93:GLU:H	2.15	0.54
21:G:1001:CLA:HBB1	21:G:1001:CLA:CHC	2.35	0.54
7:G:125:LEU:HD23	19:G:2011:BCR:H363	1.88	0.54
12:L:177:GLN:O	12:L:178:THR:HG23	2.08	0.54
2:B:571:SER:OG	2:B:574:ASP:OD1	2.25	0.54
14:1:131:LEU:HG	14:1:135:LEU:CD1	2.34	0.54
26:1:1501:LUT:C40	21:1:1001:CLA:CBB	2.85	0.54
15:2:172:ARG:NE	21:2:2011:CLA:HMC3	2.23	0.54
16:3:108:ILE:HG23	21:3:3011:CLA:CBB	2.37	0.54
21:3:3011:CLA:CGD	21:3:3011:CLA:CGA	2.85	0.54
21:4:4004:CLA:C17	21:4:4004:CLA:C14	2.85	0.54
17:4:190:ILE:N	21:4:4014:CLA:HBA1	2.21	0.54
23:A:9011:CL0:H7	21:B:9010:CLA:HBB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ARG:HG3	21:J:6015:CLA:CBB	2.38	0.54
12:L:145:LEU:HB3	12:L:186:THR:CG2	2.34	0.54
12:L:208:ASP:O	12:L:209:LEU:HD23	2.07	0.54
17:4:197:ALA:C	17:4:199:THR:H	2.10	0.54
16:3:260:HIS:CE1	16:3:261:VAL:HG12	2.42	0.54
4:D:100:PHE:HZ	4:D:158:VAL:HG11	1.69	0.54
2:B:93:ASP:OD1	2:B:95:HIS:ND1	2.23	0.54
14:1:66:LEU:HD21	21:1:1004:CLA:H42	1.88	0.54
21:1:1010:CLA:C2	21:1:1010:CLA:CBA	2.85	0.54
26:1:1501:LUT:H12	21:1:1002:CLA:CAA	2.38	0.54
15:2:109:ALA:CB	21:2:2012:CLA:CED	2.85	0.54
16:3:173:ARG:O	16:3:176:GLN:N	2.40	0.54
21:4:4008:CLA:HBC1	26:4:4501:LUT:H22	1.90	0.54
17:4:79:PRO:HD2	26:4:4502:LUT:O3	2.08	0.54
21:A:1131:CLA:C9	21:A:1131:CLA:C5	2.85	0.54
2:B:26:ALA:HA	21:B:1226:CLA:H42	1.90	0.54
17:4:197:ALA:CB	17:4:199:THR:HG22	2.38	0.54
7:G:114:LEU:CD1	21:G:1002:CLA:CGD	2.85	0.54
13:N:167:PHE:HD1	13:N:168:TRP:O	1.91	0.54
4:D:160:PRO:HD2	4:D:161:SER:H	1.72	0.54
3:C:28:MET:HE3	3:C:39:ILE:C	2.28	0.54
14:1:83:HIS:ND1	21:1:1012:CLA:HMD1	2.22	0.54
21:1:1013:CLA:H91	21:1:1013:CLA:C2D	2.37	0.54
21:2:2002:CLA:C3A	26:2:2501:LUT:C20	2.85	0.54
21:2:2002:CLA:CMA	21:2:2002:CLA:CGA	2.85	0.54
16:3:183:SER:H	16:3:184:MET:HE2	1.73	0.54
8:H:70:TRP:CE3	8:H:70:TRP:HA	2.43	0.54
8:H:70:TRP:O	12:L:162:PRO:HB3	2.08	0.54
7:G:95:ASN:H	7:G:96:GLY:C	2.11	0.54
14:1:136:VAL:HG23	14:1:137:ILE:N	2.24	0.54
15:2:155:THR:C	15:2:158:LEU:HG	2.28	0.54
21:2:2004:CLA:C2B	21:2:2004:CLA:H43	2.38	0.54
21:2:2006:CLA:C12	21:2:2006:CLA:C5	2.86	0.54
16:3:243:PHE:O	16:3:247:LEU:HD13	2.08	0.54
21:1:1009:CLA:CMB	21:4:4015:CLA:CGD	2.85	0.54
21:A:1125:CLA:O2D	21:A:1125:CLA:H2A	2.08	0.54
21:B:1220:CLA:HMD2	21:B:1221:CLA:HAB	1.90	0.54
21:B:1238:CLA:H171	12:L:140:ILE:HD13	1.89	0.54
7:G:115:LEU:C	21:G:1002:CLA:HMA3	2.27	0.54
7:G:121:ILE:HA	7:G:124:VAL:HG23	1.90	0.54
4:D:101:TYR:OH	4:D:157:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:GLN:HA	5:E:84:TYR:CE1	2.43	0.54
15:2:94:LEU:CB	15:2:96:LEU:CD2	2.86	0.54
2:B:478:LEU:HA	2:B:486:LEU:HG	1.90	0.54
14:1:223:HIS:CE1	21:1:1003:CLA:HBD	2.42	0.53
15:2:118:MET:SD	21:2:2001:CLA:CHD	2.93	0.53
21:2:2008:CLA:O2D	21:2:2008:CLA:H2A	2.08	0.53
15:2:99:ASP:N	15:2:99:ASP:OD1	2.41	0.53
16:3:165:ALA:O	16:3:168:GLY:N	2.41	0.53
21:4:4004:CLA:C1	26:4:4502:LUT:C16	2.85	0.53
17:4:214:MET:CE	21:4:4004:CLA:CHC	2.86	0.53
21:4:4008:CLA:C2	21:4:4008:CLA:CHB	2.85	0.53
2:B:411:MET:CE	21:B:1227:CLA:CHD	2.86	0.53
21:L:1501:CLA:HBA1	21:L:1501:CLA:HBD	1.90	0.53
7:G:76:ARG:NH1	21:G:1002:CLA:C1C	2.71	0.53
21:3:3003:CLA:CED	21:3:3008:CLA:CAD	2.86	0.53
5:E:77:LEU:N	5:E:77:LEU:HD12	2.24	0.53
17:4:66:TYR:OH	17:4:84:GLU:OE2	2.22	0.53
26:1:1502:LUT:H362	21:1:1006:CLA:HAB	1.89	0.53
20:1:1801:LHG:C21	20:1:1801:LHG:C17	2.86	0.53
14:1:202:GLN:HA	14:1:202:GLN:OE1	2.09	0.53
14:1:88:MET:CE	21:1:1001:CLA:HAB	2.39	0.53
15:2:227:GLU:HA	15:2:230:ASN:ND2	2.23	0.53
21:3:3013:CLA:HBD	21:3:3013:CLA:HAA2	1.90	0.53
21:4:4001:CLA:C5	21:4:4002:CLA:C1	2.85	0.53
21:4:4002:CLA:C4C	21:4:4007:CLA:CMB	2.83	0.53
21:B:1227:CLA:CBB	21:B:1240:CLA:C14	2.86	0.53
21:A:1132:CLA:C9	21:L:1503:CLA:HBB2	2.38	0.53
4:D:182:ARG:O	4:D:183:GLN:HB2	2.08	0.53
15:2:86:PRO:HA	15:2:225:THR:HG22	1.90	0.53
16:3:96:PHE:CE1	16:3:99:PRO:HG2	2.43	0.53
21:1:1009:CLA:HBB1	21:1:1009:CLA:CHC	2.38	0.53
21:1:1009:CLA:CMD	27:4:4503:NEX:C11	2.85	0.53
21:2:2002:CLA:HBA1	26:2:2501:LUT:C15	2.36	0.53
21:2:2007:CLA:H71	21:2:2007:CLA:C4	2.37	0.53
21:4:4003:CLA:C1B	26:4:4501:LUT:H42	2.38	0.53
21:4:4008:CLA:C3A	21:4:4008:CLA:CGA	2.84	0.53
21:A:1136:CLA:HBD	21:A:1136:CLA:HBA1	1.89	0.53
19:L:6020:BCR:C19	21:L:1501:CLA:CMB	2.85	0.53
8:H:135:PRO:CD	8:H:136:PRO:CD	2.81	0.53
5:E:66:ILE:HG22	5:E:67:GLY:N	2.20	0.53
14:1:143:ALA:CA	21:1:1012:CLA:HBB1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:163:GLU:OE2	21:3:3013:CLA:HBB1	2.07	0.53
17:4:226:VAL:CG2	17:4:227:THR:N	2.71	0.53
21:F:1303:CLA:CMD	21:4:4012:CLA:C1D	2.84	0.53
21:A:1125:CLA:C5	21:A:1125:CLA:C10	2.85	0.53
1:A:437:ARG:HD2	4:D:86:GLY:O	2.07	0.53
2:B:311:PRO:HB2	20:B:7004:LHG:O1	2.08	0.53
19:B:6005:BCR:H381	21:B:1203:CLA:HMC2	1.89	0.53
3:C:29:ILE:CD1	4:D:182:ARG:HB2	2.39	0.53
19:A:6002:BCR:H362	19:A:6003:BCR:C10	2.37	0.53
8:H:73:TYR:C	8:H:75:SER:H	2.10	0.53
21:1:1002:CLA:CMB	21:1:1007:CLA:C4D	2.86	0.53
14:1:190:LEU:CD2	21:1:1002:CLA:HAA1	2.38	0.53
14:1:100:LEU:HB3	21:1:1006:CLA:HED1	1.90	0.53
14:1:83:HIS:CE1	21:1:1012:CLA:HMD1	2.44	0.53
14:1:183:LYS:HD3	21:1:1002:CLA:HMC2	1.91	0.53
16:3:164:MET:HE1	21:3:3012:CLA:HBC1	1.90	0.53
17:4:171:ASP:HB3	27:4:4503:NEX:H10	1.90	0.53
21:A:1101:CLA:HMA1	21:A:1106:CLA:H203	1.89	0.53
19:A:6017:BCR:H323	21:B:9022:CLA:H141	1.90	0.53
1:A:88:ILE:HG23	19:J:6012:BCR:H282	1.90	0.53
11:K:65:LEU:HD21	11:K:104:ALA:HA	1.88	0.53
2:B:414:HIS:O	2:B:414:HIS:ND1	2.42	0.53
21:1:1003:CLA:C9	20:1:1801:LHG:H182	2.39	0.53
14:1:180:TYR:HD2	21:1:1001:CLA:O1A	1.92	0.53
16:3:173:ARG:HG2	16:3:173:ARG:HH11	1.72	0.53
16:3:171:GLU:CA	16:3:174:ARG:CG	2.86	0.53
21:3:3009:CLA:CGA	21:3:3009:CLA:HBD	2.39	0.53
21:B:9010:CLA:HAA2	21:B:9010:CLA:O2D	2.09	0.53
21:A:9013:CLA:HED3	19:F:6014:BCR:H312	1.91	0.53
1:A:331:LEU:CD1	21:A:1122:CLA:CED	2.85	0.53
12:L:61:ASN:ND2	12:L:166:LEU:CD1	2.72	0.53
16:3:96:PHE:CZ	16:3:101:TRP:HB3	2.43	0.53
21:1:1001:CLA:C5	21:1:1002:CLA:CAC	2.85	0.53
21:1:1003:CLA:C19	21:1:1003:CLA:C15	2.85	0.53
14:1:102:LEU:HD11	21:1:1006:CLA:O1D	2.09	0.53
26:1:1501:LUT:C12	21:1:1002:CLA:CBA	2.85	0.53
21:2:2005:CLA:HBC1	21:2:2010:CLA:HBB2	1.90	0.53
16:3:174:ARG:NH2	21:3:3011:CLA:C1D	2.72	0.53
17:4:102:TRP:CB	17:4:102:TRP:N	2.72	0.53
21:4:4008:CLA:H12	21:4:4008:CLA:CMA	2.38	0.53
1:A:545:HIS:O	1:A:549:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1228:CLA:CHD	21:B:1228:CLA:CBC	2.85	0.53
11:K:72:LEU:O	11:K:80:ALA:N	2.42	0.53
21:2:2001:CLA:C1D	26:2:2501:LUT:C39	2.85	0.53
21:3:3009:CLA:CBD	21:3:3009:CLA:CBA	2.85	0.53
21:4:4003:CLA:NC	21:4:4003:CLA:C4	2.72	0.53
21:B:1224:CLA:H3A	21:B:1224:CLA:CGA	2.38	0.53
21:B:9010:CLA:CHD	21:B:9010:CLA:CBC	2.85	0.53
19:L:6019:BCR:C8	19:L:6019:BCR:C33	2.85	0.53
4:D:77:PRO:CG	4:D:78:ASN:N	2.72	0.53
12:L:165:THR:HG23	12:L:166:LEU:O	2.09	0.53
14:1:223:HIS:NE2	21:1:1003:CLA:CBA	2.72	0.53
21:1:1010:CLA:C2	21:1:1010:CLA:HBA1	2.37	0.53
26:1:1502:LUT:H371	21:1:1010:CLA:HMA3	1.90	0.53
16:3:174:ARG:CZ	21:3:3011:CLA:ND	2.72	0.53
16:3:203:TYR:N	16:3:204:PRO:HD3	2.23	0.53
21:3:3001:CLA:H121	21:3:3002:CLA:HBB2	1.90	0.53
21:3:3009:CLA:HED2	21:3:3009:CLA:H2A	1.89	0.53
17:4:170:GLN:NE2	21:4:4014:CLA:CHC	2.72	0.53
17:4:99:ASN:HD22	21:4:4004:CLA:HBB2	1.73	0.53
1:A:60:ASP:OD2	20:A:7001:LHG:O2	2.27	0.53
2:B:645:VAL:HG12	21:B:1206:CLA:HAC1	1.90	0.53
2:B:523:ILE:HG21	21:B:1234:CLA:CAB	2.39	0.53
21:B:1207:CLA:CAB	9:I:14:LEU:HG	2.38	0.53
1:A:328:LYS:HD3	1:A:347:TYR:HB3	1.91	0.53
14:1:85:ARG:HE	21:1:1001:CLA:CHD	2.21	0.53
14:1:100:LEU:CD1	21:1:1014:CLA:O2A	2.57	0.53
15:2:168:TRP:HE1	21:2:2011:CLA:HBB2	1.71	0.53
21:2:2001:CLA:HHB	21:2:2014:CLA:C2A	2.39	0.53
16:3:164:MET:CE	21:3:3012:CLA:CBC	2.85	0.53
21:4:4003:CLA:CBB	26:4:4501:LUT:C18	2.85	0.53
1:A:64:PHE:CD2	21:A:1103:CLA:HMC2	2.44	0.53
13:N:118:TYR:O	13:N:119:THR:OG1	2.23	0.53
13:N:132:THR:HA	13:N:134:CYS:H	1.73	0.53
2:B:17:THR:HA	2:B:696:LYS:HB2	1.91	0.53
12:L:150:ILE:HD13	12:L:150:ILE:N	2.23	0.53
4:D:125:GLU:HG3	4:D:125:GLU:O	2.09	0.53
21:1:1007:CLA:NC	20:1:1801:LHG:HC42	2.24	0.52
14:1:195:PHE:CG	26:1:1502:LUT:C40	2.92	0.52
21:2:2003:CLA:H41	21:2:2003:CLA:C7	2.09	0.52
21:2:2011:CLA:H41	21:2:2014:CLA:NB	2.24	0.52
21:3:3011:CLA:O2A	21:3:3011:CLA:H2A	2.01	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1138:CLA:H151	21:A:1139:CLA:H43	1.90	0.52
2:B:428:PHE:CE2	21:B:1235:CLA:HAB	2.44	0.52
21:G:1002:CLA:CBC	21:G:1002:CLA:CHD	2.85	0.52
8:H:135:PRO:CG	8:H:136:PRO:HD2	2.38	0.52
21:3:3008:CLA:HBC2	21:3:3008:CLA:HHD	1.90	0.52
7:G:110:GLU:CG	7:G:111:TYR:N	2.72	0.52
16:3:246:GLY:HA2	16:3:251:VAL:O	2.10	0.52
21:1:1009:CLA:HMD3	27:4:4503:NEX:C20	2.39	0.52
21:1:1010:CLA:CMB	21:1:1013:CLA:HMB2	2.31	0.52
14:1:195:PHE:CZ	26:1:1502:LUT:C39	2.93	0.52
20:1:1801:LHG:H352	21:4:4015:CLA:HBA1	1.91	0.52
14:1:191:ALA:O	14:1:194:ALA:N	2.42	0.52
17:4:214:MET:HE3	21:4:4004:CLA:CHC	2.33	0.52
21:4:4004:CLA:C3A	21:4:4004:CLA:CGA	2.88	0.52
21:1:1009:CLA:HMB3	21:4:4015:CLA:CGD	2.39	0.52
2:B:177:HIS:CG	21:B:1210:CLA:HMC2	2.45	0.52
20:B:7004:LHG:H181	20:B:7004:LHG:H342	1.86	0.52
12:L:203:LEU:CD1	12:L:203:LEU:H	2.22	0.52
7:G:114:LEU:HD22	7:G:119:ALA:O	2.08	0.52
12:L:120:LEU:CB	12:L:126:ALA:CB	2.85	0.52
2:B:189:ALA:HA	21:B:1212:CLA:HAB	1.92	0.52
13:N:96:LYS:HG2	13:N:99:LYS:HD2	1.91	0.52
26:1:1501:LUT:C40	21:1:1001:CLA:CAB	2.85	0.52
21:1:1001:CLA:HHD	21:1:1011:CLA:O1A	2.08	0.52
20:1:1801:LHG:C38	20:1:1801:LHG:H202	2.34	0.52
14:1:195:PHE:CE1	14:1:199:CYS:SG	3.03	0.52
15:2:155:THR:HA	15:2:158:LEU:CG	2.39	0.52
21:3:3011:CLA:CGD	21:3:3011:CLA:CBA	2.88	0.52
17:4:104:MET:HE3	21:4:4001:CLA:HHC	1.90	0.52
20:A:7001:LHG:H162	21:A:1128:CLA:H72	1.92	0.52
21:A:1130:CLA:HBB1	21:A:1136:CLA:H192	1.91	0.52
21:B:1239:CLA:HBB1	21:B:1239:CLA:HHC	1.91	0.52
21:A:9012:CLA:HED1	2:B:620:LEU:HD13	1.91	0.52
18:B:5002:PQN:H301	24:B:7101:DGD:HA81	1.92	0.52
7:G:138:LEU:HD22	25:G:2021:LMG:C28	2.39	0.52
12:L:144:CYS:HB3	19:L:6019:BCR:C20	2.39	0.52
7:G:116:LYS:C	7:G:118:ALA:H	2.11	0.52
13:N:160:PHE:CE2	13:N:166:VAL:CG1	2.86	0.52
5:E:102:PRO:HD2	5:E:103:VAL:HG23	1.90	0.52
12:L:61:ASN:HD21	12:L:166:LEU:HG	1.72	0.52
14:1:184:GLU:HG3	21:1:1001:CLA:C1B	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1008:CLA:C9	21:1:1008:CLA:H51	2.40	0.52
26:1:1501:LUT:H10	21:1:1002:CLA:HBA1	1.91	0.52
15:2:118:MET:CG	15:2:119:LEU:N	2.73	0.52
15:2:120:GLY:HA2	26:2:2502:LUT:H373	1.92	0.52
15:2:172:ARG:NE	21:2:2011:CLA:CMC	2.72	0.52
21:4:4002:CLA:HAA2	21:4:4002:CLA:HBD	1.91	0.52
1:A:453:LEU:HD21	21:A:1136:CLA:HAB	1.90	0.52
1:A:336:GLY:N	1:A:339:THR:CG2	2.73	0.52
21:B:1213:CLA:C2	7:G:140:LEU:HD21	2.38	0.52
12:L:51:LYS:N	12:L:52:PRO:CD	2.72	0.52
16:3:260:HIS:HB2	21:3:3017:CLA:HBC1	1.91	0.52
21:1:1013:CLA:H61	21:1:1014:CLA:HHC	1.91	0.52
14:1:79:SER:O	14:1:82:ILE:HG22	2.09	0.52
16:3:109:ASN:HB3	21:3:3012:CLA:O1D	2.08	0.52
16:3:174:ARG:NH2	21:3:3011:CLA:C4D	2.72	0.52
19:A:6008:BCR:H19C	21:A:1124:CLA:HMB3	1.92	0.52
2:B:302:LYS:O	2:B:306:GLU:HG2	2.10	0.52
2:B:293:THR:OG1	2:B:294:ASN:N	2.42	0.52
1:A:218:TRP:HD1	1:A:303:HIS:CD2	2.28	0.52
21:1:1002:CLA:HBB1	21:1:1002:CLA:CHC	2.40	0.52
21:1:1013:CLA:C11	21:1:1013:CLA:C16	2.85	0.52
14:1:162:GLY:N	21:1:1001:CLA:CED	2.72	0.52
14:1:184:GLU:HG3	21:1:1001:CLA:C4B	2.40	0.52
15:2:168:TRP:NE1	21:2:2011:CLA:CBB	2.73	0.52
21:3:3012:CLA:C1A	21:3:3012:CLA:HED3	2.40	0.52
17:4:227:THR:CG2	17:4:234:ASN:ND2	2.73	0.52
1:A:609:ILE:N	1:A:609:ILE:CD1	2.73	0.52
19:L:6020:BCR:H19C	21:L:1501:CLA:HMB2	1.91	0.52
19:B:6004:BCR:C23	19:B:6004:BCR:H382	2.40	0.52
21:1:1006:CLA:CBA	21:1:1014:CLA:C2C	2.88	0.52
15:2:172:ARG:CZ	21:2:2011:CLA:HMC1	2.40	0.52
21:2:2001:CLA:C2D	26:2:2501:LUT:C39	2.87	0.52
15:2:259:HIS:NE2	21:2:2003:CLA:C2D	2.73	0.52
21:1:1009:CLA:HBB2	17:4:156:ILE:CG2	2.40	0.52
21:4:4004:CLA:CBC	21:4:4009:CLA:CBB	2.86	0.52
17:4:178:SER:C	21:4:4014:CLA:HMA1	2.30	0.52
6:F:215:ILE:CG2	17:4:82:LEU:HD22	2.40	0.52
2:B:289:LEU:HB3	21:B:1217:CLA:HED1	1.92	0.52
14:1:223:HIS:NE2	21:1:1003:CLA:O2A	2.43	0.52
21:2:2002:CLA:H3A	26:2:2501:LUT:H15	1.92	0.52
20:2:2801:LHG:O8	20:2:2801:LHG:H141	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4:4005:CLA:C1A	21:4:4005:CLA:CGA	2.88	0.52
21:1:1009:CLA:C2D	21:4:4005:CLA:HAC1	2.39	0.52
21:4:4014:CLA:CAA	21:4:4014:CLA:HBD	2.39	0.52
2:B:124:TRP:HB3	2:B:129:LEU:HD12	1.92	0.52
2:B:225:LEU:O	2:B:230:TRP:NE1	2.39	0.52
7:G:76:ARG:NH1	7:G:116:LYS:CE	2.73	0.52
16:3:245:GLN:HG3	21:3:3003:CLA:C2C	2.39	0.52
14:1:88:MET:CE	21:1:1001:CLA:CHC	2.85	0.52
26:1:1502:LUT:H222	21:1:1006:CLA:HMB1	1.92	0.52
21:1:1002:CLA:CAB	21:1:1007:CLA:HBD	2.28	0.52
15:2:155:THR:N	15:2:158:LEU:CD2	2.73	0.52
17:4:247:ILE:CD1	21:4:4003:CLA:CMD	2.85	0.52
17:4:163:LYS:CE	21:4:4005:CLA:HED2	2.39	0.52
17:4:225:ASN:ND2	21:4:4010:CLA:C4	2.73	0.52
21:4:4011:CLA:C12	21:4:4011:CLA:H71	2.39	0.52
19:A:6007:BCR:H372	20:A:7003:LHG:H241	1.92	0.52
21:B:1224:CLA:O1D	21:B:1225:CLA:HMA1	2.10	0.52
2:B:442:VAL:HG21	21:B:1230:CLA:HAC2	1.91	0.52
14:1:61:PHE:HD1	21:1:1009:CLA:C1	2.23	0.52
14:1:195:PHE:HE2	26:1:1502:LUT:H393	1.75	0.52
21:2:2001:CLA:CHD	26:2:2501:LUT:C39	2.85	0.52
26:2:2502:LUT:C37	26:2:2502:LUT:C28	2.87	0.52
21:4:4001:CLA:C6	26:4:4501:LUT:H371	2.37	0.52
1:A:368:LEU:HD11	21:A:1117:CLA:H71	1.92	0.52
21:B:1220:CLA:HMA1	21:B:1240:CLA:HED2	1.92	0.52
12:L:203:LEU:N	12:L:203:LEU:CD1	2.73	0.52
4:D:104:THR:CG2	4:D:129:LEU:CD2	2.86	0.52
3:C:29:ILE:HD13	4:D:182:ARG:HB2	1.91	0.52
11:K:57:MET:O	11:K:61:THR:N	2.42	0.52
14:1:111:TRP:HH2	14:1:129:GLY:O	1.92	0.51
14:1:195:PHE:CZ	26:1:1502:LUT:H391	2.45	0.51
15:2:121:ALA:C	15:2:123:GLY:H	2.13	0.51
21:2:2002:CLA:HHC	21:2:2002:CLA:CBB	2.40	0.51
21:B:9010:CLA:C3B	21:B:9022:CLA:HED2	2.39	0.51
12:L:85:ASN:C	12:L:86:LEU:HD13	2.30	0.51
12:L:158:PRO:HB3	12:L:178:THR:HG21	1.91	0.51
2:B:90:ALA:HA	2:B:113:VAL:HG12	1.91	0.51
21:1:1010:CLA:CHD	21:1:1010:CLA:CBC	2.85	0.51
21:1:1011:CLA:H142	21:1:1011:CLA:HMA1	1.92	0.51
21:1:1013:CLA:CED	21:1:1014:CLA:CMC	2.88	0.51
15:2:118:MET:HG3	15:2:119:LEU:CD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:238:HIS:NE2	21:4:4003:CLA:CGD	2.74	0.51
21:4:4004:CLA:C1	26:4:4502:LUT:H162	2.39	0.51
21:B:1226:CLA:C14	21:B:1226:CLA:C10	2.86	0.51
21:L:1501:CLA:HBA1	21:L:1501:CLA:CHA	2.41	0.51
12:L:199:TRP:HB2	19:L:6020:BCR:H321	1.92	0.51
1:A:648:THR:HG23	1:A:651:GLY:HA3	1.91	0.51
21:1:1002:CLA:CHC	21:1:1002:CLA:CBB	2.85	0.51
21:2:2002:CLA:C9	21:2:2002:CLA:H41	2.40	0.51
15:2:150:GLU:CB	21:2:2006:CLA:CMB	2.85	0.51
21:3:3012:CLA:CBC	21:3:3012:CLA:CHD	2.87	0.51
21:4:4012:CLA:H152	21:4:4012:CLA:H203	1.92	0.51
21:B:1213:CLA:CBA	21:B:1213:CLA:HBD	2.17	0.51
21:A:1130:CLA:O1A	2:B:686:PRO:HD3	2.10	0.51
4:D:101:TYR:O	4:D:132:LEU:N	2.30	0.51
16:3:256:ASN:HB3	21:3:3003:CLA:CMC	2.41	0.51
14:1:217:HIS:O	14:1:218:LEU:HG	2.11	0.51
2:B:314:ARG:O	2:B:410:ARG:NH2	2.43	0.51
2:B:199:ILE:O	2:B:202:SER:OG	2.18	0.51
21:1:1005:CLA:HED3	21:1:1012:CLA:O1A	2.10	0.51
21:2:2004:CLA:H102	21:2:2005:CLA:CMB	2.40	0.51
21:2:2009:CLA:CAB	20:2:2801:LHG:HC82	2.36	0.51
16:3:184:MET:N	16:3:184:MET:CE	2.73	0.51
16:3:203:TYR:N	16:3:204:PRO:CD	2.73	0.51
17:4:102:TRP:N	17:4:103:ALA:N	2.59	0.51
1:A:743:ILE:HG21	21:A:1126:CLA:HMC2	1.91	0.51
20:A:7003:LHG:O9	21:A:1129:CLA:H2	2.10	0.51
21:B:1206:CLA:H91	21:B:1239:CLA:H12	1.91	0.51
3:C:78:GLY:CA	4:D:134:ARG:NH1	2.73	0.51
1:A:343:HIS:N	1:A:431:LEU:HD21	2.25	0.51
12:L:155:GLU:N	12:L:156:GLY:CA	2.72	0.51
1:A:652:TRP:O	1:A:656:PHE:HB3	2.11	0.51
2:B:231:ASN:CG	7:G:143:SER:HB2	2.30	0.51
26:1:1501:LUT:C39	21:1:1001:CLA:C4	2.85	0.51
14:1:202:GLN:NE2	14:1:208:THR:CB	2.73	0.51
15:2:232:ARG:NH2	21:2:2004:CLA:CED	2.73	0.51
16:3:236:MET:O	16:3:240:LEU:N	2.41	0.51
21:3:3012:CLA:HED2	21:3:3012:CLA:CHA	2.41	0.51
1:A:92:TRP:HE1	21:A:1106:CLA:HBA1	1.75	0.51
21:A:1126:CLA:O1D	21:A:1127:CLA:HMA1	2.09	0.51
23:A:9011:CL0:H16	2:B:624:LEU:HD13	1.93	0.51
13:N:96:LYS:O	13:N:99:LYS:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:PHE:O	1:A:593:SER:OG	2.29	0.51
17:4:85:ASP:O	17:4:88:ASN:HB2	2.10	0.51
21:1:1003:CLA:C4	20:1:1801:LHG:C19	2.84	0.51
15:2:109:ALA:CA	21:2:2012:CLA:CED	2.89	0.51
15:2:110:GLU:HA	21:2:2004:CLA:HBB1	1.93	0.51
21:2:2008:CLA:CBB	26:2:2501:LUT:H183	2.41	0.51
15:2:118:MET:CB	26:2:2501:LUT:H35	2.35	0.51
21:2:2003:CLA:HBB2	26:2:2501:LUT:H42	1.89	0.51
17:4:103:ALA:O	17:4:107:VAL:N	2.36	0.51
17:4:225:ASN:ND2	21:4:4010:CLA:C5	2.73	0.51
20:B:7004:LHG:H341	20:B:7004:LHG:C18	2.38	0.51
1:A:661:ALA:O	1:A:664:VAL:HG12	2.11	0.51
2:B:293:THR:HG21	21:B:1217:CLA:OBD	2.11	0.51
15:2:86:PRO:HB2	15:2:225:THR:HA	1.92	0.51
2:B:697:PRO:O	3:C:81:TYR:OH	2.19	0.51
21:1:1008:CLA:CBD	21:1:1008:CLA:HAA1	2.40	0.51
15:2:257:PHE:CZ	21:2:2008:CLA:C4	2.94	0.51
17:4:238:HIS:NE2	21:4:4003:CLA:HED3	2.25	0.51
17:4:214:MET:HE3	21:4:4004:CLA:HMC3	1.93	0.51
21:4:4006:CLA:HMC2	26:4:4502:LUT:C22	2.30	0.51
21:F:1303:CLA:CMB	26:4:4502:LUT:H202	2.40	0.51
20:A:7003:LHG:C9	21:A:1129:CLA:CBA	2.85	0.51
20:A:7003:LHG:HC91	21:A:1129:CLA:CBA	2.40	0.51
21:B:1207:CLA:HMD3	19:I:6018:BCR:H311	1.93	0.51
21:B:1227:CLA:CBB	21:B:1240:CLA:H142	2.40	0.51
19:A:6017:BCR:C10	21:B:9022:CLA:H13	2.41	0.51
16:3:208:PHE:CB	21:3:3001:CLA:CED	2.88	0.51
16:3:174:ARG:HH22	21:3:3011:CLA:C4D	2.24	0.51
21:A:9012:CLA:H3A	21:A:9012:CLA:CGA	2.40	0.51
2:B:424:TRP:CD1	21:B:1229:CLA:HED2	2.46	0.51
1:A:604:TRP:CH2	21:B:9022:CLA:HAB	2.46	0.51
1:A:207:LEU:HA	1:A:211:LEU:HD22	1.92	0.51
14:1:198:ILE:HG13	26:1:1501:LUT:H163	1.93	0.51
14:1:64:LEU:HD12	26:1:1502:LUT:H163	1.92	0.51
21:2:2003:CLA:HBC2	21:2:2003:CLA:CHD	2.35	0.51
15:2:152:PHE:CE2	21:2:2006:CLA:H41	2.45	0.51
17:4:170:GLN:HG3	17:4:171:ASP:N	2.25	0.51
21:A:1102:CLA:HMC3	21:A:1104:CLA:HED2	1.93	0.51
2:B:711:VAL:HG21	21:B:1239:CLA:HED3	1.93	0.51
6:F:215:ILE:HG21	17:4:82:LEU:HD22	1.93	0.51
7:G:124:VAL:HG21	21:G:1002:CLA:HMD1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:107:ARG:CB	7:G:108:ALA:HB3	2.41	0.51
5:E:126:GLU:O	5:E:127:GLU:HB2	2.11	0.51
4:D:190:ARG:O	4:D:194:LYS:HD3	2.11	0.51
21:1:1006:CLA:C3B	21:1:1013:CLA:H43	2.41	0.51
14:1:89:LEU:HD21	21:1:1011:CLA:H201	1.92	0.51
16:3:170:ALA:HB1	16:3:174:ARG:CZ	2.41	0.51
17:4:110:MET:HE1	26:4:4502:LUT:H392	1.92	0.51
23:A:9011:CL0:H16	2:B:624:LEU:CD1	2.40	0.51
21:B:1220:CLA:CAB	21:B:1227:CLA:HMD2	2.40	0.51
2:B:463:ILE:HD12	21:B:1231:CLA:HMC3	1.93	0.51
23:A:9011:CL0:H7	21:B:9010:CLA:CBB	2.41	0.51
1:A:223:VAL:HG23	1:A:224:HIS:ND1	2.26	0.51
13:N:95:SER:O	13:N:95:SER:OG	2.27	0.51
14:1:128:TRP:CB	14:1:133:THR:CG2	2.89	0.50
26:1:1501:LUT:C12	21:1:1002:CLA:HAA2	2.40	0.50
21:2:2013:CLA:H122	21:2:2013:CLA:H91	1.92	0.50
21:B:1206:CLA:HMA1	21:B:1207:CLA:HBB1	1.92	0.50
10:J:27:ILE:O	10:J:31:ARG:HG3	2.11	0.50
21:L:1501:CLA:HHC	21:L:1501:CLA:CBB	2.23	0.50
7:G:92:PRO:CD	7:G:93:GLU:N	2.73	0.50
1:A:331:LEU:HA	21:A:1122:CLA:HED1	1.92	0.50
15:2:253:ILE:H	15:2:253:ILE:HD12	1.75	0.50
14:1:198:ILE:CG1	26:1:1501:LUT:H163	2.41	0.50
15:2:244:GLN:HB3	21:2:2003:CLA:HMB2	1.93	0.50
16:3:219:LYS:HG3	21:3:3001:CLA:HBA1	1.91	0.50
21:3:3009:CLA:CED	21:3:3009:CLA:H2A	2.41	0.50
19:L:6019:BCR:HC8	19:L:6019:BCR:C33	2.41	0.50
12:L:121:ARG:HB2	12:L:122:ASN:CG	2.32	0.50
12:L:52:PRO:O	12:L:54:TYR:HD2	1.94	0.50
14:1:88:MET:HE2	21:1:1001:CLA:HMC3	1.92	0.50
14:1:61:PHE:HD1	21:1:1009:CLA:H12	1.77	0.50
15:2:152:PHE:CD2	21:2:2006:CLA:H41	2.47	0.50
21:1:1008:CLA:HAA2	17:4:145:ILE:CG1	2.41	0.50
21:4:4003:CLA:C19	21:4:4008:CLA:HMD2	2.42	0.50
1:A:64:PHE:CE1	21:A:1102:CLA:HED1	2.47	0.50
21:B:1223:CLA:HMB1	21:B:1223:CLA:HBB1	1.92	0.50
2:B:463:ILE:HG22	2:B:467:HIS:CE1	2.47	0.50
21:A:1138:CLA:H172	6:F:178:GLY:HA2	1.92	0.50
10:J:2:ARG:HG3	21:J:6015:CLA:HBB2	1.92	0.50
4:D:77:PRO:CD	4:D:78:ASN:N	2.73	0.50
2:B:246:THR:HG22	2:B:248:GLN:CG	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:94:LEU:CB	15:2:96:LEU:HD21	2.41	0.50
5:E:90:VAL:HG12	5:E:105:VAL:HG22	1.93	0.50
11:K:63:LEU:O	11:K:66:PHE:HB2	2.11	0.50
14:1:211:LEU:CD2	21:1:1003:CLA:H2A	2.41	0.50
14:1:211:LEU:CD2	21:1:1003:CLA:CED	2.85	0.50
14:1:223:HIS:N	14:1:223:HIS:ND1	2.59	0.50
21:3:3011:CLA:CBC	21:3:3011:CLA:CHD	2.85	0.50
17:4:131:GLY:O	21:4:4010:CLA:HMD3	2.12	0.50
1:A:183:TRP:HB2	21:A:1109:CLA:HMC3	1.93	0.50
1:A:578:ARG:NH1	20:A:7001:LHG:O10	2.44	0.50
2:B:6:PRO:HG3	2:B:12:LEU:HD23	1.93	0.50
10:J:29:ILE:HD12	25:J:5001:LMG:H311	1.93	0.50
2:B:166:SER:HB3	7:G:102:ASP:CB	2.40	0.50
1:A:343:HIS:N	1:A:431:LEU:CD2	2.72	0.50
17:4:174:PHE:N	17:4:174:PHE:CD1	2.79	0.50
21:1:1003:CLA:H112	21:1:1003:CLA:HAB	1.92	0.50
21:1:1009:CLA:H2A	21:1:1009:CLA:O2D	2.11	0.50
15:2:155:THR:CA	15:2:158:LEU:CD1	2.85	0.50
21:3:3011:CLA:HBD	21:3:3011:CLA:CBA	2.34	0.50
21:4:4002:CLA:C3C	21:4:4007:CLA:CMB	2.85	0.50
19:B:6009:BCR:HC7	21:B:1219:CLA:HBB1	1.93	0.50
12:L:108:PHE:CE1	12:L:200:ALA:HB2	2.47	0.50
13:N:95:SER:O	13:N:97:ALA:N	2.43	0.50
6:F:96:LYS:O	6:F:100:LYS:HG2	2.12	0.50
8:H:69:GLN:HB2	12:L:66:ILE:HD13	1.93	0.50
21:1:1013:CLA:CBC	21:1:1013:CLA:CHD	2.86	0.50
14:1:142:ILE:HG22	14:1:142:ILE:O	2.11	0.50
15:2:113:HIS:CD2	21:2:2012:CLA:CMD	2.91	0.50
21:2:2009:CLA:CHC	20:2:2801:LHG:H132	2.42	0.50
16:3:160:PHE:CE1	16:3:164:MET:CG	2.86	0.50
16:3:200:ASN:C	16:3:200:ASN:HD22	2.14	0.50
17:4:238:HIS:ND1	21:4:4003:CLA:H2A	2.27	0.50
21:B:1213:CLA:H52	21:B:1213:CLA:C4C	2.42	0.50
1:A:216:LEU:HB2	1:A:307:ALA:HB1	1.94	0.50
14:1:100:LEU:HD11	21:1:1014:CLA:O2A	2.11	0.50
21:1:1013:CLA:CED	21:1:1014:CLA:HMC1	2.42	0.50
21:2:2009:CLA:CED	16:3:169:PHE:CZ	2.95	0.50
21:2:2011:CLA:CHC	21:2:2011:CLA:HBB1	2.42	0.50
16:3:200:ASN:ND2	16:3:201:PRO:N	2.60	0.50
21:4:4001:CLA:H8	26:4:4501:LUT:H372	1.94	0.50
21:1:1009:CLA:ND	21:4:4005:CLA:CAC	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:6008:BCR:H353	21:A:1125:CLA:HED1	1.90	0.50
4:D:77:PRO:HD2	4:D:78:ASN:H	1.77	0.50
1:A:590:CYS:HB2	2:B:667:TRP:HB3	1.93	0.50
1:A:596:ASP:OD1	1:A:731:ARG:NH1	2.44	0.50
26:1:1501:LUT:H392	21:1:1001:CLA:C6	2.41	0.50
26:1:1501:LUT:H173	21:1:1003:CLA:CMB	2.41	0.50
21:2:2006:CLA:HMC2	26:2:2502:LUT:H221	1.88	0.50
15:2:91:PHE:CE2	21:2:2009:CLA:HMC2	2.46	0.50
21:4:4005:CLA:HBC3	21:4:4005:CLA:HMC1	1.94	0.50
1:A:475:ASP:CG	21:A:1132:CLA:HED2	2.31	0.50
21:B:1213:CLA:HBB1	21:B:1213:CLA:HMB1	1.94	0.50
21:B:1222:CLA:HAA2	21:B:1223:CLA:OBD	2.12	0.50
19:B:6010:BCR:C10	21:B:1216:CLA:H92	2.42	0.50
6:F:201:PRO:C	6:F:202:LEU:HD23	2.31	0.50
13:N:168:TRP:CD1	16:3:262:ALA:CB	2.85	0.50
13:N:161:LYS:CE	13:N:168:TRP:HZ3	2.25	0.50
21:A:1115:CLA:H72	21:A:1115:CLA:C1C	2.42	0.50
15:2:252:PRO:CD	15:2:253:ILE:H	2.24	0.50
11:K:114:HIS:O	11:K:118:VAL:N	2.34	0.50
17:4:164:ASN:O	17:4:166:GLY:HA2	2.12	0.50
21:1:1010:CLA:HED2	21:1:1010:CLA:CHA	2.41	0.50
16:3:108:ILE:CA	16:3:111:ARG:HD2	2.33	0.50
16:3:177:ASP:CG	16:3:209:PHE:CE2	2.86	0.50
21:A:1107:CLA:HBD	21:A:1107:CLA:HBA1	1.94	0.50
1:A:189:ALA:HB1	21:A:1108:CLA:HED3	1.93	0.50
21:B:1202:CLA:HED2	21:B:1226:CLA:HBB2	1.93	0.50
7:G:76:ARG:NH1	7:G:116:LYS:NZ	2.60	0.50
13:N:106:ARG:HD3	13:N:109:THR:HA	1.94	0.50
2:B:450:GLU:OE2	6:F:129:ARG:NH1	2.45	0.50
17:4:153:TYR:CD1	17:4:153:TYR:C	2.85	0.50
14:1:186:LYS:NZ	21:1:1007:CLA:HED1	2.11	0.49
21:2:2002:CLA:H41	21:2:2002:CLA:H92	1.94	0.49
21:4:4011:CLA:CBC	21:4:4011:CLA:CHD	2.85	0.49
1:A:41:SER:HB3	1:A:44:ILE:HB	1.94	0.49
7:G:93:GLU:CD	7:G:99:THR:HB	2.32	0.49
1:A:615:HIS:CD2	21:A:1135:CLA:HMC2	2.47	0.49
21:1:1001:CLA:C3	21:1:1002:CLA:CAC	2.88	0.49
21:1:1005:CLA:C9	21:1:1005:CLA:C5	2.85	0.49
26:1:1502:LUT:C22	21:1:1006:CLA:HMB1	2.42	0.49
14:1:130:THR:CB	14:1:132:PRO:HD2	2.42	0.49
21:1:1009:CLA:CMD	20:1:1801:LHG:HC12	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:2001:CLA:HHB	21:2:2014:CLA:H2A	1.95	0.49
16:3:207:PRO:C	16:3:208:PHE:CD1	2.86	0.49
17:4:170:GLN:HE22	21:4:4014:CLA:C4B	2.24	0.49
17:4:95:ALA:CA	21:4:4012:CLA:CED	2.87	0.49
1:A:195:TRP:CH2	21:A:1108:CLA:HAA2	2.47	0.49
21:A:1106:CLA:HBB2	21:A:1126:CLA:H142	1.94	0.49
21:B:1239:CLA:CBB	21:B:1239:CLA:HHC	2.42	0.49
13:N:142:LYS:HD3	13:N:152:LEU:HD13	1.93	0.49
7:G:74:LEU:CA	7:G:78:VAL:CG1	2.85	0.49
2:B:316:GLY:N	2:B:410:ARG:NH2	2.59	0.49
17:4:137:ALA:O	17:4:141:THR:OG1	2.16	0.49
21:1:1006:CLA:CMB	21:1:1013:CLA:C2	2.88	0.49
14:1:162:GLY:N	21:1:1001:CLA:HED1	2.26	0.49
15:2:158:LEU:HD12	15:2:158:LEU:C	2.33	0.49
15:2:159:PHE:HB2	21:2:2010:CLA:HBC1	1.94	0.49
20:2:2801:LHG:HC62	20:2:2801:LHG:H142	1.94	0.49
21:1:1009:CLA:HMD3	27:4:4503:NEX:C11	2.43	0.49
21:B:1235:CLA:H172	19:F:6016:BCR:HC41	1.94	0.49
7:G:102:ASP:O	7:G:103:ALA:HB3	2.11	0.49
2:B:239:SER:OG	2:B:249:GLY:HA3	2.13	0.49
2:B:159:PRO:HA	2:B:162:LYS:HE3	1.94	0.49
26:1:1501:LUT:H392	21:1:1001:CLA:H62	1.93	0.49
21:1:1011:CLA:H102	21:1:1011:CLA:HMB2	1.94	0.49
14:1:143:ALA:N	21:1:1012:CLA:HBB1	2.27	0.49
21:3:3010:CLA:CGA	21:3:3010:CLA:C1A	2.90	0.49
17:4:109:GLY:HA3	21:4:4006:CLA:CAB	2.42	0.49
21:1:1009:CLA:HMD3	27:4:4503:NEX:H11	1.92	0.49
1:A:243:PRO:HG3	1:A:254:LEU:HD21	1.94	0.49
10:J:13:VAL:HA	10:J:16:THR:HG23	1.95	0.49
21:1:1002:CLA:O1D	21:1:1002:CLA:H12	2.11	0.49
21:1:1010:CLA:C2	21:1:1010:CLA:H92	2.42	0.49
21:2:2006:CLA:HAA2	21:2:2006:CLA:HBD	1.93	0.49
16:3:174:ARG:HA	21:3:3011:CLA:C2C	2.42	0.49
2:B:443:MET:O	2:B:447:GLY:N	2.45	0.49
14:1:105:TRP:CZ2	14:1:202:GLN:HG3	2.48	0.49
14:1:94:ILE:HG23	26:1:1502:LUT:C24	2.42	0.49
16:3:208:PHE:CB	21:3:3001:CLA:HED3	2.43	0.49
2:B:279:ALA:O	21:B:1213:CLA:HMC3	2.13	0.49
19:L:6019:BCR:H383	19:L:6019:BCR:C23	2.42	0.49
7:G:76:ARG:HG2	7:G:76:ARG:HH11	1.77	0.49
8:H:127:PRO:HB2	8:H:128:ILE:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:252:PRO:HD2	15:2:253:ILE:H	1.78	0.49
21:1:1002:CLA:HBB1	21:1:1002:CLA:HHC	1.94	0.49
14:1:145:VAL:CG1	21:1:1011:CLA:C2B	2.91	0.49
21:2:2006:CLA:H2	21:2:2006:CLA:O1A	2.13	0.49
21:2:2014:CLA:HMB3	26:2:2501:LUT:H24	1.95	0.49
17:4:104:MET:CE	21:4:4001:CLA:CMC	2.85	0.49
21:1:1009:CLA:HHC	17:4:156:ILE:HD11	1.94	0.49
20:1:1801:LHG:C35	21:4:4015:CLA:CBA	2.90	0.49
1:A:716:VAL:HG11	21:A:1138:CLA:HMB3	1.93	0.49
7:G:91:VAL:CB	7:G:92:PRO:HA	2.39	0.49
5:E:68:PRO:CG	5:E:93:VAL:HG21	2.37	0.49
5:E:89:SER:O	5:E:106:ARG:N	2.39	0.49
4:D:96:GLN:NE2	8:H:69:GLN:HB3	2.28	0.49
14:1:100:LEU:HD21	21:1:1014:CLA:CAA	2.37	0.49
21:1:1013:CLA:C7	21:1:1014:CLA:CBB	2.85	0.49
14:1:108:ALA:HB1	21:1:1006:CLA:CMA	2.41	0.49
14:1:94:ILE:CG2	26:1:1502:LUT:C38	2.90	0.49
14:1:61:PHE:CD1	21:1:1009:CLA:H12	2.47	0.49
15:2:168:TRP:C	15:2:168:TRP:CD1	2.85	0.49
15:2:228:ILE:HG22	15:2:232:ARG:NE	2.28	0.49
21:2:2008:CLA:HBB2	26:2:2501:LUT:C18	2.43	0.49
21:2:2002:CLA:H62	26:2:2501:LUT:H28	1.93	0.49
21:B:1210:CLA:HMC1	21:B:1210:CLA:HBC2	1.94	0.49
7:G:116:LYS:CG	21:G:1002:CLA:NA	2.76	0.49
7:G:94:GLN:CA	7:G:94:GLN:NE2	2.73	0.49
2:B:262:HIS:CE1	2:B:264:GLN:HB3	2.48	0.49
1:A:490:GLN:NE2	1:A:534:LEU:O	2.35	0.49
21:1:1002:CLA:HMB2	21:1:1007:CLA:C1D	2.42	0.49
21:1:1006:CLA:C4A	21:1:1013:CLA:C5	2.90	0.49
21:3:3005:CLA:NC	21:3:3012:CLA:CGA	2.76	0.49
17:4:171:ASP:CB	27:4:4503:NEX:H10	2.43	0.49
17:4:246:THR:HG21	21:4:4008:CLA:HED3	1.89	0.49
21:A:1131:CLA:HBB1	21:A:1132:CLA:H11	1.95	0.49
21:A:1132:CLA:H91	21:L:1503:CLA:HBB2	1.95	0.49
1:A:553:VAL:HG11	21:A:1137:CLA:HMB3	1.93	0.49
2:B:645:VAL:HG12	21:B:1206:CLA:HHD	1.95	0.49
2:B:428:PHE:O	2:B:432:HIS:ND1	2.33	0.49
14:1:47:ARG:NH2	14:1:51:LEU:C	2.61	0.49
7:G:116:LYS:NZ	21:G:1002:CLA:NC	2.60	0.49
8:H:135:PRO:HG2	8:H:136:PRO:HD2	1.95	0.49
1:A:648:THR:CG2	1:A:651:GLY:CA	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:138:GLU:O	14:1:142:ILE:HG12	2.12	0.49
14:1:211:LEU:HD23	14:1:211:LEU:C	2.33	0.49
14:1:223:HIS:NE2	21:1:1003:CLA:CBD	2.72	0.49
21:2:2003:CLA:H12	21:2:2003:CLA:HMA2	1.93	0.49
21:2:2010:CLA:OBD	21:2:2010:CLA:HED2	2.12	0.49
15:2:232:ARG:NH1	21:2:2004:CLA:ND	2.60	0.49
16:3:159:LEU:HD11	21:3:3013:CLA:C2D	2.42	0.49
17:4:110:MET:HE1	17:4:217:PHE:HE1	1.71	0.49
17:4:211:ARG:HA	17:4:214:MET:HE2	1.94	0.49
17:4:238:HIS:HE2	21:4:4003:CLA:HED3	1.78	0.49
18:A:5001:PQN:H201	21:A:1138:CLA:HBC1	1.95	0.49
21:B:1213:CLA:CHA	21:B:1213:CLA:CGA	2.91	0.49
20:B:7004:LHG:H161	20:B:7004:LHG:H312	1.94	0.49
6:F:202:LEU:HD13	6:F:207:VAL:HG22	1.94	0.49
1:A:654:ARG:NH2	1:A:655:ASP:OD2	2.27	0.49
3:C:77:MET:HB3	3:C:79:LEU:HG	1.94	0.49
21:1:1004:CLA:H152	21:1:1005:CLA:HMB1	1.95	0.48
21:A:9013:CLA:O1A	2:B:525:LEU:HD11	2.13	0.48
2:B:411:MET:HE3	21:B:1227:CLA:HHD	1.95	0.48
21:B:1207:CLA:HAB	9:I:14:LEU:CG	2.43	0.48
12:L:87:PRO:HD3	12:L:101:GLU:CD	2.32	0.48
17:4:168:VAL:O	17:4:179:LEU:HB2	2.13	0.48
21:4:4001:CLA:CMB	21:4:4001:CLA:HBB1	2.21	0.48
21:4:4005:CLA:HBC3	21:4:4005:CLA:CMC	2.43	0.48
1:A:401:TRP:HB3	21:A:1126:CLA:HMC3	1.95	0.48
21:A:1129:CLA:HHC	21:A:1129:CLA:CBB	2.23	0.48
16:3:241:GLY:O	16:3:245:GLN:HB2	2.12	0.48
10:J:11:ALA:CB	10:J:12:PRO:CD	2.88	0.48
1:A:615:HIS:HD2	21:A:1135:CLA:HMC1	1.77	0.48
8:H:123:GLY:O	8:H:125:ILE:HG13	2.13	0.48
21:1:1001:CLA:C3	21:1:1002:CLA:HBC1	2.43	0.48
14:1:102:LEU:CD1	21:1:1006:CLA:O1D	2.61	0.48
14:1:202:GLN:NE2	14:1:208:THR:CA	2.73	0.48
10:J:2:ARG:CG	21:J:6015:CLA:HBB2	2.43	0.48
12:L:204:LEU:HD23	12:L:207:LEU:HD21	1.95	0.48
7:G:76:ARG:HH12	21:G:1002:CLA:C1C	2.27	0.48
13:N:155:GLU:OE2	13:N:159:LYS:HD3	2.14	0.48
13:N:160:PHE:CD1	13:N:161:LYS:N	2.81	0.48
7:G:65:SER:CA	7:G:68:THR:CG2	2.85	0.48
11:K:98:PRO:HA	11:K:101:PHE:CD1	2.48	0.48
8:H:97:THR:HG21	12:L:96:LEU:HD12	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1502:LUT:C17	21:1:1004:CLA:C6	2.86	0.48
14:1:61:PHE:CE2	26:1:1502:LUT:C4	2.95	0.48
15:2:170:GLU:OE1	15:2:173:ARG:NE	2.47	0.48
21:3:3012:CLA:CED	21:3:3012:CLA:CHA	2.91	0.48
17:4:75:ASN:HB2	21:4:4004:CLA:HMD1	1.95	0.48
21:B:1205:CLA:CGA	21:B:1205:CLA:C1A	2.91	0.48
21:B:1207:CLA:H41	21:B:1207:CLA:H61	1.55	0.48
21:A:1138:CLA:H71	21:B:1229:CLA:H42	1.95	0.48
2:B:173:SER:O	2:B:177:HIS:ND1	2.31	0.48
19:B:6006:BCR:HC21	21:B:1211:CLA:HMA1	1.95	0.48
21:A:1119:CLA:H2	21:A:1123:CLA:HBB1	1.94	0.48
16:3:221:LEU:O	16:3:223:GLU:HA	2.13	0.48
14:1:111:TRP:CH2	14:1:129:GLY:O	2.66	0.48
21:1:1003:CLA:H62	20:1:1801:LHG:C18	2.43	0.48
15:2:166:ILE:O	15:2:166:ILE:HG22	2.13	0.48
21:B:1220:CLA:CMA	21:B:1240:CLA:HED2	2.44	0.48
21:B:1230:CLA:H91	21:F:1301:CLA:HMA1	1.95	0.48
2:B:299:HIS:CE1	21:B:1219:CLA:HMD1	2.48	0.48
7:G:76:ARG:NH1	21:G:1002:CLA:CHC	2.73	0.48
2:B:85:ARG:NH2	8:H:135:PRO:HD3	2.28	0.48
12:L:171:LYS:O	12:L:172:GLN:HB3	2.12	0.48
4:D:101:TYR:CE2	4:D:135:LYS:HB2	2.48	0.48
12:L:121:ARG:HB2	12:L:122:ASN:CB	2.44	0.48
1:A:279:ASP:OD1	1:A:280:PHE:N	2.46	0.48
1:A:308:ILE:HD11	21:A:1115:CLA:HMC2	1.95	0.48
8:H:124:ASP:N	8:H:124:ASP:OD1	2.47	0.48
15:2:113:HIS:CG	21:2:2004:CLA:CBB	2.96	0.48
15:2:110:GLU:HG3	21:2:2004:CLA:NB	2.29	0.48
21:2:2010:CLA:C2C	21:2:2013:CLA:HMC3	2.43	0.48
17:4:246:THR:HG21	17:4:248:VAL:CG2	2.34	0.48
21:4:4003:CLA:HBB1	26:4:4501:LUT:H182	1.90	0.48
21:B:1205:CLA:HAB	21:B:1206:CLA:HAA2	1.95	0.48
2:B:463:ILE:HG22	2:B:467:HIS:HE1	1.77	0.48
2:B:188:LEU:HD21	19:B:6004:BCR:H23C	1.95	0.48
7:G:65:SER:O	7:G:68:THR:HG23	2.14	0.48
21:A:1123:CLA:H142	21:A:1123:CLA:H111	1.66	0.48
13:N:120:VAL:HA	13:N:131:PHE:CD2	2.48	0.48
19:A:6002:BCR:H15C	19:A:6002:BCR:H351	1.69	0.48
1:A:291:THR:HG23	1:A:293:GLY:H	1.78	0.48
15:2:252:PRO:CD	15:2:253:ILE:N	2.77	0.48
2:B:439:HIS:CE1	2:B:453:ILE:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1501:LUT:C32	21:1:1001:CLA:HMC2	2.43	0.48
14:1:91:VAL:CG1	26:1:1501:LUT:H192	2.43	0.48
14:1:170:TYR:H	14:1:170:TYR:HD1	1.62	0.48
21:4:4005:CLA:CGD	21:4:4005:CLA:H2A	2.44	0.48
17:4:160:GLN:CG	21:4:4005:CLA:HMA3	2.44	0.48
1:A:354:TRP:HB3	21:A:1103:CLA:HAC1	1.96	0.48
21:A:1111:CLA:CGA	21:A:1111:CLA:H3A	2.43	0.48
1:A:434:ARG:O	1:A:438:HIS:N	2.44	0.48
2:B:5:ILE:HG12	2:B:6:PRO:HA	1.96	0.48
21:B:1224:CLA:H203	19:I:6018:BCR:H371	1.94	0.48
19:J:6012:BCR:H19C	19:J:6013:BCR:C36	2.44	0.48
12:L:173:PRO:HD2	12:L:173:PRO:O	2.13	0.48
4:D:79:THR:HB	4:D:127:PRO:HB2	1.96	0.48
1:A:308:ILE:O	1:A:312:ILE:HG22	2.13	0.48
16:3:168:GLY:O	16:3:170:ALA:N	2.46	0.48
16:3:247:LEU:HD11	21:3:3014:CLA:HAA1	1.95	0.48
21:4:4003:CLA:HAA1	21:4:4003:CLA:CBD	2.42	0.48
26:4:4501:LUT:C20	26:4:4501:LUT:C35	2.85	0.48
21:1:1009:CLA:HMD3	27:4:4503:NEX:H203	1.95	0.48
21:B:1224:CLA:H162	21:B:1224:CLA:H141	1.75	0.48
4:D:79:THR:OG1	4:D:129:LEU:HB2	2.14	0.48
8:H:68:GLY:C	8:H:70:TRP:H	2.17	0.48
16:3:96:PHE:CD1	16:3:101:TRP:HD1	2.32	0.48
1:A:267:THR:HB	1:A:277:TYR:OH	2.13	0.48
2:B:389:HIS:HA	2:B:392:ILE:HD12	1.96	0.48
21:1:1002:CLA:CMB	21:1:1007:CLA:C3D	2.92	0.48
21:1:1003:CLA:H171	21:1:1008:CLA:C7	2.44	0.48
21:2:2012:CLA:CBC	21:2:2012:CLA:CHD	2.90	0.48
17:4:171:ASP:OD1	27:4:4503:NEX:H191	2.13	0.48
17:4:110:MET:CE	17:4:217:PHE:HD1	2.26	0.48
21:4:4014:CLA:CAA	21:4:4014:CLA:CBD	2.91	0.48
17:4:171:ASP:CB	27:4:4503:NEX:C12	2.85	0.48
6:F:207:VAL:CG2	6:F:208:PHE:N	2.77	0.48
13:N:161:LYS:HD2	13:N:168:TRP:CE3	2.49	0.48
12:L:58:GLN:HB2	12:L:70:GLU:OE1	2.14	0.48
12:L:150:ILE:HG22	12:L:150:ILE:O	2.14	0.48
11:K:55:VAL:HA	11:K:58:VAL:HG22	1.95	0.48
14:1:185:VAL:O	14:1:188:GLY:N	2.46	0.48
3:C:10:THR:HA	5:E:101:TYR:CE2	2.48	0.48
15:2:110:GLU:HG3	21:2:2004:CLA:C1B	2.44	0.48
21:2:2002:CLA:HMB1	26:2:2501:LUT:H193	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:235:MET:HB3	26:2:2502:LUT:C15	2.44	0.48
21:4:4002:CLA:O1A	21:4:4002:CLA:HMA2	2.13	0.48
17:4:155:GLU:HG3	21:4:4012:CLA:C4B	2.44	0.48
26:4:4502:LUT:O23	26:4:4502:LUT:H373	2.13	0.48
21:B:1238:CLA:H18	19:I:6018:BCR:H353	1.96	0.48
12:L:104:LEU:CD2	19:L:6020:BCR:C12	2.86	0.48
1:A:41:SER:HB3	1:A:44:ILE:HG12	1.96	0.48
5:E:91:VAL:HG23	5:E:104:VAL:HG12	1.96	0.48
15:2:72:PHE:HD1	15:2:73:PRO:HD2	1.78	0.47
21:3:3001:CLA:H3A	21:3:3001:CLA:HBA2	1.53	0.47
21:3:3009:CLA:CBF	21:3:3009:CLA:CGA	2.92	0.47
21:3:3010:CLA:CHA	21:3:3010:CLA:HBA1	2.44	0.47
21:3:3001:CLA:HBC2	21:3:3011:CLA:HMA1	1.95	0.47
21:A:1136:CLA:H61	21:A:1136:CLA:H41	1.64	0.47
2:B:129:LEU:HD23	21:B:1211:CLA:HED3	1.96	0.47
21:B:1213:CLA:CBF	21:B:1214:CLA:HMC2	2.44	0.47
19:B:6005:BCR:H333	21:B:1208:CLA:H92	1.95	0.47
20:B:7004:LHG:C18	20:B:7004:LHG:C34	2.86	0.47
7:G:124:VAL:HG21	21:G:1002:CLA:CMD	2.43	0.47
12:L:159:SER:N	12:L:178:THR:CG2	2.75	0.47
21:1:1009:CLA:H2	21:4:4005:CLA:CMD	2.10	0.47
16:3:167:MET:HA	16:3:167:MET:HE2	1.92	0.47
21:A:9012:CLA:HMB3	21:B:9010:CLA:H18	1.96	0.47
21:B:1213:CLA:CHA	21:B:1213:CLA:CBA	2.93	0.47
21:B:1226:CLA:H61	21:B:1226:CLA:H41	1.59	0.47
24:B:7101:DGD:HAT1	21:B:1201:CLA:HBC1	1.96	0.47
3:C:43:PRO:HA	4:D:185:VAL:HG11	1.96	0.47
21:1:1006:CLA:C1B	21:1:1013:CLA:C2	2.93	0.47
15:2:112:VAL:HG12	15:2:116:TRP:CD1	2.49	0.47
16:3:219:LYS:HG3	21:3:3001:CLA:CBA	2.44	0.47
17:4:178:SER:C	21:4:4014:CLA:CMA	2.83	0.47
21:A:1124:CLA:O2D	21:A:1125:CLA:CAD	2.63	0.47
19:L:6019:BCR:H24C	19:L:6019:BCR:H371	1.68	0.47
5:E:79:GLN:HG2	5:E:84:TYR:CE1	2.49	0.47
21:2:2009:CLA:C1	16:3:184:MET:O	2.62	0.47
16:3:157:TYR:CD1	16:3:157:TYR:N	2.83	0.47
16:3:170:ALA:HB1	16:3:174:ARG:NH2	2.29	0.47
16:3:208:PHE:N	16:3:208:PHE:CD1	2.81	0.47
21:3:3012:CLA:CED	21:3:3012:CLA:H2A	2.18	0.47
17:4:151:PHE:HD1	27:4:4503:NEX:H221	1.78	0.47
21:A:1105:CLA:HBA2	21:A:1107:CLA:H12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:5001:PQN:H161	18:A:5001:PQN:H141	1.69	0.47
21:F:1303:CLA:HBA2	21:F:1303:CLA:HED1	1.92	0.47
19:B:6004:BCR:C35	7:G:133:ILE:HD11	2.44	0.47
17:4:66:TYR:CE1	17:4:84:GLU:HG3	2.49	0.47
20:1:1801:LHG:H351	21:4:4015:CLA:HMA2	1.95	0.47
14:1:223:HIS:N	14:1:223:HIS:HD1	2.12	0.47
17:4:170:GLN:CG	17:4:173:ILE:CG2	2.86	0.47
21:1:1009:CLA:CHD	27:4:4503:NEX:C13	2.92	0.47
21:A:1126:CLA:H203	21:A:9012:CLA:H13	1.96	0.47
2:B:182:LEU:HD13	21:B:1210:CLA:HBB	1.97	0.47
2:B:343:VAL:HG21	21:B:1223:CLA:H51	1.97	0.47
2:B:659:THR:CA	21:B:9023:CLA:HAB	2.44	0.47
19:F:6014:BCR:H15C	19:F:6014:BCR:H351	1.64	0.47
17:4:197:ALA:O	17:4:199:THR:HG22	2.15	0.47
2:B:676:GLU:HG2	3:C:81:TYR:HE1	1.80	0.47
21:1:1007:CLA:HBD	21:1:1007:CLA:HAA1	1.97	0.47
15:2:166:ILE:HD13	21:2:2012:CLA:HMC3	1.96	0.47
21:2:2003:CLA:CBC	21:2:2003:CLA:CHD	2.85	0.47
15:2:235:MET:HB3	26:2:2502:LUT:C14	2.45	0.47
16:3:106:GLU:HA	16:3:109:ASN:ND2	2.29	0.47
16:3:174:ARG:HH22	21:3:3011:CLA:C3D	2.27	0.47
21:4:4008:CLA:C2	21:4:4008:CLA:HBB	2.44	0.47
21:4:4008:CLA:OBD	21:4:4008:CLA:HED2	2.14	0.47
26:4:4502:LUT:H7	26:4:4502:LUT:H192	1.82	0.47
21:A:1140:CLA:H62	21:A:1140:CLA:H41	1.67	0.47
21:B:1208:CLA:H12	21:B:1209:CLA:C4D	2.45	0.47
10:J:29:ILE:HG23	25:J:5001:LMG:H292	1.95	0.47
7:G:114:LEU:CD2	7:G:116:LYS:HB3	2.44	0.47
4:D:166:TYR:OH	4:D:169:PRO:HD2	2.14	0.47
2:B:246:THR:CG2	2:B:248:GLN:CG	2.85	0.47
12:L:159:SER:HA	12:L:177:GLN:HB2	1.97	0.47
1:A:217:SER:O	21:A:1112:CLA:HMC3	2.15	0.47
17:4:175:LYS:O	17:4:175:LYS:HG3	2.14	0.47
14:1:211:LEU:HD21	21:1:1003:CLA:H2A	1.95	0.47
14:1:142:ILE:HG21	21:1:1012:CLA:HMC3	1.96	0.47
19:B:6009:BCR:H321	19:B:6009:BCR:HC8	1.97	0.47
9:I:11:LEU:H	9:I:11:LEU:HD12	1.80	0.47
14:1:226:ILE:N	14:1:227:GLY:CA	2.71	0.47
14:1:85:ARG:NE	21:1:1001:CLA:CHD	2.78	0.47
16:3:204:PRO:CG	16:3:209:PHE:HB3	2.44	0.47
21:A:1109:CLA:H41	21:A:1109:CLA:H62	1.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1109:CLA:H91	21:A:1109:CLA:H112	1.71	0.47
1:A:602:LEU:HD21	20:A:7001:LHG:H321	1.96	0.47
21:B:1207:CLA:HAB	9:I:14:LEU:CD2	2.44	0.47
2:B:523:ILE:HG21	21:B:1234:CLA:HAB	1.97	0.47
2:B:438:VAL:O	2:B:442:VAL:HG23	2.15	0.47
2:B:302:LYS:HD2	7:G:94:GLN:HG3	1.96	0.47
2:B:292:ARG:NH1	7:G:91:VAL:HG21	2.30	0.47
13:N:135:GLN:N	13:N:136:ASP:HA	2.29	0.47
1:A:330:ILE:HG23	1:A:331:LEU:N	2.30	0.47
3:C:28:MET:CE	3:C:39:ILE:C	2.82	0.47
21:B:1237:CLA:H41	21:B:1237:CLA:H62	1.53	0.47
14:1:149:ARG:CD	21:1:1011:CLA:C1D	2.92	0.47
15:2:150:GLU:O	21:2:2006:CLA:HMB2	2.15	0.47
21:2:2002:CLA:CMA	26:2:2501:LUT:C20	2.93	0.47
15:2:228:ILE:HG21	15:2:232:ARG:NH2	2.30	0.47
21:B:1215:CLA:H41	21:B:1215:CLA:H62	1.66	0.47
21:B:1216:CLA:H143	21:B:1216:CLA:H111	1.80	0.47
21:B:1216:CLA:CMB	21:B:1221:CLA:HMA3	2.43	0.47
2:B:174:ARG:NE	21:B:1221:CLA:HMD1	2.30	0.47
12:L:209:LEU:HA	12:L:210:PRO:HA	1.56	0.47
4:D:171:ASP:OD2	4:D:182:ARG:HG2	2.15	0.47
6:F:181:TYR:O	6:F:185:ILE:HG12	2.15	0.47
21:A:1119:CLA:HBA1	21:A:1123:CLA:C3B	2.45	0.47
2:B:286:ILE:HG13	2:B:287:GLY:N	2.30	0.47
1:A:133:ASN:HB3	1:A:141:ARG:HB3	1.96	0.47
21:1:1009:CLA:CBB	17:4:156:ILE:CG1	2.85	0.47
26:1:1501:LUT:H403	21:1:1001:CLA:CBB	2.45	0.47
16:3:167:MET:CE	16:3:167:MET:CA	2.85	0.47
17:4:104:MET:CB	26:4:4501:LUT:H35	2.44	0.47
1:A:475:ASP:HB3	21:A:1132:CLA:HED2	1.97	0.47
21:B:1227:CLA:HBA1	21:B:1240:CLA:C4	2.45	0.47
12:L:114:PHE:CZ	12:L:137:LEU:HD22	2.48	0.47
16:3:119:GLY:CA	21:3:3006:CLA:HBB1	2.45	0.47
1:A:491:TRP:HE3	1:A:492:ILE:HD12	1.80	0.47
21:1:1013:CLA:C7	21:1:1013:CLA:H41	2.41	0.47
21:1:1006:CLA:C2B	21:1:1013:CLA:H43	2.44	0.47
21:1:1006:CLA:CBA	21:1:1014:CLA:C3C	2.91	0.47
14:1:143:ALA:N	21:1:1012:CLA:CBB	2.78	0.47
14:1:46:PRO:N	21:4:4005:CLA:CBA	2.76	0.47
15:2:172:ARG:HA	21:4:4009:CLA:HED2	1.97	0.47
26:2:2501:LUT:C36	26:2:2501:LUT:C28	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:2002:CLA:HBA2	26:2:2501:LUT:C33	2.45	0.47
21:2:2002:CLA:CMA	26:2:2501:LUT:H201	2.44	0.47
17:4:171:ASP:HA	27:4:4503:NEX:H10	1.96	0.47
1:A:146:THR:HB	1:A:394:SER:OG	2.15	0.47
21:B:1227:CLA:CBA	21:B:1240:CLA:C4	2.91	0.47
21:B:1240:CLA:H62	21:B:1240:CLA:H41	1.62	0.47
19:B:6009:BCR:H351	19:B:6009:BCR:H15C	1.62	0.47
21:F:1303:CLA:HBB1	21:4:4012:CLA:H171	1.95	0.47
12:L:85:ASN:HB3	21:L:1501:CLA:HAC1	1.96	0.47
1:A:661:ALA:O	1:A:663:GLN:N	2.47	0.47
14:1:111:TRP:O	14:1:114:LEU:HD12	2.15	0.46
21:3:3010:CLA:CHD	21:3:3010:CLA:CBC	2.85	0.46
17:4:226:VAL:HG22	17:4:227:THR:H	1.80	0.46
21:4:4002:CLA:CHD	21:4:4007:CLA:CMB	2.88	0.46
21:1:1009:CLA:C3D	21:4:4005:CLA:HAC1	2.45	0.46
21:4:4009:CLA:HHC	21:4:4009:CLA:CBB	2.45	0.46
17:4:151:PHE:CD1	27:4:4503:NEX:H221	2.50	0.46
19:B:6006:BCR:H311	21:B:1225:CLA:H52	1.97	0.46
12:L:109:PHE:CE2	21:L:1502:CLA:CMB	2.98	0.46
2:B:292:ARG:HH12	7:G:107:ARG:NH2	2.10	0.46
4:D:104:THR:HG22	4:D:129:LEU:HD22	1.97	0.46
3:C:41:SER:OG	4:D:184:GLY:O	2.19	0.46
17:4:127:TRP:HE1	17:4:231:PRO:CD	2.28	0.46
2:B:519:VAL:HG11	2:B:593:TYR:HB2	1.97	0.46
21:1:1003:CLA:C15	21:1:1003:CLA:H193	2.45	0.46
14:1:131:LEU:O	14:1:135:LEU:CG	2.62	0.46
15:2:118:MET:SD	21:2:2001:CLA:C3C	3.03	0.46
21:2:2013:CLA:CBC	21:2:2013:CLA:CMC	2.86	0.46
16:3:210:ASN:N	16:3:210:ASN:OD1	2.44	0.46
26:4:4502:LUT:H27	26:4:4502:LUT:H392	1.81	0.46
21:A:1128:CLA:CHA	21:A:1128:CLA:HBA1	2.45	0.46
19:A:6017:BCR:H23C	19:A:6017:BCR:H392	1.97	0.46
2:B:411:MET:HE1	21:B:1227:CLA:C1D	2.45	0.46
2:B:708:VAL:O	2:B:712:HIS:ND1	2.48	0.46
7:G:140:LEU:C	7:G:140:LEU:CD2	2.82	0.46
2:B:406:ASN:O	2:B:410:ARG:HG2	2.15	0.46
6:F:190:LYS:O	6:F:193:GLN:HB3	2.15	0.46
14:1:96:VAL:HG22	14:1:97:PRO:HD3	1.98	0.46
21:1:1006:CLA:C2B	21:1:1013:CLA:C2	2.94	0.46
15:2:161:VAL:CG1	15:2:165:PHE:HE2	2.26	0.46
17:4:207:ILE:O	17:4:209:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1102:CLA:HBA1	21:A:1102:CLA:H3A	1.74	0.46
21:A:1136:CLA:H111	21:A:1136:CLA:H143	1.72	0.46
21:B:1204:CLA:H3A	21:B:1205:CLA:HMB3	1.97	0.46
21:B:1213:CLA:CBD	21:B:1213:CLA:CBA	2.84	0.46
21:B:1207:CLA:HED2	19:I:6020:BCR:HC7	1.97	0.46
12:L:172:GLN:C	12:L:172:GLN:HE21	2.19	0.46
14:1:177:PHE:CE2	14:1:181:LYS:CE	2.98	0.46
14:1:217:HIS:O	14:1:218:LEU:HD23	2.16	0.46
2:B:236:ASN:O	2:B:252:THR:N	2.43	0.46
1:A:519:ASP:OD1	1:A:520:LEU:N	2.48	0.46
6:F:115:PRO:O	6:F:119:ILE:HG13	2.15	0.46
14:1:137:ILE:HD12	14:1:138:GLU:N	2.31	0.46
15:2:235:MET:HE2	21:2:2004:CLA:HMC3	1.90	0.46
15:2:259:HIS:NE2	21:2:2003:CLA:CMD	2.71	0.46
17:4:102:TRP:C	17:4:102:TRP:CB	2.84	0.46
20:1:1801:LHG:C21	17:4:148:ILE:HG12	2.41	0.46
17:4:96:GLU:OE2	21:4:4004:CLA:HMA3	2.16	0.46
1:A:685:VAL:CG2	19:A:6011:BCR:H362	2.45	0.46
1:A:339:THR:HG21	20:A:7003:LHG:C2	2.45	0.46
2:B:711:VAL:HG11	21:B:1239:CLA:HED3	1.97	0.46
10:J:25:LEU:O	10:J:29:ILE:HG12	2.15	0.46
15:2:83:GLY:HA2	15:2:88:ASP:CG	2.35	0.46
13:N:101:LEU:HG	13:N:103:ASP:H	1.80	0.46
17:4:180:PRO:HD2	17:4:180:PRO:O	2.14	0.46
16:3:102:LEU:HD23	16:3:102:LEU:HA	1.75	0.46
6:F:152:GLY:O	6:F:157:TRP:NE1	2.41	0.46
21:1:1003:CLA:H41	21:1:1003:CLA:H62	1.58	0.46
21:1:1009:CLA:HHD	27:4:4503:NEX:C13	2.44	0.46
21:2:2004:CLA:C10	21:2:2005:CLA:HMB3	2.45	0.46
26:2:2501:LUT:C39	26:2:2501:LUT:H32	2.43	0.46
21:2:2005:CLA:HAB	26:2:2502:LUT:C20	2.46	0.46
21:A:1124:CLA:HMB2	21:A:1137:CLA:HBA1	1.98	0.46
19:A:6011:BCR:H351	19:A:6011:BCR:H15C	1.68	0.46
3:C:80:ALA:HB2	4:D:134:ARG:HD3	1.98	0.46
12:L:166:LEU:C	12:L:168:GLY:H	2.15	0.46
21:3:3006:CLA:H143	21:3:3006:CLA:H162	1.67	0.46
11:K:52:SER:HA	11:K:55:VAL:HG12	1.97	0.46
16:3:254:TYR:CD1	16:3:255:GLN:HG2	2.50	0.46
1:A:316:MET:O	1:A:325:HIS:ND1	2.46	0.46
21:1:1006:CLA:HMB2	21:1:1013:CLA:CMA	2.43	0.46
15:2:158:LEU:C	15:2:158:LEU:CD1	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:2007:CLA:H3A	21:2:2007:CLA:HBA1	1.69	0.46
1:A:339:THR:CG2	20:A:7003:LHG:C2	2.94	0.46
21:G:1001:CLA:CMC	21:G:1001:CLA:CBC	2.85	0.46
1:A:327:ILE:HA	1:A:330:ILE:HG22	1.98	0.46
1:A:327:ILE:O	1:A:331:LEU:HB2	2.16	0.46
1:A:458:PHE:O	1:A:462:ILE:HG12	2.15	0.46
3:C:14:CYS:SG	3:C:16:GLN:HB2	2.56	0.46
14:1:166:ASP:OD2	14:1:171:SER:HB3	2.16	0.46
14:1:85:ARG:NH2	21:1:1001:CLA:ND	2.64	0.46
14:1:207:GLY:O	14:1:211:LEU:HB2	2.16	0.46
16:3:164:MET:HE1	21:3:3012:CLA:HBC3	1.98	0.46
21:A:1108:CLA:HBB1	21:A:1111:CLA:HED2	1.97	0.46
1:A:692:PHE:HA	18:A:5001:PQN:H9	1.97	0.46
21:A:9013:CLA:H42	21:A:9013:CLA:O2A	2.15	0.46
21:B:1214:CLA:O1D	21:B:1215:CLA:HHB	2.16	0.46
12:L:207:LEU:HB3	12:L:208:ASP:H	1.54	0.46
21:A:1110:CLA:H52	16:3:89:ASP:OD2	2.15	0.46
14:1:204:ALA:C	14:1:206:PRO:HD3	2.35	0.46
21:1:1010:CLA:HED2	21:1:1010:CLA:CAD	2.45	0.46
14:1:158:LYS:O	14:1:159:LYS:HG3	2.15	0.46
21:2:2009:CLA:HBC1	21:3:3009:CLA:O2A	2.12	0.46
15:2:248:THR:O	15:2:250:THR:N	2.49	0.46
21:4:4014:CLA:HAA1	21:4:4014:CLA:CBD	2.45	0.46
19:A:6008:BCR:H282	19:A:6008:BCR:H392	1.23	0.46
21:B:1220:CLA:H41	21:B:1220:CLA:H61	1.60	0.46
12:L:105:ALA:HB2	21:L:1501:CLA:HMA1	1.96	0.46
7:G:114:LEU:CD1	7:G:116:LYS:HB3	2.45	0.46
4:D:190:ARG:O	4:D:191:SER:HB3	2.15	0.46
21:1:1006:CLA:C1B	21:1:1013:CLA:C4	2.92	0.46
21:1:1009:CLA:H71	21:1:1009:CLA:C12	2.45	0.46
14:1:64:LEU:CD1	26:1:1502:LUT:H163	2.46	0.46
10:J:2:ARG:N	15:2:98:SER:HG	2.13	0.46
17:4:234:ASN:O	17:4:238:HIS:CD2	2.68	0.46
17:4:170:GLN:NE2	21:4:4014:CLA:NB	2.64	0.46
21:B:1225:CLA:HBA2	21:B:1225:CLA:H3A	1.41	0.46
21:B:1240:CLA:CHD	21:B:1240:CLA:HBC3	2.46	0.46
23:A:9011:CL0:CBB	2:B:624:LEU:HD13	2.45	0.46
7:G:116:LYS:HG2	21:G:1002:CLA:C1B	2.45	0.46
4:D:78:ASN:C	4:D:79:THR:HG22	2.35	0.46
15:2:96:LEU:O	15:2:106:ASN:ND2	2.49	0.46
7:G:72:LEU:HD23	7:G:72:LEU:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASP:OD1	1:A:240:LYS:HG2	2.16	0.46
14:1:183:LYS:NZ	21:1:1002:CLA:CMC	2.79	0.46
21:1:1009:CLA:H162	21:1:1009:CLA:H121	1.57	0.46
14:1:94:ILE:CG2	14:1:105:TRP:CB	2.85	0.46
15:2:123:GLY:O	15:2:127:PRO:HD3	2.16	0.46
21:2:2002:CLA:HBA2	26:2:2501:LUT:C32	2.46	0.46
21:2:2003:CLA:CBB	21:2:2003:CLA:HHC	2.46	0.46
17:4:101:ARG:HB2	21:4:4011:CLA:CED	2.46	0.46
7:G:140:LEU:CD2	7:G:141:THR:N	2.78	0.46
15:2:71:TRP:CD1	15:2:90:GLY:O	2.69	0.46
6:F:95:GLU:HB2	6:F:130:PHE:CD2	2.51	0.46
21:1:1009:CLA:H3A	21:1:1009:CLA:HBA2	1.67	0.45
21:2:2003:CLA:H52	21:2:2003:CLA:H93	1.96	0.45
21:2:2014:CLA:HMB3	26:2:2501:LUT:O23	2.16	0.45
16:3:210:ASN:HB3	21:3:3001:CLA:O1D	2.15	0.45
21:A:1101:CLA:H151	19:J:6012:BCR:H14C	1.98	0.45
1:A:339:THR:HG21	20:A:7003:LHG:HC2	1.97	0.45
21:A:9012:CLA:HMB3	21:B:9010:CLA:C18	2.46	0.45
23:A:9011:CL0:CMB	21:A:9012:CLA:HMD1	2.46	0.45
7:G:116:LYS:HD3	7:G:118:ALA:N	2.31	0.45
4:D:159:PHE:HB3	4:D:160:PRO:CD	2.46	0.45
2:B:660:GLY:O	2:B:664:LEU:HG	2.16	0.45
2:B:7:ARG:HD2	2:B:7:ARG:HA	1.68	0.45
21:1:1008:CLA:C9	21:1:1008:CLA:H121	2.45	0.45
14:1:192:LEU:CD2	26:1:1502:LUT:H35	2.45	0.45
21:F:1303:CLA:C2B	26:4:4502:LUT:C20	2.92	0.45
1:A:339:THR:CG2	20:A:7003:LHG:HC2	2.47	0.45
21:B:1203:CLA:H41	21:B:1203:CLA:H61	1.54	0.45
21:B:1209:CLA:HBB1	21:B:1209:CLA:HHC	1.98	0.45
21:B:1215:CLA:CGA	21:B:1215:CLA:H3A	2.43	0.45
2:B:282:PHE:HZ	21:B:1213:CLA:HBB2	1.81	0.45
6:F:207:VAL:HG23	6:F:208:PHE:CD2	2.52	0.45
21:A:1106:CLA:CBB	19:J:6012:BCR:H363	2.46	0.45
12:L:64:PRO:HG2	12:L:65:PHE:HE1	1.66	0.45
21:G:1001:CLA:H62	21:G:1001:CLA:H41	1.64	0.45
1:A:429:ASN:OD1	1:A:431:LEU:HD23	2.16	0.45
1:A:682:ALA:HB1	1:A:745:THR:OG1	2.16	0.45
2:B:304:ILE:O	2:B:308:HIS:ND1	2.46	0.45
6:F:88:SER:OG	6:F:91:PHE:HB3	2.16	0.45
14:1:111:TRP:HH2	14:1:129:GLY:C	2.20	0.45
21:A:1106:CLA:C1C	21:A:1126:CLA:H51	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:VAL:HA	1:A:438:HIS:CE1	2.51	0.45
21:B:1214:CLA:H62	21:B:1214:CLA:H93	1.78	0.45
6:F:198:ILE:C	6:F:200:VAL:N	2.69	0.45
14:1:205:TYR:N	14:1:206:PRO:HD3	2.31	0.45
2:B:499:ASN:O	2:B:503:GLU:HG3	2.17	0.45
2:B:82:PHE:HE1	2:B:363:GLN:HG2	1.80	0.45
1:A:582:ASP:OD2	3:C:53:ARG:NH1	2.49	0.45
1:A:697:ARG:HD3	2:B:566:GLY:HA3	1.99	0.45
21:1:1013:CLA:H91	21:1:1013:CLA:H112	1.79	0.45
14:1:131:LEU:CD2	14:1:135:LEU:CD1	2.94	0.45
14:1:192:LEU:HD22	26:1:1502:LUT:C35	2.46	0.45
15:2:227:GLU:CD	21:2:2001:CLA:C4D	2.84	0.45
16:3:159:LEU:O	16:3:162:LEU:N	2.44	0.45
21:4:4001:CLA:H61	21:4:4002:CLA:H11	1.96	0.45
17:4:99:ASN:ND2	21:4:4004:CLA:CBB	2.73	0.45
21:4:4013:CLA:HBA1	21:4:4013:CLA:H3A	1.65	0.45
17:4:83:ALA:HB2	21:4:4004:CLA:O1A	2.16	0.45
21:A:1139:CLA:H72	21:A:1139:CLA:H112	1.75	0.45
21:B:1229:CLA:H191	21:B:1235:CLA:H111	1.98	0.45
19:B:6006:BCR:H282	19:B:6006:BCR:H392	1.26	0.45
7:G:114:LEU:C	7:G:116:LYS:H	2.18	0.45
2:B:242:HIS:HE1	2:B:246:THR:O	1.99	0.45
13:N:106:ARG:O	13:N:109:THR:OG1	2.25	0.45
2:B:676:GLU:HG2	3:C:81:TYR:CE1	2.52	0.45
1:A:432:LEU:O	1:A:436:LEU:HG	2.17	0.45
13:N:92:LEU:HD23	13:N:92:LEU:O	2.16	0.45
21:1:1002:CLA:H41	21:1:1002:CLA:H62	1.60	0.45
14:1:105:TRP:CE2	14:1:202:GLN:HG3	2.51	0.45
21:1:1009:CLA:CMA	20:1:1801:LHG:H282	2.47	0.45
14:1:201:GLN:NE2	14:1:211:LEU:HD13	2.30	0.45
21:2:2002:CLA:HBA2	26:2:2501:LUT:C34	2.47	0.45
10:J:2:ARG:N	15:2:98:SER:HB2	2.31	0.45
16:3:112:PHE:CZ	21:3:3012:CLA:O2D	2.69	0.45
16:3:208:PHE:HB3	21:3:3001:CLA:CED	2.47	0.45
21:4:4006:CLA:HBC1	21:4:4013:CLA:CHD	2.46	0.45
21:B:1213:CLA:CBB	21:B:1213:CLA:HMB1	2.46	0.45
21:B:1205:CLA:O1A	21:B:1224:CLA:HBD	2.16	0.45
19:L:6020:BCR:H15C	19:L:6020:BCR:H351	1.70	0.45
12:L:50:GLU:HA	12:L:51:LYS:HA	1.75	0.45
5:E:65:PRO:C	5:E:66:ILE:CG1	2.85	0.45
1:A:564:ARG:NE	4:D:114:GLU:OE2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1011:CLA:CBB	21:1:1011:CLA:HHC	2.46	0.45
14:1:146:GLU:OE1	14:1:149:ARG:CZ	2.62	0.45
14:1:88:MET:HB3	26:1:1501:LUT:H15	1.99	0.45
14:1:168:LEU:CB	14:1:170:TYR:CE1	2.85	0.45
14:1:170:TYR:HD2	14:1:180:TYR:CE2	2.29	0.45
15:2:114:SER:OG	15:2:115:ARG:N	2.49	0.45
21:2:2005:CLA:H2A	21:2:2005:CLA:O2D	2.17	0.45
21:2:2006:CLA:CMC	26:2:2502:LUT:C23	2.84	0.45
16:3:157:TYR:HD1	16:3:157:TYR:N	2.15	0.45
17:4:246:THR:CG2	17:4:247:ILE:N	2.80	0.45
21:4:4002:CLA:H11	26:4:4501:LUT:C39	2.43	0.45
21:4:4014:CLA:CBC	21:4:4014:CLA:CMC	2.93	0.45
21:A:1105:CLA:HMA1	21:A:1106:CLA:HMB3	1.99	0.45
21:A:1116:CLA:HBA2	21:A:1116:CLA:H3A	1.63	0.45
1:A:434:ARG:N	1:A:437:ARG:HG3	2.25	0.45
2:B:628:SER:CB	21:B:9010:CLA:CBC	2.94	0.45
9:I:11:LEU:O	9:I:15:LEU:N	2.49	0.45
19:I:6020:BCR:H351	19:I:6020:BCR:H15C	1.67	0.45
2:B:292:ARG:HH22	7:G:91:VAL:HG21	1.75	0.45
26:1:1501:LUT:C24	21:1:1001:CLA:CBA	2.94	0.45
21:2:2002:CLA:CBC	21:2:2002:CLA:CMC	2.92	0.45
16:3:204:PRO:HB3	16:3:209:PHE:HA	1.94	0.45
17:4:110:MET:SD	26:4:4502:LUT:H381	2.56	0.45
17:4:155:GLU:HA	17:4:155:GLU:OE1	2.16	0.45
21:A:1103:CLA:H93	21:A:1103:CLA:H62	1.75	0.45
1:A:375:HIS:ND1	21:A:1116:CLA:OBD	2.49	0.45
21:B:1213:CLA:H51	21:B:1213:CLA:H11	1.64	0.45
21:A:1138:CLA:H62	19:F:6014:BCR:H14C	1.99	0.45
12:L:53:THR:O	12:L:54:TYR:CD2	2.70	0.45
12:L:61:ASN:ND2	12:L:166:LEU:CG	2.79	0.45
1:A:715:LYS:HD2	6:F:179:ARG:HH12	1.82	0.45
8:H:129:VAL:O	8:H:130:LYS:HG2	2.17	0.45
21:1:1006:CLA:C4A	21:1:1013:CLA:H51	2.46	0.45
21:1:1009:CLA:C7	21:1:1009:CLA:H122	2.46	0.45
14:1:223:HIS:CD2	21:1:1003:CLA:O2A	2.70	0.45
14:1:46:PRO:N	21:4:4005:CLA:CGA	2.79	0.45
15:2:172:ARG:CZ	21:2:2011:CLA:CMC	2.94	0.45
21:2:2008:CLA:H3A	21:2:2008:CLA:HBA1	1.61	0.45
15:2:227:GLU:HA	15:2:230:ASN:HD21	1.82	0.45
16:3:202:ALA:C	16:3:204:PRO:CD	2.86	0.45
21:3:3002:CLA:C1	21:3:3002:CLA:H2A	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:4:77:PHE:CE2	26:4:4502:LUT:C17	2.85	0.45
19:A:6011:BCR:HC8	19:A:6011:BCR:H331	1.98	0.45
21:A:1138:CLA:HMA2	21:B:1228:CLA:HMB3	1.98	0.45
2:B:711:VAL:HG11	21:B:1239:CLA:CED	2.47	0.45
12:L:71:THR:OG1	12:L:73:VAL:HG13	2.17	0.45
7:G:116:LYS:HB2	21:G:1002:CLA:NA	2.32	0.45
2:B:243:LEU:HB2	2:B:246:THR:HB	1.98	0.45
21:A:1115:CLA:H61	21:A:1115:CLA:H41	1.67	0.45
16:3:223:GLU:C	16:3:225:LYS:H	2.19	0.45
15:2:86:PRO:CA	15:2:225:THR:HG22	2.46	0.45
2:B:410:ARG:O	2:B:414:HIS:CD2	2.70	0.45
16:3:235:ALA:HA	16:3:238:ALA:HB3	1.97	0.45
14:1:160:TYR:C	21:1:1001:CLA:CED	2.85	0.45
21:2:2009:CLA:O2D	16:3:169:PHE:CZ	2.70	0.45
17:4:247:ILE:HD13	21:4:4003:CLA:CMD	2.35	0.45
1:A:609:ILE:O	1:A:611:VAL:N	2.50	0.45
7:G:134:VAL:O	7:G:137:TYR:HB3	2.16	0.45
21:H:1000:CLA:HBA1	21:H:1000:CLA:H3A	1.56	0.45
19:L:6019:BCR:H383	19:L:6019:BCR:H23C	1.98	0.45
13:N:159:LYS:O	13:N:162:CYS:HA	2.17	0.45
16:3:90:PRO:HB3	16:3:98:GLU:O	2.15	0.45
21:1:1010:CLA:C9	21:1:1010:CLA:C3	2.85	0.45
15:2:112:VAL:O	15:2:116:TRP:CD1	2.70	0.45
21:2:2005:CLA:H3A	21:2:2005:CLA:HBA1	1.81	0.45
16:3:206:GLY:O	16:3:209:PHE:CZ	2.70	0.45
17:4:249:GLN:HE21	17:4:249:GLN:HB2	1.62	0.45
21:F:1303:CLA:CMB	21:4:4004:CLA:H101	2.47	0.45
21:4:4011:CLA:H61	21:4:4011:CLA:H2	1.67	0.45
17:4:151:PHE:CA	27:4:4503:NEX:H372	2.47	0.45
17:4:98:VAL:HG21	17:4:158:ARG:NH2	2.32	0.45
21:A:1101:CLA:H102	21:A:1101:CLA:H61	1.79	0.45
21:A:1126:CLA:O1D	21:A:1127:CLA:HBB	2.17	0.45
1:A:475:ASP:CG	21:A:1132:CLA:CED	2.85	0.45
12:L:110:LEU:O	12:L:114:PHE:HD2	2.00	0.45
7:G:116:LYS:HD3	7:G:117:SER:CA	2.46	0.45
13:N:161:LYS:HD2	13:N:168:TRP:CZ3	2.52	0.45
2:B:242:HIS:CE1	2:B:243:LEU:O	2.70	0.45
12:L:161:ALA:CB	12:L:174:ASP:HB2	2.46	0.45
11:K:54:ASN:O	11:K:58:VAL:HG13	2.16	0.45
1:A:707:ILE:O	1:A:711:HIS:ND1	2.50	0.45
14:1:82:ILE:CD1	21:1:1012:CLA:C3D	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:2004:CLA:H101	21:2:2005:CLA:HMB3	1.98	0.44
16:3:106:GLU:HA	16:3:109:ASN:HD21	1.82	0.44
17:4:96:GLU:OE1	17:4:211:ARG:HD3	2.17	0.44
21:B:1220:CLA:H141	21:B:1220:CLA:H161	1.69	0.44
21:B:1222:CLA:H3A	21:B:1222:CLA:HBA2	1.57	0.44
21:B:1240:CLA:HBA1	21:B:1240:CLA:C4A	2.46	0.44
2:B:428:PHE:CD2	21:B:1235:CLA:HAB	2.52	0.44
20:B:7004:LHG:C33	20:B:7004:LHG:H181	2.45	0.44
21:B:1235:CLA:H52	19:F:6016:BCR:H343	1.99	0.44
19:F:6016:BCR:H24C	19:F:6016:BCR:H371	1.62	0.44
7:G:64:ILE:HA	7:G:135:ALA:HB1	1.99	0.44
13:N:116:ARG:NH2	13:N:120:VAL:O	2.50	0.44
4:D:140:ALA:O	4:D:143:THR:HG22	2.17	0.44
21:1:1008:CLA:C5	21:1:1008:CLA:H92	2.39	0.44
14:1:145:VAL:O	14:1:146:GLU:CB	2.65	0.44
21:2:2005:CLA:HAB	26:2:2502:LUT:H203	1.98	0.44
21:2:2010:CLA:H142	21:2:2010:CLA:H112	1.75	0.44
21:2:2001:CLA:HHB	21:2:2014:CLA:HAA2	1.99	0.44
21:2:2009:CLA:O2D	16:3:169:PHE:CE1	2.70	0.44
16:3:177:ASP:OD2	16:3:209:PHE:CE2	2.70	0.44
17:4:171:ASP:HB2	17:4:172:PRO:HD3	1.99	0.44
21:B:1206:CLA:H3A	21:B:1207:CLA:HBB1	1.97	0.44
2:B:51:PHE:CE1	21:B:1208:CLA:HBB1	2.51	0.44
21:B:9023:CLA:CGA	21:B:9023:CLA:C3A	2.94	0.44
7:G:115:LEU:C	21:G:1002:CLA:CMA	2.85	0.44
21:3:3008:CLA:CBA	21:3:3008:CLA:HBD	2.47	0.44
21:3:3008:CLA:HBC2	21:3:3008:CLA:CHD	2.46	0.44
21:A:1123:CLA:H13	21:A:1123:CLA:HMD2	1.98	0.44
5:E:76:ILE:HB	5:E:83:TRP:O	2.17	0.44
11:K:68:GLY:HA2	11:K:69:ARG:HA	1.67	0.44
2:B:391:PRO:HG3	2:B:538:ALA:HA	1.99	0.44
2:B:476:VAL:HG12	2:B:477:LEU:H	1.81	0.44
21:1:1010:CLA:CED	21:1:1010:CLA:C4D	2.85	0.44
14:1:195:PHE:CZ	26:1:1502:LUT:H402	2.52	0.44
14:1:81:LEU:HA	14:1:84:CYS:HB2	1.98	0.44
15:2:152:PHE:CD2	21:2:2006:CLA:C4	3.01	0.44
21:2:2007:CLA:HMA3	20:2:2801:LHG:HC32	1.98	0.44
21:2:2003:CLA:CBB	26:2:2501:LUT:H41	2.46	0.44
16:3:171:GLU:CA	16:3:174:ARG:HG3	2.45	0.44
21:3:3009:CLA:HED2	21:3:3009:CLA:CHA	2.45	0.44
17:4:238:HIS:CD2	21:4:4003:CLA:O2D	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1106:CLA:H3A	21:A:1106:CLA:HBA2	1.39	0.44
21:A:1137:CLA:H41	21:A:1137:CLA:H62	1.46	0.44
21:A:9012:CLA:CED	2:B:620:LEU:CD1	2.95	0.44
1:A:92:TRP:O	1:A:96:MET:HG2	2.17	0.44
21:B:1224:CLA:H142	21:B:1224:CLA:H112	1.71	0.44
12:L:72:PRO:O	12:L:76:SER:OG	2.35	0.44
17:4:197:ALA:C	17:4:199:THR:N	2.71	0.44
13:N:160:PHE:CZ	13:N:166:VAL:CG1	2.99	0.44
12:L:53:THR:O	12:L:54:TYR:CG	2.70	0.44
21:3:3003:CLA:H41	21:3:3003:CLA:H62	1.56	0.44
2:B:316:GLY:N	2:B:410:ARG:HH21	2.14	0.44
16:3:180:LYS:HA	16:3:181:PRO:HD2	1.76	0.44
2:B:158:GLN:HB2	2:B:161:TRP:HE3	1.83	0.44
21:1:1003:CLA:H43	21:1:1008:CLA:OBD	2.18	0.44
21:1:1011:CLA:C14	21:1:1011:CLA:H171	2.44	0.44
26:1:1501:LUT:H393	26:1:1501:LUT:H27	1.88	0.44
21:3:3001:CLA:HBC1	21:3:3011:CLA:HMA1	2.00	0.44
21:4:4004:CLA:C4B	26:4:4502:LUT:H193	2.47	0.44
1:A:511:THR:HG21	21:A:1125:CLA:CBB	2.47	0.44
7:G:116:LYS:C	7:G:116:LYS:CD	2.85	0.44
4:D:130:LEU:CD2	4:D:131:LYS:N	2.73	0.44
4:D:160:PRO:CD	4:D:161:SER:H	2.31	0.44
16:3:223:GLU:C	16:3:225:LYS:N	2.70	0.44
6:F:119:ILE:O	6:F:123:ILE:HG13	2.18	0.44
15:2:263:PRO:HG2	16:3:153:TRP:HZ2	1.83	0.44
13:N:107:LEU:HD12	13:N:107:LEU:HA	1.80	0.44
14:1:85:ARG:NH2	21:1:1001:CLA:C4D	2.81	0.44
21:1:1008:CLA:C9	21:1:1008:CLA:C12	2.95	0.44
21:1:1009:CLA:O1D	20:1:1801:LHG:C6	2.65	0.44
21:1:1005:CLA:CMD	21:1:1012:CLA:ND	2.73	0.44
21:2:2011:CLA:CMC	21:2:2011:CLA:HBC2	2.40	0.44
16:3:212:LEU:HD12	16:3:212:LEU:O	2.17	0.44
17:4:243:TRP:CE2	21:4:4008:CLA:O1A	2.70	0.44
19:A:6011:BCR:H291	21:A:1126:CLA:H42	2.00	0.44
19:A:6011:BCR:H333	21:A:9013:CLA:H141	1.99	0.44
21:B:1207:CLA:CMA	8:H:117:PHE:HZ	2.31	0.44
21:B:1227:CLA:HMB2	21:B:1228:CLA:C3D	2.47	0.44
1:A:554:LEU:CD2	21:B:9023:CLA:HED3	2.47	0.44
9:I:14:LEU:HA	9:I:14:LEU:HD22	1.64	0.44
3:C:75:ARG:NE	4:D:157:ARG:NH1	2.65	0.44
7:G:78:VAL:HG13	7:G:79:PHE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:696:LYS:NZ	3:C:81:TYR:O	2.44	0.44
6:F:206:LEU:O	6:F:209:ARG:HB2	2.17	0.44
21:1:1003:CLA:H171	21:1:1008:CLA:H72	2.00	0.44
26:1:1502:LUT:H202	26:1:1502:LUT:H11	1.87	0.44
14:1:62:ASP:OD1	14:1:65:ARG:N	2.50	0.44
16:3:200:ASN:N	16:3:201:PRO:HD2	2.11	0.44
21:4:4003:CLA:H3A	21:4:4003:CLA:HBA2	1.74	0.44
21:A:1101:CLA:H41	21:A:1101:CLA:H61	1.53	0.44
1:A:410:ALA:HB1	19:A:6008:BCR:H383	1.98	0.44
21:B:1202:CLA:H91	21:B:1221:CLA:O1D	2.17	0.44
4:D:101:TYR:N	4:D:132:LEU:O	2.48	0.44
11:K:99:ALA:O	11:K:103:LEU:HG	2.17	0.44
6:F:173:TRP:C	6:F:173:TRP:CD1	2.91	0.44
1:A:567:ARG:NH2	4:D:88:THR:O	2.50	0.44
12:L:185:PHE:C	12:L:185:PHE:CD1	2.90	0.44
14:1:223:HIS:CD2	21:1:1003:CLA:OBD	2.70	0.44
14:1:102:LEU:HD11	21:1:1006:CLA:H2A	1.98	0.44
21:1:1006:CLA:CBA	21:1:1014:CLA:C1C	2.90	0.44
26:1:1502:LUT:C17	21:1:1004:CLA:C7	2.95	0.44
21:2:2010:CLA:C17	21:2:2010:CLA:H143	2.33	0.44
16:3:171:GLU:C	16:3:174:ARG:CG	2.85	0.44
16:3:203:TYR:O	16:3:203:TYR:CD1	2.70	0.44
21:4:4012:CLA:H121	21:4:4012:CLA:H192	1.96	0.44
21:A:1126:CLA:H141	21:A:1126:CLA:H161	1.80	0.44
1:A:58:HIS:HB2	20:A:7001:LHG:H111	2.00	0.44
2:B:292:ARG:CZ	7:G:91:VAL:CG2	2.85	0.44
4:D:106:GLU:HG2	4:D:127:PRO:HA	1.99	0.44
13:N:160:PHE:HA	13:N:162:CYS:N	2.32	0.44
12:L:53:THR:C	12:L:55:GLN:H	2.20	0.44
16:3:257:LEU:HD22	21:3:3003:CLA:CAB	2.47	0.44
21:J:6014:CLA:C2	21:J:6014:CLA:HBA2	2.42	0.44
13:N:90:ALA:O	13:N:94:LYS:N	2.35	0.44
13:N:130:ASN:HA	13:N:134:CYS:HB3	2.00	0.44
21:A:1112:CLA:HBA2	21:A:1114:CLA:HMB3	1.99	0.44
1:A:373:ALA:HB2	1:A:399:HIS:HB2	2.00	0.44
8:H:118:SER:HA	9:I:7:LEU:HD12	2.00	0.44
21:1:1009:CLA:H41	21:1:1009:CLA:H62	1.66	0.44
15:2:161:VAL:HG21	21:4:4008:CLA:HBA1	2.00	0.44
16:3:159:LEU:O	16:3:163:GLU:N	2.51	0.44
17:4:172:PRO:CG	17:4:173:ILE:N	2.80	0.44
21:4:4007:CLA:CHD	21:4:4007:CLA:CBC	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:1132:CLA:H43	12:L:114:PHE:CE2	2.53	0.44
2:B:517:PHE:HA	21:B:1235:CLA:HED1	2.00	0.44
2:B:655:LEU:O	2:B:659:THR:OG1	2.30	0.44
1:A:429:ASN:O	1:A:430:ASP:HB2	2.18	0.44
2:B:300:SER:O	2:B:304:ILE:HG13	2.18	0.44
3:C:11:CYS:SG	3:C:12:ILE:N	2.91	0.44
2:B:69:ALA:HB2	2:B:135:LEU:HB2	1.99	0.44
21:1:1003:CLA:H92	20:1:1801:LHG:C18	2.46	0.44
21:1:1008:CLA:O1A	21:1:1008:CLA:H2	2.17	0.44
14:1:127:PRO:O	14:1:128:TRP:CB	2.65	0.44
26:1:1501:LUT:H391	26:1:1501:LUT:H31	1.66	0.44
14:1:154:ASP:HA	14:1:155:PRO:HD2	1.72	0.44
14:1:195:PHE:CE1	26:1:1502:LUT:C40	3.01	0.44
21:2:2010:CLA:H3A	21:2:2010:CLA:HBA2	1.81	0.44
16:3:205:GLY:O	16:3:209:PHE:CE2	2.70	0.44
16:3:240:LEU:HD13	21:3:3005:CLA:CGA	2.48	0.44
21:A:1104:CLA:H101	21:A:1104:CLA:H162	2.00	0.44
21:B:1239:CLA:HBA2	21:B:1239:CLA:H3A	1.76	0.44
2:B:662:MET:HB2	21:B:9023:CLA:C1C	2.48	0.44
21:B:1207:CLA:H13	8:H:113:THR:HG22	1.99	0.44
16:3:245:GLN:HG3	21:3:3003:CLA:HMC2	2.00	0.44
13:N:120:VAL:O	13:N:120:VAL:HG23	2.18	0.44
13:N:103:ASP:HB2	13:N:104:LYS:H	1.54	0.44
1:A:397:THR:HG23	1:A:613:ILE:HG21	2.00	0.44
1:A:464:ASN:HB3	1:A:476:MET:HE3	2.00	0.44
9:I:9:VAL:O	9:I:12:VAL:HG22	2.18	0.44
14:1:160:TYR:HB2	21:1:1001:CLA:HED2	1.93	0.43
14:1:83:HIS:CD2	21:1:1004:CLA:HBB2	2.53	0.43
14:1:131:LEU:HD23	14:1:132:PRO:CA	2.49	0.43
16:3:163:GLU:OE2	21:3:3013:CLA:HHC	2.17	0.43
26:4:4501:LUT:O3	26:4:4501:LUT:H173	2.18	0.43
21:A:1129:CLA:O1A	21:A:1130:CLA:HMD1	2.18	0.43
1:A:205:HIS:CD2	21:A:1111:CLA:HMC2	2.52	0.43
1:A:408:VAL:HG21	1:A:605:MET:HE2	2.00	0.43
7:G:141:THR:HG22	25:G:2021:LMG:HC72	1.96	0.43
12:L:195:SER:O	19:L:6020:BCR:H323	2.18	0.43
14:1:47:ARG:HB3	14:1:47:ARG:HE	1.67	0.43
7:G:114:LEU:CD2	7:G:118:ALA:C	2.86	0.43
14:1:96:VAL:HG22	14:1:97:PRO:CD	2.48	0.43
2:B:548:PRO:HD2	3:C:62:PHE:CE1	2.53	0.43
14:1:180:TYR:CD2	21:1:1001:CLA:O1A	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1003:CLA:H91	21:1:1003:CLA:H122	2.00	0.43
15:2:121:ALA:C	15:2:123:GLY:N	2.72	0.43
15:2:259:HIS:HE2	21:2:2003:CLA:C2D	2.31	0.43
16:3:177:ASP:OD1	16:3:209:PHE:CE2	2.71	0.43
26:4:4501:LUT:C8	26:4:4501:LUT:C18	2.86	0.43
21:A:1109:CLA:H141	21:A:1109:CLA:H161	1.78	0.43
1:A:358:LEU:HD11	21:A:1128:CLA:CBB	2.28	0.43
1:A:684:PHE:C	1:A:684:PHE:CD1	2.91	0.43
1:A:691:MET:HE2	18:A:5001:PQN:H2M3	1.99	0.43
2:B:225:LEU:HA	2:B:230:TRP:CD1	2.53	0.43
19:B:6011:BCR:H321	21:F:1302:CLA:HMD1	2.00	0.43
6:F:167:PHE:HB2	19:F:6014:BCR:H393	2.01	0.43
12:L:202:PHE:HB3	12:L:203:LEU:HD12	2.00	0.43
21:A:1110:CLA:HED2	21:A:1110:CLA:H2A	2.00	0.43
14:1:145:VAL:HG12	21:1:1011:CLA:C3B	2.49	0.43
21:2:2002:CLA:C6	26:2:2501:LUT:C36	2.95	0.43
20:1:1801:LHG:H351	21:4:4015:CLA:HBA1	2.00	0.43
21:A:1106:CLA:HMC3	21:A:1107:CLA:CMD	2.46	0.43
21:A:1117:CLA:HMB1	21:A:1117:CLA:HBB1	2.00	0.43
1:A:688:PHE:HA	21:A:9013:CLA:HAB	1.99	0.43
2:B:51:PHE:HE1	21:B:1208:CLA:HBB1	1.82	0.43
6:F:207:VAL:HB	21:F:1301:CLA:HED2	1.99	0.43
19:I:6018:BCR:H392	19:I:6018:BCR:H282	1.26	0.43
12:L:104:LEU:C	12:L:104:LEU:HD23	2.39	0.43
14:1:48:PRO:HG2	14:1:51:LEU:HB2	2.00	0.43
7:G:76:ARG:HH11	7:G:116:LYS:HZ1	1.65	0.43
1:A:265:GLY:HA3	21:3:3017:CLA:HBA2	2.00	0.43
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.81	0.43
21:A:1115:CLA:H51	11:K:113:GLY:CA	2.48	0.43
17:4:202:ALA:C	17:4:205:LYS:H	2.20	0.43
2:B:73:ASN:HB2	2:B:76:ALA:HB3	2.00	0.43
3:C:73:THR:H	3:C:76:SER:HG	1.64	0.43
14:1:160:TYR:HB3	21:1:1001:CLA:CGD	2.47	0.43
21:2:2005:CLA:H162	21:2:2005:CLA:H203	1.85	0.43
21:2:2008:CLA:C2	21:2:2008:CLA:HMA2	2.48	0.43
16:3:168:GLY:C	16:3:170:ALA:N	2.71	0.43
21:4:4013:CLA:HMA2	27:4:4503:NEX:H222	2.00	0.43
21:A:1139:CLA:H51	21:A:1139:CLA:H11	1.83	0.43
21:B:1226:CLA:HBC2	21:B:1226:CLA:HHD	2.00	0.43
6:F:166:LEU:O	6:F:170:ILE:HG13	2.18	0.43
15:2:234:ALA:HA	15:2:237:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:95:ASN:HB2	7:G:96:GLY:HA3	1.98	0.43
6:F:114:ALA:C	6:F:116:ALA:N	2.72	0.43
11:K:76:ALA:HA	11:K:77:ASN:O	2.17	0.43
1:A:596:ASP:HA	1:A:599:PHE:HB3	2.01	0.43
3:C:17:CYS:HB2	3:C:54:CYS:HB2	2.01	0.43
26:1:1501:LUT:H12	21:1:1002:CLA:HAA2	2.00	0.43
21:2:2009:CLA:CB	21:3:3009:CLA:CBA	2.92	0.43
21:4:4004:CLA:CHC	26:4:4502:LUT:C19	2.94	0.43
21:4:4012:CLA:C19	21:4:4012:CLA:H152	2.16	0.43
21:A:1103:CLA:H2	21:A:1103:CLA:H61	1.50	0.43
1:A:315:HIS:HB3	21:A:1118:CLA:HED1	2.00	0.43
2:B:292:ARG:HH11	7:G:92:PRO:HB3	1.82	0.43
6:F:194:LYS:HZ3	6:F:200:VAL:HG11	1.84	0.43
6:F:181:TYR:OH	6:F:200:VAL:HG21	2.18	0.43
15:2:71:TRP:CD1	15:2:76:THR:HG21	2.52	0.43
21:1:1005:CLA:CE	21:1:1012:CLA:O1A	2.67	0.43
14:1:186:LYS:NZ	21:1:1007:CLA:CE	2.74	0.43
14:1:105:TRP:N	14:1:105:TRP:CD1	2.86	0.43
16:3:204:PRO:HB2	16:3:209:PHE:CB	2.48	0.43
16:3:112:PHE:HZ	21:3:3012:CLA:O2D	2.02	0.43
21:A:1101:CLA:H93	21:A:1106:CLA:H172	2.01	0.43
21:A:1132:CLA:H2A	21:A:1132:CLA:O1D	2.18	0.43
21:B:1219:CLA:HMB3	21:B:1240:CLA:C1D	2.48	0.43
21:B:1229:CLA:H3A	21:B:1229:CLA:HBA2	1.40	0.43
21:B:1235:CLA:H161	21:B:1235:CLA:H203	1.88	0.43
6:F:201:PRO:C	6:F:203:ALA:N	2.70	0.43
21:L:1501:CLA:HBA1	21:L:1501:CLA:CB	2.48	0.43
12:L:177:GLN:O	12:L:178:THR:OG1	2.21	0.43
13:N:116:ARG:HH21	13:N:122:PHE:N	2.15	0.43
6:F:152:GLY:HA2	6:F:161:ILE:HD11	2.00	0.43
14:1:90:ALA:O	14:1:93:GLY:N	2.51	0.43
14:1:186:LYS:NZ	20:1:1801:LHG:O5	2.51	0.43
21:2:2001:CLA:C2B	21:2:2014:CLA:C2A	2.85	0.43
15:2:110:GLU:CB	21:2:2004:CLA:C1B	2.90	0.43
21:2:2014:CLA:O2A	21:2:2014:CLA:H3A	2.19	0.43
17:4:151:PHE:HB3	21:4:4012:CLA:HBB2	2.01	0.43
21:4:4012:CLA:H192	21:4:4012:CLA:C13	2.48	0.43
26:4:4501:LUT:H202	26:4:4501:LUT:H11	1.86	0.43
1:A:374:GLN:NE2	21:A:1124:CLA:OBD	2.52	0.43
21:B:1227:CLA:H8	21:B:1240:CLA:C1	2.46	0.43
19:B:6006:BCR:H15C	19:B:6006:BCR:H351	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:HA	1:A:311:LEU:HD12	2.00	0.43
11:K:100:GLY:HA2	11:K:103:LEU:HB2	1.99	0.43
10:J:13:VAL:O	10:J:16:THR:HG23	2.19	0.43
2:B:529:THR:O	2:B:533:ILE:HG13	2.19	0.43
21:1:1004:CLA:H61	21:1:1004:CLA:H93	1.75	0.43
26:1:1501:LUT:H31	26:1:1501:LUT:H402	1.91	0.43
26:1:1502:LUT:H11	26:1:1502:LUT:H191	1.75	0.43
26:1:1502:LUT:H31	26:1:1502:LUT:H403	1.83	0.43
14:1:223:HIS:O	14:1:225:ASN:N	2.52	0.43
16:3:162:LEU:HA	16:3:165:ALA:CB	2.48	0.43
21:3:3001:CLA:HHD	21:3:3011:CLA:HMB3	2.00	0.43
17:4:170:GLN:NE2	21:4:4014:CLA:C1C	2.78	0.43
21:F:1303:CLA:HMB2	26:4:4502:LUT:H11	2.01	0.43
20:A:7001:LHG:H222	21:A:1104:CLA:H191	2.01	0.43
21:B:1208:CLA:H41	21:B:1208:CLA:H61	1.55	0.43
21:B:9023:CLA:H143	21:B:9023:CLA:H111	1.89	0.43
12:L:204:LEU:CD2	12:L:207:LEU:HD21	2.48	0.43
4:D:156:TYR:HB3	4:D:165:GLN:O	2.18	0.43
11:K:98:PRO:HG3	11:K:101:PHE:CE1	2.54	0.43
26:1:1502:LUT:H8	26:1:1502:LUT:C18	2.47	0.43
15:2:118:MET:HG2	15:2:119:LEU:N	2.33	0.43
15:2:119:LEU:N	15:2:119:LEU:HD12	2.34	0.43
15:2:119:LEU:N	15:2:119:LEU:CD1	2.81	0.43
16:3:162:LEU:HA	16:3:165:ALA:HB3	2.00	0.43
17:4:179:LEU:HD12	21:4:4014:CLA:H3A	2.01	0.43
26:4:4501:LUT:H28	26:4:4501:LUT:H361	2.01	0.43
21:A:1117:CLA:H3A	21:A:1117:CLA:HBA2	1.72	0.43
21:A:1131:CLA:H71	18:B:5002:PQN:C20	2.49	0.43
21:B:1207:CLA:H92	21:B:1207:CLA:H62	1.81	0.43
19:F:6016:BCR:H392	19:F:6016:BCR:H282	1.26	0.43
21:A:1129:CLA:CED	12:L:69:LEU:HD13	2.49	0.43
7:G:101:PHE:H	7:G:101:PHE:HD1	1.66	0.43
4:D:77:PRO:HD2	4:D:78:ASN:N	2.33	0.43
19:B:6004:BCR:H281	21:B:1212:CLA:NB	2.33	0.43
1:A:343:HIS:HA	1:A:346:LEU:HD12	2.00	0.43
2:B:314:ARG:C	2:B:410:ARG:NH2	2.72	0.43
2:B:100:ALA:O	2:B:104:PHE:HD1	2.02	0.43
1:A:422:TYR:CZ	1:A:424:PRO:HG3	2.54	0.43
21:1:1002:CLA:HAB	21:1:1007:CLA:CBF	2.28	0.43
21:1:1002:CLA:HED2	21:1:1002:CLA:CAD	2.49	0.43
21:1:1006:CLA:O1A	21:1:1014:CLA:C2C	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1:1010:CLA:H193	21:1:1010:CLA:H152	2.01	0.43
21:1:1011:CLA:HAA1	21:1:1011:CLA:HBD	2.00	0.43
14:1:82:ILE:CG2	14:1:83:HIS:N	2.81	0.43
21:2:2002:CLA:HBB1	21:2:2002:CLA:CHC	2.46	0.43
21:2:2006:CLA:HBA2	21:2:2013:CLA:CAD	2.49	0.43
16:3:171:GLU:OE1	21:3:3012:CLA:C1C	2.67	0.43
21:3:3001:CLA:HED2	21:3:3001:CLA:H2A	2.01	0.43
17:4:103:ALA:C	17:4:107:VAL:HG12	2.38	0.43
17:4:238:HIS:CE1	21:4:4003:CLA:O1D	2.70	0.43
17:4:163:LYS:CE	21:4:4005:CLA:HED3	2.46	0.43
21:A:9013:CLA:H3A	21:A:9013:CLA:CGA	2.49	0.43
2:B:60:TRP:HA	21:B:1204:CLA:HAB	2.01	0.43
21:B:1208:CLA:H3A	21:B:1208:CLA:HBA2	1.39	0.43
21:B:1213:CLA:CHD	21:B:1213:CLA:HBC3	2.48	0.43
7:G:138:LEU:O	7:G:142:THR:HG23	2.19	0.43
12:L:137:LEU:O	12:L:141:LEU:HG	2.18	0.43
12:L:172:GLN:C	12:L:172:GLN:NE2	2.72	0.43
21:G:1001:CLA:H51	21:G:1001:CLA:H11	1.81	0.43
2:B:77:TRP:HA	2:B:84:VAL:CG1	2.42	0.43
12:L:135:ALA:O	12:L:138:VAL:CG2	2.65	0.43
1:A:100:GLY:HA3	1:A:153:TRP:CH2	2.53	0.43
2:B:176:ASN:ND2	2:B:291:TYR:O	2.51	0.43
2:B:125:TYR:O	2:B:130:ARG:NH1	2.48	0.43
2:B:226:LEU:O	7:G:136:TYR:OH	2.23	0.43
15:2:124:ILE:C	15:2:127:PRO:HD2	2.39	0.42
16:3:171:GLU:C	16:3:174:ARG:HG3	2.40	0.42
21:3:3001:CLA:H162	21:3:3001:CLA:H143	1.75	0.42
21:4:4006:CLA:H61	21:4:4006:CLA:H41	1.86	0.42
20:A:7003:LHG:O2	20:A:7003:LHG:P	2.77	0.42
19:B:6009:BCR:HC7	21:B:1219:CLA:CBB	2.49	0.42
9:I:17:PRO:O	9:I:21:MET:HB2	2.19	0.42
12:L:110:LEU:N	12:L:110:LEU:CD2	2.81	0.42
4:D:129:LEU:CD1	4:D:129:LEU:C	2.85	0.42
12:L:164:LEU:CD2	12:L:164:LEU:N	2.72	0.42
8:H:73:TYR:C	8:H:75:SER:N	2.72	0.42
6:F:173:TRP:O	6:F:177:VAL:HG23	2.19	0.42
2:B:338:LEU:HD22	2:B:382:ILE:HG23	2.01	0.42
1:A:225:VAL:HG13	1:A:245:PRO:HB3	2.01	0.42
14:1:136:VAL:CG2	14:1:137:ILE:N	2.82	0.42
14:1:62:ASP:OD1	14:1:66:LEU:N	2.43	0.42
15:2:158:LEU:CD1	15:2:159:PHE:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:3:210:ASN:HA	16:3:214:PHE:CD2	2.53	0.42
21:3:3012:CLA:HED2	21:3:3012:CLA:C1A	2.49	0.42
17:4:171:ASP:CA	27:4:4503:NEX:C10	2.97	0.42
26:4:4501:LUT:H35	26:4:4501:LUT:C20	2.48	0.42
21:A:1130:CLA:HBC2	21:A:1137:CLA:HBC3	2.00	0.42
1:A:126:ILE:HD12	1:A:126:ILE:HA	1.90	0.42
19:A:6011:BCR:C8	19:A:6011:BCR:H331	2.49	0.42
6:F:213:TRP:O	6:F:215:ILE:N	2.51	0.42
21:A:1138:CLA:HMD3	19:F:6014:BCR:HC41	2.02	0.42
19:L:6020:BCR:C38	19:L:6020:BCR:C23	2.97	0.42
16:3:256:ASN:O	16:3:260:HIS:N	2.52	0.42
16:3:264:PRO:CB	21:3:3008:CLA:CMA	2.92	0.42
17:4:165:PRO:HA	17:4:166:GLY:HA3	1.63	0.42
2:B:102:GLU:CD	8:H:130:LYS:HG3	2.39	0.42
21:1:1010:CLA:H193	21:1:1010:CLA:C15	2.50	0.42
15:2:161:VAL:HG12	15:2:165:PHE:HD2	1.80	0.42
21:2:2003:CLA:C5	21:2:2003:CLA:H92	2.35	0.42
17:4:189:GLY:C	17:4:191:PHE:N	2.71	0.42
17:4:105:LEU:HD22	21:4:4001:CLA:HBC1	2.01	0.42
21:A:1102:CLA:H12	21:A:1109:CLA:H92	2.02	0.42
1:A:382:TYR:CE2	21:A:1127:CLA:HED2	2.54	0.42
19:A:6007:BCR:H342	19:A:6007:BCR:HC7	1.76	0.42
21:B:1207:CLA:HAC2	19:I:6018:BCR:HC7	2.01	0.42
12:L:110:LEU:HD12	12:L:137:LEU:HD23	2.00	0.42
12:L:204:LEU:HA	12:L:207:LEU:CG	2.20	0.42
3:C:75:ARG:NH2	4:D:99:GLU:OE2	2.52	0.42
21:G:1001:CLA:CMC	21:G:1001:CLA:HBC2	2.34	0.42
13:N:119:THR:C	13:N:121:GLN:N	2.72	0.42
21:A:1114:CLA:HED2	21:A:1114:CLA:H2A	2.02	0.42
17:4:132:LYS:HA	17:4:133:GLU:HA	1.83	0.42
2:B:489:GLY:HA2	2:B:493:TRP:CH2	2.55	0.42
21:1:1009:CLA:C5	21:4:4005:CLA:CMD	2.97	0.42
21:1:1009:CLA:HMB1	21:4:4015:CLA:CGD	2.49	0.42
14:1:161:PRO:HD3	21:1:1011:CLA:HMD2	2.02	0.42
14:1:149:ARG:HG3	21:1:1011:CLA:HHD	1.97	0.42
15:2:230:ASN:O	15:2:233:LEU:HB3	2.19	0.42
16:3:247:LEU:CD1	21:3:3014:CLA:HAA1	2.50	0.42
21:4:4003:CLA:C4C	21:4:4003:CLA:C4	2.97	0.42
17:4:243:TRP:HE1	21:4:4008:CLA:C1	2.32	0.42
1:A:549:ILE:CD1	21:A:1124:CLA:C1D	2.97	0.42
1:A:336:GLY:O	1:A:340:GLY:N	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1201:CLA:H2A	21:B:1201:CLA:HED2	2.01	0.42
21:L:1502:CLA:H92	21:L:1502:CLA:H62	1.80	0.42
19:L:6020:BCR:H271	19:L:6020:BCR:H393	2.01	0.42
3:C:21:CYS:SG	3:C:24:ASP:N	2.93	0.42
1:A:457:SER:CB	1:A:544:ILE:HD13	2.40	0.42
12:L:161:ALA:HB3	12:L:174:ASP:HB2	2.01	0.42
16:3:152:TYR:HB2	16:3:153:TRP:H	1.56	0.42
1:A:70:ASP:HB3	1:A:73:GLU:HB2	2.02	0.42
14:1:69:VAL:HA	14:1:70:PRO:HD3	1.88	0.42
17:4:112:LEU:HB2	17:4:113:PRO:HD3	2.00	0.42
2:B:551:LYS:NZ	2:B:552:ASP:OD1	2.47	0.42
14:1:103:GLY:O	14:1:104:ASN:CB	2.67	0.42
21:1:1009:CLA:H161	21:1:1009:CLA:H193	1.78	0.42
21:1:1010:CLA:HHC	21:1:1010:CLA:CBB	2.48	0.42
21:1:1006:CLA:HHB	21:1:1013:CLA:C1	2.49	0.42
21:1:1006:CLA:O1A	21:1:1014:CLA:C3C	2.68	0.42
21:1:1003:CLA:H42	20:1:1801:LHG:H192	1.99	0.42
21:2:2012:CLA:HBB1	21:2:2012:CLA:HMB1	2.02	0.42
16:3:104:TYR:O	16:3:108:ILE:HD12	2.18	0.42
16:3:208:PHE:HB2	21:3:3001:CLA:HED3	2.00	0.42
17:4:226:VAL:CG2	17:4:227:THR:H	2.32	0.42
17:4:145:ILE:HG21	21:4:4013:CLA:HED3	2.01	0.42
21:A:1128:CLA:H62	21:A:1128:CLA:H41	1.85	0.42
20:A:7003:LHG:HC92	21:A:1129:CLA:C1A	2.50	0.42
21:B:1202:CLA:H122	21:B:1202:CLA:HBD	2.01	0.42
21:B:1213:CLA:H142	21:B:1213:CLA:H112	1.76	0.42
19:B:6009:BCR:H343	21:B:1219:CLA:HBB2	2.00	0.42
12:L:200:ALA:O	12:L:204:LEU:HG	2.19	0.42
21:3:3008:CLA:H62	21:3:3008:CLA:H41	1.61	0.42
1:A:308:ILE:HG13	1:A:309:LEU:N	2.35	0.42
11:K:65:LEU:HD11	11:K:104:ALA:HA	2.02	0.42
4:D:81:SER:HG	8:H:57:TYR:N	2.18	0.42
14:1:184:GLU:HG3	21:1:1001:CLA:NB	2.35	0.42
14:1:224:ASN:CG	14:1:225:ASN:N	2.73	0.42
21:3:3013:CLA:HBC3	21:3:3013:CLA:CMC	2.30	0.42
21:4:4003:CLA:H192	21:4:4008:CLA:HMD2	2.01	0.42
21:A:1108:CLA:CBB	21:A:1111:CLA:HED2	2.49	0.42
1:A:433:ASP:C	1:A:434:ARG:HG3	2.40	0.42
7:G:77:PHE:CZ	21:G:1002:CLA:CMC	3.03	0.42
2:B:306:GLU:HA	2:B:320:LYS:HG2	2.01	0.42
12:L:172:GLN:HG2	12:L:173:PRO:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1:107:LYS:HD2	14:1:110:GLU:OE1	2.19	0.42
12:L:53:THR:C	12:L:55:GLN:N	2.73	0.42
21:3:3008:CLA:HBA1	21:3:3008:CLA:CBD	2.50	0.42
6:F:209:ARG:NE	17:4:80:LEU:O	2.52	0.42
21:1:1010:CLA:H92	21:1:1010:CLA:H42	2.02	0.42
21:1:1006:CLA:O1A	21:1:1014:CLA:CAC	2.67	0.42
17:4:168:VAL:HB	17:4:179:LEU:HB3	2.02	0.42
21:4:4010:CLA:H2	21:4:4010:CLA:O1A	2.20	0.42
21:A:1136:CLA:H112	21:A:1136:CLA:H91	1.83	0.42
2:B:282:PHE:CZ	21:B:1213:CLA:HBB2	2.54	0.42
2:B:422:LEU:HG	21:B:1236:CLA:CAB	2.46	0.42
21:B:9010:CLA:HBA2	21:B:9010:CLA:H3A	1.82	0.42
19:F:6016:BCR:H342	19:F:6016:BCR:HC7	1.91	0.42
19:L:6020:BCR:C27	19:L:6020:BCR:H393	2.50	0.42
4:D:170:LYS:C	4:D:172:GLY:N	2.72	0.42
8:H:77:ALA:HB2	12:L:84:SER:HB3	2.00	0.42
6:F:194:LYS:O	6:F:198:ILE:HG23	2.19	0.42
8:H:137:LYS:HA	8:H:137:LYS:HD3	1.89	0.42
6:F:157:TRP:CD1	6:F:161:ILE:HD12	2.55	0.42
21:1:1006:CLA:CBB	21:1:1006:CLA:CHC	2.91	0.42
14:1:184:GLU:CA	21:1:1001:CLA:HMB3	2.49	0.42
14:1:211:LEU:HD21	21:1:1003:CLA:O2D	2.19	0.42
20:2:2801:LHG:C23	20:2:2801:LHG:C12	2.85	0.42
20:2:2801:LHG:H122	20:2:2801:LHG:C24	2.47	0.42
17:4:247:ILE:HD13	21:4:4003:CLA:OBD	2.19	0.42
21:A:1103:CLA:HED2	21:A:1128:CLA:HBB2	2.02	0.42
21:A:1130:CLA:O1A	2:B:686:PRO:HG2	2.19	0.42
19:A:6017:BCR:H383	21:B:1239:CLA:HBC1	2.01	0.42
21:B:1209:CLA:HED2	21:B:1209:CLA:H2A	2.01	0.42
21:B:1219:CLA:H111	21:B:1219:CLA:H91	1.77	0.42
19:L:6020:BCR:C18	21:L:1501:CLA:HMB2	2.50	0.42
4:D:94:LYS:HE3	4:D:99:GLU:O	2.19	0.42
3:C:29:ILE:HG13	3:C:41:SER:HB2	2.01	0.42
12:L:130:GLY:O	12:L:133:ALA:CB	2.68	0.42
6:F:198:ILE:HG12	10:J:10:VAL:HG12	2.01	0.42
6:F:196:ILE:HG13	6:F:197:ILE:N	2.35	0.42
21:1:1009:CLA:HMC2	17:4:156:ILE:CD1	2.46	0.42
14:1:225:ASN:C	14:1:227:GLY:CA	2.85	0.42
21:3:3010:CLA:CHA	21:3:3010:CLA:CBA	2.98	0.42
21:A:1130:CLA:CAD	12:L:73:VAL:CG1	2.98	0.42
1:A:744:ALA:O	1:A:747:TRP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1227:CLA:H142	21:B:1227:CLA:H112	1.88	0.42
21:B:1207:CLA:H161	19:I:6020:BCR:HC31	2.02	0.42
1:A:745:THR:HG22	1:A:745:THR:O	2.19	0.42
2:B:199:ILE:HB	2:B:200:PRO:HD3	2.02	0.42
15:2:236:LEU:HA	15:2:236:LEU:HD23	1.79	0.42
26:1:1502:LUT:H393	26:1:1502:LUT:H27	1.84	0.42
21:2:2008:CLA:H161	21:2:2008:CLA:H122	1.82	0.42
26:2:2502:LUT:H11	26:2:2502:LUT:H191	1.80	0.42
16:3:174:ARG:HG2	16:3:174:ARG:H	1.50	0.42
21:4:4013:CLA:CMC	21:4:4013:CLA:HBC2	2.50	0.42
21:A:1103:CLA:H51	21:A:1111:CLA:H12	2.02	0.42
1:A:549:ILE:HD13	21:A:1124:CLA:C1D	2.50	0.42
1:A:64:PHE:CD2	1:A:77:LYS:HB3	2.55	0.42
23:A:9011:CL0:H10	23:A:9011:CL0:H72	1.82	0.42
21:B:1216:CLA:H91	21:B:1216:CLA:H111	1.82	0.42
21:B:1220:CLA:CMD	21:B:1221:CLA:HAB	2.49	0.42
21:B:1240:CLA:H11	21:B:1240:CLA:H52	1.89	0.42
19:I:6018:BCR:H321	19:I:6018:BCR:HC7	1.77	0.42
21:A:1107:CLA:H2	19:J:6013:BCR:H363	2.02	0.42
12:L:109:PHE:HE1	21:L:1503:CLA:CHC	2.33	0.42
7:G:116:LYS:HG3	21:G:1002:CLA:NA	2.34	0.42
8:H:76:ASP:CG	8:H:77:ALA:N	2.73	0.42
1:A:281:LEU:HA	1:A:297:THR:O	2.20	0.42
19:A:6003:BCR:H342	21:A:1110:CLA:HMC1	2.02	0.42
14:1:105:TRP:HD1	14:1:105:TRP:H	1.67	0.41
14:1:170:TYR:N	14:1:170:TYR:HD1	2.18	0.41
15:2:91:PHE:HB3	21:2:2004:CLA:C3D	2.50	0.41
16:3:214:PHE:HZ	21:3:3001:CLA:C4D	2.31	0.41
21:3:3012:CLA:CED	21:3:3012:CLA:C2A	2.85	0.41
21:4:4002:CLA:O2A	21:4:4002:CLA:HMA2	2.20	0.41
1:A:336:GLY:CA	1:A:339:THR:HG22	2.50	0.41
1:A:371:VAL:HA	21:A:1124:CLA:HED3	2.02	0.41
1:A:433:ASP:O	1:A:435:VAL:N	2.49	0.41
21:B:1219:CLA:H61	21:B:1219:CLA:H41	1.56	0.41
19:L:6020:BCR:H382	19:L:6020:BCR:C23	2.49	0.41
7:G:116:LYS:CG	21:G:1002:CLA:C4A	2.98	0.41
4:D:156:TYR:CD1	4:D:156:TYR:N	2.87	0.41
1:A:664:VAL:HG13	1:A:665:ILE:HG23	2.01	0.41
1:A:342:GLY:O	1:A:343:HIS:HB2	2.20	0.41
12:L:115:VAL:HG13	12:L:128:ALA:HA	2.02	0.41
1:A:357:GLN:HG3	21:A:1123:CLA:H151	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:O	1:A:207:LEU:HG	2.20	0.41
14:1:176:LYS:HA	14:1:179:GLU:HG2	2.01	0.41
8:H:128:ILE:HG12	8:H:128:ILE:H	1.40	0.41
2:B:443:MET:HB3	2:B:448:THR:O	2.20	0.41
1:A:268:PRO:HG3	1:A:276:LYS:HB3	2.02	0.41
17:4:71:LEU:HA	17:4:72:PRO:HD3	1.94	0.41
2:B:577:TYR:HD1	2:B:710:LEU:HD22	1.84	0.41
1:A:484:LEU:HA	1:A:484:LEU:HD12	1.90	0.41
14:1:211:LEU:HD23	21:1:1003:CLA:HED3	1.97	0.41
21:1:1013:CLA:CGD	21:1:1013:CLA:H12	2.50	0.41
14:1:102:LEU:HG	21:1:1006:CLA:O1D	2.20	0.41
26:1:1502:LUT:H7	26:1:1502:LUT:H192	1.90	0.41
15:2:159:PHE:O	15:2:163:LEU:N	2.37	0.41
16:3:207:PRO:CB	16:3:208:PHE:CD1	3.01	0.41
9:I:14:LEU:HA	9:I:17:PRO:HD2	2.02	0.41
7:G:116:LYS:C	7:G:118:ALA:N	2.73	0.41
7:G:121:ILE:O	7:G:124:VAL:N	2.53	0.41
21:3:3003:CLA:HBD	21:3:3003:CLA:HBA2	2.01	0.41
2:B:458:ILE:HD13	6:F:151:SER:HB3	2.02	0.41
6:F:154:GLN:HA	6:F:157:TRP:CD1	2.55	0.41
5:E:111:ASN:ND2	5:E:113:ALA:O	2.53	0.41
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.87	0.41
1:A:680:LEU:HD23	1:A:680:LEU:HA	1.89	0.41
2:B:576:PHE:O	2:B:580:VAL:HG23	2.20	0.41
26:1:1502:LUT:H32	21:1:1005:CLA:HBC3	2.01	0.41
21:2:2003:CLA:H141	21:2:2003:CLA:H162	1.89	0.41
21:2:2006:CLA:CED	21:2:2006:CLA:H2A	2.37	0.41
21:2:2008:CLA:H41	21:2:2008:CLA:H61	1.69	0.41
15:2:230:ASN:CG	15:2:231:GLY:N	2.73	0.41
26:4:4501:LUT:C15	26:4:4501:LUT:C40	2.96	0.41
21:4:4004:CLA:C3	26:4:4502:LUT:H162	2.47	0.41
1:A:472:ARG:NE	1:A:475:ASP:OD2	2.54	0.41
21:B:1205:CLA:H141	21:B:1205:CLA:HBA2	2.01	0.41
7:G:138:LEU:CD2	25:G:2021:LMG:C29	2.98	0.41
19:A:6002:BCR:C12	21:A:1112:CLA:HBB1	2.50	0.41
7:G:110:GLU:HG2	7:G:111:TYR:H	1.85	0.41
2:B:713:PHE:O	2:B:717:TYR:HB2	2.21	0.41
3:C:31:TRP:CH2	3:C:33:GLY:HA3	2.54	0.41
1:A:603:PHE:O	1:A:606:TYR:HB3	2.20	0.41
21:1:1012:CLA:CMC	21:1:1012:CLA:HBC2	2.45	0.41
14:1:131:LEU:CD2	14:1:135:LEU:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:2:113:HIS:HE1	21:2:2005:CLA:NB	2.19	0.41
15:2:124:ILE:CD1	26:2:2501:LUT:C17	2.99	0.41
21:2:2005:CLA:HAB	26:2:2502:LUT:C13	2.50	0.41
16:3:209:PHE:CD1	16:3:209:PHE:N	2.88	0.41
17:4:190:ILE:CA	21:4:4014:CLA:O2A	2.69	0.41
21:4:4004:CLA:CAB	26:4:4502:LUT:H203	2.46	0.41
21:A:1104:CLA:HED1	21:A:1128:CLA:H2	2.01	0.41
21:B:9023:CLA:H161	21:B:9023:CLA:H141	1.85	0.41
19:F:6016:BCR:H333	21:F:1302:CLA:H3A	2.01	0.41
4:D:198:PRO:C	4:D:199:ILE:HG23	2.40	0.41
13:N:164:SER:C	13:N:165:ASN:ND2	2.73	0.41
2:B:294:ASN:OD1	2:B:294:ASN:N	2.50	0.41
12:L:61:ASN:ND2	12:L:166:LEU:HD11	2.33	0.41
12:L:94:ASN:OD1	12:L:95:PRO:HD2	2.20	0.41
2:B:247:THR:O	2:B:247:THR:HG23	2.20	0.41
10:J:38:THR:O	10:J:40:PRO:HD3	2.21	0.41
14:1:157:LYS:CB	14:1:161:PRO:HA	2.51	0.41
14:1:224:ASN:OD1	14:1:225:ASN:N	2.54	0.41
20:2:2801:LHG:C12	20:2:2801:LHG:H252	2.51	0.41
16:3:170:ALA:C	16:3:174:ARG:NE	2.73	0.41
16:3:172:HIS:HA	21:3:3012:CLA:CBB	2.46	0.41
21:3:3005:CLA:C4C	21:3:3012:CLA:CGA	2.99	0.41
17:4:102:TRP:C	17:4:102:TRP:N	2.74	0.41
15:2:152:PHE:C	17:4:243:TRP:HZ3	2.24	0.41
1:A:551:VAL:HG11	1:A:604:TRP:CZ2	2.55	0.41
21:B:1229:CLA:HBB1	21:B:1229:CLA:HMB1	2.01	0.41
21:A:1129:CLA:CMA	12:L:71:THR:HG21	2.44	0.41
7:G:101:PHE:O	7:G:102:ASP:CB	2.69	0.41
13:N:167:PHE:CD1	13:N:168:TRP:O	2.70	0.41
11:K:72:LEU:O	11:K:73:ALA:HB3	2.21	0.41
16:3:101:TRP:C	16:3:103:ALA:H	2.24	0.41
12:L:93:VAL:HG12	12:L:94:ASN:N	2.36	0.41
2:B:549:ASP:OD1	3:C:66:ARG:NH2	2.43	0.41
1:A:208:ALA:HB2	1:A:314:GLY:HA3	2.02	0.41
21:2:2011:CLA:CBC	21:2:2011:CLA:CMC	2.89	0.41
17:4:246:THR:CG2	21:4:4008:CLA:CED	2.85	0.41
21:4:4006:CLA:CBC	21:4:4006:CLA:HHD	2.36	0.41
26:4:4502:LUT:H391	26:4:4502:LUT:H31	1.55	0.41
21:A:1116:CLA:HMD2	21:A:1125:CLA:HMB2	2.03	0.41
21:A:1117:CLA:H122	21:A:1117:CLA:H161	1.68	0.41
1:A:38:GLY:N	1:A:45:ALA:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:135:LYS:HZ2	4:D:167:LEU:HD22	1.85	0.41
12:L:120:LEU:CD1	12:L:126:ALA:CB	2.86	0.41
1:A:328:LYS:HD3	1:A:347:TYR:CB	2.51	0.41
2:B:136:TYR:O	2:B:140:ILE:HG12	2.21	0.41
8:H:81:TYR:CZ	12:L:97:LEU:HD12	2.55	0.41
21:1:1009:CLA:C12	21:1:1009:CLA:C9	2.85	0.41
14:1:89:LEU:HA	14:1:89:LEU:HD12	1.86	0.41
15:2:99:ASP:CG	15:2:102:SER:HG	2.18	0.41
16:3:163:GLU:OE1	21:3:3010:CLA:HMC2	2.20	0.41
21:3:3011:CLA:CBD	21:3:3011:CLA:CBA	2.92	0.41
17:4:171:ASP:OD2	21:4:4014:CLA:CBB	2.69	0.41
17:4:225:ASN:HD21	21:4:4010:CLA:C3	2.34	0.41
17:4:225:ASN:N	17:4:225:ASN:ND2	2.68	0.41
21:4:4001:CLA:HHC	26:4:4501:LUT:H403	2.02	0.41
18:B:5002:PQN:H292	18:B:5002:PQN:H261	1.76	0.41
21:A:1136:CLA:H171	21:L:1502:CLA:H203	2.03	0.41
2:B:309:ILE:HD11	2:B:320:LYS:HG3	2.02	0.41
12:L:172:GLN:O	12:L:172:GLN:NE2	2.54	0.41
12:L:123:THR:O	12:L:127:GLY:HA2	2.21	0.41
4:D:182:ARG:O	4:D:183:GLN:CB	2.69	0.41
1:A:429:ASN:O	1:A:430:ASP:CB	2.68	0.41
12:L:128:ALA:C	12:L:130:GLY:N	2.72	0.41
21:A:1123:CLA:H141	21:A:1123:CLA:H162	1.64	0.41
1:A:203:LEU:HD23	1:A:317:TYR:CZ	2.55	0.41
11:K:98:PRO:HG3	11:K:101:PHE:CD1	2.56	0.41
16:3:96:PHE:CG	16:3:101:TRP:CD1	3.08	0.41
21:1:1006:CLA:HAA2	21:1:1006:CLA:HBD	2.03	0.41
14:1:211:LEU:HG	21:1:1003:CLA:CED	2.35	0.41
15:2:118:MET:O	15:2:121:ALA:N	2.51	0.41
15:2:242:TRP:O	15:2:246:ILE:HG23	2.21	0.41
17:4:170:GLN:HG3	17:4:173:ILE:HB	1.98	0.41
17:4:225:ASN:ND2	21:4:4010:CLA:C3	2.84	0.41
21:4:4001:CLA:HBD	21:4:4001:CLA:HAA1	2.01	0.41
21:4:4002:CLA:CGA	21:4:4002:CLA:C3A	2.99	0.41
17:4:160:GLN:OE1	21:4:4005:CLA:C4A	2.69	0.41
26:4:4501:LUT:H191	26:4:4501:LUT:H11	1.59	0.41
21:A:1101:CLA:H12	21:A:1140:CLA:H72	2.03	0.41
21:A:1107:CLA:CBB	19:J:6012:BCR:H323	2.51	0.41
1:A:475:ASP:CB	21:A:1132:CLA:HED2	2.50	0.41
1:A:445:HIS:O	1:A:449:VAL:HG23	2.20	0.41
2:B:645:VAL:CG1	21:B:1206:CLA:HAC1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:1227:CLA:H143	21:B:1227:CLA:H162	1.78	0.41
21:B:1222:CLA:C19	21:B:1227:CLA:H201	2.49	0.41
21:B:1239:CLA:C2	21:B:1239:CLA:O1A	2.69	0.41
21:H:1000:CLA:HAB	19:L:6020:BCR:H331	2.03	0.41
7:G:114:LEU:CD2	7:G:119:ALA:O	2.69	0.41
8:H:59:ASP:C	8:H:60:LEU:HG	2.40	0.41
8:H:70:TRP:O	12:L:162:PRO:CB	2.69	0.41
21:A:1122:CLA:H92	21:A:1122:CLA:H62	1.88	0.41
11:K:80:ALA:O	11:K:84:LEU:N	2.54	0.41
15:2:118:MET:HG2	15:2:119:LEU:CD1	2.50	0.41
21:2:2005:CLA:H112	21:2:2005:CLA:H143	1.81	0.41
15:2:242:TRP:C	15:2:244:GLN:H	2.22	0.41
17:4:97:LEU:O	17:4:101:ARG:HG3	2.21	0.41
14:1:46:PRO:CA	21:4:4005:CLA:O1A	2.63	0.41
17:4:190:ILE:CB	21:4:4014:CLA:O2A	2.69	0.41
21:4:4015:CLA:HBA2	21:4:4015:CLA:H3A	1.80	0.41
21:A:1124:CLA:CHB	21:A:1137:CLA:HAA2	2.50	0.41
1:A:371:VAL:HG12	21:A:1124:CLA:HED3	2.03	0.41
21:B:1234:CLA:HBA2	21:B:1235:CLA:HAA2	2.02	0.41
2:B:348:VAL:HG21	21:B:1225:CLA:HHD	2.03	0.41
23:A:9011:CL0:CBB	2:B:624:LEU:CD1	2.98	0.41
6:F:213:TRP:C	6:F:215:ILE:N	2.74	0.41
9:I:21:MET:HE3	19:L:6019:BCR:H352	2.02	0.41
21:A:1107:CLA:HMA1	10:J:27:ILE:HD13	2.03	0.41
26:1:1501:LUT:C39	21:1:1001:CLA:C3	2.99	0.41
14:1:61:PHE:CE2	26:1:1502:LUT:H182	2.56	0.41
15:2:260:LEU:CB	21:2:2008:CLA:HED1	2.50	0.41
21:3:3005:CLA:C4C	21:3:3012:CLA:O2A	2.69	0.41
17:4:101:ARG:HB2	21:4:4011:CLA:HED1	2.03	0.41
17:4:225:ASN:C	17:4:226:VAL:CG1	2.85	0.41
17:4:230:GLY:O	17:4:234:ASN:HB2	2.20	0.41
1:A:409:GLY:HA3	21:A:1128:CLA:C2C	2.51	0.41
21:B:1202:CLA:H142	21:B:1202:CLA:H112	1.95	0.41
21:B:1227:CLA:HMB2	21:B:1228:CLA:C2D	2.51	0.41
19:B:6005:BCR:H281	21:B:1225:CLA:NC	2.36	0.41
21:B:9023:CLA:HBC2	21:B:9023:CLA:CHD	2.47	0.41
1:A:41:SER:HB3	1:A:44:ILE:CB	2.51	0.41
7:G:114:LEU:C	7:G:116:LYS:N	2.73	0.41
4:D:169:PRO:O	4:D:170:LYS:CB	2.69	0.41
14:1:107:LYS:HE3	14:1:107:LYS:HB3	1.88	0.41
1:A:280:PHE:CE1	1:A:281:LEU:HD23	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:177:GLN:O	12:L:178:THR:CB	2.68	0.41
11:K:100:GLY:O	11:K:104:ALA:HB2	2.21	0.41
12:L:96:LEU:C	12:L:96:LEU:CD2	2.85	0.41
12:L:96:LEU:O	12:L:96:LEU:HD23	2.21	0.41
12:L:78:LEU:HD12	12:L:78:LEU:C	2.38	0.41
17:4:137:ALA:O	17:4:138:SER:OG	2.34	0.41
2:B:42:LEU:HD21	2:B:330:ILE:HD11	2.03	0.41
1:A:709:TRP:HE1	6:F:229:LYS:HB3	1.86	0.41
4:D:75:LEU:HA	4:D:75:LEU:HD12	1.92	0.41
2:B:387:PHE:HB3	2:B:534:LEU:HD22	2.01	0.41
1:A:42:ARG:CZ	1:A:43:THR:HG22	2.50	0.41
21:1:1002:CLA:H52	21:1:1002:CLA:O1D	2.21	0.41
26:1:1501:LUT:H173	21:1:1003:CLA:HMB3	2.03	0.41
14:1:141:SER:O	14:1:145:VAL:HG22	2.21	0.41
16:3:158:THR:O	16:3:161:VAL:HG22	2.21	0.41
16:3:171:GLU:O	21:3:3012:CLA:CBB	2.69	0.41
17:4:226:VAL:C	17:4:228:GLY:N	2.73	0.41
17:4:186:TYR:HB3	21:4:4001:CLA:CGD	2.51	0.41
21:4:4002:CLA:H41	21:4:4002:CLA:H62	1.87	0.41
21:4:4007:CLA:HBD	21:4:4007:CLA:HAA1	2.03	0.41
21:4:4008:CLA:CBC	21:4:4008:CLA:HMC1	2.38	0.41
21:F:1303:CLA:ND	21:4:4012:CLA:H8	2.36	0.41
21:B:1229:CLA:CGA	19:F:6014:BCR:H362	2.51	0.41
2:B:712:HIS:HE1	21:B:1239:CLA:O1D	2.04	0.41
21:B:1222:CLA:H201	21:B:1240:CLA:H111	2.02	0.41
21:J:6015:CLA:C2	21:J:6015:CLA:HAA2	2.51	0.41
7:G:116:LYS:HG2	21:G:1002:CLA:C4A	2.50	0.41
4:D:130:LEU:HD23	4:D:130:LEU:C	2.41	0.41
5:E:65:PRO:O	5:E:66:ILE:HD12	2.21	0.41
8:H:134:LEU:HA	8:H:134:LEU:HD23	1.76	0.41
8:H:137:LYS:O	8:H:138:LEU:CB	2.69	0.41
1:A:656:PHE:O	1:A:660:GLN:HB2	2.21	0.41
2:B:223:GLY:N	2:B:224:PRO:HD2	2.36	0.41
21:1:1002:CLA:C2	21:1:1002:CLA:O1D	2.70	0.40
21:1:1004:CLA:H3A	21:1:1004:CLA:O2A	2.21	0.40
17:4:249:GLN:HG3	17:4:250:THR:N	2.36	0.40
21:4:4005:CLA:O2A	21:4:4005:CLA:CHA	2.69	0.40
21:4:4007:CLA:H41	21:4:4007:CLA:H61	1.87	0.40
1:A:681:GLY:O	1:A:685:VAL:HG22	2.21	0.40
2:B:526:GLY:HA2	2:B:582:TRP:CZ3	2.57	0.40
19:F:6016:BCR:H351	19:F:6016:BCR:H15C	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:J:6013:BCR:H342	19:J:6013:BCR:HC7	1.71	0.40
12:L:207:LEU:O	12:L:208:ASP:CB	2.69	0.40
12:L:56:VAL:O	12:L:57:VAL:CG1	2.69	0.40
4:D:134:ARG:O	4:D:136:GLU:N	2.46	0.40
6:F:194:LYS:O	6:F:198:ILE:CG2	2.69	0.40
1:A:203:LEU:HD11	21:A:1123:CLA:C1D	2.51	0.40
12:L:180:ASP:O	12:L:184:LYS:HG3	2.21	0.40
13:N:127:PHE:HB2	13:N:128:PRO:HD2	2.02	0.40
1:A:154:ARG:O	1:A:230:ASN:ND2	2.39	0.40
26:1:1501:LUT:H391	21:1:1001:CLA:H62	2.01	0.40
21:B:1240:CLA:HMC1	14:1:76:PHE:CZ	2.56	0.40
21:2:2010:CLA:HAA2	21:2:2010:CLA:HBD	2.03	0.40
21:2:2012:CLA:CBB	21:2:2012:CLA:HMB1	2.51	0.40
21:4:4003:CLA:CAB	26:4:4501:LUT:C18	2.99	0.40
21:4:4011:CLA:H202	21:4:4011:CLA:H161	1.92	0.40
21:4:4012:CLA:C15	21:4:4012:CLA:H203	2.50	0.40
21:B:9023:CLA:C14	19:I:6018:BCR:H331	2.50	0.40
12:L:199:TRP:O	12:L:202:PHE:HB3	2.21	0.40
14:1:173:ASP:HA	14:1:174:PRO:HD3	1.95	0.40
11:K:47:ASP:HB3	11:K:48:PHE:H	1.50	0.40
8:H:99:ARG:HG2	8:H:100:GLY:N	2.36	0.40
21:1:1002:CLA:HAB	21:1:1007:CLA:HAA1	2.02	0.40
15:2:118:MET:HE2	21:2:2001:CLA:HHD	1.99	0.40
15:2:235:MET:HE3	21:2:2004:CLA:HHC	2.02	0.40
16:3:170:ALA:C	16:3:172:HIS:N	2.73	0.40
17:4:247:ILE:O	17:4:250:THR:N	2.52	0.40
21:4:4003:CLA:C1A	21:4:4003:CLA:O2A	2.69	0.40
17:4:77:PHE:CD2	26:4:4502:LUT:H173	2.51	0.40
1:A:64:PHE:CE2	1:A:77:LYS:HB3	2.57	0.40
21:A:9012:CLA:H111	21:A:9012:CLA:H152	1.92	0.40
21:B:1225:CLA:H142	21:B:1225:CLA:H111	1.85	0.40
21:B:1230:CLA:H61	21:B:1230:CLA:H41	1.79	0.40
19:L:6019:BCR:H15C	19:L:6019:BCR:H351	1.76	0.40
19:L:6019:BCR:H382	19:L:6019:BCR:H23C	2.02	0.40
12:L:56:VAL:HG11	12:L:72:PRO:HD3	2.03	0.40
12:L:85:ASN:O	12:L:86:LEU:CB	2.69	0.40
7:G:93:GLU:OE1	7:G:99:THR:CB	2.69	0.40
12:L:64:PRO:CG	12:L:65:PHE:CD1	2.90	0.40
21:3:3003:CLA:HED1	21:3:3008:CLA:CAD	2.51	0.40
2:B:98:GLN:N	8:H:124:ASP:OD2	2.54	0.40
14:1:160:TYR:CD1	21:1:1001:CLA:O1D	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1501:LUT:C14	21:1:1002:CLA:HBD	2.51	0.40
21:1:1008:CLA:H91	21:1:1008:CLA:C12	2.43	0.40
20:1:1801:LHG:H371	21:4:4015:CLA:CMA	2.51	0.40
14:1:201:GLN:HB3	14:1:211:LEU:HD13	2.03	0.40
15:2:161:VAL:HG12	15:2:165:PHE:HE2	1.78	0.40
15:2:168:TRP:CA	21:4:4009:CLA:O1A	2.70	0.40
21:2:2009:CLA:HED3	21:2:2009:CLA:H2A	1.99	0.40
21:2:2011:CLA:H111	21:2:2011:CLA:H91	1.73	0.40
26:2:2501:LUT:H15	26:2:2501:LUT:H201	1.83	0.40
21:2:2014:CLA:CMB	26:2:2501:LUT:O23	2.70	0.40
16:3:206:GLY:O	16:3:209:PHE:CE1	2.74	0.40
16:3:237:LEU:HD23	16:3:240:LEU:HD23	2.03	0.40
17:4:102:TRP:N	17:4:103:ALA:H	2.20	0.40
17:4:160:GLN:HG2	21:4:4005:CLA:HMA3	2.04	0.40
17:4:163:LYS:HE2	21:4:4005:CLA:HED2	2.01	0.40
17:4:170:GLN:HG3	17:4:171:ASP:H	1.86	0.40
21:4:4006:CLA:H93	21:4:4006:CLA:H112	1.87	0.40
15:2:171:GLY:O	21:4:4009:CLA:HED1	2.21	0.40
21:A:1136:CLA:C4C	21:A:1136:CLA:H42	2.51	0.40
1:A:339:THR:CG2	20:A:7003:LHG:O2	2.69	0.40
21:B:1213:CLA:CHA	21:B:1213:CLA:HBA1	2.51	0.40
7:G:121:ILE:HG23	7:G:122:VAL:N	2.36	0.40
7:G:99:THR:O	7:G:101:PHE:HD1	2.04	0.40
1:A:281:LEU:O	1:A:281:LEU:HD12	2.21	0.40
14:1:217:HIS:O	14:1:218:LEU:CG	2.69	0.40
21:J:6014:CLA:CGA	21:J:6014:CLA:C1A	3.00	0.40
8:H:63:ILE:HD12	12:L:170:LYS:CE	2.43	0.40
6:F:109:TYR:O	6:F:110:ALA:CB	2.70	0.40
2:B:474:PHE:HB3	2:B:476:VAL:HG23	2.03	0.40
14:1:103:GLY:O	14:1:104:ASN:HB2	2.20	0.40
4:D:202:LYS:O	4:D:203:PHE:CB	2.69	0.40
2:B:649:MET:HA	2:B:652:PHE:HB3	2.04	0.40
21:1:1006:CLA:O1A	21:1:1014:CLA:CMC	2.70	0.40
14:1:186:LYS:CE	21:1:1007:CLA:O2D	2.69	0.40
26:1:1502:LUT:C8	26:1:1502:LUT:H181	2.49	0.40
14:1:186:LYS:NZ	20:1:1801:LHG:P	2.94	0.40
21:3:3002:CLA:HAA2	21:3:3002:CLA:HBD	2.03	0.40
21:4:4002:CLA:CED	21:4:4002:CLA:HBA2	2.52	0.40
1:A:92:TRP:CD1	21:A:1104:CLA:HBC1	2.57	0.40
21:B:1228:CLA:CBB	21:B:1228:CLA:HHC	2.51	0.40
2:B:433:THR:HG22	21:B:9010:CLA:H192	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ARG:HB3	15:2:99:ASP:OD1	2.20	0.40
12:L:186:THR:O	12:L:189:PHE:N	2.55	0.40
21:A:1130:CLA:C3D	12:L:73:VAL:HG11	2.52	0.40
12:L:171:LYS:O	12:L:172:GLN:CB	2.69	0.40
12:L:50:GLU:C	12:L:52:PRO:HD3	2.42	0.40
16:3:256:ASN:O	16:3:260:HIS:HB3	2.21	0.40
12:L:166:LEU:O	12:L:167:THR:CB	2.69	0.40
5:E:74:VAL:HG21	5:E:90:VAL:CG1	2.52	0.40
2:B:200:PRO:HB3	2:B:205:GLU:OE2	2.22	0.40
16:3:185:GLY:O	16:3:186:LYS:CB	2.70	0.40
1:A:629:ASN:HB3	1:A:630:ASP:H	1.75	0.40
4:D:89:GLY:HA3	4:D:117:THR:HG22	2.03	0.40
1:A:649:ILE:HD13	1:A:649:ILE:HA	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	719/721 (100%)	666 (93%)	44 (6%)	9 (1%)	15	53
2	B	729/731 (100%)	702 (96%)	24 (3%)	3 (0%)	39	80
3	C	78/80 (98%)	69 (88%)	8 (10%)	1 (1%)	15	53
4	D	135/137 (98%)	104 (77%)	17 (13%)	14 (10%)	1	3
5	E	61/63 (97%)	51 (84%)	7 (12%)	3 (5%)	3	16
6	F	150/152 (99%)	128 (85%)	17 (11%)	5 (3%)	5	26
7	G	82/84 (98%)	65 (79%)	10 (12%)	7 (8%)	1	5
8	H	80/82 (98%)	67 (84%)	6 (8%)	7 (9%)	1	4
9	I	24/26 (92%)	23 (96%)	1 (4%)	0	100	100
10	J	38/40 (95%)	36 (95%)	0	2 (5%)	2	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	62/72 (86%)	50 (81%)	10 (16%)	2 (3%)	5	27
12	L	161/163 (99%)	135 (84%)	14 (9%)	12 (8%)	1	6
13	N	83/85 (98%)	44 (53%)	20 (24%)	19 (23%)	0	0
14	1	167/182 (92%)	146 (87%)	10 (6%)	11 (7%)	1	8
15	2	140/199 (70%)	112 (80%)	18 (13%)	10 (7%)	1	7
16	3	145/275 (53%)	98 (68%)	26 (18%)	21 (14%)	0	1
17	4	193/196 (98%)	152 (79%)	22 (11%)	19 (10%)	1	3
All	All	3047/3288 (93%)	2648 (87%)	254 (8%)	145 (5%)	3	17

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	LYS
4	D	77	PRO
5	E	66	ILE
5	E	102	PRO
7	G	92	PRO
7	G	100	HIS
7	G	104	GLY
7	G	117	SER
7	G	118	ALA
8	H	80	PRO
8	H	135	PRO
10	J	11	ALA
12	L	57	VAL
12	L	173	PRO
12	L	206	VAL
13	N	96	LYS
13	N	97	ALA
13	N	144	PRO
13	N	148	GLU
13	N	150	LEU
14	1	151	MET
14	1	155	PRO
14	1	206	PRO
15	2	77	PRO
15	2	96	LEU
15	2	154	ASP
15	2	249	GLY
16	3	90	PRO

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Mol	Chain	Res	Type
16	3	200	ASN
16	3	201	PRO
16	3	243	PHE
17	4	207	ILE
17	4	208	ALA
17	4	228	GLY
1	A	430	ASP
1	A	662	SER
4	D	170	LYS
6	F	138	LEU
6	F	140	CYS
7	G	106	GLU
7	G	108	ALA
8	H	74	GLY
12	L	68	SER
12	L	86	LEU
12	L	90	ARG
12	L	122	ASN
13	N	94	LYS
13	N	114	PHE
13	N	118	TYR
13	N	124	THR
13	N	125	CYS
13	N	126	LYS
13	N	128	PRO
13	N	132	THR
13	N	151	GLU
14	1	174	PRO
15	2	153	THR
16	3	99	PRO
16	3	171	GLU
16	3	172	HIS
16	3	184	MET
16	3	215	GLY
16	3	221	LEU
17	4	200	LEU
17	4	230	GLY
17	4	240	SER
1	A	121	GLN
1	A	610	SER
2	B	74	PHE
2	B	492	ILE

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Mol	Chain	Res	Type
4	D	115	MET
4	D	128	ASN
4	D	148	LYS
4	D	168	HIS
4	D	203	PHE
6	F	205	ARG
8	H	83	PRO
10	J	40	PRO
11	K	74	PRO
11	K	77	ASN
13	N	117	ALA
13	N	121	GLN
13	N	140	GLN
13	N	158	ASP
14	1	148	GLN
15	2	88	ASP
15	2	92	ASP
16	3	150	TYR
16	3	169	PHE
16	3	173	ARG
16	3	224	LEU
16	3	242	TYR
17	4	171	ASP
17	4	177	TYR
17	4	180	PRO
17	4	183	GLU
17	4	195	ASN
17	4	196	PHE
17	4	198	PRO
17	4	242	PRO
4	D	120	ALA
4	D	199	ILE
8	H	77	ALA
8	H	99	ARG
12	L	128	ALA
12	L	178	THR
12	L	208	ASP
15	2	247	TYR
16	3	218	GLU
16	3	219	LYS
16	3	245	GLN
17	4	103	ALA

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Mol	Chain	Res	Type
2	B	559	CYS
3	C	62	PHE
4	D	159	PHE
4	D	171	ASP
4	D	185	VAL
5	E	68	PRO
6	F	189	LYS
6	F	201	PRO
13	N	115	ALA
14	1	129	GLY
14	1	154	ASP
14	1	205	TYR
14	1	225	ASN
15	2	69	PRO
16	3	232	GLY
17	4	227	THR
1	A	238	ASP
4	D	183	GLN
8	H	78	PRO
14	1	152	GLU
16	3	181	PRO
15	2	74	GLY
17	4	187	PRO
12	L	172	GLN
1	A	127	VAL
1	A	267	THR
4	D	160	PRO
17	4	226	VAL
17	4	241	ASP
1	A	48	PRO
12	L	60	ILE
16	3	264	PRO
14	1	127	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	583/584 (100%)	553 (95%)	30 (5%)	29	69
2	B	596/600 (99%)	577 (97%)	19 (3%)	46	82
3	C	69/69 (100%)	65 (94%)	4 (6%)	25	63
4	D	114/117 (97%)	99 (87%)	15 (13%)	5	22
5	E	56/56 (100%)	47 (84%)	9 (16%)	3	14
6	F	124/125 (99%)	114 (92%)	10 (8%)	15	47
7	G	65/66 (98%)	52 (80%)	13 (20%)	1	8
8	H	67/68 (98%)	52 (78%)	15 (22%)	1	5
9	I	22/22 (100%)	19 (86%)	3 (14%)	5	20
10	J	33/33 (100%)	30 (91%)	3 (9%)	12	41
11	K	46/52 (88%)	41 (89%)	5 (11%)	8	30
12	L	126/129 (98%)	113 (90%)	13 (10%)	9	33
13	N	73/73 (100%)	62 (85%)	11 (15%)	3	17
14	1	123/148 (83%)	106 (86%)	17 (14%)	4	20
15	2	108/162 (67%)	92 (85%)	16 (15%)	4	17
16	3	103/213 (48%)	76 (74%)	27 (26%)	0	3
17	4	134/162 (83%)	113 (84%)	21 (16%)	3	15
All	All	2442/2679 (91%)	2211 (90%)	231 (10%)	11	38

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	PHE
1	A	42	ARG
1	A	49	ASP
1	A	78	VAL
1	A	89	ILE
1	A	90	PHE
1	A	110	LEU
1	A	115	HIS
1	A	141	ARG
1	A	159	THR
1	A	167	THR
1	A	172	LEU
1	A	185	HIS
1	A	188	LYS
1	A	257	GLN

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Mol	Chain	Res	Type
1	A	258	LEU
1	A	272	LEU
1	A	309	LEU
1	A	315	HIS
1	A	341	GLN
1	A	364	MET
1	A	433	ASP
1	A	472	ARG
1	A	565	SER
1	A	630	ASP
1	A	638	THR
1	A	644	GLN
1	A	678	PHE
1	A	685	VAL
1	A	728	VAL
2	B	5	ILE
2	B	85	ARG
2	B	164	SER
2	B	172	GLU
2	B	220	GLN
2	B	275	HIS
2	B	280	ILE
2	B	292	ARG
2	B	332	PHE
2	B	354	SER
2	B	427	LEU
2	B	441	ASP
2	B	444	LEU
2	B	481	THR
2	B	486	LEU
2	B	574	ASP
2	B	577	TYR
2	B	636	THR
2	B	694	ARG
3	C	11	CYS
3	C	16	GLN
3	C	46	GLU
3	C	53	ARG
4	D	79	THR
4	D	91	LEU
4	D	93	ARG
4	D	99	GLU

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Mol	Chain	Res	Type
4	D	115	MET
4	D	117	THR
4	D	124	ARG
4	D	128	ASN
4	D	149	TYR
4	D	154	GLN
4	D	156	TYR
4	D	190	ARG
4	D	199	ILE
4	D	206	LYS
4	D	207	GLN
5	E	68	PRO
5	E	74	VAL
5	E	78	ARG
5	E	80	GLU
5	E	92	THR
5	E	95	GLN
5	E	109	LYS
5	E	119	ASN
5	E	123	ASP
6	F	82	LEU
6	F	87	GLU
6	F	179	ARG
6	F	198	ILE
6	F	200	VAL
6	F	213	TRP
6	F	218	TYR
6	F	222	LEU
6	F	225	GLU
6	F	227	VAL
7	G	66	LEU
7	G	68	THR
7	G	74	LEU
7	G	93	GLU
7	G	94	GLN
7	G	101	PHE
7	G	105	ASP
7	G	111	TYR
7	G	114	LEU
7	G	116	LYS
7	G	117	SER
7	G	140	LEU

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Mol	Chain	Res	Type
7	G	141	THR
8	H	58	PHE
8	H	59	ASP
8	H	60	LEU
8	H	62	ASP
8	H	70	TRP
8	H	73	TYR
8	H	83	PRO
8	H	99	ARG
8	H	101	LEU
8	H	113	THR
8	H	114	LEU
8	H	124	ASP
8	H	126	LEU
8	H	128	ILE
8	H	135	PRO
9	I	7	LEU
9	I	11	LEU
9	I	14	LEU
10	J	8	LEU
10	J	15	SER
10	J	16	THR
11	K	47	ASP
11	K	54	ASN
11	K	64	MET
11	K	102	THR
11	K	118	VAL
12	L	51	LYS
12	L	64	PRO
12	L	66	ILE
12	L	102	VAL
12	L	120	LEU
12	L	123	THR
12	L	125	TYR
12	L	163	SER
12	L	164	LEU
12	L	165	THR
12	L	167	THR
12	L	172	GLN
12	L	176	LEU
13	N	87	VAL
13	N	91	TYR

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Mol	Chain	Res	Type
13	N	96	LYS
13	N	99	LYS
13	N	103	ASP
13	N	106	ARG
13	N	120	VAL
13	N	130	ASN
13	N	150	LEU
13	N	155	GLU
13	N	158	ASP
14	1	47	ARG
14	1	66	LEU
14	1	94	ILE
14	1	102	LEU
14	1	105	TRP
14	1	111	TRP
14	1	114	LEU
14	1	131	LEU
14	1	137	ILE
14	1	145	VAL
14	1	147	HIS
14	1	148	GLN
14	1	154	ASP
14	1	170	TYR
14	1	173	ASP
14	1	203	SER
14	1	221	PRO
15	2	63	VAL
15	2	70	LEU
15	2	72	PHE
15	2	91	PHE
15	2	96	LEU
15	2	98	SER
15	2	99	ASP
15	2	111	LEU
15	2	113	HIS
15	2	126	ILE
15	2	153	THR
15	2	158	LEU
15	2	163	LEU
15	2	243	PHE
15	2	252	PRO
15	2	254	ASP

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Mol	Chain	Res	Type
16	3	87	LEU
16	3	91	GLU
16	3	96	PHE
16	3	101	TRP
16	3	102	LEU
16	3	111	ARG
16	3	121	ILE
16	3	153	TRP
16	3	161	VAL
16	3	162	LEU
16	3	166	LEU
16	3	169	PHE
16	3	172	HIS
16	3	173	ARG
16	3	174	ARG
16	3	184	MET
16	3	200	ASN
16	3	209	PHE
16	3	216	LYS
16	3	225	LYS
16	3	236	MET
16	3	242	TYR
16	3	245	GLN
16	3	251	VAL
16	3	255	GLN
16	3	260	HIS
16	3	261	VAL
17	4	66	TYR
17	4	80	LEU
17	4	141	THR
17	4	151	PHE
17	4	156	ILE
17	4	170	GLN
17	4	173	ILE
17	4	174	PHE
17	4	179	LEU
17	4	186	TYR
17	4	196	PHE
17	4	199	THR
17	4	200	LEU
17	4	221	ILE
17	4	226	VAL

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Mol	Chain	Res	Type
17	4	234	ASN
17	4	239	ILE
17	4	243	TRP
17	4	245	ASN
17	4	247	ILE
17	4	249	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	303	HIS
1	A	615	HIS
2	B	115	ASN
4	D	96	GLN
4	D	128	ASN
7	G	94	GLN
8	H	69	GLN
12	L	58	GLN
12	L	85	ASN
12	L	122	ASN
12	L	172	GLN
14	1	201	GLN
14	1	202	GLN
14	1	217	HIS
15	2	113	HIS
15	2	255	ASN
16	3	200	ASN
16	3	256	ASN
17	4	99	ASN
17	4	170	GLN
17	4	225	ASN
17	4	234	ASN
17	4	244	HIS
17	4	249	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

200 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	CLA	1	1001	14	45,63,73	1.91	12 (26%)	49,101,113	2.42	19 (38%)
21	CLA	1	1002	-	46,64,73	1.90	11 (23%)	50,102,113	2.44	17 (34%)
21	CLA	1	1003	14	55,73,73	1.68	12 (21%)	61,113,113	2.29	18 (29%)
21	CLA	1	1004	14	55,73,73	1.64	13 (23%)	61,113,113	2.28	14 (22%)
21	CLA	1	1005	-	46,64,73	1.82	12 (26%)	50,102,113	2.28	16 (32%)
21	CLA	1	1006	-	37,55,73	2.18	12 (32%)	42,91,113	2.74	16 (38%)
21	CLA	1	1007	20	45,63,73	1.89	12 (26%)	49,101,113	2.14	14 (28%)
21	CLA	1	1008	-	55,73,73	1.65	13 (23%)	61,113,113	2.18	13 (21%)
21	CLA	1	1009	-	55,73,73	1.65	11 (20%)	61,113,113	2.76	19 (31%)
21	CLA	1	1010	-	55,73,73	1.70	12 (21%)	61,113,113	2.01	13 (21%)
21	CLA	1	1011	-	55,73,73	1.68	13 (23%)	61,113,113	2.39	17 (27%)
21	CLA	1	1012	14	40,58,73	2.01	12 (30%)	44,95,113	2.36	17 (38%)
21	CLA	1	1013	-	55,73,73	1.73	12 (21%)	61,113,113	2.05	15 (24%)
21	CLA	1	1014	-	32,53,73	2.17	11 (34%)	37,89,113	2.68	11 (29%)
26	LUT	1	1501	-	41,43,43	2.39	2 (4%)	51,60,60	3.89	27 (52%)
26	LUT	1	1502	-	41,43,43	2.34	4 (9%)	51,60,60	4.41	28 (54%)
20	LHG	1	1801	21	48,48,48	0.87	2 (4%)	49,54,54	1.16	3 (6%)
21	CLA	2	2001	15	18,35,73	2.85	11 (61%)	22,60,113	3.54	14 (63%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	2002	-	50,68,73	1.81	13 (26%)	55,107,113	2.34	16 (29%)
21	CLA	2	2003	-	55,73,73	1.78	12 (21%)	61,113,113	2.25	15 (24%)
21	CLA	2	2004	15	50,67,73	1.97	14 (28%)	56,105,113	2.31	14 (25%)
21	CLA	2	2005	-	55,73,73	1.65	10 (18%)	61,113,113	1.96	11 (18%)
21	CLA	2	2006	-	47,65,73	1.91	12 (25%)	50,103,113	2.38	13 (26%)
21	CLA	2	2007	20	45,63,73	1.85	12 (26%)	49,101,113	2.38	15 (30%)
21	CLA	2	2008	-	55,73,73	1.79	12 (21%)	61,113,113	2.28	16 (26%)
21	CLA	2	2009	15	36,54,73	2.21	12 (33%)	41,90,113	2.37	13 (31%)
21	CLA	2	2010	-	55,73,73	1.74	12 (21%)	61,113,113	2.15	14 (22%)
21	CLA	2	2011	-	50,68,73	1.81	13 (26%)	55,107,113	2.46	14 (25%)
21	CLA	2	2012	15	55,73,73	1.68	13 (23%)	61,113,113	2.04	15 (24%)
21	CLA	2	2013	-	55,73,73	1.63	12 (21%)	61,113,113	2.26	15 (24%)
21	CLA	2	2014	-	32,53,73	2.09	12 (37%)	37,89,113	2.73	14 (37%)
26	LUT	2	2501	-	41,43,43	2.39	3 (7%)	51,60,60	3.42	16 (31%)
26	LUT	2	2502	-	41,43,43	2.43	3 (7%)	51,60,60	2.43	14 (27%)
20	LHG	2	2801	21	35,35,48	1.10	3 (8%)	36,41,54	1.14	3 (8%)
21	CLA	3	3001	-	55,73,73	1.83	12 (21%)	61,113,113	2.05	11 (18%)
21	CLA	3	3002	-	45,63,73	2.04	11 (24%)	49,101,113	2.35	12 (24%)
21	CLA	3	3003	-	50,68,73	1.94	12 (24%)	55,107,113	2.05	13 (23%)
21	CLA	3	3004	-	32,53,73	2.25	11 (34%)	37,89,113	2.22	9 (24%)
21	CLA	3	3005	21	32,53,73	2.28	10 (31%)	37,89,113	2.41	9 (24%)
21	CLA	3	3006	-	55,73,73	1.85	12 (21%)	61,113,113	2.06	12 (19%)
21	CLA	3	3008	-	55,73,73	1.76	12 (21%)	61,113,113	2.15	17 (27%)
21	CLA	3	3009	-	36,54,73	2.31	12 (33%)	41,90,113	2.56	17 (41%)
21	CLA	3	3010	-	42,60,73	2.08	12 (28%)	45,97,113	2.45	14 (31%)
21	CLA	3	3011	-	36,54,73	2.31	12 (33%)	41,90,113	2.42	12 (29%)
21	CLA	3	3012	21,16	32,53,73	2.12	11 (34%)	37,89,113	3.06	17 (45%)
21	CLA	3	3013	-	40,58,73	2.13	13 (32%)	44,95,113	2.82	15 (34%)
21	CLA	3	3014	-	32,53,73	2.18	10 (31%)	37,89,113	2.49	14 (37%)
21	CLA	3	3015	-	32,53,73	2.28	11 (34%)	37,89,113	2.28	10 (27%)
21	CLA	3	3016	-	32,53,73	2.28	11 (34%)	37,89,113	2.29	9 (24%)
21	CLA	3	3017	-	32,53,73	2.25	11 (34%)	37,89,113	2.36	9 (24%)
21	CLA	4	4001	17	55,73,73	1.69	11 (20%)	61,113,113	2.26	14 (22%)
21	CLA	4	4002	-	46,64,73	1.91	13 (28%)	50,102,113	2.45	13 (26%)
21	CLA	4	4003	17	55,73,73	1.69	13 (23%)	61,113,113	1.87	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	4004	-	55,73,73	1.69	13 (23%)	61,113,113	2.27	13 (21%)
21	CLA	4	4005	17	32,53,73	2.08	12 (37%)	37,89,113	3.23	18 (48%)
21	CLA	4	4006	-	55,73,73	1.77	12 (21%)	61,113,113	2.29	21 (34%)
21	CLA	4	4007	-	55,73,73	1.69	12 (21%)	61,113,113	2.02	12 (19%)
21	CLA	4	4008	-	38,56,73	1.95	11 (28%)	42,92,113	3.17	19 (45%)
21	CLA	4	4009	17	40,58,73	1.93	11 (27%)	44,95,113	2.54	11 (25%)
21	CLA	4	4010	-	40,58,73	1.99	10 (25%)	44,95,113	2.65	15 (34%)
21	CLA	4	4011	-	55,73,73	1.59	13 (23%)	61,113,113	2.43	17 (27%)
21	CLA	4	4012	-	55,73,73	1.72	12 (21%)	61,113,113	2.16	13 (21%)
21	CLA	4	4013	-	41,59,73	1.83	12 (29%)	44,96,113	2.79	15 (34%)
21	CLA	4	4014	17	32,53,73	2.20	11 (34%)	37,89,113	2.56	14 (37%)
21	CLA	4	4015	-	36,54,73	2.11	10 (27%)	41,90,113	2.32	14 (34%)
26	LUT	4	4501	-	41,43,43	2.32	1 (2%)	51,60,60	3.75	24 (47%)
26	LUT	4	4502	-	41,43,43	2.37	5 (12%)	51,60,60	3.54	26 (50%)
27	NEX	4	4503	-	39,46,46	3.03	12 (30%)	48,70,70	2.27	17 (35%)
28	G3P	4	4505	-	9,9,9	0.60	0	10,12,12	0.66	0
21	CLA	A	1101	-	55,73,73	1.85	12 (21%)	61,113,113	2.08	12 (19%)
21	CLA	A	1102	-	40,58,73	2.16	12 (30%)	44,95,113	2.53	13 (29%)
21	CLA	A	1103	-	55,73,73	1.84	12 (21%)	61,113,113	2.03	14 (22%)
21	CLA	A	1104	1	55,73,73	1.83	11 (20%)	61,113,113	2.05	12 (19%)
21	CLA	A	1105	-	41,59,73	2.14	12 (29%)	44,96,113	2.34	13 (29%)
21	CLA	A	1106	1	55,73,73	1.86	12 (21%)	61,113,113	2.11	12 (19%)
21	CLA	A	1107	1	41,59,73	2.14	11 (26%)	44,96,113	2.45	13 (29%)
21	CLA	A	1108	-	36,54,73	2.38	12 (33%)	41,90,113	2.29	12 (29%)
21	CLA	A	1109	-	55,73,73	1.86	12 (21%)	61,113,113	2.02	14 (22%)
21	CLA	A	1110	-	45,63,73	2.00	12 (26%)	49,101,113	2.27	13 (26%)
21	CLA	A	1111	-	50,68,73	1.93	12 (24%)	55,107,113	2.15	13 (23%)
21	CLA	A	1112	-	36,54,73	2.37	13 (36%)	41,90,113	2.29	13 (31%)
21	CLA	A	1113	-	36,54,73	2.38	12 (33%)	41,90,113	2.31	12 (29%)
21	CLA	A	1114	-	36,54,73	2.41	12 (33%)	41,90,113	2.33	11 (26%)
21	CLA	A	1115	-	46,64,73	2.02	13 (28%)	50,102,113	2.12	10 (20%)
21	CLA	A	1116	-	44,62,73	2.05	13 (29%)	47,99,113	2.24	13 (27%)
21	CLA	A	1117	-	55,73,73	1.86	12 (21%)	61,113,113	2.07	12 (19%)
21	CLA	A	1118	-	36,54,73	2.31	12 (33%)	41,90,113	2.57	14 (34%)
21	CLA	A	1119	-	55,73,73	1.84	11 (20%)	61,113,113	2.02	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	1120	-	36,54,73	2.37	12 (33%)	41,90,113	2.29	12 (29%)
21	CLA	A	1121	-	36,54,73	2.38	11 (30%)	41,90,113	2.44	11 (26%)
21	CLA	A	1122	-	49,67,73	1.95	12 (24%)	53,105,113	2.22	11 (20%)
21	CLA	A	1123	-	55,73,73	1.86	13 (23%)	61,113,113	2.16	13 (21%)
21	CLA	A	1124	-	45,63,73	2.05	12 (26%)	49,101,113	2.24	12 (24%)
21	CLA	A	1125	-	45,63,73	1.78	11 (24%)	49,101,113	2.45	14 (28%)
21	CLA	A	1126	-	55,73,73	1.83	13 (23%)	61,113,113	2.06	15 (24%)
21	CLA	A	1127	-	55,73,73	1.84	12 (21%)	61,113,113	2.03	12 (19%)
21	CLA	A	1128	-	55,73,73	1.81	11 (20%)	61,113,113	2.06	14 (22%)
21	CLA	A	1129	-	40,58,73	2.13	11 (27%)	44,95,113	2.39	13 (29%)
21	CLA	A	1130	-	36,54,73	2.35	11 (30%)	41,90,113	2.25	12 (29%)
21	CLA	A	1131	-	55,73,73	1.69	12 (21%)	61,113,113	2.27	13 (21%)
21	CLA	A	1132	-	55,73,73	1.71	12 (21%)	61,113,113	2.02	14 (22%)
21	CLA	A	1133	-	36,54,73	2.25	12 (33%)	41,90,113	2.41	14 (34%)
21	CLA	A	1134	1	36,54,73	2.37	12 (33%)	41,90,113	2.35	11 (26%)
21	CLA	A	1135	-	41,59,73	2.12	12 (29%)	44,96,113	2.48	14 (31%)
21	CLA	A	1136	-	55,73,73	1.84	12 (21%)	61,113,113	2.10	14 (22%)
21	CLA	A	1137	-	45,63,73	2.02	12 (26%)	49,101,113	2.34	13 (26%)
21	CLA	A	1138	-	55,73,73	1.86	12 (21%)	61,113,113	2.02	13 (21%)
21	CLA	A	1139	-	55,73,73	1.85	12 (21%)	61,113,113	1.97	12 (19%)
21	CLA	A	1140	-	55,73,73	1.87	12 (21%)	61,113,113	2.03	12 (19%)
21	CLA	A	1141	20	41,59,73	2.16	13 (31%)	44,96,113	2.33	10 (22%)
21	CLA	A	1142	-	31,52,73	2.17	10 (32%)	37,88,113	2.29	9 (24%)
21	CLA	A	1143	-	32,53,73	2.28	11 (34%)	37,89,113	2.24	9 (24%)
18	PQN	A	5001	-	34,34,34	1.43	2 (5%)	44,45,45	1.08	2 (4%)
19	BCR	A	6002	-	41,41,41	2.80	6 (14%)	56,56,56	6.65	22 (39%)
19	BCR	A	6003	-	41,41,41	2.87	6 (14%)	56,56,56	6.34	25 (44%)
19	BCR	A	6007	-	41,41,41	2.74	6 (14%)	56,56,56	6.60	28 (50%)
19	BCR	A	6008	-	41,41,41	2.62	6 (14%)	56,56,56	7.61	38 (67%)
19	BCR	A	6011	-	41,41,41	2.77	6 (14%)	56,56,56	7.75	34 (60%)
19	BCR	A	6017	-	41,41,41	2.70	6 (14%)	56,56,56	6.40	25 (44%)
20	LHG	A	7001	-	48,48,48	0.92	2 (4%)	49,54,54	1.08	3 (6%)
20	LHG	A	7003	21	48,48,48	0.93	2 (4%)	49,54,54	1.01	3 (6%)
22	SF4	A	8001	-	0,12,12	0.00	-	0,24,24	0.00	-
23	CL0	A	9011	-	55,73,73	1.60	11 (20%)	61,113,113	2.26	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	9012	-	55,73,73	1.76	12 (21%)	61,113,113	2.16	15 (24%)
21	CLA	A	9013	-	55,73,73	1.67	11 (20%)	61,113,113	2.28	16 (26%)
21	CLA	B	1201	-	36,54,73	2.37	11 (30%)	41,90,113	2.39	12 (29%)
21	CLA	B	1202	-	55,73,73	1.85	12 (21%)	61,113,113	2.09	12 (19%)
21	CLA	B	1203	2	50,68,73	1.93	11 (22%)	55,107,113	2.09	11 (20%)
21	CLA	B	1204	-	45,63,73	2.04	12 (26%)	49,101,113	2.26	14 (28%)
21	CLA	B	1205	-	55,73,73	1.84	12 (21%)	61,113,113	2.19	12 (19%)
21	CLA	B	1206	2	55,73,73	1.82	12 (21%)	61,113,113	2.14	14 (22%)
21	CLA	B	1207	-	55,73,73	1.84	12 (21%)	61,113,113	2.15	13 (21%)
21	CLA	B	1208	-	45,63,73	2.05	13 (28%)	49,101,113	2.12	9 (18%)
21	CLA	B	1209	-	36,54,73	2.36	13 (36%)	41,90,113	2.28	11 (26%)
21	CLA	B	1210	-	55,73,73	1.90	12 (21%)	61,113,113	2.07	13 (21%)
21	CLA	B	1211	-	55,73,73	1.86	12 (21%)	61,113,113	2.08	13 (21%)
21	CLA	B	1212	-	36,54,73	2.38	12 (33%)	41,90,113	2.35	13 (31%)
21	CLA	B	1213	-	50,68,73	1.78	12 (24%)	55,107,113	2.27	14 (25%)
21	CLA	B	1214	-	49,67,73	1.95	11 (22%)	53,105,113	2.13	15 (28%)
21	CLA	B	1215	-	50,68,73	1.92	12 (24%)	55,107,113	2.17	12 (21%)
21	CLA	B	1216	-	55,73,73	1.83	12 (21%)	61,113,113	2.05	13 (21%)
21	CLA	B	1217	-	36,54,73	2.36	12 (33%)	41,90,113	2.36	13 (31%)
21	CLA	B	1218	-	50,68,73	1.93	11 (22%)	55,107,113	2.21	12 (21%)
21	CLA	B	1219	-	50,68,73	1.91	12 (24%)	55,107,113	2.11	15 (27%)
21	CLA	B	1220	-	55,73,73	1.85	11 (20%)	61,113,113	2.03	14 (22%)
21	CLA	B	1221	-	44,62,73	2.06	12 (27%)	47,99,113	2.44	13 (27%)
21	CLA	B	1222	-	55,73,73	1.86	12 (21%)	61,113,113	2.09	13 (21%)
21	CLA	B	1223	-	55,73,73	1.83	12 (21%)	61,113,113	2.15	12 (19%)
21	CLA	B	1224	-	55,73,73	1.85	12 (21%)	61,113,113	2.12	11 (18%)
21	CLA	B	1225	-	55,73,73	1.86	12 (21%)	61,113,113	2.05	12 (19%)
21	CLA	B	1226	-	55,73,73	1.67	11 (20%)	61,113,113	2.33	11 (18%)
21	CLA	B	1227	-	55,73,73	1.61	13 (23%)	61,113,113	2.31	16 (26%)
21	CLA	B	1228	-	41,59,73	1.98	12 (29%)	44,96,113	2.47	14 (31%)
21	CLA	B	1229	-	55,73,73	1.86	13 (23%)	61,113,113	2.05	11 (18%)
21	CLA	B	1230	-	48,66,73	1.96	12 (25%)	52,104,113	2.31	14 (26%)
21	CLA	B	1231	-	36,54,73	2.37	12 (33%)	41,90,113	2.37	11 (26%)
21	CLA	B	1234	-	50,68,73	1.94	12 (24%)	55,107,113	2.16	12 (21%)
21	CLA	B	1235	-	55,73,73	1.85	11 (20%)	61,113,113	2.07	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1236	-	45,63,73	2.03	11 (24%)	49,101,113	2.31	12 (24%)
21	CLA	B	1237	-	50,68,73	1.92	12 (24%)	55,107,113	2.11	13 (23%)
21	CLA	B	1238	-	55,73,73	1.86	12 (21%)	61,113,113	2.04	11 (18%)
21	CLA	B	1239	-	55,73,73	1.63	10 (18%)	61,113,113	2.31	17 (27%)
21	CLA	B	1240	20	55,73,73	1.70	13 (23%)	61,113,113	2.30	19 (31%)
18	PQN	B	5002	-	34,34,34	1.41	2 (5%)	44,45,45	1.01	4 (9%)
19	BCR	B	6004	-	41,41,41	2.88	7 (17%)	56,56,56	6.39	27 (48%)
19	BCR	B	6005	-	41,41,41	2.71	6 (14%)	56,56,56	7.00	28 (50%)
19	BCR	B	6006	-	41,41,41	2.76	6 (14%)	56,56,56	7.97	34 (60%)
19	BCR	B	6009	-	41,41,41	2.70	6 (14%)	56,56,56	6.27	22 (39%)
19	BCR	B	6010	-	41,41,41	2.70	6 (14%)	56,56,56	6.74	22 (39%)
19	BCR	B	6011	-	25,25,41	3.32	5 (20%)	33,33,56	8.25	16 (48%)
20	LHG	B	7004	21	48,48,48	0.94	3 (6%)	49,54,54	1.06	4 (8%)
24	DGD	B	7101	-	62,62,67	0.87	1 (1%)	76,76,81	1.39	11 (14%)
21	CLA	B	9010	-	55,73,73	1.70	12 (21%)	61,113,113	2.11	16 (26%)
21	CLA	B	9022	-	55,73,73	1.73	13 (23%)	61,113,113	2.48	19 (31%)
21	CLA	B	9023	-	55,73,73	1.67	12 (21%)	61,113,113	2.02	16 (26%)
22	SF4	C	8002	3	0,12,12	0.00	-	0,24,24	0.00	-
22	SF4	C	8003	-	0,12,12	0.00	-	0,24,24	0.00	-
21	CLA	F	1301	-	32,53,73	2.25	11 (34%)	37,89,113	2.23	8 (21%)
21	CLA	F	1302	-	36,54,73	2.38	12 (33%)	41,90,113	2.28	11 (26%)
21	CLA	F	1303	-	54,72,73	1.72	13 (24%)	61,111,113	1.97	16 (26%)
19	BCR	F	6014	-	41,41,41	2.68	6 (14%)	56,56,56	7.79	35 (62%)
19	BCR	F	6016	-	41,41,41	2.80	6 (14%)	56,56,56	7.75	36 (64%)
21	CLA	G	1001	-	45,63,73	1.88	13 (28%)	49,101,113	2.49	15 (30%)
21	CLA	G	1002	-	36,54,73	2.22	13 (36%)	41,90,113	2.54	15 (36%)
19	BCR	G	2011	-	41,41,41	2.93	6 (14%)	56,56,56	6.64	26 (46%)
25	LMG	G	2021	-	23,23,55	1.23	2 (8%)	31,31,63	1.83	6 (19%)
21	CLA	H	1000	8	36,54,73	2.30	12 (33%)	41,90,113	2.55	13 (31%)
19	BCR	I	6018	-	41,41,41	2.63	6 (14%)	56,56,56	7.65	33 (58%)
19	BCR	I	6020	-	41,41,41	2.81	6 (14%)	56,56,56	6.62	22 (39%)
21	CLA	J	1302	-	51,69,73	1.92	11 (21%)	56,108,113	2.19	13 (23%)
25	LMG	J	5001	-	35,35,55	1.07	2 (5%)	43,43,63	1.13	3 (6%)
19	BCR	J	6012	-	41,41,41	2.71	6 (14%)	56,56,56	7.48	30 (53%)
19	BCR	J	6013	-	41,41,41	2.78	6 (14%)	56,56,56	6.79	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	J	6014	-	51,69,73	1.93	12 (23%)	56,108,113	2.15	13 (23%)
21	CLA	J	6015	-	45,63,73	2.02	13 (28%)	49,101,113	2.37	15 (30%)
21	CLA	L	1501	12	36,54,73	2.34	11 (30%)	41,90,113	2.29	12 (29%)
21	CLA	L	1502	-	55,73,73	1.83	12 (21%)	61,113,113	2.04	13 (21%)
21	CLA	L	1503	-	40,58,73	2.13	12 (30%)	44,95,113	2.41	13 (29%)
19	BCR	L	6019	-	41,41,41	2.82	6 (14%)	56,56,56	6.34	26 (46%)
19	BCR	L	6020	-	41,41,41	2.80	6 (14%)	56,56,56	6.37	24 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	1	1001	14	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	1	1002	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	1	1003	14	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1004	14	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1005	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	1	1006	-	3/3/16/25	0/16/114/135	0/0/9/9
21	CLA	1	1007	20	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	1	1008	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1009	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1010	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1011	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1012	14	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	1	1013	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	1	1014	-	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	1	1501	-	1/1/12/27	0/29/67/67	0/2/2/2
26	LUT	1	1502	-	1/1/12/27	0/29/67/67	0/2/2/2
20	LHG	1	1801	21	-	0/53/53/53	0/0/0/0
21	CLA	2	2001	15	3/3/8/25	0/0/75/135	0/0/9/9
21	CLA	2	2002	-	3/3/19/25	1/31/129/135	0/0/9/9
21	CLA	2	2003	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2004	15	3/3/18/25	0/31/125/135	0/0/9/9
21	CLA	2	2005	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	2	2006	-	3/3/18/25	1/28/126/135	0/0/9/9
21	CLA	2	2007	20	3/3/18/25	1/25/123/135	0/0/9/9
21	CLA	2	2008	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2009	15	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	2	2010	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2011	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	2	2012	15	3/3/20/25	1/37/135/135	0/0/9/9
21	CLA	2	2013	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	2	2014	-	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	2	2501	-	1/1/12/27	0/29/67/67	0/2/2/2
26	LUT	2	2502	-	1/1/12/27	1/29/67/67	0/2/2/2
20	LHG	2	2801	21	-	2/40/40/53	0/0/0/0
21	CLA	3	3001	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	3	3002	-	2/2/18/25	0/25/123/135	0/0/9/9
21	CLA	3	3003	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	3	3004	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3005	21	2/2/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3006	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	3	3008	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	3	3009	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	3	3010	-	3/3/17/25	0/22/120/135	0/0/9/9
21	CLA	3	3011	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	3	3012	21,16	3/3/16/25	1/11/111/135	0/0/9/9
21	CLA	3	3013	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	3	3014	-	2/2/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3015	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3016	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	3	3017	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	4	4001	17	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4002	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	4	4003	17	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4004	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4005	17	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	4	4006	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	4007	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4008	-	3/3/16/25	0/17/115/135	0/0/9/9
21	CLA	4	4009	17	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	4	4010	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	4	4011	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4012	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	4	4013	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	4	4014	17	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	4	4015	-	3/3/16/25	0/15/113/135	0/0/9/9
26	LUT	4	4501	-	1/1/12/27	0/29/67/67	0/2/2/2
26	LUT	4	4502	-	1/1/12/27	0/29/67/67	0/2/2/2
27	NEX	4	4503	-	-	1/27/83/83	0/2/3/3
28	G3P	4	4505	-	-	0/8/8/8	0/0/0/0
21	CLA	A	1101	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1102	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	A	1103	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1104	1	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1105	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	A	1106	1	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1107	1	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	A	1108	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1109	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1110	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1111	-	2/2/19/25	0/31/129/135	0/0/9/9
21	CLA	A	1112	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1113	-	2/2/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1114	-	2/2/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1115	-	3/3/18/25	0/27/125/135	0/0/9/9
21	CLA	A	1116	-	2/2/17/25	0/24/122/135	0/0/9/9
21	CLA	A	1117	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1118	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1119	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1120	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1121	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1122	-	3/3/18/25	0/30/128/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	1123	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1124	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1125	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1126	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1127	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1128	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1129	-	3/3/17/25	0/19/117/135	0/0/9/9
21	CLA	A	1130	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1131	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1132	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1133	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1134	1	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	A	1135	-	1/1/17/25	0/21/119/135	0/0/9/9
21	CLA	A	1136	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1137	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	A	1138	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1139	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1140	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	1141	20	3/3/17/25	1/21/119/135	0/0/9/9
21	CLA	A	1142	-	3/3/16/25	0/11/109/135	0/0/9/9
21	CLA	A	1143	-	3/3/16/25	0/11/111/135	0/0/9/9
18	PQN	A	5001	-	-	0/23/43/43	0/2/2/2
19	BCR	A	6002	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6003	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6007	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6008	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6011	-	-	0/29/63/63	0/2/2/2
19	BCR	A	6017	-	-	0/29/63/63	0/2/2/2
20	LHG	A	7001	-	-	0/53/53/53	0/0/0/0
20	LHG	A	7003	21	-	0/53/53/53	0/0/0/0
22	SF4	A	8001	-	-	0/0/48/48	0/6/5/5
23	CL0	A	9011	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	9012	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	A	9013	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1201	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1202	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1203	2	2/2/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1204	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	B	1205	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1206	2	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1207	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1208	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	B	1209	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1210	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1211	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1212	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1213	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1214	-	2/2/18/25	0/30/128/135	0/0/9/9
21	CLA	B	1215	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1216	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1217	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1218	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1219	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1220	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1221	-	3/3/17/25	0/24/122/135	0/0/9/9
21	CLA	B	1222	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1223	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1224	-	2/2/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1225	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1226	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1227	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1228	-	3/3/17/25	0/21/119/135	0/0/9/9
21	CLA	B	1229	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1230	-	3/3/18/25	0/29/127/135	0/0/9/9
21	CLA	B	1231	-	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	B	1234	-	2/2/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1235	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1236	-	2/2/18/25	0/25/123/135	0/0/9/9
21	CLA	B	1237	-	3/3/19/25	0/31/129/135	0/0/9/9
21	CLA	B	1238	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1239	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	1240	20	3/3/20/25	0/37/135/135	0/0/9/9
18	PQN	B	5002	-	-	0/23/43/43	0/2/2/2
19	BCR	B	6004	-	-	1/29/63/63	0/2/2/2
19	BCR	B	6005	-	-	2/29/63/63	0/2/2/2
19	BCR	B	6006	-	-	0/29/63/63	0/2/2/2
19	BCR	B	6009	-	-	0/29/63/63	0/2/2/2
19	BCR	B	6010	-	-	0/29/63/63	0/2/2/2
19	BCR	B	6011	-	-	0/18/35/63	0/1/1/2
20	LHG	B	7004	21	-	0/53/53/53	0/0/0/0
24	DGD	B	7101	-	-	0/50/90/95	0/2/2/2
21	CLA	B	9010	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	9022	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	B	9023	-	3/3/20/25	0/37/135/135	0/0/9/9
22	SF4	C	8002	3	-	0/0/48/48	0/6/5/5
22	SF4	C	8003	-	-	0/0/48/48	0/6/5/5
21	CLA	F	1301	-	3/3/16/25	0/11/111/135	0/0/9/9
21	CLA	F	1302	-	2/2/16/25	0/15/113/135	0/0/9/9
21	CLA	F	1303	-	3/3/19/25	0/35/133/135	0/0/9/9
19	BCR	F	6014	-	-	0/29/63/63	0/2/2/2
19	BCR	F	6016	-	-	0/29/63/63	0/2/2/2
21	CLA	G	1001	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	G	1002	-	3/3/16/25	0/15/113/135	0/0/9/9
19	BCR	G	2011	-	-	1/29/63/63	0/2/2/2
25	LMG	G	2021	-	-	1/16/36/70	0/1/1/1
21	CLA	H	1000	8	2/2/16/25	0/15/113/135	0/0/9/9
19	BCR	I	6018	-	-	0/29/63/63	0/2/2/2
19	BCR	I	6020	-	-	0/29/63/63	0/2/2/2
21	CLA	J	1302	-	2/2/19/25	0/33/131/135	0/0/9/9
25	LMG	J	5001	-	-	0/30/50/70	0/1/1/1
19	BCR	J	6012	-	-	0/29/63/63	0/2/2/2
19	BCR	J	6013	-	-	0/29/63/63	0/2/2/2
21	CLA	J	6014	-	3/3/19/25	0/33/131/135	0/0/9/9
21	CLA	J	6015	-	3/3/18/25	0/25/123/135	0/0/9/9
21	CLA	L	1501	12	3/3/16/25	0/15/113/135	0/0/9/9
21	CLA	L	1502	-	3/3/20/25	0/37/135/135	0/0/9/9
21	CLA	L	1503	-	3/3/17/25	0/19/117/135	0/0/9/9
19	BCR	L	6019	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BCR	L	6020	-	-	0/29/63/63	0/2/2/2

All (2052) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	6003	BCR	C8-C9	-8.58	1.26	1.45
19	B	6011	BCR	C8-C9	-8.47	1.27	1.45
19	G	2011	BCR	C8-C9	-8.45	1.27	1.45
19	A	6002	BCR	C11-C10	-8.21	1.18	1.43
19	L	6019	BCR	C11-C10	-8.19	1.18	1.43
19	G	2011	BCR	C11-C10	-8.17	1.18	1.43
19	A	6011	BCR	C11-C10	-8.15	1.18	1.43
19	B	6011	BCR	C11-C10	-8.14	1.18	1.43
19	L	6020	BCR	C11-C10	-8.13	1.18	1.43
19	I	6020	BCR	C11-C10	-8.13	1.18	1.43
19	B	6006	BCR	C11-C10	-8.11	1.18	1.43
19	J	6013	BCR	C11-C10	-8.10	1.18	1.43
19	A	6011	BCR	C8-C9	-8.09	1.28	1.45
19	A	6003	BCR	C11-C10	-8.09	1.18	1.43
19	B	6004	BCR	C11-C10	-8.08	1.18	1.43
19	F	6016	BCR	C11-C10	-8.07	1.18	1.43
19	A	6007	BCR	C11-C10	-8.01	1.18	1.43
19	A	6017	BCR	C8-C9	-7.99	1.28	1.45
19	F	6016	BCR	C8-C9	-7.99	1.28	1.45
19	I	6018	BCR	C8-C9	-7.99	1.28	1.45
19	B	6004	BCR	C10-C9	-7.99	1.25	1.35
19	L	6019	BCR	C8-C9	-7.98	1.28	1.45
19	I	6020	BCR	C8-C9	-7.98	1.28	1.45
19	B	6005	BCR	C11-C10	-7.97	1.19	1.43
19	A	6002	BCR	C8-C9	-7.94	1.28	1.45
19	B	6009	BCR	C8-C9	-7.91	1.28	1.45
19	J	6012	BCR	C11-C10	-7.90	1.19	1.43
19	B	6004	BCR	C8-C9	-7.87	1.28	1.45
19	F	6014	BCR	C8-C9	-7.87	1.28	1.45
19	L	6020	BCR	C8-C9	-7.84	1.28	1.45
19	B	6010	BCR	C11-C10	-7.84	1.19	1.43
19	A	6008	BCR	C8-C9	-7.83	1.28	1.45
19	B	6006	BCR	C8-C9	-7.83	1.28	1.45
19	B	6009	BCR	C11-C10	-7.81	1.19	1.43
19	A	6007	BCR	C8-C9	-7.80	1.28	1.45
19	B	6005	BCR	C8-C9	-7.80	1.28	1.45
19	J	6012	BCR	C8-C9	-7.79	1.28	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	6014	BCR	C11-C10	-7.78	1.19	1.43
19	A	6017	BCR	C11-C10	-7.77	1.19	1.43
19	J	6013	BCR	C8-C9	-7.76	1.28	1.45
19	B	6011	BCR	C10-C9	-7.75	1.25	1.35
19	G	2011	BCR	C16-C17	-7.73	1.19	1.43
19	A	6008	BCR	C11-C10	-7.73	1.19	1.43
19	B	6010	BCR	C8-C9	-7.72	1.28	1.45
19	I	6018	BCR	C11-C10	-7.71	1.19	1.43
19	L	6019	BCR	C10-C9	-7.71	1.25	1.35
19	G	2011	BCR	C20-C21	-7.66	1.20	1.43
19	G	2011	BCR	C10-C9	-7.63	1.25	1.35
19	F	6016	BCR	C10-C9	-7.61	1.25	1.35
19	A	6003	BCR	C20-C21	-7.58	1.20	1.43
19	A	6003	BCR	C16-C17	-7.55	1.20	1.43
19	A	6003	BCR	C10-C9	-7.55	1.25	1.35
19	L	6020	BCR	C10-C9	-7.54	1.25	1.35
19	B	6004	BCR	C20-C21	-7.53	1.20	1.43
19	J	6013	BCR	C20-C21	-7.52	1.20	1.43
19	I	6020	BCR	C20-C21	-7.50	1.20	1.43
19	L	6020	BCR	C20-C21	-7.50	1.20	1.43
19	A	6002	BCR	C20-C21	-7.49	1.20	1.43
19	J	6013	BCR	C16-C17	-7.46	1.20	1.43
19	B	6006	BCR	C20-C21	-7.46	1.20	1.43
19	B	6009	BCR	C20-C21	-7.45	1.20	1.43
19	L	6019	BCR	C20-C21	-7.44	1.20	1.43
19	A	6002	BCR	C10-C9	-7.43	1.25	1.35
19	B	6004	BCR	C16-C17	-7.41	1.20	1.43
19	I	6020	BCR	C10-C9	-7.41	1.26	1.35
19	I	6020	BCR	C16-C17	-7.41	1.20	1.43
19	F	6016	BCR	C20-C21	-7.40	1.20	1.43
19	F	6016	BCR	C16-C17	-7.40	1.20	1.43
19	B	6006	BCR	C16-C17	-7.39	1.20	1.43
19	A	6011	BCR	C20-C21	-7.39	1.20	1.43
19	A	6007	BCR	C20-C21	-7.37	1.20	1.43
19	F	6014	BCR	C16-C17	-7.36	1.20	1.43
19	A	6002	BCR	C16-C17	-7.36	1.20	1.43
19	B	6011	BCR	C16-C17	-7.35	1.20	1.43
19	A	6008	BCR	C20-C21	-7.34	1.21	1.43
19	L	6020	BCR	C16-C17	-7.34	1.21	1.43
19	F	6014	BCR	C20-C21	-7.32	1.21	1.43
19	B	6010	BCR	C20-C21	-7.32	1.21	1.43
19	L	6019	BCR	C16-C17	-7.31	1.21	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	6017	BCR	C16-C17	-7.31	1.21	1.43
19	I	6018	BCR	C16-C17	-7.29	1.21	1.43
19	A	6008	BCR	C16-C17	-7.27	1.21	1.43
19	A	6007	BCR	C16-C17	-7.27	1.21	1.43
19	B	6005	BCR	C20-C21	-7.26	1.21	1.43
19	I	6018	BCR	C20-C21	-7.24	1.21	1.43
19	A	6011	BCR	C16-C17	-7.24	1.21	1.43
19	B	6005	BCR	C16-C17	-7.23	1.21	1.43
19	J	6012	BCR	C16-C17	-7.23	1.21	1.43
19	B	6006	BCR	C10-C9	-7.23	1.26	1.35
19	A	6011	BCR	C10-C9	-7.23	1.26	1.35
19	J	6012	BCR	C20-C21	-7.22	1.21	1.43
19	A	6017	BCR	C20-C21	-7.20	1.21	1.43
19	A	6007	BCR	C10-C9	-7.18	1.26	1.35
19	B	6009	BCR	C16-C17	-7.18	1.21	1.43
27	4	4503	NEX	C34-C33	-7.18	1.26	1.35
19	J	6013	BCR	C10-C9	-7.15	1.26	1.35
19	B	6010	BCR	C16-C17	-7.15	1.21	1.43
19	B	6010	BCR	C10-C9	-7.14	1.26	1.35
19	J	6012	BCR	C10-C9	-7.12	1.26	1.35
27	4	4503	NEX	C30-C29	-6.99	1.26	1.35
19	B	6005	BCR	C10-C9	-6.96	1.26	1.35
19	B	6009	BCR	C10-C9	-6.86	1.26	1.35
19	A	6017	BCR	C10-C9	-6.83	1.26	1.35
19	F	6014	BCR	C10-C9	-6.59	1.27	1.35
27	4	4503	NEX	C14-C13	-6.45	1.27	1.35
19	I	6018	BCR	C10-C9	-6.08	1.27	1.35
27	4	4503	NEX	C31-C32	-6.01	1.18	1.34
27	4	4503	NEX	C35-C15	-5.95	1.19	1.35
19	A	6008	BCR	C10-C9	-5.83	1.28	1.35
27	4	4503	NEX	C10-C9	-5.22	1.28	1.35
21	2	2004	CLA	CAD-CBD	-5.19	1.48	1.54
27	4	4503	NEX	C11-C12	-4.69	1.22	1.34
21	B	1226	CLA	C1C-NC	-4.62	1.30	1.37
27	4	4503	NEX	C28-C29	-4.61	1.35	1.45
21	A	9013	CLA	C1C-NC	-4.39	1.30	1.37
23	A	9011	CL0	C1C-NC	-4.27	1.30	1.37
21	4	4012	CLA	C1C-NC	-4.20	1.30	1.37
21	B	9022	CLA	C4C-NC	-4.18	1.31	1.37
23	A	9011	CL0	C4C-NC	-4.17	1.31	1.37
21	B	9010	CLA	C4C-NC	-4.14	1.31	1.37
21	4	4012	CLA	C4C-NC	-4.11	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	9010	CLA	C1C-NC	-3.92	1.31	1.37
21	B	1239	CLA	C1C-NC	-3.86	1.31	1.37
21	4	4011	CLA	C1C-NC	-3.86	1.31	1.37
21	B	1239	CLA	C4C-NC	-3.85	1.31	1.37
21	B	9023	CLA	C1C-NC	-3.84	1.31	1.37
21	4	4011	CLA	C4C-NC	-3.83	1.31	1.37
21	B	1228	CLA	C4C-NC	-3.83	1.31	1.37
21	2	2004	CLA	CAD-C3D	-3.81	1.46	1.51
21	B	1228	CLA	C1C-NC	-3.77	1.31	1.37
19	B	6011	BCR	C11-C12	-3.77	1.24	1.34
21	F	1303	CLA	C1C-NC	-3.76	1.31	1.37
21	4	4010	CLA	C4C-NC	-3.73	1.31	1.37
21	B	1226	CLA	C4C-NC	-3.72	1.31	1.37
21	B	1240	CLA	C1C-NC	-3.71	1.31	1.37
21	1	1009	CLA	C1C-NC	-3.70	1.31	1.37
21	1	1008	CLA	C1C-NC	-3.66	1.31	1.37
21	4	4006	CLA	C4C-NC	-3.63	1.31	1.37
21	4	4001	CLA	C1C-NC	-3.61	1.31	1.37
21	4	4010	CLA	C1C-NC	-3.61	1.31	1.37
21	1	1002	CLA	C4C-NC	-3.60	1.31	1.37
21	1	1001	CLA	C1C-NC	-3.60	1.31	1.37
21	4	4005	CLA	C1C-NC	-3.58	1.31	1.37
21	1	1009	CLA	C4C-NC	-3.52	1.32	1.37
21	A	9013	CLA	C4C-NC	-3.51	1.32	1.37
21	B	9022	CLA	C1C-NC	-3.49	1.31	1.37
21	1	1003	CLA	C1C-NC	-3.49	1.31	1.37
21	B	9023	CLA	C4C-NC	-3.47	1.32	1.37
21	A	9012	CLA	C4C-NC	-3.47	1.32	1.37
21	1	1002	CLA	C1C-NC	-3.46	1.31	1.37
21	2	2001	CLA	CAD-CBD	-3.42	1.49	1.54
21	4	4015	CLA	C1C-NC	-3.41	1.32	1.37
21	1	1008	CLA	C4C-NC	-3.41	1.32	1.37
21	4	4009	CLA	C4C-NC	-3.39	1.32	1.37
21	1	1004	CLA	C1C-NC	-3.36	1.32	1.37
21	4	4002	CLA	C4C-NC	-3.35	1.32	1.37
21	4	4002	CLA	C1C-NC	-3.33	1.32	1.37
19	A	6002	BCR	C11-C12	-3.32	1.25	1.34
21	4	4015	CLA	C4C-NC	-3.31	1.32	1.37
21	2	2013	CLA	C1C-NC	-3.30	1.32	1.37
19	G	2011	BCR	C11-C12	-3.29	1.25	1.34
19	F	6016	BCR	C11-C12	-3.28	1.25	1.34
26	2	2502	LUT	C1-C6	-3.27	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	6019	BCR	C11-C12	-3.27	1.25	1.34
21	1	1007	CLA	C4C-NC	-3.25	1.32	1.37
21	B	1213	CLA	C1C-NC	-3.25	1.32	1.37
21	1	1001	CLA	C4C-NC	-3.24	1.32	1.37
19	B	6004	BCR	C11-C12	-3.23	1.26	1.34
19	I	6020	BCR	C11-C12	-3.23	1.26	1.34
21	G	1001	CLA	C1C-NC	-3.23	1.32	1.37
21	B	1227	CLA	C4C-NC	-3.23	1.32	1.37
19	L	6020	BCR	C11-C12	-3.22	1.26	1.34
21	B	1240	CLA	C4C-NC	-3.22	1.32	1.37
19	J	6013	BCR	C11-C12	-3.22	1.26	1.34
19	B	6006	BCR	C11-C12	-3.20	1.26	1.34
21	1	1003	CLA	C4C-NC	-3.20	1.32	1.37
21	2	2012	CLA	C1C-NC	-3.20	1.32	1.37
21	4	4004	CLA	C1C-NC	-3.20	1.32	1.37
21	4	4001	CLA	C4C-NC	-3.20	1.32	1.37
21	G	1001	CLA	C4C-NC	-3.18	1.32	1.37
21	B	1227	CLA	C1C-NC	-3.18	1.32	1.37
21	2	2005	CLA	C1C-NC	-3.17	1.32	1.37
21	2	2011	CLA	C1C-NC	-3.16	1.32	1.37
21	1	1013	CLA	C1C-NC	-3.16	1.32	1.37
21	1	1010	CLA	C1C-NC	-3.15	1.32	1.37
21	1	1012	CLA	C1C-NC	-3.14	1.32	1.37
21	A	9012	CLA	C1C-NC	-3.14	1.32	1.37
21	2	2011	CLA	C4C-NC	-3.13	1.32	1.37
21	A	1125	CLA	C1C-NC	-3.13	1.32	1.37
21	2	2012	CLA	C4C-NC	-3.13	1.32	1.37
21	G	1002	CLA	C1C-NC	-3.12	1.32	1.37
21	4	4008	CLA	C1C-NC	-3.10	1.32	1.37
21	4	4003	CLA	C1C-NC	-3.10	1.32	1.37
19	A	6007	BCR	C11-C12	-3.10	1.26	1.34
21	4	4008	CLA	C4C-NC	-3.10	1.32	1.37
21	2	2005	CLA	C4C-NC	-3.10	1.32	1.37
21	4	4009	CLA	C1C-NC	-3.10	1.32	1.37
21	2	2009	CLA	C1C-NC	-3.10	1.32	1.37
19	A	6003	BCR	C11-C12	-3.08	1.26	1.34
21	1	1007	CLA	C1C-NC	-3.08	1.32	1.37
21	1	1011	CLA	C4C-NC	-3.08	1.32	1.37
21	2	2013	CLA	C4C-NC	-3.08	1.32	1.37
21	1	1012	CLA	C4C-NC	-3.07	1.32	1.37
21	1	1005	CLA	C1C-NC	-3.06	1.32	1.37
19	A	6011	BCR	C11-C12	-3.04	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	2004	CLA	C1C-NC	-3.02	1.32	1.37
21	A	1132	CLA	C1C-NC	-3.00	1.32	1.37
21	4	4004	CLA	C4C-NC	-2.99	1.32	1.37
21	1	1004	CLA	C4C-NC	-2.98	1.32	1.37
19	B	6010	BCR	C11-C12	-2.98	1.26	1.34
19	B	6005	BCR	C11-C12	-2.96	1.26	1.34
21	F	1303	CLA	C4C-NC	-2.95	1.33	1.37
19	J	6012	BCR	C11-C12	-2.95	1.26	1.34
21	3	3013	CLA	C1C-NC	-2.95	1.32	1.37
26	1	1502	LUT	C5-C6	-2.93	1.29	1.34
21	4	4013	CLA	C4C-NC	-2.90	1.33	1.37
21	4	4006	CLA	C1C-NC	-2.90	1.32	1.37
21	A	1125	CLA	C4C-NC	-2.88	1.33	1.37
21	B	1228	CLA	C2A-C1A	-2.88	1.46	1.52
21	1	1011	CLA	C1C-NC	-2.87	1.32	1.37
21	3	3011	CLA	C1C-NC	-2.86	1.32	1.37
21	3	3011	CLA	C4C-NC	-2.85	1.33	1.37
21	2	2001	CLA	C1C-NC	-2.84	1.32	1.37
19	F	6014	BCR	C11-C12	-2.83	1.27	1.34
19	B	6009	BCR	C11-C12	-2.82	1.27	1.34
21	2	2004	CLA	C4C-NC	-2.82	1.33	1.37
21	2	2011	CLA	C2A-C1A	-2.80	1.46	1.52
21	3	3012	CLA	C4C-NC	-2.80	1.33	1.37
21	3	3009	CLA	C4C-NC	-2.80	1.33	1.37
21	2	2007	CLA	C1C-NC	-2.80	1.33	1.37
21	1	1005	CLA	C4C-NC	-2.80	1.33	1.37
26	1	1502	LUT	C1-C6	-2.79	1.49	1.53
21	2	2010	CLA	C4C-NC	-2.79	1.33	1.37
21	3	3009	CLA	C1C-NC	-2.78	1.33	1.37
21	3	3013	CLA	C4C-NC	-2.77	1.33	1.37
21	2	2014	CLA	C4C-NC	-2.77	1.33	1.37
21	A	1131	CLA	C1C-NC	-2.75	1.33	1.37
21	2	2010	CLA	C1C-NC	-2.74	1.33	1.37
21	G	1002	CLA	C4C-NC	-2.73	1.33	1.37
21	2	2014	CLA	C1C-NC	-2.73	1.33	1.37
21	2	2008	CLA	C1C-NC	-2.72	1.33	1.37
19	A	6008	BCR	C11-C12	-2.71	1.27	1.34
21	2	2007	CLA	C4C-NC	-2.71	1.33	1.37
21	1	1006	CLA	C4C-NC	-2.70	1.33	1.37
21	1	1006	CLA	C1C-NC	-2.68	1.33	1.37
21	4	4013	CLA	C1C-NC	-2.67	1.33	1.37
21	2	2009	CLA	C4C-NC	-2.64	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1133	CLA	C4C-NC	-2.64	1.33	1.37
21	3	3008	CLA	C1C-NC	-2.64	1.33	1.37
19	A	6017	BCR	C11-C12	-2.64	1.27	1.34
21	2	2002	CLA	C1C-NC	-2.63	1.33	1.37
21	4	4002	CLA	C2A-C1A	-2.61	1.47	1.52
21	2	2003	CLA	C1C-NC	-2.61	1.33	1.37
21	B	1213	CLA	C4C-NC	-2.60	1.33	1.37
21	1	1004	CLA	C2A-C1A	-2.59	1.47	1.52
21	3	3010	CLA	C4C-NC	-2.59	1.33	1.37
21	1	1010	CLA	C4C-NC	-2.59	1.33	1.37
21	F	1303	CLA	O2A-CGA	-2.58	1.31	1.42
19	I	6018	BCR	C11-C12	-2.57	1.27	1.34
21	1	1013	CLA	C4C-NC	-2.56	1.33	1.37
21	A	1131	CLA	C4C-NC	-2.56	1.33	1.37
21	1	1014	CLA	C1C-NC	-2.55	1.33	1.37
21	A	1133	CLA	C1C-NC	-2.53	1.33	1.37
26	1	1501	LUT	C1-C6	-2.49	1.50	1.53
21	4	4011	CLA	C2A-C1A	-2.49	1.47	1.52
21	2	2004	CLA	CBD-CGD	-2.49	1.46	1.52
21	A	1132	CLA	C4C-NC	-2.46	1.33	1.37
21	B	1240	CLA	C2A-C1A	-2.45	1.47	1.52
21	1	1008	CLA	C2A-C1A	-2.45	1.47	1.52
21	3	3008	CLA	C4C-NC	-2.45	1.33	1.37
24	B	7101	DGD	O2G-C2G	-2.44	1.40	1.46
21	4	4005	CLA	C4C-NC	-2.38	1.33	1.37
21	A	1109	CLA	C1C-NC	-2.35	1.33	1.37
21	4	4012	CLA	C2A-C1A	-2.35	1.47	1.52
21	4	4005	CLA	C2A-C1A	-2.35	1.47	1.52
21	2	2006	CLA	C4C-NC	-2.34	1.34	1.37
21	B	1210	CLA	C1C-NC	-2.34	1.33	1.37
21	3	3010	CLA	C1C-NC	-2.32	1.33	1.37
21	4	4004	CLA	C2A-C1A	-2.31	1.47	1.52
21	B	9022	CLA	O2D-CED	-2.30	1.39	1.45
21	4	4007	CLA	C1C-NC	-2.30	1.33	1.37
27	4	4503	NEX	O24-C25	-2.29	1.42	1.46
21	2	2001	CLA	CAD-C3D	-2.29	1.47	1.51
21	B	9023	CLA	C2A-C1A	-2.28	1.47	1.52
21	A	1110	CLA	C1C-NC	-2.27	1.33	1.37
21	F	1301	CLA	C1C-NC	-2.27	1.33	1.37
21	4	4003	CLA	C4C-NC	-2.26	1.34	1.37
21	2	2001	CLA	C4C-NC	-2.26	1.33	1.37
21	A	9012	CLA	C2A-C1A	-2.26	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1009	CLA	C2A-C1A	-2.25	1.47	1.52
21	G	1002	CLA	C2A-C1A	-2.24	1.47	1.52
21	J	6015	CLA	C1C-NC	-2.24	1.34	1.37
21	4	4007	CLA	C4C-NC	-2.24	1.34	1.37
21	G	1001	CLA	C2A-C1A	-2.24	1.47	1.52
21	A	1139	CLA	C1C-NC	-2.23	1.34	1.37
21	2	2008	CLA	C4C-NC	-2.23	1.34	1.37
21	J	6015	CLA	C4C-NC	-2.22	1.34	1.37
21	B	1219	CLA	C1C-NC	-2.21	1.34	1.37
21	B	1223	CLA	C1C-NC	-2.20	1.34	1.37
21	B	1217	CLA	C1C-NC	-2.20	1.34	1.37
21	A	1118	CLA	C1C-NC	-2.20	1.34	1.37
21	1	1007	CLA	C2A-C1A	-2.19	1.47	1.52
21	A	1137	CLA	C1C-NC	-2.18	1.34	1.37
21	3	3014	CLA	C1C-NC	-2.18	1.34	1.37
21	B	1225	CLA	C1C-NC	-2.18	1.34	1.37
21	B	1231	CLA	C1C-NC	-2.18	1.34	1.37
21	4	4014	CLA	C4C-NC	-2.17	1.34	1.37
21	L	1502	CLA	C1C-NC	-2.17	1.34	1.37
21	3	3003	CLA	C1C-NC	-2.17	1.34	1.37
21	B	1207	CLA	C1C-NC	-2.17	1.34	1.37
21	A	1129	CLA	C1C-NC	-2.17	1.34	1.37
21	A	1140	CLA	C1C-NC	-2.17	1.34	1.37
21	B	1230	CLA	C1C-NC	-2.17	1.34	1.37
21	B	9010	CLA	C3A-C4A	-2.17	1.44	1.51
21	B	1222	CLA	C1C-NC	-2.16	1.34	1.37
21	A	1111	CLA	C1C-NC	-2.16	1.34	1.37
21	B	1205	CLA	C1C-NC	-2.16	1.34	1.37
21	B	1209	CLA	C1C-NC	-2.16	1.34	1.37
21	A	1130	CLA	C1C-NC	-2.16	1.34	1.37
21	H	1000	CLA	C1C-NC	-2.16	1.34	1.37
21	A	1104	CLA	C1C-NC	-2.15	1.34	1.37
21	A	1113	CLA	C1C-NC	-2.15	1.34	1.37
21	B	1218	CLA	C1C-NC	-2.14	1.34	1.37
21	A	1141	CLA	C1C-NC	-2.14	1.34	1.37
19	B	6004	BCR	C30-C25	-2.14	1.50	1.53
21	B	1204	CLA	C1C-NC	-2.14	1.34	1.37
21	A	1101	CLA	C1C-NC	-2.13	1.34	1.37
21	B	1238	CLA	C1C-NC	-2.13	1.34	1.37
20	2	2801	LHG	O7-C5	-2.13	1.41	1.46
21	2	2012	CLA	C2A-C1A	-2.12	1.48	1.52
21	4	4003	CLA	C2A-C1A	-2.11	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1117	CLA	C1C-NC	-2.11	1.34	1.37
21	B	9022	CLA	C2A-C1A	-2.11	1.48	1.52
21	A	1106	CLA	C1C-NC	-2.11	1.34	1.37
21	A	1128	CLA	C1C-NC	-2.11	1.34	1.37
21	L	1503	CLA	C1C-NC	-2.11	1.34	1.37
21	B	1212	CLA	C1C-NC	-2.10	1.34	1.37
21	B	1211	CLA	C1C-NC	-2.10	1.34	1.37
21	B	1229	CLA	C1C-NC	-2.10	1.34	1.37
21	B	1206	CLA	C1C-NC	-2.10	1.34	1.37
21	B	1214	CLA	C1C-NC	-2.10	1.34	1.37
21	A	1124	CLA	C1C-NC	-2.09	1.34	1.37
21	A	1121	CLA	C1C-NC	-2.09	1.34	1.37
21	A	1135	CLA	C1C-NC	-2.09	1.34	1.37
21	2	2002	CLA	C4C-NC	-2.09	1.34	1.37
21	F	1302	CLA	C1C-NC	-2.08	1.34	1.37
21	B	1234	CLA	C1C-NC	-2.08	1.34	1.37
21	B	1235	CLA	C1C-NC	-2.08	1.34	1.37
21	A	1127	CLA	C1C-NC	-2.08	1.34	1.37
21	B	1237	CLA	C1C-NC	-2.08	1.34	1.37
21	B	1236	CLA	C1C-NC	-2.08	1.34	1.37
21	A	1136	CLA	C1C-NC	-2.07	1.34	1.37
21	B	1221	CLA	C1C-NC	-2.07	1.34	1.37
21	A	1126	CLA	C1C-NC	-2.07	1.34	1.37
21	A	1134	CLA	C1C-NC	-2.07	1.34	1.37
21	B	1216	CLA	C1C-NC	-2.07	1.34	1.37
23	A	9011	CL0	C3A-C4A	-2.07	1.45	1.51
21	3	3017	CLA	C1C-NC	-2.06	1.34	1.37
26	4	4502	LUT	C1-C6	-2.06	1.50	1.53
21	A	1105	CLA	C1C-NC	-2.06	1.34	1.37
21	A	1116	CLA	C1C-NC	-2.06	1.34	1.37
21	L	1501	CLA	C1C-NC	-2.06	1.34	1.37
21	B	1203	CLA	C1C-NC	-2.06	1.34	1.37
21	A	1103	CLA	C1C-NC	-2.05	1.34	1.37
21	1	1002	CLA	C2A-C1A	-2.05	1.48	1.52
21	A	1112	CLA	C1C-NC	-2.05	1.34	1.37
21	A	1138	CLA	C1C-NC	-2.05	1.34	1.37
21	1	1011	CLA	C2A-C1A	-2.05	1.48	1.52
21	A	1114	CLA	C1C-NC	-2.05	1.34	1.37
21	B	1215	CLA	C1C-NC	-2.04	1.34	1.37
21	3	3016	CLA	C1C-NC	-2.04	1.34	1.37
21	A	1107	CLA	C1C-NC	-2.04	1.34	1.37
21	B	1224	CLA	C1C-NC	-2.04	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1123	CLA	C1C-NC	-2.04	1.34	1.37
21	3	3006	CLA	C1C-NC	-2.04	1.34	1.37
21	A	1108	CLA	C1C-NC	-2.04	1.34	1.37
26	2	2501	LUT	C1-C6	-2.04	1.50	1.53
21	A	1115	CLA	C1C-NC	-2.04	1.34	1.37
21	B	1226	CLA	O2D-CED	-2.03	1.40	1.45
21	3	3015	CLA	C1C-NC	-2.03	1.34	1.37
20	B	7004	LHG	P-O4	-2.03	1.46	1.54
21	2	2006	CLA	C1C-NC	-2.03	1.34	1.37
21	A	1122	CLA	C1C-NC	-2.03	1.34	1.37
21	B	1202	CLA	C1C-NC	-2.03	1.34	1.37
21	A	1142	CLA	C1C-NC	-2.03	1.34	1.37
21	A	1143	CLA	C1C-NC	-2.03	1.34	1.37
21	3	3012	CLA	C1C-NC	-2.02	1.34	1.37
21	B	1208	CLA	C1C-NC	-2.02	1.34	1.37
26	4	4502	LUT	C22-C21	-2.02	1.52	1.54
21	B	1227	CLA	C2A-C1A	-2.01	1.48	1.52
21	A	1120	CLA	C1C-NC	-2.00	1.34	1.37
21	3	3004	CLA	C1C-NC	-2.00	1.34	1.37
21	L	1502	CLA	C4C-C3C	2.00	1.48	1.45
21	B	1209	CLA	C1C-C2C	2.01	1.48	1.44
26	4	4502	LUT	C28-C29	2.01	1.50	1.45
21	A	1126	CLA	C1C-C2C	2.01	1.48	1.44
21	1	1008	CLA	CHD-C4C	2.01	1.45	1.41
21	B	1229	CLA	C1C-C2C	2.02	1.48	1.44
26	1	1502	LUT	C28-C29	2.02	1.50	1.45
21	3	3003	CLA	C1C-C2C	2.02	1.48	1.44
21	1	1011	CLA	C3D-C2D	2.02	1.45	1.40
21	A	1123	CLA	C1C-C2C	2.02	1.48	1.44
21	A	1112	CLA	C1C-C2C	2.02	1.48	1.44
21	4	4006	CLA	CHD-C4C	2.02	1.45	1.41
21	4	4012	CLA	C1B-CHB	2.03	1.45	1.39
21	J	6014	CLA	C1C-C2C	2.03	1.48	1.44
21	A	1141	CLA	C1C-C2C	2.03	1.48	1.44
21	4	4014	CLA	C4C-C3C	2.04	1.48	1.45
23	A	9011	CL0	C1B-CHB	2.04	1.45	1.39
21	B	1223	CLA	C4C-C3C	2.04	1.48	1.45
21	A	1116	CLA	C1C-C2C	2.04	1.48	1.44
21	4	4002	CLA	C3D-C2D	2.04	1.45	1.40
21	4	4002	CLA	C4B-CHC	2.04	1.45	1.39
21	B	1228	CLA	CHD-C4C	2.04	1.45	1.41
21	B	1228	CLA	C1B-CHB	2.04	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1102	CLA	C4C-C3C	2.04	1.48	1.45
21	B	1201	CLA	C4C-C3C	2.04	1.48	1.45
21	G	1001	CLA	C3D-C2D	2.05	1.45	1.40
21	2	2001	CLA	C3C-C4C	2.05	1.48	1.43
21	4	4009	CLA	CHD-C4C	2.05	1.46	1.41
21	B	1208	CLA	C4C-C3C	2.06	1.48	1.45
21	A	1102	CLA	C1C-C2C	2.06	1.48	1.44
21	B	1208	CLA	C1C-C2C	2.06	1.48	1.44
21	A	1116	CLA	C4C-C3C	2.06	1.48	1.45
21	1	1010	CLA	CHD-C4C	2.07	1.46	1.41
21	B	1215	CLA	C4C-C3C	2.07	1.48	1.45
21	1	1001	CLA	C3D-C2D	2.07	1.45	1.40
21	4	4006	CLA	C3D-C2D	2.08	1.45	1.40
21	L	1503	CLA	C4C-C3C	2.08	1.48	1.45
21	B	1230	CLA	C4C-C3C	2.08	1.48	1.45
21	B	1229	CLA	C4C-C3C	2.08	1.48	1.45
21	B	1219	CLA	C4C-C3C	2.08	1.48	1.45
21	B	1238	CLA	C4C-C3C	2.08	1.48	1.45
21	A	1137	CLA	C4C-C3C	2.09	1.48	1.45
21	4	4013	CLA	CHD-C4C	2.09	1.46	1.41
21	1	1009	CLA	CHD-C4C	2.10	1.46	1.41
21	B	1221	CLA	C4C-C3C	2.10	1.48	1.45
21	A	1112	CLA	C4C-C3C	2.10	1.48	1.45
21	J	6014	CLA	C4C-C3C	2.10	1.48	1.45
21	2	2013	CLA	CHD-C4C	2.10	1.46	1.41
21	A	1115	CLA	C1C-C2C	2.11	1.48	1.44
21	A	1136	CLA	C4C-C3C	2.11	1.48	1.45
21	4	4011	CLA	C3D-C2D	2.11	1.45	1.40
21	4	4008	CLA	CHD-C4C	2.11	1.46	1.41
21	A	1115	CLA	C4C-C3C	2.12	1.48	1.45
21	B	1202	CLA	C4C-C3C	2.12	1.48	1.45
23	A	9011	CL0	OBD-CAD	2.12	1.25	1.22
21	B	1239	CLA	C4B-CHC	2.12	1.45	1.39
21	3	3001	CLA	C4C-C3C	2.12	1.48	1.45
21	A	1105	CLA	C4C-C3C	2.12	1.48	1.45
21	3	3001	CLA	C1C-C2C	2.13	1.48	1.44
21	G	1002	CLA	CHD-C4C	2.13	1.46	1.41
21	B	1204	CLA	C4C-C3C	2.13	1.48	1.45
21	1	1012	CLA	C3D-C2D	2.13	1.45	1.40
21	A	1108	CLA	C4C-C3C	2.13	1.48	1.45
21	B	1237	CLA	C4C-C3C	2.13	1.48	1.45
21	F	1303	CLA	C3D-C2D	2.14	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1140	CLA	C4C-C3C	2.14	1.48	1.45
21	1	1007	CLA	CHD-C4C	2.15	1.46	1.41
21	B	1222	CLA	C4C-C3C	2.15	1.48	1.45
21	A	1117	CLA	C4C-C3C	2.15	1.48	1.45
21	G	1001	CLA	CHD-C4C	2.15	1.46	1.41
21	B	1209	CLA	C4C-C3C	2.15	1.48	1.45
21	B	1216	CLA	C4C-C3C	2.16	1.48	1.45
21	B	1211	CLA	C4C-C3C	2.16	1.48	1.45
21	F	1303	CLA	CHD-C4C	2.16	1.46	1.41
21	A	1124	CLA	C4C-C3C	2.17	1.48	1.45
21	B	9023	CLA	C3D-C2D	2.17	1.45	1.40
21	A	1106	CLA	C1C-C2C	2.17	1.48	1.44
21	A	1138	CLA	C4C-C3C	2.17	1.48	1.45
21	3	3009	CLA	CHD-C4C	2.17	1.46	1.41
21	A	1103	CLA	C4C-C3C	2.17	1.48	1.45
21	3	3002	CLA	C4C-C3C	2.18	1.49	1.45
21	B	1240	CLA	CHD-C4C	2.18	1.46	1.41
21	A	1126	CLA	C4C-C3C	2.18	1.49	1.45
21	A	1135	CLA	C4C-C3C	2.18	1.49	1.45
21	3	3005	CLA	C4C-C3C	2.18	1.49	1.45
21	1	1002	CLA	CHD-C4C	2.18	1.46	1.41
21	B	1225	CLA	C4C-C3C	2.18	1.49	1.45
21	A	1143	CLA	C4C-C3C	2.19	1.49	1.45
21	B	1217	CLA	C4C-C3C	2.19	1.49	1.45
21	A	1125	CLA	C3D-C2D	2.19	1.45	1.40
21	B	1220	CLA	C4C-C3C	2.19	1.49	1.45
21	1	1014	CLA	C4C-C3C	2.20	1.49	1.45
21	1	1013	CLA	CHD-C4C	2.20	1.46	1.41
21	F	1301	CLA	C4C-C3C	2.20	1.49	1.45
21	B	1227	CLA	CHD-C4C	2.20	1.46	1.41
21	1	1005	CLA	C3D-C2D	2.20	1.45	1.40
21	A	1101	CLA	C4C-C3C	2.20	1.49	1.45
21	B	1205	CLA	C4C-C3C	2.22	1.49	1.45
21	2	2002	CLA	C1B-CHB	2.22	1.46	1.39
21	B	9022	CLA	C4B-CHC	2.22	1.46	1.39
21	B	1231	CLA	C4C-C3C	2.22	1.49	1.45
21	A	1123	CLA	C4C-C3C	2.22	1.49	1.45
21	4	4005	CLA	C4B-CHC	2.22	1.46	1.39
21	A	1111	CLA	C4C-C3C	2.22	1.49	1.45
21	1	1010	CLA	C3D-C2D	2.23	1.45	1.40
21	B	1212	CLA	C4C-C3C	2.23	1.49	1.45
21	1	1001	CLA	CHD-C4C	2.23	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1110	CLA	C4C-C3C	2.23	1.49	1.45
21	A	1120	CLA	C4C-C3C	2.23	1.49	1.45
21	2	2010	CLA	C3D-C2D	2.23	1.45	1.40
21	B	1227	CLA	C4B-CHC	2.24	1.46	1.39
21	B	1207	CLA	C4C-C3C	2.24	1.49	1.45
21	2	2014	CLA	C1B-CHB	2.24	1.46	1.39
21	3	3015	CLA	C4C-C3C	2.24	1.49	1.45
21	A	1118	CLA	C4C-C3C	2.24	1.49	1.45
21	A	1113	CLA	C4C-C3C	2.25	1.49	1.45
21	3	3013	CLA	C4C-C3C	2.25	1.49	1.45
21	1	1011	CLA	C4B-CHC	2.25	1.46	1.39
21	A	9013	CLA	C4B-CHC	2.25	1.46	1.39
21	B	1210	CLA	C4C-C3C	2.26	1.49	1.45
21	A	1114	CLA	C4C-C3C	2.26	1.49	1.45
21	A	1134	CLA	C4C-C3C	2.26	1.49	1.45
21	3	3004	CLA	C4C-C3C	2.26	1.49	1.45
21	1	1003	CLA	C1B-CHB	2.27	1.46	1.39
21	B	1234	CLA	C4C-C3C	2.27	1.49	1.45
21	B	9010	CLA	C4B-CHC	2.27	1.46	1.39
25	G	2021	LMG	O8-C28	2.27	1.45	1.33
21	A	1139	CLA	C4C-C3C	2.27	1.49	1.45
21	3	3017	CLA	C4C-C3C	2.27	1.49	1.45
21	4	4003	CLA	CHD-C4C	2.28	1.46	1.41
21	A	1142	CLA	C4C-C3C	2.28	1.49	1.45
21	4	4011	CLA	C4B-CHC	2.28	1.46	1.39
21	3	3006	CLA	C4C-C3C	2.28	1.49	1.45
21	A	1122	CLA	C4C-C3C	2.29	1.49	1.45
21	A	1109	CLA	C4C-C3C	2.29	1.49	1.45
21	B	9022	CLA	C1B-CHB	2.29	1.46	1.39
21	A	9012	CLA	C3D-C2D	2.30	1.45	1.40
21	4	4002	CLA	CHD-C4C	2.31	1.46	1.41
21	3	3016	CLA	C4C-C3C	2.31	1.49	1.45
21	1	1012	CLA	CHD-C4C	2.31	1.46	1.41
21	1	1005	CLA	CHD-C4C	2.32	1.46	1.41
21	4	4011	CLA	C3B-C2B	2.32	1.43	1.40
21	A	1119	CLA	C4C-C3C	2.32	1.49	1.45
21	4	4012	CLA	C3D-C2D	2.32	1.45	1.40
21	B	1239	CLA	C3B-C2B	2.32	1.43	1.40
21	G	1002	CLA	C3D-C2D	2.32	1.45	1.40
21	4	4008	CLA	C4B-CHC	2.33	1.46	1.39
21	2	2011	CLA	C4B-CHC	2.33	1.46	1.39
21	4	4010	CLA	C4B-CHC	2.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	9010	CLA	C1B-CHB	2.33	1.46	1.39
21	B	1224	CLA	C4C-C3C	2.33	1.49	1.45
21	F	1302	CLA	C4C-C3C	2.33	1.49	1.45
21	B	1239	CLA	OBD-CAD	2.34	1.25	1.22
21	A	1127	CLA	C4C-C3C	2.34	1.49	1.45
21	1	1001	CLA	C4B-CHC	2.34	1.46	1.39
21	2	2008	CLA	C3D-C2D	2.35	1.45	1.40
21	2	2001	CLA	C2C-C1C	2.35	1.48	1.43
21	B	1227	CLA	C3D-C2D	2.35	1.45	1.40
27	4	4503	NEX	C11-C10	2.35	1.51	1.43
21	B	9023	CLA	C4B-CHC	2.36	1.46	1.39
21	4	4011	CLA	CHD-C4C	2.36	1.46	1.41
21	2	2008	CLA	CHD-C4C	2.36	1.46	1.41
21	2	2014	CLA	C4B-CHC	2.36	1.46	1.39
21	2	2011	CLA	CHD-C4C	2.37	1.46	1.41
21	A	9013	CLA	C1B-CHB	2.37	1.46	1.39
21	2	2007	CLA	CHD-C4C	2.37	1.46	1.41
21	4	4006	CLA	C1B-CHB	2.37	1.46	1.39
21	A	1141	CLA	C4C-C3C	2.38	1.49	1.45
21	J	1302	CLA	C4C-C3C	2.38	1.49	1.45
21	B	1240	CLA	C3D-C2D	2.39	1.45	1.40
21	2	2012	CLA	C1B-CHB	2.39	1.46	1.39
21	B	1206	CLA	C4C-C3C	2.39	1.49	1.45
21	1	1013	CLA	C3D-C2D	2.39	1.45	1.40
21	1	1004	CLA	C3D-C2D	2.39	1.45	1.40
21	H	1000	CLA	C4C-C3C	2.40	1.49	1.45
21	2	2014	CLA	C4C-C3C	2.41	1.49	1.45
21	1	1011	CLA	CHD-C4C	2.41	1.46	1.41
21	3	3009	CLA	C3D-C2D	2.41	1.45	1.40
21	G	1002	CLA	C4B-CHC	2.41	1.46	1.39
21	A	9013	CLA	OBD-CAD	2.42	1.26	1.22
21	2	2003	CLA	C3D-C2D	2.42	1.45	1.40
21	1	1008	CLA	OBD-CAD	2.42	1.26	1.22
21	F	1303	CLA	C4B-CHC	2.42	1.46	1.39
21	B	1240	CLA	C4B-CHC	2.42	1.46	1.39
21	B	1226	CLA	C3D-C2D	2.43	1.46	1.40
21	3	3017	CLA	C3D-C2D	2.43	1.46	1.40
23	A	9011	CL0	C3B-C2B	2.44	1.43	1.40
21	4	4013	CLA	C3B-C2B	2.44	1.43	1.40
21	4	4004	CLA	CHD-C4C	2.44	1.46	1.41
21	2	2001	CLA	CHD-C4C	2.44	1.46	1.41
21	4	4005	CLA	C3D-C2D	2.44	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	2003	CLA	C4B-CHC	2.45	1.46	1.39
21	4	4013	CLA	C3D-C2D	2.45	1.46	1.40
21	4	4005	CLA	C1B-CHB	2.45	1.46	1.39
21	B	9023	CLA	C1B-CHB	2.46	1.46	1.39
21	2	2013	CLA	C4B-CHC	2.46	1.46	1.39
21	4	4001	CLA	C1B-CHB	2.46	1.46	1.39
23	A	9011	CL0	C4B-CHC	2.46	1.46	1.39
21	2	2012	CLA	C4B-CHC	2.46	1.46	1.39
21	1	1005	CLA	C4B-CHC	2.46	1.46	1.39
21	1	1006	CLA	C4B-CHC	2.47	1.46	1.39
21	2	2009	CLA	CHD-C4C	2.47	1.47	1.41
21	4	4005	CLA	CHD-C4C	2.47	1.47	1.41
21	1	1008	CLA	C1B-CHB	2.47	1.46	1.39
21	1	1008	CLA	C3D-C2D	2.47	1.46	1.40
21	3	3008	CLA	C4B-CHC	2.48	1.46	1.39
21	2	2012	CLA	C3D-C2D	2.48	1.46	1.40
21	2	2013	CLA	C3D-C2D	2.48	1.46	1.40
21	2	2002	CLA	C3D-C2D	2.48	1.46	1.40
21	2	2012	CLA	CHD-C4C	2.48	1.47	1.41
21	1	1009	CLA	C1B-CHB	2.49	1.46	1.39
21	2	2009	CLA	C1B-CHB	2.49	1.46	1.39
21	4	4004	CLA	C3D-C2D	2.49	1.46	1.40
21	3	3012	CLA	C3D-C2D	2.49	1.46	1.40
21	4	4015	CLA	C1B-CHB	2.49	1.46	1.39
21	2	2005	CLA	C4B-CHC	2.50	1.46	1.39
21	3	3013	CLA	C4B-CHC	2.50	1.46	1.39
21	3	3011	CLA	C3D-C2D	2.50	1.46	1.40
21	3	3012	CLA	C4B-CHC	2.50	1.46	1.39
21	2	2007	CLA	C4B-CHC	2.50	1.46	1.39
21	1	1013	CLA	C1B-CHB	2.50	1.46	1.39
21	A	1107	CLA	C3D-C2D	2.51	1.46	1.40
21	2	2009	CLA	C4B-CHC	2.51	1.46	1.39
23	A	9011	CL0	C3C-C2C	2.51	1.42	1.36
21	A	1125	CLA	OBD-CAD	2.51	1.26	1.22
21	J	6015	CLA	C4B-CHC	2.51	1.46	1.39
21	4	4013	CLA	C4B-CHC	2.52	1.46	1.39
21	2	2004	CLA	CHD-C4C	2.52	1.47	1.41
21	2	2005	CLA	OBD-CAD	2.52	1.26	1.22
21	2	2011	CLA	C1B-CHB	2.52	1.46	1.39
21	4	4012	CLA	OBD-CAD	2.53	1.26	1.22
21	2	2010	CLA	CHD-C4C	2.53	1.47	1.41
21	3	3010	CLA	CHD-C4C	2.53	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1213	CLA	CHD-C4C	2.53	1.47	1.41
21	A	1125	CLA	C4B-CHC	2.54	1.46	1.39
21	B	1213	CLA	C1B-CHB	2.54	1.46	1.39
21	2	2002	CLA	C4B-CHC	2.54	1.46	1.39
26	2	2501	LUT	C23-C24	2.54	1.52	1.50
21	4	4012	CLA	C4B-CHC	2.56	1.46	1.39
21	2	2002	CLA	C4C-C3C	2.56	1.49	1.45
21	G	1001	CLA	C4B-CHC	2.56	1.46	1.39
21	A	1132	CLA	C1B-CHB	2.56	1.46	1.39
21	3	3008	CLA	C3D-C2D	2.57	1.46	1.40
21	B	9022	CLA	OBD-CAD	2.57	1.26	1.22
21	2	2011	CLA	C3D-C2D	2.57	1.46	1.40
21	B	9010	CLA	C3D-C2D	2.57	1.46	1.40
21	4	4008	CLA	C1B-CHB	2.57	1.46	1.39
21	1	1004	CLA	OBD-CAD	2.57	1.26	1.22
21	4	4007	CLA	C3B-C2B	2.57	1.43	1.40
21	4	4004	CLA	C4B-CHC	2.58	1.46	1.39
21	3	3011	CLA	CHD-C4C	2.58	1.47	1.41
21	A	1131	CLA	C4B-CHC	2.59	1.47	1.39
21	F	1303	CLA	OBD-CAD	2.60	1.26	1.22
21	3	3011	CLA	C1B-CHB	2.60	1.47	1.39
21	1	1004	CLA	C3B-C2B	2.61	1.43	1.40
21	1	1004	CLA	C1B-CHB	2.62	1.47	1.39
21	1	1003	CLA	C4B-CHC	2.62	1.47	1.39
21	A	1133	CLA	CHD-C4C	2.62	1.47	1.41
21	4	4011	CLA	C1B-CHB	2.62	1.47	1.39
21	2	2007	CLA	C3D-C2D	2.63	1.46	1.40
21	4	4007	CLA	C1B-CHB	2.63	1.47	1.39
21	2	2004	CLA	C4B-CHC	2.64	1.47	1.39
21	J	6015	CLA	C3D-C2D	2.65	1.46	1.40
21	B	1227	CLA	C1B-CHB	2.66	1.47	1.39
21	2	2009	CLA	C3D-C2D	2.66	1.46	1.40
21	4	4014	CLA	C3D-C2D	2.66	1.46	1.40
21	3	3012	CLA	C1B-CHB	2.66	1.47	1.39
21	1	1004	CLA	CHD-C4C	2.67	1.47	1.41
21	1	1004	CLA	C4B-CHC	2.67	1.47	1.39
21	1	1003	CLA	C3D-C2D	2.67	1.46	1.40
21	B	1213	CLA	C3D-C2D	2.67	1.46	1.40
21	2	2006	CLA	C4B-CHC	2.67	1.47	1.39
21	1	1008	CLA	C4B-CHC	2.67	1.47	1.39
21	A	1132	CLA	CHD-C4C	2.67	1.47	1.41
21	4	4009	CLA	C4B-CHC	2.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1226	CLA	C1B-CHB	2.68	1.47	1.39
21	1	1014	CLA	C4B-CHC	2.68	1.47	1.39
21	1	1002	CLA	C4B-CHC	2.69	1.47	1.39
21	4	4009	CLA	C1B-CHB	2.69	1.47	1.39
21	3	3009	CLA	C4B-CHC	2.70	1.47	1.39
21	3	3008	CLA	CHD-C4C	2.70	1.47	1.41
21	A	1125	CLA	C1B-CHB	2.71	1.47	1.39
21	4	4006	CLA	C4B-CHC	2.71	1.47	1.39
21	J	6015	CLA	C4C-C3C	2.71	1.49	1.45
21	4	4010	CLA	C1B-CHB	2.71	1.47	1.39
21	A	1131	CLA	CHD-C4C	2.71	1.47	1.41
21	B	1226	CLA	O2D-CGD	2.72	1.40	1.33
27	4	4503	NEX	C12-C13	2.72	1.51	1.45
21	3	3001	CLA	C3D-C2D	2.72	1.46	1.40
21	B	9010	CLA	OBD-CAD	2.72	1.26	1.22
21	2	2010	CLA	C1B-CHB	2.72	1.47	1.39
21	B	1222	CLA	C1B-CHB	2.73	1.47	1.39
21	4	4003	CLA	C3D-C2D	2.73	1.46	1.40
21	1	1006	CLA	CHD-C4C	2.73	1.47	1.41
21	3	3003	CLA	CHD-C4C	2.73	1.47	1.41
21	4	4015	CLA	OBD-CAD	2.74	1.26	1.22
21	4	4011	CLA	C3C-C2C	2.74	1.42	1.36
21	A	1133	CLA	C1B-CHB	2.74	1.47	1.39
21	3	3001	CLA	CHD-C4C	2.74	1.47	1.41
21	B	1223	CLA	C3D-C2D	2.74	1.46	1.40
21	B	1228	CLA	C4B-CHC	2.74	1.47	1.39
21	4	4003	CLA	C4B-CHC	2.75	1.47	1.39
21	2	2010	CLA	OBD-CAD	2.75	1.26	1.22
21	B	1206	CLA	C4B-CHC	2.75	1.47	1.39
26	4	4502	LUT	C23-C24	2.76	1.52	1.50
21	4	4001	CLA	CHD-C4C	2.76	1.47	1.41
21	F	1303	CLA	C1B-CHB	2.76	1.47	1.39
21	A	9012	CLA	C4B-CHC	2.76	1.47	1.39
21	A	1118	CLA	C4B-CHC	2.76	1.47	1.39
21	1	1007	CLA	OBD-CAD	2.76	1.26	1.22
21	B	1239	CLA	C1B-CHB	2.76	1.47	1.39
21	A	9013	CLA	C3D-C2D	2.77	1.46	1.40
21	A	1132	CLA	C3D-C2D	2.77	1.46	1.40
21	2	2006	CLA	CHD-C4C	2.77	1.47	1.41
21	4	4001	CLA	C4B-CHC	2.77	1.47	1.39
21	1	1012	CLA	C4B-CHC	2.77	1.47	1.39
21	3	3004	CLA	C3D-C2D	2.78	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	2013	CLA	C1B-CHB	2.78	1.47	1.39
21	B	1221	CLA	CHD-C4C	2.78	1.47	1.41
21	1	1003	CLA	CHD-C4C	2.78	1.47	1.41
21	3	3014	CLA	C1B-CHB	2.78	1.47	1.39
21	B	1224	CLA	C1B-CHB	2.79	1.47	1.39
21	A	1107	CLA	CHD-C4C	2.79	1.47	1.41
21	3	3010	CLA	C3D-C2D	2.79	1.46	1.40
21	4	4007	CLA	C3D-C2D	2.79	1.46	1.40
21	1	1010	CLA	C1B-CHB	2.80	1.47	1.39
21	2	2004	CLA	C3D-C2D	2.80	1.46	1.37
21	A	1133	CLA	C3D-C2D	2.80	1.46	1.40
21	2	2008	CLA	C1B-CHB	2.80	1.47	1.39
21	A	1131	CLA	C1B-CHB	2.81	1.47	1.39
21	3	3010	CLA	C1B-CHB	2.81	1.47	1.39
21	3	3013	CLA	CHD-C4C	2.81	1.47	1.41
21	1	1010	CLA	C4B-CHC	2.81	1.47	1.39
21	H	1000	CLA	C4B-CHC	2.81	1.47	1.39
21	B	1223	CLA	CHD-C4C	2.81	1.47	1.41
21	J	1302	CLA	C1B-CHB	2.82	1.47	1.39
21	4	4013	CLA	OBD-CAD	2.82	1.26	1.22
21	2	2014	CLA	CHD-C4C	2.82	1.47	1.41
21	A	1118	CLA	C3D-C2D	2.82	1.46	1.40
21	1	1006	CLA	C3D-C2D	2.82	1.46	1.40
21	A	1123	CLA	C3D-C2D	2.82	1.46	1.40
21	A	1106	CLA	CHD-C4C	2.82	1.47	1.41
21	A	1121	CLA	CHD-C4C	2.83	1.47	1.41
21	A	1122	CLA	C1B-CHB	2.83	1.47	1.39
21	4	4013	CLA	C1B-CHB	2.83	1.47	1.39
21	3	3003	CLA	C3D-C2D	2.83	1.46	1.40
21	1	1001	CLA	C1B-CHB	2.83	1.47	1.39
21	A	9012	CLA	C1B-CHB	2.83	1.47	1.39
21	A	1131	CLA	C3D-C2D	2.83	1.46	1.40
21	2	2003	CLA	C4C-C3C	2.84	1.50	1.45
21	L	1501	CLA	CHD-C4C	2.84	1.47	1.41
21	A	1129	CLA	C3D-C2D	2.84	1.46	1.40
21	B	1209	CLA	C3D-C2D	2.84	1.46	1.40
21	B	1229	CLA	CHD-C4C	2.84	1.47	1.41
21	B	1210	CLA	C3D-C2D	2.85	1.47	1.40
21	A	1138	CLA	C1B-CHB	2.85	1.47	1.39
21	A	1122	CLA	C3D-C2D	2.85	1.47	1.40
21	B	1216	CLA	C1B-CHB	2.85	1.47	1.39
21	B	1202	CLA	C3D-C2D	2.85	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1102	CLA	C3D-C2D	2.85	1.47	1.40
21	L	1501	CLA	C3D-C2D	2.86	1.47	1.40
21	B	1207	CLA	C4B-CHC	2.86	1.47	1.39
21	4	4004	CLA	C1B-CHB	2.86	1.47	1.39
21	A	1112	CLA	C3D-C2D	2.86	1.47	1.40
21	A	1139	CLA	C3D-C2D	2.86	1.47	1.40
21	A	1110	CLA	C4B-CHC	2.86	1.47	1.39
21	B	1209	CLA	CHD-C4C	2.87	1.47	1.41
21	B	1211	CLA	C3D-C2D	2.87	1.47	1.40
21	B	1208	CLA	C3D-C2D	2.87	1.47	1.40
21	1	1014	CLA	C3D-C2D	2.87	1.47	1.40
21	F	1301	CLA	C3D-C2D	2.88	1.47	1.40
21	A	1132	CLA	C4B-CHC	2.88	1.47	1.39
21	A	1109	CLA	C1B-CHB	2.88	1.47	1.39
21	A	1101	CLA	C1B-CHB	2.88	1.47	1.39
21	B	1202	CLA	CHD-C4C	2.88	1.47	1.41
21	4	4012	CLA	C3B-C2B	2.88	1.44	1.40
21	2	2008	CLA	C4B-CHC	2.88	1.47	1.39
21	A	1104	CLA	C3D-C2D	2.88	1.47	1.40
21	A	1110	CLA	C1B-CHB	2.88	1.47	1.39
21	G	1002	CLA	C1B-CHB	2.89	1.47	1.39
21	B	1230	CLA	C3D-C2D	2.89	1.47	1.40
21	4	4015	CLA	C4B-CHC	2.89	1.47	1.39
21	B	1238	CLA	C3D-C2D	2.89	1.47	1.40
21	A	1126	CLA	C1B-CHB	2.89	1.47	1.39
21	B	9022	CLA	C3D-C2D	2.89	1.47	1.40
21	B	1205	CLA	C3D-C2D	2.89	1.47	1.40
21	A	1133	CLA	C4B-CHC	2.90	1.47	1.39
21	3	3014	CLA	C4B-CHC	2.90	1.47	1.39
21	L	1502	CLA	C3D-C2D	2.90	1.47	1.40
21	B	1217	CLA	C3D-C2D	2.90	1.47	1.40
21	3	3008	CLA	C1B-CHB	2.90	1.47	1.39
21	A	1111	CLA	C1B-CHB	2.90	1.47	1.39
21	B	9023	CLA	C3B-C2B	2.90	1.44	1.40
21	A	1137	CLA	C1B-CHB	2.90	1.47	1.39
21	G	1001	CLA	C1B-CHB	2.90	1.47	1.39
21	B	1204	CLA	C3D-C2D	2.90	1.47	1.40
21	2	2002	CLA	CHD-C4C	2.90	1.48	1.41
21	4	4003	CLA	OBD-CAD	2.90	1.26	1.22
21	B	1218	CLA	C3D-C2D	2.90	1.47	1.40
21	B	1207	CLA	C3D-C2D	2.91	1.47	1.40
21	B	1214	CLA	CHD-C4C	2.91	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	2004	CLA	C1B-CHB	2.91	1.47	1.39
21	A	1113	CLA	C3D-C2D	2.91	1.47	1.40
21	B	1237	CLA	C3D-C2D	2.91	1.47	1.40
21	B	1210	CLA	CHD-C4C	2.91	1.48	1.41
21	A	1138	CLA	C3D-C2D	2.91	1.47	1.40
21	F	1301	CLA	CHD-C4C	2.91	1.48	1.41
21	L	1503	CLA	CHD-C4C	2.91	1.48	1.41
21	1	1012	CLA	OBD-CAD	2.91	1.26	1.22
21	B	1225	CLA	C3D-C2D	2.91	1.47	1.40
21	A	1105	CLA	C3D-C2D	2.91	1.47	1.40
21	2	2005	CLA	C1B-CHB	2.92	1.47	1.39
21	B	1220	CLA	C3D-C2D	2.92	1.47	1.40
21	A	1102	CLA	C1B-CHB	2.92	1.47	1.39
21	B	1208	CLA	CHD-C4C	2.92	1.48	1.41
21	A	1111	CLA	C3D-C2D	2.92	1.47	1.40
21	3	3002	CLA	C3D-C2D	2.92	1.47	1.40
21	A	1108	CLA	C1B-CHB	2.93	1.47	1.39
21	A	1119	CLA	C1B-CHB	2.93	1.47	1.39
21	A	1103	CLA	C1B-CHB	2.93	1.47	1.39
21	A	1127	CLA	C1B-CHB	2.93	1.47	1.39
21	L	1503	CLA	C3D-C2D	2.93	1.47	1.40
21	A	1128	CLA	C3D-C2D	2.93	1.47	1.40
21	A	1128	CLA	CHD-C4C	2.93	1.48	1.41
21	A	1115	CLA	CHD-C4C	2.93	1.48	1.41
21	B	1230	CLA	CHD-C4C	2.93	1.48	1.41
21	A	1106	CLA	C1B-CHB	2.94	1.47	1.39
21	B	1201	CLA	C3D-C2D	2.94	1.47	1.40
21	A	1130	CLA	C3D-C2D	2.94	1.47	1.40
21	A	1143	CLA	C3D-C2D	2.94	1.47	1.40
21	B	1238	CLA	C1B-CHB	2.94	1.47	1.39
21	B	1201	CLA	C1B-CHB	2.94	1.47	1.39
21	3	3002	CLA	C1B-CHB	2.94	1.47	1.39
21	B	1231	CLA	C3D-C2D	2.94	1.47	1.40
21	2	2006	CLA	C3D-C2D	2.94	1.47	1.40
21	B	1217	CLA	CHD-C4C	2.94	1.48	1.41
21	B	1222	CLA	C3D-C2D	2.94	1.47	1.40
21	A	1126	CLA	CHD-C4C	2.94	1.48	1.41
21	B	1236	CLA	CHD-C4C	2.94	1.48	1.41
21	B	1235	CLA	C3D-C2D	2.94	1.47	1.40
21	A	1130	CLA	CHD-C4C	2.94	1.48	1.41
21	A	1121	CLA	C3D-C2D	2.94	1.47	1.40
21	A	1117	CLA	C3D-C2D	2.94	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1219	CLA	C1B-CHB	2.94	1.48	1.39
21	A	1104	CLA	CHD-C4C	2.95	1.48	1.41
21	A	1116	CLA	C1B-CHB	2.95	1.48	1.39
21	A	1126	CLA	C3D-C2D	2.95	1.47	1.40
21	3	3014	CLA	C3D-C2D	2.95	1.47	1.40
21	A	1139	CLA	C1B-CHB	2.95	1.48	1.39
21	A	1109	CLA	C3D-C2D	2.95	1.47	1.40
21	L	1502	CLA	CHD-C4C	2.95	1.48	1.41
21	B	1235	CLA	C1B-CHB	2.95	1.48	1.39
21	A	1124	CLA	C1B-CHB	2.95	1.48	1.39
21	B	1236	CLA	C3D-C2D	2.95	1.47	1.40
21	J	6014	CLA	C3D-C2D	2.95	1.47	1.40
21	B	1224	CLA	C3D-C2D	2.95	1.47	1.40
21	B	1203	CLA	C3D-C2D	2.95	1.47	1.40
21	3	3001	CLA	C1B-CHB	2.96	1.48	1.39
21	B	1237	CLA	CHD-C4C	2.96	1.48	1.41
21	B	1213	CLA	C4B-CHC	2.96	1.48	1.39
21	F	1302	CLA	CHD-C4C	2.96	1.48	1.41
21	B	1211	CLA	C1B-CHB	2.96	1.48	1.39
21	A	1129	CLA	CHD-C4C	2.96	1.48	1.41
21	B	1240	CLA	C1B-CHB	2.96	1.48	1.39
21	B	1220	CLA	C1B-CHB	2.96	1.48	1.39
21	A	1116	CLA	C3D-C2D	2.96	1.47	1.40
21	3	3016	CLA	C1B-CHB	2.96	1.48	1.39
21	L	1503	CLA	C4B-CHC	2.96	1.48	1.39
21	B	1207	CLA	C1B-CHB	2.96	1.48	1.39
21	A	1108	CLA	C3D-C2D	2.96	1.47	1.40
21	B	1229	CLA	C3D-C2D	2.96	1.47	1.40
21	3	3012	CLA	CHD-C4C	2.97	1.48	1.41
21	B	1203	CLA	CHD-C4C	2.97	1.48	1.41
21	A	1117	CLA	C1B-CHB	2.97	1.48	1.39
21	B	1214	CLA	C3D-C2D	2.97	1.47	1.40
21	B	1202	CLA	C1B-CHB	2.97	1.48	1.39
21	A	1102	CLA	CHD-C4C	2.97	1.48	1.41
21	A	1120	CLA	C1B-CHB	2.97	1.48	1.39
21	F	1301	CLA	C1B-CHB	2.97	1.48	1.39
21	3	3005	CLA	C3D-C2D	2.97	1.47	1.40
21	A	1137	CLA	C3D-C2D	2.97	1.47	1.40
21	B	1219	CLA	CHD-C4C	2.97	1.48	1.41
21	B	1215	CLA	C1B-CHB	2.97	1.48	1.39
21	3	3016	CLA	C3D-C2D	2.97	1.47	1.40
21	A	1140	CLA	C3D-C2D	2.97	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1136	CLA	C3D-C2D	2.97	1.47	1.40
21	A	1112	CLA	CHD-C4C	2.97	1.48	1.41
21	3	3006	CLA	C1B-CHB	2.97	1.48	1.39
21	A	1135	CLA	C3D-C2D	2.97	1.47	1.40
21	B	1216	CLA	C3D-C2D	2.97	1.47	1.40
21	A	1127	CLA	C3D-C2D	2.97	1.47	1.40
21	A	1136	CLA	C1B-CHB	2.97	1.48	1.39
21	1	1012	CLA	C1B-CHB	2.97	1.48	1.39
21	4	4007	CLA	C4B-CHC	2.98	1.48	1.39
21	A	1124	CLA	C3D-C2D	2.98	1.47	1.40
21	A	1106	CLA	C3D-C2D	2.98	1.47	1.40
21	B	1215	CLA	CHD-C4C	2.98	1.48	1.41
21	A	1139	CLA	CHD-C4C	2.98	1.48	1.41
21	B	1221	CLA	C3D-C2D	2.98	1.47	1.40
21	A	1115	CLA	C3D-C2D	2.98	1.47	1.40
21	B	1234	CLA	C3D-C2D	2.98	1.47	1.40
21	A	1114	CLA	C1B-CHB	2.98	1.48	1.39
21	B	1228	CLA	OBD-CAD	2.98	1.26	1.22
21	3	3006	CLA	C3D-C2D	2.98	1.47	1.40
21	A	1101	CLA	C3D-C2D	2.98	1.47	1.40
21	A	1123	CLA	CHD-C4C	2.98	1.48	1.41
21	B	1225	CLA	CHD-C4C	2.98	1.48	1.41
21	A	1114	CLA	C3D-C2D	2.98	1.47	1.40
21	A	1105	CLA	CHD-C4C	2.98	1.48	1.41
21	3	3002	CLA	CHD-C4C	2.98	1.48	1.41
21	A	1112	CLA	C1B-CHB	2.98	1.48	1.39
21	A	1143	CLA	CHD-C4C	2.99	1.48	1.41
21	2	2010	CLA	C4B-CHC	2.99	1.48	1.39
21	A	9012	CLA	OBD-CAD	2.99	1.26	1.22
21	B	1212	CLA	C3D-C2D	2.99	1.47	1.40
21	B	1201	CLA	CHD-C4C	2.99	1.48	1.41
21	B	1206	CLA	C3D-C2D	2.99	1.47	1.40
21	B	1212	CLA	C1B-CHB	2.99	1.48	1.39
21	A	1142	CLA	C3D-C2D	2.99	1.47	1.40
21	B	1211	CLA	CHD-C4C	2.99	1.48	1.41
21	4	4011	CLA	OBD-CAD	2.99	1.26	1.22
21	A	1141	CLA	C3D-C2D	2.99	1.47	1.40
21	2	2003	CLA	C1B-CHB	2.99	1.48	1.39
21	A	1113	CLA	CHD-C4C	2.99	1.48	1.41
21	B	1217	CLA	C4B-CHC	2.99	1.48	1.39
21	A	1119	CLA	C3D-C2D	2.99	1.47	1.40
21	A	1115	CLA	C1B-CHB	3.00	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1215	CLA	C4B-CHC	3.00	1.48	1.39
21	3	3009	CLA	C1B-CHB	3.00	1.48	1.39
21	A	1134	CLA	C3D-C2D	3.00	1.47	1.40
21	A	1120	CLA	C3D-C2D	3.00	1.47	1.40
21	B	1236	CLA	C1B-CHB	3.00	1.48	1.39
21	B	1219	CLA	C3D-C2D	3.00	1.47	1.40
21	A	1136	CLA	CHD-C4C	3.00	1.48	1.41
21	B	1238	CLA	CHD-C4C	3.00	1.48	1.41
21	B	1222	CLA	CHD-C4C	3.01	1.48	1.41
21	F	1302	CLA	C1B-CHB	3.01	1.48	1.39
21	B	1221	CLA	C1B-CHB	3.01	1.48	1.39
21	B	1205	CLA	C1B-CHB	3.01	1.48	1.39
21	B	1226	CLA	C3C-C2C	3.01	1.43	1.36
21	B	1235	CLA	CHD-C4C	3.01	1.48	1.41
21	3	3005	CLA	C1B-CHB	3.01	1.48	1.39
21	B	1214	CLA	C1B-CHB	3.01	1.48	1.39
21	H	1000	CLA	C3D-C2D	3.01	1.47	1.40
21	2	2014	CLA	C3D-C2D	3.01	1.47	1.40
21	A	1143	CLA	C1B-CHB	3.01	1.48	1.39
21	A	1116	CLA	CHD-C4C	3.01	1.48	1.41
21	A	1118	CLA	CHD-C4C	3.01	1.48	1.41
21	A	1142	CLA	C1B-CHB	3.01	1.48	1.39
21	A	1135	CLA	C1B-CHB	3.01	1.48	1.39
21	4	4004	CLA	C3B-C2B	3.01	1.44	1.40
21	B	1237	CLA	C1B-CHB	3.02	1.48	1.39
21	A	1103	CLA	C3D-C2D	3.02	1.47	1.40
21	B	1237	CLA	C4B-CHC	3.02	1.48	1.39
21	B	1210	CLA	C1B-CHB	3.02	1.48	1.39
21	A	1127	CLA	CHD-C4C	3.02	1.48	1.41
21	1	1009	CLA	CHC-C1C	3.02	1.44	1.35
21	3	3014	CLA	CHD-C4C	3.02	1.48	1.41
21	A	1110	CLA	C3D-C2D	3.02	1.47	1.40
21	A	1141	CLA	C1B-CHB	3.02	1.48	1.39
26	2	2502	LUT	C23-C24	3.02	1.52	1.50
21	A	1140	CLA	CHD-C4C	3.02	1.48	1.41
21	B	1204	CLA	C1B-CHB	3.02	1.48	1.39
21	J	6014	CLA	CHD-C4C	3.02	1.48	1.41
21	F	1302	CLA	C3D-C2D	3.02	1.47	1.40
21	B	1204	CLA	CHD-C4C	3.02	1.48	1.41
21	B	1216	CLA	C4B-CHC	3.02	1.48	1.39
21	1	1009	CLA	OBD-CAD	3.03	1.27	1.22
21	3	3015	CLA	C3D-C2D	3.03	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1117	CLA	CHD-C4C	3.03	1.48	1.41
21	B	1217	CLA	C1B-CHB	3.03	1.48	1.39
21	3	3017	CLA	C1B-CHB	3.03	1.48	1.39
21	B	1205	CLA	CHD-C4C	3.03	1.48	1.41
21	A	1111	CLA	C4B-CHC	3.03	1.48	1.39
21	A	1117	CLA	C4B-CHC	3.03	1.48	1.39
21	B	1209	CLA	C1B-CHB	3.03	1.48	1.39
21	1	1005	CLA	C1B-CHB	3.03	1.48	1.39
21	J	1302	CLA	C4B-CHC	3.03	1.48	1.39
21	B	1218	CLA	CHD-C4C	3.03	1.48	1.41
21	A	1135	CLA	C4B-CHC	3.04	1.48	1.39
21	B	1216	CLA	CHD-C4C	3.04	1.48	1.41
21	B	1231	CLA	C1B-CHB	3.04	1.48	1.39
21	A	1104	CLA	C1B-CHB	3.04	1.48	1.39
21	4	4003	CLA	C1B-CHB	3.04	1.48	1.39
21	B	1206	CLA	C1B-CHB	3.04	1.48	1.39
21	2	2013	CLA	OBD-CAD	3.04	1.27	1.22
21	3	3013	CLA	C1B-CHB	3.04	1.48	1.39
21	3	3004	CLA	CHD-C4C	3.04	1.48	1.41
21	A	1137	CLA	CHD-C4C	3.04	1.48	1.41
21	1	1014	CLA	CHD-C4C	3.04	1.48	1.41
21	A	1134	CLA	C1B-CHB	3.04	1.48	1.39
21	A	1140	CLA	C1B-CHB	3.04	1.48	1.39
21	A	1124	CLA	CHD-C4C	3.04	1.48	1.41
21	3	3004	CLA	C1B-CHB	3.04	1.48	1.39
21	A	1105	CLA	C1B-CHB	3.04	1.48	1.39
21	B	1227	CLA	C3B-C2B	3.04	1.44	1.40
21	B	1224	CLA	CHD-C4C	3.04	1.48	1.41
21	B	1215	CLA	C3D-C2D	3.05	1.47	1.40
21	B	1230	CLA	C1B-CHB	3.05	1.48	1.39
21	A	1119	CLA	C4B-CHC	3.05	1.48	1.39
21	3	3016	CLA	CHD-C4C	3.05	1.48	1.41
21	B	1234	CLA	C1B-CHB	3.05	1.48	1.39
21	B	1231	CLA	CHD-C4C	3.05	1.48	1.41
21	3	3015	CLA	C1B-CHB	3.05	1.48	1.39
21	4	4002	CLA	CHC-C1C	3.05	1.44	1.35
21	3	3005	CLA	CHD-C4C	3.05	1.48	1.41
21	J	6014	CLA	C1B-CHB	3.05	1.48	1.39
21	A	1111	CLA	CHD-C4C	3.05	1.48	1.41
21	A	1135	CLA	CHD-C4C	3.05	1.48	1.41
21	A	1113	CLA	C1B-CHB	3.05	1.48	1.39
21	A	1128	CLA	C4B-CHC	3.05	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1220	CLA	CHD-C4C	3.05	1.48	1.41
21	B	1221	CLA	C4B-CHC	3.05	1.48	1.39
21	3	3015	CLA	CHD-C4C	3.06	1.48	1.41
21	A	1120	CLA	CHD-C4C	3.06	1.48	1.41
21	A	1101	CLA	C4B-CHC	3.06	1.48	1.39
21	A	1109	CLA	CHD-C4C	3.06	1.48	1.41
21	B	1212	CLA	C4B-CHC	3.06	1.48	1.39
21	1	1006	CLA	C1B-CHB	3.06	1.48	1.39
21	4	4014	CLA	C1B-CHB	3.06	1.48	1.39
21	B	1225	CLA	C1B-CHB	3.06	1.48	1.39
21	4	4014	CLA	C4B-CHC	3.06	1.48	1.39
21	B	1212	CLA	CHD-C4C	3.06	1.48	1.41
21	B	1218	CLA	C1B-CHB	3.06	1.48	1.39
21	J	1302	CLA	C3D-C2D	3.07	1.47	1.40
21	L	1501	CLA	C4B-CHC	3.07	1.48	1.39
21	A	1110	CLA	CHD-C4C	3.07	1.48	1.41
21	A	1141	CLA	CHD-C4C	3.07	1.48	1.41
21	A	1101	CLA	CHD-C4C	3.07	1.48	1.41
21	3	3006	CLA	CHD-C4C	3.07	1.48	1.41
21	B	1223	CLA	C4B-CHC	3.07	1.48	1.39
21	H	1000	CLA	CHD-C4C	3.07	1.48	1.41
21	A	1142	CLA	CHD-C4C	3.07	1.48	1.41
21	3	3003	CLA	C1B-CHB	3.07	1.48	1.39
21	B	1207	CLA	CHD-C4C	3.07	1.48	1.41
21	B	1223	CLA	C1B-CHB	3.07	1.48	1.39
21	A	1123	CLA	C1B-CHB	3.07	1.48	1.39
21	B	1203	CLA	C1B-CHB	3.07	1.48	1.39
21	A	1103	CLA	C4B-CHC	3.08	1.48	1.39
21	B	1227	CLA	OBD-CAD	3.08	1.27	1.22
21	B	1236	CLA	C4B-CHC	3.08	1.48	1.39
21	A	1108	CLA	CHD-C4C	3.08	1.48	1.41
21	A	1124	CLA	C4B-CHC	3.08	1.48	1.39
21	A	1134	CLA	C4B-CHC	3.08	1.48	1.39
21	A	1134	CLA	CHD-C4C	3.08	1.48	1.41
21	A	1130	CLA	C4B-CHC	3.08	1.48	1.39
21	A	1109	CLA	C4B-CHC	3.08	1.48	1.39
21	3	3001	CLA	C4B-CHC	3.08	1.48	1.39
21	A	1119	CLA	CHD-C4C	3.08	1.48	1.41
21	B	1234	CLA	CHD-C4C	3.09	1.48	1.41
21	4	4007	CLA	OBD-CAD	3.09	1.27	1.22
21	B	1211	CLA	C4B-CHC	3.09	1.48	1.39
21	B	1224	CLA	C4B-CHC	3.09	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1222	CLA	C4B-CHC	3.09	1.48	1.39
21	1	1013	CLA	C4B-CHC	3.09	1.48	1.39
21	A	1137	CLA	C4B-CHC	3.09	1.48	1.39
21	A	1142	CLA	C4B-CHC	3.09	1.48	1.39
21	B	1202	CLA	C4B-CHC	3.09	1.48	1.39
21	A	1108	CLA	C4B-CHC	3.10	1.48	1.39
21	F	1303	CLA	C3C-C2C	3.10	1.43	1.36
21	B	1205	CLA	C4B-CHC	3.10	1.48	1.39
21	3	3016	CLA	C4B-CHC	3.10	1.48	1.39
21	B	1230	CLA	C4B-CHC	3.10	1.48	1.39
21	A	1114	CLA	CHD-C4C	3.10	1.48	1.41
21	A	1103	CLA	CHD-C4C	3.10	1.48	1.41
21	B	1231	CLA	C4B-CHC	3.10	1.48	1.39
21	3	3013	CLA	C3D-C2D	3.10	1.47	1.40
21	B	1228	CLA	C3C-C2C	3.10	1.43	1.36
21	B	1225	CLA	C4B-CHC	3.10	1.48	1.39
21	A	1138	CLA	C4B-CHC	3.10	1.48	1.39
21	A	1136	CLA	C4B-CHC	3.10	1.48	1.39
21	A	1138	CLA	CHD-C4C	3.10	1.48	1.41
21	B	1226	CLA	CHC-C1C	3.10	1.45	1.35
21	A	1107	CLA	C1B-CHB	3.11	1.48	1.39
21	3	3002	CLA	C4B-CHC	3.11	1.48	1.39
21	B	1214	CLA	C4B-CHC	3.11	1.48	1.39
21	F	1301	CLA	C4B-CHC	3.11	1.48	1.39
21	A	1143	CLA	C4B-CHC	3.11	1.48	1.39
21	B	1234	CLA	C4B-CHC	3.11	1.48	1.39
21	B	1206	CLA	CHD-C4C	3.11	1.48	1.41
21	3	3004	CLA	C4B-CHC	3.11	1.48	1.39
21	J	1302	CLA	CHD-C4C	3.11	1.48	1.41
21	2	2007	CLA	C1B-CHB	3.11	1.48	1.39
21	A	1114	CLA	C4B-CHC	3.11	1.48	1.39
21	J	6014	CLA	C4B-CHC	3.12	1.48	1.39
21	3	3017	CLA	C4B-CHC	3.12	1.48	1.39
21	1	1007	CLA	C1B-CHB	3.12	1.48	1.39
21	A	1123	CLA	C4B-CHC	3.12	1.48	1.39
21	B	1208	CLA	C1B-CHB	3.12	1.48	1.39
21	A	1130	CLA	C1B-CHB	3.12	1.48	1.39
21	L	1502	CLA	C4B-CHC	3.12	1.48	1.39
21	1	1003	CLA	OBD-CAD	3.12	1.27	1.22
21	3	3010	CLA	C4B-CHC	3.12	1.48	1.39
21	B	1210	CLA	C4B-CHC	3.12	1.48	1.39
21	F	1302	CLA	C4B-CHC	3.13	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1120	CLA	C4B-CHC	3.13	1.48	1.39
21	A	1128	CLA	C1B-CHB	3.13	1.48	1.39
21	B	1229	CLA	C1B-CHB	3.13	1.48	1.39
21	A	1139	CLA	C4B-CHC	3.13	1.48	1.39
21	B	1235	CLA	C4B-CHC	3.13	1.48	1.39
21	H	1000	CLA	C1B-CHB	3.13	1.48	1.39
21	3	3005	CLA	C4B-CHC	3.13	1.48	1.39
21	B	1229	CLA	C4B-CHC	3.14	1.48	1.39
21	3	3006	CLA	C4B-CHC	3.14	1.48	1.39
21	F	1303	CLA	C3B-C2B	3.14	1.44	1.40
21	B	1203	CLA	C4B-CHC	3.14	1.48	1.39
21	A	1121	CLA	C4B-CHC	3.14	1.48	1.39
21	A	1102	CLA	C4B-CHC	3.14	1.48	1.39
21	B	1204	CLA	C4B-CHC	3.14	1.48	1.39
21	L	1502	CLA	C1B-CHB	3.14	1.48	1.39
21	B	1201	CLA	C4B-CHC	3.14	1.48	1.39
21	A	1127	CLA	C4B-CHC	3.14	1.48	1.39
21	B	1219	CLA	C4B-CHC	3.15	1.48	1.39
21	B	1220	CLA	C4B-CHC	3.15	1.48	1.39
21	A	1121	CLA	C1B-CHB	3.15	1.48	1.39
21	A	1140	CLA	C4B-CHC	3.15	1.48	1.39
21	B	1218	CLA	C4B-CHC	3.15	1.48	1.39
21	3	3015	CLA	C4B-CHC	3.15	1.48	1.39
21	4	4002	CLA	C1B-CHB	3.15	1.48	1.39
21	A	1113	CLA	C4B-CHC	3.15	1.48	1.39
21	4	4008	CLA	OBD-CAD	3.15	1.27	1.22
21	A	1129	CLA	C4B-CHC	3.16	1.48	1.39
21	1	1007	CLA	C4B-CHC	3.16	1.48	1.39
21	A	1112	CLA	C4B-CHC	3.16	1.48	1.39
21	A	1106	CLA	C4B-CHC	3.16	1.48	1.39
21	3	3003	CLA	C4B-CHC	3.17	1.48	1.39
21	A	1104	CLA	C4B-CHC	3.17	1.48	1.39
21	B	9010	CLA	C3C-C2C	3.17	1.43	1.36
21	B	1238	CLA	C4B-CHC	3.17	1.48	1.39
21	4	4005	CLA	OBD-CAD	3.17	1.27	1.22
21	4	4009	CLA	OBD-CAD	3.18	1.27	1.22
21	A	1105	CLA	C4B-CHC	3.18	1.48	1.39
21	B	9022	CLA	CHC-C1C	3.18	1.45	1.35
21	A	1129	CLA	C1B-CHB	3.18	1.48	1.39
21	A	1126	CLA	C4B-CHC	3.18	1.48	1.39
21	4	4001	CLA	OBD-CAD	3.18	1.27	1.22
21	3	3017	CLA	CHD-C4C	3.19	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	4007	CLA	CHD-C4C	3.19	1.48	1.41
21	4	4001	CLA	C3B-C2B	3.19	1.44	1.40
21	A	1122	CLA	CHD-C4C	3.19	1.48	1.41
21	B	1226	CLA	OBD-CAD	3.20	1.27	1.22
21	B	9023	CLA	OBD-CAD	3.20	1.27	1.22
21	J	6015	CLA	CHD-C4C	3.22	1.48	1.41
21	A	9013	CLA	CHC-C1C	3.22	1.45	1.35
21	A	1118	CLA	C1B-CHB	3.22	1.48	1.39
21	B	1227	CLA	O2D-CGD	3.22	1.41	1.33
21	B	1209	CLA	C4B-CHC	3.23	1.48	1.39
21	4	4011	CLA	CHC-C1C	3.23	1.45	1.35
21	1	1014	CLA	C1B-CHB	3.24	1.48	1.39
21	1	1004	CLA	C3C-C2C	3.24	1.43	1.36
21	A	1116	CLA	C4B-CHC	3.24	1.48	1.39
21	2	2013	CLA	C3C-C2C	3.24	1.43	1.36
21	2	2012	CLA	OBD-CAD	3.24	1.27	1.22
21	B	1208	CLA	C4B-CHC	3.24	1.48	1.39
21	L	1503	CLA	C1B-CHB	3.25	1.48	1.39
21	L	1501	CLA	C1B-CHB	3.26	1.48	1.39
21	A	1122	CLA	C4B-CHC	3.26	1.48	1.39
21	1	1005	CLA	OBD-CAD	3.27	1.27	1.22
23	A	9011	CL0	O2D-CGD	3.27	1.41	1.33
21	A	1141	CLA	C4B-CHC	3.28	1.48	1.39
20	1	1801	LHG	O7-C7	3.28	1.44	1.34
21	A	1115	CLA	C4B-CHC	3.29	1.48	1.39
21	1	1003	CLA	C3B-C2B	3.29	1.44	1.40
21	A	1107	CLA	C4B-CHC	3.30	1.48	1.39
21	4	4005	CLA	CHC-C1C	3.30	1.45	1.35
21	2	2006	CLA	C1B-CHB	3.31	1.49	1.39
21	B	1228	CLA	O2D-CGD	3.33	1.41	1.33
21	4	4010	CLA	C3B-C2B	3.34	1.44	1.40
21	1	1013	CLA	C3B-C2B	3.35	1.44	1.40
21	3	3011	CLA	C4B-CHC	3.35	1.49	1.39
21	1	1008	CLA	C3B-C2B	3.35	1.44	1.40
21	1	1011	CLA	OBD-CAD	3.35	1.27	1.22
21	2	2011	CLA	C3B-C2B	3.36	1.44	1.40
21	J	6015	CLA	C1B-CHB	3.36	1.49	1.39
21	B	1240	CLA	OBD-CAD	3.36	1.27	1.22
21	A	1131	CLA	OBD-CAD	3.38	1.27	1.22
21	2	2001	CLA	C2D-C3D	3.39	1.45	1.40
21	3	3013	CLA	CHC-C1C	3.39	1.45	1.35
21	2	2009	CLA	OBD-CAD	3.40	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	2801	LHG	O7-C7	3.40	1.44	1.34
21	4	4008	CLA	CHC-C1C	3.41	1.46	1.35
21	1	1011	CLA	C1B-CHB	3.42	1.49	1.39
21	1	1008	CLA	O2D-CGD	3.42	1.41	1.33
21	B	1226	CLA	C3B-C2B	3.43	1.44	1.40
21	4	4009	CLA	C3C-C2C	3.43	1.44	1.36
21	2	2012	CLA	C3B-C2B	3.44	1.44	1.40
21	A	9013	CLA	C3C-C2C	3.44	1.44	1.36
21	4	4006	CLA	C3B-C2B	3.47	1.44	1.40
21	4	4012	CLA	C3C-C2C	3.47	1.44	1.36
21	1	1009	CLA	C3C-C2C	3.48	1.44	1.36
21	G	1001	CLA	OBD-CAD	3.48	1.27	1.22
21	1	1008	CLA	C3C-C2C	3.49	1.44	1.36
21	1	1002	CLA	OBD-CAD	3.50	1.27	1.22
21	B	1239	CLA	CHC-C1C	3.50	1.46	1.35
21	B	9023	CLA	C3C-C2C	3.51	1.44	1.36
21	B	1239	CLA	C3C-C2C	3.52	1.44	1.36
21	B	1227	CLA	CHC-C1C	3.53	1.46	1.35
21	4	4005	CLA	C3C-C2C	3.53	1.44	1.36
21	4	4010	CLA	CHC-C1C	3.53	1.46	1.35
21	1	1001	CLA	C3C-C2C	3.54	1.44	1.36
21	1	1003	CLA	C3C-C2C	3.54	1.44	1.36
21	4	4010	CLA	OBD-CAD	3.54	1.27	1.22
21	1	1013	CLA	OBD-CAD	3.54	1.27	1.22
21	1	1006	CLA	CHC-C1C	3.54	1.46	1.35
21	1	1011	CLA	C3C-C2C	3.55	1.44	1.36
20	B	7004	LHG	O7-C7	3.55	1.44	1.34
21	3	3008	CLA	OBD-CAD	3.56	1.27	1.22
21	4	4014	CLA	CHD-C4C	3.56	1.49	1.41
21	A	1132	CLA	OBD-CAD	3.57	1.27	1.22
21	B	9023	CLA	CHC-C1C	3.58	1.46	1.35
21	1	1004	CLA	O2D-CGD	3.58	1.42	1.33
21	B	1240	CLA	CHC-C1C	3.59	1.46	1.35
21	4	4015	CLA	O2D-CGD	3.59	1.42	1.33
21	2	2014	CLA	CHC-C1C	3.60	1.46	1.35
21	2	2005	CLA	C3B-C2B	3.60	1.45	1.40
21	2	2007	CLA	OBD-CAD	3.60	1.27	1.22
21	1	1011	CLA	CHC-C1C	3.61	1.46	1.35
21	4	4008	CLA	O2D-CGD	3.61	1.42	1.33
21	B	1223	CLA	OBD-CAD	3.61	1.27	1.22
21	2	2011	CLA	O2D-CGD	3.62	1.42	1.33
21	2	2014	CLA	OBD-CAD	3.62	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	9022	CLA	C3C-C2C	3.62	1.44	1.36
21	4	4015	CLA	C3B-C2B	3.63	1.45	1.40
21	4	4004	CLA	O2D-CGD	3.63	1.42	1.33
21	2	2003	CLA	CHC-C1C	3.63	1.46	1.35
21	2	2005	CLA	CHC-C1C	3.63	1.46	1.35
21	1	1003	CLA	CHC-C1C	3.63	1.46	1.35
21	B	9010	CLA	CHC-C1C	3.63	1.46	1.35
21	F	1303	CLA	CHC-C1C	3.64	1.46	1.35
21	4	4004	CLA	C3C-C2C	3.64	1.44	1.36
21	4	4001	CLA	C3C-C2C	3.64	1.44	1.36
21	B	1228	CLA	C3B-C2B	3.64	1.45	1.40
21	B	1213	CLA	OBD-CAD	3.64	1.27	1.22
21	B	1227	CLA	C3C-C2C	3.64	1.44	1.36
21	4	4012	CLA	CHC-C1C	3.65	1.46	1.35
20	A	7003	LHG	O7-C7	3.65	1.45	1.34
21	4	4008	CLA	C3C-C2C	3.65	1.44	1.36
21	G	1002	CLA	OBD-CAD	3.65	1.27	1.22
21	B	9010	CLA	O2D-CGD	3.66	1.42	1.33
21	1	1001	CLA	CHC-C1C	3.67	1.46	1.35
21	B	1228	CLA	CHC-C1C	3.68	1.46	1.35
21	4	4014	CLA	C3C-C2C	3.68	1.44	1.36
21	3	3012	CLA	CHC-C1C	3.69	1.46	1.35
23	A	9011	CL0	CHC-C1C	3.69	1.46	1.35
23	A	9011	CL0	O2A-C1	3.70	1.57	1.46
20	B	7004	LHG	O8-C23	3.71	1.44	1.33
21	J	6015	CLA	CHC-C1C	3.71	1.46	1.35
21	1	1001	CLA	OBD-CAD	3.71	1.28	1.22
21	1	1001	CLA	C3B-C2B	3.71	1.45	1.40
21	B	1213	CLA	C3B-C2B	3.71	1.45	1.40
21	2	2013	CLA	C3B-C2B	3.72	1.45	1.40
21	A	1125	CLA	C3B-C2B	3.72	1.45	1.40
21	3	3008	CLA	CHC-C1C	3.72	1.47	1.35
21	2	2002	CLA	OBD-CAD	3.73	1.28	1.22
21	A	9013	CLA	O2A-C1	3.73	1.57	1.46
21	1	1007	CLA	C3B-C2B	3.73	1.45	1.40
21	2	2005	CLA	C3C-C2C	3.73	1.44	1.36
21	2	2009	CLA	C3B-C2B	3.73	1.45	1.40
21	4	4009	CLA	C3B-C2B	3.74	1.45	1.40
21	H	1000	CLA	C3B-C2B	3.74	1.45	1.40
21	4	4001	CLA	O2D-CGD	3.74	1.42	1.33
21	4	4013	CLA	C3C-C2C	3.75	1.44	1.36
21	1	1005	CLA	C3C-C2C	3.75	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	3012	CLA	C3B-C2B	3.75	1.45	1.40
21	1	1009	CLA	O2D-CGD	3.75	1.42	1.33
21	G	1001	CLA	CHC-C1C	3.75	1.47	1.35
21	2	2003	CLA	CHD-C4C	3.75	1.50	1.41
21	4	4003	CLA	O2D-CGD	3.76	1.42	1.33
21	2	2012	CLA	C3C-C2C	3.76	1.44	1.36
21	4	4003	CLA	C3B-C2B	3.76	1.45	1.40
21	A	9013	CLA	C3B-C2B	3.76	1.45	1.40
21	2	2011	CLA	CHC-C1C	3.77	1.47	1.35
21	B	1239	CLA	O2D-CGD	3.77	1.42	1.33
21	1	1012	CLA	C3C-C2C	3.78	1.44	1.36
21	B	1240	CLA	C3C-C2C	3.78	1.44	1.36
21	4	4004	CLA	CHC-C1C	3.78	1.47	1.35
21	A	1131	CLA	CHC-C1C	3.78	1.47	1.35
21	4	4013	CLA	CHC-C1C	3.78	1.47	1.35
21	B	1240	CLA	C3B-C2B	3.78	1.45	1.40
21	2	2007	CLA	CHC-C1C	3.79	1.47	1.35
21	2	2013	CLA	CHC-C1C	3.81	1.47	1.35
21	1	1005	CLA	C3B-C2B	3.81	1.45	1.40
21	2	2004	CLA	CHC-C1C	3.81	1.47	1.35
21	3	3009	CLA	C3C-C2C	3.81	1.44	1.36
21	A	1125	CLA	C3C-C2C	3.81	1.44	1.36
21	4	4002	CLA	OBD-CAD	3.81	1.28	1.22
21	2	2011	CLA	C3C-C2C	3.82	1.44	1.36
21	1	1009	CLA	O2A-C1	3.82	1.58	1.46
21	A	9012	CLA	O2D-CGD	3.82	1.42	1.33
21	2	2006	CLA	C3C-C2C	3.83	1.45	1.36
21	A	1133	CLA	OBD-CAD	3.83	1.28	1.22
21	G	1002	CLA	CHC-C1C	3.83	1.47	1.35
21	3	3011	CLA	C3B-C2B	3.83	1.45	1.40
21	A	9012	CLA	C3C-C2C	3.84	1.45	1.36
21	B	1240	CLA	O2A-C1	3.84	1.58	1.46
21	B	1206	CLA	CHC-C1C	3.85	1.47	1.35
21	1	1010	CLA	C3C-C2C	3.85	1.45	1.36
21	2	2003	CLA	OBD-CAD	3.85	1.28	1.22
25	J	5001	LMG	O7-C10	3.85	1.45	1.34
21	B	9023	CLA	O2D-CGD	3.85	1.43	1.33
21	3	3010	CLA	CHC-C1C	3.85	1.47	1.35
21	G	1001	CLA	C3C-C2C	3.85	1.45	1.36
21	2	2012	CLA	O2D-CGD	3.86	1.43	1.33
21	1	1002	CLA	CHC-C1C	3.86	1.47	1.35
21	1	1004	CLA	CHC-C1C	3.86	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	4011	CLA	O2D-CGD	3.86	1.43	1.33
21	4	4001	CLA	CHC-C1C	3.86	1.47	1.35
20	1	1801	LHG	O8-C23	3.87	1.45	1.33
21	1	1014	CLA	CHC-C1C	3.87	1.47	1.35
21	1	1007	CLA	C3C-C2C	3.87	1.45	1.36
21	2	2012	CLA	CHC-C1C	3.87	1.47	1.35
21	B	9010	CLA	C3B-C2B	3.87	1.45	1.40
21	4	4007	CLA	CHC-C1C	3.88	1.47	1.35
21	2	2007	CLA	C3C-C2C	3.88	1.45	1.36
21	2	2014	CLA	C3C-C2C	3.88	1.45	1.36
21	2	2011	CLA	OBD-CAD	3.88	1.28	1.22
21	A	1132	CLA	C3C-C2C	3.88	1.45	1.36
21	A	1118	CLA	CHC-C1C	3.88	1.47	1.35
21	B	1213	CLA	C3C-C2C	3.88	1.45	1.36
21	3	3009	CLA	C3B-C2B	3.89	1.45	1.40
21	A	9013	CLA	O2D-CGD	3.89	1.43	1.33
21	B	9010	CLA	O2A-C1	3.89	1.58	1.46
21	2	2004	CLA	C3C-C2C	3.90	1.45	1.36
21	1	1005	CLA	CHC-C1C	3.90	1.47	1.35
21	2	2006	CLA	OBD-CAD	3.90	1.28	1.22
21	2	2006	CLA	CHC-C1C	3.90	1.47	1.35
21	1	1008	CLA	CHC-C1C	3.90	1.47	1.35
21	4	4015	CLA	C3C-C2C	3.90	1.45	1.36
20	A	7003	LHG	O8-C23	3.90	1.45	1.33
21	1	1002	CLA	C3C-C2C	3.90	1.45	1.36
21	4	4013	CLA	O2D-CGD	3.91	1.43	1.33
21	4	4009	CLA	CHC-C1C	3.91	1.47	1.35
21	1	1010	CLA	C3B-C2B	3.91	1.45	1.40
21	2	2002	CLA	CHC-C1C	3.92	1.47	1.35
21	A	1125	CLA	CHC-C1C	3.92	1.47	1.35
20	A	7001	LHG	O7-C7	3.92	1.46	1.34
21	1	1012	CLA	CHC-C1C	3.93	1.47	1.35
21	H	1000	CLA	CHC-C1C	3.93	1.47	1.35
21	4	4004	CLA	OBD-CAD	3.93	1.28	1.22
21	4	4014	CLA	OBD-CAD	3.93	1.28	1.22
21	2	2009	CLA	CHC-C1C	3.94	1.47	1.35
21	4	4003	CLA	CHC-C1C	3.94	1.47	1.35
21	1	1006	CLA	C3C-C2C	3.95	1.45	1.36
21	1	1014	CLA	C3C-C2C	3.96	1.45	1.36
21	2	2004	CLA	C3B-C2B	3.96	1.45	1.40
21	3	3009	CLA	CHC-C1C	3.97	1.47	1.35
21	1	1014	CLA	C3B-C2B	3.98	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	2010	CLA	C3C-C2C	3.98	1.45	1.36
21	1	1010	CLA	CHC-C1C	3.98	1.47	1.35
21	B	1213	CLA	CHC-C1C	3.98	1.47	1.35
21	A	9012	CLA	CHC-C1C	3.99	1.47	1.35
21	4	4006	CLA	CHC-C1C	3.99	1.47	1.35
21	2	2002	CLA	C3C-C2C	3.99	1.45	1.36
21	2	2008	CLA	C3C-C2C	3.99	1.45	1.36
21	B	1207	CLA	CHC-C1C	4.01	1.47	1.35
21	3	3014	CLA	CHC-C1C	4.01	1.47	1.35
21	1	1007	CLA	O2D-CGD	4.01	1.43	1.33
21	4	4012	CLA	O2D-CGD	4.02	1.43	1.33
21	A	1133	CLA	CHC-C1C	4.02	1.47	1.35
21	G	1002	CLA	C3C-C2C	4.02	1.45	1.36
21	4	4010	CLA	C3C-C2C	4.02	1.45	1.36
21	2	2007	CLA	C3B-C2B	4.02	1.45	1.40
21	2	2002	CLA	O2D-CGD	4.04	1.43	1.33
21	B	9022	CLA	O2D-CGD	4.04	1.43	1.33
21	B	1240	CLA	O2D-CGD	4.04	1.43	1.33
21	2	2004	CLA	O2D-CGD	4.05	1.43	1.33
21	A	1110	CLA	CHC-C1C	4.05	1.48	1.35
21	2	2010	CLA	CHC-C1C	4.06	1.48	1.35
21	F	1301	CLA	CHC-C1C	4.06	1.48	1.35
21	B	1223	CLA	CHC-C1C	4.06	1.48	1.35
21	A	1126	CLA	OBD-CAD	4.06	1.28	1.22
21	B	1217	CLA	OBD-CAD	4.07	1.28	1.22
21	B	1221	CLA	CHC-C1C	4.07	1.48	1.35
21	1	1002	CLA	C3B-C2B	4.07	1.45	1.40
21	A	1129	CLA	OBD-CAD	4.08	1.28	1.22
21	B	9022	CLA	O2A-C1	4.08	1.58	1.46
21	B	1216	CLA	CHC-C1C	4.08	1.48	1.35
21	B	1217	CLA	CHC-C1C	4.08	1.48	1.35
21	4	4011	CLA	O2A-C1	4.08	1.58	1.46
21	B	1231	CLA	CHC-C1C	4.08	1.48	1.35
21	A	1130	CLA	OBD-CAD	4.08	1.28	1.22
21	A	1109	CLA	CHC-C1C	4.09	1.48	1.35
21	3	3001	CLA	CHC-C1C	4.09	1.48	1.35
21	A	1137	CLA	CHC-C1C	4.09	1.48	1.35
21	A	1132	CLA	O2D-CGD	4.09	1.43	1.33
21	B	1210	CLA	OBD-CAD	4.09	1.28	1.22
21	A	1135	CLA	CHC-C1C	4.09	1.48	1.35
21	4	4008	CLA	C3B-C2B	4.10	1.45	1.40
21	A	1134	CLA	CHC-C1C	4.10	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	1003	CLA	O2A-C1	4.10	1.58	1.46
21	A	1128	CLA	OBD-CAD	4.10	1.28	1.22
21	B	1215	CLA	CHC-C1C	4.10	1.48	1.35
21	A	1113	CLA	CHC-C1C	4.10	1.48	1.35
21	A	1139	CLA	CHC-C1C	4.10	1.48	1.35
21	B	1237	CLA	CHC-C1C	4.11	1.48	1.35
21	B	1204	CLA	OBD-CAD	4.11	1.28	1.22
21	L	1501	CLA	OBD-CAD	4.11	1.28	1.22
21	3	3017	CLA	CHC-C1C	4.11	1.48	1.35
21	A	1111	CLA	CHC-C1C	4.11	1.48	1.35
21	L	1502	CLA	OBD-CAD	4.11	1.28	1.22
21	A	1104	CLA	CHC-C1C	4.12	1.48	1.35
21	B	1205	CLA	CHC-C1C	4.12	1.48	1.35
21	A	1131	CLA	C3B-C2B	4.12	1.45	1.40
21	A	1121	CLA	CHC-C1C	4.12	1.48	1.35
21	4	4010	CLA	O2D-CGD	4.13	1.43	1.33
21	3	3002	CLA	CHC-C1C	4.13	1.48	1.35
21	2	2009	CLA	C3C-C2C	4.13	1.45	1.36
21	J	1302	CLA	CHC-C1C	4.13	1.48	1.35
21	A	1142	CLA	CHC-C1C	4.13	1.48	1.35
21	B	1225	CLA	CHC-C1C	4.13	1.48	1.35
21	A	1132	CLA	C3B-C2B	4.13	1.45	1.40
21	B	1212	CLA	CHC-C1C	4.13	1.48	1.35
21	2	2008	CLA	OBD-CAD	4.13	1.28	1.22
21	3	3011	CLA	OBD-CAD	4.13	1.28	1.22
21	3	3016	CLA	CHC-C1C	4.14	1.48	1.35
21	B	9023	CLA	O2A-C1	4.14	1.59	1.46
21	A	1120	CLA	CHC-C1C	4.14	1.48	1.35
21	A	1135	CLA	OBD-CAD	4.14	1.28	1.22
21	A	1132	CLA	O2A-C1	4.14	1.59	1.46
21	B	1229	CLA	CHC-C1C	4.14	1.48	1.35
21	B	1209	CLA	CHC-C1C	4.14	1.48	1.35
21	G	1001	CLA	C3B-C2B	4.14	1.45	1.40
21	A	1123	CLA	CHC-C1C	4.15	1.48	1.35
21	A	1114	CLA	CHC-C1C	4.15	1.48	1.35
21	B	1219	CLA	OBD-CAD	4.15	1.28	1.22
21	A	1124	CLA	CHC-C1C	4.15	1.48	1.35
21	3	3015	CLA	CHC-C1C	4.15	1.48	1.35
21	B	1203	CLA	OBD-CAD	4.15	1.28	1.22
21	A	1143	CLA	CHC-C1C	4.15	1.48	1.35
21	A	1119	CLA	CHC-C1C	4.15	1.48	1.35
21	L	1503	CLA	OBD-CAD	4.16	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1132	CLA	CHC-C1C	4.16	1.48	1.35
21	L	1503	CLA	CHC-C1C	4.16	1.48	1.35
20	A	7001	LHG	O8-C23	4.16	1.45	1.33
21	3	3004	CLA	CHC-C1C	4.16	1.48	1.35
21	A	1133	CLA	C3C-C2C	4.16	1.45	1.36
21	A	1108	CLA	CHC-C1C	4.16	1.48	1.35
21	4	4007	CLA	C3C-C2C	4.16	1.45	1.36
21	A	1131	CLA	C3C-C2C	4.16	1.45	1.36
21	F	1302	CLA	CHC-C1C	4.16	1.48	1.35
21	A	1125	CLA	O2D-CGD	4.16	1.43	1.33
21	B	1236	CLA	CHC-C1C	4.16	1.48	1.35
21	2	2003	CLA	C3B-C2B	4.16	1.45	1.40
21	J	6014	CLA	CHC-C1C	4.17	1.48	1.35
21	3	3006	CLA	CHC-C1C	4.17	1.48	1.35
21	A	1117	CLA	CHC-C1C	4.17	1.48	1.35
21	B	1218	CLA	CHC-C1C	4.17	1.48	1.35
21	B	1219	CLA	CHC-C1C	4.17	1.48	1.35
21	A	1140	CLA	CHC-C1C	4.17	1.48	1.35
21	B	1213	CLA	O2D-CGD	4.17	1.43	1.33
21	B	1230	CLA	CHC-C1C	4.17	1.48	1.35
21	B	1235	CLA	OBD-CAD	4.17	1.28	1.22
21	A	1127	CLA	CHC-C1C	4.17	1.48	1.35
21	A	1103	CLA	CHC-C1C	4.17	1.48	1.35
21	B	9022	CLA	C3B-C2B	4.17	1.45	1.40
21	3	3001	CLA	OBD-CAD	4.18	1.28	1.22
21	G	1002	CLA	C3B-C2B	4.18	1.45	1.40
21	A	1101	CLA	CHC-C1C	4.18	1.48	1.35
25	J	5001	LMG	O8-C28	4.18	1.45	1.33
21	A	1131	CLA	O2D-CGD	4.18	1.43	1.33
21	A	1106	CLA	CHC-C1C	4.18	1.48	1.35
21	B	1234	CLA	CHC-C1C	4.18	1.48	1.35
21	2	2008	CLA	CHC-C1C	4.18	1.48	1.35
21	B	1224	CLA	CHC-C1C	4.18	1.48	1.35
21	A	1136	CLA	CHC-C1C	4.19	1.48	1.35
21	B	1202	CLA	CHC-C1C	4.19	1.48	1.35
21	A	9012	CLA	O2A-C1	4.19	1.59	1.46
21	3	3012	CLA	OBD-CAD	4.19	1.28	1.22
21	B	1204	CLA	CHC-C1C	4.19	1.48	1.35
21	B	1201	CLA	CHC-C1C	4.19	1.48	1.35
21	1	1011	CLA	C3B-C2B	4.19	1.45	1.40
21	1	1006	CLA	O2A-C1	4.19	1.61	1.46
21	B	1210	CLA	CHC-C1C	4.19	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1211	CLA	CHC-C1C	4.20	1.48	1.35
21	4	4009	CLA	O2A-C1	4.20	1.59	1.46
21	L	1501	CLA	CHC-C1C	4.20	1.48	1.35
21	B	1238	CLA	CHC-C1C	4.20	1.48	1.35
21	1	1003	CLA	O2D-CGD	4.20	1.43	1.33
21	4	4003	CLA	C3C-C2C	4.21	1.45	1.36
21	A	1118	CLA	C3B-C2B	4.21	1.45	1.40
21	2	2008	CLA	C3B-C2B	4.21	1.45	1.40
21	B	1208	CLA	CHC-C1C	4.21	1.48	1.35
21	F	1302	CLA	OBD-CAD	4.21	1.28	1.22
21	B	1220	CLA	CHC-C1C	4.21	1.48	1.35
21	B	1235	CLA	CHC-C1C	4.21	1.48	1.35
21	B	1203	CLA	CHC-C1C	4.21	1.48	1.35
21	A	1122	CLA	CHC-C1C	4.21	1.48	1.35
21	3	3014	CLA	C3C-C2C	4.22	1.45	1.36
21	4	4002	CLA	C3C-C2C	4.22	1.45	1.36
21	1	1013	CLA	CHC-C1C	4.22	1.48	1.35
21	1	1010	CLA	OBD-CAD	4.22	1.28	1.22
21	A	1138	CLA	CHC-C1C	4.22	1.48	1.35
21	B	1214	CLA	CHC-C1C	4.22	1.48	1.35
21	4	4009	CLA	O2D-CGD	4.22	1.44	1.33
21	B	1234	CLA	OBD-CAD	4.22	1.28	1.22
21	B	1222	CLA	CHC-C1C	4.22	1.48	1.35
21	B	1214	CLA	OBD-CAD	4.22	1.28	1.22
21	1	1005	CLA	O2D-CGD	4.22	1.44	1.33
21	A	1102	CLA	CHC-C1C	4.22	1.48	1.35
21	3	3010	CLA	OBD-CAD	4.23	1.28	1.22
21	3	3014	CLA	OBD-CAD	4.23	1.28	1.22
21	A	1105	CLA	CHC-C1C	4.23	1.48	1.35
21	4	4015	CLA	CHC-C1C	4.23	1.48	1.35
21	B	1202	CLA	OBD-CAD	4.23	1.28	1.22
21	A	1116	CLA	CHC-C1C	4.23	1.48	1.35
21	G	1001	CLA	O2D-CGD	4.23	1.44	1.33
21	3	3017	CLA	OBD-CAD	4.23	1.28	1.22
21	A	1129	CLA	CHC-C1C	4.24	1.48	1.35
21	A	1141	CLA	CHC-C1C	4.24	1.48	1.35
21	A	1128	CLA	CHC-C1C	4.24	1.48	1.35
21	L	1502	CLA	CHC-C1C	4.25	1.48	1.35
21	B	1211	CLA	OBD-CAD	4.25	1.28	1.22
21	1	1007	CLA	O2A-C1	4.25	1.59	1.46
21	A	1112	CLA	CHC-C1C	4.25	1.48	1.35
21	A	1115	CLA	CHC-C1C	4.25	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1107	CLA	OBD-CAD	4.26	1.28	1.22
21	B	1236	CLA	OBD-CAD	4.26	1.28	1.22
21	A	1126	CLA	CHC-C1C	4.26	1.48	1.35
21	A	1118	CLA	OBD-CAD	4.26	1.28	1.22
21	3	3005	CLA	CHC-C1C	4.26	1.48	1.35
21	A	1119	CLA	OBD-CAD	4.26	1.28	1.22
21	A	1115	CLA	OBD-CAD	4.26	1.28	1.22
21	A	1133	CLA	C3B-C2B	4.26	1.45	1.40
21	B	1221	CLA	OBD-CAD	4.26	1.28	1.22
21	A	1106	CLA	C3C-C2C	4.26	1.45	1.36
21	A	1136	CLA	OBD-CAD	4.27	1.28	1.22
21	F	1301	CLA	OBD-CAD	4.27	1.28	1.22
21	B	1230	CLA	OBD-CAD	4.27	1.28	1.22
21	3	3011	CLA	C3C-C2C	4.27	1.45	1.36
21	4	4014	CLA	CHC-C1C	4.28	1.48	1.35
21	A	1123	CLA	OBD-CAD	4.28	1.28	1.22
21	A	1109	CLA	OBD-CAD	4.28	1.28	1.22
21	B	1209	CLA	OBD-CAD	4.28	1.28	1.22
21	A	1108	CLA	OBD-CAD	4.29	1.28	1.22
21	A	1130	CLA	CHC-C1C	4.29	1.48	1.35
21	3	3003	CLA	CHC-C1C	4.29	1.48	1.35
21	A	1111	CLA	OBD-CAD	4.29	1.28	1.22
21	A	1104	CLA	OBD-CAD	4.29	1.28	1.22
21	1	1007	CLA	CHC-C1C	4.29	1.48	1.35
21	A	1116	CLA	OBD-CAD	4.29	1.28	1.22
21	1	1009	CLA	C3B-C2B	4.29	1.46	1.40
21	A	1140	CLA	OBD-CAD	4.29	1.28	1.22
21	B	1238	CLA	OBD-CAD	4.29	1.28	1.22
21	1	1010	CLA	O2A-C1	4.30	1.59	1.46
21	A	1112	CLA	OBD-CAD	4.30	1.28	1.22
21	B	1218	CLA	OBD-CAD	4.30	1.28	1.22
21	4	4002	CLA	O2A-C1	4.30	1.59	1.46
21	3	3004	CLA	OBD-CAD	4.30	1.28	1.22
21	3	3003	CLA	OBD-CAD	4.31	1.28	1.22
21	B	1206	CLA	OBD-CAD	4.31	1.28	1.22
21	A	1131	CLA	O2A-C1	4.31	1.59	1.46
21	2	2007	CLA	O2A-C1	4.31	1.59	1.46
21	B	1237	CLA	OBD-CAD	4.31	1.28	1.22
21	A	1124	CLA	OBD-CAD	4.31	1.28	1.22
21	3	3013	CLA	C3C-C2C	4.32	1.46	1.36
21	4	4004	CLA	O2A-C1	4.32	1.59	1.46
21	A	1102	CLA	OBD-CAD	4.32	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1231	CLA	OBD-CAD	4.32	1.28	1.22
21	A	1106	CLA	OBD-CAD	4.32	1.28	1.22
21	2	2002	CLA	C3B-C2B	4.32	1.46	1.40
21	A	1127	CLA	OBD-CAD	4.32	1.29	1.22
21	A	1114	CLA	OBD-CAD	4.32	1.29	1.22
21	H	1000	CLA	OBD-CAD	4.32	1.29	1.22
21	A	1125	CLA	O2A-C1	4.32	1.59	1.46
21	A	1142	CLA	OBD-CAD	4.32	1.29	1.22
21	B	1208	CLA	OBD-CAD	4.33	1.29	1.22
21	3	3005	CLA	OBD-CAD	4.33	1.29	1.22
21	B	1207	CLA	OBD-CAD	4.33	1.29	1.22
21	A	1101	CLA	OBD-CAD	4.33	1.29	1.22
21	A	1107	CLA	CHC-C1C	4.33	1.48	1.35
21	2	2007	CLA	O2D-CGD	4.33	1.44	1.33
21	3	3002	CLA	OBD-CAD	4.33	1.29	1.22
21	B	1212	CLA	OBD-CAD	4.33	1.29	1.22
21	B	1225	CLA	OBD-CAD	4.33	1.29	1.22
21	1	1011	CLA	O2D-CGD	4.33	1.44	1.33
21	B	1205	CLA	OBD-CAD	4.33	1.29	1.22
21	A	1128	CLA	C3C-C2C	4.33	1.46	1.36
21	3	3011	CLA	O2D-CGD	4.33	1.44	1.33
21	A	1103	CLA	C3C-C2C	4.34	1.46	1.36
21	2	2006	CLA	O2A-C1	4.34	1.59	1.46
21	A	1139	CLA	OBD-CAD	4.34	1.29	1.22
21	J	6014	CLA	OBD-CAD	4.34	1.29	1.22
21	A	1134	CLA	OBD-CAD	4.34	1.29	1.22
21	B	1201	CLA	OBD-CAD	4.34	1.29	1.22
21	J	6015	CLA	OBD-CAD	4.34	1.29	1.22
21	A	1103	CLA	OBD-CAD	4.34	1.29	1.22
21	A	1117	CLA	OBD-CAD	4.34	1.29	1.22
21	B	1216	CLA	OBD-CAD	4.34	1.29	1.22
21	A	1110	CLA	OBD-CAD	4.34	1.29	1.22
21	A	1141	CLA	OBD-CAD	4.34	1.29	1.22
21	A	1121	CLA	OBD-CAD	4.35	1.29	1.22
21	A	1120	CLA	OBD-CAD	4.35	1.29	1.22
20	2	2801	LHG	O8-C23	4.35	1.46	1.33
21	A	1113	CLA	OBD-CAD	4.35	1.29	1.22
21	3	3016	CLA	OBD-CAD	4.35	1.29	1.22
21	B	1214	CLA	C3C-C2C	4.35	1.46	1.36
21	A	1137	CLA	OBD-CAD	4.35	1.29	1.22
21	G	1002	CLA	O2D-CGD	4.36	1.44	1.33
21	A	1105	CLA	OBD-CAD	4.36	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1122	CLA	OBD-CAD	4.36	1.29	1.22
21	4	4002	CLA	O2D-CGD	4.36	1.44	1.33
21	G	1001	CLA	O2A-C1	4.36	1.59	1.46
21	J	1302	CLA	OBD-CAD	4.36	1.29	1.22
21	B	1220	CLA	OBD-CAD	4.37	1.29	1.22
21	B	1222	CLA	OBD-CAD	4.37	1.29	1.22
21	B	1229	CLA	OBD-CAD	4.37	1.29	1.22
21	1	1013	CLA	C3C-C2C	4.37	1.46	1.36
21	F	1303	CLA	O2D-CGD	4.37	1.44	1.33
21	A	1129	CLA	C3C-C2C	4.37	1.46	1.36
21	1	1005	CLA	O2A-C1	4.37	1.59	1.46
21	B	1215	CLA	OBD-CAD	4.38	1.29	1.22
21	3	3015	CLA	OBD-CAD	4.38	1.29	1.22
21	A	1138	CLA	OBD-CAD	4.38	1.29	1.22
21	2	2013	CLA	O2D-CGD	4.38	1.44	1.33
21	3	3006	CLA	OBD-CAD	4.38	1.29	1.22
21	A	1143	CLA	OBD-CAD	4.38	1.29	1.22
21	B	1206	CLA	C3C-C2C	4.39	1.46	1.36
21	3	3013	CLA	O2A-C1	4.39	1.59	1.46
21	B	1227	CLA	O2A-C1	4.39	1.59	1.46
21	B	1224	CLA	OBD-CAD	4.39	1.29	1.22
21	2	2003	CLA	O2A-C1	4.39	1.59	1.46
21	4	4006	CLA	OBD-CAD	4.39	1.29	1.22
21	B	1213	CLA	O2A-C1	4.40	1.59	1.46
21	2	2013	CLA	O2A-C1	4.41	1.59	1.46
21	1	1012	CLA	O2D-CGD	4.41	1.44	1.33
21	4	4003	CLA	O2A-C1	4.41	1.59	1.46
21	4	4013	CLA	O2A-C1	4.41	1.59	1.46
21	2	2010	CLA	C3B-C2B	4.41	1.46	1.40
21	4	4006	CLA	C3C-C2C	4.42	1.46	1.36
21	A	1111	CLA	C3C-C2C	4.42	1.46	1.36
21	B	1221	CLA	C3C-C2C	4.42	1.46	1.36
21	2	2014	CLA	C3B-C2B	4.42	1.46	1.40
21	3	3010	CLA	C3C-C2C	4.42	1.46	1.36
21	L	1503	CLA	C3C-C2C	4.42	1.46	1.36
21	L	1501	CLA	C3C-C2C	4.42	1.46	1.36
21	1	1004	CLA	O2A-C1	4.42	1.59	1.46
21	3	3013	CLA	O2D-CGD	4.43	1.44	1.33
21	3	3003	CLA	C3C-C2C	4.44	1.46	1.36
21	A	1133	CLA	O2D-CGD	4.45	1.44	1.33
21	A	1126	CLA	O2A-C1	4.45	1.60	1.46
21	1	1012	CLA	O2A-C1	4.45	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1118	CLA	C3C-C2C	4.45	1.46	1.36
21	J	6015	CLA	O2D-CGD	4.45	1.44	1.33
21	B	1239	CLA	O2A-C1	4.45	1.60	1.46
21	B	1215	CLA	C3C-C2C	4.45	1.46	1.36
21	1	1013	CLA	O2D-CGD	4.46	1.44	1.33
21	4	4006	CLA	O2A-C1	4.46	1.60	1.46
21	4	4008	CLA	O2A-C1	4.46	1.60	1.46
21	2	2004	CLA	O2A-C1	4.46	1.60	1.46
21	1	1002	CLA	O2A-C1	4.47	1.60	1.46
21	A	1110	CLA	O2A-C1	4.47	1.60	1.46
21	4	4007	CLA	O2A-C1	4.47	1.60	1.46
21	B	1201	CLA	C3C-C2C	4.47	1.46	1.36
21	2	2014	CLA	O2D-CGD	4.47	1.44	1.33
21	A	1121	CLA	C3C-C2C	4.48	1.46	1.36
21	A	1116	CLA	C3C-C2C	4.48	1.46	1.36
21	1	1014	CLA	OBD-CAD	4.49	1.29	1.22
21	B	1231	CLA	C3C-C2C	4.49	1.46	1.36
21	B	1205	CLA	C3C-C2C	4.49	1.46	1.36
21	A	1110	CLA	C3B-C2B	4.49	1.46	1.40
21	A	1130	CLA	C3C-C2C	4.49	1.46	1.36
21	A	1104	CLA	C3C-C2C	4.49	1.46	1.36
21	3	3002	CLA	C3C-C2C	4.50	1.46	1.36
21	H	1000	CLA	C3C-C2C	4.50	1.46	1.36
21	L	1502	CLA	C3C-C2C	4.50	1.46	1.36
21	A	1137	CLA	C3C-C2C	4.50	1.46	1.36
21	A	1136	CLA	O2A-C1	4.50	1.60	1.46
21	A	1112	CLA	C3C-C2C	4.50	1.46	1.36
21	A	1114	CLA	C3C-C2C	4.51	1.46	1.36
21	A	1110	CLA	C3C-C2C	4.51	1.46	1.36
21	3	3006	CLA	C3C-C2C	4.51	1.46	1.36
21	A	1120	CLA	C3C-C2C	4.51	1.46	1.36
21	3	3008	CLA	O2D-CGD	4.51	1.44	1.33
21	B	1230	CLA	C3C-C2C	4.51	1.46	1.36
21	A	1124	CLA	C3C-C2C	4.51	1.46	1.36
21	B	1217	CLA	C3C-C2C	4.51	1.46	1.36
21	A	1107	CLA	C3C-C2C	4.51	1.46	1.36
21	4	4014	CLA	C3B-C2B	4.51	1.46	1.40
21	B	1203	CLA	C3C-C2C	4.52	1.46	1.36
21	4	4001	CLA	O2A-C1	4.52	1.60	1.46
21	A	1101	CLA	C3C-C2C	4.52	1.46	1.36
25	G	2021	LMG	O7-C10	4.53	1.45	1.35
21	B	1237	CLA	C3C-C2C	4.53	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1104	CLA	O2A-C1	4.53	1.60	1.46
21	A	1141	CLA	O2A-C1	4.53	1.60	1.46
21	4	4005	CLA	O2D-CGD	4.53	1.44	1.33
21	A	1115	CLA	C3C-C2C	4.53	1.46	1.36
21	A	1127	CLA	O2A-C1	4.53	1.60	1.46
21	B	1218	CLA	O2A-C1	4.53	1.60	1.46
21	A	1142	CLA	C3C-C2C	4.54	1.46	1.36
21	J	1302	CLA	C3C-C2C	4.54	1.46	1.36
21	B	1216	CLA	C3C-C2C	4.54	1.46	1.36
21	3	3013	CLA	OBD-CAD	4.54	1.29	1.22
21	1	1002	CLA	O2D-CGD	4.54	1.44	1.33
21	F	1302	CLA	C3C-C2C	4.54	1.46	1.36
21	A	1134	CLA	C3C-C2C	4.54	1.46	1.36
21	3	3004	CLA	C3C-C2C	4.54	1.46	1.36
21	B	1214	CLA	O2A-C1	4.54	1.60	1.46
21	B	1212	CLA	C3C-C2C	4.54	1.46	1.36
21	A	1117	CLA	C3C-C2C	4.54	1.46	1.36
21	L	1502	CLA	O2A-C1	4.55	1.60	1.46
21	3	3015	CLA	C3C-C2C	4.55	1.46	1.36
21	A	1127	CLA	C3C-C2C	4.55	1.46	1.36
21	B	1230	CLA	O2A-C1	4.55	1.60	1.46
21	B	1202	CLA	O2A-C1	4.55	1.60	1.46
21	A	1116	CLA	O2A-C1	4.55	1.60	1.46
21	B	1209	CLA	C3C-C2C	4.56	1.46	1.36
21	A	1140	CLA	C3C-C2C	4.56	1.46	1.36
21	B	1229	CLA	C3C-C2C	4.56	1.46	1.36
21	B	1234	CLA	C3C-C2C	4.56	1.46	1.36
21	2	2002	CLA	O2A-C1	4.56	1.60	1.46
21	A	1105	CLA	C3C-C2C	4.56	1.46	1.36
21	B	1207	CLA	C3C-C2C	4.56	1.46	1.36
21	A	1119	CLA	C3C-C2C	4.56	1.46	1.36
21	A	1126	CLA	C3C-C2C	4.56	1.46	1.36
21	A	1101	CLA	O2A-C1	4.56	1.60	1.46
21	A	1113	CLA	C3C-C2C	4.56	1.46	1.36
21	A	1143	CLA	C3C-C2C	4.57	1.46	1.36
21	1	1006	CLA	OBD-CAD	4.57	1.29	1.22
21	A	1103	CLA	O2A-C1	4.57	1.60	1.46
21	B	1219	CLA	C3C-C2C	4.57	1.46	1.36
21	3	3008	CLA	C3C-C2C	4.57	1.46	1.36
21	B	1206	CLA	C3B-C2B	4.57	1.46	1.40
21	B	1236	CLA	O2A-C1	4.57	1.60	1.46
21	B	1218	CLA	C3C-C2C	4.57	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1223	CLA	C3C-C2C	4.58	1.46	1.36
21	A	1128	CLA	O2A-C1	4.58	1.60	1.46
21	B	1219	CLA	O2A-C1	4.58	1.60	1.46
21	3	3017	CLA	C3C-C2C	4.58	1.46	1.36
21	4	4002	CLA	C3B-C2B	4.58	1.46	1.40
21	B	1234	CLA	O2A-C1	4.58	1.60	1.46
21	J	6014	CLA	C3C-C2C	4.58	1.46	1.36
21	B	1222	CLA	O2A-C1	4.58	1.60	1.46
21	A	1108	CLA	C3C-C2C	4.58	1.46	1.36
21	B	1220	CLA	O2A-C1	4.58	1.60	1.46
21	3	3016	CLA	C3C-C2C	4.58	1.46	1.36
21	B	1238	CLA	C3C-C2C	4.58	1.46	1.36
21	B	1225	CLA	C3C-C2C	4.58	1.46	1.36
21	B	1208	CLA	C3C-C2C	4.58	1.46	1.36
21	A	1129	CLA	O2A-C1	4.58	1.60	1.46
21	3	3011	CLA	CHC-C1C	4.58	1.49	1.35
21	F	1301	CLA	C3C-C2C	4.58	1.46	1.36
21	A	1105	CLA	O2A-C1	4.58	1.60	1.46
21	2	2012	CLA	O2A-C1	4.58	1.60	1.46
21	B	1216	CLA	O2A-C1	4.59	1.60	1.46
21	B	1229	CLA	O2A-C1	4.59	1.60	1.46
21	3	3005	CLA	C3C-C2C	4.59	1.46	1.36
21	B	1219	CLA	C3B-C2B	4.59	1.46	1.40
21	3	3001	CLA	C3C-C2C	4.59	1.46	1.36
21	B	1236	CLA	C3C-C2C	4.59	1.46	1.36
21	A	1115	CLA	O2A-C1	4.59	1.60	1.46
21	3	3006	CLA	O2A-C1	4.59	1.60	1.46
21	B	1207	CLA	O2A-C1	4.59	1.60	1.46
21	B	1223	CLA	O2A-C1	4.59	1.60	1.46
21	B	1202	CLA	C3C-C2C	4.59	1.46	1.36
21	B	1235	CLA	C3C-C2C	4.59	1.46	1.36
21	A	1122	CLA	O2A-C1	4.59	1.60	1.46
21	A	1102	CLA	O2A-C1	4.60	1.60	1.46
21	A	1138	CLA	O2A-C1	4.60	1.60	1.46
21	A	1123	CLA	C3C-C2C	4.60	1.46	1.36
21	2	2005	CLA	O2A-C1	4.60	1.60	1.46
21	1	1011	CLA	O2A-C1	4.60	1.60	1.46
21	B	1220	CLA	C3C-C2C	4.60	1.46	1.36
21	1	1001	CLA	O2A-C1	4.60	1.60	1.46
21	B	1210	CLA	O2A-C1	4.61	1.60	1.46
21	A	1124	CLA	O2A-C1	4.61	1.60	1.46
21	3	3001	CLA	O2A-C1	4.61	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1119	CLA	O2A-C1	4.61	1.60	1.46
21	2	2010	CLA	O2A-C1	4.61	1.60	1.46
21	A	1139	CLA	C3C-C2C	4.61	1.46	1.36
21	A	1135	CLA	O2A-C1	4.61	1.60	1.46
21	A	1102	CLA	C3C-C2C	4.61	1.46	1.36
21	B	1211	CLA	C3C-C2C	4.61	1.46	1.36
21	B	1221	CLA	O2A-C1	4.62	1.60	1.46
21	B	1226	CLA	O2A-C1	4.62	1.60	1.46
21	B	1216	CLA	C3B-C2B	4.62	1.46	1.40
21	3	3012	CLA	C3C-C2C	4.62	1.46	1.36
21	A	1123	CLA	O2A-C1	4.62	1.60	1.46
21	B	1203	CLA	O2A-C1	4.62	1.60	1.46
21	A	1137	CLA	O2A-C1	4.62	1.60	1.46
21	B	1218	CLA	O2D-CGD	4.62	1.45	1.33
21	A	1109	CLA	C3C-C2C	4.63	1.46	1.36
21	A	1106	CLA	O2A-C1	4.63	1.60	1.46
21	4	4012	CLA	O2A-C1	4.63	1.60	1.46
21	B	1222	CLA	C3C-C2C	4.63	1.46	1.36
21	A	1138	CLA	C3C-C2C	4.63	1.46	1.36
21	B	1206	CLA	O2A-C1	4.63	1.60	1.46
21	A	1122	CLA	C3B-C2B	4.63	1.46	1.40
21	2	2003	CLA	O2D-CGD	4.64	1.45	1.33
21	A	1137	CLA	C3B-C2B	4.64	1.46	1.40
21	L	1503	CLA	O2A-C1	4.64	1.60	1.46
21	A	1127	CLA	C3B-C2B	4.64	1.46	1.40
21	A	1141	CLA	C3C-C2C	4.64	1.46	1.36
21	A	1122	CLA	C3C-C2C	4.64	1.46	1.36
21	3	3003	CLA	O2A-C1	4.65	1.60	1.46
21	A	1139	CLA	O2A-C1	4.65	1.60	1.46
21	A	1128	CLA	O2D-CGD	4.65	1.45	1.33
21	B	1237	CLA	O2A-C1	4.65	1.60	1.46
21	B	1224	CLA	O2A-C1	4.65	1.60	1.46
21	A	1136	CLA	C3C-C2C	4.65	1.46	1.36
21	B	1204	CLA	O2A-C1	4.65	1.60	1.46
21	B	1215	CLA	C3B-C2B	4.65	1.46	1.40
21	A	1135	CLA	C3C-C2C	4.66	1.46	1.36
21	B	1205	CLA	O2A-C1	4.66	1.60	1.46
21	B	1208	CLA	O2A-C1	4.67	1.60	1.46
21	B	1235	CLA	O2A-C1	4.67	1.60	1.46
21	2	2001	CLA	C3B-C4B	4.67	1.48	1.40
21	B	1204	CLA	C3C-C2C	4.68	1.46	1.36
21	A	1109	CLA	O2A-C1	4.68	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	J	1302	CLA	O2A-C1	4.69	1.60	1.46
21	1	1006	CLA	C3B-C2B	4.69	1.46	1.40
21	A	1117	CLA	O2A-C1	4.69	1.60	1.46
21	B	1224	CLA	C3C-C2C	4.69	1.46	1.36
21	B	1215	CLA	O2A-C1	4.70	1.60	1.46
21	L	1501	CLA	O2D-CGD	4.70	1.45	1.33
21	B	1211	CLA	O2A-C1	4.70	1.60	1.46
21	B	1225	CLA	O2A-C1	4.70	1.60	1.46
21	B	1222	CLA	O2D-CGD	4.70	1.45	1.33
21	A	1130	CLA	O2D-CGD	4.71	1.45	1.33
21	2	2009	CLA	O2D-CGD	4.71	1.45	1.33
21	J	6015	CLA	C3C-C2C	4.71	1.46	1.36
21	4	4014	CLA	O2D-CGD	4.71	1.45	1.33
21	3	3010	CLA	O2A-C1	4.71	1.60	1.46
21	4	4010	CLA	O2A-C1	4.73	1.60	1.46
21	2	2005	CLA	O2D-CGD	4.73	1.45	1.33
21	3	3008	CLA	O2A-C1	4.73	1.60	1.46
21	J	1302	CLA	C3B-C2B	4.73	1.46	1.40
21	L	1502	CLA	O2D-CGD	4.74	1.45	1.33
21	1	1012	CLA	C3B-C2B	4.75	1.46	1.40
21	B	1220	CLA	C3B-C2B	4.75	1.46	1.40
21	J	6015	CLA	O2A-C1	4.75	1.60	1.46
21	A	1129	CLA	O2D-CGD	4.75	1.45	1.33
21	A	1107	CLA	O2A-C1	4.76	1.61	1.46
21	B	1237	CLA	C3B-C2B	4.76	1.46	1.40
21	A	1116	CLA	C3B-C2B	4.76	1.46	1.40
21	A	1128	CLA	C3B-C2B	4.76	1.46	1.40
21	B	1238	CLA	O2A-C1	4.77	1.61	1.46
21	J	6015	CLA	C3B-C2B	4.77	1.46	1.40
21	B	1225	CLA	C3B-C2B	4.77	1.46	1.40
21	A	1129	CLA	C3B-C2B	4.78	1.46	1.40
21	1	1010	CLA	O2D-CGD	4.78	1.45	1.33
21	3	3002	CLA	O2A-C1	4.78	1.61	1.46
21	3	3004	CLA	O2D-CGD	4.79	1.45	1.33
21	1	1008	CLA	O2A-C1	4.79	1.61	1.46
21	L	1503	CLA	O2D-CGD	4.79	1.45	1.33
21	B	1224	CLA	C3B-C2B	4.79	1.46	1.40
21	A	1102	CLA	O2D-CGD	4.79	1.45	1.33
21	B	1209	CLA	C3B-C2B	4.79	1.46	1.40
21	J	6014	CLA	O2A-C1	4.79	1.61	1.46
21	B	1228	CLA	O2A-C1	4.80	1.61	1.46
21	B	1230	CLA	C3B-C2B	4.80	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1141	CLA	C3B-C2B	4.80	1.46	1.40
21	3	3009	CLA	OBD-CAD	4.80	1.29	1.22
21	A	1101	CLA	O2D-CGD	4.81	1.45	1.33
21	1	1001	CLA	O2D-CGD	4.81	1.45	1.33
21	F	1301	CLA	C3B-C2B	4.81	1.46	1.40
21	A	1135	CLA	C3B-C2B	4.81	1.46	1.40
21	A	1111	CLA	O2A-C1	4.81	1.61	1.46
21	B	1221	CLA	O2D-CGD	4.81	1.45	1.33
21	3	3014	CLA	C3B-C2B	4.82	1.46	1.40
21	A	1139	CLA	C3B-C2B	4.82	1.46	1.40
21	A	1130	CLA	C3B-C2B	4.82	1.46	1.40
21	B	1231	CLA	C3B-C2B	4.82	1.46	1.40
21	B	1209	CLA	O2D-CGD	4.82	1.45	1.33
21	B	1205	CLA	C3B-C2B	4.82	1.46	1.40
21	B	1204	CLA	C3B-C2B	4.82	1.46	1.40
21	L	1503	CLA	C3B-C2B	4.82	1.46	1.40
21	A	1119	CLA	C3B-C2B	4.83	1.46	1.40
21	B	1236	CLA	O2D-CGD	4.84	1.45	1.33
21	A	1134	CLA	C3B-C2B	4.84	1.46	1.40
21	3	3001	CLA	O2D-CGD	4.84	1.45	1.33
21	2	2001	CLA	C3C-C2C	4.85	1.46	1.35
21	L	1501	CLA	C3B-C2B	4.85	1.46	1.40
21	3	3008	CLA	C3B-C2B	4.85	1.46	1.40
21	A	1113	CLA	O2D-CGD	4.85	1.45	1.33
21	A	1140	CLA	C3B-C2B	4.85	1.46	1.40
21	4	4007	CLA	O2D-CGD	4.85	1.45	1.33
21	A	1115	CLA	C3B-C2B	4.85	1.46	1.40
21	A	1136	CLA	C3B-C2B	4.86	1.46	1.40
21	A	1111	CLA	C3B-C2B	4.86	1.46	1.40
21	B	1235	CLA	C3B-C2B	4.86	1.46	1.40
21	A	1109	CLA	C3B-C2B	4.86	1.46	1.40
21	B	1208	CLA	C3B-C2B	4.86	1.46	1.40
21	L	1502	CLA	C3B-C2B	4.86	1.46	1.40
21	B	1229	CLA	O2D-CGD	4.86	1.45	1.33
21	B	1214	CLA	O2D-CGD	4.87	1.45	1.33
21	J	6014	CLA	C3B-C2B	4.87	1.46	1.40
21	A	1104	CLA	C3B-C2B	4.87	1.46	1.40
21	3	3017	CLA	O2D-CGD	4.87	1.45	1.33
21	3	3015	CLA	C3B-C2B	4.87	1.46	1.40
21	A	1126	CLA	C3B-C2B	4.87	1.46	1.40
21	A	1107	CLA	O2D-CGD	4.87	1.45	1.33
21	A	1118	CLA	O2D-CGD	4.88	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1123	CLA	O2D-CGD	4.88	1.45	1.33
21	B	1205	CLA	O2D-CGD	4.88	1.45	1.33
21	A	1120	CLA	C3B-C2B	4.88	1.46	1.40
21	A	1122	CLA	O2D-CGD	4.88	1.45	1.33
21	A	1119	CLA	O2D-CGD	4.88	1.45	1.33
21	3	3012	CLA	O2D-CGD	4.88	1.45	1.33
21	A	1105	CLA	C3B-C2B	4.88	1.46	1.40
21	3	3002	CLA	C3B-C2B	4.88	1.46	1.40
21	A	1111	CLA	O2D-CGD	4.89	1.45	1.33
21	A	1124	CLA	O2D-CGD	4.89	1.45	1.33
21	B	1235	CLA	O2D-CGD	4.89	1.45	1.33
21	2	2006	CLA	O2D-CGD	4.89	1.45	1.33
21	B	1230	CLA	O2D-CGD	4.90	1.45	1.33
21	1	1013	CLA	O2A-C1	4.90	1.61	1.46
21	A	1134	CLA	O2D-CGD	4.90	1.45	1.33
21	B	1201	CLA	O2D-CGD	4.90	1.45	1.33
21	A	1121	CLA	O2D-CGD	4.90	1.45	1.33
21	B	1211	CLA	O2D-CGD	4.90	1.45	1.33
21	3	3016	CLA	C3B-C2B	4.90	1.46	1.40
21	A	1104	CLA	O2D-CGD	4.91	1.45	1.33
21	A	1140	CLA	O2A-C1	4.91	1.61	1.46
21	B	1219	CLA	O2D-CGD	4.91	1.45	1.33
21	A	1137	CLA	O2D-CGD	4.91	1.45	1.33
21	B	1203	CLA	O2D-CGD	4.91	1.45	1.33
21	B	1231	CLA	O2D-CGD	4.91	1.45	1.33
21	1	1006	CLA	O2D-CGD	4.91	1.45	1.33
21	B	1212	CLA	O2D-CGD	4.91	1.45	1.33
21	A	1112	CLA	O2D-CGD	4.92	1.45	1.33
21	A	1135	CLA	O2D-CGD	4.92	1.45	1.33
21	F	1302	CLA	C3B-C2B	4.92	1.46	1.40
21	B	1217	CLA	O2D-CGD	4.92	1.45	1.33
21	A	1112	CLA	C3B-C2B	4.92	1.46	1.40
21	B	1208	CLA	O2D-CGD	4.92	1.45	1.33
21	A	1116	CLA	O2D-CGD	4.92	1.45	1.33
21	B	1220	CLA	O2D-CGD	4.92	1.45	1.33
21	A	1126	CLA	O2D-CGD	4.93	1.45	1.33
21	J	6014	CLA	O2D-CGD	4.93	1.45	1.33
21	A	1106	CLA	O2D-CGD	4.93	1.45	1.33
21	3	3004	CLA	C3B-C2B	4.93	1.46	1.40
21	B	1207	CLA	O2D-CGD	4.93	1.45	1.33
21	B	1223	CLA	O2D-CGD	4.93	1.45	1.33
21	3	3005	CLA	C3B-C2B	4.93	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	1120	CLA	O2D-CGD	4.94	1.45	1.33
21	3	3010	CLA	C3B-C2B	4.94	1.46	1.40
21	F	1301	CLA	O2D-CGD	4.94	1.45	1.33
21	B	1202	CLA	O2D-CGD	4.94	1.45	1.33
21	3	3017	CLA	C3B-C2B	4.94	1.46	1.40
21	A	1127	CLA	O2D-CGD	4.94	1.45	1.33
21	B	1234	CLA	O2D-CGD	4.94	1.45	1.33
21	B	1237	CLA	O2D-CGD	4.94	1.45	1.33
21	A	1139	CLA	O2D-CGD	4.95	1.45	1.33
21	3	3006	CLA	C3B-C2B	4.95	1.46	1.40
21	A	1113	CLA	C3B-C2B	4.95	1.46	1.40
21	A	1105	CLA	O2D-CGD	4.95	1.45	1.33
21	B	1224	CLA	O2D-CGD	4.95	1.45	1.33
21	A	1103	CLA	C3B-C2B	4.95	1.46	1.40
21	B	1206	CLA	O2D-CGD	4.95	1.45	1.33
21	3	3014	CLA	O2D-CGD	4.95	1.45	1.33
21	1	1014	CLA	O2D-CGD	4.95	1.45	1.33
21	F	1302	CLA	O2D-CGD	4.95	1.45	1.33
21	2	2006	CLA	C3B-C2B	4.96	1.46	1.40
21	3	3010	CLA	O2D-CGD	4.96	1.45	1.33
21	H	1000	CLA	O2D-CGD	4.96	1.45	1.33
21	B	1218	CLA	C3B-C2B	4.96	1.46	1.40
21	2	2008	CLA	O2A-C1	4.96	1.61	1.46
21	A	1136	CLA	O2D-CGD	4.96	1.45	1.33
21	B	1238	CLA	O2D-CGD	4.96	1.45	1.33
21	B	1238	CLA	C3B-C2B	4.96	1.46	1.40
21	B	1236	CLA	C3B-C2B	4.96	1.46	1.40
21	B	1216	CLA	O2D-CGD	4.97	1.45	1.33
21	B	1215	CLA	O2D-CGD	4.97	1.45	1.33
21	B	1217	CLA	C3B-C2B	4.97	1.46	1.40
21	B	1210	CLA	O2D-CGD	4.97	1.45	1.33
21	A	1114	CLA	O2D-CGD	4.97	1.45	1.33
21	3	3006	CLA	O2D-CGD	4.97	1.45	1.33
21	A	1143	CLA	O2D-CGD	4.97	1.45	1.33
21	A	1110	CLA	O2D-CGD	4.97	1.45	1.33
21	A	1142	CLA	O2D-CGD	4.97	1.45	1.33
21	B	1203	CLA	C3B-C2B	4.97	1.46	1.40
21	A	1103	CLA	O2D-CGD	4.98	1.45	1.33
21	J	1302	CLA	O2D-CGD	4.98	1.45	1.33
21	A	1141	CLA	O2D-CGD	4.98	1.45	1.33
21	3	3015	CLA	O2D-CGD	4.98	1.45	1.33
21	A	1138	CLA	C3B-C2B	4.99	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	3005	CLA	O2D-CGD	4.99	1.45	1.33
21	3	3002	CLA	O2D-CGD	4.99	1.45	1.33
21	A	1115	CLA	O2D-CGD	4.99	1.45	1.33
21	A	1143	CLA	C3B-C2B	4.99	1.46	1.40
21	F	1303	CLA	O2A-C1	4.99	1.59	1.42
21	A	1140	CLA	O2D-CGD	4.99	1.45	1.33
21	A	1117	CLA	O2D-CGD	4.99	1.45	1.33
21	B	1212	CLA	C3B-C2B	4.99	1.46	1.40
21	B	1234	CLA	C3B-C2B	5.00	1.46	1.40
21	3	3016	CLA	O2D-CGD	5.00	1.46	1.33
21	A	1108	CLA	O2D-CGD	5.00	1.46	1.33
21	3	3003	CLA	C3B-C2B	5.00	1.46	1.40
21	A	1109	CLA	O2D-CGD	5.00	1.46	1.33
21	B	1204	CLA	O2D-CGD	5.01	1.46	1.33
21	B	1225	CLA	O2D-CGD	5.01	1.46	1.33
21	B	1210	CLA	C3C-C2C	5.01	1.47	1.36
21	A	1138	CLA	O2D-CGD	5.01	1.46	1.33
21	B	1201	CLA	C3B-C2B	5.02	1.46	1.40
21	A	9012	CLA	C3B-C2B	5.02	1.46	1.40
21	2	2003	CLA	C3C-C2C	5.02	1.47	1.36
21	2	2011	CLA	O2A-C1	5.02	1.61	1.46
21	3	3001	CLA	C3B-C2B	5.03	1.46	1.40
21	A	1121	CLA	C3B-C2B	5.03	1.47	1.40
21	B	1207	CLA	C3B-C2B	5.04	1.47	1.40
21	A	1108	CLA	C3B-C2B	5.05	1.47	1.40
21	A	1102	CLA	C3B-C2B	5.06	1.47	1.40
21	4	4005	CLA	C3B-C2B	5.08	1.47	1.40
21	3	3009	CLA	O2D-CGD	5.08	1.46	1.33
21	3	3013	CLA	C3B-C2B	5.09	1.47	1.40
21	B	1211	CLA	C3B-C2B	5.11	1.47	1.40
21	2	2010	CLA	O2D-CGD	5.11	1.46	1.33
21	A	1124	CLA	C3B-C2B	5.15	1.47	1.40
21	A	1117	CLA	C3B-C2B	5.15	1.47	1.40
21	A	1107	CLA	C3B-C2B	5.16	1.47	1.40
21	3	3003	CLA	O2D-CGD	5.18	1.46	1.33
21	4	4006	CLA	O2D-CGD	5.21	1.46	1.33
21	A	1101	CLA	C3B-C2B	5.22	1.47	1.40
21	B	1202	CLA	C3B-C2B	5.22	1.47	1.40
21	A	1123	CLA	C3B-C2B	5.28	1.47	1.40
21	B	1222	CLA	C3B-C2B	5.29	1.47	1.40
21	B	1229	CLA	C3B-C2B	5.31	1.47	1.40
18	B	5002	PQN	C10-C5	5.32	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	1214	CLA	C3B-C2B	5.33	1.47	1.40
21	B	1221	CLA	C3B-C2B	5.35	1.47	1.40
21	A	1114	CLA	C3B-C2B	5.35	1.47	1.40
18	A	5001	PQN	C10-C5	5.39	1.49	1.40
21	A	1106	CLA	C3B-C2B	5.43	1.47	1.40
21	2	2001	CLA	C2B-C1B	5.44	1.49	1.40
21	B	1210	CLA	C3B-C2B	5.50	1.47	1.40
21	B	1223	CLA	C3B-C2B	5.50	1.47	1.40
21	2	2008	CLA	O2D-CGD	5.51	1.47	1.33
21	4	4015	CLA	O2A-C1	5.69	1.59	1.45
18	B	5002	PQN	C3-C2	5.89	1.49	1.35
18	A	5001	PQN	C3-C2	5.95	1.49	1.35
27	4	4503	NEX	C7-C8	6.12	1.43	1.32
21	B	1209	CLA	O2A-C1	6.18	1.60	1.45
21	A	1130	CLA	O2A-C1	6.18	1.60	1.45
21	B	1201	CLA	O2A-C1	6.19	1.60	1.45
21	A	1120	CLA	O2A-C1	6.19	1.60	1.45
21	A	1121	CLA	O2A-C1	6.19	1.60	1.45
21	A	1108	CLA	O2A-C1	6.19	1.60	1.45
21	A	1134	CLA	O2A-C1	6.19	1.60	1.45
21	A	1133	CLA	O2A-C1	6.20	1.60	1.45
21	A	1113	CLA	O2A-C1	6.20	1.60	1.45
21	A	1118	CLA	O2A-C1	6.20	1.60	1.45
21	B	1231	CLA	O2A-C1	6.22	1.60	1.45
21	B	1212	CLA	O2A-C1	6.22	1.60	1.45
21	F	1302	CLA	O2A-C1	6.23	1.60	1.45
21	H	1000	CLA	O2A-C1	6.23	1.60	1.45
21	A	1112	CLA	O2A-C1	6.24	1.60	1.45
21	2	2009	CLA	O2A-C1	6.24	1.60	1.45
21	A	1114	CLA	O2A-C1	6.24	1.60	1.45
21	L	1501	CLA	O2A-C1	6.25	1.60	1.45
21	B	1217	CLA	O2A-C1	6.26	1.60	1.45
21	G	1002	CLA	O2A-C1	6.27	1.60	1.45
21	3	3011	CLA	O2A-C1	6.40	1.60	1.45
21	3	3009	CLA	O2A-C1	6.46	1.61	1.45
26	4	4502	LUT	C24-C25	12.93	1.50	1.33
26	1	1502	LUT	C24-C25	12.97	1.50	1.33
26	4	4501	LUT	C24-C25	13.05	1.50	1.33
26	1	1501	LUT	C24-C25	13.73	1.51	1.33
26	2	2502	LUT	C24-C25	13.78	1.51	1.33
26	2	2501	LUT	C24-C25	14.17	1.51	1.33

All (2891) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1502	LUT	C23-C24-C25	-21.29	105.32	125.22
26	2	2501	LUT	C23-C24-C25	-20.23	106.31	125.22
19	F	6016	BCR	C32-C1-C6	-18.88	80.71	110.30
19	B	6006	BCR	C32-C1-C6	-18.68	81.02	110.30
26	4	4501	LUT	C23-C24-C25	-18.63	107.81	125.22
26	1	1501	LUT	C23-C24-C25	-17.48	108.88	125.22
19	A	6011	BCR	C31-C1-C6	-17.22	83.30	110.30
19	F	6014	BCR	C31-C1-C6	-16.32	84.72	110.30
19	A	6008	BCR	C31-C1-C6	-16.31	84.73	110.30
19	I	6018	BCR	C31-C1-C6	-16.12	85.03	110.30
19	I	6018	BCR	C32-C1-C6	-15.91	85.36	110.30
26	4	4502	LUT	C23-C24-C25	-15.51	110.72	125.22
19	A	6008	BCR	C32-C1-C6	-15.17	86.52	110.30
19	F	6014	BCR	C32-C1-C6	-15.09	86.64	110.30
19	B	6006	BCR	C29-C30-C25	-14.16	87.95	110.36
19	A	6011	BCR	C32-C1-C6	-14.08	88.22	110.30
19	F	6014	BCR	C29-C30-C25	-13.93	88.30	110.36
19	I	6018	BCR	C29-C30-C25	-13.84	88.46	110.36
19	A	6008	BCR	C29-C30-C25	-13.15	89.54	110.36
19	F	6016	BCR	C29-C30-C25	-11.97	91.42	110.36
19	B	6006	BCR	C31-C1-C6	-11.50	92.28	110.30
19	A	6011	BCR	C29-C30-C25	-11.46	92.22	110.36
19	F	6016	BCR	C31-C1-C6	-11.25	92.67	110.30
26	2	2502	LUT	C23-C24-C25	-10.69	115.23	125.22
19	B	6006	BCR	C2-C1-C6	-10.27	94.10	110.36
26	1	1501	LUT	C7-C8-C9	-10.13	110.78	126.22
19	F	6016	BCR	C2-C1-C6	-10.10	94.37	110.36
19	A	6008	BCR	C2-C1-C6	-9.90	94.69	110.36
19	I	6018	BCR	C2-C1-C6	-9.82	94.82	110.36
19	F	6014	BCR	C2-C1-C6	-9.65	95.08	110.36
19	A	6011	BCR	C2-C1-C6	-9.29	95.66	110.36
21	B	9022	CLA	OBD-CAD-CBD	-8.71	112.80	125.94
21	2	2001	CLA	C3B-C2B-C1B	-8.63	98.74	106.29
19	A	6011	BCR	C40-C30-C29	-7.73	81.11	108.79
19	B	6004	BCR	C24-C23-C22	-7.56	114.69	126.22
19	F	6016	BCR	C40-C30-C29	-7.55	81.74	108.79
19	F	6014	BCR	C39-C30-C29	-7.46	82.07	108.79
19	J	6013	BCR	C7-C8-C9	-7.35	115.01	126.22
26	4	4502	LUT	C7-C8-C9	-7.31	115.07	126.22
19	I	6018	BCR	C40-C30-C29	-7.27	82.73	108.79
19	A	6008	BCR	C40-C30-C29	-7.25	82.83	108.79
19	B	6006	BCR	C40-C30-C29	-7.17	83.11	108.79
21	A	9012	CLA	OBD-CAD-CBD	-7.03	115.33	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	6007	BCR	C7-C8-C9	-6.81	115.84	126.22
19	A	6011	BCR	C38-C26-C25	-6.67	118.05	124.61
21	2	2011	CLA	O2A-CGA-O1A	-6.65	106.32	123.49
19	J	6013	BCR	C15-C14-C13	-6.61	117.65	127.20
26	1	1502	LUT	C11-C10-C9	-6.45	117.88	127.20
19	B	6006	BCR	C7-C8-C9	-6.37	116.51	126.22
21	4	4008	CLA	O2A-CGA-O1A	-6.36	107.09	123.49
19	A	6007	BCR	C15-C14-C13	-6.33	118.05	127.20
19	A	6002	BCR	C24-C23-C22	-6.33	116.57	126.22
21	4	4008	CLA	OBD-CAD-C3D	-6.32	115.46	128.35
21	4	4005	CLA	OBD-CAD-C3D	-6.20	115.69	128.35
21	4	4014	CLA	OBD-CAD-CBD	-6.20	116.58	125.94
21	1	1002	CLA	C3B-CAB-CBB	-6.12	113.79	126.32
21	3	3012	CLA	C1C-C2C-C3C	-6.12	99.59	106.91
21	B	1226	CLA	O2A-CGA-O1A	-6.10	107.75	123.49
21	1	1011	CLA	O2A-CGA-O1A	-6.09	107.77	123.49
19	F	6014	BCR	C38-C26-C25	-6.06	118.65	124.61
19	B	6005	BCR	C15-C14-C13	-6.05	118.46	127.20
21	4	4012	CLA	O2A-CGA-O1A	-6.02	107.96	123.49
26	1	1502	LUT	C18-C5-C6	-6.02	118.70	124.61
26	4	4502	LUT	C31-C30-C29	-6.01	118.52	127.20
19	L	6020	BCR	C24-C23-C22	-5.96	117.13	126.22
21	4	4011	CLA	O2A-CGA-O1A	-5.91	108.23	123.49
19	F	6016	BCR	C24-C23-C22	-5.89	117.24	126.22
19	A	6008	BCR	C24-C23-C22	-5.87	117.27	126.22
19	A	6007	BCR	C24-C23-C22	-5.82	117.34	126.22
19	J	6012	BCR	C7-C8-C9	-5.82	117.34	126.22
26	1	1502	LUT	C7-C8-C9	-5.82	117.34	126.22
19	B	6010	BCR	C38-C26-C25	-5.79	118.92	124.61
21	B	1213	CLA	O2A-CGA-O1A	-5.78	108.59	123.49
21	B	1202	CLA	O2A-CGA-O1A	-5.77	108.61	123.49
19	J	6012	BCR	C24-C23-C22	-5.76	117.43	126.22
21	A	1125	CLA	O2A-CGA-O1A	-5.76	108.62	123.49
26	4	4501	LUT	C7-C8-C9	-5.75	117.45	126.22
21	3	3012	CLA	O1D-CGD-CBD	-5.73	116.41	124.62
26	4	4501	LUT	C31-C30-C29	-5.72	118.93	127.20
19	A	6003	BCR	C24-C23-C22	-5.71	117.51	126.22
19	B	6005	BCR	C38-C26-C25	-5.69	119.01	124.61
21	4	4011	CLA	C1C-C2C-C3C	-5.69	100.11	106.91
19	B	6005	BCR	C33-C5-C6	-5.67	119.03	124.61
26	1	1501	LUT	C22-C23-C24	-5.67	105.08	111.75
21	A	9013	CLA	O2A-CGA-O1A	-5.67	108.86	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1132	CLA	O2A-CGA-O1A	-5.64	108.94	123.49
21	3	3002	CLA	O2A-CGA-O1A	-5.64	108.95	123.49
21	2	2013	CLA	O2A-CGA-O1A	-5.63	108.97	123.49
19	B	6005	BCR	C7-C8-C9	-5.61	117.67	126.22
21	4	4013	CLA	C1C-C2C-C3C	-5.58	100.23	106.91
19	A	6011	BCR	C39-C30-C29	-5.57	88.85	108.79
21	B	1239	CLA	O2A-CGA-O1A	-5.54	109.20	123.49
19	B	6009	BCR	C38-C26-C25	-5.52	119.18	124.61
21	1	1001	CLA	O2A-CGA-O1A	-5.52	109.25	123.49
21	A	1131	CLA	O2A-CGA-O1A	-5.51	109.27	123.49
21	2	2002	CLA	O2A-CGA-O1A	-5.49	109.32	123.49
21	3	3013	CLA	C1C-C2C-C3C	-5.47	100.36	106.91
19	F	6016	BCR	C38-C26-C25	-5.47	119.23	124.61
21	A	1101	CLA	O2A-CGA-O1A	-5.47	109.38	123.49
21	2	2004	CLA	O2A-CGA-O1A	-5.47	109.39	123.49
19	A	6008	BCR	C3-C4-C5	-5.45	105.22	113.87
21	2	2004	CLA	C3B-CAB-CBB	-5.43	115.21	126.32
21	3	3010	CLA	O2A-CGA-O1A	-5.43	109.49	123.49
21	1	1009	CLA	O1D-CGD-CBD	-5.42	116.86	124.62
26	1	1502	LUT	C1-C6-C5	-5.40	114.74	122.66
19	B	6005	BCR	C24-C23-C22	-5.39	118.00	126.22
19	J	6012	BCR	C33-C5-C6	-5.39	119.31	124.61
21	1	1002	CLA	C1C-C2C-C3C	-5.39	100.46	106.91
21	G	1001	CLA	O2A-CGA-O1A	-5.36	109.66	123.49
19	B	6009	BCR	C24-C23-C22	-5.36	118.05	126.22
21	4	4004	CLA	O2A-CGA-O1A	-5.35	109.68	123.49
19	F	6016	BCR	C39-C30-C29	-5.33	89.69	108.79
21	4	4002	CLA	C1C-C2C-C3C	-5.32	100.54	106.91
19	A	6008	BCR	C7-C8-C9	-5.31	118.13	126.22
21	2	2001	CLA	C3C-C2C-C1C	-5.28	101.29	107.23
21	3	3010	CLA	C1C-C2C-C3C	-5.28	100.59	106.91
19	A	6008	BCR	C38-C26-C25	-5.28	119.42	124.61
21	1	1005	CLA	O2A-CGA-O1A	-5.28	109.87	123.49
26	4	4501	LUT	C18-C5-C6	-5.28	119.42	124.61
19	F	6016	BCR	C7-C8-C9	-5.26	118.20	126.22
19	A	6008	BCR	C39-C30-C29	-5.26	89.96	108.79
21	B	1235	CLA	O2A-CGA-O1A	-5.25	109.95	123.49
21	1	1009	CLA	C1C-C2C-C3C	-5.24	100.64	106.91
19	J	6013	BCR	C38-C26-C25	-5.24	119.46	124.61
21	4	4009	CLA	C1C-C2C-C3C	-5.23	100.65	106.91
21	1	1001	CLA	C1C-C2C-C3C	-5.22	100.66	106.91
19	B	6006	BCR	C38-C26-C25	-5.22	119.48	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4010	CLA	C1C-C2C-C3C	-5.21	100.68	106.91
21	4	4013	CLA	O2A-CGA-O1A	-5.20	110.07	123.49
21	3	3008	CLA	C1C-C2C-C3C	-5.18	100.71	106.91
21	1	1004	CLA	O2A-CGA-O1A	-5.18	110.12	123.49
21	1	1006	CLA	O2A-CGA-O1A	-5.18	110.12	123.49
21	2	2006	CLA	O2A-CGA-O1A	-5.17	110.14	123.49
21	4	4005	CLA	C1C-C2C-C3C	-5.17	100.72	106.91
21	3	3003	CLA	O2A-CGA-O1A	-5.16	110.17	123.49
21	A	1118	CLA	C1C-C2C-C3C	-5.15	100.75	106.91
21	4	4001	CLA	O2A-CGA-O1A	-5.15	110.20	123.49
19	J	6013	BCR	C24-C23-C22	-5.15	118.37	126.22
19	A	6008	BCR	C15-C14-C13	-5.15	119.77	127.20
26	4	4501	LUT	C11-C10-C9	-5.14	119.77	127.20
19	I	6018	BCR	C3-C4-C5	-5.14	105.71	113.87
21	B	1227	CLA	C1C-C2C-C3C	-5.14	100.76	106.91
19	I	6018	BCR	C39-C30-C29	-5.14	90.39	108.79
21	B	1224	CLA	O2A-CGA-O1A	-5.13	110.26	123.49
21	A	1111	CLA	O2A-CGA-O1A	-5.12	110.27	123.49
19	B	6006	BCR	C39-C30-C29	-5.11	90.47	108.79
19	F	6016	BCR	C3-C4-C5	-5.11	105.76	113.87
26	1	1501	LUT	C31-C30-C29	-5.11	119.82	127.20
21	4	4009	CLA	O2A-CGA-O1A	-5.09	110.36	123.49
21	H	1000	CLA	C3B-CAB-CBB	-5.08	115.91	126.32
21	4	4008	CLA	C1C-C2C-C3C	-5.08	100.83	106.91
21	J	6015	CLA	C1C-C2C-C3C	-5.08	100.83	106.91
19	A	6017	BCR	C38-C26-C25	-5.08	119.62	124.61
19	F	6014	BCR	C7-C8-C9	-5.08	118.48	126.22
21	A	1109	CLA	O2A-CGA-O1A	-5.07	110.41	123.49
21	B	1205	CLA	O2A-CGA-O1A	-5.07	110.41	123.49
21	J	6014	CLA	O2A-CGA-O1A	-5.06	110.43	123.49
21	3	3014	CLA	C1C-C2C-C3C	-5.06	100.86	106.91
19	B	6011	BCR	C15-C14-C13	-5.05	119.90	127.20
21	1	1009	CLA	O2A-CGA-O1A	-5.05	110.45	123.49
19	B	6006	BCR	C3-C4-C5	-5.05	105.85	113.87
21	4	4005	CLA	C3B-CAB-CBB	-5.05	115.98	126.32
21	4	4012	CLA	C3B-CAB-CBB	-5.05	115.98	126.32
21	2	2012	CLA	C1C-C2C-C3C	-5.05	100.87	106.91
21	1	1007	CLA	O2A-CGA-O1A	-5.04	110.49	123.49
19	B	6004	BCR	C34-C9-C10	-5.04	115.46	122.90
21	B	1237	CLA	O2A-CGA-O1A	-5.04	110.50	123.49
21	J	1302	CLA	O2A-CGA-O1A	-5.03	110.52	123.49
19	F	6016	BCR	C28-C27-C26	-5.02	105.89	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	9011	CL0	O2A-CGA-O1A	-5.02	110.53	123.49
21	G	1002	CLA	C1C-C2C-C3C	-5.02	100.91	106.91
21	4	4006	CLA	C1C-C2C-C3C	-5.01	100.92	106.91
21	1	1011	CLA	C1C-C2C-C3C	-5.01	100.92	106.91
21	B	1240	CLA	O2A-CGA-O1A	-5.01	110.57	123.49
21	3	3013	CLA	O2A-CGA-O1A	-5.00	110.58	123.49
21	A	1125	CLA	OBD-CAD-C3D	-5.00	118.16	128.35
21	A	1129	CLA	O2A-CGA-O1A	-4.99	110.62	123.49
19	I	6018	BCR	C38-C26-C25	-4.99	119.71	124.61
21	1	1003	CLA	C1C-C2C-C3C	-4.98	100.95	106.91
21	B	1211	CLA	O2A-CGA-O1A	-4.98	110.64	123.49
21	B	1206	CLA	C1C-C2C-C3C	-4.98	100.95	106.91
21	1	1006	CLA	C1C-C2C-C3C	-4.98	100.95	106.91
21	B	1222	CLA	O2A-CGA-O1A	-4.97	110.66	123.49
21	4	4008	CLA	CAA-C2A-C3A	-4.97	98.93	113.22
27	4	4503	NEX	C20-C13-C14	-4.97	115.56	122.90
21	B	1210	CLA	O2A-CGA-O1A	-4.95	110.73	123.49
19	L	6019	BCR	C24-C23-C22	-4.94	118.69	126.22
21	A	9012	CLA	O2A-CGA-O1A	-4.94	110.75	123.49
21	B	9010	CLA	C1C-C2C-C3C	-4.93	101.01	106.91
21	4	4001	CLA	C1C-C2C-C3C	-4.93	101.02	106.91
19	I	6020	BCR	C7-C8-C9	-4.93	118.71	126.22
21	A	1133	CLA	C1C-C2C-C3C	-4.91	101.03	106.91
21	A	1124	CLA	O2A-CGA-O1A	-4.91	110.82	123.49
21	4	4011	CLA	C3B-CAB-CBB	-4.91	116.27	126.32
21	4	4007	CLA	C1C-C2C-C3C	-4.90	101.04	106.91
21	3	3009	CLA	C1C-C2C-C3C	-4.90	101.05	106.91
21	2	2008	CLA	O2A-CGA-O1A	-4.89	110.86	123.49
21	B	1207	CLA	C1C-C2C-C3C	-4.89	101.06	106.91
21	3	3017	CLA	C1C-C2C-C3C	-4.89	101.06	106.91
21	2	2012	CLA	C3B-CAB-CBB	-4.88	116.33	126.32
21	1	1012	CLA	O2A-CGA-O1A	-4.88	110.90	123.49
19	B	6006	BCR	C28-C27-C26	-4.87	106.14	113.87
21	2	2004	CLA	CGD-CBD-CHA	-4.87	100.87	112.68
21	2	2007	CLA	C1C-C2C-C3C	-4.87	101.08	106.91
21	1	1009	CLA	CMB-C2B-C1B	-4.87	120.31	128.36
21	A	1110	CLA	O2A-CGA-O1A	-4.87	110.92	123.49
21	B	9022	CLA	C1C-C2C-C3C	-4.86	101.10	106.91
19	B	6010	BCR	C15-C14-C13	-4.85	120.19	127.20
21	H	1000	CLA	C1C-C2C-C3C	-4.85	101.11	106.91
21	4	4006	CLA	C3B-CAB-CBB	-4.85	116.40	126.32
19	A	6003	BCR	C38-C26-C25	-4.85	119.85	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1004	CLA	C1C-C2C-C3C	-4.85	101.11	106.91
21	B	1218	CLA	O2A-CGA-O1A	-4.84	111.00	123.49
21	1	1009	CLA	C3B-CAB-CBB	-4.83	116.43	126.32
21	B	1223	CLA	O2A-CGA-O1A	-4.83	111.03	123.49
21	B	1225	CLA	O2A-CGA-O1A	-4.82	111.05	123.49
21	A	1122	CLA	O2A-CGA-O1A	-4.82	111.06	123.49
21	B	9010	CLA	O2A-CGA-O1A	-4.81	111.07	123.49
21	B	1204	CLA	O2A-CGA-O1A	-4.81	111.07	123.49
21	2	2003	CLA	O2A-CGA-O1A	-4.80	111.09	123.49
21	A	1137	CLA	C1C-C2C-C3C	-4.80	101.17	106.91
21	B	1228	CLA	O2A-CGA-O1A	-4.80	111.10	123.49
21	1	1014	CLA	O1D-CGD-CBD	-4.80	117.74	124.62
21	2	2014	CLA	C1C-C2C-C3C	-4.80	101.17	106.91
21	B	1218	CLA	C1C-C2C-C3C	-4.79	101.17	106.91
21	2	2010	CLA	O2A-CGA-O1A	-4.79	111.12	123.49
21	4	4013	CLA	C3B-CAB-CBB	-4.79	116.52	126.32
21	B	1215	CLA	C1C-C2C-C3C	-4.78	101.19	106.91
21	2	2011	CLA	C1C-C2C-C3C	-4.78	101.19	106.91
21	F	1303	CLA	C3B-CAB-CBB	-4.76	116.57	126.32
21	4	4001	CLA	O1D-CGD-CBD	-4.76	117.80	124.62
21	B	1236	CLA	C1C-C2C-C3C	-4.75	101.22	106.91
21	4	4005	CLA	OBD-CAD-CBD	-4.75	118.77	125.94
21	2	2010	CLA	C1C-C2C-C3C	-4.74	101.23	106.91
21	A	1126	CLA	O2A-CGA-O1A	-4.74	111.27	123.49
21	B	1229	CLA	O2A-CGA-O1A	-4.74	111.27	123.49
21	B	9022	CLA	C3B-CAB-CBB	-4.73	116.63	126.32
21	3	3011	CLA	O2D-CGD-O1D	-4.73	114.02	123.79
21	A	1116	CLA	O2A-CGA-O1A	-4.73	111.29	123.49
21	4	4004	CLA	C3B-CAB-CBB	-4.73	116.65	126.32
21	B	1220	CLA	O2A-CGA-O1A	-4.72	111.30	123.49
21	A	1135	CLA	C1C-C2C-C3C	-4.72	101.26	106.91
21	L	1502	CLA	O2A-CGA-O1A	-4.72	111.32	123.49
21	3	3006	CLA	O2A-CGA-O1A	-4.72	111.32	123.49
21	B	1230	CLA	O2A-CGA-O1A	-4.72	111.32	123.49
21	B	1202	CLA	C1C-C2C-C3C	-4.72	101.27	106.91
21	A	1121	CLA	C1C-C2C-C3C	-4.71	101.27	106.91
21	2	2002	CLA	C1C-C2C-C3C	-4.71	101.27	106.91
21	B	1226	CLA	C1C-C2C-C3C	-4.71	101.28	106.91
19	I	6018	BCR	C7-C8-C9	-4.71	119.04	126.22
21	B	1203	CLA	O2A-CGA-O1A	-4.71	111.34	123.49
21	B	1207	CLA	O2A-CGA-O1A	-4.70	111.35	123.49
21	A	1106	CLA	O2A-CGA-O1A	-4.70	111.36	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	6008	BCR	C33-C5-C6	-4.69	120.00	124.61
21	A	1102	CLA	C1C-C2C-C3C	-4.69	101.30	106.91
19	F	6014	BCR	C33-C5-C6	-4.69	120.00	124.61
19	I	6018	BCR	C28-C27-C26	-4.68	106.43	113.87
21	A	1125	CLA	C1C-C2C-C3C	-4.68	101.31	106.91
19	A	6011	BCR	C28-C27-C26	-4.68	106.44	113.87
21	B	1208	CLA	O2A-CGA-O1A	-4.68	111.41	123.49
21	2	2013	CLA	C3B-CAB-CBB	-4.68	116.75	126.32
21	A	1102	CLA	O2A-CGA-O1A	-4.68	111.42	123.49
21	2	2012	CLA	O2A-CGA-O1A	-4.67	111.43	123.49
21	A	1107	CLA	O2A-CGA-O1A	-4.67	111.44	123.49
21	B	1217	CLA	C1C-C2C-C3C	-4.67	101.33	106.91
21	B	1221	CLA	O2A-CGA-O1A	-4.67	111.45	123.49
21	2	2006	CLA	C1C-C2C-C3C	-4.66	101.33	106.91
21	A	1104	CLA	O2A-CGA-O1A	-4.66	111.47	123.49
21	B	9022	CLA	O2A-CGA-O1A	-4.66	111.47	123.49
21	B	1205	CLA	C1C-C2C-C3C	-4.65	101.35	106.91
21	A	1123	CLA	O2A-CGA-O1A	-4.65	111.50	123.49
21	B	1223	CLA	C1C-C2C-C3C	-4.64	101.35	106.91
21	3	3016	CLA	C1C-C2C-C3C	-4.64	101.36	106.91
21	A	1127	CLA	O2A-CGA-O1A	-4.64	111.53	123.49
21	B	1213	CLA	C3B-CAB-CBB	-4.63	116.83	126.32
21	B	1206	CLA	O2A-CGA-O1A	-4.63	111.53	123.49
21	F	1301	CLA	C1C-C2C-C3C	-4.63	101.37	106.91
21	A	1138	CLA	O2A-CGA-O1A	-4.63	111.53	123.49
21	B	1235	CLA	C1C-C2C-C3C	-4.63	101.37	106.91
19	B	6009	BCR	C3-C4-C5	-4.62	106.53	113.87
21	G	1001	CLA	C1C-C2C-C3C	-4.62	101.38	106.91
21	A	1134	CLA	C1C-C2C-C3C	-4.62	101.38	106.91
21	L	1503	CLA	C1C-C2C-C3C	-4.62	101.38	106.91
21	A	1136	CLA	O2A-CGA-O1A	-4.62	111.56	123.49
21	A	1119	CLA	O2A-CGA-O1A	-4.62	111.57	123.49
21	A	1105	CLA	O2A-CGA-O1A	-4.62	111.58	123.49
21	B	1221	CLA	C1C-C2C-C3C	-4.62	101.39	106.91
19	B	6009	BCR	C33-C5-C6	-4.61	120.07	124.61
21	B	1238	CLA	O2A-CGA-O1A	-4.61	111.58	123.49
21	A	1128	CLA	C1C-C2C-C3C	-4.61	101.39	106.91
21	B	1228	CLA	C1C-C2C-C3C	-4.61	101.40	106.91
21	L	1501	CLA	C1C-C2C-C3C	-4.61	101.40	106.91
21	A	1140	CLA	C1C-C2C-C3C	-4.61	101.40	106.91
21	J	6014	CLA	C1C-C2C-C3C	-4.60	101.40	106.91
21	A	1139	CLA	C1C-C2C-C3C	-4.60	101.40	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1106	CLA	C1C-C2C-C3C	-4.60	101.41	106.91
21	B	1219	CLA	O2A-CGA-O1A	-4.60	111.62	123.49
21	A	1113	CLA	C1C-C2C-C3C	-4.60	101.41	106.91
21	A	1114	CLA	C1C-C2C-C3C	-4.60	101.41	106.91
21	B	1234	CLA	C1C-C2C-C3C	-4.60	101.41	106.91
21	1	1013	CLA	O2A-CGA-O1A	-4.60	111.63	123.49
21	B	1216	CLA	C1C-C2C-C3C	-4.59	101.41	106.91
21	B	1231	CLA	C1C-C2C-C3C	-4.59	101.42	106.91
26	1	1502	LUT	C31-C30-C29	-4.59	120.57	127.20
21	J	1302	CLA	C1C-C2C-C3C	-4.59	101.42	106.91
21	A	1135	CLA	O2A-CGA-O1A	-4.59	111.65	123.49
21	B	1229	CLA	C1C-C2C-C3C	-4.59	101.42	106.91
21	B	1225	CLA	C1C-C2C-C3C	-4.59	101.42	106.91
21	B	1214	CLA	O2A-CGA-O1A	-4.58	111.66	123.49
21	A	1122	CLA	C1C-C2C-C3C	-4.58	101.43	106.91
21	A	1138	CLA	C1C-C2C-C3C	-4.58	101.43	106.91
21	A	1104	CLA	C1C-C2C-C3C	-4.58	101.43	106.91
21	A	1120	CLA	C1C-C2C-C3C	-4.58	101.43	106.91
21	B	1239	CLA	C1C-C2C-C3C	-4.58	101.44	106.91
21	2	2009	CLA	C1C-C2C-C3C	-4.58	101.44	106.91
21	A	1142	CLA	C1C-C2C-C3C	-4.58	101.44	106.91
19	B	6010	BCR	C7-C8-C9	-4.57	119.25	126.22
21	A	1115	CLA	O2A-CGA-O1A	-4.57	111.69	123.49
21	2	2003	CLA	C1C-C2C-C3C	-4.57	101.44	106.91
19	B	6011	BCR	C33-C5-C6	-4.57	120.12	124.61
21	A	1131	CLA	C1C-C2C-C3C	-4.57	101.44	106.91
21	B	1215	CLA	O2A-CGA-O1A	-4.57	111.70	123.49
21	B	1219	CLA	C1C-C2C-C3C	-4.57	101.44	106.91
21	A	1119	CLA	C1C-C2C-C3C	-4.57	101.45	106.91
21	A	1136	CLA	C1C-C2C-C3C	-4.56	101.45	106.91
21	A	1108	CLA	C1C-C2C-C3C	-4.56	101.46	106.91
19	G	2011	BCR	C36-C18-C17	-4.56	116.17	122.90
21	1	1008	CLA	O2A-CGA-O1A	-4.55	111.75	123.49
21	3	3004	CLA	C1C-C2C-C3C	-4.55	101.47	106.91
21	A	1143	CLA	C1C-C2C-C3C	-4.55	101.47	106.91
21	B	1238	CLA	C1C-C2C-C3C	-4.55	101.47	106.91
21	A	1117	CLA	C1C-C2C-C3C	-4.55	101.47	106.91
21	A	1124	CLA	C1C-C2C-C3C	-4.55	101.47	106.91
21	A	1141	CLA	O2A-CGA-O1A	-4.54	111.76	123.49
19	J	6013	BCR	C34-C9-C10	-4.54	116.19	122.90
21	A	1123	CLA	C1C-C2C-C3C	-4.54	101.48	106.91
21	B	9023	CLA	O2A-CGA-O1A	-4.54	111.78	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	6018	BCR	C15-C14-C13	-4.53	120.65	127.20
21	3	3001	CLA	C1C-C2C-C3C	-4.53	101.49	106.91
21	3	3015	CLA	C1C-C2C-C3C	-4.53	101.49	106.91
21	B	1220	CLA	C1C-C2C-C3C	-4.53	101.49	106.91
21	B	1216	CLA	O2A-CGA-O1A	-4.53	111.80	123.49
21	3	3002	CLA	C1C-C2C-C3C	-4.53	101.50	106.91
21	B	1208	CLA	C1C-C2C-C3C	-4.53	101.50	106.91
21	B	1234	CLA	O2A-CGA-O1A	-4.52	111.82	123.49
21	1	1005	CLA	C1C-C2C-C3C	-4.52	101.50	106.91
19	F	6014	BCR	C40-C30-C29	-4.52	92.60	108.79
21	2	2013	CLA	C1C-C2C-C3C	-4.52	101.50	106.91
21	A	1117	CLA	O2A-CGA-O1A	-4.52	111.84	123.49
21	B	1227	CLA	O2A-CGA-O1A	-4.51	111.84	123.49
19	J	6012	BCR	C36-C18-C17	-4.51	116.23	122.90
19	G	2011	BCR	C33-C5-C6	-4.51	120.17	124.61
19	J	6012	BCR	C38-C26-C25	-4.51	120.17	124.61
21	B	1201	CLA	C1C-C2C-C3C	-4.51	101.51	106.91
21	2	2007	CLA	O2A-CGA-O1A	-4.50	111.87	123.49
21	2	2005	CLA	C1C-C2C-C3C	-4.50	101.53	106.91
19	F	6014	BCR	C24-C23-C22	-4.50	119.36	126.22
19	A	6007	BCR	C33-C5-C6	-4.50	120.19	124.61
21	1	1012	CLA	C1C-C2C-C3C	-4.49	101.53	106.91
21	B	1237	CLA	C1C-C2C-C3C	-4.49	101.54	106.91
21	B	1212	CLA	C1C-C2C-C3C	-4.49	101.54	106.91
21	B	1240	CLA	C1C-C2C-C3C	-4.49	101.54	106.91
21	B	1204	CLA	C1C-C2C-C3C	-4.49	101.54	106.91
21	A	1129	CLA	C1C-C2C-C3C	-4.49	101.54	106.91
21	3	3006	CLA	C1C-C2C-C3C	-4.49	101.54	106.91
21	2	2009	CLA	O2A-CGA-O1A	-4.49	108.22	123.02
21	A	1128	CLA	O2A-CGA-O1A	-4.49	111.91	123.49
21	B	1222	CLA	C1C-C2C-C3C	-4.48	101.55	106.91
21	L	1502	CLA	C1C-C2C-C3C	-4.48	101.55	106.91
21	B	1203	CLA	C1C-C2C-C3C	-4.48	101.55	106.91
21	A	1130	CLA	C1C-C2C-C3C	-4.48	101.55	106.91
21	1	1008	CLA	C1C-C2C-C3C	-4.47	101.56	106.91
21	1	1014	CLA	C3B-CAB-CBB	-4.47	117.16	126.32
21	2	2004	CLA	C1C-C2C-C3C	-4.47	101.56	106.91
21	3	3005	CLA	C1C-C2C-C3C	-4.47	101.56	106.91
21	B	1213	CLA	C1C-C2C-C3C	-4.47	101.56	106.91
21	1	1010	CLA	O2A-CGA-O1A	-4.46	111.97	123.49
21	A	1103	CLA	C1C-C2C-C3C	-4.46	101.57	106.91
21	B	1226	CLA	O2D-CGD-O1D	-4.46	114.58	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	9013	CLA	C1C-C2C-C3C	-4.46	101.58	106.91
21	B	1211	CLA	C1C-C2C-C3C	-4.45	101.58	106.91
21	B	1236	CLA	O2A-CGA-O1A	-4.45	112.00	123.49
21	L	1503	CLA	O2A-CGA-O1A	-4.45	112.00	123.49
21	4	4010	CLA	C3B-CAB-CBB	-4.45	117.21	126.32
21	A	1105	CLA	C1C-C2C-C3C	-4.45	101.59	106.91
19	I	6020	BCR	C33-C5-C6	-4.45	120.24	124.61
21	1	1010	CLA	C1C-C2C-C3C	-4.45	101.59	106.91
19	A	6008	BCR	C28-C27-C26	-4.44	106.82	113.87
21	B	1209	CLA	C1C-C2C-C3C	-4.42	101.62	106.91
21	B	1210	CLA	C1C-C2C-C3C	-4.42	101.62	106.91
21	3	3003	CLA	C1C-C2C-C3C	-4.42	101.62	106.91
21	A	1109	CLA	C1C-C2C-C3C	-4.42	101.62	106.91
21	3	3008	CLA	O2A-CGA-O1A	-4.41	112.11	123.49
19	A	6002	BCR	C33-C5-C6	-4.40	120.29	124.61
21	4	4012	CLA	C1C-C2C-C3C	-4.39	101.66	106.91
21	4	4006	CLA	O2A-CGA-O1A	-4.39	112.16	123.49
21	1	1003	CLA	CAA-C2A-C3A	-4.39	100.60	113.22
21	1	1013	CLA	C1C-C2C-C3C	-4.39	101.66	106.91
21	B	1224	CLA	C1C-C2C-C3C	-4.38	101.67	106.91
21	F	1302	CLA	C1C-C2C-C3C	-4.38	101.67	106.91
19	B	6004	BCR	C15-C14-C13	-4.38	120.87	127.20
19	A	6011	BCR	C24-C23-C22	-4.38	119.54	126.22
21	3	3011	CLA	C3B-CAB-CBB	-4.37	117.37	126.32
21	4	4009	CLA	O1D-CGD-CBD	-4.37	118.36	124.62
19	F	6016	BCR	C33-C5-C6	-4.37	120.31	124.61
21	B	1230	CLA	C1C-C2C-C3C	-4.37	101.69	106.91
21	1	1007	CLA	C1C-C2C-C3C	-4.37	101.69	106.91
21	4	4005	CLA	CAA-C2A-C1A	-4.36	97.08	112.47
21	A	1139	CLA	O2A-CGA-O1A	-4.35	112.26	123.49
21	A	1110	CLA	C1C-C2C-C3C	-4.35	101.70	106.91
21	A	9013	CLA	CAA-C2A-C3A	-4.35	100.71	113.22
21	1	1010	CLA	C3B-CAB-CBB	-4.35	117.42	126.32
21	A	1115	CLA	C1C-C2C-C3C	-4.34	101.72	106.91
21	2	2005	CLA	O2A-CGA-O1A	-4.33	112.31	123.49
19	L	6019	BCR	C33-C5-C6	-4.33	120.36	124.61
21	4	4010	CLA	CAA-C2A-C3A	-4.32	100.79	113.22
21	4	4015	CLA	C1C-C2C-C3C	-4.32	101.74	106.91
21	A	1101	CLA	C1C-C2C-C3C	-4.32	101.74	106.91
23	A	9011	CL0	C1C-C2C-C3C	-4.32	101.74	106.91
27	4	4503	NEX	C39-C29-C30	-4.32	116.52	122.90
21	A	1140	CLA	O2A-CGA-O1A	-4.31	112.36	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1141	CLA	C1C-C2C-C3C	-4.31	101.75	106.91
21	B	9023	CLA	C1C-C2C-C3C	-4.31	101.75	106.91
26	2	2502	LUT	C7-C8-C9	-4.31	119.65	126.22
19	B	6004	BCR	C27-C26-C25	-4.30	117.30	122.78
21	4	4010	CLA	O2A-CGA-O1A	-4.30	112.40	123.49
19	J	6013	BCR	C33-C5-C6	-4.30	120.39	124.61
21	A	1116	CLA	C1C-C2C-C3C	-4.30	101.77	106.91
21	A	1127	CLA	C1C-C2C-C3C	-4.30	101.77	106.91
26	1	1502	LUT	C35-C34-C33	-4.30	120.99	127.20
19	I	6020	BCR	C38-C26-C25	-4.29	120.39	124.61
21	A	1112	CLA	C1C-C2C-C3C	-4.29	101.78	106.91
21	A	1126	CLA	C1C-C2C-C3C	-4.28	101.78	106.91
19	A	6017	BCR	C24-C23-C22	-4.27	119.71	126.22
21	A	1103	CLA	O2A-CGA-O1A	-4.26	112.50	123.49
26	2	2501	LUT	C35-C34-C33	-4.24	121.07	127.20
19	A	6002	BCR	C7-C8-C9	-4.24	119.76	126.22
21	A	9012	CLA	OBD-CAD-C3D	-4.24	119.71	128.35
26	1	1501	LUT	C11-C10-C9	-4.23	121.08	127.20
19	A	6011	BCR	C3-C4-C5	-4.22	107.17	113.87
26	4	4501	LUT	C11-C12-C13	-4.22	113.90	126.32
21	4	4015	CLA	C3B-CAB-CBB	-4.21	117.71	126.32
21	4	4015	CLA	O2A-CGA-O1A	-4.21	109.14	123.02
19	A	6017	BCR	C35-C13-C14	-4.21	116.69	122.90
26	1	1502	LUT	O23-C23-C24	-4.20	103.70	110.21
21	2	2009	CLA	O1D-CGD-CBD	-4.20	118.61	124.62
21	4	4008	CLA	O2D-CGD-O1D	-4.19	115.14	123.79
21	4	4004	CLA	C1C-C2C-C3C	-4.19	101.90	106.91
19	A	6017	BCR	C36-C18-C17	-4.19	116.72	122.90
26	4	4502	LUT	C11-C10-C9	-4.18	121.15	127.20
21	A	1132	CLA	C1C-C2C-C3C	-4.18	101.91	106.91
19	J	6012	BCR	C15-C14-C13	-4.17	121.17	127.20
19	A	6017	BCR	C33-C5-C6	-4.17	120.51	124.61
21	3	3001	CLA	O2A-CGA-O1A	-4.17	112.74	123.49
21	4	4014	CLA	C1C-C2C-C3C	-4.17	101.93	106.91
21	2	2014	CLA	O2D-CGD-O1D	-4.16	115.20	123.79
21	4	4007	CLA	O2A-CGA-O1A	-4.16	112.77	123.49
21	1	1014	CLA	C1C-C2C-C3C	-4.15	101.94	106.91
21	A	1131	CLA	C3B-CAB-CBB	-4.15	117.83	126.32
21	1	1004	CLA	C3B-CAB-CBB	-4.14	117.84	126.32
21	B	1214	CLA	C1C-C2C-C3C	-4.13	101.96	106.91
21	2	2008	CLA	OBD-CAD-C3D	-4.13	119.92	128.35
19	G	2011	BCR	C24-C23-C22	-4.13	119.92	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	6004	BCR	C33-C5-C6	-4.13	120.55	124.61
19	G	2011	BCR	C37-C22-C21	-4.12	116.81	122.90
26	2	2502	LUT	C11-C10-C9	-4.12	121.25	127.20
21	A	1107	CLA	C1C-C2C-C3C	-4.12	101.98	106.91
19	B	6005	BCR	C36-C18-C17	-4.11	116.83	122.90
21	J	6015	CLA	O2A-CGA-O1A	-4.11	112.89	123.49
21	A	1111	CLA	C1C-C2C-C3C	-4.10	102.01	106.91
19	A	6003	BCR	C4-C5-C6	-4.09	117.57	122.78
21	2	2011	CLA	CAA-C2A-C1A	-4.09	98.06	112.47
19	A	6007	BCR	C38-C26-C25	-4.08	120.60	124.61
19	L	6020	BCR	C33-C5-C6	-4.08	120.60	124.61
23	A	9011	CL0	C3B-CAB-CBB	-4.07	117.99	126.32
21	2	2003	CLA	OBD-CAD-CBD	-4.07	119.80	125.94
21	4	4006	CLA	OBD-CAD-C3D	-4.06	120.06	128.35
19	B	6006	BCR	C34-C9-C10	-4.06	116.90	122.90
19	B	6006	BCR	C33-C5-C6	-4.06	120.62	124.61
26	2	2501	LUT	C7-C8-C9	-4.06	120.03	126.22
19	L	6019	BCR	C7-C8-C9	-4.05	120.04	126.22
19	J	6012	BCR	C37-C22-C21	-4.04	116.94	122.90
21	3	3011	CLA	C1C-C2C-C3C	-4.03	102.08	106.91
21	4	4014	CLA	OBD-CAD-C3D	-4.03	120.12	128.35
21	4	4002	CLA	O2A-CGA-O1A	-4.03	113.10	123.49
19	A	6003	BCR	C7-C8-C9	-4.02	120.08	126.22
19	A	6011	BCR	C7-C8-C9	-4.02	120.09	126.22
26	4	4501	LUT	C35-C34-C33	-4.01	121.40	127.20
19	B	6010	BCR	C33-C5-C6	-4.01	120.67	124.61
19	B	6004	BCR	C7-C8-C9	-4.00	120.11	126.22
21	A	1125	CLA	C3B-CAB-CBB	-4.00	118.13	126.32
21	1	1002	CLA	O2A-CGA-O1A	-4.00	113.18	123.49
21	A	9012	CLA	C3B-CAB-CBB	-3.99	118.15	126.32
21	B	1227	CLA	O1D-CGD-CBD	-3.99	118.90	124.62
26	4	4502	LUT	C35-C34-C33	-3.99	121.44	127.20
21	2	2003	CLA	O2D-CGD-O1D	-3.97	115.58	123.79
21	A	1137	CLA	O2A-CGA-O1A	-3.97	113.24	123.49
21	2	2003	CLA	CGD-CBD-CAD	-3.97	97.19	110.62
26	1	1502	LUT	C31-C32-C33	-3.95	114.68	126.32
21	G	1001	CLA	CAA-C2A-C1A	-3.94	98.56	112.47
21	2	2011	CLA	O2D-CGD-O1D	-3.94	115.65	123.79
19	G	2011	BCR	C15-C14-C13	-3.93	121.51	127.20
19	A	6017	BCR	C37-C22-C21	-3.93	117.09	122.90
21	B	9023	CLA	C3B-CAB-CBB	-3.93	118.27	126.32
21	4	4007	CLA	C3B-CAB-CBB	-3.93	118.28	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	F	6014	BCR	C3-C4-C5	-3.92	107.64	113.87
21	4	4004	CLA	O1D-CGD-CBD	-3.91	119.02	124.62
21	B	1227	CLA	C3B-CAB-CBB	-3.88	118.37	126.32
21	1	1008	CLA	O2D-CGD-O1D	-3.84	115.86	123.79
21	1	1003	CLA	OBD-CAD-CBD	-3.84	120.14	125.94
26	1	1502	LUT	C11-C12-C13	-3.83	115.04	126.32
21	2	2008	CLA	C3B-CAB-CBB	-3.83	118.48	126.32
21	A	9012	CLA	C1C-C2C-C3C	-3.83	102.33	106.91
21	2	2008	CLA	O2D-CGD-O1D	-3.83	115.88	123.79
21	4	4005	CLA	CAC-C3C-C2C	-3.83	120.80	127.51
21	4	4003	CLA	O2A-CGA-O1A	-3.82	113.62	123.49
19	L	6019	BCR	C37-C22-C21	-3.82	117.26	122.90
21	B	1228	CLA	C3B-CAB-CBB	-3.82	118.51	126.32
21	L	1503	CLA	C1-C2-C3	-3.81	120.47	126.71
21	2	2008	CLA	C1C-C2C-C3C	-3.80	102.36	106.91
19	A	6017	BCR	C7-C8-C9	-3.80	120.43	126.22
21	4	4003	CLA	C1C-C2C-C3C	-3.80	102.37	106.91
21	A	1133	CLA	O2A-CGA-O1A	-3.79	110.53	123.02
26	2	2501	LUT	C15-C14-C13	-3.79	121.73	127.20
21	1	1006	CLA	C3B-CAB-CBB	-3.79	118.57	126.32
21	A	1102	CLA	C1-C2-C3	-3.78	120.51	126.71
21	B	1240	CLA	OBD-CAD-CBD	-3.77	120.24	125.94
21	1	1004	CLA	OBD-CAD-CBD	-3.77	120.25	125.94
26	4	4502	LUT	C19-C9-C10	-3.76	117.34	122.90
21	1	1008	CLA	C3B-CAB-CBB	-3.74	118.66	126.32
19	G	2011	BCR	C8-C7-C6	-3.73	116.10	127.32
21	B	1240	CLA	O2D-CGD-O1D	-3.73	116.09	123.79
21	3	3008	CLA	OBD-CAD-C3D	-3.73	120.75	128.35
21	B	1224	CLA	O1D-CGD-CBD	-3.72	119.28	124.62
21	4	4006	CLA	CBC-CAC-C3C	-3.72	101.02	112.39
21	2	2005	CLA	C3B-CAB-CBB	-3.72	118.70	126.32
21	3	3014	CLA	CBC-CAC-C3C	-3.70	101.08	112.39
19	J	6012	BCR	C34-C9-C10	-3.70	117.43	122.90
19	B	6005	BCR	C34-C9-C10	-3.69	117.45	122.90
21	1	1014	CLA	CGD-CBD-CAD	-3.69	98.13	110.62
21	2	2010	CLA	C3B-CAB-CBB	-3.68	118.78	126.32
21	2	2007	CLA	C3B-CAB-CBB	-3.68	118.79	126.32
21	A	1134	CLA	O2A-CGA-O1A	-3.68	110.89	123.02
21	3	3009	CLA	O1D-CGD-CBD	-3.66	119.38	124.62
21	B	1213	CLA	CAA-C2A-C3A	-3.66	102.70	113.22
21	4	4010	CLA	C1-C2-C3	-3.65	120.73	126.71
19	A	6007	BCR	C34-C9-C10	-3.65	117.51	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4003	CLA	O2D-CGD-O1D	-3.65	116.26	123.79
21	A	1132	CLA	C3B-CAB-CBB	-3.65	118.86	126.32
21	A	1125	CLA	OBD-CAD-CBD	-3.64	120.44	125.94
21	A	1107	CLA	O1D-CGD-CBD	-3.64	119.40	124.62
21	A	1102	CLA	O1D-CGD-CBD	-3.64	119.40	124.62
19	B	6006	BCR	C24-C23-C22	-3.64	120.67	126.22
21	2	2014	CLA	C3B-CAB-CBB	-3.64	118.88	126.32
21	2	2006	CLA	C3B-CAB-CBB	-3.64	118.88	126.32
19	I	6018	BCR	C37-C22-C21	-3.63	117.54	122.90
21	B	1201	CLA	O1D-CGD-CBD	-3.63	119.42	124.62
21	A	1113	CLA	O2A-CGA-O1A	-3.63	111.05	123.02
21	A	1112	CLA	O2A-CGA-O1A	-3.63	111.05	123.02
21	1	1011	CLA	C3B-CAB-CBB	-3.63	118.89	126.32
21	L	1501	CLA	O2A-CGA-O1A	-3.63	111.06	123.02
21	A	1133	CLA	C3B-CAB-CBB	-3.63	118.90	126.32
21	B	1217	CLA	O2A-CGA-O1A	-3.62	111.07	123.02
21	B	1201	CLA	O2A-CGA-O1A	-3.62	111.07	123.02
21	3	3008	CLA	C3B-CAB-CBB	-3.62	118.90	126.32
26	1	1501	LUT	C15-C14-C13	-3.62	121.96	127.20
21	A	1121	CLA	O2A-CGA-O1A	-3.62	111.09	123.02
21	4	4006	CLA	O1D-CGD-CBD	-3.61	119.44	124.62
21	A	1108	CLA	O2A-CGA-O1A	-3.61	111.11	123.02
21	B	1209	CLA	O2A-CGA-O1A	-3.61	111.12	123.02
21	F	1302	CLA	O2A-CGA-O1A	-3.61	111.12	123.02
21	B	1231	CLA	O2A-CGA-O1A	-3.60	111.14	123.02
21	A	1120	CLA	O2A-CGA-O1A	-3.60	111.14	123.02
19	B	6005	BCR	C37-C22-C21	-3.59	117.60	122.90
19	I	6020	BCR	C3-C4-C5	-3.58	108.18	113.87
21	4	4013	CLA	O1D-CGD-CBD	-3.58	119.49	124.62
21	4	4001	CLA	C3B-CAB-CBB	-3.58	119.00	126.32
21	H	1000	CLA	O2A-CGA-O1A	-3.57	111.23	123.02
21	A	1130	CLA	O2A-CGA-O1A	-3.57	111.25	123.02
19	I	6018	BCR	C33-C5-C6	-3.57	121.10	124.61
21	A	1118	CLA	O2A-CGA-O1A	-3.57	111.26	123.02
21	B	1205	CLA	O1D-CGD-CBD	-3.56	119.53	124.62
21	2	2010	CLA	O1D-CGD-CBD	-3.55	119.53	124.62
19	L	6019	BCR	C38-C26-C25	-3.55	121.12	124.61
21	2	2011	CLA	C3B-CAB-CBB	-3.54	119.07	126.32
21	L	1503	CLA	C3B-CAB-CBB	-3.53	119.09	126.32
21	B	1240	CLA	C3B-CAB-CBB	-3.53	119.09	126.32
19	A	6003	BCR	C3-C4-C5	-3.52	108.28	113.87
26	2	2501	LUT	C18-C5-C6	-3.52	121.15	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	G	1001	CLA	C3B-CAB-CBB	-3.52	119.12	126.32
21	2	2001	CLA	C3A-C4A-CHB	-3.50	120.52	124.06
21	B	1228	CLA	O2D-CGD-O1D	-3.50	116.57	123.79
21	B	9010	CLA	C3B-CAB-CBB	-3.49	119.18	126.32
21	A	1123	CLA	O1D-CGD-CBD	-3.49	119.62	124.62
26	1	1501	LUT	C31-C32-C33	-3.49	116.05	126.32
21	B	1230	CLA	O1D-CGD-CBD	-3.48	119.63	124.62
26	2	2502	LUT	C17-C1-C6	-3.48	104.85	110.30
21	A	1114	CLA	O2A-CGA-O1A	-3.48	111.55	123.02
21	B	1212	CLA	O2A-CGA-O1A	-3.48	111.55	123.02
24	B	7101	DGD	O3G-C3G-C2G	-3.47	102.73	110.99
21	1	1012	CLA	O1D-CGD-CBD	-3.46	119.66	124.62
21	3	3013	CLA	C1-C2-C3	-3.46	121.04	126.71
26	4	4501	LUT	C22-C23-C24	-3.46	107.69	111.75
21	A	1122	CLA	O2D-CGD-O1D	-3.45	116.66	123.79
21	2	2014	CLA	CAA-C2A-C3A	-3.45	103.31	113.22
26	4	4502	LUT	C40-C33-C34	-3.44	117.81	122.90
21	3	3009	CLA	C3B-CAB-CBB	-3.44	119.28	126.32
26	1	1501	LUT	C18-C5-C6	-3.44	121.23	124.61
26	4	4502	LUT	C18-C5-C6	-3.44	121.23	124.61
21	F	1303	CLA	C1C-C2C-C3C	-3.43	102.81	106.91
21	G	1002	CLA	OBD-CAD-C3D	-3.43	121.36	128.35
21	G	1002	CLA	O2A-CGA-O1A	-3.42	111.73	123.02
25	G	2021	LMG	C1-O6-C5	-3.42	107.10	113.75
21	G	1001	CLA	OBD-CAD-C3D	-3.42	121.37	128.35
21	2	2013	CLA	O1D-CGD-CBD	-3.42	119.72	124.62
21	B	1221	CLA	O1D-CGD-CBD	-3.42	119.72	124.62
23	A	9011	CL0	O2D-CGD-O1D	-3.42	116.73	123.79
21	3	3001	CLA	O1D-CGD-CBD	-3.41	119.74	124.62
21	B	1239	CLA	O1D-CGD-CBD	-3.40	119.74	124.62
21	B	1218	CLA	O1D-CGD-CBD	-3.40	119.74	124.62
19	L	6020	BCR	C38-C26-C25	-3.40	121.26	124.61
26	1	1501	LUT	C35-C34-C33	-3.40	122.29	127.20
26	4	4502	LUT	C31-C32-C33	-3.39	116.35	126.32
26	2	2502	LUT	C18-C5-C6	-3.38	121.28	124.61
26	1	1501	LUT	C19-C9-C10	-3.38	117.90	122.90
21	G	1002	CLA	C3B-CAB-CBB	-3.38	119.40	126.32
19	B	6010	BCR	C24-C23-C22	-3.38	121.07	126.22
21	A	1126	CLA	O1D-CGD-CBD	-3.37	119.79	124.62
21	A	1129	CLA	C1-C2-C3	-3.37	121.18	126.71
26	1	1501	LUT	C20-C13-C14	-3.37	117.92	122.90
21	B	1239	CLA	C3B-CAB-CBB	-3.37	119.43	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1224	CLA	C3B-CAB-CBB	-3.36	119.44	126.32
26	1	1501	LUT	C11-C12-C13	-3.36	116.43	126.32
21	B	1228	CLA	CAA-C2A-C3A	-3.36	103.56	113.22
21	2	2002	CLA	C6-C5-C3	-3.36	105.12	112.48
19	A	6002	BCR	C38-C26-C25	-3.35	121.31	124.61
21	A	1106	CLA	O1D-CGD-CBD	-3.35	119.81	124.62
21	G	1001	CLA	CAA-C2A-C3A	-3.35	103.58	113.22
19	L	6019	BCR	C28-C27-C26	-3.35	108.56	113.87
19	A	6007	BCR	C3-C4-C5	-3.34	108.56	113.87
26	1	1502	LUT	O3-C3-C2	-3.34	103.07	109.91
21	1	1003	CLA	O2A-CGA-O1A	-3.34	114.88	123.49
21	3	3013	CLA	O1D-CGD-CBD	-3.33	119.84	124.62
19	I	6020	BCR	C24-C23-C22	-3.33	121.14	126.22
21	A	9013	CLA	O1D-CGD-CBD	-3.33	119.85	124.62
26	4	4502	LUT	C20-C13-C14	-3.33	117.98	122.90
19	A	6003	BCR	C33-C5-C6	-3.33	121.34	124.61
23	A	9011	CL0	OBD-CAD-CBD	-3.32	120.93	125.94
26	4	4501	LUT	C31-C32-C33	-3.31	116.56	126.32
19	A	6008	BCR	C37-C22-C21	-3.31	118.01	122.90
19	I	6018	BCR	C23-C24-C25	-3.31	117.37	127.32
21	1	1012	CLA	C1-C2-C3	-3.31	121.28	126.71
26	1	1502	LUT	C20-C13-C14	-3.31	118.02	122.90
26	4	4501	LUT	C15-C14-C13	-3.30	122.43	127.20
21	A	1136	CLA	CAA-C2A-C3A	-3.30	103.72	113.22
21	2	2007	CLA	C6-C5-C3	-3.30	105.24	112.48
19	B	6011	BCR	C3-C4-C5	-3.30	108.63	113.87
21	B	1237	CLA	C3B-CAB-CBB	-3.30	119.57	126.32
19	A	6002	BCR	C3-C4-C5	-3.29	108.64	113.87
24	B	7101	DGD	O5D-C6D-C5D	-3.29	103.12	109.08
21	A	1121	CLA	O1D-CGD-CBD	-3.28	119.92	124.62
21	3	3011	CLA	O2A-CGA-O1A	-3.28	112.21	123.02
21	1	1013	CLA	C3B-CAB-CBB	-3.28	119.61	126.32
26	1	1502	LUT	C15-C14-C13	-3.28	122.47	127.20
21	1	1005	CLA	C3B-CAB-CBB	-3.27	119.62	126.32
21	1	1004	CLA	O2D-CGD-O1D	-3.27	117.04	123.79
19	F	6014	BCR	C15-C14-C13	-3.27	122.48	127.20
21	3	3009	CLA	O2A-CGA-O1A	-3.27	112.25	123.02
21	A	1133	CLA	OBD-CAD-C3D	-3.27	121.69	128.35
19	B	6010	BCR	C3-C4-C5	-3.26	108.69	113.87
21	A	9013	CLA	C3B-CAB-CBB	-3.26	119.64	126.32
19	A	6003	BCR	C28-C27-C26	-3.26	108.70	113.87
19	B	6004	BCR	C36-C18-C17	-3.26	118.09	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1118	CLA	O1D-CGD-CBD	-3.25	119.96	124.62
26	4	4502	LUT	C15-C14-C13	-3.25	122.50	127.20
21	1	1009	CLA	CAA-C2A-C1A	-3.25	101.01	112.47
21	F	1303	CLA	OBD-CAD-CBD	-3.24	121.04	125.94
19	A	6007	BCR	C36-C18-C17	-3.23	118.12	122.90
21	L	1502	CLA	C3B-CAB-CBB	-3.22	119.72	126.32
19	B	6011	BCR	C7-C8-C9	-3.22	121.31	126.22
19	A	6003	BCR	C8-C7-C6	-3.22	117.64	127.32
26	1	1502	LUT	C40-C33-C34	-3.22	118.15	122.90
19	J	6012	BCR	C30-C25-C26	-3.21	117.94	122.66
21	1	1004	CLA	CAA-C2A-C1A	-3.21	101.14	112.47
19	A	6017	BCR	C3-C4-C5	-3.21	108.78	113.87
21	G	1001	CLA	O2D-CGD-O1D	-3.20	117.18	123.79
21	B	1211	CLA	O1D-CGD-CBD	-3.20	120.04	124.62
21	2	2009	CLA	C3B-CAB-CBB	-3.19	119.79	126.32
21	B	1227	CLA	CAA-C2A-C3A	-3.19	104.05	113.22
26	1	1501	LUT	C40-C33-C34	-3.19	118.19	122.90
21	A	1126	CLA	C3B-CAB-CBB	-3.18	119.81	126.32
21	B	1205	CLA	C3B-CAB-CBB	-3.17	119.82	126.32
21	A	1133	CLA	OBD-CAD-CBD	-3.17	121.15	125.94
21	3	3017	CLA	CMD-C2D-C3D	-3.16	118.90	125.09
21	B	1212	CLA	C3B-CAB-CBB	-3.16	119.85	126.32
21	B	1236	CLA	O1D-CGD-CBD	-3.16	120.10	124.62
21	B	1236	CLA	C3B-CAB-CBB	-3.16	119.86	126.32
21	1	1007	CLA	CAA-CBA-CGA	-3.16	104.08	113.32
21	4	4001	CLA	OBD-CAD-CBD	-3.16	121.17	125.94
21	A	1112	CLA	C3B-CAB-CBB	-3.16	119.86	126.32
21	A	1108	CLA	O1D-CGD-CBD	-3.15	120.10	124.62
21	A	1117	CLA	O1D-CGD-CBD	-3.15	120.10	124.62
21	A	1118	CLA	C3B-CAB-CBB	-3.15	119.87	126.32
21	4	4004	CLA	O2D-CGD-O1D	-3.15	117.29	123.79
21	2	2003	CLA	C3B-CAB-CBB	-3.14	119.88	126.32
21	A	1137	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
21	4	4008	CLA	C3B-CAB-CBB	-3.14	119.90	126.32
21	A	1131	CLA	O2D-CGD-O1D	-3.14	117.31	123.79
21	3	3009	CLA	CGD-CBD-CAD	-3.14	99.99	110.62
19	B	6009	BCR	C7-C8-C9	-3.13	121.44	126.22
21	4	4013	CLA	O2D-CGD-O1D	-3.13	117.32	123.79
21	B	1216	CLA	C3B-CAB-CBB	-3.13	119.92	126.32
21	A	1125	CLA	O2D-CGD-O1D	-3.13	117.33	123.79
21	A	1137	CLA	CAA-CBA-CGA	-3.13	104.17	113.32
21	4	4005	CLA	CBC-CAC-C3C	-3.12	102.88	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1226	CLA	C3B-CAB-CBB	-3.11	119.95	126.32
21	A	1129	CLA	C3B-CAB-CBB	-3.11	119.95	126.32
21	B	1207	CLA	O2D-CGD-O1D	-3.11	117.36	123.79
21	B	1222	CLA	CAA-C2A-C3A	-3.11	104.28	113.22
21	2	2001	CLA	C2C-C3C-C4C	-3.11	103.74	107.23
21	1	1012	CLA	OBD-CAD-C3D	-3.10	122.03	128.35
19	A	6017	BCR	C30-C25-C26	-3.10	118.11	122.66
26	2	2502	LUT	C31-C30-C29	-3.10	122.72	127.20
21	B	9022	CLA	OBD-CAD-C3D	-3.09	122.04	128.35
19	L	6019	BCR	C36-C18-C17	-3.09	118.33	122.90
21	H	1000	CLA	O1D-CGD-CBD	-3.09	120.19	124.62
21	2	2013	CLA	OBD-CAD-C3D	-3.09	122.05	128.35
21	B	1220	CLA	C3B-CAB-CBB	-3.09	120.00	126.32
21	3	3012	CLA	C3B-CAB-CBB	-3.09	120.00	126.32
19	B	6009	BCR	C36-C18-C17	-3.09	118.34	122.90
21	A	1128	CLA	C3B-CAB-CBB	-3.08	120.01	126.32
21	B	1231	CLA	O1D-CGD-CBD	-3.08	120.21	124.62
21	4	4015	CLA	OBD-CAD-C3D	-3.08	122.07	128.35
21	3	3003	CLA	C3B-CAB-CBB	-3.08	120.02	126.32
21	B	1225	CLA	O1D-CGD-CBD	-3.08	120.21	124.62
21	4	4003	CLA	OBD-CAD-CBD	-3.07	121.30	125.94
21	1	1013	CLA	OBD-CAD-C3D	-3.07	122.08	128.35
19	F	6014	BCR	C36-C18-C17	-3.06	118.38	122.90
21	1	1001	CLA	CAA-C2A-C3A	-3.06	104.42	113.22
21	1	1002	CLA	O1D-CGD-CBD	-3.06	120.24	124.62
21	A	1131	CLA	O1D-CGD-CBD	-3.05	120.25	124.62
19	L	6020	BCR	C34-C9-C10	-3.05	118.39	122.90
21	B	9010	CLA	OBD-CAD-CBD	-3.05	121.33	125.94
26	4	4501	LUT	O3-C3-C2	-3.05	103.66	109.91
21	3	3017	CLA	O1D-CGD-CBD	-3.05	120.25	124.62
26	1	1502	LUT	C39-C29-C30	-3.05	118.40	122.90
21	B	1235	CLA	C3B-CAB-CBB	-3.04	120.09	126.32
21	4	4009	CLA	C1-C2-C3	-3.04	121.72	126.71
21	4	4006	CLA	OBD-CAD-CBD	-3.04	121.35	125.94
23	A	9011	CL0	CGD-CBD-CAD	-3.04	100.33	110.62
21	A	1128	CLA	O1D-CGD-CBD	-3.04	120.27	124.62
19	F	6016	BCR	C2-C3-C4	-3.03	103.88	111.53
21	B	1209	CLA	O1D-CGD-CBD	-3.03	120.28	124.62
21	3	3005	CLA	C3B-CAB-CBB	-3.03	120.13	126.32
19	B	6005	BCR	C3-C4-C5	-3.02	109.07	113.87
21	B	1203	CLA	C3B-CAB-CBB	-3.02	120.14	126.32
19	A	6011	BCR	C34-C9-C10	-3.02	118.45	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1215	CLA	O1D-CGD-CBD	-3.02	120.30	124.62
21	B	1217	CLA	C3B-CAB-CBB	-3.01	120.16	126.32
21	B	1223	CLA	O1D-CGD-CBD	-3.01	120.31	124.62
21	B	1212	CLA	O1D-CGD-CBD	-3.01	120.31	124.62
21	2	2008	CLA	O1D-CGD-CBD	-3.01	120.31	124.62
19	A	6002	BCR	C36-C18-C17	-3.00	118.47	122.90
21	L	1501	CLA	C3B-CAB-CBB	-3.00	120.18	126.32
21	3	3010	CLA	O1D-CGD-CBD	-3.00	120.33	124.62
21	2	2007	CLA	O1D-CGD-CBD	-3.00	120.33	124.62
21	2	2001	CLA	C3A-C2A-C1A	-2.99	100.58	104.58
21	2	2003	CLA	CMD-C2D-C3D	-2.99	119.24	125.09
21	3	3005	CLA	O1D-CGD-CBD	-2.99	120.34	124.62
21	A	1135	CLA	OBD-CAD-C3D	-2.98	122.26	128.35
21	A	1135	CLA	O1D-CGD-CBD	-2.98	120.35	124.62
21	3	3008	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
19	A	6003	BCR	C37-C22-C21	-2.98	118.50	122.90
21	A	1101	CLA	O2D-CGD-O1D	-2.98	117.64	123.79
21	B	1238	CLA	C3B-CAB-CBB	-2.98	120.22	126.32
21	3	3004	CLA	O1D-CGD-CBD	-2.98	120.36	124.62
21	4	4005	CLA	CHC-C1C-C2C	-2.97	118.53	126.35
21	3	3012	CLA	CMD-C2D-C3D	-2.97	119.27	125.09
19	I	6020	BCR	C36-C18-C17	-2.97	118.51	122.90
21	A	1136	CLA	O1D-CGD-CBD	-2.97	120.37	124.62
21	B	1214	CLA	O1D-CGD-CBD	-2.97	120.37	124.62
21	4	4014	CLA	C3B-CAB-CBB	-2.97	120.25	126.32
21	B	1229	CLA	O1D-CGD-CBD	-2.96	120.38	124.62
21	1	1003	CLA	O2D-CGD-O1D	-2.96	117.67	123.79
21	4	4011	CLA	CBC-CAC-C3C	-2.96	103.36	112.39
21	B	1215	CLA	C3B-CAB-CBB	-2.96	120.26	126.32
21	1	1009	CLA	CHC-C1C-C2C	-2.96	118.57	126.35
21	1	1001	CLA	C3B-CAB-CBB	-2.95	120.27	126.32
19	A	6003	BCR	C15-C14-C13	-2.95	122.93	127.20
26	2	2502	LUT	C8-C7-C6	-2.95	118.45	127.32
21	4	4012	CLA	O1D-CGD-CBD	-2.95	120.39	124.62
21	J	6015	CLA	O2D-CGD-O1D	-2.95	117.70	123.79
21	1	1014	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
26	4	4501	LUT	C20-C13-C14	-2.95	118.55	122.90
21	1	1011	CLA	O1D-CGD-CBD	-2.94	120.40	124.62
21	3	3013	CLA	O2D-CGD-O1D	-2.94	117.72	123.79
21	J	1302	CLA	O1D-CGD-CBD	-2.94	120.41	124.62
21	4	4005	CLA	O1D-CGD-CBD	-2.94	120.41	124.62
19	L	6019	BCR	C34-C9-C10	-2.94	118.57	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1112	CLA	O1D-CGD-CBD	-2.93	120.42	124.62
21	B	1230	CLA	C3B-CAB-CBB	-2.93	120.32	126.32
21	A	1114	CLA	O1D-CGD-CBD	-2.93	120.42	124.62
21	A	1105	CLA	O1D-CGD-CBD	-2.93	120.42	124.62
21	3	3006	CLA	O1D-CGD-CBD	-2.93	120.42	124.62
19	L	6019	BCR	C15-C14-C13	-2.93	122.97	127.20
21	1	1011	CLA	O2D-CGD-O1D	-2.93	117.75	123.79
21	3	3001	CLA	O2D-CGD-O1D	-2.92	117.76	123.79
21	2	2008	CLA	C4-C3-C2	-2.92	117.78	123.50
19	B	6005	BCR	C7-C6-C5	-2.92	114.69	121.37
21	B	1217	CLA	O1D-CGD-CBD	-2.92	120.44	124.62
21	B	1213	CLA	O2D-CGD-O1D	-2.91	117.77	123.79
21	A	1129	CLA	O1D-CGD-CBD	-2.91	120.45	124.62
21	B	1234	CLA	O1D-CGD-CBD	-2.91	120.46	124.62
19	F	6014	BCR	C28-C27-C26	-2.91	109.25	113.87
26	4	4502	LUT	C11-C12-C13	-2.91	117.77	126.32
21	4	4001	CLA	CBC-CAC-C3C	-2.90	103.53	112.39
21	A	1143	CLA	C3B-CAB-CBB	-2.90	120.39	126.32
21	A	1119	CLA	C3B-CAB-CBB	-2.89	120.40	126.32
21	3	3014	CLA	C3B-CAB-CBB	-2.89	120.41	126.32
21	1	1009	CLA	CMD-C2D-C3D	-2.89	119.44	125.09
26	2	2501	LUT	C2-C3-C4	-2.88	105.21	110.32
21	4	4010	CLA	O1D-CGD-CBD	-2.88	120.49	124.62
21	2	2005	CLA	OBD-CAD-C3D	-2.88	122.48	128.35
21	A	1110	CLA	O1D-CGD-CBD	-2.88	120.50	124.62
21	2	2001	CLA	C2A-C3A-C4A	-2.88	101.02	103.90
21	2	2006	CLA	O2D-CGD-O1D	-2.87	117.86	123.79
21	A	1134	CLA	O1D-CGD-CBD	-2.87	120.50	124.62
21	3	3005	CLA	O2D-CGD-O1D	-2.87	117.86	123.79
19	J	6012	BCR	C28-C27-C26	-2.87	109.31	113.87
21	3	3016	CLA	O2D-CGD-O1D	-2.87	117.87	123.79
21	A	1132	CLA	CAA-C2A-C3A	-2.87	104.97	113.22
21	B	1204	CLA	C3B-CAB-CBB	-2.87	120.45	126.32
21	B	1240	CLA	C4-C3-C2	-2.86	117.88	123.50
21	B	1227	CLA	O2D-CGD-O1D	-2.86	117.88	123.79
21	4	4012	CLA	CAA-C2A-C1A	-2.86	102.39	112.47
19	B	6009	BCR	C15-C14-C13	-2.86	123.07	127.20
21	4	4011	CLA	O2D-CGD-O1D	-2.85	117.90	123.79
19	F	6014	BCR	C37-C22-C21	-2.84	118.70	122.90
26	1	1501	LUT	O3-C3-C2	-2.84	104.09	109.91
21	1	1003	CLA	C3B-CAB-CBB	-2.84	120.51	126.32
21	A	1141	CLA	O1D-CGD-CBD	-2.83	120.56	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1107	CLA	C3B-CAB-CBB	-2.82	120.54	126.32
21	J	6014	CLA	O1D-CGD-CBD	-2.82	120.58	124.62
26	2	2502	LUT	C39-C29-C30	-2.82	118.73	122.90
21	A	1103	CLA	O2D-CGD-O1D	-2.82	117.97	123.79
21	B	9010	CLA	CMA-C3A-C2A	-2.81	101.89	114.35
19	J	6012	BCR	C3-C4-C5	-2.81	109.40	113.87
19	F	6016	BCR	C37-C22-C21	-2.81	118.75	122.90
21	1	1006	CLA	O2D-CGD-O1D	-2.81	117.98	123.79
21	B	1238	CLA	O1D-CGD-CBD	-2.81	120.59	124.62
21	A	1142	CLA	O1D-CGD-CBD	-2.81	120.60	124.62
23	A	9011	CL0	CAA-C2A-C3A	-2.81	105.15	113.22
21	3	3008	CLA	O1D-CGD-CBD	-2.81	120.60	124.62
26	4	4502	LUT	C39-C29-C30	-2.80	118.76	122.90
21	A	1138	CLA	O1D-CGD-CBD	-2.80	120.61	124.62
21	B	1221	CLA	O2D-CGD-O1D	-2.80	118.01	123.79
21	1	1004	CLA	O1D-CGD-CBD	-2.80	120.61	124.62
21	J	6014	CLA	C3B-CAB-CBB	-2.80	120.59	126.32
21	B	1201	CLA	C3B-CAB-CBB	-2.80	120.59	126.32
21	B	1227	CLA	OBD-CAD-CBD	-2.80	121.72	125.94
19	L	6020	BCR	C37-C22-C21	-2.79	118.78	122.90
21	3	3002	CLA	O1D-CGD-CBD	-2.79	120.62	124.62
21	A	1130	CLA	C3B-CAB-CBB	-2.79	120.61	126.32
21	A	1124	CLA	O1D-CGD-CBD	-2.79	120.62	124.62
21	A	1127	CLA	O1D-CGD-CBD	-2.79	120.63	124.62
21	B	1237	CLA	O1D-CGD-CBD	-2.79	120.63	124.62
21	J	6015	CLA	C3B-CAB-CBB	-2.78	120.62	126.32
21	1	1006	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
21	A	1121	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
19	A	6007	BCR	C37-C22-C21	-2.78	118.80	122.90
21	3	3015	CLA	C3B-CAB-CBB	-2.78	120.64	126.32
21	J	6015	CLA	OBD-CAD-CBD	-2.78	121.75	125.94
21	A	1123	CLA	O2D-CGD-O1D	-2.77	118.06	123.79
21	F	1301	CLA	O1D-CGD-CBD	-2.77	120.66	124.62
21	3	3002	CLA	C3B-CAB-CBB	-2.76	120.66	126.32
21	A	1110	CLA	C3B-CAB-CBB	-2.76	120.67	126.32
21	A	1104	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
21	2	2014	CLA	CHC-C1C-C2C	-2.76	119.09	126.35
21	3	3016	CLA	C3B-CAB-CBB	-2.76	120.67	126.32
21	B	1235	CLA	O1D-CGD-CBD	-2.75	120.68	124.62
21	B	1222	CLA	O1D-CGD-CBD	-2.75	120.69	124.62
19	A	6011	BCR	C36-C18-C17	-2.74	118.85	122.90
26	4	4501	LUT	C19-C9-C10	-2.74	118.85	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1239	CLA	O2D-CGD-O1D	-2.74	118.13	123.79
21	L	1502	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
19	A	6008	BCR	C4-C5-C6	-2.74	119.29	122.78
21	F	1302	CLA	C3B-CAB-CBB	-2.74	120.72	126.32
21	1	1005	CLA	OBD-CAD-CBD	-2.73	121.81	125.94
21	1	1007	CLA	C3B-CAB-CBB	-2.73	120.73	126.32
26	2	2501	LUT	C31-C32-C33	-2.73	118.29	126.32
21	1	1005	CLA	OBD-CAD-C3D	-2.73	122.79	128.35
21	A	1102	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
21	4	4014	CLA	C2A-C1A-CHA	-2.72	118.87	123.89
20	1	1801	LHG	C6-C5-C4	-2.72	105.71	112.07
21	G	1002	CLA	O2D-CGD-O1D	-2.71	118.18	123.79
21	B	1216	CLA	O1D-CGD-CBD	-2.71	120.73	124.62
21	1	1013	CLA	C4-C3-C2	-2.71	118.18	123.50
19	F	6016	BCR	C7-C6-C5	-2.71	115.17	121.37
20	A	7001	LHG	C5-O7-C7	-2.71	111.39	117.89
21	4	4011	CLA	CAA-CBA-CGA	-2.71	105.40	113.32
19	B	6009	BCR	C37-C22-C21	-2.70	118.91	122.90
21	A	1135	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
21	J	1302	CLA	C3B-CAB-CBB	-2.70	120.79	126.32
21	2	2004	CLA	O1D-CGD-CBD	-2.70	119.09	124.42
21	A	1119	CLA	O1D-CGD-CBD	-2.70	120.75	124.62
21	3	3014	CLA	CHD-C4C-C3C	-2.70	120.77	124.94
21	A	1138	CLA	C3B-CAB-CBB	-2.69	120.81	126.32
19	B	6011	BCR	C1-C6-C5	-2.69	118.71	122.66
23	A	9011	CL0	CMA-C3A-C2A	-2.69	102.46	114.35
21	B	1204	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
21	A	1140	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
19	A	6011	BCR	C15-C14-C13	-2.68	123.33	127.20
21	4	4011	CLA	C4-C3-C2	-2.68	118.25	123.50
21	A	1120	CLA	O1D-CGD-CBD	-2.68	120.79	124.62
21	A	1136	CLA	C3B-CAB-CBB	-2.67	120.85	126.32
19	L	6020	BCR	C36-C18-C17	-2.67	118.95	122.90
24	B	7101	DGD	CDB-CCB-CBB	-2.67	100.74	114.53
21	A	1115	CLA	O1D-CGD-CBD	-2.67	120.80	124.62
21	B	1206	CLA	O1D-CGD-CBD	-2.67	120.80	124.62
26	2	2501	LUT	C17-C1-C6	-2.67	106.12	110.30
21	A	1126	CLA	C6-C5-C3	-2.66	106.64	112.48
21	B	9022	CLA	CAA-C2A-C3A	-2.66	105.56	113.22
19	B	6006	BCR	C15-C14-C13	-2.66	123.35	127.20
21	A	1120	CLA	C3B-CAB-CBB	-2.66	120.87	126.32
27	4	4503	NEX	C18-C5-C4	-2.66	107.65	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1234	CLA	C3B-CAB-CBB	-2.66	120.87	126.32
21	J	6015	CLA	CHC-C1C-C2C	-2.66	119.36	126.35
21	B	1228	CLA	C4-C3-C2	-2.66	118.28	123.50
21	B	1205	CLA	O2D-CGD-O1D	-2.66	118.30	123.79
21	3	3015	CLA	O1D-CGD-CBD	-2.65	120.82	124.62
21	2	2014	CLA	OBD-CAD-C3D	-2.65	122.95	128.35
21	4	4005	CLA	O2D-CGD-O1D	-2.65	118.32	123.79
21	2	2002	CLA	CHC-C1C-C2C	-2.65	119.39	126.35
21	B	1216	CLA	CAA-C2A-C3A	-2.65	105.61	113.22
19	B	6006	BCR	C2-C3-C4	-2.64	104.87	111.53
21	A	1113	CLA	O2D-CGD-O1D	-2.64	118.33	123.79
21	B	9023	CLA	CAA-C2A-C3A	-2.64	105.62	113.22
21	3	3004	CLA	C3B-CAB-CBB	-2.64	120.91	126.32
21	4	4006	CLA	CHD-C4C-C3C	-2.64	120.86	124.94
21	3	3013	CLA	CHC-C1C-C2C	-2.64	119.41	126.35
21	A	1125	CLA	CHD-C4C-C3C	-2.64	120.86	124.94
21	A	1111	CLA	C3B-CAB-CBB	-2.64	120.92	126.32
21	A	1134	CLA	C3B-CAB-CBB	-2.63	120.93	126.32
21	B	1219	CLA	O1D-CGD-CBD	-2.63	120.85	124.62
21	A	1116	CLA	O1D-CGD-CBD	-2.63	120.85	124.62
21	L	1503	CLA	O1D-CGD-CBD	-2.63	120.85	124.62
20	B	7004	LHG	C5-O7-C7	-2.63	111.59	117.89
19	A	6008	BCR	C35-C13-C14	-2.62	119.03	122.90
19	A	6003	BCR	C36-C18-C17	-2.62	119.03	122.90
21	1	1008	CLA	CBC-CAC-C3C	-2.62	104.38	112.39
21	3	3014	CLA	O1D-CGD-CBD	-2.61	120.88	124.62
21	A	1103	CLA	C3B-CAB-CBB	-2.61	120.98	126.32
26	4	4502	LUT	O3-C3-C2	-2.61	104.57	109.91
21	B	1210	CLA	OBD-CAD-C3D	-2.60	123.04	128.35
21	2	2003	CLA	CHC-C1C-C2C	-2.60	119.51	126.35
19	B	6010	BCR	C37-C22-C21	-2.60	119.06	122.90
21	2	2002	CLA	CAC-C3C-C2C	-2.60	122.96	127.51
27	4	4503	NEX	C40-C33-C34	-2.59	119.07	122.90
21	B	9022	CLA	CGD-CBD-CAD	-2.59	101.84	110.62
21	2	2011	CLA	C4-C3-C2	-2.59	118.42	123.50
21	2	2011	CLA	CHC-C1C-C2C	-2.58	119.56	126.35
21	A	1128	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
21	3	3012	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
21	4	4012	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
21	4	4007	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
19	L	6020	BCR	C3-C4-C5	-2.58	109.77	113.87
21	1	1012	CLA	C3B-CAB-CBB	-2.58	121.04	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1202	CLA	O1D-CGD-CBD	-2.58	120.93	124.62
21	A	1121	CLA	C3B-CAB-CBB	-2.58	121.04	126.32
21	F	1302	CLA	O1D-CGD-CBD	-2.57	120.93	124.62
21	B	1231	CLA	C3B-CAB-CBB	-2.57	121.05	126.32
21	B	1218	CLA	O2D-CGD-O1D	-2.57	118.48	123.79
21	A	1130	CLA	O1D-CGD-CBD	-2.57	120.94	124.62
21	B	1230	CLA	CAA-CBA-CGA	-2.57	105.79	113.32
21	B	1226	CLA	CHC-C1C-C2C	-2.57	119.60	126.35
19	B	6006	BCR	C23-C24-C25	-2.57	119.61	127.32
21	A	1133	CLA	O2D-CGD-O1D	-2.56	118.50	123.79
21	1	1003	CLA	O1D-CGD-CBD	-2.56	120.96	124.62
21	2	2013	CLA	O2D-CGD-O1D	-2.56	118.51	123.79
26	2	2501	LUT	C20-C13-C14	-2.55	119.13	122.90
21	2	2008	CLA	CHD-C4C-C3C	-2.55	121.01	124.94
19	A	6011	BCR	C37-C22-C21	-2.54	119.14	122.90
21	A	1106	CLA	O2D-CGD-O1D	-2.54	118.54	123.79
27	4	4503	NEX	C17-C1-C6	-2.54	108.20	110.48
21	B	9022	CLA	C11-C12-C13	-2.54	107.06	115.49
21	B	1223	CLA	OBD-CAD-C3D	-2.54	123.17	128.35
21	1	1011	CLA	CBC-CAC-C3C	-2.54	104.65	112.39
21	2	2002	CLA	C3B-CAB-CBB	-2.54	121.13	126.32
27	4	4503	NEX	C19-C9-C10	-2.53	119.16	122.90
21	B	1209	CLA	O2D-CGD-O1D	-2.53	118.56	123.79
19	B	6004	BCR	C37-C22-C21	-2.53	119.16	122.90
21	2	2002	CLA	O1D-CGD-CBD	-2.53	120.99	124.62
26	1	1501	LUT	C38-C25-C24	-2.53	118.00	123.59
21	1	1001	CLA	O1D-CGD-CBD	-2.53	121.00	124.62
19	A	6007	BCR	C27-C26-C25	-2.52	119.56	122.78
21	4	4010	CLA	O2D-CGD-O1D	-2.52	118.59	123.79
21	B	1203	CLA	O1D-CGD-CBD	-2.52	121.01	124.62
21	A	1111	CLA	O1D-CGD-CBD	-2.52	121.02	124.62
21	1	1002	CLA	CBA-CAA-C2A	-2.51	106.64	113.73
21	B	1210	CLA	O1D-CGD-CBD	-2.51	121.02	124.62
21	B	1211	CLA	C3B-CAB-CBB	-2.51	121.18	126.32
21	1	1005	CLA	CAA-CBA-CGA	-2.51	105.97	113.32
21	4	4001	CLA	C4-C3-C2	-2.51	118.58	123.50
21	2	2010	CLA	CMD-C2D-C3D	-2.51	120.19	125.09
21	B	1236	CLA	O2D-CGD-O1D	-2.50	118.62	123.79
21	4	4014	CLA	O2D-CGD-O1D	-2.50	118.62	123.79
21	L	1501	CLA	O1D-CGD-CBD	-2.50	121.04	124.62
19	I	6020	BCR	C15-C14-C13	-2.50	123.58	127.20
21	4	4002	CLA	CHC-C1C-C2C	-2.50	119.78	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1240	CLA	CAA-C2A-C3A	-2.50	106.03	113.22
21	L	1502	CLA	O2D-CGD-O1D	-2.50	118.64	123.79
19	B	6011	BCR	C4-C5-C6	-2.49	119.60	122.78
21	B	1202	CLA	O2D-CGD-O1D	-2.49	118.64	123.79
19	L	6020	BCR	C7-C8-C9	-2.49	122.42	126.22
21	B	9010	CLA	O2D-CGD-O1D	-2.49	118.64	123.79
19	A	6011	BCR	C24-C25-C26	-2.49	115.67	121.37
21	4	4013	CLA	OBD-CAD-C3D	-2.49	123.27	128.35
24	B	7101	DGD	O6D-C1D-O3G	-2.49	104.06	110.05
21	3	3003	CLA	O1D-CGD-CBD	-2.49	121.06	124.62
21	1	1001	CLA	C4-C3-C2	-2.49	118.62	123.50
21	B	1230	CLA	O2D-CGD-O1D	-2.49	118.66	123.79
21	A	1137	CLA	O2D-CGD-O1D	-2.49	118.66	123.79
19	B	6010	BCR	C34-C9-C10	-2.48	119.23	122.90
21	B	1208	CLA	O1D-CGD-CBD	-2.48	121.06	124.62
21	1	1011	CLA	CHC-C1C-C2C	-2.48	119.82	126.35
21	B	1222	CLA	C3B-CAB-CBB	-2.48	121.24	126.32
21	3	3014	CLA	OBD-CAD-C3D	-2.48	123.29	128.35
21	2	2007	CLA	CHC-C1C-C2C	-2.48	119.83	126.35
21	J	6014	CLA	C4-C3-C2	-2.48	118.64	123.50
21	B	1227	CLA	OBD-CAD-C3D	-2.47	123.31	128.35
21	B	1220	CLA	O1D-CGD-CBD	-2.47	121.08	124.62
21	G	1002	CLA	CHC-C1C-C2C	-2.47	119.86	126.35
21	A	1108	CLA	C3B-CAB-CBB	-2.47	121.27	126.32
21	1	1001	CLA	CMD-C2D-C3D	-2.46	120.27	125.09
21	B	1239	CLA	CHD-C4C-C3C	-2.46	121.14	124.94
21	B	1211	CLA	O2D-CGD-O1D	-2.46	118.70	123.79
21	A	1118	CLA	O2D-CGD-O1D	-2.46	118.71	123.79
21	1	1009	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
21	A	1128	CLA	CAA-C2A-C3A	-2.46	106.16	113.22
21	1	1005	CLA	O1D-CGD-CBD	-2.45	121.11	124.62
21	A	1143	CLA	O2D-CGD-O1D	-2.45	118.73	123.79
21	B	1204	CLA	O2D-CGD-O1D	-2.44	118.75	123.79
21	A	1134	CLA	O2D-CGD-O1D	-2.44	118.75	123.79
21	B	1201	CLA	O2D-CGD-O1D	-2.44	118.75	123.79
21	4	4005	CLA	CMD-C2D-C3D	-2.44	120.32	125.09
21	B	1228	CLA	CAA-C2A-C1A	-2.43	103.89	112.47
21	4	4004	CLA	CAA-C2A-C3A	-2.43	106.23	113.22
19	B	6005	BCR	C35-C13-C14	-2.43	119.31	122.90
21	G	1002	CLA	CAA-C2A-C1A	-2.43	103.91	112.47
21	B	1218	CLA	C3B-CAB-CBB	-2.43	121.35	126.32
19	B	6006	BCR	C36-C18-C17	-2.43	119.32	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	H	1000	CLA	O2D-CGD-O1D	-2.43	118.78	123.79
21	3	3006	CLA	C3B-CAB-CBB	-2.43	121.35	126.32
21	2	2004	CLA	CBD-CHA-C1A	-2.43	127.48	128.59
21	B	1238	CLA	O2D-CGD-O1D	-2.42	118.78	123.79
21	L	1503	CLA	O2D-CGD-O1D	-2.42	118.78	123.79
21	B	1212	CLA	O2D-CGD-O1D	-2.42	118.79	123.79
19	B	6004	BCR	C38-C26-C25	-2.42	122.23	124.61
21	A	1130	CLA	O2D-CGD-O1D	-2.42	118.79	123.79
19	A	6008	BCR	C34-C9-C10	-2.42	119.33	122.90
21	4	4013	CLA	OBD-CAD-CBD	-2.41	122.30	125.94
21	3	3012	CLA	CBC-CAC-C3C	-2.41	105.03	112.39
21	A	1116	CLA	O2D-CGD-O1D	-2.41	118.81	123.79
21	A	1141	CLA	O2D-CGD-O1D	-2.41	118.82	123.79
21	A	1135	CLA	O2D-CGD-O1D	-2.41	118.82	123.79
21	A	1117	CLA	O2D-CGD-O1D	-2.41	118.82	123.79
21	4	4015	CLA	O1D-CGD-CBD	-2.41	121.17	124.62
21	4	4012	CLA	C4-C3-C2	-2.40	118.78	123.50
21	2	2008	CLA	CHA-C1A-NA	-2.40	120.15	126.06
21	4	4014	CLA	CMD-C2D-C3D	-2.40	120.39	125.09
21	A	1109	CLA	CAA-C2A-C3A	-2.40	106.31	113.22
21	A	1139	CLA	C6-C5-C3	-2.40	107.22	112.48
21	1	1013	CLA	O2D-CGD-O1D	-2.40	118.84	123.79
21	L	1501	CLA	OBD-CAD-C3D	-2.40	123.46	128.35
21	A	1111	CLA	O2D-CGD-O1D	-2.40	118.84	123.79
19	L	6019	BCR	C27-C26-C25	-2.40	119.73	122.78
19	G	2011	BCR	C27-C26-C25	-2.40	119.73	122.78
21	B	1229	CLA	O2D-CGD-O1D	-2.39	118.84	123.79
19	G	2011	BCR	C38-C26-C25	-2.39	122.25	124.61
21	B	1219	CLA	C3B-CAB-CBB	-2.39	121.42	126.32
21	4	4002	CLA	O2D-CGD-O1D	-2.39	118.85	123.79
21	B	1234	CLA	O2D-CGD-O1D	-2.39	118.85	123.79
21	3	3012	CLA	OBD-CAD-C3D	-2.39	123.48	128.35
21	F	1303	CLA	OBD-CAD-C3D	-2.39	123.48	128.35
21	4	4002	CLA	O1D-CGD-CBD	-2.39	121.20	124.62
21	A	1112	CLA	O2D-CGD-O1D	-2.39	118.86	123.79
21	A	1102	CLA	C3B-CAB-CBB	-2.38	121.44	126.32
21	A	9013	CLA	CMA-C3A-C2A	-2.38	103.80	114.35
21	B	1235	CLA	O2D-CGD-O1D	-2.38	118.87	123.79
21	3	3006	CLA	O2D-CGD-O1D	-2.38	118.88	123.79
21	A	9012	CLA	C4C-C3C-C2C	-2.37	103.10	106.94
26	1	1502	LUT	C38-C25-C24	-2.37	118.36	123.59
21	3	3012	CLA	OBD-CAD-CBD	-2.37	122.36	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4002	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
21	2	2012	CLA	O2D-CGD-O1D	-2.37	118.90	123.79
19	J	6012	BCR	C31-C1-C6	-2.37	106.59	110.30
21	4	4015	CLA	O2D-CGD-O1D	-2.36	118.91	123.79
20	2	2801	LHG	C5-O7-C7	-2.36	112.22	117.89
19	F	6014	BCR	C7-C6-C5	-2.36	115.96	121.37
21	A	1129	CLA	O2D-CGD-O1D	-2.36	118.92	123.79
21	1	1010	CLA	OBD-CAD-CBD	-2.36	122.38	125.94
21	B	1231	CLA	O2D-CGD-O1D	-2.36	118.93	123.79
26	2	2502	LUT	C35-C34-C33	-2.35	123.80	127.20
21	1	1008	CLA	C4-C3-C2	-2.35	118.88	123.50
21	1	1012	CLA	CBC-CAC-C3C	-2.35	105.21	112.39
21	A	1123	CLA	OBD-CAD-C3D	-2.35	123.55	128.35
18	A	5001	PQN	C11-C12-C13	-2.35	122.71	126.70
21	4	4009	CLA	OBD-CAD-C3D	-2.35	123.56	128.35
21	B	1212	CLA	CAA-C2A-C3A	-2.35	106.47	113.22
21	A	1136	CLA	O2D-CGD-O1D	-2.35	118.95	123.79
19	J	6013	BCR	C31-C1-C6	-2.35	106.63	110.30
21	B	1240	CLA	CHC-C1C-C2C	-2.34	120.19	126.35
21	B	9023	CLA	O1D-CGD-CBD	-2.34	121.27	124.62
21	B	1223	CLA	O2D-CGD-O1D	-2.34	118.96	123.79
21	A	1127	CLA	O2D-CGD-O1D	-2.34	118.96	123.79
21	A	1107	CLA	CAA-C2A-C3A	-2.34	106.50	113.22
19	J	6013	BCR	C3-C4-C5	-2.33	110.17	113.87
21	1	1010	CLA	O1D-CGD-CBD	-2.33	121.28	124.62
21	3	3008	CLA	C4-C3-C2	-2.33	118.93	123.50
21	1	1001	CLA	OBD-CAD-CBD	-2.33	122.43	125.94
21	1	1007	CLA	O1D-CGD-CBD	-2.32	121.29	124.62
26	1	1502	LUT	C37-C21-C22	-2.32	105.24	109.35
21	A	1113	CLA	O1D-CGD-CBD	-2.32	121.29	124.62
19	B	6006	BCR	C7-C6-C5	-2.32	116.06	121.37
21	B	1240	CLA	OBD-CAD-C3D	-2.32	123.62	128.35
24	B	7101	DGD	O2D-C2D-C1D	-2.32	104.93	110.02
19	J	6013	BCR	C36-C18-C17	-2.32	119.47	122.90
21	3	3012	CLA	CHC-C1C-C2C	-2.32	120.25	126.35
21	A	1114	CLA	O2D-CGD-O1D	-2.32	119.00	123.79
21	A	1103	CLA	CAA-C2A-C3A	-2.32	106.55	113.22
21	A	1135	CLA	C3B-CAB-CBB	-2.32	121.58	126.32
21	1	1009	CLA	C1C-NC-C4C	-2.32	103.45	106.27
21	A	1109	CLA	O2D-CGD-O1D	-2.32	119.01	123.79
21	3	3009	CLA	OBD-CAD-C3D	-2.31	123.63	128.35
21	J	6014	CLA	O2D-CGD-O1D	-2.31	119.02	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	2009	CLA	CAA-C2A-C3A	-2.31	106.58	113.22
21	A	1104	CLA	O2D-CGD-O1D	-2.31	119.03	123.79
21	B	1210	CLA	O2D-CGD-O1D	-2.30	119.03	123.79
21	G	1002	CLA	O1D-CGD-CBD	-2.30	121.33	124.62
21	2	2004	CLA	O2D-CGD-O1D	-2.30	119.04	123.79
21	A	1132	CLA	O2D-CGD-O1D	-2.30	119.05	123.79
21	4	4003	CLA	CAA-CBA-CGA	-2.30	106.59	113.32
21	A	1105	CLA	O2D-CGD-O1D	-2.29	119.05	123.79
19	G	2011	BCR	C34-C9-C10	-2.29	119.51	122.90
21	B	1206	CLA	CAA-C2A-C3A	-2.29	106.63	113.22
21	B	9023	CLA	C16-C15-C13	-2.29	107.90	115.49
21	B	1214	CLA	C4-C3-C2	-2.29	119.01	123.50
21	A	1140	CLA	O2D-CGD-O1D	-2.29	119.07	123.79
21	3	3015	CLA	O2D-CGD-O1D	-2.29	119.07	123.79
21	B	1225	CLA	C3B-CAB-CBB	-2.28	121.64	126.32
21	B	1216	CLA	O2D-CGD-O1D	-2.28	119.07	123.79
21	B	1215	CLA	O2D-CGD-O1D	-2.28	119.08	123.79
21	A	1138	CLA	O2D-CGD-O1D	-2.28	119.08	123.79
21	1	1001	CLA	CHC-C1C-C2C	-2.28	120.36	126.35
21	2	2005	CLA	CHC-C1C-C2C	-2.28	120.36	126.35
21	1	1001	CLA	CBC-CAC-C3C	-2.28	105.44	112.39
21	2	2007	CLA	O2D-CGD-O1D	-2.28	119.09	123.79
21	B	1217	CLA	O2D-CGD-O1D	-2.28	119.09	123.79
21	1	1011	CLA	C16-C15-C13	-2.28	107.94	115.49
27	4	4503	NEX	O23-C23-C24	-2.27	105.26	109.91
21	4	4014	CLA	CBC-CAC-C3C	-2.27	105.46	112.39
19	A	6002	BCR	C15-C14-C13	-2.27	123.92	127.20
21	A	1104	CLA	CAA-C2A-C3A	-2.27	106.69	113.22
21	L	1501	CLA	O2D-CGD-O1D	-2.27	119.11	123.79
21	B	1206	CLA	C3B-CAB-CBB	-2.27	121.68	126.32
18	B	5002	PQN	C11-C12-C13	-2.27	122.86	126.70
21	3	3008	CLA	CBC-CAC-C3C	-2.26	105.49	112.39
21	3	3008	CLA	CHC-C1C-C2C	-2.26	120.41	126.35
21	1	1006	CLA	CHC-C1C-C2C	-2.26	120.41	126.35
21	A	1139	CLA	O1D-CGD-CBD	-2.26	121.38	124.62
19	B	6004	BCR	C39-C30-C25	-2.26	106.76	110.30
21	4	4013	CLA	CBC-CAC-C3C	-2.26	105.50	112.39
19	B	6011	BCR	C8-C7-C6	-2.26	120.54	127.32
21	1	1007	CLA	CGD-CBD-CAD	-2.26	102.97	110.62
21	1	1002	CLA	CMD-C2D-C3D	-2.26	120.67	125.09
21	A	1126	CLA	CAA-C2A-C3A	-2.26	106.73	113.22
21	B	1222	CLA	O2D-CGD-O1D	-2.26	119.13	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1012	CLA	OBD-CAD-CBD	-2.26	122.53	125.94
26	1	1501	LUT	C39-C29-C30	-2.26	119.57	122.90
21	A	1126	CLA	CAA-CBA-CGA	-2.25	106.72	113.32
19	J	6012	BCR	C27-C26-C25	-2.25	119.91	122.78
21	2	2005	CLA	O1D-CGD-CBD	-2.25	121.40	124.62
19	L	6019	BCR	C32-C1-C6	-2.25	106.78	110.30
21	A	9012	CLA	CHD-C4C-C3C	-2.25	121.47	124.94
19	F	6014	BCR	C24-C25-C26	-2.25	116.22	121.37
24	B	7101	DGD	CFB-CEB-CDB	-2.24	102.94	114.53
21	1	1013	CLA	CHD-C4C-C3C	-2.24	121.48	124.94
26	4	4502	LUT	C17-C1-C6	-2.24	106.79	110.30
21	B	1206	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
21	J	1302	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
21	1	1002	CLA	C4-C3-C2	-2.24	119.11	123.50
21	A	9013	CLA	OBD-CAD-C3D	-2.23	123.80	128.35
21	3	3003	CLA	CHD-C4C-C3C	-2.23	121.49	124.94
21	B	1204	CLA	OBD-CAD-C3D	-2.23	123.80	128.35
21	B	1214	CLA	O2D-CGD-O1D	-2.23	119.18	123.79
21	3	3009	CLA	O2D-CGD-O1D	-2.23	119.18	123.79
21	3	3013	CLA	OBD-CAD-CBD	-2.23	122.57	125.94
21	B	9023	CLA	CBA-CAA-C2A	-2.23	107.44	113.73
21	B	1217	CLA	CAA-C2A-C3A	-2.23	106.80	113.22
23	A	9011	CL0	CHA-C1A-NA	-2.23	120.57	126.06
21	A	1142	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
21	2	2009	CLA	CHA-C1A-NA	-2.23	120.58	126.06
21	A	1110	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
21	A	1115	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
21	2	2012	CLA	CAA-C2A-C3A	-2.23	106.81	113.22
21	J	6015	CLA	O1D-CGD-CBD	-2.23	121.43	124.62
21	B	1219	CLA	OBD-CAD-C3D	-2.23	123.81	128.35
21	A	1133	CLA	CBC-CAC-C3C	-2.23	105.60	112.39
19	A	6017	BCR	C28-C27-C26	-2.22	110.34	113.87
21	A	1105	CLA	C3B-CAB-CBB	-2.22	121.77	126.32
21	B	1239	CLA	CAA-CBA-CGA	-2.22	106.81	113.32
21	4	4010	CLA	CAA-C2A-C1A	-2.22	104.64	112.47
21	4	4006	CLA	CHC-C1C-C2C	-2.22	120.51	126.35
19	A	6008	BCR	C36-C18-C17	-2.22	119.63	122.90
21	4	4008	CLA	CHA-C1A-NA	-2.21	120.61	126.06
21	B	9022	CLA	O2D-CGD-O1D	-2.21	119.22	123.79
21	4	4010	CLA	CHC-C1C-C2C	-2.21	120.54	126.35
21	B	1202	CLA	C3B-CAB-CBB	-2.21	121.79	126.32
21	3	3002	CLA	O2D-CGD-O1D	-2.21	119.23	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	1303	CLA	C4C-C3C-C2C	-2.21	103.36	106.94
21	1	1010	CLA	CHD-C4C-C3C	-2.21	121.53	124.94
21	B	1219	CLA	OBD-CAD-CBD	-2.21	122.61	125.94
21	G	1002	CLA	CAA-CBA-CGA	-2.21	106.86	113.32
19	F	6016	BCR	C36-C18-C17	-2.21	119.64	122.90
21	B	1239	CLA	C4-C3-C2	-2.20	119.18	123.50
21	A	1109	CLA	C4-C3-C2	-2.20	119.18	123.50
21	1	1011	CLA	CGD-CBD-CAD	-2.20	103.17	110.62
21	A	1131	CLA	CAA-CBA-CGA	-2.20	106.88	113.32
21	3	3005	CLA	OBD-CAD-C3D	-2.20	123.87	128.35
19	A	6007	BCR	C35-C13-C14	-2.20	119.66	122.90
21	4	4006	CLA	CAC-C3C-C4C	-2.20	121.64	124.83
21	1	1004	CLA	C4-C3-C2	-2.20	119.19	123.50
21	A	1118	CLA	CHC-C1C-C2C	-2.19	120.58	126.35
21	B	1206	CLA	CHC-C1C-C2C	-2.19	120.58	126.35
21	B	1219	CLA	CAA-C2A-C3A	-2.19	106.91	113.22
26	2	2501	LUT	C38-C25-C24	-2.19	118.75	123.59
21	1	1013	CLA	CBA-CAA-C2A	-2.19	107.56	113.73
21	B	1230	CLA	C4-C3-C2	-2.19	119.21	123.50
24	B	7101	DGD	CBB-CAB-C9B	-2.19	103.25	114.53
21	G	1001	CLA	O1D-CGD-CBD	-2.18	121.49	124.62
21	A	1120	CLA	O2D-CGD-O1D	-2.18	119.28	123.79
21	B	1220	CLA	O2D-CGD-O1D	-2.18	119.29	123.79
19	J	6013	BCR	C35-C13-C14	-2.18	119.68	122.90
21	G	1002	CLA	OBD-CAD-CBD	-2.18	122.65	125.94
26	4	4501	LUT	C39-C29-C30	-2.17	119.69	122.90
21	B	1207	CLA	CMA-C3A-C2A	-2.17	104.73	114.35
21	L	1502	CLA	CAA-C2A-C3A	-2.17	106.97	113.22
21	3	3012	CLA	CAA-CBA-CGA	-2.17	104.16	113.02
26	1	1501	LUT	C3-C4-C5	-2.17	107.39	111.86
21	1	1009	CLA	O2D-CGD-O1D	-2.17	119.31	123.79
21	A	1109	CLA	O1D-CGD-CBD	-2.17	121.52	124.62
21	A	9012	CLA	O2D-CGD-O1D	-2.17	119.32	123.79
21	B	1225	CLA	O2D-CGD-O1D	-2.16	119.32	123.79
21	A	1107	CLA	CMD-C2D-C3D	-2.16	120.86	125.09
26	1	1502	LUT	C1-C2-C3	-2.16	108.34	113.41
21	B	1239	CLA	C6-C7-C8	-2.16	108.32	115.49
21	A	9013	CLA	C4C-C3C-C2C	-2.15	103.45	106.94
21	F	1302	CLA	O2D-CGD-O1D	-2.15	119.34	123.79
21	3	3014	CLA	CHC-C1C-C2C	-2.15	120.69	126.35
21	A	1132	CLA	C4-C3-C2	-2.15	119.28	123.50
21	A	1122	CLA	O1D-CGD-CBD	-2.15	121.54	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	G	2011	BCR	C7-C8-C9	-2.15	122.94	126.22
21	J	6015	CLA	CMD-C2D-C3D	-2.15	120.89	125.09
21	A	1137	CLA	C4-C3-C2	-2.15	119.29	123.50
21	4	4015	CLA	CHD-C4C-C3C	-2.15	121.63	124.94
21	1	1006	CLA	CAA-C2A-C1A	-2.15	104.91	112.47
21	3	3008	CLA	CMD-C2D-C3D	-2.14	120.89	125.09
21	B	1214	CLA	OBD-CAD-C3D	-2.14	123.98	128.35
21	1	1003	CLA	OBD-CAD-C3D	-2.14	123.98	128.35
21	F	1301	CLA	O2D-CGD-O1D	-2.14	119.37	123.79
21	1	1010	CLA	OBD-CAD-C3D	-2.14	123.98	128.35
24	B	7101	DGD	C3D-C4D-C5D	-2.14	106.47	110.20
21	A	1130	CLA	CAA-C2A-C3A	-2.14	107.06	113.22
21	B	1237	CLA	C4-C3-C2	-2.14	119.30	123.50
21	B	1240	CLA	CAA-C2A-C1A	-2.14	104.94	112.47
21	A	1127	CLA	C4-C3-C2	-2.13	119.31	123.50
26	2	2501	LUT	C3-C4-C5	-2.13	107.47	111.86
19	A	6007	BCR	C30-C25-C26	-2.13	119.54	122.66
21	3	3009	CLA	CMD-C2D-C3D	-2.13	120.93	125.09
21	F	1303	CLA	CHC-C1C-C2C	-2.13	120.76	126.35
21	4	4011	CLA	C16-C15-C13	-2.13	108.44	115.49
21	A	1124	CLA	C3B-CAB-CBB	-2.13	121.97	126.32
21	4	4008	CLA	CMD-C2D-C3D	-2.12	120.93	125.09
21	A	1119	CLA	O2D-CGD-O1D	-2.12	119.41	123.79
21	A	1124	CLA	O2D-CGD-O1D	-2.12	119.41	123.79
21	A	1110	CLA	CHC-C1C-C2C	-2.12	120.78	126.35
21	B	9022	CLA	CHA-C1A-NA	-2.12	120.85	126.06
21	2	2009	CLA	CHC-C1C-C2C	-2.12	120.79	126.35
21	3	3017	CLA	O2D-CGD-O1D	-2.11	119.42	123.79
21	4	4003	CLA	C4C-C3C-C2C	-2.11	103.51	106.94
21	B	1201	CLA	CAA-C2A-C3A	-2.11	107.14	113.22
21	4	4011	CLA	CMD-C2D-C3D	-2.11	120.96	125.09
21	A	1116	CLA	C3B-CAB-CBB	-2.11	122.00	126.32
21	B	1207	CLA	O1D-CGD-CBD	-2.11	121.60	124.62
21	2	2006	CLA	O1D-CGD-CBD	-2.11	121.60	124.62
21	4	4008	CLA	CHC-C1C-C2C	-2.11	120.81	126.35
21	4	4002	CLA	C3B-CAB-CBB	-2.11	122.01	126.32
21	2	2012	CLA	CBC-CAC-C3C	-2.10	105.97	112.39
21	A	1112	CLA	CAA-C2A-C3A	-2.10	107.18	113.22
19	A	6002	BCR	C34-C9-C10	-2.10	119.80	122.90
19	F	6016	BCR	C34-C9-C10	-2.10	119.80	122.90
21	3	3010	CLA	O2D-CGD-O1D	-2.10	119.46	123.79
21	A	1143	CLA	O1D-CGD-CBD	-2.10	121.61	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	3010	CLA	CHC-C1C-C2C	-2.10	120.83	126.35
19	A	6011	BCR	C29-C28-C27	-2.10	106.25	111.53
26	4	4501	LUT	C40-C33-C34	-2.10	119.81	122.90
21	B	1235	CLA	CAA-C2A-C3A	-2.10	107.19	113.22
21	3	3014	CLA	OBD-CAD-CBD	-2.09	122.78	125.94
21	A	9013	CLA	C7-C6-C5	-2.09	106.88	113.06
21	B	9022	CLA	C16-C15-C13	-2.09	108.55	115.49
18	B	5002	PQN	C12-C11-C3	-2.09	105.36	111.64
19	L	6020	BCR	C30-C25-C26	-2.09	119.59	122.66
25	G	2021	LMG	O7-C10-O9	-2.09	118.74	122.92
19	I	6020	BCR	C34-C9-C10	-2.09	119.81	122.90
21	2	2012	CLA	CHC-C1C-C2C	-2.09	120.86	126.35
21	1	1012	CLA	CMD-C2D-C3D	-2.09	121.00	125.09
21	B	1240	CLA	CAA-CBA-CGA	-2.09	107.20	113.32
21	A	1101	CLA	O1D-CGD-CBD	-2.09	121.63	124.62
26	2	2502	LUT	C10-C11-C12	-2.09	116.77	123.13
21	1	1001	CLA	OBD-CAD-C3D	-2.09	124.10	128.35
19	L	6019	BCR	C31-C1-C6	-2.09	107.03	110.30
21	A	1107	CLA	O2D-CGD-O1D	-2.08	119.49	123.79
19	I	6020	BCR	C23-C24-C25	-2.08	121.06	127.32
21	1	1001	CLA	CGD-CBD-CAD	-2.08	103.57	110.62
21	A	1140	CLA	C3B-CAB-CBB	-2.08	122.06	126.32
25	G	2021	LMG	C8-O7-C10	-2.08	113.99	117.92
21	B	1239	CLA	CMA-C3A-C2A	-2.08	105.15	114.35
19	A	6002	BCR	C31-C1-C6	-2.08	107.04	110.30
21	B	1219	CLA	C4-C3-C2	-2.08	119.42	123.50
21	1	1005	CLA	C4-C3-C2	-2.08	119.43	123.50
21	3	3014	CLA	O2D-CGD-O1D	-2.08	119.50	123.79
21	F	1303	CLA	O2D-CGD-O1D	-2.07	119.51	123.79
19	J	6013	BCR	C37-C22-C21	-2.07	119.84	122.90
21	B	1204	CLA	C4-C3-C2	-2.07	119.44	123.50
21	A	1116	CLA	C4-C3-C2	-2.07	119.44	123.50
21	2	2001	CLA	CAD-CBD-CHA	-2.07	102.45	105.61
19	J	6012	BCR	C7-C6-C5	-2.07	116.64	121.37
21	B	1221	CLA	OBD-CAD-C3D	-2.06	124.14	128.35
21	1	1005	CLA	O2D-CGD-O1D	-2.06	119.53	123.79
19	B	6005	BCR	C31-C1-C6	-2.06	107.07	110.30
21	A	1128	CLA	C6-C5-C3	-2.06	107.96	112.48
24	B	7101	DGD	C3G-C2G-C1G	-2.06	107.25	112.07
19	G	2011	BCR	C31-C1-C6	-2.06	107.07	110.30
21	1	1014	CLA	CHC-C1C-C2C	-2.06	120.93	126.35
21	2	2014	CLA	OBD-CAD-CBD	-2.06	122.83	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4003	CLA	C3B-CAB-CBB	-2.06	122.11	126.32
19	A	6007	BCR	C28-C27-C26	-2.06	110.60	113.87
21	2	2010	CLA	OBD-CAD-C3D	-2.05	124.16	128.35
19	B	6010	BCR	C35-C13-C14	-2.05	119.87	122.90
19	I	6020	BCR	C30-C25-C26	-2.05	119.64	122.66
21	B	1237	CLA	O2D-CGD-O1D	-2.05	119.55	123.79
21	B	1213	CLA	C6-C5-C3	-2.05	107.98	112.48
21	1	1011	CLA	CAA-C2A-C1A	-2.05	105.23	112.47
21	A	1103	CLA	O1D-CGD-CBD	-2.05	121.68	124.62
21	4	4004	CLA	C4-C3-C2	-2.04	119.49	123.50
21	2	2012	CLA	CMD-C2D-C3D	-2.04	121.09	125.09
21	B	1211	CLA	CAA-C2A-C3A	-2.04	107.34	113.22
21	A	1125	CLA	CHA-C1A-NA	-2.04	121.04	126.06
21	1	1003	CLA	C4-C3-C2	-2.04	119.50	123.50
19	L	6020	BCR	C27-C26-C25	-2.04	120.18	122.78
21	B	1210	CLA	C4C-C3C-C2C	-2.04	103.64	106.94
21	B	9022	CLA	CHC-C1C-C2C	-2.04	121.00	126.35
19	B	6009	BCR	C7-C6-C5	-2.03	116.72	121.37
21	3	3011	CLA	CMD-C2D-C3D	-2.03	121.11	125.09
21	4	4006	CLA	CAA-C2A-C1A	-2.03	105.31	112.47
21	A	1133	CLA	CHC-C1C-C2C	-2.03	121.01	126.35
19	F	6016	BCR	C29-C28-C27	-2.03	106.41	111.53
21	2	2011	CLA	C2A-C1A-CHA	-2.03	120.15	123.89
24	B	7101	DGD	CAB-C9B-C8B	-2.03	104.06	114.53
19	A	6007	BCR	C31-C1-C6	-2.03	107.12	110.30
24	B	7101	DGD	C5B-C4B-C3B	-2.03	104.06	114.53
19	J	6012	BCR	C35-C13-C14	-2.03	119.91	122.90
21	A	1126	CLA	C4-C3-C2	-2.03	119.53	123.50
21	B	1214	CLA	C3B-CAB-CBB	-2.02	122.17	126.32
21	H	1000	CLA	CHC-C1C-C2C	-2.02	121.03	126.35
21	A	1109	CLA	CHC-C1C-C2C	-2.02	121.03	126.35
21	J	1302	CLA	OBD-CAD-C3D	-2.02	124.23	128.35
21	1	1006	CLA	CAA-C2A-C3A	-2.02	107.40	113.22
21	4	4007	CLA	CGD-CBD-CAD	-2.02	103.77	110.62
21	B	1227	CLA	C4-C3-C2	-2.02	119.53	123.50
21	B	1219	CLA	O2D-CGD-O1D	-2.02	119.62	123.79
19	L	6020	BCR	C8-C7-C6	-2.02	121.25	127.32
21	4	4009	CLA	C3B-CAB-CBB	-2.02	122.19	126.32
21	A	1118	CLA	CBC-CAC-C3C	-2.02	106.23	112.39
21	B	1203	CLA	O2D-CGD-O1D	-2.02	119.63	123.79
21	1	1006	CLA	CMD-C2D-C3D	-2.01	121.15	125.09
21	B	9010	CLA	CHC-C1C-C2C	-2.01	121.05	126.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	2004	CLA	CAA-C2A-C3A	-2.01	107.42	113.22
21	3	3009	CLA	CHC-C1C-C2C	-2.01	121.06	126.35
21	A	1113	CLA	C3B-CAB-CBB	-2.01	122.20	126.32
21	A	1108	CLA	O2D-CGD-O1D	-2.01	119.65	123.79
21	2	2013	CLA	CBC-CAC-C3C	-2.01	106.27	112.39
19	B	6010	BCR	C23-C24-C25	-2.00	121.30	127.32
21	B	1239	CLA	C4C-C3C-C2C	-2.00	103.69	106.94
21	4	4015	CLA	CMD-C2D-C3D	-2.00	121.18	125.09
21	3	3015	CLA	CAC-C3C-C4C	2.00	127.73	124.83
19	B	6004	BCR	C12-C13-C14	2.00	122.21	118.98
21	F	1301	CLA	CMB-C2B-C3B	2.00	129.01	125.09
21	B	1220	CLA	CAC-C3C-C4C	2.01	127.74	124.83
26	2	2501	LUT	C32-C33-C34	2.01	122.22	118.98
21	A	1117	CLA	CAC-C3C-C4C	2.01	127.75	124.83
27	4	4503	NEX	C31-C32-C33	2.01	132.25	126.32
21	B	9023	CLA	CHB-C4A-NA	2.02	127.30	124.51
21	A	1108	CLA	CED-O2D-CGD	2.02	120.72	115.99
21	3	3001	CLA	CAC-C3C-C4C	2.02	127.76	124.83
21	1	1013	CLA	CAA-C2A-C1A	2.02	119.60	112.47
21	4	4011	CLA	CMB-C2B-C1B	2.02	131.71	128.36
21	B	1208	CLA	CMB-C2B-C3B	2.02	129.04	125.09
26	2	2502	LUT	C18-C5-C4	2.02	117.93	114.24
21	A	1120	CLA	C4A-NA-C1A	2.02	108.97	106.36
21	4	4010	CLA	C5-C3-C4	2.03	119.62	114.64
21	B	1215	CLA	C4A-NA-C1A	2.03	108.98	106.36
21	B	1225	CLA	CAC-C3C-C4C	2.03	127.78	124.83
21	A	9013	CLA	CGD-CBD-CAD	2.03	117.51	110.62
26	2	2501	LUT	C12-C13-C14	2.03	122.26	118.98
21	A	1133	CLA	CMB-C2B-C3B	2.03	129.07	125.09
21	2	2003	CLA	CAC-C3C-C4C	2.04	127.78	124.83
21	A	1134	CLA	C4A-NA-C1A	2.04	108.99	106.36
21	B	1222	CLA	CAC-C3C-C4C	2.04	127.79	124.83
21	L	1503	CLA	C5-C3-C4	2.04	119.65	114.64
19	J	6013	BCR	C33-C5-C4	2.04	117.29	113.43
21	A	1124	CLA	CAC-C3C-C4C	2.04	127.79	124.83
21	A	1112	CLA	C4A-NA-C1A	2.04	109.00	106.36
21	1	1009	CLA	C4A-NA-C1A	2.04	109.00	106.36
21	B	1220	CLA	CED-O2D-CGD	2.04	120.77	115.99
21	A	1142	CLA	C4A-NA-C1A	2.04	109.00	106.36
21	2	2010	CLA	C4A-NA-C1A	2.04	109.00	106.36
21	3	3015	CLA	C4A-NA-C1A	2.04	109.00	106.36
21	4	4005	CLA	CMB-C2B-C3B	2.05	129.09	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1135	CLA	CMB-C2B-C3B	2.05	129.09	125.09
21	A	1116	CLA	CAC-C3C-C4C	2.05	127.81	124.83
21	A	1108	CLA	C4A-NA-C1A	2.05	109.01	106.36
21	A	1143	CLA	C4A-NA-C1A	2.05	109.01	106.36
21	3	3012	CLA	CMC-C2C-C3C	2.05	131.91	125.94
21	4	4007	CLA	CMB-C2B-C1B	2.06	131.77	128.36
21	4	4006	CLA	CHB-C4A-NA	2.06	127.36	124.51
21	B	1204	CLA	C4A-NA-C1A	2.06	109.02	106.36
21	A	1104	CLA	C4A-NA-C1A	2.06	109.02	106.36
21	B	1217	CLA	CAC-C3C-C4C	2.06	127.82	124.83
19	G	2011	BCR	C29-C28-C27	2.06	116.73	111.53
26	2	2501	LUT	C18-C5-C4	2.06	118.00	114.24
21	3	3011	CLA	C1-O2A-CGA	2.06	123.84	116.21
21	A	1114	CLA	C4A-NA-C1A	2.06	109.03	106.36
21	B	1240	CLA	CMC-C2C-C1C	2.06	128.21	125.02
18	B	5002	PQN	C2M-C2-C1	2.07	119.62	116.27
21	A	1122	CLA	CAC-C3C-C4C	2.07	127.83	124.83
21	4	4012	CLA	CMC-C2C-C1C	2.07	128.22	125.02
21	B	1217	CLA	C4A-NA-C1A	2.07	109.03	106.36
21	B	1240	CLA	CMB-C2B-C3B	2.07	129.13	125.09
19	F	6016	BCR	C23-C22-C21	2.07	122.31	118.98
19	A	6003	BCR	C19-C18-C17	2.07	122.32	118.98
26	4	4502	LUT	C18-C5-C4	2.07	118.02	114.24
21	A	1138	CLA	CED-O2D-CGD	2.07	120.86	115.99
21	A	1135	CLA	C4A-NA-C1A	2.08	109.04	106.36
21	3	3016	CLA	CAC-C3C-C4C	2.08	127.84	124.83
21	4	4013	CLA	CAC-C3C-C4C	2.08	127.85	124.83
21	2	2002	CLA	CGD-CBD-CAD	2.08	117.67	110.62
21	G	1002	CLA	CMC-C2C-C1C	2.08	128.24	125.02
21	A	1129	CLA	C5-C3-C4	2.08	119.75	114.64
21	A	1117	CLA	C4A-NA-C1A	2.08	109.05	106.36
21	B	1204	CLA	CMB-C2B-C3B	2.08	129.16	125.09
21	A	1104	CLA	CMB-C2B-C3B	2.08	129.16	125.09
21	A	1105	CLA	CMB-C2B-C3B	2.08	129.16	125.09
19	G	2011	BCR	C30-C25-C24	2.08	121.65	115.82
21	B	1209	CLA	CMB-C2B-C3B	2.08	129.16	125.09
19	A	6002	BCR	C29-C28-C27	2.09	116.79	111.53
21	A	1142	CLA	CMB-C2B-C3B	2.09	129.40	125.14
21	B	1230	CLA	CMB-C2B-C3B	2.09	129.17	125.09
21	2	2007	CLA	CMB-C2B-C3B	2.09	129.17	125.09
21	A	1105	CLA	C4A-NA-C1A	2.09	109.06	106.36
21	3	3017	CLA	CAC-C3C-C4C	2.09	127.86	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1201	CLA	C4A-NA-C1A	2.09	109.06	106.36
21	B	1231	CLA	CED-O2D-CGD	2.09	120.89	115.99
21	1	1005	CLA	CMB-C2B-C3B	2.09	129.18	125.09
21	2	2006	CLA	CAC-C3C-C4C	2.09	127.87	124.83
21	B	1211	CLA	C4A-NA-C1A	2.09	109.06	106.36
21	B	1229	CLA	C4A-NA-C1A	2.10	109.07	106.36
21	A	1139	CLA	CMB-C2B-C3B	2.10	129.19	125.09
21	B	1220	CLA	C4A-NA-C1A	2.10	109.07	106.36
21	A	1106	CLA	C4A-NA-C1A	2.10	109.07	106.36
21	B	1216	CLA	CAC-C3C-C4C	2.10	127.88	124.83
21	A	1110	CLA	C4A-NA-C1A	2.10	109.08	106.36
19	A	6008	BCR	C30-C25-C26	2.10	125.75	122.66
26	4	4501	LUT	C8-C7-C6	2.10	133.64	127.32
21	F	1302	CLA	CMB-C2B-C3B	2.11	129.21	125.09
21	3	3010	CLA	CED-O2D-CGD	2.11	120.93	115.99
21	F	1303	CLA	O2A-CGA-CBA	2.11	118.31	109.87
21	B	1237	CLA	CAC-C3C-C4C	2.11	127.89	124.83
21	L	1502	CLA	CMB-C2B-C3B	2.11	129.22	125.09
19	B	6004	BCR	C29-C30-C25	2.11	113.71	110.36
21	H	1000	CLA	C4A-NA-C1A	2.11	109.09	106.36
21	A	1102	CLA	C5-C3-C4	2.12	119.84	114.64
20	A	7003	LHG	O4-P-O5	2.12	124.00	112.53
21	B	1237	CLA	C4A-NA-C1A	2.12	109.09	106.36
21	B	1226	CLA	CMB-C2B-C3B	2.12	129.23	125.09
19	I	6018	BCR	C35-C13-C12	2.12	121.62	118.10
21	1	1009	CLA	CMC-C2C-C1C	2.12	128.30	125.02
21	A	1121	CLA	CMB-C2B-C3B	2.12	129.24	125.09
19	L	6019	BCR	C33-C5-C4	2.12	117.45	113.43
21	B	9022	CLA	C4A-NA-C1A	2.12	109.10	106.36
21	L	1501	CLA	CMB-C2B-C3B	2.12	129.24	125.09
21	4	4001	CLA	CHB-C4A-NA	2.12	127.45	124.51
21	3	3013	CLA	CMC-C2C-C1C	2.12	128.31	125.02
21	A	1113	CLA	CMB-C2B-C3B	2.13	129.25	125.09
21	3	3004	CLA	C4A-NA-C1A	2.13	109.11	106.36
21	B	1209	CLA	C4A-NA-C1A	2.13	109.11	106.36
19	B	6009	BCR	C38-C26-C27	2.13	117.47	113.43
21	F	1301	CLA	C4A-NA-C1A	2.13	109.11	106.36
21	B	1207	CLA	CAC-C3C-C4C	2.13	127.93	124.83
21	A	1113	CLA	C4A-NA-C1A	2.14	109.12	106.36
21	3	3004	CLA	CMB-C2B-C3B	2.14	129.26	125.09
21	1	1002	CLA	OBD-CAD-CBD	2.14	129.16	125.94
21	B	1223	CLA	C4A-NA-C1A	2.14	109.12	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	6014	CLA	CMB-C2B-C3B	2.14	129.27	125.09
21	B	1219	CLA	CMB-C2B-C3B	2.14	129.27	125.09
21	A	1137	CLA	C4A-NA-C1A	2.14	109.12	106.36
21	B	1236	CLA	C4A-NA-C1A	2.14	109.12	106.36
21	A	1139	CLA	CAC-C3C-C4C	2.14	127.94	124.83
21	A	1136	CLA	CMB-C2B-C3B	2.14	129.28	125.09
21	3	3015	CLA	CMB-C2B-C3B	2.14	129.28	125.09
21	A	1136	CLA	C4A-NA-C1A	2.15	109.13	106.36
21	2	2003	CLA	CMC-C2C-C3C	2.15	132.18	125.94
21	4	4015	CLA	C4A-NA-C1A	2.15	109.13	106.36
21	B	1212	CLA	C4A-NA-C1A	2.15	109.13	106.36
21	A	1111	CLA	CMC-C2C-C1C	2.15	128.35	125.02
21	A	1105	CLA	CAC-C3C-C4C	2.15	127.95	124.83
21	A	1101	CLA	C4A-NA-C1A	2.15	109.14	106.36
21	3	3016	CLA	C4A-NA-C1A	2.15	109.14	106.36
21	2	2005	CLA	CMC-C2C-C1C	2.15	128.35	125.02
21	A	1122	CLA	CMB-C2B-C3B	2.15	129.30	125.09
21	B	1225	CLA	CMB-C2B-C3B	2.15	129.30	125.09
21	3	3011	CLA	C4A-NA-C1A	2.16	109.15	106.36
26	1	1502	LUT	C15-C35-C34	2.16	128.16	123.39
21	J	6014	CLA	C4A-NA-C1A	2.16	109.15	106.36
21	B	1218	CLA	C4A-NA-C1A	2.16	109.15	106.36
19	A	6011	BCR	C32-C1-C2	2.16	116.52	108.79
21	4	4008	CLA	CMB-C2B-C3B	2.16	129.31	125.09
21	A	1140	CLA	C4A-NA-C1A	2.16	109.15	106.36
21	A	1119	CLA	CAC-C3C-C4C	2.16	127.97	124.83
19	A	6011	BCR	C30-C25-C26	2.16	125.83	122.66
21	A	1109	CLA	CAC-C3C-C4C	2.16	127.97	124.83
21	A	1113	CLA	CAC-C3C-C4C	2.16	127.97	124.83
21	A	1128	CLA	CMB-C2B-C3B	2.16	129.32	125.09
19	F	6016	BCR	C35-C13-C12	2.16	121.70	118.10
21	2	2011	CLA	CAC-C3C-C4C	2.17	127.97	124.83
21	A	1120	CLA	CAC-C3C-C4C	2.17	127.97	124.83
21	A	1123	CLA	C4A-NA-C1A	2.17	109.16	106.36
19	B	6009	BCR	C23-C22-C21	2.17	122.48	118.98
21	B	1220	CLA	CMB-C2B-C3B	2.17	129.33	125.09
21	A	1139	CLA	C4A-NA-C1A	2.17	109.16	106.36
21	4	4004	CLA	CMC-C2C-C1C	2.17	128.38	125.02
21	A	1129	CLA	CMB-C2B-C3B	2.17	129.33	125.09
21	B	1235	CLA	C4A-NA-C1A	2.17	109.16	106.36
21	B	1235	CLA	CMB-C2B-C3B	2.17	129.34	125.09
21	3	3009	CLA	CMB-C2B-C3B	2.17	129.34	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	2004	CLA	CMB-C2B-C3B	2.18	129.34	125.09
21	3	3014	CLA	C4A-NA-C1A	2.18	109.17	106.36
19	F	6016	BCR	C30-C25-C26	2.18	125.86	122.66
21	A	1140	CLA	CMB-C2B-C3B	2.18	129.35	125.09
27	4	4503	NEX	C31-C30-C29	2.18	130.35	127.20
21	B	1212	CLA	CAC-C3C-C4C	2.18	128.00	124.83
21	A	1115	CLA	CMB-C2B-C3B	2.18	129.35	125.09
21	A	1120	CLA	CMB-C2B-C3B	2.18	129.36	125.09
21	B	1214	CLA	C4A-NA-C1A	2.18	109.18	106.36
21	3	3002	CLA	CMB-C2B-C3B	2.18	129.36	125.09
21	4	4001	CLA	C4-C3-C5	2.18	118.74	115.41
21	3	3006	CLA	CMB-C2B-C3B	2.19	129.36	125.09
21	3	3017	CLA	CMB-C2B-C3B	2.19	129.37	125.09
21	A	1114	CLA	CAC-C3C-C4C	2.19	128.01	124.83
21	A	9013	CLA	CMB-C2B-C3B	2.19	129.37	125.09
21	A	1143	CLA	CMB-C2B-C3B	2.19	129.38	125.09
21	1	1007	CLA	CED-O2D-CGD	2.19	121.14	115.99
21	2	2013	CLA	CED-O2D-CGD	2.19	121.14	115.99
21	B	1213	CLA	C4A-NA-C1A	2.19	109.19	106.36
20	2	2801	LHG	O8-C23-C24	2.20	118.59	111.90
21	A	1135	CLA	CMC-C2C-C1C	2.20	128.42	125.02
21	A	1137	CLA	CAC-C3C-C4C	2.20	128.02	124.83
21	A	1128	CLA	C4-C3-C5	2.20	118.76	115.41
21	B	1218	CLA	CMB-C2B-C3B	2.20	129.39	125.09
20	B	7004	LHG	O4-P-O5	2.20	124.45	112.53
21	1	1014	CLA	CMC-C2C-C1C	2.20	128.43	125.02
21	A	1130	CLA	CMB-C2B-C3B	2.20	129.40	125.09
21	A	1123	CLA	CAC-C3C-C4C	2.20	128.03	124.83
21	A	1109	CLA	CMB-C2B-C3B	2.21	129.41	125.09
21	B	1210	CLA	CED-O2D-CGD	2.21	121.17	115.99
21	B	1215	CLA	CMB-C2B-C3B	2.21	129.41	125.09
21	2	2007	CLA	CMC-C2C-C1C	2.21	128.44	125.02
21	B	9022	CLA	CMC-C2C-C1C	2.21	128.44	125.02
21	A	1106	CLA	CAC-C3C-C4C	2.22	128.05	124.83
21	B	1236	CLA	CMB-C2B-C3B	2.22	129.43	125.09
21	4	4008	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	L	6020	BCR	C33-C5-C4	2.22	117.64	113.43
21	2	2012	CLA	CMB-C2B-C3B	2.22	129.43	125.09
21	A	1103	CLA	C4A-NA-C1A	2.22	109.23	106.36
21	3	3009	CLA	C1-O2A-CGA	2.22	124.42	116.21
19	L	6020	BCR	C23-C22-C21	2.22	122.57	118.98
21	B	1203	CLA	CMB-C2B-C3B	2.23	129.44	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	6004	BCR	C8-C9-C10	2.23	122.57	118.98
21	1	1012	CLA	CED-O2D-CGD	2.23	121.21	115.99
27	4	4503	NEX	C20-C13-C12	2.23	121.81	118.10
26	4	4501	LUT	C12-C13-C14	2.23	122.58	118.98
21	3	3004	CLA	CAC-C3C-C4C	2.23	128.07	124.83
21	B	1212	CLA	CMB-C2B-C3B	2.23	129.46	125.09
21	A	1110	CLA	CAC-C3C-C4C	2.24	128.07	124.83
21	B	1231	CLA	CAC-C3C-C4C	2.24	128.08	124.83
21	1	1008	CLA	C4A-NA-C1A	2.24	109.26	106.36
21	3	3010	CLA	CBA-CAA-C2A	2.24	120.06	113.73
21	B	1207	CLA	C4A-NA-C1A	2.24	109.26	106.36
19	A	6003	BCR	C23-C22-C21	2.25	122.60	118.98
21	A	1111	CLA	C4A-NA-C1A	2.25	109.26	106.36
19	B	6011	BCR	C36-C18-C19	2.25	120.17	114.64
19	B	6005	BCR	C30-C25-C24	2.25	122.12	115.82
21	3	3012	CLA	CMC-C2C-C1C	2.25	128.50	125.02
21	3	3003	CLA	CMB-C2B-C3B	2.25	129.49	125.09
21	B	1202	CLA	C4A-NA-C1A	2.25	109.27	106.36
21	4	4011	CLA	CAA-C2A-C3A	2.26	119.70	113.22
21	A	1134	CLA	CAC-C3C-C4C	2.26	128.10	124.83
21	2	2008	CLA	C4A-NA-C1A	2.26	109.28	106.36
21	3	3005	CLA	CMB-C2B-C3B	2.26	129.51	125.09
21	3	3016	CLA	CMB-C2B-C3B	2.26	129.51	125.09
21	A	1112	CLA	CMB-C2B-C3B	2.26	129.51	125.09
27	4	4503	NEX	C12-C13-C14	2.26	122.63	118.98
21	A	1118	CLA	CAC-C3C-C4C	2.26	128.12	124.83
21	B	1214	CLA	CAC-C3C-C4C	2.26	128.12	124.83
21	J	6015	CLA	CMB-C2B-C3B	2.27	129.52	125.09
21	A	1112	CLA	CAC-C3C-C4C	2.27	128.12	124.83
21	B	1210	CLA	CAC-C3C-C2C	2.27	131.49	127.51
21	2	2007	CLA	C4-C3-C5	2.27	118.87	115.41
21	4	4006	CLA	CMC-C2C-C3C	2.27	132.54	125.94
21	A	1127	CLA	CMB-C2B-C3B	2.27	129.53	125.09
21	B	1230	CLA	C4A-NA-C1A	2.27	109.30	106.36
21	A	1110	CLA	CMB-C2B-C3B	2.27	129.53	125.09
21	A	1109	CLA	C4A-NA-C1A	2.27	109.30	106.36
21	B	1209	CLA	CAC-C3C-C4C	2.28	128.13	124.83
21	3	3008	CLA	CMC-C2C-C1C	2.28	128.54	125.02
21	B	1205	CLA	C4A-NA-C1A	2.28	109.30	106.36
21	A	1116	CLA	CMB-C2B-C3B	2.28	129.54	125.09
21	1	1007	CLA	C4A-NA-C1A	2.28	109.31	106.36
21	4	4001	CLA	CAC-C3C-C4C	2.28	128.14	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1142	CLA	CAC-C3C-C4C	2.28	128.14	124.83
21	1	1003	CLA	CMB-C2B-C3B	2.28	129.55	125.09
21	1	1012	CLA	CMB-C2B-C3B	2.28	129.55	125.09
21	1	1007	CLA	CAC-C3C-C4C	2.29	128.15	124.83
21	2	2010	CLA	CED-O2D-CGD	2.29	121.35	115.99
21	2	2014	CLA	CMC-C2C-C1C	2.29	128.56	125.02
19	A	6007	BCR	C23-C22-C21	2.29	122.67	118.98
21	1	1004	CLA	C4A-NA-C1A	2.29	109.32	106.36
21	A	1126	CLA	CAC-C3C-C4C	2.29	128.16	124.83
21	B	1205	CLA	CAC-C3C-C4C	2.29	128.16	124.83
21	L	1503	CLA	CAC-C3C-C4C	2.30	128.16	124.83
19	B	6004	BCR	C33-C5-C4	2.30	117.78	113.43
21	A	1126	CLA	C4-C3-C5	2.30	118.92	115.41
21	2	2012	CLA	CMC-C2C-C1C	2.30	128.58	125.02
21	B	1234	CLA	CMB-C2B-C3B	2.30	129.59	125.09
21	A	1101	CLA	CAC-C3C-C4C	2.30	128.17	124.83
21	3	3003	CLA	C4A-NA-C1A	2.30	109.33	106.36
21	B	1221	CLA	CAC-C3C-C4C	2.30	128.17	124.83
21	B	1234	CLA	CAC-C3C-C4C	2.30	128.17	124.83
21	A	1138	CLA	C4A-NA-C1A	2.30	109.34	106.36
21	B	1217	CLA	CMB-C2B-C3B	2.30	129.59	125.09
21	4	4012	CLA	CMB-C2B-C3B	2.31	129.60	125.09
19	J	6012	BCR	C33-C5-C4	2.31	117.80	113.43
21	A	1132	CLA	C4A-NA-C1A	2.31	109.34	106.36
21	2	2006	CLA	CMB-C2B-C3B	2.31	129.60	125.09
21	1	1012	CLA	CMC-C2C-C1C	2.31	128.59	125.02
21	B	1206	CLA	C4A-NA-C1A	2.31	109.34	106.36
21	B	9010	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	B	6004	BCR	C34-C9-C8	2.31	121.94	118.10
21	B	1207	CLA	CMB-C2B-C3B	2.31	129.62	125.09
21	1	1001	CLA	CMC-C2C-C1C	2.32	128.60	125.02
19	F	6014	BCR	C32-C1-C2	2.32	117.08	108.79
21	A	1111	CLA	CMB-C2B-C3B	2.32	129.62	125.09
21	4	4003	CLA	C4-C3-C5	2.32	118.95	115.41
21	2	2009	CLA	CED-O2D-CGD	2.32	121.43	115.99
21	3	3009	CLA	CED-O2D-CGD	2.33	121.45	115.99
19	F	6014	BCR	C23-C22-C21	2.33	122.73	118.98
21	B	1227	CLA	CMB-C2B-C1B	2.33	132.22	128.36
21	4	4005	CLA	C4A-NA-C1A	2.33	109.37	106.36
26	1	1501	LUT	C18-C5-C4	2.34	118.50	114.24
21	1	1001	CLA	CAC-C3C-C4C	2.34	128.23	124.83
21	A	1103	CLA	CAC-C3C-C4C	2.34	128.23	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1131	CLA	CMC-C2C-C1C	2.34	128.65	125.02
21	A	1132	CLA	CMB-C2B-C3B	2.35	129.68	125.09
21	3	3001	CLA	C4A-NA-C1A	2.35	109.39	106.36
21	4	4002	CLA	CMB-C2B-C3B	2.35	129.69	125.09
21	3	3010	CLA	CMC-C2C-C1C	2.35	128.66	125.02
19	B	6005	BCR	C33-C5-C4	2.35	117.89	113.43
21	3	3002	CLA	C4A-NA-C1A	2.36	109.40	106.36
21	H	1000	CLA	CAC-C3C-C4C	2.36	128.25	124.83
21	2	2007	CLA	CAC-C3C-C4C	2.36	128.25	124.83
21	1	1012	CLA	C5-C3-C4	2.36	120.44	114.64
21	B	9023	CLA	CAC-C3C-C4C	2.36	128.25	124.83
21	A	1102	CLA	C4A-NA-C1A	2.36	109.41	106.36
20	B	7004	LHG	O8-C23-C24	2.36	119.09	111.90
19	A	6008	BCR	C38-C26-C27	2.36	117.90	113.43
19	F	6016	BCR	C38-C26-C27	2.36	117.91	113.43
21	3	3013	CLA	C4A-NA-C1A	2.37	109.42	106.36
21	3	3014	CLA	CMC-C2C-C1C	2.37	128.69	125.02
21	3	3006	CLA	CAC-C3C-C4C	2.37	128.28	124.83
21	F	1303	CLA	CMB-C2B-C3B	2.37	129.73	125.09
19	A	6011	BCR	C38-C26-C27	2.38	117.93	113.43
21	A	9012	CLA	C4-C3-C5	2.38	119.03	115.41
21	A	1118	CLA	CMB-C2B-C1B	2.38	132.30	128.36
21	4	4011	CLA	C4A-NA-C1A	2.38	109.43	106.36
21	B	1224	CLA	CAC-C3C-C4C	2.38	128.28	124.83
19	B	6010	BCR	C33-C5-C4	2.38	117.95	113.43
21	B	1223	CLA	CMC-C2C-C1C	2.38	128.71	125.02
21	B	1213	CLA	C4-C3-C5	2.39	119.06	115.41
19	A	6002	BCR	C33-C5-C4	2.39	117.96	113.43
23	A	9011	CL0	C4A-NA-C1A	2.40	109.46	106.36
21	A	1125	CLA	CMB-C2B-C3B	2.40	129.78	125.09
21	B	1238	CLA	CMB-C2B-C3B	2.40	129.78	125.09
21	2	2004	CLA	CMC-C2C-C1C	2.40	128.73	125.02
21	B	1213	CLA	CMB-C2B-C3B	2.40	129.78	125.09
25	J	5001	LMG	O1-C1-C2	2.40	111.07	108.04
19	A	6008	BCR	C23-C22-C21	2.40	122.86	118.98
19	L	6019	BCR	C2-C1-C6	2.40	114.17	110.36
21	B	1221	CLA	C4A-NA-C1A	2.41	109.47	106.36
19	A	6002	BCR	C38-C26-C27	2.41	117.99	113.43
21	B	1202	CLA	CMC-C2C-C1C	2.42	128.76	125.02
19	G	2011	BCR	C38-C26-C27	2.42	118.01	113.43
21	3	3009	CLA	O2A-CGA-CBA	2.42	122.44	112.36
21	B	1228	CLA	C4A-NA-C1A	2.42	109.48	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4006	CLA	CMB-C2B-C3B	2.43	129.83	125.09
21	A	1131	CLA	CMB-C2B-C3B	2.43	129.84	125.09
21	A	1121	CLA	C4A-NA-C1A	2.43	109.50	106.36
21	1	1003	CLA	CHB-C4A-NA	2.43	127.87	124.51
21	A	1118	CLA	C4A-NA-C1A	2.43	109.50	106.36
23	A	9011	CL0	CHB-C4A-NA	2.44	127.88	124.51
19	A	6007	BCR	C33-C5-C4	2.44	118.05	113.43
21	2	2008	CLA	CMC-C2C-C1C	2.44	128.79	125.02
21	A	1101	CLA	CMC-C2C-C1C	2.44	128.79	125.02
21	B	1205	CLA	C4-C3-C5	2.44	119.14	115.41
21	J	1302	CLA	CAC-C3C-C4C	2.45	128.38	124.83
21	B	1216	CLA	CMB-C2B-C3B	2.45	129.88	125.09
21	A	1136	CLA	CBA-CAA-C2A	2.45	120.64	113.73
21	2	2001	CLA	C2B-C3B-C4B	2.45	108.43	106.29
21	B	1240	CLA	CAC-C3C-C4C	2.46	128.40	124.83
21	3	3014	CLA	CMB-C2B-C3B	2.46	129.89	125.09
21	B	1224	CLA	CMC-C2C-C1C	2.46	128.82	125.02
21	A	1118	CLA	CMC-C2C-C1C	2.46	128.83	125.02
19	F	6014	BCR	C19-C18-C17	2.46	122.95	118.98
25	G	2021	LMG	O6-C5-C6	2.46	112.58	106.36
21	3	3010	CLA	C4-C3-C5	2.47	119.18	115.41
21	3	3001	CLA	CMC-C2C-C1C	2.48	128.85	125.02
26	4	4501	LUT	C28-C29-C30	2.48	122.98	118.98
21	4	4010	CLA	CMB-C2B-C3B	2.48	129.94	125.09
21	3	3012	CLA	CMB-C2B-C3B	2.48	129.95	125.09
19	B	6010	BCR	C38-C26-C27	2.49	118.14	113.43
21	A	1130	CLA	C4A-NA-C1A	2.49	109.58	106.36
21	1	1002	CLA	CED-O2D-CGD	2.49	121.84	115.99
21	L	1502	CLA	C4-C3-C5	2.49	119.22	115.41
21	1	1010	CLA	CMC-C2C-C1C	2.49	128.88	125.02
21	1	1013	CLA	C4-C3-C5	2.50	119.22	115.41
21	A	1136	CLA	CMC-C2C-C1C	2.50	128.89	125.02
21	A	1138	CLA	CMB-C2B-C3B	2.50	129.98	125.09
21	1	1006	CLA	CMC-C2C-C1C	2.50	128.89	125.02
21	4	4010	CLA	C4A-NA-C1A	2.50	109.60	106.36
21	1	1003	CLA	C4A-NA-C1A	2.50	109.60	106.36
21	3	3011	CLA	CMC-C2C-C1C	2.51	128.90	125.02
21	B	1230	CLA	CMC-C2C-C1C	2.51	128.90	125.02
21	F	1302	CLA	CAC-C3C-C4C	2.51	128.47	124.83
21	B	1211	CLA	CMC-C2C-C1C	2.51	128.91	125.02
21	B	1210	CLA	C4-C3-C5	2.51	119.24	115.41
21	4	4015	CLA	CMC-C2C-C1C	2.51	128.91	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1119	CLA	CMB-C2B-C3B	2.52	130.01	125.09
21	J	1302	CLA	C4-C3-C5	2.52	119.25	115.41
21	A	1107	CLA	CMC-C2C-C1C	2.53	128.93	125.02
21	B	1237	CLA	C4-C3-C5	2.53	119.27	115.41
21	1	1008	CLA	CAC-C3C-C4C	2.53	128.50	124.83
21	2	2009	CLA	C4A-NA-C1A	2.53	109.63	106.36
21	1	1002	CLA	CAC-C3C-C4C	2.53	128.50	124.83
21	B	1204	CLA	CMC-C2C-C1C	2.53	128.94	125.02
21	B	1207	CLA	CMC-C2C-C1C	2.53	128.94	125.02
21	B	1211	CLA	CMB-C2B-C3B	2.53	130.04	125.09
21	H	1000	CLA	CMC-C2C-C1C	2.54	128.94	125.02
21	4	4012	CLA	C4A-NA-C1A	2.54	109.64	106.36
21	A	1129	CLA	C4A-NA-C1A	2.55	109.65	106.36
26	1	1501	LUT	C32-C33-C34	2.55	123.09	118.98
21	B	1201	CLA	CMB-C2B-C3B	2.55	130.08	125.09
19	B	6009	BCR	C19-C18-C17	2.55	123.10	118.98
21	B	1216	CLA	CMC-C2C-C1C	2.55	128.97	125.02
21	3	3013	CLA	C5-C3-C4	2.55	120.92	114.64
21	A	1127	CLA	CAC-C3C-C4C	2.56	128.54	124.83
21	3	3013	CLA	CMB-C2B-C3B	2.56	130.09	125.09
21	F	1303	CLA	CMC-C2C-C1C	2.56	128.98	125.02
21	J	6015	CLA	CAC-C3C-C4C	2.57	128.56	124.83
21	A	1141	CLA	CAC-C3C-C4C	2.57	128.56	124.83
21	B	1239	CLA	CMC-C2C-C1C	2.57	129.00	125.02
21	3	3011	CLA	CMB-C2B-C3B	2.57	130.12	125.09
21	L	1502	CLA	CMC-C2C-C1C	2.57	129.00	125.02
21	B	1227	CLA	C4-C3-C5	2.57	119.33	115.41
21	3	3012	CLA	CED-O2D-CGD	2.58	122.03	115.99
26	4	4502	LUT	C32-C33-C34	2.58	123.14	118.98
21	B	1237	CLA	CMC-C2C-C1C	2.58	129.02	125.02
21	B	1213	CLA	CAC-C3C-C4C	2.58	128.58	124.83
19	I	6018	BCR	C32-C1-C2	2.59	118.05	108.79
21	A	1133	CLA	C4A-NA-C1A	2.59	109.70	106.36
21	4	4008	CLA	CAC-C3C-C4C	2.59	128.59	124.83
21	A	1111	CLA	CAC-C3C-C4C	2.59	128.59	124.83
19	B	6009	BCR	C33-C5-C4	2.59	118.34	113.43
21	3	3013	CLA	CAC-C3C-C4C	2.59	128.59	124.83
19	L	6020	BCR	C19-C18-C17	2.60	123.17	118.98
26	1	1502	LUT	C1-C6-C7	2.60	123.09	115.82
21	L	1502	CLA	C4A-NA-C1A	2.60	109.72	106.36
21	F	1301	CLA	CMC-C2C-C1C	2.60	129.04	125.02
21	J	6015	CLA	C4A-NA-C1A	2.60	109.72	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4013	CLA	C4-C3-C5	2.60	118.63	115.68
21	2	2013	CLA	C4-C3-C5	2.60	119.38	115.41
21	B	1234	CLA	C4-C3-C5	2.60	119.38	115.41
21	3	3008	CLA	CMB-C2B-C3B	2.60	130.18	125.09
21	4	4013	CLA	C4A-NA-C1A	2.60	109.72	106.36
21	B	9023	CLA	CMB-C2B-C3B	2.60	130.18	125.09
21	B	1206	CLA	CMC-C2C-C1C	2.61	129.05	125.02
21	A	1108	CLA	CMB-C2B-C3B	2.61	130.19	125.09
21	A	1139	CLA	CMC-C2C-C1C	2.61	129.06	125.02
21	3	3003	CLA	CED-O2D-CGD	2.62	122.12	115.99
21	1	1014	CLA	CAC-C3C-C4C	2.62	128.64	124.83
21	B	1212	CLA	CMC-C2C-C1C	2.62	129.08	125.02
21	A	1107	CLA	CMB-C2B-C3B	2.62	130.22	125.09
21	A	1117	CLA	CMC-C2C-C1C	2.63	129.09	125.02
21	1	1009	CLA	CAC-C3C-C4C	2.63	128.65	124.83
21	B	1202	CLA	CMB-C2B-C3B	2.64	130.24	125.09
21	B	1224	CLA	CMB-C2B-C3B	2.64	130.24	125.09
21	A	1111	CLA	C4-C3-C5	2.64	119.44	115.41
21	B	1222	CLA	CMC-C2C-C1C	2.64	129.11	125.02
19	I	6018	BCR	C33-C5-C4	2.65	118.45	113.43
21	3	3010	CLA	CMB-C2B-C3B	2.65	130.27	125.09
19	B	6011	BCR	C1-C6-C7	2.66	123.25	115.82
21	A	1122	CLA	CMC-C2C-C1C	2.66	129.14	125.02
21	2	2011	CLA	C4A-NA-C1A	2.66	109.80	106.36
21	A	1103	CLA	CMB-C2B-C3B	2.66	130.30	125.09
21	A	1102	CLA	CMB-C2B-C3B	2.67	130.30	125.09
21	3	3017	CLA	CMC-C2C-C1C	2.67	129.15	125.02
21	3	3016	CLA	CMC-C2C-C1C	2.67	129.15	125.02
21	1	1011	CLA	C4-C3-C5	2.67	119.48	115.41
21	1	1006	CLA	C4A-NA-C1A	2.67	109.81	106.36
21	A	1140	CLA	CMC-C2C-C1C	2.67	129.15	125.02
21	2	2012	CLA	C4A-NA-C1A	2.67	109.81	106.36
21	A	1119	CLA	CMC-C2C-C1C	2.67	129.15	125.02
21	A	1139	CLA	C4-C3-C5	2.67	119.49	115.41
21	1	1011	CLA	CAC-C3C-C4C	2.68	128.72	124.83
21	A	1108	CLA	CMC-C2C-C1C	2.68	129.16	125.02
21	4	4003	CLA	C4A-NA-C1A	2.68	109.82	106.36
21	1	1005	CLA	C4-C3-C5	2.68	119.50	115.41
21	3	3006	CLA	C4-C3-C5	2.68	119.50	115.41
21	A	1123	CLA	CMB-C2B-C3B	2.68	130.34	125.09
21	2	2014	CLA	CHB-C4A-NA	2.68	128.22	124.51
21	G	1001	CLA	CMC-C2C-C1C	2.68	129.17	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	F	1302	CLA	CMC-C2C-C1C	2.68	129.17	125.02
21	A	1106	CLA	C4-C3-C5	2.68	119.51	115.41
19	L	6019	BCR	C23-C22-C21	2.69	123.31	118.98
21	L	1501	CLA	C4A-NA-C1A	2.69	109.84	106.36
21	3	3015	CLA	CMC-C2C-C1C	2.69	129.18	125.02
21	B	1212	CLA	O2A-CGA-CBA	2.69	123.58	112.36
21	2	2006	CLA	C4A-NA-C1A	2.69	109.84	106.36
21	J	1302	CLA	CMC-C2C-C1C	2.69	129.19	125.02
19	J	6012	BCR	C30-C25-C24	2.70	123.36	115.82
21	L	1503	CLA	C4A-NA-C1A	2.70	109.84	106.36
21	A	9012	CLA	C4A-NA-C1A	2.70	109.85	106.36
19	L	6020	BCR	C38-C26-C27	2.70	118.55	113.43
21	4	4007	CLA	CMC-C2C-C1C	2.71	129.21	125.02
21	2	2004	CLA	C4A-NA-C1A	2.71	109.86	106.36
19	A	6017	BCR	C33-C5-C4	2.71	118.56	113.43
21	A	1123	CLA	C4-C3-C5	2.71	119.55	115.41
21	B	1219	CLA	CMC-C2C-C1C	2.71	129.22	125.02
21	B	1238	CLA	CMC-C2C-C1C	2.71	129.22	125.02
21	B	1205	CLA	CMC-C2C-C1C	2.71	129.22	125.02
21	B	1206	CLA	CAC-C3C-C4C	2.71	128.77	124.83
21	A	1130	CLA	CMC-C2C-C1C	2.72	129.23	125.02
21	1	1003	CLA	CMC-C2C-C1C	2.72	129.23	125.02
21	A	1124	CLA	CMB-C2B-C3B	2.73	130.42	125.09
21	B	1217	CLA	CMC-C2C-C1C	2.73	129.24	125.02
21	J	6014	CLA	CMC-C2C-C1C	2.73	129.24	125.02
19	B	6004	BCR	C2-C1-C6	2.73	114.68	110.36
21	1	1008	CLA	CMC-C2C-C1C	2.73	129.25	125.02
21	2	2002	CLA	CMB-C2B-C3B	2.73	130.43	125.09
21	B	1229	CLA	C4-C3-C5	2.73	119.58	115.41
21	A	1138	CLA	C4-C3-C5	2.73	119.58	115.41
21	A	1128	CLA	C4A-NA-C1A	2.74	109.89	106.36
21	3	3004	CLA	CMC-C2C-C1C	2.74	129.25	125.02
21	B	1211	CLA	C4-C3-C5	2.74	119.59	115.41
21	B	1235	CLA	CMC-C2C-C1C	2.74	129.25	125.02
21	B	1227	CLA	CMC-C2C-C1C	2.74	129.26	125.02
21	3	3005	CLA	CMC-C2C-C1C	2.74	129.26	125.02
21	A	1114	CLA	O2A-CGA-CBA	2.74	123.77	112.36
21	3	3003	CLA	CMC-C2C-C1C	2.74	129.26	125.02
19	A	6008	BCR	C31-C1-C2	2.74	118.60	108.79
21	B	1229	CLA	CMB-C2B-C3B	2.74	130.45	125.09
21	3	3002	CLA	C4-C3-C5	2.74	119.60	115.41
21	B	1231	CLA	CMC-C2C-C1C	2.74	129.27	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1234	CLA	CMC-C2C-C1C	2.74	129.27	125.02
21	1	1003	CLA	CAC-C3C-C4C	2.75	128.81	124.83
21	A	1113	CLA	CMC-C2C-C1C	2.75	129.27	125.02
21	A	1141	CLA	CMC-C2C-C1C	2.75	129.27	125.02
21	B	9010	CLA	CMB-C2B-C3B	2.75	130.47	125.09
21	A	1124	CLA	CMC-C2C-C1C	2.75	129.28	125.02
21	3	3002	CLA	CMC-C2C-C1C	2.75	129.28	125.02
21	B	1203	CLA	CMC-C2C-C1C	2.76	129.29	125.02
21	A	1104	CLA	CMC-C2C-C1C	2.76	129.29	125.02
21	2	2002	CLA	CMC-C2C-C1C	2.76	129.29	125.02
21	1	1011	CLA	CMC-C2C-C1C	2.76	129.29	125.02
21	4	4015	CLA	CMB-C2B-C3B	2.76	130.49	125.09
21	B	1208	CLA	CMC-C2C-C1C	2.76	129.30	125.02
21	1	1005	CLA	CMC-C2C-C1C	2.76	129.30	125.02
25	J	5001	LMG	O8-C28-C29	2.77	120.33	111.90
21	A	1143	CLA	CMC-C2C-C1C	2.77	129.30	125.02
21	A	1123	CLA	CMC-C2C-C1C	2.77	129.31	125.02
21	B	9010	CLA	C4-C3-C5	2.78	119.65	115.41
21	A	1114	CLA	CMC-C2C-C1C	2.78	129.32	125.02
21	B	1225	CLA	CMC-C2C-C1C	2.78	129.32	125.02
21	B	1222	CLA	C4-C3-C5	2.78	119.65	115.41
21	4	4003	CLA	CAC-C3C-C4C	2.78	128.87	124.83
21	A	1126	CLA	CMB-C2B-C3B	2.78	130.53	125.09
21	B	1214	CLA	C4-C3-C5	2.78	119.66	115.41
21	3	3006	CLA	CMC-C2C-C1C	2.79	129.33	125.02
21	A	1131	CLA	C4A-NA-C1A	2.79	109.96	106.36
21	A	1122	CLA	C4-C3-C5	2.79	119.67	115.41
21	A	1133	CLA	CMC-C2C-C1C	2.79	129.34	125.02
21	A	1134	CLA	CMC-C2C-C1C	2.79	129.34	125.02
21	4	4015	CLA	O2A-CGA-CBA	2.79	124.00	112.36
19	F	6014	BCR	C40-C30-C39	2.79	117.32	108.37
21	B	1209	CLA	CMC-C2C-C1C	2.79	129.34	125.02
21	3	3012	CLA	C4A-NA-C1A	2.79	109.97	106.36
21	4	4002	CLA	C4-C3-C5	2.80	119.68	115.41
26	4	4502	LUT	C12-C13-C14	2.80	123.49	118.98
21	2	2010	CLA	CMC-C2C-C1C	2.80	129.35	125.02
21	H	1000	CLA	CMB-C2B-C1B	2.80	132.99	128.36
21	A	1108	CLA	O2A-CGA-CBA	2.80	124.04	112.36
21	B	1229	CLA	CMC-C2C-C1C	2.80	129.36	125.02
19	A	6008	BCR	C32-C1-C2	2.80	118.83	108.79
21	A	1121	CLA	O2A-CGA-CBA	2.80	124.05	112.36
21	B	1206	CLA	C4-C3-C5	2.80	119.69	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1112	CLA	O2A-CGA-CBA	2.81	124.07	112.36
21	B	1218	CLA	CMC-C2C-C1C	2.81	129.37	125.02
21	B	1217	CLA	O2A-CGA-CBA	2.81	124.07	112.36
19	J	6013	BCR	C38-C26-C27	2.81	118.76	113.43
21	B	1209	CLA	O2A-CGA-CBA	2.81	124.08	112.36
21	B	1220	CLA	CMC-C2C-C1C	2.81	129.37	125.02
21	A	1127	CLA	CMC-C2C-C1C	2.81	129.38	125.02
21	B	1214	CLA	CMB-C2B-C3B	2.82	130.59	125.09
21	A	1142	CLA	CMC-C2C-C1C	2.82	129.38	125.02
21	1	1005	CLA	C4A-NA-C1A	2.82	110.00	106.36
21	A	1118	CLA	O2A-CGA-CBA	2.82	124.10	112.36
21	3	3009	CLA	CMC-C2C-C1C	2.82	129.38	125.02
19	I	6018	BCR	C31-C1-C2	2.82	118.88	108.79
21	4	4004	CLA	C4A-NA-C1A	2.82	110.00	106.36
26	1	1501	LUT	C28-C29-C30	2.82	123.53	118.98
21	A	1138	CLA	CMC-C2C-C1C	2.82	129.39	125.02
21	B	1238	CLA	C4-C3-C5	2.82	119.72	115.41
21	A	1119	CLA	C4-C3-C5	2.82	119.72	115.41
21	3	3010	CLA	C4A-NA-C1A	2.82	110.01	106.36
21	B	1231	CLA	O2A-CGA-CBA	2.82	124.13	112.36
21	A	1120	CLA	CMC-C2C-C1C	2.82	129.39	125.02
19	I	6020	BCR	C33-C5-C4	2.82	118.78	113.43
21	G	1001	CLA	C4-C3-C5	2.83	119.73	115.41
26	2	2502	LUT	C22-C23-C24	2.83	115.08	111.75
21	B	1218	CLA	C4-C3-C5	2.83	119.73	115.41
21	1	1014	CLA	C4A-NA-C1A	2.83	110.02	106.36
21	J	1302	CLA	CMB-C2B-C3B	2.83	130.63	125.09
21	B	1236	CLA	CMC-C2C-C1C	2.84	129.41	125.02
21	2	2011	CLA	CAA-CBA-CGA	2.84	121.62	113.32
21	1	1002	CLA	C4A-NA-C1A	2.84	110.03	106.36
21	4	4014	CLA	CMB-C2B-C3B	2.84	130.64	125.09
21	4	4006	CLA	CED-O2D-CGD	2.84	122.65	115.99
19	I	6018	BCR	C38-C26-C27	2.84	118.81	113.43
21	A	1130	CLA	O2A-CGA-CBA	2.84	124.20	112.36
21	A	1137	CLA	CMC-C2C-C1C	2.85	129.43	125.02
21	A	1113	CLA	O2A-CGA-CBA	2.85	124.24	112.36
21	A	9012	CLA	CMC-C2C-C1C	2.85	129.43	125.02
21	A	1124	CLA	C4-C3-C5	2.86	119.77	115.41
21	B	1201	CLA	O2A-CGA-CBA	2.86	124.26	112.36
21	G	1002	CLA	O2A-CGA-CBA	2.86	124.27	112.36
21	L	1501	CLA	CMC-C2C-C1C	2.86	129.45	125.02
21	L	1501	CLA	O2A-CGA-CBA	2.86	124.29	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1224	CLA	C4-C3-C5	2.86	119.78	115.41
21	3	3008	CLA	C4A-NA-C1A	2.87	110.06	106.36
21	2	2009	CLA	CMB-C2B-C3B	2.87	130.70	125.09
21	B	1215	CLA	CMC-C2C-C1C	2.87	129.46	125.02
21	F	1302	CLA	O2A-CGA-CBA	2.87	124.33	112.36
19	A	6017	BCR	C30-C25-C24	2.87	123.86	115.82
21	2	2007	CLA	C4A-NA-C1A	2.87	110.08	106.36
21	A	1129	CLA	CMC-C2C-C1C	2.87	129.47	125.02
21	2	2002	CLA	C4-C3-C5	2.87	119.80	115.41
21	A	1132	CLA	CMC-C2C-C1C	2.88	129.47	125.02
21	A	1101	CLA	CMB-C2B-C3B	2.88	130.72	125.09
21	L	1503	CLA	CMC-C2C-C1C	2.88	129.47	125.02
21	A	1128	CLA	CMC-C2C-C1C	2.88	129.48	125.02
20	A	7001	LHG	O8-C23-C24	2.88	120.68	111.90
21	H	1000	CLA	O2A-CGA-CBA	2.88	124.38	112.36
21	A	1117	CLA	CMB-C2B-C3B	2.88	130.73	125.09
21	B	1223	CLA	CMB-C2B-C3B	2.88	130.73	125.09
21	B	1208	CLA	C4-C3-C5	2.89	119.81	115.41
21	B	9023	CLA	C4A-NA-C1A	2.89	110.09	106.36
19	A	6003	BCR	C38-C26-C27	2.89	118.90	113.43
21	A	1125	CLA	CMC-C2C-C1C	2.89	129.49	125.02
19	A	6007	BCR	C8-C9-C10	2.89	123.64	118.98
21	4	4008	CLA	C4A-NA-C1A	2.89	110.10	106.36
21	A	1120	CLA	O2A-CGA-CBA	2.89	124.42	112.36
26	1	1502	LUT	C12-C13-C14	2.90	123.65	118.98
21	A	1102	CLA	CMC-C2C-C1C	2.91	129.52	125.02
21	1	1012	CLA	C4A-NA-C1A	2.91	110.12	106.36
26	4	4501	LUT	C8-C9-C10	2.91	123.67	118.98
21	A	1103	CLA	C4-C3-C5	2.91	119.86	115.41
21	3	3009	CLA	C4A-NA-C1A	2.91	110.13	106.36
21	4	4014	CLA	CAA-C2A-C3A	2.91	121.59	113.22
21	A	1117	CLA	C4-C3-C5	2.91	119.86	115.41
19	F	6014	BCR	C30-C25-C26	2.92	126.94	122.66
21	A	1103	CLA	CMC-C2C-C1C	2.92	129.54	125.02
21	A	9012	CLA	CMB-C2B-C3B	2.92	130.80	125.09
21	A	9013	CLA	CMC-C2C-C1C	2.92	129.54	125.02
19	B	6006	BCR	C8-C9-C10	2.92	123.69	118.98
19	B	6005	BCR	C1-C6-C7	2.92	124.01	115.82
21	A	1121	CLA	CMC-C2C-C1C	2.93	129.55	125.02
21	B	1226	CLA	C4-C3-C5	2.93	119.88	115.41
21	A	1134	CLA	O2A-CGA-CBA	2.93	124.56	112.36
21	B	1227	CLA	C4A-NA-C1A	2.93	110.14	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	6015	CLA	C4-C3-C5	2.93	119.88	115.41
21	B	1235	CLA	C4-C3-C5	2.94	119.89	115.41
19	B	6005	BCR	C38-C26-C27	2.94	119.01	113.43
21	1	1009	CLA	O2A-CGA-CBA	2.95	120.88	111.90
19	A	6003	BCR	C35-C13-C12	2.95	123.00	118.10
21	2	2013	CLA	C4A-NA-C1A	2.95	110.17	106.36
21	B	9010	CLA	CAC-C3C-C4C	2.95	129.12	124.83
21	B	1201	CLA	CMC-C2C-C1C	2.95	129.59	125.02
21	A	1115	CLA	CMC-C2C-C1C	2.96	129.60	125.02
21	A	1126	CLA	CMC-C2C-C1C	2.97	129.62	125.02
21	4	4008	CLA	CAA-CBA-CGA	2.98	122.03	113.32
19	I	6020	BCR	C38-C26-C27	2.98	119.07	113.43
20	A	7003	LHG	O7-C7-C8	2.98	118.00	111.53
21	A	1127	CLA	C4-C3-C5	2.98	119.96	115.41
21	A	1125	CLA	C4A-NA-C1A	2.98	110.22	106.36
21	2	2013	CLA	CAC-C3C-C4C	2.98	129.16	124.83
19	A	6008	BCR	C35-C13-C12	2.98	123.06	118.10
21	B	1221	CLA	CMB-C2B-C3B	2.99	130.93	125.09
21	1	1007	CLA	C4-C3-C5	2.99	119.98	115.41
21	1	1013	CLA	CMC-C2C-C1C	3.00	129.65	125.02
21	B	1221	CLA	C4-C3-C5	3.00	119.98	115.41
21	1	1009	CLA	C4-C3-C5	3.00	119.99	115.41
21	B	1236	CLA	C4-C3-C5	3.00	120.00	115.41
19	G	2011	BCR	C33-C5-C4	3.01	119.13	113.43
21	B	9023	CLA	CMC-C2C-C1C	3.02	129.69	125.02
19	L	6019	BCR	C38-C26-C27	3.02	119.15	113.43
21	B	1240	CLA	C4A-NA-C1A	3.02	110.26	106.36
21	2	2001	CLA	CAD-C3D-C2D	3.02	140.13	132.80
21	1	1003	CLA	O2A-CGA-CBA	3.02	121.11	111.90
21	4	4004	CLA	C4-C3-C5	3.03	120.03	115.41
21	A	1105	CLA	CMC-C2C-C1C	3.03	129.71	125.02
21	B	1223	CLA	C4-C3-C5	3.03	120.03	115.41
21	A	1133	CLA	O2A-CGA-CBA	3.03	125.01	112.36
21	2	2010	CLA	CMB-C2B-C3B	3.03	131.02	125.09
21	1	1010	CLA	C4-C3-C5	3.04	120.04	115.41
21	A	1114	CLA	CMB-C2B-C3B	3.04	131.03	125.09
21	2	2003	CLA	C4A-NA-C1A	3.04	110.29	106.36
19	B	6006	BCR	C38-C26-C27	3.04	119.19	113.43
21	B	1221	CLA	CMC-C2C-C1C	3.04	129.72	125.02
21	B	1202	CLA	C4-C3-C5	3.04	120.05	115.41
23	A	9011	CL0	CMC-C2C-C1C	3.04	129.73	125.02
21	A	1109	CLA	C4-C3-C5	3.04	120.06	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	2014	CLA	CMB-C2B-C3B	3.05	131.05	125.09
21	B	9010	CLA	C4A-NA-C1A	3.05	110.30	106.36
21	A	1104	CLA	C4-C3-C5	3.05	120.07	115.41
21	B	1216	CLA	C4-C3-C5	3.05	120.07	115.41
21	B	1228	CLA	C4-C3-C5	3.06	119.15	115.68
21	B	1213	CLA	CMC-C2C-C1C	3.06	129.75	125.02
19	B	6010	BCR	C19-C18-C17	3.06	123.92	118.98
21	1	1004	CLA	CAC-C3C-C4C	3.06	129.27	124.83
21	A	1112	CLA	CMC-C2C-C1C	3.06	129.76	125.02
26	4	4501	LUT	C30-C31-C32	3.07	132.48	123.13
21	B	1228	CLA	CMB-C2B-C3B	3.07	131.09	125.09
21	4	4003	CLA	O2A-CGA-CBA	3.07	121.26	111.90
21	A	1116	CLA	C4-C3-C5	3.07	120.10	115.41
21	B	1204	CLA	C4-C3-C5	3.08	120.11	115.41
21	4	4014	CLA	CAC-C3C-C4C	3.08	129.30	124.83
21	F	1303	CLA	C1-O2A-CGA	3.09	122.39	112.37
19	A	6007	BCR	C19-C18-C17	3.10	123.97	118.98
20	1	1801	LHG	O8-C23-C24	3.10	121.34	111.90
21	3	3003	CLA	C4-C3-C5	3.10	120.14	115.41
27	4	4503	NEX	C26-O24-C25	3.12	64.93	61.25
21	3	3008	CLA	C4-C3-C5	3.13	120.18	115.41
21	2	2012	CLA	C4-C3-C5	3.13	120.19	115.41
21	4	4005	CLA	CMC-C2C-C1C	3.14	129.87	125.02
21	3	3011	CLA	O2A-CGA-CBA	3.14	125.44	112.36
19	A	6002	BCR	C19-C18-C17	3.15	124.05	118.98
19	F	6014	BCR	C31-C1-C2	3.15	120.06	108.79
21	A	1116	CLA	CMC-C2C-C1C	3.15	129.90	125.02
21	G	1001	CLA	CMB-C2B-C3B	3.16	131.26	125.09
21	B	9010	CLA	CMC-C2C-C1C	3.17	129.93	125.02
21	B	9023	CLA	C4-C3-C5	3.18	120.27	115.41
21	B	1227	CLA	O2A-CGA-CBA	3.18	121.59	111.90
20	A	7003	LHG	O8-C23-C24	3.18	121.59	111.90
21	G	1002	CLA	C4A-NA-C1A	3.18	110.48	106.36
21	B	1207	CLA	C4-C3-C5	3.20	120.29	115.41
21	A	1106	CLA	CMB-C2B-C3B	3.20	131.34	125.09
21	B	1210	CLA	CMB-C2B-C3B	3.20	131.34	125.09
21	B	9022	CLA	C4-C3-C5	3.20	120.29	115.41
21	B	1203	CLA	C4-C3-C5	3.20	120.30	115.41
21	4	4006	CLA	C4-C3-C5	3.21	120.31	115.41
21	4	4009	CLA	C4A-NA-C1A	3.23	110.53	106.36
21	B	1214	CLA	CMC-C2C-C1C	3.23	130.01	125.02
19	A	6011	BCR	C31-C1-C2	3.23	120.35	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1502	LUT	C8-C9-C10	3.23	124.19	118.98
21	1	1010	CLA	C4A-NA-C1A	3.24	110.54	106.36
26	4	4502	LUT	C28-C29-C30	3.24	124.20	118.98
21	B	1239	CLA	C4-C3-C5	3.24	120.35	115.41
21	B	9022	CLA	CMB-C2B-C3B	3.24	131.43	125.09
21	F	1303	CLA	C4A-NA-C1A	3.25	110.56	106.36
21	A	9013	CLA	C4A-NA-C1A	3.25	110.56	106.36
21	B	1215	CLA	C4-C3-C5	3.25	120.37	115.41
21	B	1225	CLA	C4-C3-C5	3.25	120.38	115.41
21	4	4008	CLA	CMC-C2C-C1C	3.26	130.07	125.02
19	L	6019	BCR	C19-C18-C17	3.27	124.25	118.98
21	3	3001	CLA	C4-C3-C5	3.28	120.42	115.41
21	4	4014	CLA	CMC-C2C-C1C	3.28	130.10	125.02
21	1	1001	CLA	C4A-NA-C1A	3.29	110.61	106.36
21	4	4008	CLA	O2A-C1-C2	3.29	120.03	109.28
21	J	6015	CLA	O2A-CGA-CBA	3.31	121.98	111.90
21	A	1101	CLA	C4-C3-C5	3.31	120.46	115.41
21	A	1110	CLA	C4-C3-C5	3.31	120.46	115.41
21	A	1132	CLA	CAC-C3C-C4C	3.31	129.63	124.83
21	4	4006	CLA	CAC-C3C-C2C	3.32	133.32	127.51
21	2	2001	CLA	C2C-C1C-NC	3.32	116.21	109.44
21	F	1303	CLA	O2A-C1-C2	3.34	124.55	109.40
26	1	1501	LUT	C37-C21-C36	3.34	112.95	107.91
21	2	2008	CLA	CMB-C2B-C3B	3.35	131.64	125.09
21	4	4006	CLA	O2A-CGA-CBA	3.35	122.12	111.90
21	2	2014	CLA	CAC-C3C-C4C	3.36	129.70	124.83
21	B	1222	CLA	CMB-C2B-C3B	3.36	131.66	125.09
21	B	1240	CLA	O2A-CGA-CBA	3.38	122.18	111.90
21	2	2005	CLA	C4A-NA-C1A	3.38	110.72	106.36
19	A	6017	BCR	C38-C26-C27	3.38	119.83	113.43
19	A	6007	BCR	C38-C26-C27	3.38	119.84	113.43
21	A	1132	CLA	C4-C3-C5	3.38	120.57	115.41
26	1	1502	LUT	C32-C33-C34	3.39	124.44	118.98
21	B	1219	CLA	C4-C3-C5	3.40	120.60	115.41
19	B	6004	BCR	C19-C18-C17	3.40	124.46	118.98
21	2	2009	CLA	O2A-CGA-CBA	3.40	126.55	112.36
21	B	1240	CLA	C4-C3-C5	3.40	120.61	115.41
21	1	1001	CLA	C4-C3-C5	3.41	120.62	115.41
19	J	6012	BCR	C38-C26-C27	3.42	119.92	113.43
21	B	1239	CLA	C4A-NA-C1A	3.43	110.79	106.36
26	2	2501	LUT	C2-C1-C6	3.43	115.97	110.49
21	2	2006	CLA	C4-C3-C5	3.44	120.66	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1103	CLA	O2A-CGA-CBA	3.44	122.37	111.90
21	J	6014	CLA	C4-C3-C5	3.44	120.66	115.41
21	1	1007	CLA	CMC-C2C-C1C	3.44	130.35	125.02
19	J	6012	BCR	C8-C9-C10	3.45	124.54	118.98
21	2	2008	CLA	C4-C3-C5	3.46	120.69	115.41
21	1	1006	CLA	CMB-C2B-C3B	3.46	131.85	125.09
21	2	2002	CLA	C4A-NA-C1A	3.46	110.83	106.36
21	4	4007	CLA	C4A-NA-C1A	3.46	110.84	106.36
21	1	1011	CLA	C4A-NA-C1A	3.47	110.84	106.36
26	2	2502	LUT	C2-C1-C6	3.47	116.02	110.49
26	4	4502	LUT	C2-C1-C6	3.48	116.04	110.49
21	4	4007	CLA	O2A-CGA-CBA	3.48	122.51	111.90
21	B	1220	CLA	C4-C3-C5	3.49	120.73	115.41
21	B	1221	CLA	O2A-CGA-CBA	3.49	122.54	111.90
18	B	5002	PQN	C14-C13-C15	3.50	120.75	115.41
21	3	3001	CLA	O2A-CGA-CBA	3.51	122.58	111.90
21	4	4007	CLA	C4-C3-C5	3.51	120.77	115.41
21	A	1128	CLA	O2A-CGA-CBA	3.52	122.61	111.90
21	1	1013	CLA	C4A-NA-C1A	3.53	110.92	106.36
21	B	1226	CLA	C4A-NA-C1A	3.55	110.94	106.36
21	1	1002	CLA	CMC-C2C-C1C	3.56	130.52	125.02
21	2	2008	CLA	O2A-CGA-CBA	3.56	122.74	111.90
21	B	1216	CLA	O2A-CGA-CBA	3.57	122.76	111.90
21	4	4002	CLA	O2A-CGA-CBA	3.57	122.77	111.90
21	2	2014	CLA	C4A-NA-C1A	3.57	110.98	106.36
21	1	1002	CLA	C4-C3-C5	3.58	120.87	115.41
21	A	1131	CLA	C4-C3-C5	3.58	120.88	115.41
21	A	1136	CLA	O2A-CGA-CBA	3.59	122.83	111.90
21	A	1137	CLA	C4-C3-C5	3.59	120.89	115.41
21	A	1135	CLA	C4-C3-C5	3.59	119.75	115.68
19	B	6006	BCR	C40-C30-C39	3.60	119.89	108.37
21	2	2006	CLA	CMC-C2C-C1C	3.60	130.59	125.02
21	4	4011	CLA	CMC-C2C-C1C	3.61	130.60	125.02
19	B	6011	BCR	C33-C5-C4	3.61	120.28	113.43
21	1	1002	CLA	CMB-C2B-C3B	3.61	132.16	125.09
21	A	1115	CLA	C4-C3-C5	3.62	120.93	115.41
21	G	1001	CLA	C4A-NA-C1A	3.62	111.03	106.36
23	A	9011	CL0	O2A-CGA-CBA	3.62	122.93	111.90
26	4	4502	LUT	C10-C11-C12	3.62	134.17	123.13
21	1	1001	CLA	O2D-CGD-CBD	3.65	116.30	111.30
26	4	4502	LUT	C8-C9-C10	3.65	124.87	118.98
19	I	6018	BCR	C40-C30-C39	3.65	120.08	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	4502	LUT	C38-C25-C26	3.66	118.78	116.04
21	B	9010	CLA	O2A-CGA-CBA	3.66	123.05	111.90
19	B	6005	BCR	C23-C22-C21	3.66	124.88	118.98
21	A	1105	CLA	C4-C3-C5	3.66	119.83	115.68
21	1	1003	CLA	C4-C3-C5	3.67	121.01	115.41
27	4	4503	NEX	C1-C2-C3	3.68	122.04	113.41
21	1	1008	CLA	C4-C3-C5	3.68	121.03	115.41
21	A	1115	CLA	O2A-CGA-CBA	3.69	123.14	111.90
21	2	2007	CLA	O2A-CGA-CBA	3.69	123.15	111.90
21	2	2012	CLA	O2A-CGA-CBA	3.70	123.17	111.90
21	1	1012	CLA	O2A-CGA-CBA	3.70	123.18	111.90
21	A	1135	CLA	O2A-CGA-CBA	3.71	123.20	111.90
21	B	1219	CLA	O2A-CGA-CBA	3.71	123.21	111.90
21	2	2003	CLA	C4-C3-C5	3.71	121.08	115.41
21	2	2001	CLA	C2D-C1D-ND	3.71	115.33	110.22
19	B	6004	BCR	C38-C26-C27	3.71	120.47	113.43
21	B	1234	CLA	O2A-CGA-CBA	3.74	123.28	111.90
21	A	1127	CLA	O2A-CGA-CBA	3.74	123.30	111.90
21	B	1236	CLA	O2A-CGA-CBA	3.74	123.31	111.90
20	B	7004	LHG	O7-C7-C8	3.75	119.68	111.53
19	A	6008	BCR	C40-C30-C39	3.75	120.40	108.37
26	1	1501	LUT	C2-C1-C6	3.77	116.50	110.49
19	I	6018	BCR	C23-C22-C21	3.77	125.05	118.98
21	B	1228	CLA	CMC-C2C-C1C	3.77	130.85	125.02
21	A	1141	CLA	O2A-CGA-CBA	3.77	123.39	111.90
21	A	1140	CLA	C4-C3-C5	3.78	121.18	115.41
21	2	2013	CLA	CMC-C2C-C1C	3.81	130.91	125.02
21	1	1004	CLA	CMC-C2C-C1C	3.81	130.91	125.02
21	L	1503	CLA	O2A-CGA-CBA	3.81	123.52	111.90
21	4	4010	CLA	O2A-CGA-CBA	3.82	123.54	111.90
21	4	4009	CLA	CMC-C2C-C1C	3.82	130.93	125.02
21	B	9022	CLA	O2A-CGA-CBA	3.82	123.55	111.90
21	2	2005	CLA	O2A-CGA-CBA	3.84	123.59	111.90
19	A	6008	BCR	C33-C5-C4	3.84	120.71	113.43
21	2	2010	CLA	C4-C3-C5	3.84	121.28	115.41
19	J	6013	BCR	C8-C9-C10	3.85	125.19	118.98
21	A	1117	CLA	O2A-CGA-CBA	3.86	123.66	111.90
21	A	1141	CLA	C4-C3-C5	3.87	120.06	115.68
21	A	1136	CLA	C4-C3-C5	3.87	121.32	115.41
21	A	1106	CLA	O2A-CGA-CBA	3.87	123.70	111.90
21	A	9012	CLA	O2D-CGD-CBD	3.88	116.61	111.30
21	L	1502	CLA	O2A-CGA-CBA	3.88	123.73	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	1002	CLA	O2A-CGA-CBA	3.88	123.74	111.90
19	I	6020	BCR	C19-C18-C17	3.89	125.25	118.98
21	3	3008	CLA	O2A-CGA-CBA	3.90	123.78	111.90
21	A	1102	CLA	O2A-CGA-CBA	3.90	123.79	111.90
21	B	1214	CLA	O2A-CGA-CBA	3.91	123.80	111.90
21	2	2003	CLA	O2A-CGA-CBA	3.91	123.82	111.90
21	B	1220	CLA	O2A-CGA-CBA	3.92	123.83	111.90
21	3	3006	CLA	O2A-CGA-CBA	3.92	123.83	111.90
21	1	1010	CLA	O2A-CGA-CBA	3.92	123.84	111.90
19	B	6005	BCR	C8-C9-C10	3.92	125.30	118.98
20	2	2801	LHG	O7-C7-C8	3.92	120.05	111.53
21	A	1107	CLA	C4-C3-C5	3.92	120.13	115.68
26	1	1501	LUT	C10-C11-C12	3.92	135.09	123.13
26	4	4501	LUT	C10-C11-C12	3.93	135.09	123.13
21	A	1119	CLA	O2A-CGA-CBA	3.93	123.87	111.90
21	1	1006	CLA	O2A-C1-C2	3.94	123.21	108.42
27	4	4503	NEX	C11-C12-C13	3.94	137.91	126.32
21	B	1206	CLA	O2A-CGA-CBA	3.94	123.90	111.90
21	A	1123	CLA	O2A-CGA-CBA	3.94	123.91	111.90
21	B	1238	CLA	O2A-CGA-CBA	3.95	123.93	111.90
21	4	4005	CLA	CGD-CBD-CAD	3.95	124.01	110.62
21	1	1007	CLA	O2D-CGD-CBD	3.95	116.72	111.30
26	1	1501	LUT	C30-C31-C32	3.96	135.19	123.13
21	B	1207	CLA	O2A-CGA-CBA	3.96	123.97	111.90
26	4	4501	LUT	C2-C3-C4	3.98	117.36	110.32
21	4	4006	CLA	C4A-NA-C1A	3.98	111.50	106.36
26	1	1501	LUT	C8-C9-C10	3.98	125.40	118.98
19	A	6011	BCR	C40-C30-C39	3.98	121.13	108.37
19	F	6016	BCR	C40-C30-C39	3.98	121.13	108.37
21	A	9012	CLA	O2A-CGA-CBA	3.98	124.04	111.90
21	A	1105	CLA	O2A-CGA-CBA	3.99	124.04	111.90
21	A	1110	CLA	O2A-CGA-CBA	3.99	124.05	111.90
25	J	5001	LMG	O7-C10-C11	3.99	120.20	111.53
21	4	4011	CLA	C4-C3-C5	4.00	121.51	115.41
23	A	9011	CL0	CAC-C3C-C4C	4.00	130.63	124.83
21	A	1139	CLA	O2A-CGA-CBA	4.00	124.09	111.90
21	B	1208	CLA	O2A-CGA-CBA	4.01	124.11	111.90
19	F	6016	BCR	C32-C1-C2	4.01	123.14	108.79
19	B	6006	BCR	C32-C1-C2	4.01	123.15	108.79
21	B	1203	CLA	O2A-CGA-CBA	4.02	124.14	111.90
21	G	1001	CLA	O2A-CGA-CBA	4.03	124.17	111.90
21	B	1230	CLA	C4-C3-C5	4.03	121.56	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4004	CLA	O2A-CGA-CBA	4.03	124.18	111.90
21	A	1116	CLA	O2A-CGA-CBA	4.03	124.18	111.90
21	A	1104	CLA	O2A-CGA-CBA	4.03	124.18	111.90
26	1	1502	LUT	C28-C29-C30	4.03	125.48	118.98
21	A	1138	CLA	O2A-CGA-CBA	4.03	124.19	111.90
26	1	1502	LUT	C10-C11-C12	4.04	135.44	123.13
19	A	6003	BCR	C33-C5-C4	4.04	121.09	113.43
26	1	1501	LUT	C8-C7-C6	4.05	139.47	127.32
21	B	1205	CLA	O2A-CGA-CBA	4.05	124.24	111.90
21	A	1101	CLA	O2A-CGA-CBA	4.06	124.27	111.90
19	G	2011	BCR	C23-C22-C21	4.06	125.53	118.98
19	A	6017	BCR	C23-C22-C21	4.10	125.58	118.98
21	B	1218	CLA	O2A-CGA-CBA	4.10	124.38	111.90
19	B	6006	BCR	C32-C1-C31	4.11	121.53	108.37
21	B	1229	CLA	O2A-CGA-CBA	4.11	124.42	111.90
19	F	6016	BCR	C32-C1-C31	4.11	121.55	108.37
21	3	3003	CLA	O2A-CGA-CBA	4.12	124.46	111.90
21	B	1223	CLA	O2A-CGA-CBA	4.12	124.46	111.90
18	A	5001	PQN	C14-C13-C15	4.13	121.71	115.41
21	1	1013	CLA	O2A-CGA-CBA	4.14	124.52	111.90
21	B	1204	CLA	O2A-CGA-CBA	4.16	124.56	111.90
21	A	1106	CLA	CMC-C2C-C1C	4.16	131.45	125.02
26	4	4502	LUT	C37-C21-C36	4.16	114.17	107.91
21	A	1124	CLA	O2A-CGA-CBA	4.18	124.65	111.90
21	A	1126	CLA	O2A-CGA-CBA	4.19	124.66	111.90
21	2	2013	CLA	O2A-CGA-CBA	4.20	124.68	111.90
21	B	1225	CLA	O2A-CGA-CBA	4.20	124.69	111.90
21	B	1211	CLA	O2A-CGA-CBA	4.21	124.71	111.90
21	A	1107	CLA	O2A-CGA-CBA	4.21	124.73	111.90
21	1	1006	CLA	O2A-CGA-CBA	4.21	124.74	111.90
21	3	3010	CLA	O2A-CGA-CBA	4.22	124.75	111.90
21	A	1132	CLA	O2A-CGA-CBA	4.22	124.75	111.90
21	B	1228	CLA	O2A-CGA-CBA	4.22	124.76	111.90
21	B	1237	CLA	O2A-CGA-CBA	4.22	124.77	111.90
21	F	1303	CLA	CAC-C3C-C4C	4.23	130.97	124.83
23	A	9011	CL0	C4-C3-C5	4.23	121.87	115.41
21	A	1137	CLA	O2A-CGA-CBA	4.25	124.84	111.90
21	B	1215	CLA	O2A-CGA-CBA	4.26	124.89	111.90
21	B	1230	CLA	O2A-CGA-CBA	4.27	124.90	111.90
20	A	7001	LHG	O7-C7-C8	4.28	120.82	111.53
21	B	1210	CLA	O2A-CGA-CBA	4.28	124.93	111.90
21	4	4009	CLA	O2A-CGA-CBA	4.28	124.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	9023	CLA	O2A-CGA-CBA	4.30	125.01	111.90
21	J	6014	CLA	O2A-CGA-CBA	4.33	125.09	111.90
21	4	4001	CLA	CMC-C2C-C1C	4.33	131.72	125.02
21	A	1129	CLA	O2A-CGA-CBA	4.34	125.11	111.90
21	J	1302	CLA	O2A-CGA-CBA	4.34	125.12	111.90
21	A	1122	CLA	O2A-CGA-CBA	4.34	125.12	111.90
21	B	1235	CLA	O2A-CGA-CBA	4.37	125.22	111.90
19	A	6008	BCR	C32-C1-C31	4.37	122.39	108.37
21	1	1001	CLA	O2A-CGA-CBA	4.40	125.30	111.90
21	A	1109	CLA	O2A-CGA-CBA	4.41	125.35	111.90
19	J	6012	BCR	C23-C22-C21	4.42	126.10	118.98
21	3	3013	CLA	O2A-CGA-CBA	4.44	125.42	111.90
25	G	2021	LMG	O1-C1-C2	4.44	113.64	108.04
21	B	1222	CLA	O2A-CGA-CBA	4.46	125.48	111.90
21	A	1140	CLA	O2A-CGA-CBA	4.46	125.49	111.90
21	4	4013	CLA	O2A-CGA-CBA	4.47	125.51	111.90
21	4	4002	CLA	C4A-NA-C1A	4.47	112.14	106.36
19	F	6014	BCR	C32-C1-C31	4.47	122.71	108.37
21	2	2006	CLA	O2A-CGA-CBA	4.49	125.57	111.90
21	4	4013	CLA	CMC-C2C-C1C	4.49	131.96	125.02
26	4	4501	LUT	C18-C5-C4	4.50	122.45	114.24
20	1	1801	LHG	O7-C7-C8	4.50	121.32	111.53
27	4	4503	NEX	C11-C10-C9	4.51	133.70	127.20
19	I	6018	BCR	C32-C1-C31	4.51	122.81	108.37
21	1	1004	CLA	O2A-CGA-CBA	4.51	125.66	111.90
27	4	4503	NEX	C35-C34-C33	4.53	133.75	127.20
21	1	1002	CLA	O2D-CGD-CBD	4.54	117.53	111.30
21	2	2010	CLA	O2A-CGA-CBA	4.55	125.76	111.90
21	A	1131	CLA	O2A-CGA-CBA	4.57	125.83	111.90
19	A	6011	BCR	C32-C1-C31	4.57	123.03	108.37
21	1	1007	CLA	O2A-CGA-CBA	4.58	125.85	111.90
21	B	9023	CLA	O2D-CGD-CBD	4.58	117.59	111.30
19	B	6005	BCR	C19-C18-C17	4.59	126.37	118.98
19	A	6017	BCR	C19-C18-C17	4.61	126.41	118.98
21	2	2004	CLA	O2A-CGA-CBA	4.61	125.95	111.90
21	B	1224	CLA	O2A-CGA-CBA	4.62	125.97	111.90
21	1	1005	CLA	O2A-CGA-CBA	4.64	126.02	111.90
21	B	1202	CLA	O2A-CGA-CBA	4.64	126.04	111.90
21	1	1008	CLA	O2A-CGA-CBA	4.65	126.06	111.90
21	1	1010	CLA	O2D-CGD-CBD	4.67	117.71	111.30
19	G	2011	BCR	C19-C18-C17	4.71	126.57	118.98
21	4	4011	CLA	O2A-CGA-CBA	4.72	126.30	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4001	CLA	O2A-CGA-CBA	4.75	126.37	111.90
21	2	2002	CLA	CAC-C3C-C4C	4.75	131.73	124.83
19	A	6017	BCR	C12-C13-C14	4.76	126.65	118.98
21	A	1111	CLA	O2A-CGA-CBA	4.76	126.42	111.90
21	B	1226	CLA	O2A-CGA-CBA	4.90	126.82	111.90
21	3	3011	CLA	C2C-C1C-NC	4.97	113.94	110.24
26	2	2502	LUT	C38-C25-C26	4.97	119.75	116.04
21	2	2002	CLA	O2D-CGD-CBD	4.97	118.11	111.30
21	2	2001	CLA	C2B-C1B-NB	4.98	114.56	110.09
21	B	9010	CLA	O2D-CGD-CBD	4.99	118.14	111.30
26	4	4502	LUT	C8-C7-C6	4.99	142.31	127.32
21	2	2011	CLA	O2A-CGA-CBA	5.01	127.17	111.90
21	2	2001	CLA	C3C-C4C-NC	5.05	114.53	110.09
21	A	1125	CLA	O2A-CGA-CBA	5.05	127.29	111.90
21	2	2001	CLA	CBD-CAD-C3D	5.06	107.97	104.39
21	2	2002	CLA	O2A-CGA-CBA	5.08	127.39	111.90
21	B	1213	CLA	O2A-CGA-CBA	5.09	127.41	111.90
21	4	4012	CLA	O2A-CGA-CBA	5.11	127.47	111.90
21	1	1011	CLA	O2A-CGA-CBA	5.15	127.59	111.90
21	B	9022	CLA	O2D-CGD-CBD	5.16	118.38	111.30
21	A	1132	CLA	O2D-CGD-CBD	5.18	118.41	111.30
19	A	6011	BCR	C39-C30-C25	5.19	118.44	110.30
21	A	1139	CLA	O2D-CGD-CBD	5.20	118.43	111.30
25	G	2021	LMG	O7-C10-C11	5.21	120.94	111.10
21	F	1303	CLA	O2D-CGD-CBD	5.22	118.46	111.30
21	A	9013	CLA	O2A-CGA-CBA	5.27	127.95	111.90
21	2	2012	CLA	O2D-CGD-CBD	5.28	118.54	111.30
21	3	3002	CLA	O2A-CGA-CBA	5.29	128.01	111.90
21	2	2005	CLA	O2D-CGD-CBD	5.29	118.56	111.30
19	G	2011	BCR	C20-C19-C18	5.32	141.98	126.32
21	B	1239	CLA	O2A-CGA-CBA	5.32	128.12	111.90
26	1	1502	LUT	C30-C31-C32	5.34	139.42	123.13
21	1	1012	CLA	O2D-CGD-CBD	5.40	118.70	111.30
19	A	6017	BCR	C20-C19-C18	5.40	142.22	126.32
19	I	6020	BCR	C20-C19-C18	5.44	142.33	126.32
19	B	6005	BCR	C20-C19-C18	5.46	142.39	126.32
19	I	6018	BCR	C40-C30-C25	5.51	118.94	110.30
21	4	4003	CLA	O2D-CGD-CBD	5.52	118.87	111.30
19	J	6012	BCR	C20-C19-C18	5.54	142.61	126.32
21	4	4008	CLA	O2A-CGA-CBA	5.54	128.78	111.90
19	A	6008	BCR	C40-C30-C25	5.54	119.00	110.30
21	2	2004	CLA	O2D-CGD-CBD	5.55	121.78	111.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	4007	CLA	O2D-CGD-CBD	5.55	118.91	111.30
26	4	4501	LUT	C38-C25-C26	5.60	120.23	116.04
19	F	6016	BCR	C40-C30-C25	5.61	119.11	110.30
21	4	4005	CLA	CAC-C3C-C4C	5.61	132.98	124.83
26	4	4502	LUT	C30-C31-C32	5.63	140.29	123.13
21	3	3003	CLA	O2D-CGD-CBD	5.64	119.04	111.30
21	2	2009	CLA	O2D-CGD-CBD	5.64	119.04	111.30
19	B	6006	BCR	C40-C30-C25	5.67	119.19	110.30
23	A	9011	CL0	O2D-CGD-CBD	5.68	119.09	111.30
19	F	6016	BCR	C39-C30-C25	5.70	119.23	110.30
26	2	2501	LUT	C38-C25-C26	5.70	120.30	116.04
19	J	6012	BCR	C19-C18-C17	5.71	128.18	118.98
21	3	3008	CLA	O2D-CGD-CBD	5.71	119.14	111.30
21	1	1013	CLA	O2D-CGD-CBD	5.73	119.16	111.30
21	3	3004	CLA	O2D-CGD-CBD	5.73	119.16	111.30
21	4	4014	CLA	C2C-C1C-NC	5.76	114.53	110.24
21	A	9013	CLA	O2D-CGD-CBD	5.77	119.21	111.30
21	B	1208	CLA	O2D-CGD-CBD	5.81	119.27	111.30
21	A	1125	CLA	O2D-CGD-CBD	5.81	119.27	111.30
26	1	1502	LUT	C18-C5-C4	5.86	124.93	114.24
21	1	1005	CLA	O2D-CGD-CBD	5.87	119.35	111.30
21	4	4014	CLA	O2D-CGD-CBD	5.87	119.35	111.30
21	B	1203	CLA	O2D-CGD-CBD	5.88	119.36	111.30
21	2	2003	CLA	O2D-CGD-CBD	5.88	119.37	111.30
27	4	4503	NEX	C2-C1-C6	5.89	114.78	109.24
21	A	1133	CLA	O2D-CGD-CBD	5.89	119.38	111.30
21	1	1009	CLA	CMB-C2B-C3B	5.95	136.72	125.09
21	A	1109	CLA	O2D-CGD-CBD	5.96	119.47	111.30
21	B	1213	CLA	O2D-CGD-CBD	5.96	119.48	111.30
21	B	1219	CLA	O2D-CGD-CBD	6.00	119.53	111.30
21	3	3016	CLA	O2D-CGD-CBD	6.04	119.58	111.30
19	A	6011	BCR	C40-C30-C25	6.05	119.79	110.30
21	3	3014	CLA	O2D-CGD-CBD	6.06	119.61	111.30
21	B	1220	CLA	O2D-CGD-CBD	6.06	119.61	111.30
21	4	4012	CLA	O2D-CGD-CBD	6.09	119.65	111.30
21	A	1143	CLA	O2D-CGD-CBD	6.09	119.66	111.30
21	4	4015	CLA	C2C-C1C-NC	6.12	114.80	110.24
21	F	1302	CLA	O2D-CGD-CBD	6.14	119.73	111.30
21	A	9012	CLA	C2C-C1C-NC	6.14	114.82	110.24
21	1	1007	CLA	C2C-C1C-NC	6.19	114.85	110.24
19	A	6008	BCR	C39-C30-C25	6.19	120.01	110.30
21	B	1237	CLA	O2D-CGD-CBD	6.21	119.82	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1119	CLA	O2D-CGD-CBD	6.23	119.84	111.30
21	L	1501	CLA	O2D-CGD-CBD	6.23	119.85	111.30
21	4	4015	CLA	O2D-CGD-CBD	6.26	119.89	111.30
21	4	4002	CLA	O2D-CGD-CBD	6.27	119.90	111.30
21	2	2008	CLA	C2C-C1C-NC	6.27	114.91	110.24
26	1	1501	LUT	C38-C25-C26	6.28	120.74	116.04
21	A	1120	CLA	O2D-CGD-CBD	6.29	119.93	111.30
21	B	1210	CLA	O2D-CGD-CBD	6.30	119.94	111.30
21	A	1126	CLA	O2D-CGD-CBD	6.31	119.95	111.30
21	4	4006	CLA	O2D-CGD-CBD	6.31	119.95	111.30
21	A	1124	CLA	O2D-CGD-CBD	6.31	119.96	111.30
19	B	6006	BCR	C39-C30-C25	6.31	120.20	110.30
21	4	4011	CLA	O2D-CGD-CBD	6.32	119.97	111.30
21	F	1301	CLA	O2D-CGD-CBD	6.32	119.97	111.30
21	B	1228	CLA	C2C-C1C-NC	6.33	114.96	110.24
19	A	6003	BCR	C20-C19-C18	6.35	145.00	126.32
21	A	1115	CLA	O2D-CGD-CBD	6.35	120.01	111.30
19	A	6017	BCR	C11-C12-C13	6.35	145.01	126.32
19	I	6018	BCR	C39-C30-C25	6.36	120.27	110.30
21	B	1206	CLA	O2D-CGD-CBD	6.37	120.03	111.30
21	2	2014	CLA	O2D-CGD-CBD	6.38	120.05	111.30
21	2	2010	CLA	O2D-CGD-CBD	6.39	120.07	111.30
19	A	6007	BCR	C20-C19-C18	6.40	145.16	126.32
21	3	3015	CLA	O2D-CGD-CBD	6.42	120.11	111.30
21	3	3002	CLA	O2D-CGD-CBD	6.43	120.13	111.30
21	A	1111	CLA	O2D-CGD-CBD	6.45	120.14	111.30
19	L	6019	BCR	C20-C19-C18	6.45	145.30	126.32
21	A	1140	CLA	O2D-CGD-CBD	6.45	120.15	111.30
21	B	1222	CLA	O2D-CGD-CBD	6.47	120.18	111.30
21	B	1216	CLA	O2D-CGD-CBD	6.48	120.20	111.30
21	3	3010	CLA	O2D-CGD-CBD	6.49	120.20	111.30
21	4	4006	CLA	C2C-C1C-NC	6.50	115.08	110.24
21	A	1142	CLA	O2D-CGD-CBD	6.50	120.22	111.30
21	A	1108	CLA	O2D-CGD-CBD	6.52	120.24	111.30
21	A	1130	CLA	O2D-CGD-CBD	6.54	120.27	111.30
21	4	4001	CLA	C2C-C1C-NC	6.56	115.13	110.24
21	A	1104	CLA	O2D-CGD-CBD	6.56	120.31	111.30
21	A	1138	CLA	O2D-CGD-CBD	6.57	120.31	111.30
21	A	1110	CLA	O2D-CGD-CBD	6.57	120.31	111.30
21	3	3017	CLA	O2D-CGD-CBD	6.58	120.32	111.30
21	A	1116	CLA	O2D-CGD-CBD	6.59	120.33	111.30
21	A	1103	CLA	O2D-CGD-CBD	6.60	120.35	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	L	1503	CLA	O2D-CGD-CBD	6.60	120.35	111.30
21	A	1113	CLA	O2D-CGD-CBD	6.61	120.37	111.30
21	3	3003	CLA	C2C-C1C-NC	6.62	115.17	110.24
21	J	6014	CLA	O2D-CGD-CBD	6.63	120.40	111.30
21	A	1127	CLA	O2D-CGD-CBD	6.64	120.41	111.30
21	J	1302	CLA	O2D-CGD-CBD	6.65	120.42	111.30
21	4	4012	CLA	C2C-C1C-NC	6.65	115.19	110.24
21	B	1202	CLA	O2D-CGD-CBD	6.66	120.43	111.30
21	B	1235	CLA	O2D-CGD-CBD	6.67	120.45	111.30
21	B	1214	CLA	O2D-CGD-CBD	6.67	120.45	111.30
21	B	1225	CLA	O2D-CGD-CBD	6.68	120.46	111.30
21	1	1013	CLA	C2C-C1C-NC	6.68	115.21	110.24
21	B	1217	CLA	O2D-CGD-CBD	6.68	120.46	111.30
21	B	1204	CLA	O2D-CGD-CBD	6.69	120.47	111.30
21	G	1002	CLA	O2D-CGD-CBD	6.69	120.47	111.30
21	F	1303	CLA	C2C-C1C-NC	6.70	115.23	110.24
19	F	6014	BCR	C39-C30-C25	6.71	120.83	110.30
21	A	1105	CLA	O2D-CGD-CBD	6.73	120.53	111.30
21	2	2006	CLA	O2D-CGD-CBD	6.74	120.54	111.30
19	F	6014	BCR	C20-C19-C18	6.75	146.20	126.32
21	A	1114	CLA	O2D-CGD-CBD	6.76	120.58	111.30
21	2	2007	CLA	O2D-CGD-CBD	6.77	120.58	111.30
21	A	1141	CLA	O2D-CGD-CBD	6.79	120.61	111.30
21	B	1215	CLA	O2D-CGD-CBD	6.79	120.62	111.30
21	B	1238	CLA	O2D-CGD-CBD	6.80	120.62	111.30
21	A	1129	CLA	O2D-CGD-CBD	6.80	120.64	111.30
21	B	1224	CLA	O2D-CGD-CBD	6.81	120.64	111.30
21	L	1502	CLA	O2D-CGD-CBD	6.83	120.67	111.30
21	B	1234	CLA	O2D-CGD-CBD	6.84	120.69	111.30
21	A	1136	CLA	O2D-CGD-CBD	6.84	120.69	111.30
21	3	3006	CLA	O2D-CGD-CBD	6.85	120.70	111.30
19	L	6020	BCR	C20-C19-C18	6.86	146.52	126.32
21	A	1112	CLA	O2D-CGD-CBD	6.87	120.72	111.30
21	B	1228	CLA	O2D-CGD-CBD	6.87	120.73	111.30
21	B	1223	CLA	O2D-CGD-CBD	6.87	120.73	111.30
21	A	1101	CLA	O2D-CGD-CBD	6.87	120.73	111.30
21	1	1005	CLA	C2C-C1C-NC	6.88	115.36	110.24
21	A	1134	CLA	O2D-CGD-CBD	6.88	120.75	111.30
21	4	4005	CLA	O2D-CGD-CBD	6.91	120.78	111.30
21	B	1229	CLA	O2D-CGD-CBD	6.91	120.78	111.30
19	B	6010	BCR	C20-C19-C18	6.92	146.69	126.32
21	1	1012	CLA	C2C-C1C-NC	6.94	115.41	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	6015	CLA	O2D-CGD-CBD	6.95	120.83	111.30
21	A	1135	CLA	O2D-CGD-CBD	6.95	120.83	111.30
19	B	6009	BCR	C20-C19-C18	6.96	146.82	126.32
21	B	1231	CLA	O2D-CGD-CBD	6.97	120.86	111.30
21	4	4003	CLA	C2C-C1C-NC	6.99	115.44	110.24
21	A	1132	CLA	C2C-C1C-NC	6.99	115.45	110.24
21	4	4004	CLA	C2C-C1C-NC	7.00	115.45	110.24
21	B	1212	CLA	O2D-CGD-CBD	7.00	120.91	111.30
21	4	4010	CLA	O2D-CGD-CBD	7.01	120.92	111.30
19	A	6008	BCR	C20-C19-C18	7.01	146.96	126.32
21	B	1214	CLA	C2C-C1C-NC	7.03	115.47	110.24
21	2	2013	CLA	C2C-C1C-NC	7.03	115.48	110.24
21	B	1213	CLA	C2C-C1C-NC	7.03	115.48	110.24
19	F	6014	BCR	C40-C30-C25	7.06	121.36	110.30
21	A	1112	CLA	C2C-C1C-NC	7.07	115.51	110.24
21	A	1125	CLA	C2C-C1C-NC	7.07	115.51	110.24
21	G	1001	CLA	C2C-C1C-NC	7.09	115.52	110.24
21	A	1115	CLA	C2C-C1C-NC	7.09	115.52	110.24
21	H	1000	CLA	O2D-CGD-CBD	7.09	121.03	111.30
21	B	1207	CLA	O2D-CGD-CBD	7.10	121.04	111.30
21	A	1130	CLA	C2C-C1C-NC	7.11	115.53	110.24
21	A	1106	CLA	C2C-C1C-NC	7.12	115.54	110.24
21	A	1129	CLA	C2C-C1C-NC	7.12	115.55	110.24
21	A	1117	CLA	O2D-CGD-CBD	7.12	121.07	111.30
21	A	1107	CLA	O2D-CGD-CBD	7.15	121.11	111.30
21	B	1209	CLA	O2D-CGD-CBD	7.19	121.16	111.30
19	I	6018	BCR	C20-C19-C18	7.19	147.48	126.32
21	3	3001	CLA	C2C-C1C-NC	7.20	115.60	110.24
19	B	6004	BCR	C20-C19-C18	7.20	147.51	126.32
21	A	1128	CLA	C2C-C1C-NC	7.21	115.61	110.24
21	A	1137	CLA	O2D-CGD-CBD	7.23	121.22	111.30
21	L	1502	CLA	C2C-C1C-NC	7.25	115.64	110.24
21	A	1126	CLA	C2C-C1C-NC	7.25	115.64	110.24
21	A	1116	CLA	C2C-C1C-NC	7.25	115.64	110.24
21	2	2009	CLA	C2C-C1C-NC	7.25	115.64	110.24
21	B	1211	CLA	O2D-CGD-CBD	7.26	121.26	111.30
21	1	1008	CLA	C2C-C1C-NC	7.27	115.65	110.24
21	A	1128	CLA	O2D-CGD-CBD	7.27	121.27	111.30
21	B	1236	CLA	O2D-CGD-CBD	7.28	121.28	111.30
21	A	1107	CLA	C2C-C1C-NC	7.28	115.66	110.24
21	1	1003	CLA	O2D-CGD-CBD	7.29	121.30	111.30
21	3	3009	CLA	O2D-CGD-CBD	7.29	121.30	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1239	CLA	C2C-C1C-NC	7.30	115.68	110.24
21	G	1001	CLA	O2D-CGD-CBD	7.31	121.32	111.30
21	A	1118	CLA	O2D-CGD-CBD	7.31	121.32	111.30
19	A	6002	BCR	C20-C19-C18	7.31	147.83	126.32
21	B	1222	CLA	C2C-C1C-NC	7.32	115.69	110.24
21	2	2011	CLA	O2D-CGD-CBD	7.32	121.35	111.30
21	4	4009	CLA	O2D-CGD-CBD	7.33	121.35	111.30
21	1	1006	CLA	O2D-CGD-CBD	7.33	121.36	111.30
21	B	1235	CLA	C2C-C1C-NC	7.34	115.70	110.24
21	B	1230	CLA	C2C-C1C-NC	7.34	115.71	110.24
21	1	1004	CLA	C2C-C1C-NC	7.34	115.71	110.24
21	B	1201	CLA	C2C-C1C-NC	7.34	115.71	110.24
21	A	1138	CLA	C2C-C1C-NC	7.36	115.72	110.24
21	B	1208	CLA	C2C-C1C-NC	7.36	115.72	110.24
21	B	9023	CLA	C2C-C1C-NC	7.36	115.72	110.24
21	A	1131	CLA	C2C-C1C-NC	7.37	115.73	110.24
21	1	1010	CLA	C2C-C1C-NC	7.39	115.75	110.24
21	4	4001	CLA	O2D-CGD-CBD	7.41	121.46	111.30
21	A	1133	CLA	C2C-C1C-NC	7.41	115.76	110.24
21	B	1211	CLA	C2C-C1C-NC	7.41	115.76	110.24
21	A	1111	CLA	C2C-C1C-NC	7.42	115.77	110.24
21	B	9010	CLA	C2C-C1C-NC	7.45	115.79	110.24
21	L	1501	CLA	C2C-C1C-NC	7.45	115.79	110.24
21	4	4009	CLA	C2C-C1C-NC	7.45	115.79	110.24
21	B	1204	CLA	C2C-C1C-NC	7.46	115.80	110.24
21	B	1209	CLA	C2C-C1C-NC	7.46	115.80	110.24
21	A	1127	CLA	C2C-C1C-NC	7.49	115.82	110.24
19	J	6013	BCR	C20-C19-C18	7.50	148.38	126.32
21	B	1238	CLA	C2C-C1C-NC	7.50	115.83	110.24
21	A	1105	CLA	C2C-C1C-NC	7.50	115.83	110.24
21	A	1141	CLA	C2C-C1C-NC	7.52	115.84	110.24
21	A	1103	CLA	C2C-C1C-NC	7.52	115.84	110.24
21	B	1237	CLA	C2C-C1C-NC	7.52	115.84	110.24
21	A	1122	CLA	C2C-C1C-NC	7.53	115.85	110.24
21	1	1002	CLA	C2C-C1C-NC	7.53	115.85	110.24
21	2	2010	CLA	C2C-C1C-NC	7.54	115.85	110.24
21	A	1106	CLA	O2D-CGD-CBD	7.54	121.64	111.30
21	2	2006	CLA	C2C-C1C-NC	7.54	115.86	110.24
21	B	1218	CLA	C2C-C1C-NC	7.55	115.86	110.24
19	B	6006	BCR	C20-C19-C18	7.56	148.56	126.32
21	A	1108	CLA	C2C-C1C-NC	7.56	115.87	110.24
21	A	1136	CLA	C2C-C1C-NC	7.56	115.87	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1101	CLA	C2C-C1C-NC	7.56	115.87	110.24
21	B	1220	CLA	C2C-C1C-NC	7.56	115.87	110.24
21	B	1203	CLA	C2C-C1C-NC	7.57	115.88	110.24
21	2	2013	CLA	O2D-CGD-CBD	7.59	121.71	111.30
21	B	1230	CLA	O2D-CGD-CBD	7.59	121.71	111.30
21	B	1219	CLA	C2C-C1C-NC	7.61	115.91	110.24
21	2	2004	CLA	C2C-C1C-NC	7.61	115.91	110.24
21	B	1229	CLA	C2C-C1C-NC	7.61	115.91	110.24
23	A	9011	CL0	C2C-C1C-NC	7.61	115.91	110.24
21	A	1124	CLA	C2C-C1C-NC	7.62	115.92	110.24
21	B	1212	CLA	C2C-C1C-NC	7.62	115.92	110.24
21	B	1218	CLA	O2D-CGD-CBD	7.64	121.78	111.30
21	A	1122	CLA	O2D-CGD-CBD	7.65	121.79	111.30
21	4	4008	CLA	O2D-CGD-CBD	7.65	121.79	111.30
21	A	1117	CLA	C2C-C1C-NC	7.65	115.94	110.24
21	3	3005	CLA	C2C-C1C-NC	7.65	115.94	110.24
21	3	3005	CLA	O2D-CGD-CBD	7.65	121.80	111.30
21	B	1224	CLA	C2C-C1C-NC	7.65	115.94	110.24
21	J	6014	CLA	C2C-C1C-NC	7.66	115.94	110.24
21	2	2012	CLA	C2C-C1C-NC	7.67	115.95	110.24
21	1	1011	CLA	O2D-CGD-CBD	7.67	121.82	111.30
21	A	1102	CLA	C2C-C1C-NC	7.67	115.95	110.24
21	B	1201	CLA	O2D-CGD-CBD	7.68	121.83	111.30
21	L	1503	CLA	C2C-C1C-NC	7.68	115.96	110.24
21	1	1008	CLA	O2D-CGD-CBD	7.69	121.84	111.30
21	B	1216	CLA	C2C-C1C-NC	7.70	115.97	110.24
21	2	2005	CLA	C2C-C1C-NC	7.71	115.98	110.24
21	B	1236	CLA	C2C-C1C-NC	7.71	115.98	110.24
21	A	1143	CLA	C2C-C1C-NC	7.72	115.99	110.24
21	3	3002	CLA	C2C-C1C-NC	7.72	115.99	110.24
21	B	1240	CLA	O2D-CGD-CBD	7.73	121.90	111.30
19	A	6011	BCR	C20-C19-C18	7.73	149.08	126.32
21	3	3006	CLA	C2C-C1C-NC	7.74	116.01	110.24
21	A	1109	CLA	C2C-C1C-NC	7.75	116.01	110.24
21	A	1110	CLA	C2C-C1C-NC	7.76	116.02	110.24
21	A	1121	CLA	C2C-C1C-NC	7.77	116.02	110.24
21	B	1225	CLA	C2C-C1C-NC	7.77	116.02	110.24
21	B	1215	CLA	C2C-C1C-NC	7.78	116.04	110.24
21	3	3015	CLA	C2C-C1C-NC	7.79	116.04	110.24
19	F	6016	BCR	C20-C19-C18	7.79	149.24	126.32
21	A	1119	CLA	C2C-C1C-NC	7.80	116.05	110.24
21	A	1120	CLA	C2C-C1C-NC	7.80	116.05	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	1114	CLA	C2C-C1C-NC	7.81	116.05	110.24
21	3	3004	CLA	C2C-C1C-NC	7.81	116.06	110.24
21	F	1302	CLA	C2C-C1C-NC	7.81	116.06	110.24
21	A	1121	CLA	O2D-CGD-CBD	7.82	122.03	111.30
21	A	1140	CLA	C2C-C1C-NC	7.82	116.07	110.24
21	B	1202	CLA	C2C-C1C-NC	7.83	116.07	110.24
21	4	4013	CLA	C2C-C1C-NC	7.84	116.08	110.24
21	A	1104	CLA	C2C-C1C-NC	7.84	116.08	110.24
19	A	6017	BCR	C11-C10-C9	7.85	138.54	127.20
21	B	1231	CLA	C2C-C1C-NC	7.86	116.10	110.24
21	A	1142	CLA	C2C-C1C-NC	7.87	116.10	110.24
21	B	1234	CLA	C2C-C1C-NC	7.89	116.11	110.24
21	B	1239	CLA	O2D-CGD-CBD	7.89	122.12	111.30
21	A	1139	CLA	C2C-C1C-NC	7.89	116.12	110.24
21	A	1123	CLA	C2C-C1C-NC	7.91	116.13	110.24
21	B	1210	CLA	C2C-C1C-NC	7.91	116.13	110.24
21	B	1205	CLA	O2D-CGD-CBD	7.92	122.17	111.30
21	A	1137	CLA	C2C-C1C-NC	7.94	116.15	110.24
21	3	3010	CLA	C2C-C1C-NC	7.95	116.16	110.24
21	3	3017	CLA	C2C-C1C-NC	7.95	116.17	110.24
21	B	1226	CLA	O2D-CGD-CBD	7.96	122.22	111.30
21	F	1301	CLA	C2C-C1C-NC	7.96	116.17	110.24
21	A	1134	CLA	C2C-C1C-NC	7.98	116.18	110.24
21	B	1221	CLA	O2D-CGD-CBD	7.99	122.27	111.30
21	B	1227	CLA	C2C-C1C-NC	7.99	116.19	110.24
21	3	3009	CLA	C2C-C1C-NC	8.00	116.20	110.24
21	1	1014	CLA	O2D-CGD-CBD	8.00	122.28	111.30
21	2	2002	CLA	C2C-C1C-NC	8.01	116.21	110.24
21	A	1123	CLA	O2D-CGD-CBD	8.03	122.31	111.30
21	B	1205	CLA	C2C-C1C-NC	8.03	116.22	110.24
21	3	3016	CLA	C2C-C1C-NC	8.03	116.22	110.24
21	B	1217	CLA	C2C-C1C-NC	8.04	116.23	110.24
21	1	1004	CLA	O2D-CGD-CBD	8.04	122.33	111.30
21	4	4007	CLA	C2C-C1C-NC	8.06	116.24	110.24
21	A	1113	CLA	C2C-C1C-NC	8.06	116.25	110.24
21	J	1302	CLA	C2C-C1C-NC	8.08	116.26	110.24
21	B	1240	CLA	C2C-C1C-NC	8.08	116.26	110.24
21	1	1014	CLA	C2C-C1C-NC	8.09	116.27	110.24
21	3	3013	CLA	O2D-CGD-CBD	8.11	122.42	111.30
21	A	1102	CLA	O2D-CGD-CBD	8.11	122.43	111.30
21	A	1131	CLA	O2D-CGD-CBD	8.12	122.44	111.30
21	3	3001	CLA	O2D-CGD-CBD	8.14	122.47	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	1221	CLA	C2C-C1C-NC	8.15	116.31	110.24
21	A	1135	CLA	C2C-C1C-NC	8.19	116.34	110.24
21	3	3008	CLA	C2C-C1C-NC	8.19	116.34	110.24
21	A	9013	CLA	C2C-C1C-NC	8.21	116.35	110.24
21	2	2011	CLA	C2C-C1C-NC	8.23	116.37	110.24
21	2	2007	CLA	C2C-C1C-NC	8.27	116.40	110.24
21	1	1011	CLA	C2C-C1C-NC	8.28	116.41	110.24
19	A	6008	BCR	C11-C12-C13	8.29	150.72	126.32
21	G	1002	CLA	C2C-C1C-NC	8.30	116.42	110.24
21	B	1223	CLA	C2C-C1C-NC	8.31	116.43	110.24
21	4	4010	CLA	C2C-C1C-NC	8.35	116.46	110.24
21	2	2003	CLA	C2C-C1C-NC	8.40	116.49	110.24
19	B	6004	BCR	C11-C12-C13	8.41	151.06	126.32
21	B	9022	CLA	C2C-C1C-NC	8.41	116.50	110.24
21	3	3014	CLA	C2C-C1C-NC	8.42	116.52	110.24
21	B	1207	CLA	C2C-C1C-NC	8.43	116.52	110.24
21	4	4005	CLA	C2C-C1C-NC	8.44	116.53	110.24
21	1	1003	CLA	C2C-C1C-NC	8.52	116.59	110.24
21	1	1006	CLA	C2C-C1C-NC	8.55	116.61	110.24
21	B	1206	CLA	C2C-C1C-NC	8.59	116.64	110.24
21	J	6015	CLA	C2C-C1C-NC	8.61	116.65	110.24
21	4	4013	CLA	O2D-CGD-CBD	8.66	123.17	111.30
21	B	1227	CLA	O2D-CGD-CBD	8.68	123.21	111.30
26	1	1502	LUT	C38-C25-C26	8.68	122.53	116.04
19	J	6012	BCR	C11-C12-C13	8.69	151.91	126.32
21	B	1226	CLA	C2C-C1C-NC	8.75	116.76	110.24
21	1	1001	CLA	C2C-C1C-NC	8.79	116.79	110.24
21	H	1000	CLA	C2C-C1C-NC	8.80	116.79	110.24
21	3	3011	CLA	O2D-CGD-CBD	8.85	123.44	111.30
19	I	6018	BCR	C11-C12-C13	8.86	152.39	126.32
21	A	1118	CLA	C2C-C1C-NC	8.98	116.93	110.24
21	3	3012	CLA	C2C-C1C-NC	8.98	116.93	110.24
19	L	6019	BCR	C11-C12-C13	9.00	152.81	126.32
21	2	2014	CLA	C2C-C1C-NC	9.01	116.95	110.24
21	4	4004	CLA	O2D-CGD-CBD	9.01	123.66	111.30
21	1	1009	CLA	O2D-CGD-CBD	9.01	123.67	111.30
21	4	4011	CLA	C2C-C1C-NC	9.05	116.98	110.24
19	B	6010	BCR	C11-C12-C13	9.08	153.03	126.32
21	2	2008	CLA	O2D-CGD-CBD	9.11	123.80	111.30
21	4	4008	CLA	C2C-C1C-NC	9.18	117.08	110.24
19	G	2011	BCR	C11-C12-C13	9.36	153.86	126.32
19	A	6003	BCR	C11-C12-C13	9.43	154.09	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	6018	BCR	C11-C10-C9	9.49	140.90	127.20
19	B	6009	BCR	C11-C10-C9	9.49	140.90	127.20
19	L	6020	BCR	C11-C12-C13	9.59	154.55	126.32
19	B	6009	BCR	C11-C12-C13	9.70	154.87	126.32
21	4	4002	CLA	C2C-C1C-NC	9.70	117.47	110.24
19	A	6008	BCR	C11-C10-C9	9.71	141.22	127.20
19	J	6012	BCR	C21-C20-C19	9.74	152.83	123.13
19	I	6020	BCR	C11-C12-C13	9.77	155.07	126.32
19	J	6013	BCR	C11-C12-C13	9.78	155.09	126.32
19	A	6007	BCR	C11-C12-C13	9.86	155.34	126.32
19	B	6005	BCR	C11-C12-C13	9.95	155.61	126.32
21	3	3012	CLA	O2D-CGD-CBD	10.05	125.09	111.30
19	A	6011	BCR	C11-C12-C13	10.14	156.16	126.32
21	3	3013	CLA	C2C-C1C-NC	10.18	117.83	110.24
19	B	6011	BCR	C11-C12-C13	10.26	156.52	126.32
19	A	6002	BCR	C11-C12-C13	10.28	156.59	126.32
19	F	6016	BCR	C11-C12-C13	10.40	156.93	126.32
19	G	2011	BCR	C11-C10-C9	10.71	142.67	127.20
21	1	1009	CLA	C2C-C1C-NC	10.76	118.25	110.24
19	F	6014	BCR	C11-C12-C13	10.84	158.21	126.32
19	B	6006	BCR	C11-C12-C13	11.13	159.09	126.32
19	A	6002	BCR	C16-C15-C14	11.14	148.02	123.39
19	B	6004	BCR	C11-C10-C9	11.47	143.77	127.20
19	I	6020	BCR	C16-C15-C14	11.55	148.94	123.39
19	L	6020	BCR	C16-C15-C14	11.60	149.03	123.39
19	B	6006	BCR	C21-C20-C19	11.65	158.65	123.13
19	A	6017	BCR	C16-C15-C14	11.68	149.22	123.39
19	F	6016	BCR	C16-C15-C14	11.84	149.57	123.39
19	L	6019	BCR	C16-C15-C14	11.89	149.69	123.39
19	A	6003	BCR	C16-C15-C14	11.93	149.77	123.39
19	A	6011	BCR	C21-C20-C19	12.23	160.40	123.13
19	L	6019	BCR	C11-C10-C9	12.25	144.90	127.20
19	F	6014	BCR	C16-C15-C14	12.39	150.79	123.39
19	B	6006	BCR	C16-C15-C14	12.45	150.93	123.39
19	L	6020	BCR	C11-C10-C9	12.46	145.19	127.20
19	B	6010	BCR	C21-C20-C19	12.47	161.15	123.13
19	J	6013	BCR	C21-C20-C19	12.49	161.20	123.13
19	B	6004	BCR	C21-C20-C19	12.57	161.45	123.13
19	J	6012	BCR	C11-C10-C9	12.58	145.36	127.20
19	B	6009	BCR	C16-C15-C14	12.60	151.25	123.39
19	F	6016	BCR	C21-C20-C19	12.62	161.61	123.13
19	A	6002	BCR	C11-C10-C9	12.80	145.68	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	6011	BCR	C16-C15-C14	12.86	151.83	123.39
19	A	6002	BCR	C21-C20-C19	12.88	162.38	123.13
19	A	6011	BCR	C11-C10-C9	12.96	145.92	127.20
19	B	6009	BCR	C21-C20-C19	13.01	162.78	123.13
19	G	2011	BCR	C16-C15-C14	13.01	152.16	123.39
19	L	6020	BCR	C21-C20-C19	13.05	162.91	123.13
19	F	6014	BCR	C11-C10-C9	13.19	146.25	127.20
19	F	6014	BCR	C21-C20-C19	13.38	163.92	123.13
19	A	6003	BCR	C11-C10-C9	13.43	146.59	127.20
19	B	6005	BCR	C11-C10-C9	13.43	146.59	127.20
19	B	6010	BCR	C11-C10-C9	13.44	146.61	127.20
19	A	6008	BCR	C21-C20-C19	13.45	164.12	123.13
19	F	6016	BCR	C11-C10-C9	13.47	146.66	127.20
19	A	6007	BCR	C21-C20-C19	13.56	164.47	123.13
19	A	6007	BCR	C11-C10-C9	13.61	146.86	127.20
19	I	6018	BCR	C21-C20-C19	13.62	164.66	123.13
19	B	6011	BCR	C16-C15-C14	13.65	153.58	123.39
19	L	6019	BCR	C21-C20-C19	13.71	164.91	123.13
19	A	6003	BCR	C21-C20-C19	13.74	165.02	123.13
19	I	6020	BCR	C15-C16-C17	13.83	153.97	123.39
19	B	6005	BCR	C15-C16-C17	13.86	154.03	123.39
19	I	6020	BCR	C21-C20-C19	13.86	165.38	123.13
19	I	6020	BCR	C11-C10-C9	13.95	147.34	127.20
19	B	6004	BCR	C16-C15-C14	14.09	154.55	123.39
19	J	6012	BCR	C16-C15-C14	14.25	154.90	123.39
19	G	2011	BCR	C15-C16-C17	14.60	155.67	123.39
19	B	6005	BCR	C21-C20-C19	14.63	167.73	123.13
19	B	6010	BCR	C16-C15-C14	14.74	155.99	123.39
19	A	6008	BCR	C16-C15-C14	14.79	156.10	123.39
19	G	2011	BCR	C21-C20-C19	14.79	168.23	123.13
19	A	6017	BCR	C21-C20-C19	14.94	168.66	123.13
19	J	6012	BCR	C15-C16-C17	15.06	156.69	123.39
19	B	6006	BCR	C11-C10-C9	15.31	149.32	127.20
19	I	6018	BCR	C16-C15-C14	15.32	157.26	123.39
19	B	6010	BCR	C15-C16-C17	15.56	157.81	123.39
19	J	6013	BCR	C15-C16-C17	15.57	157.81	123.39
19	J	6013	BCR	C16-C15-C14	15.59	157.87	123.39
19	A	6007	BCR	C16-C15-C14	15.70	158.11	123.39
19	B	6011	BCR	C11-C10-C9	15.91	150.18	127.20
19	J	6013	BCR	C11-C10-C9	15.93	150.21	127.20
19	A	6017	BCR	C10-C11-C12	15.98	171.84	123.13
19	B	6005	BCR	C16-C15-C14	16.04	158.87	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	6011	BCR	C15-C16-C17	16.12	159.04	123.39
19	A	6008	BCR	C10-C11-C12	16.20	172.50	123.13
19	B	6011	BCR	C15-C16-C17	16.62	160.15	123.39
19	B	6004	BCR	C15-C16-C17	16.67	160.25	123.39
19	B	6006	BCR	C10-C11-C12	16.72	174.10	123.13
19	B	6009	BCR	C10-C11-C12	16.75	174.18	123.13
19	B	6004	BCR	C10-C11-C12	16.76	174.22	123.13
19	A	6008	BCR	C15-C16-C17	16.76	160.46	123.39
19	I	6018	BCR	C10-C11-C12	16.80	174.36	123.13
19	J	6013	BCR	C10-C11-C12	16.85	174.49	123.13
19	J	6012	BCR	C10-C11-C12	16.89	174.61	123.13
19	A	6017	BCR	C15-C16-C17	16.89	160.75	123.39
19	A	6003	BCR	C10-C11-C12	17.02	175.02	123.13
19	A	6011	BCR	C10-C11-C12	17.06	175.13	123.13
19	F	6016	BCR	C10-C11-C12	17.11	175.29	123.13
19	I	6018	BCR	C15-C16-C17	17.13	161.28	123.39
19	A	6007	BCR	C10-C11-C12	17.20	175.57	123.13
19	B	6010	BCR	C10-C11-C12	17.26	175.75	123.13
19	B	6005	BCR	C10-C11-C12	17.26	175.76	123.13
19	I	6020	BCR	C10-C11-C12	17.53	176.57	123.13
19	A	6002	BCR	C10-C11-C12	17.63	176.86	123.13
19	B	6006	BCR	C15-C16-C17	17.68	162.49	123.39
19	F	6014	BCR	C10-C11-C12	17.83	177.49	123.13
19	G	2011	BCR	C20-C21-C22	17.84	152.97	127.20
19	A	6017	BCR	C20-C21-C22	17.90	153.05	127.20
19	F	6016	BCR	C15-C16-C17	18.07	163.35	123.39
19	B	6005	BCR	C20-C21-C22	18.11	153.36	127.20
19	L	6020	BCR	C10-C11-C12	18.29	178.89	123.13
19	B	6009	BCR	C15-C16-C17	18.41	164.11	123.39
19	B	6011	BCR	C10-C11-C12	18.50	179.53	123.13
19	L	6019	BCR	C10-C11-C12	18.56	179.71	123.13
19	G	2011	BCR	C10-C11-C12	18.62	179.90	123.13
19	A	6007	BCR	C15-C16-C17	18.70	164.75	123.39
19	A	6003	BCR	C16-C17-C18	18.78	154.32	127.20
19	I	6018	BCR	C20-C21-C22	18.82	154.38	127.20
19	F	6014	BCR	C15-C16-C17	18.82	165.02	123.39
19	L	6019	BCR	C15-C16-C17	18.84	165.05	123.39
19	L	6020	BCR	C15-C16-C17	19.06	165.53	123.39
19	A	6007	BCR	C16-C17-C18	19.10	154.78	127.20
19	L	6019	BCR	C16-C17-C18	19.10	154.78	127.20
19	A	6003	BCR	C20-C21-C22	19.11	154.79	127.20
19	A	6003	BCR	C15-C16-C17	19.24	165.94	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	6002	BCR	C15-C16-C17	19.40	166.30	123.39
19	L	6019	BCR	C20-C21-C22	19.47	155.32	127.20
19	L	6020	BCR	C16-C17-C18	19.72	155.68	127.20
19	A	6002	BCR	C16-C17-C18	19.73	155.70	127.20
19	A	6007	BCR	C20-C21-C22	19.85	155.87	127.20
19	I	6020	BCR	C20-C21-C22	19.85	155.87	127.20
19	A	6008	BCR	C20-C21-C22	19.91	155.96	127.20
19	L	6020	BCR	C20-C21-C22	20.13	156.28	127.20
19	B	6009	BCR	C20-C21-C22	20.16	156.32	127.20
19	B	6009	BCR	C16-C17-C18	20.45	156.73	127.20
19	F	6014	BCR	C20-C21-C22	20.53	156.84	127.20
19	B	6004	BCR	C16-C17-C18	20.54	156.86	127.20
19	F	6014	BCR	C16-C17-C18	20.57	156.91	127.20
19	B	6004	BCR	C20-C21-C22	20.68	157.06	127.20
19	A	6008	BCR	C16-C17-C18	20.93	157.43	127.20
19	F	6016	BCR	C20-C21-C22	20.95	157.45	127.20
19	B	6006	BCR	C16-C17-C18	21.24	157.87	127.20
19	J	6013	BCR	C20-C21-C22	22.02	159.00	127.20
19	B	6010	BCR	C20-C21-C22	22.12	159.14	127.20
19	F	6016	BCR	C16-C17-C18	22.16	159.20	127.20
19	J	6013	BCR	C16-C17-C18	22.33	159.45	127.20
19	A	6011	BCR	C16-C17-C18	22.35	159.49	127.20
19	I	6018	BCR	C16-C17-C18	22.35	159.49	127.20
19	A	6011	BCR	C20-C21-C22	23.49	161.12	127.20
19	B	6006	BCR	C20-C21-C22	24.09	161.98	127.20
19	A	6002	BCR	C20-C21-C22	24.72	162.91	127.20
19	B	6010	BCR	C16-C17-C18	25.30	163.74	127.20
19	A	6017	BCR	C16-C17-C18	25.86	164.54	127.20
19	I	6020	BCR	C16-C17-C18	27.03	166.24	127.20
19	G	2011	BCR	C16-C17-C18	27.32	166.66	127.20
19	B	6005	BCR	C16-C17-C18	28.37	168.17	127.20
19	J	6012	BCR	C20-C21-C22	28.70	168.65	127.20
19	J	6012	BCR	C16-C17-C18	29.97	170.48	127.20
19	B	6011	BCR	C16-C17-C18	30.86	159.60	127.42

All (457) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	4	4010	CLA	NC
21	4	4010	CLA	ND
21	4	4010	CLA	NA
21	B	1203	CLA	ND

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Mol	Chain	Res	Type	Atom
21	B	1203	CLA	NA
21	4	4004	CLA	NC
21	4	4004	CLA	ND
21	4	4004	CLA	NA
21	B	1206	CLA	NC
21	B	1206	CLA	ND
21	B	1206	CLA	NA
21	A	1136	CLA	NC
21	A	1136	CLA	ND
21	A	1136	CLA	NA
21	B	1215	CLA	NC
21	B	1215	CLA	ND
21	B	1215	CLA	NA
21	A	1139	CLA	NC
21	A	1139	CLA	ND
21	A	1139	CLA	NA
21	G	1001	CLA	NC
21	G	1001	CLA	ND
21	G	1001	CLA	NA
21	2	2004	CLA	NC
21	2	2004	CLA	ND
21	2	2004	CLA	NA
21	4	4014	CLA	NC
21	4	4014	CLA	ND
21	4	4014	CLA	NA
21	B	1211	CLA	NC
21	B	1211	CLA	ND
21	B	1211	CLA	NA
21	A	1114	CLA	ND
21	A	1114	CLA	NA
21	A	1141	CLA	NC
21	A	1141	CLA	ND
21	A	1141	CLA	NA
21	A	1122	CLA	NC
21	A	1122	CLA	ND
21	A	1122	CLA	NA
21	B	1227	CLA	NC
21	B	1227	CLA	ND
21	B	1227	CLA	NA
21	B	1231	CLA	NC
21	B	1231	CLA	ND
21	B	1231	CLA	NA

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Mol	Chain	Res	Type	Atom
21	J	6014	CLA	NC
21	J	6014	CLA	ND
21	J	6014	CLA	NA
21	A	1127	CLA	NC
21	A	1127	CLA	ND
21	A	1127	CLA	NA
21	3	3005	CLA	ND
21	3	3005	CLA	NA
26	4	4502	LUT	C26
21	2	2012	CLA	NC
21	2	2012	CLA	ND
21	2	2012	CLA	NA
21	B	1218	CLA	NC
21	B	1218	CLA	ND
21	B	1218	CLA	NA
21	B	1230	CLA	NC
21	B	1230	CLA	ND
21	B	1230	CLA	NA
21	B	1240	CLA	NC
21	B	1240	CLA	ND
21	B	1240	CLA	NA
21	3	3015	CLA	NC
21	3	3015	CLA	ND
21	3	3015	CLA	NA
21	1	1003	CLA	NC
21	1	1003	CLA	ND
21	1	1003	CLA	NA
21	A	1121	CLA	NC
21	A	1121	CLA	ND
21	A	1121	CLA	NA
21	A	1101	CLA	ND
21	A	1101	CLA	NA
21	3	3010	CLA	NC
21	3	3010	CLA	ND
21	3	3010	CLA	NA
21	A	1108	CLA	NC
21	A	1108	CLA	ND
21	A	1108	CLA	NA
21	3	3004	CLA	NC
21	3	3004	CLA	ND
21	3	3004	CLA	NA
21	A	1117	CLA	NC

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Mol	Chain	Res	Type	Atom
21	A	1117	CLA	ND
21	A	1117	CLA	NA
21	A	1123	CLA	ND
21	A	1123	CLA	NA
21	B	1204	CLA	NC
21	B	1204	CLA	ND
21	B	1204	CLA	NA
21	A	1126	CLA	ND
21	A	1126	CLA	NA
21	A	1102	CLA	NC
21	A	1102	CLA	ND
21	A	1102	CLA	NA
21	A	1107	CLA	NC
21	A	1107	CLA	ND
21	A	1107	CLA	NA
21	3	3008	CLA	NC
21	3	3008	CLA	ND
21	3	3008	CLA	NA
21	1	1010	CLA	NC
21	1	1010	CLA	ND
21	1	1010	CLA	NA
21	A	1124	CLA	NC
21	A	1124	CLA	ND
21	A	1124	CLA	NA
21	3	3017	CLA	NC
21	3	3017	CLA	ND
21	3	3017	CLA	NA
21	H	1000	CLA	ND
21	H	1000	CLA	NA
21	2	2007	CLA	NC
21	2	2007	CLA	ND
21	2	2007	CLA	NA
21	4	4006	CLA	NC
21	4	4006	CLA	ND
21	4	4006	CLA	NA
21	B	1226	CLA	NC
21	B	1226	CLA	ND
21	B	1226	CLA	NA
21	A	1134	CLA	NC
21	A	1134	CLA	ND
21	A	1134	CLA	NA
21	3	3003	CLA	NC

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Mol	Chain	Res	Type	Atom
21	3	3003	CLA	ND
21	3	3003	CLA	NA
21	B	1239	CLA	NC
21	B	1239	CLA	ND
21	B	1239	CLA	NA
21	B	1229	CLA	NC
21	B	1229	CLA	ND
21	B	1229	CLA	NA
21	1	1012	CLA	NC
21	1	1012	CLA	ND
21	1	1012	CLA	NA
21	2	2006	CLA	NC
21	2	2006	CLA	ND
21	2	2006	CLA	NA
21	4	4005	CLA	NC
21	4	4005	CLA	ND
21	4	4005	CLA	NA
26	2	2502	LUT	C26
21	4	4009	CLA	NC
21	4	4009	CLA	ND
21	4	4009	CLA	NA
21	A	1132	CLA	NC
21	A	1132	CLA	ND
21	A	1132	CLA	NA
21	A	1116	CLA	ND
21	A	1116	CLA	NA
21	L	1503	CLA	NC
21	L	1503	CLA	ND
21	L	1503	CLA	NA
21	F	1301	CLA	NC
21	F	1301	CLA	ND
21	F	1301	CLA	NA
21	3	3001	CLA	NC
21	3	3001	CLA	NA
21	3	3001	CLA	ND
21	A	1130	CLA	NC
21	A	1130	CLA	ND
21	A	1130	CLA	NA
21	B	1237	CLA	NC
21	B	1237	CLA	ND
21	B	1237	CLA	NA
21	A	1110	CLA	NC

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Mol	Chain	Res	Type	Atom
21	A	1110	CLA	ND
21	A	1110	CLA	NA
21	3	3012	CLA	NC
21	3	3012	CLA	ND
21	3	3012	CLA	NA
21	A	1137	CLA	NC
21	A	1137	CLA	ND
21	A	1137	CLA	NA
21	2	2011	CLA	NC
21	2	2011	CLA	ND
21	2	2011	CLA	NA
21	4	4015	CLA	NC
21	4	4015	CLA	ND
21	4	4015	CLA	NA
21	B	1213	CLA	NC
21	B	1213	CLA	ND
21	B	1213	CLA	NA
21	B	9010	CLA	NC
21	B	9010	CLA	ND
21	B	9010	CLA	NA
21	A	1142	CLA	NC
21	A	1142	CLA	ND
21	A	1142	CLA	NA
21	A	9012	CLA	NC
21	A	9012	CLA	ND
21	A	9012	CLA	NA
21	B	1220	CLA	NC
21	B	1220	CLA	ND
21	B	1220	CLA	NA
21	A	1104	CLA	ND
21	A	1104	CLA	NA
21	1	1008	CLA	NC
21	1	1008	CLA	ND
21	1	1008	CLA	NA
21	1	1001	CLA	NC
21	1	1001	CLA	ND
21	1	1001	CLA	NA
21	4	4012	CLA	NC
21	4	4012	CLA	ND
21	4	4012	CLA	NA
21	F	1302	CLA	ND
21	F	1302	CLA	NA

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Mol	Chain	Res	Type	Atom
21	3	3011	CLA	NC
21	3	3011	CLA	ND
21	3	3011	CLA	NA
21	A	1105	CLA	NC
21	A	1105	CLA	ND
21	A	1105	CLA	NA
21	3	3013	CLA	NC
21	3	3013	CLA	ND
21	3	3013	CLA	NA
21	B	1225	CLA	NC
21	B	1225	CLA	ND
21	B	1225	CLA	NA
21	4	4007	CLA	NC
21	4	4007	CLA	ND
21	4	4007	CLA	NA
21	2	2001	CLA	NC
21	2	2001	CLA	ND
21	2	2001	CLA	NA
21	3	3016	CLA	NC
21	3	3016	CLA	ND
21	3	3016	CLA	NA
21	A	1138	CLA	NC
21	A	1138	CLA	ND
21	A	1138	CLA	NA
21	A	1109	CLA	NC
21	A	1109	CLA	ND
21	A	1109	CLA	NA
21	1	1011	CLA	NC
21	1	1011	CLA	ND
21	1	1011	CLA	NA
21	3	3014	CLA	ND
21	3	3014	CLA	NA
21	1	1014	CLA	NC
21	1	1014	CLA	ND
21	1	1014	CLA	NA
21	B	1208	CLA	NC
21	B	1208	CLA	ND
21	B	1208	CLA	NA
21	A	1113	CLA	ND
21	A	1113	CLA	NA
26	2	2501	LUT	C26
21	B	1202	CLA	NC

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Mol	Chain	Res	Type	Atom
21	B	1202	CLA	NA
21	B	1202	CLA	ND
21	2	2008	CLA	NC
21	2	2008	CLA	ND
21	2	2008	CLA	NA
21	1	1005	CLA	NC
21	1	1005	CLA	ND
21	1	1005	CLA	NA
21	B	1209	CLA	NC
21	B	1209	CLA	ND
21	B	1209	CLA	NA
21	A	1133	CLA	NC
21	A	1133	CLA	ND
21	A	1133	CLA	NA
21	A	1118	CLA	NC
21	A	1118	CLA	ND
21	A	1118	CLA	NA
21	A	1112	CLA	NC
21	A	1112	CLA	ND
21	A	1112	CLA	NA
21	B	1221	CLA	NC
21	B	1221	CLA	ND
21	B	1221	CLA	NA
23	A	9011	CL0	NC
23	A	9011	CL0	ND
23	A	9011	CL0	NA
21	B	1210	CLA	NC
21	B	1210	CLA	ND
21	B	1210	CLA	NA
21	4	4003	CLA	NC
21	4	4003	CLA	ND
21	4	4003	CLA	NA
21	F	1303	CLA	NC
21	F	1303	CLA	ND
21	F	1303	CLA	NA
21	2	2002	CLA	NC
21	2	2002	CLA	ND
21	2	2002	CLA	NA
21	4	4008	CLA	NC
21	4	4008	CLA	ND
21	4	4008	CLA	NA
21	1	1002	CLA	NC

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Mol	Chain	Res	Type	Atom
21	1	1002	CLA	ND
21	1	1002	CLA	NA
21	4	4011	CLA	NC
21	4	4011	CLA	ND
21	4	4011	CLA	NA
21	1	1007	CLA	NC
21	1	1007	CLA	ND
21	1	1007	CLA	NA
21	B	9022	CLA	NC
21	B	9022	CLA	ND
21	B	9022	CLA	NA
21	A	1143	CLA	NC
21	A	1143	CLA	ND
21	A	1143	CLA	NA
21	B	1235	CLA	NC
21	B	1235	CLA	ND
21	B	1235	CLA	NA
21	A	1128	CLA	NC
21	A	1128	CLA	ND
21	A	1128	CLA	NA
21	4	4001	CLA	NC
21	4	4001	CLA	ND
21	4	4001	CLA	NA
21	2	2013	CLA	NC
21	2	2013	CLA	ND
21	2	2013	CLA	NA
21	B	9023	CLA	NC
21	B	9023	CLA	ND
21	B	9023	CLA	NA
21	A	1140	CLA	NC
21	A	1140	CLA	ND
21	A	1140	CLA	NA
21	1	1013	CLA	NC
21	1	1013	CLA	ND
21	1	1013	CLA	NA
21	B	1214	CLA	ND
21	B	1214	CLA	NA
21	3	3002	CLA	ND
21	3	3002	CLA	NA
21	A	1131	CLA	NC
21	A	1131	CLA	ND
21	A	1131	CLA	NA

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Mol	Chain	Res	Type	Atom
21	A	1106	CLA	NC
21	A	1106	CLA	ND
21	A	1106	CLA	NA
21	B	1212	CLA	NC
21	B	1212	CLA	ND
21	B	1212	CLA	NA
21	B	1201	CLA	NC
21	B	1201	CLA	ND
21	B	1201	CLA	NA
21	B	1222	CLA	NC
21	B	1222	CLA	ND
21	B	1222	CLA	NA
21	2	2003	CLA	NC
21	2	2003	CLA	ND
21	2	2003	CLA	NA
21	2	2010	CLA	NC
21	2	2010	CLA	ND
21	2	2010	CLA	NA
21	J	6015	CLA	NC
21	J	6015	CLA	ND
21	J	6015	CLA	NA
21	A	1119	CLA	NC
21	A	1119	CLA	ND
21	A	1119	CLA	NA
21	B	1228	CLA	NC
21	B	1228	CLA	ND
21	B	1228	CLA	NA
21	B	1207	CLA	NC
21	B	1207	CLA	ND
21	B	1207	CLA	NA
21	1	1004	CLA	NC
21	1	1004	CLA	ND
21	1	1004	CLA	NA
21	B	1223	CLA	ND
21	B	1223	CLA	NA
21	2	2009	CLA	NC
21	2	2009	CLA	ND
21	2	2009	CLA	NA
21	1	1009	CLA	NC
21	1	1009	CLA	ND
21	1	1009	CLA	NA
21	L	1502	CLA	NC

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Mol	Chain	Res	Type	Atom
21	L	1502	CLA	ND
21	L	1502	CLA	NA
26	4	4501	LUT	C26
21	G	1002	CLA	NC
21	G	1002	CLA	ND
21	G	1002	CLA	NA
21	B	1236	CLA	ND
21	B	1236	CLA	NA
21	2	2014	CLA	NC
21	2	2014	CLA	ND
21	2	2014	CLA	NA
21	A	1135	CLA	NA
21	A	1115	CLA	NC
21	A	1115	CLA	ND
21	A	1115	CLA	NA
21	A	1111	CLA	ND
21	A	1111	CLA	NA
21	1	1006	CLA	NC
21	1	1006	CLA	ND
21	1	1006	CLA	NA
21	B	1238	CLA	NC
21	B	1238	CLA	ND
21	B	1238	CLA	NA
21	J	1302	CLA	ND
21	J	1302	CLA	NA
21	B	1217	CLA	NC
21	B	1217	CLA	ND
21	B	1217	CLA	NA
21	A	1129	CLA	NC
21	A	1129	CLA	ND
21	A	1129	CLA	NA
21	L	1501	CLA	NC
21	L	1501	CLA	ND
21	L	1501	CLA	NA
21	2	2005	CLA	NC
21	2	2005	CLA	ND
21	2	2005	CLA	NA
21	4	4002	CLA	NC
21	4	4002	CLA	ND
21	4	4002	CLA	NA
21	4	4013	CLA	NC
21	4	4013	CLA	ND

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Mol	Chain	Res	Type	Atom
21	4	4013	CLA	NA
21	B	1216	CLA	NC
21	B	1216	CLA	ND
21	B	1216	CLA	NA
21	B	1219	CLA	NC
21	B	1219	CLA	ND
21	B	1219	CLA	NA
21	A	1125	CLA	NC
21	A	1125	CLA	ND
21	A	1125	CLA	NA
26	1	1502	LUT	C26
21	A	1120	CLA	NC
21	A	1120	CLA	ND
21	A	1120	CLA	NA
21	3	3009	CLA	NC
21	3	3009	CLA	ND
21	3	3009	CLA	NA
21	B	1224	CLA	ND
21	B	1224	CLA	NA
21	A	1103	CLA	ND
21	A	1103	CLA	NA
21	3	3006	CLA	NC
21	3	3006	CLA	ND
21	3	3006	CLA	NA
26	1	1501	LUT	C26
21	B	1234	CLA	ND
21	B	1234	CLA	NA
21	A	9013	CLA	NC
21	A	9013	CLA	ND
21	A	9013	CLA	NA
21	B	1205	CLA	NC
21	B	1205	CLA	ND
21	B	1205	CLA	NA

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B	6004	BCR	C10-C11-C12-C13
19	G	2011	BCR	C10-C11-C12-C13
27	4	4503	NEX	C34-C35-C15-C14
26	2	2502	LUT	C28-C27-C26-C21
19	B	6005	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	B	6005	BCR	C11-C10-C9-C34
25	G	2021	LMG	C7-O1-C1-O6
21	A	1141	CLA	CGA-O2A-C1-C2
21	2	2002	CLA	CGA-O2A-C1-C2
21	2	2006	CLA	CGA-O2A-C1-C2
21	2	2007	CLA	CED-O2D-CGD-CBD
21	2	2012	CLA	CED-O2D-CGD-CBD
20	2	2801	LHG	C5-O7-C7-O9
20	2	2801	LHG	C5-O7-C7-C8
21	3	3012	CLA	CED-O2D-CGD-CBD

There are no ring outliers.

190 monomers are involved in 2349 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	1	1001	CLA	72	0
21	1	1002	CLA	71	0
21	1	1003	CLA	52	0
21	1	1004	CLA	29	0
21	1	1005	CLA	20	0
21	1	1006	CLA	61	0
21	1	1007	CLA	22	0
21	1	1008	CLA	26	0
21	1	1009	CLA	72	0
21	1	1010	CLA	28	0
21	1	1011	CLA	19	0
21	1	1012	CLA	25	0
21	1	1013	CLA	69	0
21	1	1014	CLA	29	0
26	1	1501	LUT	51	0
26	1	1502	LUT	61	0
20	1	1801	LHG	41	0
21	2	2001	CLA	19	0
21	2	2002	CLA	49	0
21	2	2003	CLA	41	0
21	2	2004	CLA	36	0
21	2	2005	CLA	24	0
21	2	2006	CLA	23	0
21	2	2007	CLA	8	0
21	2	2008	CLA	21	0
21	2	2009	CLA	25	0
21	2	2010	CLA	20	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	2011	CLA	22	0
21	2	2012	CLA	26	0
21	2	2013	CLA	22	0
21	2	2014	CLA	15	0
26	2	2501	LUT	65	0
26	2	2502	LUT	24	0
20	2	2801	LHG	23	0
21	3	3001	CLA	25	0
21	3	3002	CLA	3	0
21	3	3003	CLA	12	0
21	3	3005	CLA	4	0
21	3	3006	CLA	3	0
21	3	3008	CLA	18	0
21	3	3009	CLA	22	0
21	3	3010	CLA	17	0
21	3	3011	CLA	35	0
21	3	3012	CLA	35	0
21	3	3013	CLA	15	0
21	3	3014	CLA	4	0
21	3	3017	CLA	5	0
21	4	4001	CLA	53	0
21	4	4002	CLA	46	0
21	4	4003	CLA	38	0
21	4	4004	CLA	46	0
21	4	4005	CLA	48	0
21	4	4006	CLA	20	0
21	4	4007	CLA	15	0
21	4	4008	CLA	29	0
21	4	4009	CLA	11	0
21	4	4010	CLA	10	0
21	4	4011	CLA	21	0
21	4	4012	CLA	32	0
21	4	4013	CLA	16	0
21	4	4014	CLA	32	0
21	4	4015	CLA	18	0
26	4	4501	LUT	41	0
26	4	4502	LUT	54	0
27	4	4503	NEX	43	0
21	A	1101	CLA	7	0
21	A	1102	CLA	7	0
21	A	1103	CLA	7	0
21	A	1104	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1105	CLA	2	0
21	A	1106	CLA	11	0
21	A	1107	CLA	7	0
21	A	1108	CLA	4	0
21	A	1109	CLA	9	0
21	A	1110	CLA	3	0
21	A	1111	CLA	6	0
21	A	1112	CLA	3	0
21	A	1113	CLA	1	0
21	A	1114	CLA	3	0
21	A	1115	CLA	7	0
21	A	1116	CLA	3	0
21	A	1117	CLA	7	0
21	A	1118	CLA	4	0
21	A	1119	CLA	3	0
21	A	1120	CLA	2	0
21	A	1121	CLA	1	0
21	A	1122	CLA	7	0
21	A	1123	CLA	8	0
21	A	1124	CLA	9	0
21	A	1125	CLA	18	0
21	A	1126	CLA	14	0
21	A	1127	CLA	4	0
21	A	1128	CLA	15	0
21	A	1129	CLA	23	0
21	A	1130	CLA	17	0
21	A	1131	CLA	8	0
21	A	1132	CLA	16	0
21	A	1133	CLA	4	0
21	A	1135	CLA	5	0
21	A	1136	CLA	10	0
21	A	1137	CLA	9	0
21	A	1138	CLA	9	0
21	A	1139	CLA	3	0
21	A	1140	CLA	5	0
21	A	1141	CLA	4	0
18	A	5001	PQN	4	0
19	A	6002	BCR	3	0
19	A	6003	BCR	2	0
19	A	6007	BCR	2	0
19	A	6008	BCR	7	0
19	A	6011	BCR	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	6017	BCR	6	0
20	A	7001	LHG	10	0
20	A	7003	LHG	16	0
23	A	9011	CL0	15	0
21	A	9012	CLA	19	0
21	A	9013	CLA	11	0
21	B	1201	CLA	2	0
21	B	1202	CLA	4	0
21	B	1203	CLA	3	0
21	B	1204	CLA	3	0
21	B	1205	CLA	7	0
21	B	1206	CLA	13	0
21	B	1207	CLA	15	0
21	B	1208	CLA	7	0
21	B	1209	CLA	7	0
21	B	1210	CLA	8	0
21	B	1211	CLA	3	0
21	B	1212	CLA	2	0
21	B	1213	CLA	26	0
21	B	1214	CLA	6	0
21	B	1215	CLA	4	0
21	B	1216	CLA	5	0
21	B	1217	CLA	5	0
21	B	1218	CLA	2	0
21	B	1219	CLA	7	0
21	B	1220	CLA	10	0
21	B	1221	CLA	7	0
21	B	1222	CLA	7	0
21	B	1223	CLA	5	0
21	B	1224	CLA	8	0
21	B	1225	CLA	8	0
21	B	1226	CLA	11	0
21	B	1227	CLA	26	0
21	B	1228	CLA	8	0
21	B	1229	CLA	10	0
21	B	1230	CLA	5	0
21	B	1231	CLA	3	0
21	B	1234	CLA	6	0
21	B	1235	CLA	8	0
21	B	1236	CLA	4	0
21	B	1237	CLA	1	0
21	B	1238	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	1239	CLA	13	0
21	B	1240	CLA	21	0
18	B	5002	PQN	6	0
19	B	6004	BCR	8	0
19	B	6005	BCR	4	0
19	B	6006	BCR	5	0
19	B	6009	BCR	5	0
19	B	6010	BCR	2	0
19	B	6011	BCR	1	0
20	B	7004	LHG	16	0
24	B	7101	DGD	4	0
21	B	9010	CLA	21	0
21	B	9022	CLA	9	0
21	B	9023	CLA	13	0
21	F	1301	CLA	3	0
21	F	1302	CLA	3	0
21	F	1303	CLA	21	0
19	F	6014	BCR	6	0
19	F	6016	BCR	8	0
21	G	1001	CLA	16	0
21	G	1002	CLA	44	0
19	G	2011	BCR	14	0
25	G	2021	LMG	12	0
21	H	1000	CLA	5	0
19	I	6018	BCR	10	0
19	I	6020	BCR	4	0
21	J	1302	CLA	1	0
25	J	5001	LMG	3	0
19	J	6012	BCR	5	0
19	J	6013	BCR	3	0
21	J	6014	CLA	4	0
21	J	6015	CLA	11	0
21	L	1501	CLA	25	0
21	L	1502	CLA	8	0
21	L	1503	CLA	18	0
19	L	6019	BCR	19	0
19	L	6020	BCR	16	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	721/721 (100%)	0.21	44 (6%) 25 9	34, 73, 146, 307	0
2	B	731/731 (100%)	0.01	37 (5%) 32 12	30, 58, 139, 288	0
3	C	80/80 (100%)	-0.04	2 (2%) 61 30	42, 62, 98, 112	0
4	D	137/137 (100%)	0.48	19 (13%) 4 1	52, 80, 137, 204	0
5	E	63/63 (100%)	0.99	12 (19%) 2 1	42, 86, 124, 170	0
6	F	152/152 (100%)	-0.22	4 (2%) 59 29	44, 73, 135, 225	0
7	G	84/84 (100%)	-0.22	1 (1%) 81 55	63, 98, 122, 147	0
8	H	82/82 (100%)	0.51	8 (9%) 10 4	57, 97, 150, 184	0
9	I	26/26 (100%)	0.32	0 100 100	47, 68, 91, 112	0
10	J	40/40 (100%)	-0.59	0 100 100	47, 69, 110, 138	0
11	K	66/72 (91%)	4.26	43 (65%) 0 0	171, 246, 287, 303	0
12	L	163/163 (100%)	-0.13	5 (3%) 52 24	51, 79, 157, 195	0
13	N	85/85 (100%)	2.62	44 (51%) 0 0	177, 229, 289, 321	0
14	1	171/182 (93%)	0.40	19 (11%) 7 3	63, 103, 176, 315	0
15	2	146/199 (73%)	0.91	33 (22%) 1 1	74, 125, 214, 316	0
16	3	151/275 (54%)	1.55	45 (29%) 1 0	109, 193, 274, 335	0
17	4	196/196 (100%)	0.21	12 (6%) 25 9	59, 93, 182, 301	0
All	All	3094/3288 (94%)	0.39	328 (10%) 8 3	30, 80, 228, 335	0

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	102	THR	20.2
14	1	152	GLU	16.4
16	3	265	VAL	15.3
1	A	43	THR	15.1

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Mol	Chain	Res	Type	RSRZ
15	2	76	THR	14.7
1	A	42	ARG	13.4
13	N	115	ALA	12.8
17	4	123	ASN	12.4
11	K	62	THR	11.4
15	2	75	SER	11.4
13	N	170	TRP	11.1
2	B	486	LEU	10.9
11	K	65	LEU	10.5
11	K	60	SER	10.2
2	B	487	ASN	9.7
16	3	264	PRO	9.6
2	B	488	ALA	9.4
15	2	249	GLY	9.3
11	K	63	LEU	9.3
11	K	103	LEU	9.1
16	3	154	ALA	8.9
2	B	483	SER	8.8
11	K	59	ALA	8.8
11	K	100	GLY	8.7
13	N	116	ARG	8.6
14	1	222	TRP	8.4
11	K	101	PHE	8.3
13	N	110	SER	8.3
16	3	226	LEU	8.3
15	2	131	THR	8.1
15	2	74	GLY	8.0
11	K	56	ILE	8.0
11	K	68	GLY	7.9
13	N	129	GLU	7.8
11	K	55	VAL	7.7
13	N	114	PHE	7.7
16	3	259	ASP	7.6
13	N	134	CYS	7.6
11	K	64	MET	7.6
14	1	103	GLY	7.3
11	K	77	ASN	7.3
16	3	223	GLU	7.3
2	B	214	ASP	7.1
13	N	125	CYS	6.9
17	4	193	PRO	6.8
1	A	630	ASP	6.7

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Mol	Chain	Res	Type	RSRZ
13	N	144	PRO	6.7
11	K	53	THR	6.7
14	1	114	LEU	6.6
16	3	250	GLY	6.6
13	N	169	LYS	6.5
2	B	480	SER	6.5
11	K	111	THR	6.5
2	B	482	ASN	6.4
1	A	160	SER	6.3
16	3	263	ASP	6.3
13	N	113	ASN	6.3
11	K	47	ASP	6.3
17	4	124	VAL	6.1
11	K	116	ILE	6.0
16	3	151	ASN	6.0
13	N	136	ASP	6.0
16	3	93	THR	5.9
2	B	470	THR	5.8
15	2	64	ALA	5.7
11	K	107	LEU	5.6
5	E	67	GLY	5.5
11	K	104	ALA	5.5
13	N	126	LYS	5.4
14	1	151	MET	5.3
11	K	58	VAL	5.2
16	3	210	ASN	5.2
11	K	52	SER	5.2
17	4	120	GLY	5.0
13	N	128	PRO	5.0
15	2	127	PRO	4.9
16	3	202	ALA	4.9
2	B	489	GLY	4.9
16	3	225	LYS	4.9
16	3	249	THR	4.8
16	3	256	ASN	4.8
4	D	76	ASP	4.8
13	N	108	ALA	4.7
13	N	127	PHE	4.7
11	K	106	THR	4.7
15	2	247	TYR	4.6
1	A	352	THR	4.6
11	K	70	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
16	3	220	SER	4.6
13	N	141	LYS	4.6
1	A	257	GLN	4.6
4	D	81	SER	4.5
11	K	112	VAL	4.5
16	3	211	PRO	4.4
11	K	51	SER	4.4
15	2	63	VAL	4.4
1	A	41	SER	4.4
16	3	222	LYS	4.4
11	K	105	ASP	4.4
15	2	69	PRO	4.4
13	N	130	ASN	4.3
2	B	502	ASN	4.3
2	B	210	ASN	4.3
2	B	478	LEU	4.3
8	H	131	GLY	4.2
13	N	137	LEU	4.2
4	D	183	GLN	4.2
2	B	215	VAL	4.2
15	2	84	SER	4.1
4	D	75	LEU	4.1
16	3	262	ALA	4.1
11	K	54	ASN	4.1
16	3	203	TYR	4.1
14	1	217	HIS	4.1
16	3	252	GLY	4.1
1	A	348	GLU	4.1
13	N	122	PHE	4.1
13	N	100	GLU	4.1
2	B	485	ALA	4.1
14	1	131	LEU	4.0
17	4	196	PHE	4.0
4	D	184	GLY	4.0
15	2	154	ASP	4.0
2	B	492	ILE	4.0
16	3	122	ALA	4.0
13	N	109	THR	3.9
2	B	241	ASN	3.9
16	3	224	LEU	3.9
16	3	209	PHE	3.9
11	K	67	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
4	D	74	GLU	3.9
15	2	248	THR	3.9
5	E	73	LYS	3.9
15	2	77	PRO	3.9
1	A	265	GLY	3.9
1	A	69	SER	3.9
1	A	245	PRO	3.8
15	2	65	GLU	3.8
11	K	48	PHE	3.8
13	N	97	ALA	3.8
2	B	484	PRO	3.7
8	H	135	PRO	3.7
5	E	65	PRO	3.7
11	K	113	GLY	3.7
15	2	83	GLY	3.7
16	3	253	PRO	3.7
1	A	46	LYS	3.7
13	N	87	VAL	3.7
2	B	507	SER	3.6
11	K	89	ARG	3.6
13	N	99	LYS	3.6
11	K	109	CYS	3.6
16	3	149	THR	3.6
2	B	501	ILE	3.6
11	K	61	THR	3.6
13	N	112	ALA	3.6
14	1	150	SER	3.5
15	2	66	PRO	3.5
4	D	156	TYR	3.5
8	H	117	PHE	3.5
13	N	132	THR	3.5
13	N	149	ASP	3.5
11	K	57	MET	3.5
6	F	187	ASP	3.4
16	3	155	ASP	3.4
1	A	628	ILE	3.4
1	A	635	THR	3.4
5	E	72	ALA	3.4
1	A	40	PHE	3.4
1	A	641	ASN	3.3
3	C	34	CYS	3.3
13	N	111	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
16	3	130	GLY	3.3
1	A	244	LEU	3.3
2	B	213	LEU	3.3
13	N	107	LEU	3.3
4	D	127	PRO	3.3
11	K	66	PHE	3.3
7	G	88	ALA	3.2
1	A	629	ASN	3.2
13	N	106	ARG	3.2
1	A	426	THR	3.2
1	A	427	ARG	3.2
16	3	255	GLN	3.2
14	1	147	HIS	3.2
13	N	140	GLN	3.1
4	D	79	THR	3.1
2	B	490	ARG	3.1
11	K	88	ALA	3.1
5	E	66	ILE	3.1
15	2	68	ARG	3.1
15	2	70	LEU	3.1
13	N	117	ALA	3.1
5	E	95	GLN	3.1
15	2	82	ASP	3.1
13	N	162	CYS	3.1
1	A	502	THR	3.1
16	3	178	TRP	3.1
16	3	260	HIS	3.1
2	B	342	GLY	3.1
2	B	211	ASN	3.0
1	A	627	SER	3.0
2	B	475	ASP	3.0
13	N	148	GLU	3.0
2	B	479	SER	3.0
15	2	250	THR	3.0
4	D	73	PRO	3.0
11	K	78	ARG	3.0
6	F	227	VAL	3.0
16	3	204	PRO	3.0
2	B	505	SER	2.9
16	3	153	TRP	2.9
11	K	117	GLY	2.9
15	2	179	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
15	2	91	PHE	2.9
12	L	170	LYS	2.9
14	1	128	TRP	2.9
2	B	321	GLY	2.9
17	4	194	LEU	2.9
16	3	216	LYS	2.9
13	N	143	VAL	2.9
1	A	623	ASP	2.8
14	1	110	GLU	2.8
1	A	423	ASP	2.8
13	N	96	LYS	2.8
15	2	67	ASP	2.8
16	3	219	LYS	2.8
13	N	163	GLY	2.8
4	D	77	PRO	2.8
15	2	242	TRP	2.8
15	2	130	LEU	2.8
17	4	200	LEU	2.8
6	F	228	ALA	2.7
2	B	491	SER	2.7
4	D	78	ASN	2.7
11	K	108	ALA	2.7
16	3	205	GLY	2.7
15	2	155	THR	2.7
2	B	346	SER	2.7
14	1	107	LYS	2.6
5	E	99	THR	2.6
16	3	230	LYS	2.6
2	B	504	ASN	2.6
4	D	166	TYR	2.6
14	1	174	PRO	2.6
8	H	122	SER	2.6
1	A	315	HIS	2.6
13	N	124	THR	2.5
14	1	92	PRO	2.5
16	3	207	PRO	2.5
1	A	506	GLY	2.5
5	E	86	GLY	2.5
2	B	493	TRP	2.5
1	A	250	LEU	2.5
15	2	85	LEU	2.5
17	4	69	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
5	E	74	VAL	2.5
6	F	226	LEU	2.5
8	H	119	THR	2.5
14	1	134	ILE	2.5
16	3	102	LEU	2.5
1	A	326	GLY	2.4
1	A	559	GLY	2.4
5	E	126	GLU	2.4
12	L	52	PRO	2.4
15	2	78	PRO	2.4
1	A	323	ILE	2.4
13	N	93	GLU	2.4
14	1	148	GLN	2.4
15	2	126	ILE	2.4
17	4	192	ASN	2.4
17	4	207	ILE	2.4
4	D	82	PRO	2.4
16	3	156	ASN	2.4
11	K	96	GLY	2.4
4	D	104	THR	2.4
1	A	38	GLY	2.4
4	D	155	PHE	2.4
15	2	246	ILE	2.3
1	A	253	ASP	2.3
16	3	251	VAL	2.3
1	A	505	PRO	2.3
1	A	633	VAL	2.3
8	H	132	PRO	2.3
17	4	195	ASN	2.3
13	N	123	GLY	2.3
1	A	290	LEU	2.3
8	H	118	SER	2.3
1	A	501	GLY	2.3
4	D	171	ASP	2.3
16	3	150	TYR	2.3
1	A	518	GLY	2.3
14	1	153	LYS	2.2
2	B	473	GLY	2.2
1	A	631	GLN	2.2
16	3	248	VAL	2.2
2	B	499	ASN	2.2
11	K	82	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	349	ILE	2.2
14	1	176	LYS	2.2
1	A	67	HIS	2.2
16	3	127	GLY	2.2
4	D	158	VAL	2.1
13	N	95	SER	2.1
12	L	158	PRO	2.1
1	A	339	THR	2.1
15	2	222	GLU	2.1
12	L	169	ARG	2.1
11	K	84	LEU	2.1
14	1	71	GLU	2.1
13	N	145	PHE	2.1
1	A	638	THR	2.1
2	B	481	THR	2.1
16	3	181	PRO	2.1
4	D	167	LEU	2.1
2	B	249	GLY	2.1
5	E	71	GLY	2.1
1	A	44	ILE	2.0
2	B	384	THR	2.0
5	E	94	ASP	2.0
15	2	88	ASP	2.0
1	A	159	THR	2.0
3	C	17	CYS	2.0
12	L	211	TYR	2.0
13	N	168	TRP	2.0
8	H	128	ILE	2.0
17	4	125	PRO	2.0
2	B	477	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	NEX	4	4503	44/44	0.58	0.66	9.28	72,110,128,133	0
19	BCR	J	6013	40/40	0.57	0.60	7.89	119,143,153,153	0
20	LHG	B	7004	49/49	0.88	0.41	7.15	68,98,111,124	0
21	CLA	J	1302	61/65	0.71	0.33	6.49	59,117,149,153	0
21	CLA	1	1013	65/65	0.66	0.70	3.86	94,119,138,148	0
19	BCR	A	6002	40/40	0.73	0.46	3.66	72,103,133,133	0
21	CLA	2	2008	65/65	0.61	0.45	3.62	103,135,158,161	0
19	BCR	A	6007	40/40	0.80	0.33	3.35	69,91,97,98	0
21	CLA	3	3004	45/65	0.55	0.65	3.14	260,267,271,309	0
19	BCR	A	6003	40/40	0.74	0.43	3.14	80,97,123,124	0
21	CLA	4	4007	65/65	0.56	0.39	3.10	103,123,140,244	0
21	CLA	3	3014	45/65	0.53	0.66	2.96	242,261,265,271	0
21	CLA	2	2005	65/65	0.90	0.32	2.92	89,112,126,128	0
21	CLA	4	4005	45/65	0.56	0.32	2.84	107,130,142,144	0
21	CLA	1	1008	65/65	0.89	0.27	2.80	64,84,124,129	0
20	LHG	1	1801	49/49	0.87	0.23	2.67	68,88,119,122	0
26	LUT	1	1502	42/42	0.87	0.34	2.55	65,87,109,118	0
21	CLA	1	1009	65/65	0.79	0.28	2.53	58,78,104,108	0
21	CLA	B	1216	65/65	0.90	0.23	2.47	43,56,94,97	0
21	CLA	A	1110	55/65	0.73	0.37	2.36	129,148,161,166	0
21	CLA	F	1302	46/65	0.90	0.30	2.34	52,85,98,151	0
26	LUT	2	2501	42/42	0.74	0.40	2.32	106,121,131,138	0
19	BCR	I	6020	40/40	0.92	0.26	2.30	44,51,65,75	0
21	CLA	A	1126	65/65	0.88	0.35	2.29	59,79,95,106	0
19	BCR	B	6004	40/40	0.86	0.43	2.23	54,75,81,82	0
21	CLA	B	1240	65/65	0.91	0.28	2.21	42,72,83,97	0
21	CLA	1	1006	47/65	0.56	0.49	2.11	116,133,148,152	0
19	BCR	J	6012	40/40	0.92	0.26	2.10	45,67,98,109	0
21	CLA	B	1206	65/65	0.93	0.27	2.08	38,50,78,84	0
21	CLA	4	4001	65/65	0.80	0.60	1.96	73,91,124,131	0
19	BCR	G	2011	40/40	0.88	0.31	1.91	55,78,120,121	0
20	LHG	A	7001	49/49	0.91	0.31	1.90	47,72,94,97	0
21	CLA	F	1301	45/65	0.91	0.20	1.86	48,63,77,148	0
21	CLA	B	1215	60/65	0.88	0.36	1.85	51,69,81,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	BCR	A	6008	40/40	0.76	0.39	1.84	57,87,105,112	0
19	BCR	B	6009	40/40	0.86	0.31	1.83	30,52,68,73	0
21	CLA	A	1107	51/65	0.85	0.28	1.80	52,74,99,104	0
26	LUT	4	4502	42/42	0.90	0.27	1.75	56,76,84,88	0
21	CLA	4	4012	65/65	0.93	0.22	1.62	54,62,89,107	0
21	CLA	1	1007	55/65	0.91	0.36	1.45	76,100,121,139	0
21	CLA	A	1106	65/65	0.93	0.25	1.40	39,55,76,81	0
18	PQN	B	5002	33/33	0.90	0.31	1.40	41,50,76,79	0
21	CLA	G	1001	55/65	0.89	0.31	1.35	74,93,113,123	0
21	CLA	A	1138	65/65	0.93	0.23	1.33	32,49,60,65	0
19	BCR	L	6019	40/40	0.86	0.35	1.33	40,59,79,87	0
21	CLA	B	1224	65/65	0.90	0.29	1.31	32,54,93,95	0
21	CLA	L	1501	46/65	0.93	0.34	1.30	66,80,103,115	0
21	CLA	A	1117	65/65	0.93	0.38	1.30	59,78,92,123	0
26	LUT	1	1501	42/42	0.86	0.29	1.28	83,94,104,107	0
25	LMG	J	5001	35/55	0.86	0.31	1.27	62,91,103,104	0
21	CLA	B	1212	46/65	0.87	0.49	1.25	64,85,98,109	0
21	CLA	G	1002	46/65	0.84	0.25	1.25	112,128,140,145	0
21	CLA	B	9022	65/65	0.93	0.24	1.17	32,47,62,86	0
21	CLA	F	1303	64/65	0.91	0.29	1.16	52,65,104,149	0
19	BCR	B	6006	40/40	0.78	0.40	1.11	45,63,110,110	0
21	CLA	B	1214	59/65	0.90	0.34	1.09	44,61,102,119	0
23	CL0	A	9011	65/65	0.95	0.24	1.07	30,39,53,73	0
21	CLA	3	3006	65/65	0.51	0.48	1.07	144,177,194,197	0
21	CLA	A	1132	65/65	0.94	0.21	1.04	39,50,80,85	0
21	CLA	B	1236	55/65	0.93	0.25	1.01	51,61,122,125	0
19	BCR	B	6005	40/40	0.79	0.36	1.00	51,69,122,123	0
21	CLA	B	1209	46/65	0.93	0.18	0.98	52,63,84,96	0
18	PQN	A	5001	33/33	0.93	0.28	0.97	38,57,67,71	0
21	CLA	4	4014	45/65	0.83	0.35	0.97	71,105,128,134	0
21	CLA	A	1122	59/65	0.89	0.23	0.97	57,78,98,103	0
21	CLA	A	9012	65/65	0.91	0.26	0.96	36,63,75,78	0
24	DGD	B	7101	61/66	0.87	0.26	0.95	40,70,96,104	0
21	CLA	A	1112	46/65	0.84	0.36	0.93	68,88,99,101	0
21	CLA	A	1137	55/65	0.91	0.33	0.93	63,81,99,106	0
21	CLA	4	4004	65/65	0.88	0.31	0.91	56,81,91,96	0
21	CLA	A	1131	65/65	0.94	0.28	0.89	39,55,72,90	0
21	CLA	A	1111	60/65	0.88	0.26	0.88	60,86,114,117	0
21	CLA	3	3005	45/65	0.65	0.39	0.88	197,209,213,274	0
21	CLA	B	9023	65/65	0.93	0.28	0.87	36,54,62,89	0
21	CLA	3	3003	60/65	0.63	0.55	0.85	190,224,234,252	0
21	CLA	4	4010	50/65	0.87	0.24	0.85	57,93,132,147	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	L	1502	65/65	0.90	0.23	0.84	54,66,88,91	0
21	CLA	2	2007	55/65	0.82	0.36	0.83	113,130,142,149	0
19	BCR	B	6010	40/40	0.80	0.33	0.82	47,67,81,88	0
21	CLA	B	1210	65/65	0.90	0.24	0.81	46,56,73,101	0
21	CLA	B	1220	65/65	0.94	0.23	0.80	32,48,101,106	0
21	CLA	1	1010	65/65	0.74	0.42	0.78	108,123,152,154	0
21	CLA	4	4011	65/65	0.91	0.26	0.78	66,74,104,108	0
21	CLA	2	2013	65/65	0.86	0.27	0.77	91,119,135,146	0
19	BCR	A	6011	40/40	0.89	0.27	0.74	32,48,74,81	0
21	CLA	A	1141	51/65	0.88	0.28	0.73	91,124,133,137	0
21	CLA	A	1109	65/65	0.88	0.30	0.70	81,105,133,147	0
21	CLA	2	2012	65/65	0.91	0.23	0.69	72,88,117,121	0
19	BCR	F	6016	40/40	0.94	0.23	0.69	35,51,76,82	0
21	CLA	A	1139	65/65	0.92	0.20	0.68	33,51,81,88	0
21	CLA	A	1124	55/65	0.87	0.31	0.65	48,60,83,91	0
21	CLA	A	1136	65/65	0.86	0.26	0.63	59,82,108,155	0
21	CLA	B	1229	65/65	0.94	0.22	0.63	36,50,73,85	0
26	LUT	4	4501	42/42	0.76	0.42	0.62	77,95,99,107	0
21	CLA	B	1202	65/65	0.94	0.22	0.62	33,53,71,92	0
19	BCR	A	6017	40/40	0.90	0.29	0.61	34,52,79,93	0
26	LUT	2	2502	42/42	0.83	0.31	0.58	83,99,106,109	0
21	CLA	A	1103	65/65	0.91	0.25	0.58	63,80,90,111	0
21	CLA	A	1127	65/65	0.92	0.32	0.58	52,63,79,85	0
21	CLA	A	1104	65/65	0.92	0.28	0.57	47,69,81,87	0
21	CLA	A	1116	54/65	0.88	0.27	0.54	73,89,105,111	0
21	CLA	B	1234	60/65	0.88	0.29	0.54	39,56,98,104	0
21	CLA	B	1217	46/65	0.93	0.19	0.54	52,70,92,109	0
20	LHG	A	7003	49/49	0.87	0.27	0.52	81,113,121,123	0
21	CLA	A	1135	51/65	0.88	0.29	0.49	47,62,87,88	0
21	CLA	A	1105	51/65	0.92	0.22	0.49	67,81,98,103	0
21	CLA	J	6015	55/65	0.48	0.31	0.49	122,143,159,160	0
21	CLA	B	1230	58/65	0.90	0.23	0.46	38,59,73,77	0
21	CLA	B	1237	60/65	0.90	0.27	0.44	41,60,87,101	0
21	CLA	A	1133	46/65	0.84	0.25	0.42	77,90,112,119	0
21	CLA	1	1004	65/65	0.92	0.19	0.41	57,77,83,113	0
20	LHG	2	2801	36/49	0.79	0.39	0.39	112,132,147,150	0
21	CLA	B	1204	55/65	0.94	0.18	0.35	38,61,77,78	0
21	CLA	1	1003	65/65	0.87	0.19	0.32	53,72,97,108	0
21	CLA	A	1119	65/65	0.87	0.28	0.32	78,91,99,105	0
19	BCR	L	6020	40/40	0.92	0.19	0.32	60,75,82,83	0
21	CLA	B	1201	46/65	0.95	0.21	0.31	34,46,78,91	0
21	CLA	A	1129	50/65	0.86	0.25	0.28	51,83,90,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	BCR	F	6014	40/40	0.93	0.22	0.27	38,56,64,66	0
21	CLA	A	9013	65/65	0.91	0.25	0.26	35,61,71,110	0
21	CLA	2	2011	60/65	0.87	0.17	0.26	80,97,144,158	0
21	CLA	B	1239	65/65	0.93	0.23	0.25	32,47,65,73	0
21	CLA	B	1235	65/65	0.95	0.20	0.23	36,53,68,73	0
21	CLA	A	1128	65/65	0.93	0.24	0.23	44,66,81,96	0
21	CLA	4	4006	65/65	0.53	0.34	0.23	116,133,155,160	0
21	CLA	2	2006	57/65	0.54	0.32	0.22	140,162,183,256	0
21	CLA	B	1227	65/65	0.93	0.20	0.19	39,63,89,92	0
21	CLA	A	1140	65/65	0.93	0.22	0.18	35,50,73,99	0
21	CLA	B	1221	54/65	0.93	0.22	0.16	33,57,71,86	0
21	CLA	A	1130	46/65	0.93	0.21	0.16	48,60,88,109	0
21	CLA	B	1238	65/65	0.92	0.24	0.15	35,51,74,86	0
21	CLA	2	2010	65/65	0.80	0.29	0.15	103,118,134,151	0
21	CLA	1	1001	55/65	0.91	0.23	0.13	81,103,129,170	0
21	CLA	B	1205	65/65	0.95	0.20	0.10	33,46,70,83	0
21	CLA	4	4009	50/65	0.91	0.20	0.09	64,83,103,105	0
21	CLA	B	1208	55/65	0.91	0.22	0.09	49,68,96,99	0
21	CLA	L	1503	50/65	0.87	0.22	0.04	58,77,98,105	0
21	CLA	B	1213	60/65	0.89	0.22	0.00	67,81,103,106	0
21	CLA	A	1123	65/65	0.86	0.29	-0.05	58,84,97,103	0
21	CLA	B	1207	65/65	0.93	0.19	-0.06	40,62,83,98	0
21	CLA	B	1211	65/65	0.91	0.22	-0.09	56,68,81,90	0
21	CLA	B	1225	65/65	0.93	0.23	-0.10	31,46,60,71	0
21	CLA	B	1218	60/65	0.91	0.20	-0.11	54,78,101,102	0
21	CLA	1	1011	65/65	0.87	0.27	-0.12	89,109,115,118	0
21	CLA	2	2003	65/65	0.61	0.31	-0.15	136,144,159,185	0
21	CLA	A	1101	65/65	0.93	0.20	-0.16	43,63,91,95	0
22	SF4	A	8001	8/8	0.96	0.21	-0.17	50,64,71,75	0
21	CLA	B	1226	65/65	0.95	0.23	-0.17	28,43,71,73	0
21	CLA	3	3011	46/65	0.76	0.31	-0.18	131,154,160,195	0
21	CLA	2	2004	59/65	0.87	0.23	-0.18	84,101,110,116	0
21	CLA	1	1012	50/65	0.91	0.22	-0.21	78,95,113,175	0
21	CLA	B	1219	60/65	0.88	0.23	-0.22	50,81,101,103	0
21	CLA	3	3013	50/65	0.73	0.26	-0.25	107,132,148,153	0
21	CLA	A	1134	46/65	0.85	0.28	-0.26	93,103,131,137	0
21	CLA	A	1108	46/65	0.84	0.23	-0.26	103,120,136,146	0
25	LMG	G	2021	23/55	0.62	0.31	-0.30	160,168,177,180	0
21	CLA	B	9010	65/65	0.96	0.19	-0.31	29,39,57,72	0
21	CLA	A	1113	46/65	0.85	0.29	-0.35	95,112,136,139	0
21	CLA	3	3001	65/65	0.67	0.38	-0.40	187,204,220,223	0
21	CLA	4	4008	48/65	0.85	0.16	-0.45	66,92,107,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	CLA	4	4013	51/65	0.92	0.17	-0.45	63,77,101,104	0
21	CLA	A	1118	46/65	0.88	0.26	-0.47	109,118,126,135	0
21	CLA	A	1102	50/65	0.94	0.18	-0.48	43,63,91,95	0
21	CLA	4	4003	65/65	0.89	0.16	-0.53	61,86,100,116	0
21	CLA	B	1222	65/65	0.89	0.30	-0.55	28,47,85,87	0
21	CLA	2	2009	46/65	0.81	0.30	-0.56	82,101,128,141	0
21	CLA	A	1115	56/65	0.86	0.24	-0.59	85,107,132,161	0
21	CLA	B	1203	60/65	0.95	0.20	-0.59	30,43,69,74	0
21	CLA	3	3017	45/65	0.58	0.50	-0.61	224,249,260,262	0
21	CLA	B	1223	65/65	0.92	0.28	-0.61	31,50,60,63	0
21	CLA	3	3012	45/65	0.77	0.18	-0.63	163,196,205,208	0
21	CLA	A	1125	55/65	0.89	0.24	-0.65	54,73,89,99	0
21	CLA	A	1114	46/65	0.88	0.30	-0.73	93,114,120,124	0
21	CLA	B	1231	46/65	0.88	0.24	-0.79	49,76,87,92	0
21	CLA	A	1121	46/65	0.85	0.24	-0.80	103,130,154,160	0
21	CLA	B	1228	51/65	0.95	0.16	-0.83	33,45,66,92	0
21	CLA	2	2001	27/65	0.90	0.15	-0.96	105,120,130,131	0
22	SF4	C	8002	8/8	0.98	0.13	-1.12	53,65,79,92	0
22	SF4	C	8003	8/8	0.98	0.10	-1.25	53,63,89,92	0
21	CLA	1	1014	45/65	0.53	0.69	-	115,160,167,171	0
21	CLA	4	4015	46/65	0.92	0.17	-	51,65,83,108	0
21	CLA	3	3015	45/65	0.32	1.17	-	250,262,271,285	0
21	CLA	A	1143	46/65	0.52	0.92	-	198,214,217,262	0
21	CLA	4	4002	56/65	0.84	0.32	-	76,94,112,128	0
19	BCR	B	6011	25/40	0.71	0.32	-	77,111,118,120	0
21	CLA	J	6014	61/65	0.61	0.25	-	191,215,220,289	0
21	CLA	3	3016	45/65	0.42	0.78	-	172,203,215,248	0
21	CLA	A	1142	44/65	0.57	0.28	-	186,199,202,274	0
28	G3P	4	4505	10/10	0.89	0.24	-	94,125,132,135	0
21	CLA	A	1120	46/65	0.77	0.49	-	97,128,144,149	0
21	CLA	3	3009	46/65	0.81	0.24	-	138,174,190,191	0
21	CLA	2	2014	45/65	0.70	0.24	-	104,135,145,168	0
21	CLA	2	2002	60/65	0.81	0.33	-	112,142,151,201	0
21	CLA	1	1005	56/65	0.92	0.21	-	54,69,80,85	0
19	BCR	I	6018	40/40	0.83	0.30	-	37,61,79,86	0
21	CLA	1	1002	56/65	0.88	0.32	-	101,113,133,140	0
21	CLA	3	3008	65/65	0.72	0.25	-	149,167,183,187	0
21	CLA	H	1000	46/65	0.89	0.39	-	69,106,123,134	0
21	CLA	3	3010	52/65	0.67	0.32	-	115,168,179,182	0
21	CLA	3	3002	55/65	0.75	0.47	-	181,189,204,206	0

6.5 Other polymers [i](#)

There are no such residues in this entry.