



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:37 PM GMT

PDB ID : 4V62
Title : Crystal Structure of cyanobacterial Photosystem II
Authors : Guskov, A.; Gabdulkhakov, A.; Kern, J.; Broser, M.; Zouni, A.; Saenger, W.
Deposited on : 2008-01-17
Resolution : 2.90 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

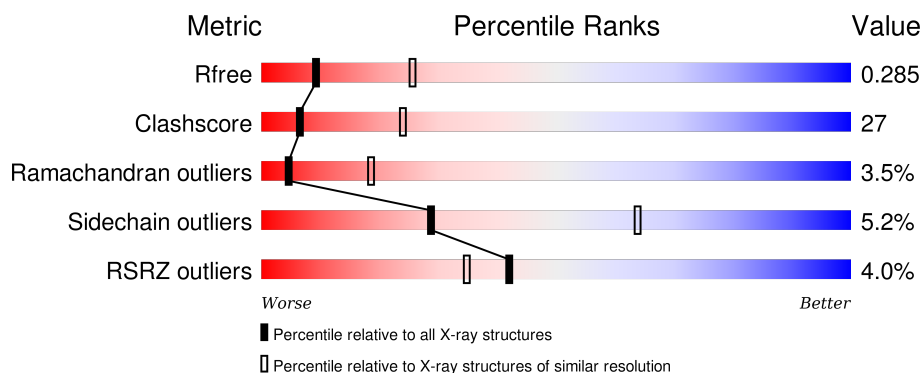
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	AA	344	<div> <div>2%</div> <div>51% 42% . .</div> </div>
1	BA	344	<div> <div>%</div> <div>50% 43% 5% .</div> </div>
2	AB	510	<div> <div>2%</div> <div>56% 35% . . .</div> </div>
2	BB	510	<div> <div>2%</div> <div>55% 36% . . .</div> </div>
3	AC	473	<div> <div>3%</div> <div>45% 43% 6% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	BC	473	
4	AD	352	
4	BD	352	
5	AE	84	
5	BE	84	
6	AF	45	
6	BF	45	
7	AH	66	
7	BH	66	
8	AI	38	
8	BI	38	
9	AJ	40	
9	BJ	40	
10	AK	37	
10	BK	37	
11	AL	37	
11	BL	37	
12	AM	36	
12	BM	36	
13	AO	247	
13	BO	247	
14	AT	32	
14	BT	32	
15	AU	104	
15	BU	104	

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Mol	Chain	Length	Quality of chain
16	AV	137	
16	BV	137	
17	Ay	46	
17	By	46	
18	AX	50	
18	BX	50	
19	AY	28	
19	BY	28	
20	AZ	62	
20	BZ	62	

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
22	CLA	AA	402	X	-	-	-
22	CLA	AA	403	X	-	-	-
22	CLA	AA	404	X	-	-	-
22	CLA	AA	406	X	-	-	X
22	CLA	AB	601	X	-	-	X
22	CLA	AB	602	X	-	-	-
22	CLA	AB	603	X	-	-	-
22	CLA	AB	604	X	-	-	X
22	CLA	AB	605	X	-	-	-
22	CLA	AB	606	X	-	-	-
22	CLA	AB	607	X	-	-	-
22	CLA	AB	608	X	-	-	-
22	CLA	AB	609	X	-	-	X
22	CLA	AB	610	X	-	-	-
22	CLA	AB	611	X	-	-	-
22	CLA	AB	612	X	-	-	-
22	CLA	AB	613	X	-	-	-
22	CLA	AB	614	X	-	-	-
22	CLA	AB	615	X	-	-	-
22	CLA	AB	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	AC	501	X	-	-	-
22	CLA	AC	502	X	-	-	-
22	CLA	AC	503	X	-	-	X
22	CLA	AC	504	X	-	-	X
22	CLA	AC	505	X	-	-	-
22	CLA	AC	506	X	-	-	-
22	CLA	AC	507	X	-	-	X
22	CLA	AC	508	X	-	-	-
22	CLA	AC	509	X	-	-	-
22	CLA	AC	510	X	-	-	-
22	CLA	AC	511	X	-	-	-
22	CLA	AC	512	X	-	-	X
22	CLA	AC	513	X	-	-	-
22	CLA	AD	402	X	-	-	X
22	CLA	AD	404	X	-	-	X
22	CLA	BA	403	X	-	-	-
22	CLA	BA	404	X	-	-	-
22	CLA	BA	405	X	-	-	X
22	CLA	BA	407	X	-	-	X
22	CLA	BB	604	X	-	-	-
22	CLA	BB	605	X	-	-	-
22	CLA	BB	606	X	-	-	-
22	CLA	BB	607	X	-	-	-
22	CLA	BB	608	X	-	-	-
22	CLA	BB	609	X	-	-	-
22	CLA	BB	610	X	-	-	-
22	CLA	BB	611	X	-	-	-
22	CLA	BB	612	X	-	-	X
22	CLA	BB	613	X	-	-	-
22	CLA	BB	614	X	-	-	-
22	CLA	BB	615	X	-	-	-
22	CLA	BB	616	X	-	-	-
22	CLA	BB	617	X	-	-	-
22	CLA	BB	618	X	-	-	-
22	CLA	BB	619	X	-	-	-
22	CLA	BC	501	X	-	-	-
22	CLA	BC	502	X	-	-	-
22	CLA	BC	503	X	-	-	-
22	CLA	BC	504	X	-	-	-
22	CLA	BC	505	X	-	-	-
22	CLA	BC	506	X	-	-	-
22	CLA	BC	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	BC	508	X	-	-	-
22	CLA	BC	509	X	-	-	-
22	CLA	BC	510	X	-	-	-
22	CLA	BC	511	X	-	-	-
22	CLA	BC	512	X	-	-	-
22	CLA	BC	513	X	-	-	X
22	CLA	BD	402	X	-	-	-
22	CLA	BD	404	X	-	-	-
23	PHO	BD	403	-	-	-	X
24	PL9	AA	407	-	-	-	X
24	PL9	AJ	101	-	-	-	X
24	PL9	BA	408	-	-	-	X
24	PL9	BJ	101	-	-	-	X
26	BCR	AH	101	-	-	-	X
26	BCR	AJ	102	-	-	-	X
26	BCR	AK	102	-	-	-	X
26	BCR	AZ	101	-	-	-	X
26	BCR	BJ	102	-	-	-	X
26	BCR	BK	102	-	-	-	X
27	DGD	AA	410	X	-	-	-
27	DGD	AB	626	X	-	-	X
27	DGD	AC	516	X	-	-	-
27	DGD	AC	517	X	-	-	X
27	DGD	AC	518	X	-	-	-
27	DGD	AD	410	X	-	-	X
27	DGD	AH	102	X	-	-	-
27	DGD	BA	411	X	-	-	X
27	DGD	BB	602	X	-	-	X
27	DGD	BC	516	X	-	-	-
27	DGD	BC	517	X	-	-	-
27	DGD	BC	518	X	-	-	-
27	DGD	BD	410	X	-	-	X
27	DGD	BH	101	X	-	-	-
28	LHG	AC	521	-	-	-	X
28	LHG	BC	521	-	-	-	X
29	SQD	AA	415	-	-	-	X
29	SQD	AF	101	-	-	-	X
29	SQD	BA	401	-	-	-	X
29	SQD	BF	101	-	-	-	X
30	LMG	AA	413	X	-	-	-
30	LMG	AA	416	X	-	-	X
30	LMG	AB	621	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	LMG	AB	622	X	-	-	-
30	LMG	AB	623	X	-	-	X
30	LMG	AC	519	X	-	-	-
30	LMG	AC	520	X	-	-	X
30	LMG	AD	407	X	-	-	-
30	LMG	AD	408	X	-	-	X
30	LMG	AE	102	X	-	-	-
30	LMG	AI	101	X	-	-	-
30	LMG	AM	101	X	-	-	-
30	LMG	BA	414	X	-	-	-
30	LMG	BB	623	X	-	-	-
30	LMG	BB	624	X	-	-	-
30	LMG	BC	519	X	-	-	-
30	LMG	BC	520	X	-	-	X
30	LMG	BD	407	X	-	-	X
30	LMG	BD	408	X	-	-	X
30	LMG	BE	102	X	-	-	X
30	LMG	BI	101	X	-	-	-
30	LMG	BM	102	X	-	-	-
31	CL	AA	414	-	-	-	X
31	CL	BA	415	-	-	-	X
32	LMT	AB	625	-	-	-	X
32	LMT	AB	627	-	-	-	X
32	LMT	AD	411	-	-	-	X
32	LMT	AI	102	-	-	-	X
32	LMT	AT	101	-	-	-	X
32	LMT	BD	411	-	-	-	X
32	LMT	BI	102	-	-	-	X
32	LMT	BT	101	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50234 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	BA	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	BB	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

- Molecule 3 is a protein called Photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	BC	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
AC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
AC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
AC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
AC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8

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Chain	Residue	Modelled	Actual	Comment	Reference
AC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
AC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
AC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
AC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8
BC	2	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	3	THR	-	SEE REMARK 999	UNP Q8DIF8
BC	4	LEU	-	SEE REMARK 999	UNP Q8DIF8
BC	5	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	6	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	7	GLN	-	SEE REMARK 999	UNP Q8DIF8
BC	8	LYS	-	SEE REMARK 999	UNP Q8DIF8
BC	9	ARG	-	SEE REMARK 999	UNP Q8DIF8
BC	10	TYR	-	SEE REMARK 999	UNP Q8DIF8
BC	11	SER	-	SEE REMARK 999	UNP Q8DIF8
BC	12	PRO	-	SEE REMARK 999	UNP Q8DIF8
BC	13	VAL	-	SEE REMARK 999	UNP Q8DIF8

- Molecule 4 is a protein called Photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	BD	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	AE	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	BE	82	Total	C	N	O	0	0	0
			666	434	108	124			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	BF	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			
7	BH	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	BI	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	BJ	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	AK	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	BK	37	Total	C	N	O	0	0	0
			293	204	43	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	BL	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	BM	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			
13	BO	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	BT	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AU	97	Total	C	N	O		0	0	0
			774	491	129	154				
15	BU	97	Total	C	N	O		0	0	0
			774	491	129	154				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			
16	BV	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

- Molecule 17 is a protein called Protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Ay	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	By	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

- Molecule 18 is a protein called Photosystem II PsbX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AX	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	BX	37	Total	C	N	O	0	0	0
			270	182	41	47			

- Molecule 19 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	AY	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	BY	28	Total	C	N	O	0	0	0
			140	84	28	28			

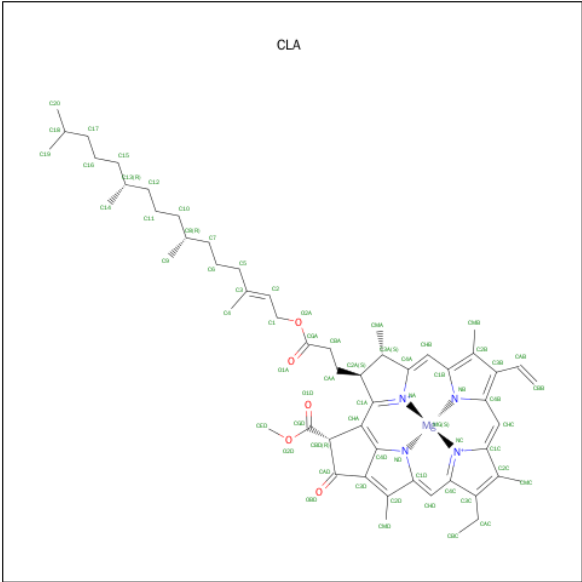
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
20	BZ	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	AA	1	Total	Fe	0	0
			1	1		
21	BA	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AA	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	AB	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	AD	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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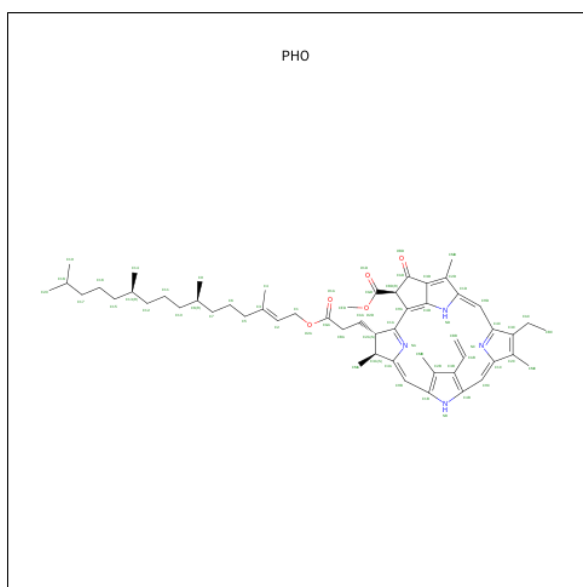
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BA	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BB	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	BC	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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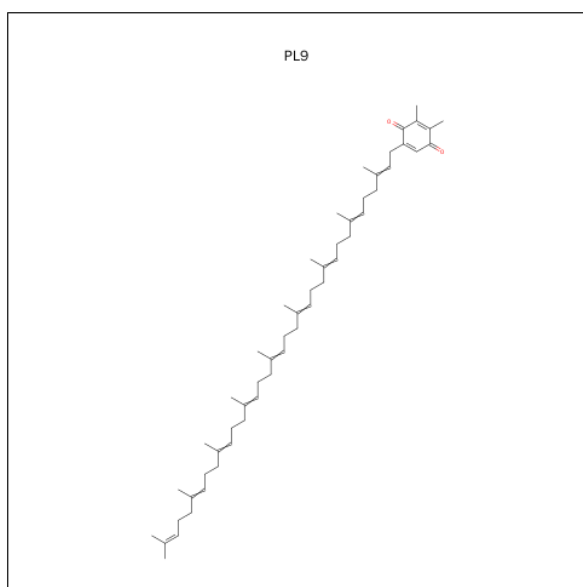
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BC	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	BD	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



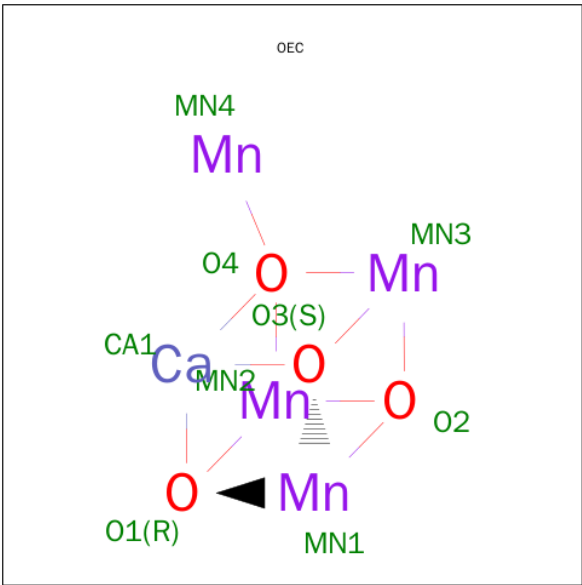
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	AA	1	Total	C	N	O	0	0
			64	55	4	5		
23	AD	1	Total	C	N	O	0	0
			64	55	4	5		
23	BA	1	Total	C	N	O	0	0
			64	55	4	5		
23	BD	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



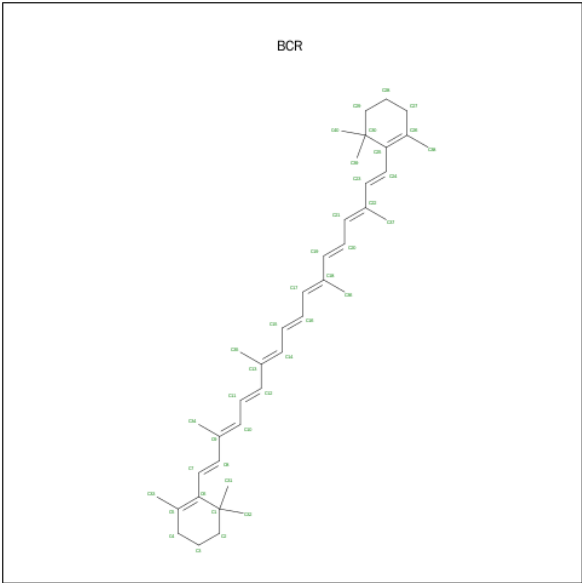
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	AA	1	Total	C	O	0	0
			45	43	2		
24	AD	1	Total	C	O	0	0
			55	53	2		
24	AJ	1	Total	C	O	0	0
			35	33	2		
24	BA	1	Total	C	O	0	0
			45	43	2		
24	BD	1	Total	C	O	0	0
			55	53	2		
24	BJ	1	Total	C	O	0	0
			35	33	2		

- Molecule 25 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	AA	1	Total	Ca	Mn	0	0
			5	1	4		
25	BA	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	AA	1	Total	C	0	0
			40	40		
26	AB	1	Total	C	0	0
			40	40		

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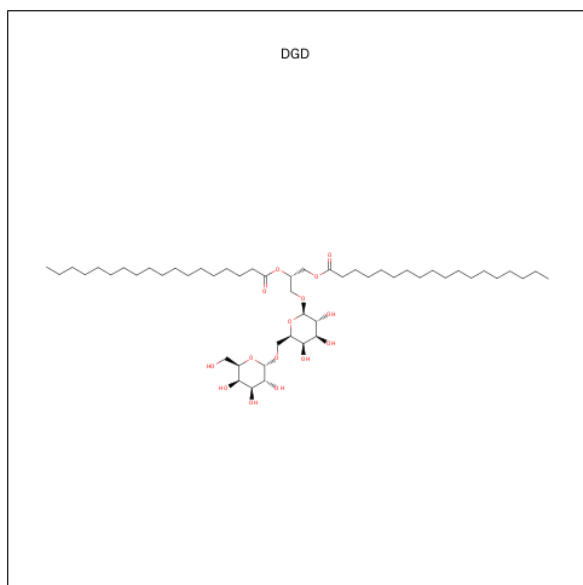
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AB	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AC	1	Total C 40 40	0	0
26	AD	1	Total C 40 40	0	0
26	AH	1	Total C 40 40	0	0
26	AJ	1	Total C 40 40	0	0
26	AK	1	Total C 40 40	0	0
26	AT	1	Total C 40 40	0	0
26	AZ	1	Total C 40 40	0	0
26	BA	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BB	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BC	1	Total C 40 40	0	0
26	BD	1	Total C 40 40	0	0
26	BJ	1	Total C 40 40	0	0
26	BK	1	Total C 40 40	0	0
26	BX	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	BZ	1	Total C 40 40	0	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



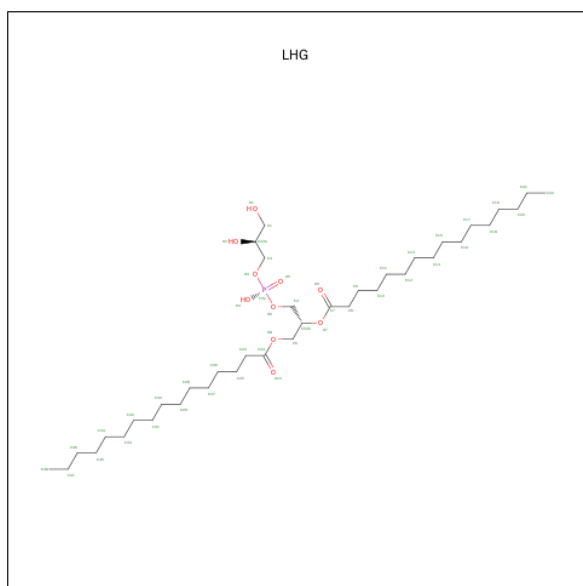
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	AA	1	Total C O 56 41 15	0	0
27	AB	1	Total C O 52 37 15	0	0
27	AC	1	Total C O 53 38 15	0	0
27	AC	1	Total C O 62 47 15	0	0
27	AC	1	Total C O 66 51 15	0	0
27	AD	1	Total C O 63 48 15	0	0
27	AH	1	Total C O 58 43 15	0	0
27	BA	1	Total C O 56 41 15	0	0
27	BB	1	Total C O 52 37 15	0	0
27	BC	1	Total C O 53 38 15	0	0

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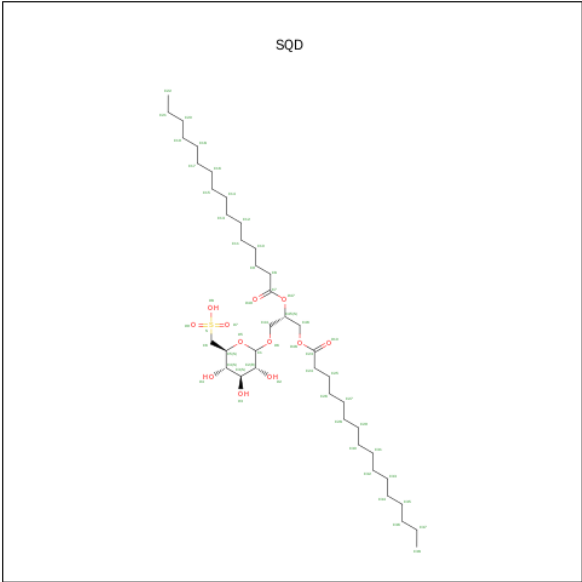
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	BC	1	Total	C	O	0	0
			62	47	15		
27	BC	1	Total	C	O	0	0
			66	51	15		
27	BD	1	Total	C	O	0	0
			63	48	15		
27	BH	1	Total	C	O	0	0
			58	43	15		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



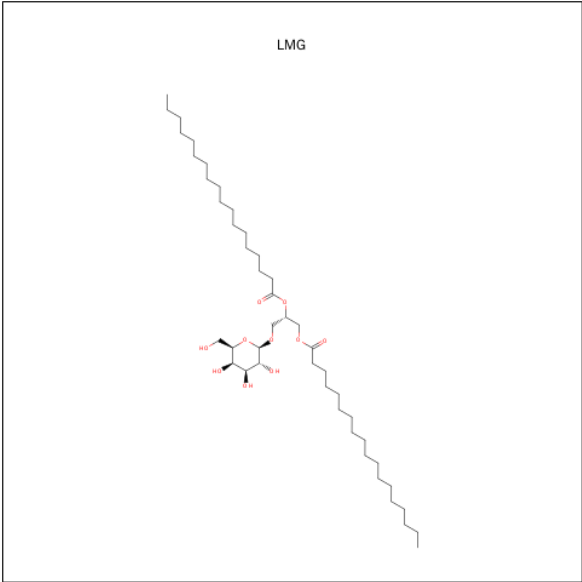
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	AA	1	Total	C	O	P	0	0
			39	28	10	1		
28	AC	1	Total	C	O	P	0	0
			37	26	10	1		
28	BA	1	Total	C	O	P	0	0
			39	28	10	1		
28	BC	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	AA	1	Total	C	O	S	0	0
			51	38	12	1		
29	AA	1	Total	C	O	S	0	0
			54	41	12	1		
29	AD	1	Total	C	O	S	0	0
			43	30	12	1		
29	AF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BA	1	Total	C	O	S	0	0
			54	41	12	1		
29	BA	1	Total	C	O	S	0	0
			51	38	12	1		
29	BB	1	Total	C	O	S	0	0
			47	34	12	1		
29	BD	1	Total	C	O	S	0	0
			43	30	12	1		
29	BF	1	Total	C	O	S	0	0
			45	32	12	1		
29	BL	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 30 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	AA	1	Total	C	O	0	0
			51	41	10		
30	AA	1	Total	C	O	0	0
			42	32	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			49	39	10		
30	AB	1	Total	C	O	0	0
			42	32	10		
30	AC	1	Total	C	O	0	0
			48	38	10		
30	AC	1	Total	C	O	0	0
			45	35	10		
30	AD	1	Total	C	O	0	0
			46	36	10		
30	AD	1	Total	C	O	0	0
			48	38	10		
30	AE	1	Total	C	O	0	0
			44	34	10		
30	AI	1	Total	C	O	0	0
			43	33	10		
30	AM	1	Total	C	O	0	0
			42	32	10		
30	BA	1	Total	C	O	0	0
			51	41	10		
30	BB	1	Total	C	O	0	0
			49	39	10		

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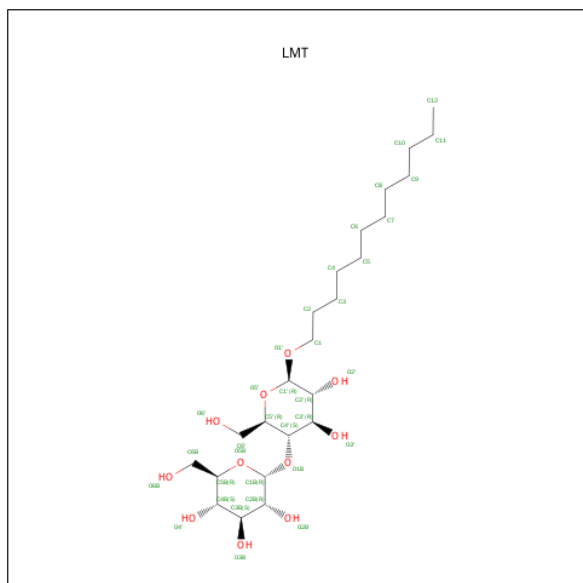
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	BB	1	Total	C	O	0	0
			49	39	10		
30	BC	1	Total	C	O	0	0
			48	38	10		
30	BC	1	Total	C	O	0	0
			45	35	10		
30	BD	1	Total	C	O	0	0
			46	36	10		
30	BD	1	Total	C	O	0	0
			48	38	10		
30	BE	1	Total	C	O	0	0
			44	34	10		
30	BI	1	Total	C	O	0	0
			43	33	10		
30	BM	1	Total	C	O	0	0
			42	32	10		

- Molecule 31 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

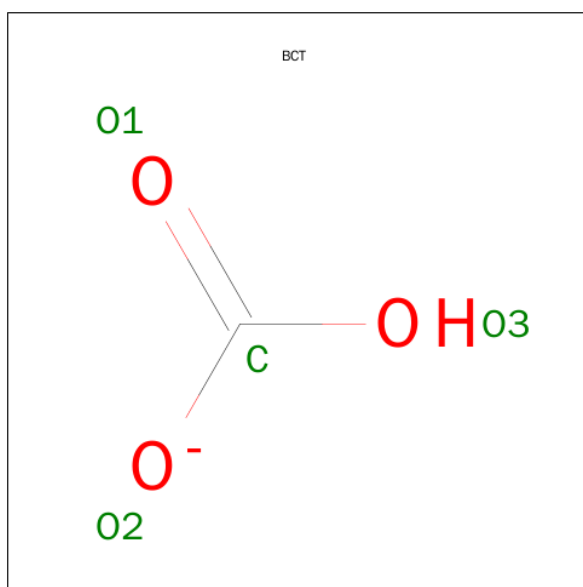
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	AA	1	Total	Cl	0	0
			1	1		
31	BA	1	Total	Cl	0	0
			1	1		

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



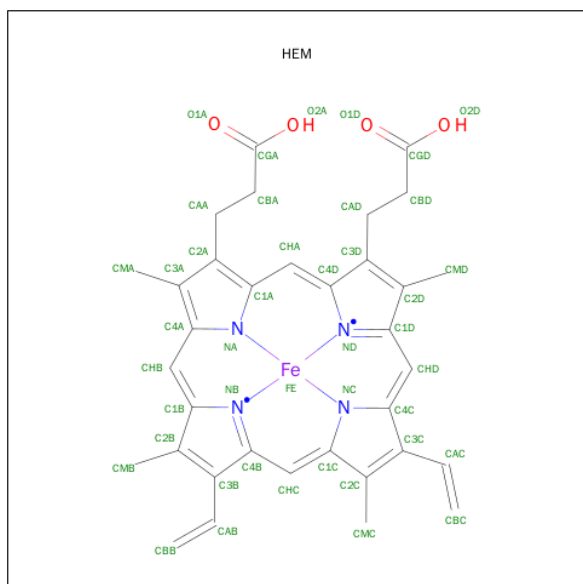
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AB	1	Total	C	O	0	0
			35	24	11		
32	AD	1	Total	C	O	0	0
			31	20	11		
32	AI	1	Total	C	O	0	0
			35	24	11		
32	AM	1	Total	C	O	0	0
			35	24	11		
32	AT	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BB	1	Total	C	O	0	0
			35	24	11		
32	BD	1	Total	C	O	0	0
			31	20	11		
32	BI	1	Total	C	O	0	0
			35	24	11		
32	BM	1	Total	C	O	0	0
			35	24	11		
32	BT	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	AD	1	Total	C	O	0	0
			4	1	3		
33	BD	1	Total	C	O	0	0
			4	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	AE	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	AV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	BE	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
34	BV	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

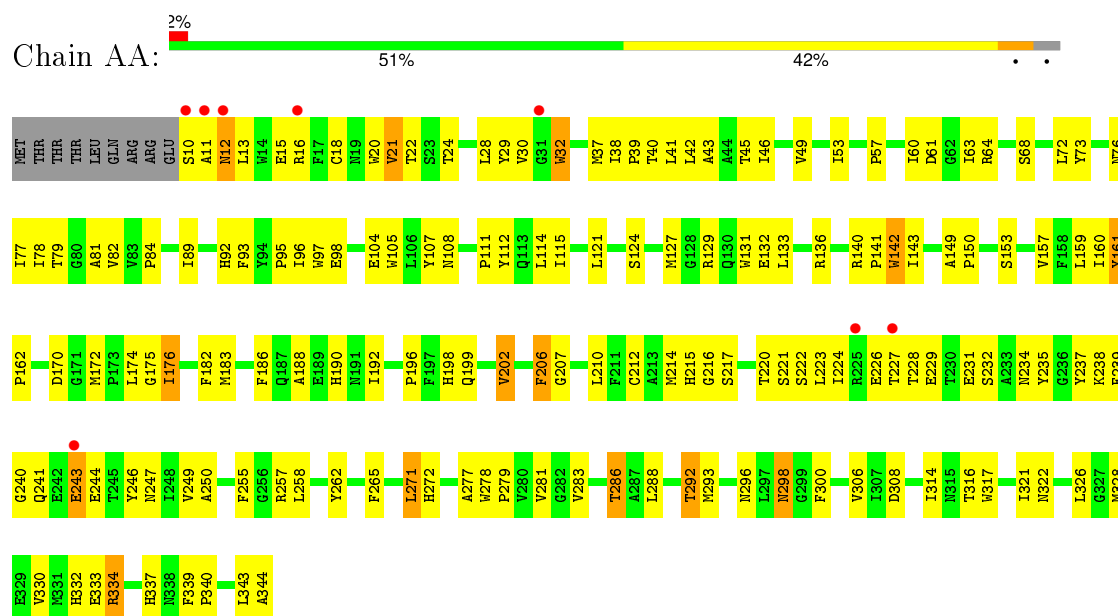
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	AO	1	Total 1	Ca 1	0	0
35	BO	1	Total 1	Ca 1	0	0
35	AK	1	Total 1	Ca 1	0	0
35	BK	1	Total 1	Ca 1	0	0

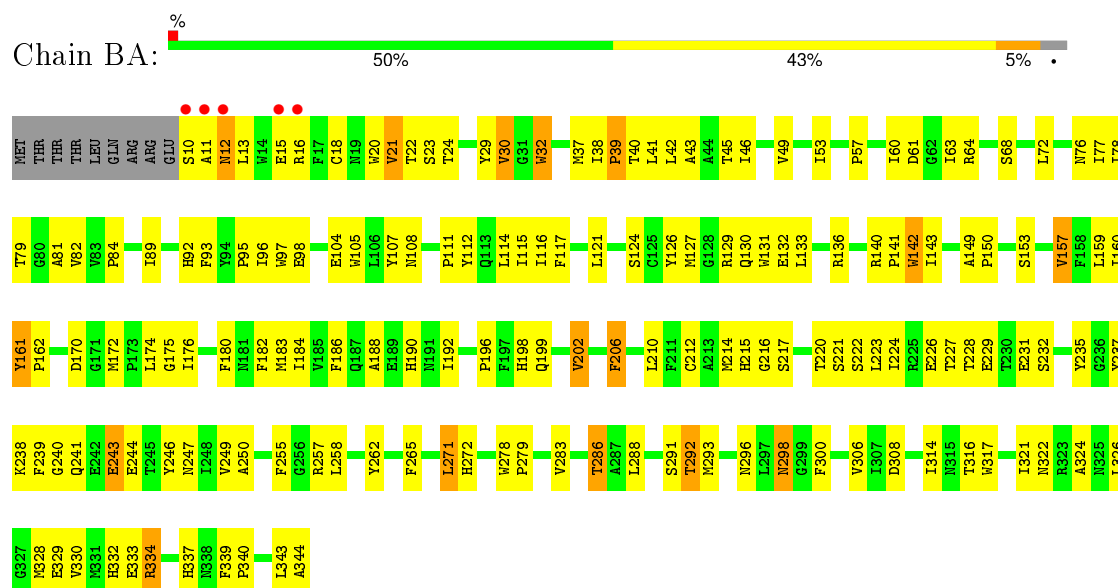
3 Residue-property plots

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 ($RSRZ > 2$). 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.

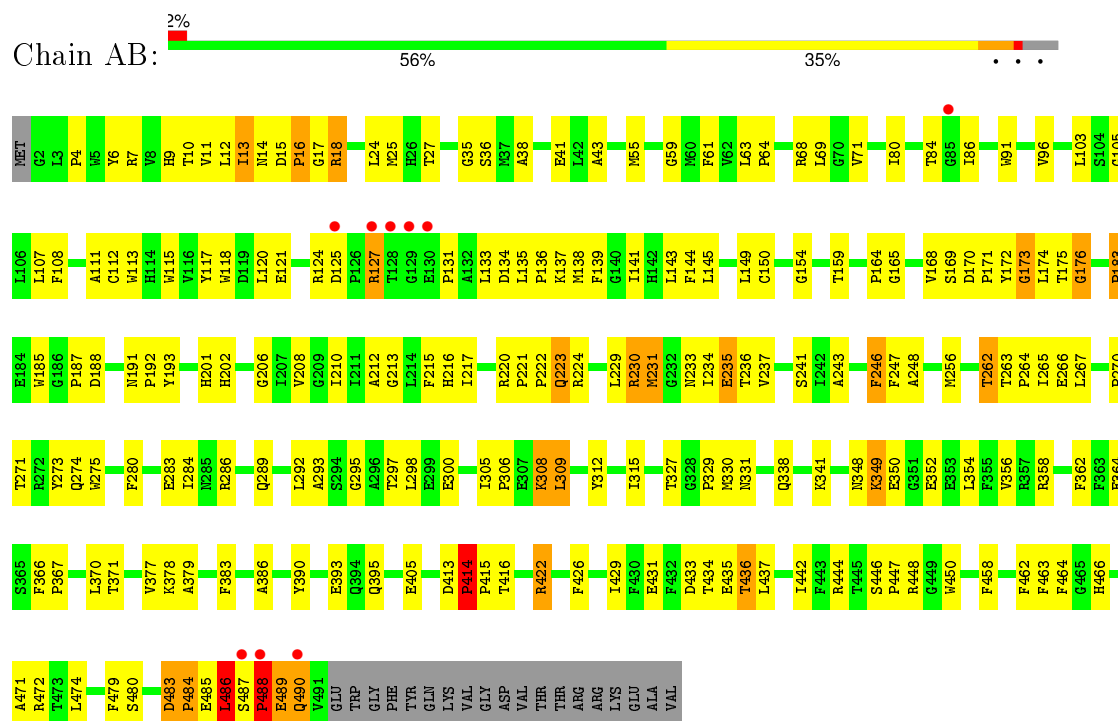
• Molecule 1: Photosystem Q(B) protein



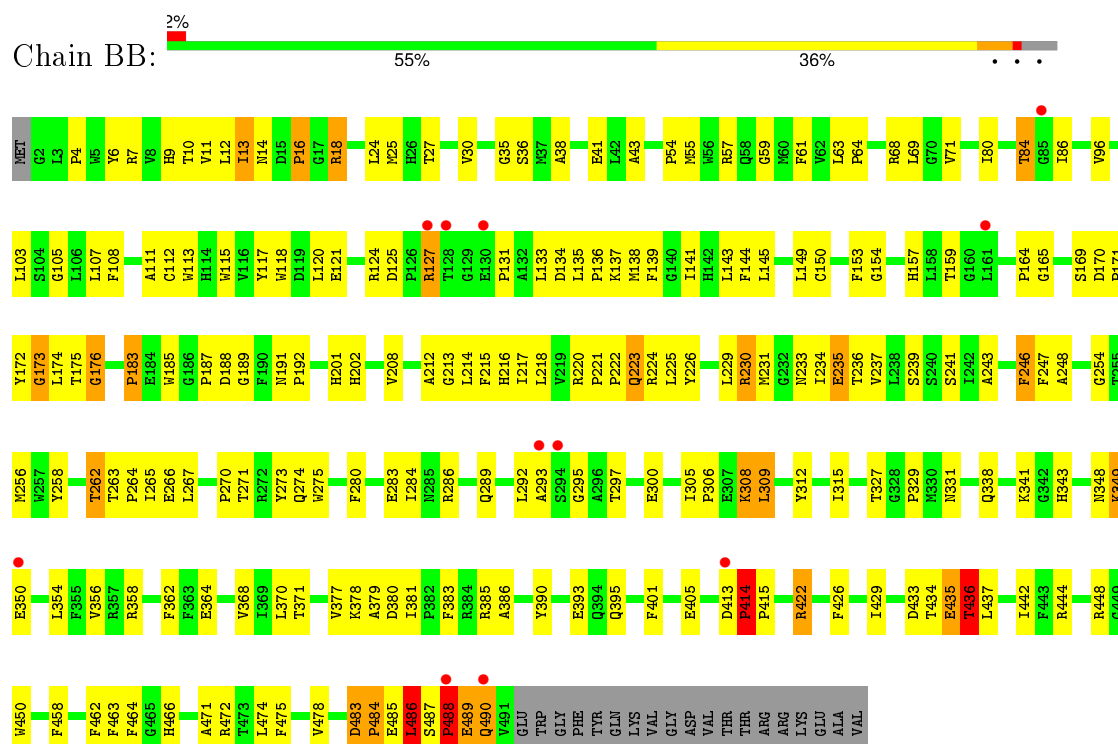
• Molecule 1: Photosystem Q(B) protein



- Molecule 2: Photosystem II core light harvesting protein

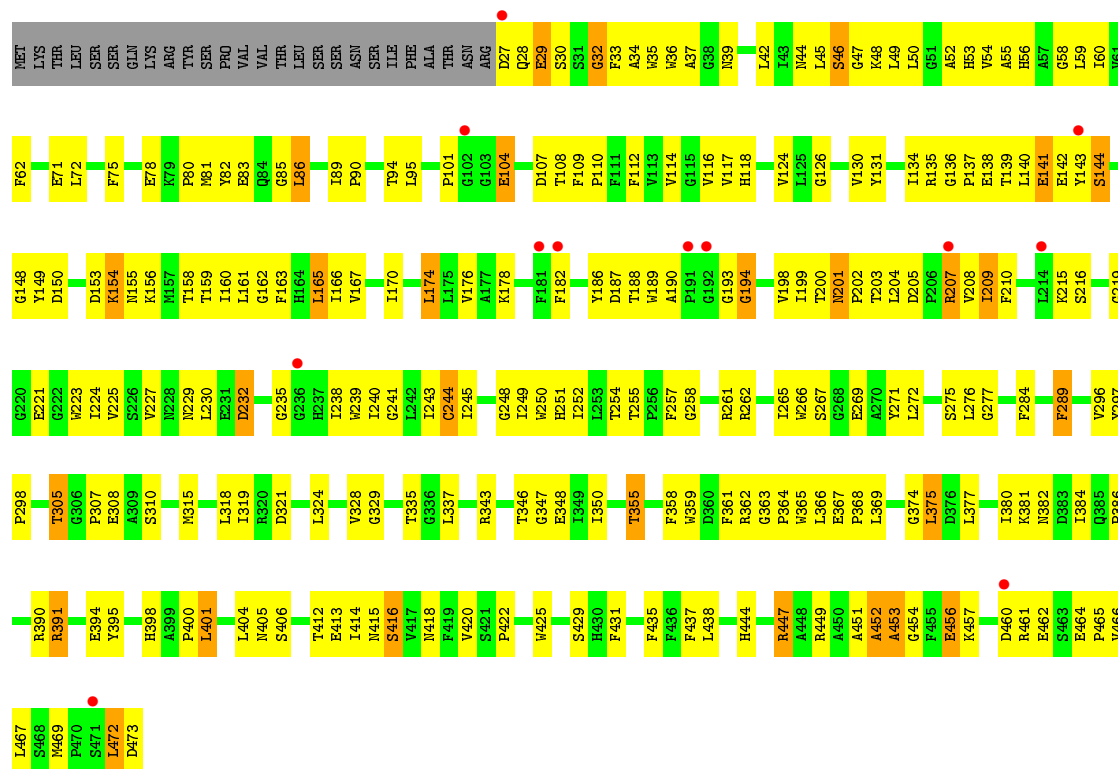


- Molecule 2: Photosystem II core light harvesting protein



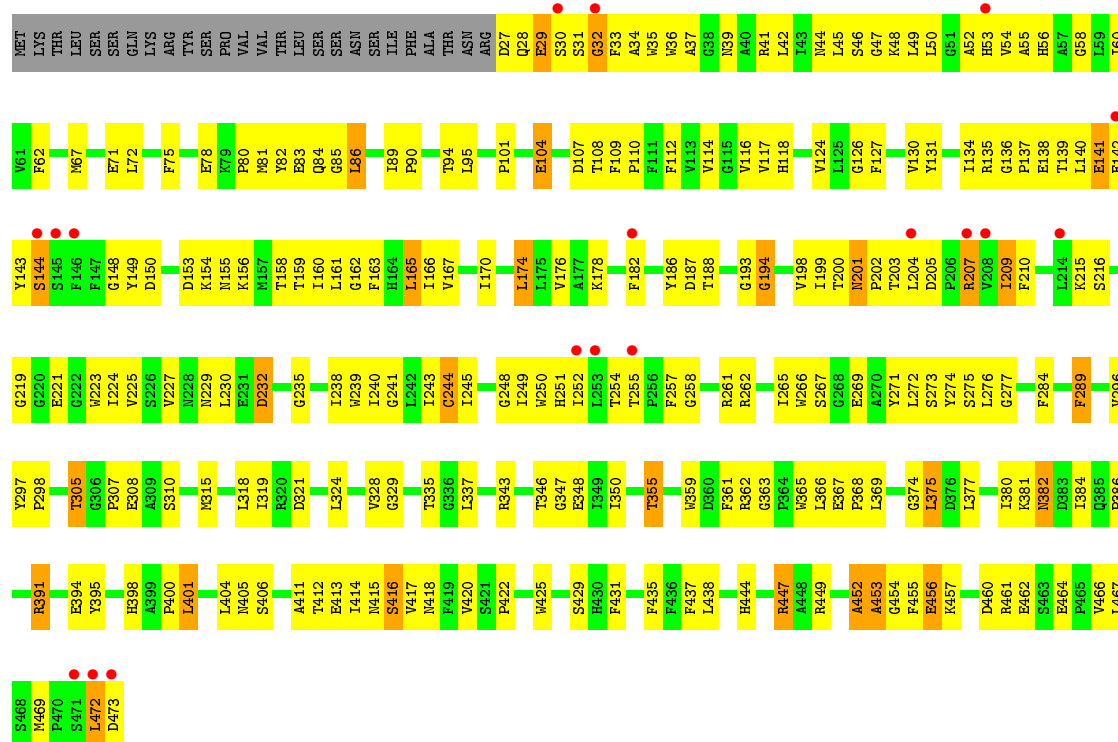
- Molecule 3: Photosystem II CP43 protein



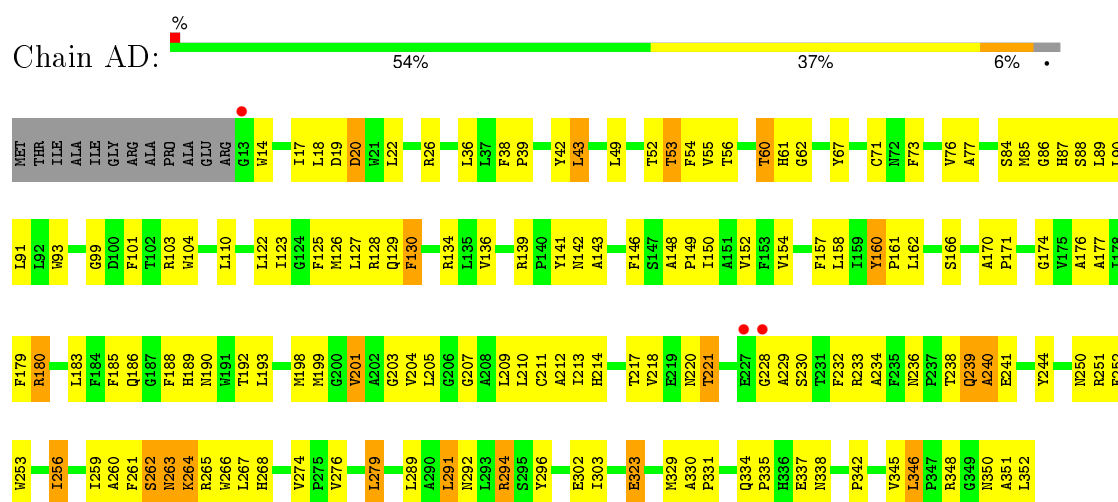


• Molecule 3: Photosystem II CP43 protein

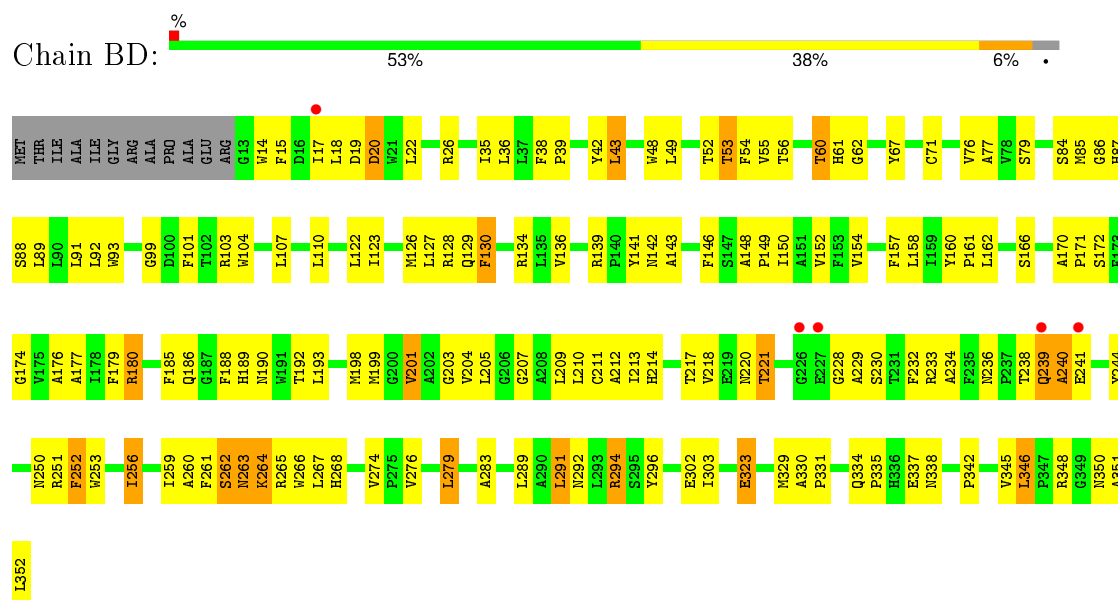
Chain BC: 4% 45% 44% 6% 5%



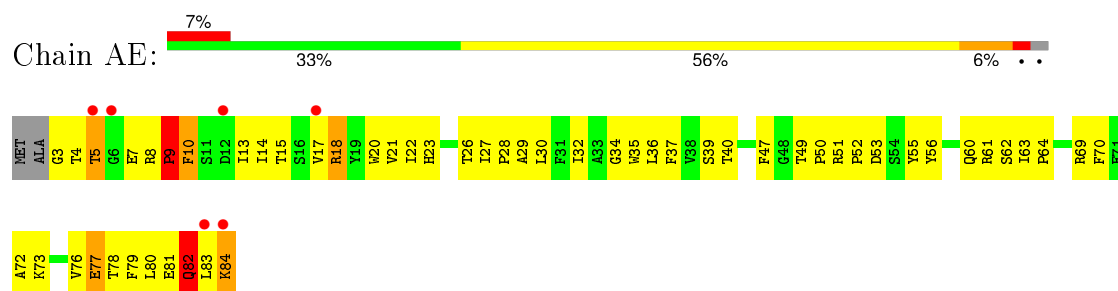
• Molecule 4: Photosystem II reaction center D2 protein



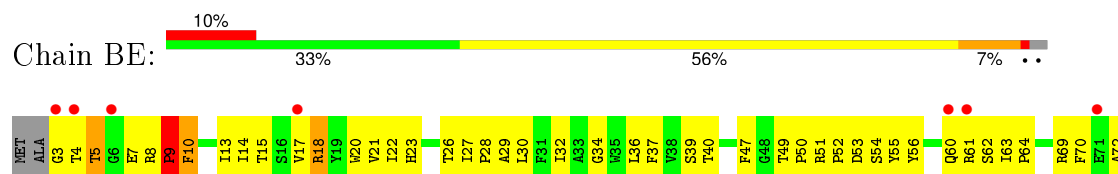
• Molecule 4: Photosystem II reaction center D2 protein

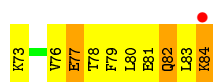


• Molecule 5: Cytochrome b559 subunit alpha

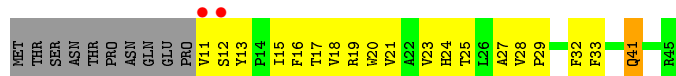


• Molecule 5: Cytochrome b559 subunit alpha

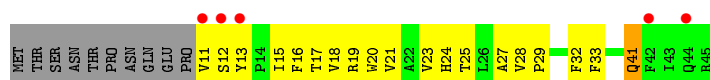




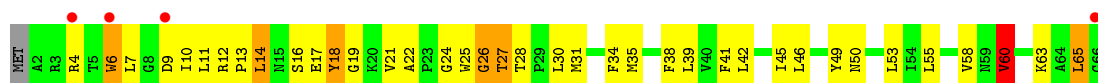
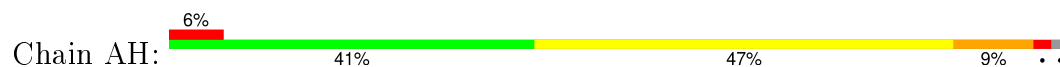
- Molecule 6: Cytochrome b559 subunit beta



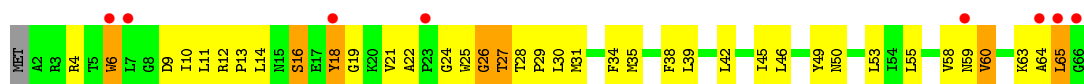
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

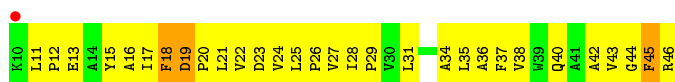
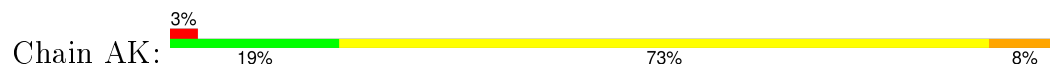




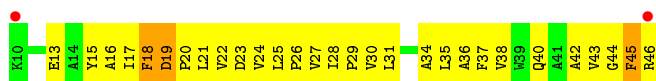
- Molecule 9: Photosystem II reaction center protein J



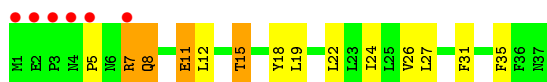
- Molecule 10: Photosystem II reaction center protein K



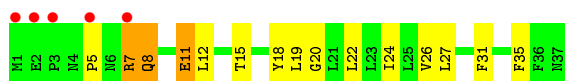
- Molecule 10: Photosystem II reaction center protein K



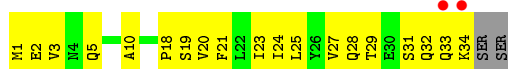
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



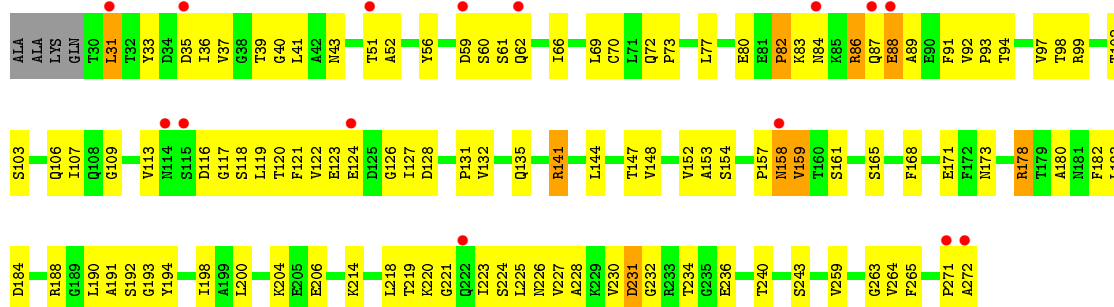
- Molecule 12: Photosystem II reaction center protein M





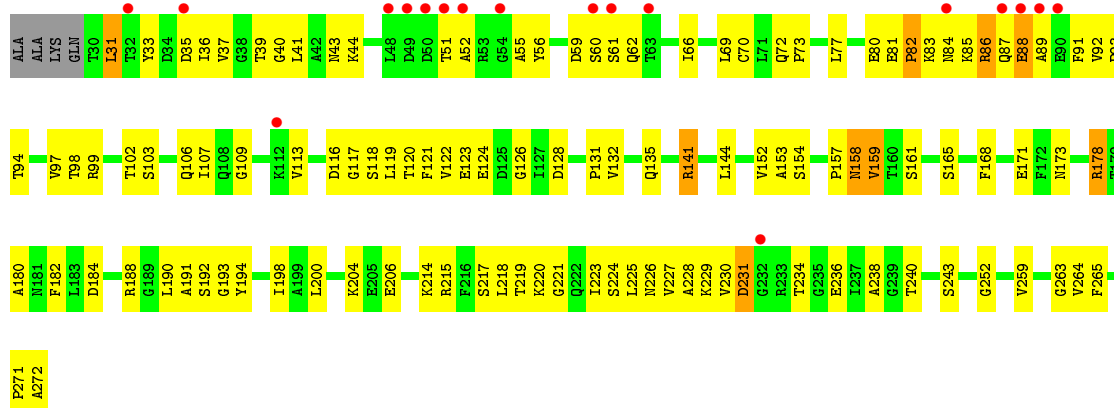
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain AO: 6% 53% 42%



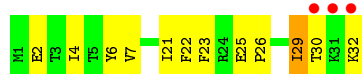
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain BO: 7% 51% 43%



- Molecule 14: Photosystem II reaction center protein T

Chain AT: 9% 63% 34%

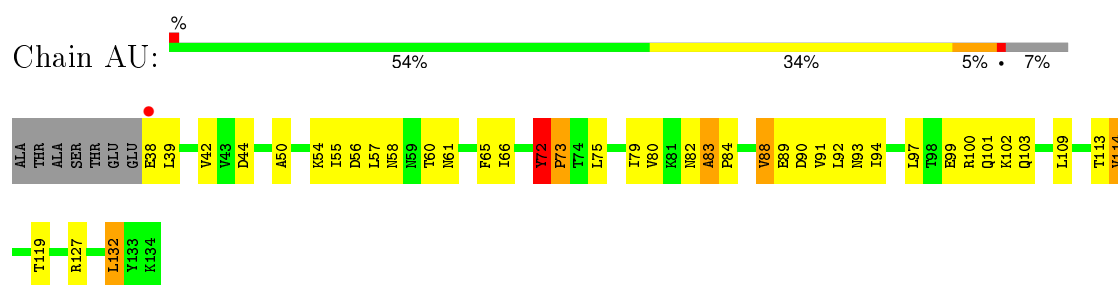


- Molecule 14: Photosystem II reaction center protein T

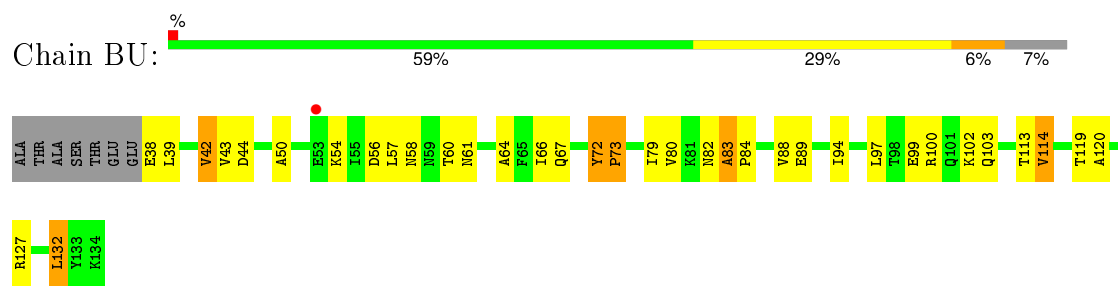
Chain BT: 6% 63% 34%



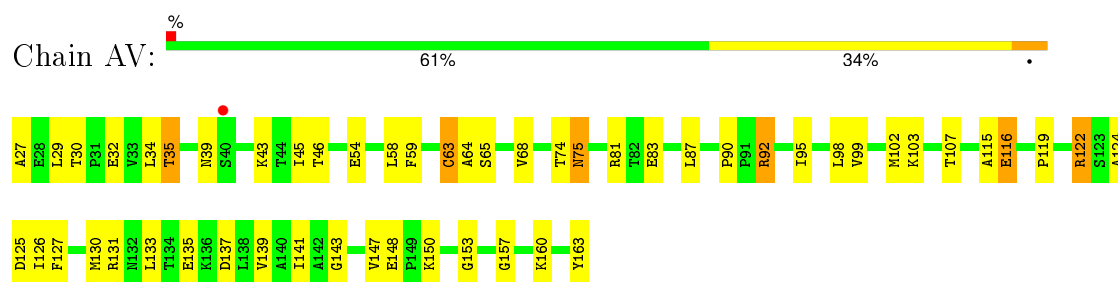
- Molecule 15: Photosystem II 12 kDa extrinsic protein



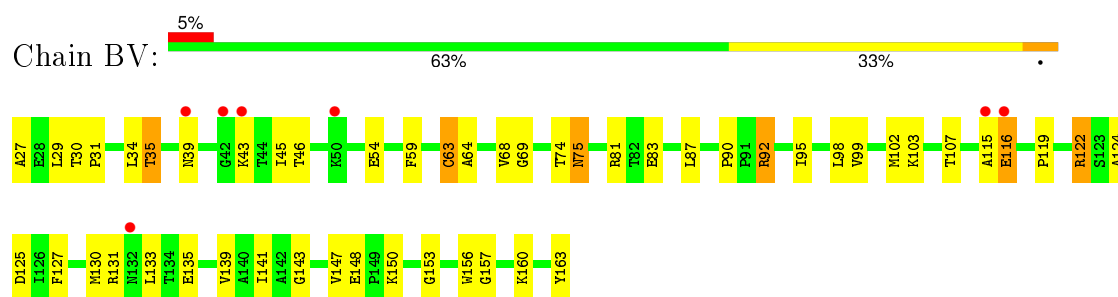
- Molecule 15: Photosystem II 12 kDa extrinsic protein



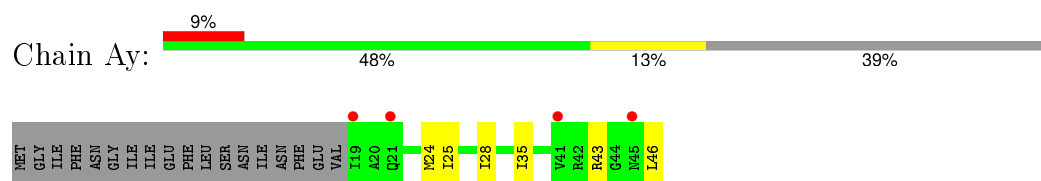
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

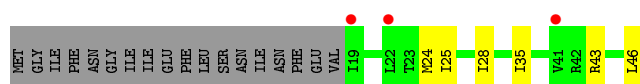


- Molecule 17: Protein ycf12

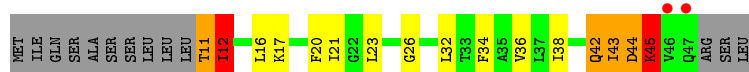


- Molecule 17: Protein ycf12

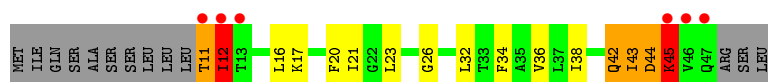
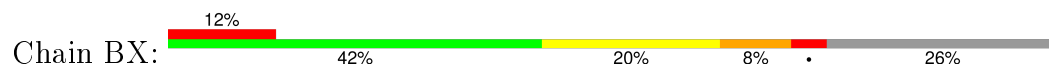




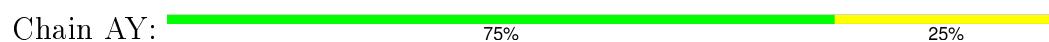
• Molecule 18: Photosystem II PsbX protein



• Molecule 18: Photosystem II PsbX protein



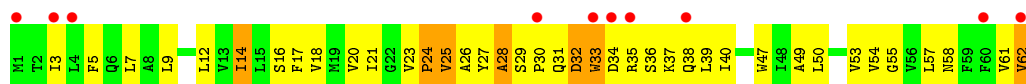
• Molecule 19: Photosystem II protein Y



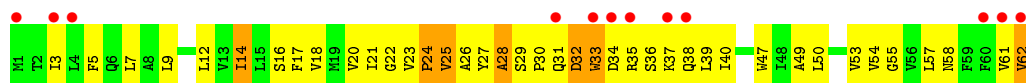
• Molecule 19: Photosystem II protein Y



• Molecule 20: Photosystem II reaction center protein Z



• Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (10.00-2.90) 99.3 (20.00-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.292 0.246 , 0.285	Depositor DCC
R_{free} test set	3784 reflections (2.04%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 193457 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50234	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, HEM, SQD, 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	AA	0.44	0/2713	0.66	0/3700
1	BA	0.43	0/2713	0.65	0/3700
2	AB	0.44	0/3986	0.67	3/5433 (0.1%)
2	BB	0.43	0/3986	0.66	3/5433 (0.1%)
3	AC	0.41	0/3556	0.64	1/4842 (0.0%)
3	BC	0.39	0/3556	0.63	1/4842 (0.0%)
4	AD	0.47	0/2801	0.65	0/3818
4	BD	0.45	0/2801	0.65	0/3818
5	AE	0.45	0/685	0.71	0/933
5	BE	0.45	0/685	0.70	0/933
6	AF	0.45	0/291	0.59	0/397
6	BF	0.47	0/291	0.57	0/397
7	AH	0.42	0/520	0.73	1/709 (0.1%)
7	BH	0.40	0/520	0.72	1/709 (0.1%)
8	AI	0.51	0/293	0.68	0/395
8	BI	0.50	0/293	0.67	0/395
9	AJ	0.43	0/255	0.69	0/346
9	BJ	0.45	0/255	0.66	0/346
10	AK	0.43	0/303	0.63	0/416
10	BK	0.44	0/303	0.61	0/416
11	AL	0.39	0/311	0.65	0/422
11	BL	0.41	0/311	0.65	0/422
12	AM	0.44	0/270	0.70	0/367
12	BM	0.45	0/270	0.67	0/367
13	AO	0.44	0/1876	0.70	0/2548
13	BO	0.43	0/1876	0.70	0/2548
14	AT	0.50	0/284	0.62	0/381
14	BT	0.48	0/284	0.62	0/381
15	AU	0.42	0/785	0.73	1/1064 (0.1%)
15	BU	0.40	0/785	0.73	0/1064
16	AV	0.38	0/1081	0.65	0/1468
16	BV	0.37	0/1081	0.64	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Ay	0.46	0/202	0.73	0/272
17	By	0.41	0/202	0.74	0/272
18	AX	0.43	0/273	0.63	0/370
18	BX	0.41	0/273	0.63	0/370
20	AZ	0.45	0/490	0.69	0/669
20	BZ	0.47	0/490	0.70	0/669
All	All	0.43	0/41950	0.66	11/57100 (0.0%)

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
1	AA	0	1
1	BA	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BB	486	LEU	CA-CB-CG	7.12	131.67	115.30
2	AB	486	LEU	CA-CB-CG	6.99	131.39	115.30
2	AB	488	PRO	N-CA-C	5.86	127.33	112.10
2	AB	489	GLU	N-CA-C	5.76	126.56	111.00
7	AH	65	LEU	CA-CB-CG	5.72	128.45	115.30
7	BH	65	LEU	CA-CB-CG	5.72	128.45	115.30
2	BB	488	PRO	N-CA-C	5.71	126.94	112.10
2	BB	489	GLU	N-CA-C	5.65	126.25	111.00
3	AC	32	GLY	N-CA-C	-5.54	99.24	113.10
3	BC	32	GLY	N-CA-C	-5.09	100.37	113.10
15	AU	72	TYR	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	161	TYR	Sidechain
1	BA	161	TYR	Sidechain

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	AA	2628	0	2524	179	0
1	BA	2628	0	2524	179	0
2	AB	3850	0	3718	224	0
2	BB	3850	0	3718	227	0
3	AC	3444	0	3365	258	0
3	BC	3444	0	3365	263	0
4	AD	2706	0	2608	177	0
4	BD	2706	0	2608	184	0
5	AE	666	0	651	71	0
5	BE	666	0	651	74	0
6	AF	282	0	291	28	0
6	BF	282	0	291	29	0
7	AH	507	0	521	52	0
7	BH	507	0	521	50	0
8	AI	286	0	308	15	0
8	BI	286	0	308	18	0
9	AJ	249	0	262	28	0
9	BJ	249	0	262	26	0
10	AK	293	0	305	42	0
10	BK	293	0	305	44	0
11	AL	304	0	316	15	0
11	BL	304	0	316	17	0
12	AM	267	0	289	27	0
12	BM	267	0	289	26	0
13	AO	1845	0	1801	115	0
13	BO	1845	0	1801	118	0
14	AT	275	0	288	21	0
14	BT	275	0	288	20	0
15	AU	774	0	773	46	0
15	BU	774	0	773	42	0
16	AV	1060	0	1068	42	0
16	BV	1060	0	1068	39	0
17	Ay	201	0	226	0	0
17	By	201	0	226	0	0
18	AX	270	0	299	27	0
18	BX	270	0	299	25	0
19	AY	140	0	32	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	BY	140	0	32	6	0
20	AZ	479	0	516	54	0
20	BZ	479	0	516	55	0
21	AA	1	0	0	0	0
21	BA	1	0	0	0	0
22	AA	260	0	288	18	0
22	AB	1040	0	1152	77	0
22	AC	845	0	936	61	0
22	AD	130	0	144	11	0
22	BA	260	0	288	18	0
22	BB	1040	0	1152	83	0
22	BC	845	0	936	62	0
22	BD	130	0	144	12	0
23	AA	64	0	74	5	0
23	AD	64	0	74	2	0
23	BA	64	0	74	5	0
23	BD	64	0	74	5	0
24	AA	45	0	61	5	0
24	AD	55	0	80	9	0
24	AJ	35	0	45	0	0
24	BA	45	0	61	6	0
24	BD	55	0	80	8	0
24	BJ	35	0	45	0	0
25	AA	5	0	0	0	0
25	BA	5	0	0	0	0
26	AA	40	0	56	6	0
26	AB	160	0	224	10	0
26	AC	80	0	112	15	0
26	AD	40	0	56	3	0
26	AH	40	0	56	5	0
26	AJ	40	0	56	5	0
26	AK	40	0	56	13	0
26	AT	40	0	56	8	0
26	AZ	40	0	56	5	0
26	BA	40	0	56	3	0
26	BB	120	0	168	5	0
26	BC	80	0	112	17	0
26	BD	40	0	56	3	0
26	BJ	40	0	56	5	0
26	BK	40	0	56	13	0
26	BX	40	0	56	6	0
26	BZ	40	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	AA	56	0	70	0	0
27	AB	52	0	62	3	0
27	AC	181	0	245	19	0
27	AD	63	0	87	0	0
27	AH	58	0	74	1	0
27	BA	56	0	70	0	0
27	BB	52	0	62	3	0
27	BC	181	0	245	21	0
27	BD	63	0	87	0	0
27	BH	58	0	74	1	0
28	AA	39	0	51	3	0
28	AC	37	0	44	5	0
28	BA	39	0	51	4	0
28	BC	37	0	44	4	0
29	AA	105	0	145	10	0
29	AD	43	0	49	2	0
29	AF	45	0	53	2	0
29	BA	105	0	145	6	0
29	BB	47	0	60	2	0
29	BD	43	0	49	2	0
29	BF	45	0	53	1	0
29	BL	47	0	60	2	0
30	AA	93	0	126	5	0
30	AB	140	0	190	4	0
30	AC	93	0	126	6	0
30	AD	94	0	128	9	0
30	AE	44	0	58	4	0
30	AI	43	0	56	3	0
30	AM	42	0	54	4	0
30	BA	51	0	72	2	0
30	BB	98	0	136	2	0
30	BC	93	0	126	8	0
30	BD	94	0	128	10	0
30	BE	44	0	58	4	0
30	BI	43	0	56	3	0
30	BM	42	0	54	4	0
31	AA	1	0	0	0	0
31	BA	1	0	0	0	0
32	AB	105	0	138	6	0
32	AD	31	0	35	2	0
32	AI	35	0	46	4	0
32	AM	35	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	AT	35	0	46	3	0
32	BB	105	0	138	5	0
32	BD	31	0	35	1	0
32	BI	35	0	46	3	0
32	BM	35	0	46	1	0
32	BT	35	0	46	3	0
33	AD	4	0	0	1	0
33	BD	4	0	0	1	0
34	AE	43	0	30	5	0
34	AV	43	0	30	3	0
34	BE	43	0	30	6	0
34	BV	43	0	30	3	0
35	AK	1	0	0	0	0
35	AO	1	0	0	0	0
35	BK	1	0	0	0	0
35	BO	1	0	0	0	0
All	All	50234	0	51364	2715	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 27.

All (2715) 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)
16:AV:63:CYS:SG	34:AV:201:HEM:HAB	1.85	1.16
15:BU:83:ALA:HB1	15:BU:84:PRO:HD2	1.23	1.16
9:AJ:15:THR:HG21	10:AK:38:VAL:HG13	1.23	1.16
16:BV:63:CYS:SG	34:BV:201:HEM:HAB	1.85	1.15
9:BJ:15:THR:HG21	10:BK:38:VAL:HG13	1.24	1.13
2:BB:68:ARG:HH22	22:BB:607:CLA:HED1	1.13	1.11
15:AU:83:ALA:HB1	15:AU:84:PRO:HD2	1.22	1.09
2:AB:68:ARG:HH22	22:AB:604:CLA:HED1	1.12	1.07
1:AA:129:ARG:HH21	4:AD:256:ILE:HD12	1.19	1.06
2:BB:121:GLU:HG2	7:BH:4:ARG:HG2	1.36	1.05
2:AB:121:GLU:HG2	7:AH:4:ARG:HG2	1.36	1.04
13:BO:178:ARG:HG3	13:BO:178:ARG:HH11	1.17	1.04
13:AO:178:ARG:HG3	13:AO:178:ARG:HH11	1.18	1.04
13:AO:82:PRO:HG3	13:AO:89:ALA:HB2	1.37	1.03
3:BC:254:THR:HG22	3:BC:255:THR:H	1.23	1.03
3:AC:254:THR:HG22	3:AC:255:THR:H	1.18	1.03
1:BA:317:TRP:CZ3	4:BD:180:ARG:HD3	1.96	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:129:ARG:HH21	4:BD:256:ILE:HD12	1.20	1.00
13:BO:82:PRO:HG3	13:BO:89:ALA:HB2	1.40	1.00
2:AB:149:LEU:HG	22:AB:603:CLA:HBC1	1.44	1.00
1:AA:317:TRP:CZ3	4:AD:180:ARG:HD3	1.95	0.99
12:AM:33:GLN:HB3	12:BM:33:GLN:HB3	1.43	0.97
4:AD:26:ARG:HD3	6:AF:18:VAL:HG11	1.47	0.97
13:AO:230:VAL:HG12	13:AO:231:ASP:H	1.30	0.97
2:BB:149:LEU:HG	22:BB:606:CLA:HBC1	1.45	0.96
13:BO:230:VAL:HG12	13:BO:231:ASP:H	1.32	0.94
13:AO:69:LEU:HB3	13:AO:107:ILE:HB	1.49	0.94
15:AU:83:ALA:HB1	15:AU:84:PRO:CD	1.98	0.93
14:AT:29:ILE:HD12	14:AT:29:ILE:H	1.33	0.92
4:BD:26:ARG:HD3	6:BF:18:VAL:HG11	1.48	0.92
2:BB:271:THR:HG22	2:BB:273:TYR:H	1.35	0.92
15:BU:83:ALA:HB1	15:BU:84:PRO:CD	2.00	0.91
13:BO:69:LEU:HB3	13:BO:107:ILE:HB	1.51	0.91
2:BB:414:PRO:HB2	2:BB:415:PRO:HD3	1.53	0.90
14:BT:29:ILE:H	14:BT:29:ILE:HD12	1.34	0.90
2:BB:68:ARG:NH2	22:BB:607:CLA:HED1	1.87	0.90
13:BO:178:ARG:CG	13:BO:178:ARG:HH11	1.84	0.90
3:BC:473:ASP:HB2	14:BT:26:PRO:HB3	1.54	0.90
3:AC:473:ASP:HB2	14:AT:26:PRO:HB3	1.53	0.89
1:AA:72:LEU:HD13	30:AA:416:LMG:H111	1.55	0.89
1:AA:317:TRP:HZ3	4:AD:180:ARG:HD3	1.37	0.89
22:BB:611:CLA:HMD1	22:BB:613:CLA:HAB	1.53	0.89
22:AD:404:CLA:H42	18:AX:26:GLY:HA3	1.53	0.89
13:BO:69:LEU:HD12	13:BO:70:CYS:H	1.37	0.88
3:AC:224:ILE:O	3:AC:227:VAL:HG23	1.73	0.88
22:BD:404:CLA:H42	18:BX:26:GLY:HA3	1.56	0.88
2:AB:68:ARG:NH2	22:AB:604:CLA:HED1	1.88	0.88
13:AO:178:ARG:HH11	13:AO:178:ARG:CG	1.88	0.87
5:BE:18:ARG:HD2	5:BE:22:ILE:HD11	1.55	0.87
7:BH:12:ARG:HD3	7:BH:12:ARG:O	1.74	0.87
15:AU:72:TYR:HB3	15:AU:73:PRO:HD3	1.57	0.87
2:AB:414:PRO:HB2	2:AB:415:PRO:HD3	1.55	0.87
22:AB:608:CLA:HMD1	22:AB:610:CLA:HAB	1.55	0.86
22:AB:608:CLA:HAB	4:AD:123:ILE:HG23	1.58	0.86
11:BL:5:PRO:HA	11:BL:7:ARG:HH22	1.38	0.86
2:AB:271:THR:HG22	2:AB:273:TYR:H	1.39	0.86
3:AC:305:THR:HG22	3:AC:308:GLU:H	1.40	0.86
4:AD:129:GLN:NE2	4:AD:143:ALA:HA	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:69:LEU:HD12	13:AO:70:CYS:H	1.39	0.85
1:BA:317:TRP:HZ3	4:BD:180:ARG:HD3	1.36	0.85
3:BC:155:ASN:HD21	3:BC:255:THR:HB	1.39	0.85
3:AC:447:ARG:HH11	3:AC:447:ARG:HG2	1.40	0.85
18:AX:12:ILE:HG12	18:AX:16:LEU:HD12	1.56	0.85
3:BC:224:ILE:O	3:BC:227:VAL:HG23	1.76	0.85
7:AH:12:ARG:O	7:AH:12:ARG:HD3	1.76	0.84
34:BE:101:HEM:HBC2	6:BF:27:ALA:HB1	1.58	0.84
11:BL:8:GLN:N	11:BL:8:GLN:HE21	1.74	0.84
2:BB:120:LEU:HD13	22:BB:619:CLA:HMD2	1.60	0.84
34:AE:101:HEM:HBC2	6:AF:27:ALA:HB1	1.59	0.84
3:BC:447:ARG:HH11	3:BC:447:ARG:HG2	1.40	0.84
5:AE:18:ARG:HD2	5:AE:22:ILE:HD11	1.60	0.84
11:AL:5:PRO:HA	11:AL:7:ARG:HH22	1.39	0.84
3:BC:39:ASN:HB2	22:BC:508:CLA:HBA1	1.57	0.84
3:BC:305:THR:HG23	3:BC:307:PRO:HD2	1.59	0.84
3:BC:449:ARG:HE	22:BC:505:CLA:HED1	1.42	0.84
3:AC:155:ASN:HD21	3:AC:255:THR:HB	1.40	0.84
22:BB:611:CLA:HAB	4:BD:123:ILE:HG23	1.60	0.84
3:AC:305:THR:HG23	3:AC:307:PRO:HD2	1.60	0.84
3:BC:305:THR:HG22	3:BC:308:GLU:H	1.40	0.84
15:BU:72:TYR:HB3	15:BU:73:PRO:HD3	1.59	0.83
4:BD:148:ALA:HB3	4:BD:149:PRO:HD3	1.60	0.83
20:BZ:36:SER:HA	20:BZ:39:LEU:HG	1.60	0.83
11:AL:8:GLN:HE21	11:AL:8:GLN:N	1.75	0.83
3:AC:39:ASN:HB2	22:AC:508:CLA:HBA1	1.58	0.83
22:BA:403:CLA:H152	23:BA:406:PHO:H51	1.60	0.83
3:BC:166:ILE:HG23	3:BC:245:ILE:HG23	1.60	0.83
3:AC:449:ARG:HE	22:AC:505:CLA:HED1	1.43	0.83
2:BB:68:ARG:HH22	22:BB:607:CLA:CED	1.91	0.83
2:AB:68:ARG:HH22	22:AB:604:CLA:CED	1.92	0.83
2:BB:124:ARG:HE	2:BB:131:PRO:HD3	1.42	0.83
1:BA:41:LEU:HD13	23:BA:406:PHO:H2	1.61	0.82
18:BX:12:ILE:HG12	18:BX:16:LEU:HD12	1.61	0.82
2:AB:124:ARG:HE	2:AB:131:PRO:HD3	1.43	0.82
3:AC:166:ILE:HG23	3:AC:245:ILE:HG23	1.61	0.81
2:BB:489:GLU:HB2	5:BE:3:GLY:N	1.95	0.81
4:BD:129:GLN:NE2	4:BD:143:ALA:HA	1.97	0.80
2:AB:489:GLU:HB2	5:AE:3:GLY:N	1.96	0.80
13:AO:83:LYS:HG2	13:AO:84:ASN:H	1.46	0.80
22:AA:402:CLA:H152	23:AA:405:PHO:H51	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AD:406:BCR:H403	9:AJ:25:VAL:HG21	1.64	0.80
20:AZ:36:SER:HA	20:AZ:39:LEU:HG	1.64	0.80
1:AA:41:LEU:HD13	23:AA:405:PHO:H2	1.62	0.79
3:AC:254:THR:HG22	3:AC:255:THR:N	1.96	0.79
1:BA:258:LEU:HD12	4:BD:128:ARG:HD3	1.65	0.79
4:AD:148:ALA:HB3	4:AD:149:PRO:HD3	1.63	0.79
13:AO:230:VAL:HG12	13:AO:231:ASP:N	1.98	0.79
13:BO:218:LEU:HD22	15:BU:119:THR:HG21	1.65	0.79
2:AB:348:ASN:HB3	2:AB:354:LEU:HD21	1.65	0.78
2:AB:187:PRO:HB3	22:AB:601:CLA:HMB2	1.65	0.78
2:AB:24:LEU:HD21	22:AB:616:CLA:HAB	1.65	0.78
1:AA:12:ASN:HD22	1:AA:15:GLU:HB2	1.49	0.78
5:AE:84:LYS:HB2	5:AE:84:LYS:NZ	1.97	0.78
4:BD:60:THR:HG23	4:BD:61:HIS:CD2	2.18	0.78
2:AB:271:THR:HG22	2:AB:273:TYR:N	1.98	0.78
13:BO:83:LYS:HG2	13:BO:84:ASN:H	1.47	0.78
13:BO:31:LEU:HB2	13:BO:36:ILE:HD11	1.66	0.78
1:BA:12:ASN:HD22	1:BA:15:GLU:HB2	1.49	0.78
2:AB:120:LEU:HD13	22:AB:616:CLA:HMD2	1.64	0.78
2:BB:271:THR:HG22	2:BB:273:TYR:N	1.98	0.78
11:BL:5:PRO:HA	11:BL:7:ARG:NH2	1.99	0.78
24:BA:408:PL9:H33	4:BD:38:PHE:HD1	1.47	0.77
1:BA:192:ILE:HA	1:BA:293:MET:HE3	1.67	0.77
2:BB:124:ARG:HH11	2:BB:124:ARG:HG3	1.49	0.77
26:BD:406:BCR:H403	9:BJ:25:VAL:HG21	1.64	0.77
2:BB:187:PRO:HB3	22:BB:604:CLA:HMB2	1.65	0.77
24:AA:407:PL9:H33	4:AD:38:PHE:HD1	1.48	0.77
2:BB:24:LEU:HD21	22:BB:619:CLA:HAB	1.67	0.76
22:BC:501:CLA:HMB3	26:BC:515:BCR:H403	1.67	0.76
2:AB:329:PRO:HB3	22:AB:607:CLA:HED1	1.65	0.76
26:BC:514:BCR:H353	26:BK:102:BCR:H321	1.68	0.76
5:BE:84:LYS:NZ	5:BE:84:LYS:HB2	2.00	0.76
2:BB:329:PRO:HB3	22:BB:610:CLA:HED1	1.67	0.76
2:BB:188:ASP:HA	7:BH:58:VAL:HG23	1.68	0.76
13:AO:31:LEU:HB2	13:AO:36:ILE:HD11	1.67	0.76
1:AA:258:LEU:HD12	4:AD:128:ARG:HD3	1.66	0.76
3:AC:42:LEU:HD13	22:AC:511:CLA:HMA3	1.68	0.76
1:AA:57:PRO:HG3	1:AA:68:SER:HB3	1.66	0.76
20:AZ:32:ASP:HB2	20:AZ:35:ARG:HG2	1.67	0.76
3:BC:42:LEU:HD13	22:BC:511:CLA:HMA3	1.67	0.75
2:AB:134:ASP:OD2	2:AB:137:LYS:HE3	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:244:TYR:OH	4:BD:264:LYS:HE3	1.86	0.75
1:AA:192:ILE:HA	1:AA:293:MET:HE3	1.68	0.75
3:AC:391:ARG:NH1	3:AC:391:ARG:HB2	2.02	0.75
5:BE:18:ARG:HB3	5:BE:18:ARG:HH11	1.50	0.75
18:AX:12:ILE:O	18:AX:12:ILE:HG23	1.85	0.75
2:BB:134:ASP:OD2	2:BB:137:LYS:HE3	1.87	0.75
1:BA:57:PRO:HG3	1:BA:68:SER:HB3	1.68	0.75
22:AC:501:CLA:HMB3	26:AC:515:BCR:H403	1.69	0.75
2:AB:483:ASP:CG	2:AB:484:PRO:HD2	2.07	0.75
3:BC:254:THR:HG22	3:BC:255:THR:N	2.00	0.75
20:AZ:49:ALA:O	20:AZ:53:VAL:HG23	1.86	0.75
2:BB:150:CYS:HB2	22:BB:606:CLA:HMC3	1.68	0.74
1:BA:214:MET:CE	1:BA:214:MET:HA	2.17	0.74
11:AL:5:PRO:HA	11:AL:7:ARG:NH2	2.00	0.74
3:AC:155:ASN:HA	3:AC:158:THR:HG22	1.69	0.74
13:BO:230:VAL:HG12	13:BO:231:ASP:N	2.02	0.74
3:AC:241:GLY:O	3:AC:245:ILE:HG13	1.88	0.74
1:AA:214:MET:HA	1:AA:214:MET:CE	2.17	0.74
2:AB:137:LYS:HD2	7:AH:14:LEU:O	1.87	0.74
4:AD:244:TYR:OH	4:AD:264:LYS:HE3	1.88	0.74
4:AD:148:ALA:HB2	4:AD:276:VAL:HG13	1.70	0.74
5:BE:17:VAL:O	5:BE:21:VAL:HG23	1.87	0.74
6:AF:17:THR:HG23	6:AF:20:TRP:H	1.53	0.74
2:AB:135:LEU:HD23	2:AB:138:MET:HE3	1.70	0.74
5:AE:18:ARG:HH11	5:AE:18:ARG:HB3	1.52	0.73
13:BO:69:LEU:HD12	13:BO:70:CYS:N	2.03	0.73
3:AC:240:ILE:O	3:AC:244:CYS:HB2	1.88	0.73
4:AD:60:THR:HG23	4:AD:61:HIS:CD2	2.23	0.73
26:AC:514:BCR:H353	26:AK:102:BCR:H321	1.69	0.73
13:AO:218:LEU:HD22	15:AU:119:THR:HG21	1.69	0.73
3:BC:155:ASN:HA	3:BC:158:THR:HG22	1.70	0.73
3:BC:241:GLY:O	3:BC:245:ILE:HG13	1.87	0.73
2:AB:483:ASP:CB	2:AB:484:PRO:HD2	2.17	0.73
2:BB:286:ARG:HG2	2:BB:286:ARG:HH11	1.54	0.73
4:BD:88:SER:HB2	5:BE:69:ARG:NH2	2.02	0.73
13:AO:92:VAL:CG1	13:AO:93:PRO:HD2	2.19	0.73
5:AE:17:VAL:O	5:AE:21:VAL:HG23	1.88	0.73
12:AM:20:VAL:HG21	12:BM:20:VAL:HG21	1.69	0.73
2:BB:483:ASP:CG	2:BB:484:PRO:HD2	2.08	0.73
18:AX:34:PHE:O	18:AX:38:ILE:HG12	1.88	0.73
2:BB:135:LEU:HA	2:BB:138:MET:HE3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:35:ASP:C	13:BO:36:ILE:HD12	2.09	0.73
2:BB:348:ASN:HB3	2:BB:354:LEU:HD21	1.71	0.73
22:BD:404:CLA:H43	18:BX:23:LEU:HA	1.71	0.73
3:AC:254:THR:CG2	3:AC:255:THR:H	2.00	0.72
1:AA:41:LEU:O	1:AA:45:THR:HG22	1.88	0.72
16:BV:63:CYS:SG	34:BV:201:HEM:CAB	2.74	0.72
3:AC:305:THR:CG2	3:AC:308:GLU:H	2.02	0.72
20:BZ:32:ASP:CG	20:BZ:33:TRP:H	1.92	0.72
20:BZ:32:ASP:HB2	20:BZ:35:ARG:HG2	1.71	0.72
3:AC:415:ASN:O	3:AC:416:SER:HB3	1.89	0.72
3:AC:405:ASN:HD22	27:AC:518:DGD:HD5	1.54	0.72
3:BC:240:ILE:O	3:BC:244:CYS:HB2	1.89	0.72
1:AA:129:ARG:NH2	4:AD:256:ILE:HD12	2.01	0.72
20:AZ:32:ASP:CG	20:AZ:33:TRP:H	1.90	0.72
3:BC:391:ARG:HB2	3:BC:391:ARG:NH1	2.04	0.72
1:BA:41:LEU:O	1:BA:45:THR:HG22	1.89	0.72
3:AC:361:PHE:HA	27:AC:516:DGD:HE61	1.72	0.72
3:BC:305:THR:CG2	3:BC:308:GLU:H	2.02	0.72
2:BB:483:ASP:CB	2:BB:484:PRO:HD2	2.19	0.72
13:AO:69:LEU:HD12	13:AO:70:CYS:N	2.05	0.72
13:AO:86:ARG:NH1	13:AO:87:GLN:HA	2.05	0.72
13:BO:86:ARG:NH1	13:BO:87:GLN:HA	2.05	0.72
3:AC:391:ARG:HH11	3:AC:391:ARG:HB2	1.55	0.71
3:AC:29:GLU:HB3	10:AK:46:ARG:NH1	2.04	0.71
2:AB:27:THR:HG22	2:AB:107:LEU:HD13	1.72	0.71
2:AB:68:ARG:NH1	2:AB:262:THR:HG23	2.04	0.71
2:AB:188:ASP:HA	7:AH:58:VAL:HG23	1.72	0.71
5:AE:56:TYR:O	16:AV:27:ALA:HB2	1.90	0.71
12:AM:33:GLN:HB3	12:BM:33:GLN:CB	2.19	0.71
3:BC:405:ASN:HD22	27:BC:518:DGD:HD5	1.55	0.71
22:AD:404:CLA:H43	18:AX:23:LEU:HA	1.71	0.71
13:BO:92:VAL:CG1	13:BO:93:PRO:HD2	2.20	0.71
2:AB:124:ARG:HG3	2:AB:124:ARG:HH11	1.55	0.71
14:AT:29:ILE:CD1	14:AT:29:ILE:H	1.95	0.71
1:BA:129:ARG:NH2	4:BD:256:ILE:HA	2.06	0.71
2:BB:68:ARG:NH1	2:BB:262:THR:HG23	2.06	0.70
3:BC:29:GLU:HB3	10:BK:46:ARG:NH1	2.06	0.70
2:AB:150:CYS:HB2	22:AB:603:CLA:HMC3	1.72	0.70
4:BD:148:ALA:HB2	4:BD:276:VAL:HG13	1.71	0.70
3:AC:348:GLU:OE2	13:AO:37:VAL:HA	1.91	0.70
3:AC:187:ASP:HB2	3:AC:230:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AH:38:PHE:HB2	26:AH:101:BCR:H10C	1.74	0.70
13:BO:77:LEU:HD23	13:BO:93:PRO:HA	1.72	0.70
15:AU:38:GLU:HG2	15:AU:39:LEU:N	2.05	0.70
1:AA:129:ARG:NH2	4:AD:256:ILE:HA	2.06	0.70
16:AV:63:CYS:SG	34:AV:201:HEM:CAB	2.74	0.70
2:BB:27:THR:HG22	2:BB:107:LEU:HD13	1.72	0.70
1:BA:93:PHE:CD2	1:BA:95:PRO:HD3	2.26	0.70
4:BD:192:THR:HG23	22:BD:402:CLA:HBC2	1.74	0.70
3:BC:158:THR:O	3:BC:251:HIS:HB3	1.92	0.70
5:BE:26:THR:HB	34:BE:101:HEM:HBB2	1.74	0.70
13:AO:77:LEU:HD23	13:AO:93:PRO:HA	1.74	0.70
4:BD:39:PRO:O	4:BD:43:LEU:HD22	1.91	0.70
13:AO:35:ASP:C	13:AO:36:ILE:HD12	2.12	0.70
13:AO:87:GLN:O	13:AO:88:GLU:HB3	1.91	0.70
18:BX:12:ILE:O	18:BX:12:ILE:HG23	1.89	0.70
16:AV:115:ALA:CB	16:AV:122:ARG:HD2	2.22	0.70
2:BB:137:LYS:HD2	7:BH:14:LEU:O	1.92	0.69
1:AA:93:PHE:CD2	1:AA:95:PRO:HD3	2.26	0.69
30:AB:623:LMG:H111	1:BA:72:LEU:HD13	1.74	0.69
3:BC:85:GLY:N	27:BC:517:DGD:HE4	2.06	0.69
1:BA:332:HIS:CD2	1:BA:333:GLU:HG3	2.27	0.69
6:BF:17:THR:HG23	6:BF:20:TRP:H	1.57	0.69
4:AD:55:VAL:HG21	4:AD:110:LEU:HD12	1.74	0.69
7:BH:38:PHE:HB2	26:BX:101:BCR:H10C	1.73	0.69
4:AD:152:VAL:HG21	4:AD:279:LEU:HD12	1.72	0.69
4:AD:122:LEU:HD11	23:AD:403:PHO:H92	1.74	0.69
13:AO:33:TYR:O	13:AO:37:VAL:HG23	1.92	0.69
5:BE:56:TYR:O	16:BV:27:ALA:HB2	1.92	0.69
4:BD:152:VAL:HG21	4:BD:279:LEU:HD12	1.74	0.69
3:AC:158:THR:O	3:AC:251:HIS:HB3	1.92	0.69
5:AE:26:THR:HB	34:AE:101:HEM:HBB2	1.74	0.69
3:AC:85:GLY:N	27:AC:517:DGD:HE4	2.07	0.69
5:AE:81:GLU:O	5:AE:83:LEU:N	2.24	0.69
18:BX:34:PHE:O	18:BX:38:ILE:HG12	1.91	0.69
16:BV:115:ALA:CB	16:BV:122:ARG:HD2	2.23	0.69
3:BC:254:THR:CG2	3:BC:255:THR:H	2.04	0.69
12:AM:33:GLN:CB	12:BM:33:GLN:HB3	2.19	0.69
2:BB:135:LEU:HD23	2:BB:138:MET:HE3	1.74	0.69
4:AD:39:PRO:O	4:AD:43:LEU:HD22	1.93	0.69
3:BC:348:GLU:OE2	13:BO:37:VAL:HA	1.93	0.69
4:AD:129:GLN:HE22	4:AD:143:ALA:HA	1.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:33:TYR:O	13:BO:37:VAL:HG23	1.92	0.69
4:AD:87:HIS:HD2	4:AD:162:LEU:HD23	1.58	0.69
2:BB:264:PRO:HG2	2:BB:267:LEU:HD12	1.74	0.69
15:BU:54:LYS:HB2	15:BU:113:THR:HG23	1.75	0.68
13:BO:178:ARG:CG	13:BO:178:ARG:NH1	2.53	0.68
4:AD:261:PHE:HB2	24:AD:405:PL9:H522	1.74	0.68
15:BU:38:GLU:HG2	15:BU:39:LEU:N	2.08	0.68
5:AE:15:THR:HG23	9:AJ:8:ILE:O	1.92	0.68
1:BA:129:ARG:NH2	4:BD:256:ILE:HD12	2.02	0.68
20:AZ:30:PRO:HG3	20:AZ:33:TRP:HZ3	1.58	0.68
7:AH:6:TRP:CE2	7:AH:10:ILE:HD11	2.27	0.68
4:AD:192:THR:HG23	22:AD:402:CLA:HBC2	1.74	0.68
1:AA:40:THR:HG21	1:AA:121:LEU:HD23	1.73	0.68
2:AB:4:PRO:HD2	2:AB:7:ARG:HD2	1.74	0.68
20:AZ:32:ASP:HB3	20:AZ:35:ARG:NH1	2.08	0.68
2:BB:284:ILE:HG12	2:BB:309:LEU:CD1	2.23	0.68
10:AK:19:ASP:N	10:AK:20:PRO:HD2	2.09	0.68
3:BC:166:ILE:O	3:BC:170:ILE:HG13	1.93	0.68
2:AB:135:LEU:HA	2:AB:138:MET:HE3	1.74	0.68
13:AO:206:GLU:H	13:AO:206:GLU:CD	1.97	0.68
2:BB:135:LEU:HB2	2:BB:136:PRO:HD3	1.75	0.68
1:AA:332:HIS:CD2	1:AA:333:GLU:HG3	2.27	0.68
1:AA:238:LYS:HD2	14:AT:32:LYS:HB3	1.76	0.68
4:BD:122:LEU:HD11	23:BD:403:PHO:H92	1.76	0.68
2:BB:103:LEU:HD21	22:BB:608:CLA:HMC3	1.75	0.68
22:AA:404:CLA:HAB	22:AD:402:CLA:H72	1.76	0.68
20:AZ:28:ALA:O	20:AZ:30:PRO:HD3	1.93	0.68
2:BB:315:ILE:HG22	2:BB:426:PHE:HB3	1.76	0.68
2:BB:4:PRO:HD2	2:BB:7:ARG:HD2	1.74	0.68
12:BM:31:SER:HB3	30:BM:102:LMG:HC71	1.76	0.68
2:AB:284:ILE:HG12	2:AB:309:LEU:CD1	2.23	0.68
22:BA:405:CLA:HAB	22:BD:402:CLA:H72	1.76	0.68
4:AD:279:LEU:HG	23:AD:403:PHO:HBC3	1.76	0.68
2:BB:135:LEU:HD23	2:BB:138:MET:CE	2.24	0.68
3:BC:415:ASN:O	3:BC:416:SER:HB3	1.94	0.68
4:BD:250:ASN:HD22	4:BD:262:SER:HB3	1.58	0.67
3:BC:305:THR:HG22	3:BC:308:GLU:CB	2.24	0.67
5:AE:81:GLU:C	5:AE:83:LEU:H	1.96	0.67
5:BE:81:GLU:C	5:BE:83:LEU:H	1.97	0.67
4:BD:180:ARG:HH11	4:BD:180:ARG:CG	2.07	0.67
4:AD:180:ARG:CG	4:AD:180:ARG:HH11	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BZ:33:TRP:O	20:BZ:37:LYS:HB2	1.93	0.67
2:BB:331:ASN:HB3	2:BB:437:LEU:HD12	1.75	0.67
3:AC:42:LEU:HD21	22:AC:511:CLA:H2A	1.74	0.67
3:BC:361:PHE:HA	27:BC:516:DGD:HE61	1.77	0.67
20:AZ:33:TRP:O	20:AZ:33:TRP:CD1	2.48	0.67
2:AB:483:ASP:OD2	2:AB:484:PRO:HD2	1.94	0.67
2:AB:264:PRO:HG2	2:AB:267:LEU:HD12	1.75	0.67
10:BK:19:ASP:N	10:BK:20:PRO:HD2	2.10	0.67
2:AB:135:LEU:HD23	2:AB:138:MET:CE	2.25	0.67
7:BH:6:TRP:CE2	7:BH:10:ILE:HD11	2.29	0.67
6:BF:11:VAL:HG12	6:BF:12:SER:N	2.09	0.67
24:BA:408:PL9:H33	4:BD:38:PHE:CD1	2.29	0.67
2:AB:270:PRO:HG3	2:AB:312:TYR:HD2	1.59	0.67
5:BE:27:ILE:HB	5:BE:28:PRO:HD3	1.77	0.67
13:BO:206:GLU:CD	13:BO:206:GLU:H	1.97	0.67
3:AC:472:LEU:HD12	3:AC:473:ASP:H	1.59	0.67
3:BC:215:LYS:HB3	3:BC:223:TRP:HA	1.77	0.67
3:AC:166:ILE:O	3:AC:170:ILE:HG13	1.94	0.67
1:AA:183:MET:HA	22:AA:402:CLA:HMD2	1.76	0.67
3:BC:391:ARG:HB2	3:BC:391:ARG:HH11	1.59	0.67
3:BC:75:PHE:HD1	3:BC:86:LEU:HD21	1.60	0.67
12:AM:31:SER:HB3	30:AM:101:LMG:HC71	1.77	0.67
6:AF:11:VAL:HG12	6:AF:12:SER:H	1.59	0.67
1:BA:174:LEU:HD22	23:BA:406:PHO:H151	1.75	0.67
4:BD:186:GLN:HB2	22:BD:402:CLA:HBC1	1.77	0.67
3:BC:155:ASN:HD21	3:BC:255:THR:CB	2.07	0.67
3:AC:215:LYS:HB3	3:AC:223:TRP:HA	1.77	0.67
2:AB:271:THR:CG2	2:AB:273:TYR:H	2.08	0.67
2:AB:133:LEU:HB3	2:AB:138:MET:CE	2.24	0.67
22:AB:602:CLA:H42	7:AH:45:ILE:HD11	1.76	0.67
2:BB:356:VAL:HG22	2:BB:370:LEU:HD21	1.77	0.67
3:AC:377:LEU:O	3:AC:381:LYS:HB2	1.95	0.67
5:AE:78:THR:O	5:AE:81:GLU:HB2	1.94	0.67
1:BA:32:TRP:HA	1:BA:32:TRP:CE3	2.30	0.67
3:BC:161:LEU:HG	3:BC:165:LEU:HD12	1.77	0.66
3:BC:449:ARG:HE	22:BC:505:CLA:CED	2.07	0.66
2:BB:483:ASP:OD2	2:BB:484:PRO:HD2	1.95	0.66
13:BO:92:VAL:HG12	13:BO:93:PRO:HD2	1.78	0.66
5:BE:81:GLU:O	5:BE:83:LEU:N	2.27	0.66
1:AA:161:TYR:HB3	1:AA:162:PRO:HD3	1.77	0.66
3:BC:377:LEU:O	3:BC:381:LYS:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:75:PHE:HD1	3:AC:86:LEU:HD21	1.59	0.66
2:BB:284:ILE:HG23	2:BB:305:ILE:HD12	1.76	0.66
6:BF:11:VAL:HG12	6:BF:12:SER:H	1.59	0.66
3:BC:42:LEU:HD21	22:BC:511:CLA:H2A	1.77	0.66
22:AC:507:CLA:H112	26:AC:515:BCR:H362	1.78	0.66
12:AM:23:ILE:HD13	30:AM:101:LMG:H182	1.78	0.66
3:AC:150:ASP:HB3	3:AC:153:ASP:HB2	1.77	0.66
2:AB:141:ILE:CG2	22:AB:615:CLA:HBB1	2.26	0.66
22:AC:505:CLA:HBA1	22:AC:505:CLA:HBD	1.77	0.66
15:AU:83:ALA:CB	15:AU:84:PRO:HD2	2.14	0.66
1:BA:183:MET:HA	22:BA:403:CLA:HMD2	1.76	0.66
5:BE:18:ARG:O	5:BE:22:ILE:HG13	1.95	0.66
5:BE:84:LYS:HZ2	5:BE:84:LYS:HB2	1.61	0.66
5:BE:15:THR:HG23	9:BJ:8:ILE:O	1.95	0.66
6:AF:11:VAL:HG12	6:AF:12:SER:N	2.09	0.66
1:BA:238:LYS:HD2	14:BT:32:LYS:HB3	1.76	0.66
11:BL:7:ARG:O	11:BL:7:ARG:HD2	1.96	0.66
3:AC:305:THR:HG22	3:AC:308:GLU:CB	2.26	0.66
3:BC:114:VAL:HG22	30:BC:520:LMG:H152	1.77	0.66
3:BC:30:SER:HB2	10:BK:46:ARG:O	1.95	0.66
1:BA:40:THR:HG21	1:BA:121:LEU:HD23	1.77	0.66
3:BC:89:ILE:N	3:BC:90:PRO:HD2	2.11	0.66
1:BA:343:LEU:O	1:BA:344:ALA:HB2	1.96	0.66
20:BZ:30:PRO:HG3	20:BZ:33:TRP:HZ3	1.60	0.66
3:AC:277:GLY:C	22:AC:505:CLA:HBC2	2.15	0.66
4:BD:279:LEU:HG	23:BD:403:PHO:HBC3	1.76	0.66
3:BC:277:GLY:C	22:BC:505:CLA:HBC2	2.16	0.66
2:BB:133:LEU:HB3	2:BB:138:MET:CE	2.26	0.66
2:AB:356:VAL:HG22	2:AB:370:LEU:CD2	2.26	0.66
13:BO:120:THR:HG22	13:BO:154:SER:OG	1.96	0.66
1:BA:77:ILE:HD11	14:BT:6:TYR:HB3	1.78	0.66
22:BC:505:CLA:HBA1	22:BC:505:CLA:HBD	1.78	0.65
2:BB:490:GLN:O	2:BB:490:GLN:OE1	2.15	0.65
4:AD:250:ASN:HD22	4:AD:262:SER:HB3	1.62	0.65
2:BB:327:THR:HG22	22:BB:610:CLA:H12	1.78	0.65
20:AZ:33:TRP:O	20:AZ:37:LYS:HB2	1.95	0.65
24:AA:407:PL9:H33	4:AD:38:PHE:CD1	2.31	0.65
5:BE:78:THR:O	5:BE:81:GLU:HB2	1.96	0.65
1:AA:81:ALA:HB2	1:AA:175:GLY:HA3	1.78	0.65
2:AB:224:ARG:HG2	7:AH:24:GLY:O	1.96	0.65
3:AC:161:LEU:HG	3:AC:165:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:89:ILE:N	3:AC:90:PRO:HD2	2.11	0.65
3:AC:55:ALA:HB1	26:AC:514:BCR:H373	1.78	0.65
20:BZ:33:TRP:CD1	20:BZ:33:TRP:O	2.50	0.65
1:AA:32:TRP:HA	1:AA:32:TRP:CE3	2.31	0.65
2:BB:247:PHE:HE1	22:BB:605:CLA:H101	1.61	0.65
13:AO:144:LEU:HD13	13:AO:259:VAL:HG11	1.78	0.65
2:AB:331:ASN:HB3	2:AB:437:LEU:HD12	1.79	0.65
2:BB:86:ILE:O	2:BB:86:ILE:HD12	1.96	0.65
2:BB:270:PRO:HG3	2:BB:312:TYR:HD2	1.61	0.65
2:BB:386:ALA:HB3	15:BU:132:LEU:HD11	1.79	0.65
3:AC:155:ASN:HD21	3:AC:255:THR:CB	2.07	0.65
13:AO:92:VAL:HG12	13:AO:93:PRO:HD2	1.78	0.65
3:AC:30:SER:HB2	10:AK:46:ARG:O	1.95	0.65
2:BB:356:VAL:HG22	2:BB:370:LEU:CD2	2.27	0.65
4:BD:103:ARG:HG3	5:BE:73:LYS:HG3	1.78	0.65
20:BZ:49:ALA:O	20:BZ:53:VAL:HG23	1.96	0.65
9:AJ:14:ALA:CB	26:AK:102:BCR:H393	2.27	0.65
4:BD:261:PHE:HB2	24:BD:405:PL9:H522	1.78	0.65
22:BC:507:CLA:H112	26:BC:515:BCR:H362	1.78	0.65
13:BO:87:GLN:O	13:BO:88:GLU:HB3	1.96	0.65
2:AB:222:PRO:HG3	7:AH:27:THR:H	1.61	0.65
2:AB:271:THR:HB	2:AB:274:GLN:HG3	1.78	0.65
22:BC:512:CLA:H143	22:BC:513:CLA:H162	1.79	0.65
20:BZ:28:ALA:O	20:BZ:30:PRO:HD3	1.97	0.65
2:AB:248:ALA:HA	22:AB:603:CLA:H42	1.79	0.65
11:AL:7:ARG:HD2	11:AL:7:ARG:O	1.97	0.65
13:AO:120:THR:HG22	13:AO:154:SER:OG	1.96	0.65
3:BC:187:ASP:HB2	3:BC:230:LEU:HD12	1.78	0.65
2:AB:490:GLN:O	2:AB:490:GLN:OE1	2.15	0.65
2:AB:247:PHE:HE1	22:AB:602:CLA:H101	1.62	0.64
22:BC:511:CLA:H151	20:BZ:20:VAL:HG13	1.78	0.64
27:BC:518:DGD:HD2	9:BJ:32:ALA:O	1.97	0.64
3:BC:55:ALA:HB1	26:BC:514:BCR:H373	1.77	0.64
14:BT:29:ILE:HD12	14:BT:29:ILE:N	2.10	0.64
3:AC:186:TYR:HE2	3:AC:188:THR:HG22	1.62	0.64
2:AB:86:ILE:HD12	2:AB:86:ILE:O	1.97	0.64
2:BB:271:THR:CG2	2:BB:273:TYR:H	2.08	0.64
22:BB:611:CLA:HMA1	4:BD:130:PHE:CE1	2.32	0.64
4:AD:88:SER:HB2	5:AE:69:ARG:NH2	2.11	0.64
2:AB:139:PHE:CZ	2:AB:143:LEU:HD22	2.32	0.64
4:BD:87:HIS:HD2	4:BD:162:LEU:HD23	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:449:ARG:HE	22:AC:505:CLA:CED	2.08	0.64
15:BU:94:ILE:O	15:BU:97:LEU:HG	1.98	0.64
3:BC:472:LEU:HD12	3:BC:473:ASP:H	1.62	0.64
3:BC:156:LYS:O	3:BC:160:ILE:HG13	1.97	0.64
13:AO:86:ARG:C	13:AO:86:ARG:HD2	2.18	0.64
2:AB:103:LEU:HD21	22:AB:605:CLA:HMC3	1.78	0.64
2:BB:271:THR:HB	2:BB:274:GLN:HG3	1.80	0.64
2:AB:327:THR:HG22	22:AB:607:CLA:H12	1.78	0.64
2:AB:135:LEU:HB2	2:AB:136:PRO:HD3	1.79	0.64
15:BU:58:ASN:ND2	15:BU:114:VAL:HG13	2.13	0.64
22:AC:511:CLA:H151	20:AZ:20:VAL:HG13	1.78	0.64
5:BE:26:THR:O	5:BE:29:ALA:HB3	1.97	0.64
4:BD:129:GLN:HE22	4:BD:143:ALA:HA	1.61	0.64
1:AA:174:LEU:HD22	23:AA:405:PHO:H151	1.78	0.64
22:BC:511:CLA:H171	20:BZ:20:VAL:HA	1.80	0.64
15:AU:66:ILE:O	15:AU:66:ILE:HG22	1.98	0.64
22:BC:505:CLA:CMD	22:BC:507:CLA:HAB	2.28	0.64
15:BU:66:ILE:HG22	15:BU:66:ILE:O	1.97	0.64
7:AH:35:MET:HE2	26:AH:101:BCR:HC21	1.80	0.64
13:AO:36:ILE:HG23	13:AO:41:LEU:HB3	1.80	0.64
1:AA:57:PRO:HG3	1:AA:68:SER:CB	2.28	0.64
2:AB:379:ALA:HA	2:AB:390:TYR:HB3	1.80	0.64
13:AO:117:GLY:O	13:AO:159:VAL:HG12	1.98	0.64
2:AB:286:ARG:HH11	2:AB:286:ARG:HG2	1.62	0.64
2:AB:284:ILE:HG23	2:AB:305:ILE:HD12	1.80	0.63
16:AV:143:GLY:O	16:AV:147:VAL:HG23	1.97	0.63
2:BB:379:ALA:HA	2:BB:390:TYR:HB3	1.79	0.63
12:BM:23:ILE:HD13	30:BM:102:LMG:H182	1.79	0.63
3:BC:204:LEU:HD21	3:BC:238:ILE:HG21	1.79	0.63
3:AC:209:ILE:HG23	26:AC:515:BCR:H382	1.81	0.63
3:BC:141:GLU:H	3:BC:141:GLU:CD	2.02	0.63
3:AC:310:SER:OG	3:AC:355:THR:HG23	1.98	0.63
13:BO:144:LEU:HD13	13:BO:259:VAL:HG11	1.80	0.63
2:BB:141:ILE:CG2	22:BB:618:CLA:HBB1	2.27	0.63
2:AB:386:ALA:HB3	15:AU:132:LEU:HD11	1.80	0.63
2:BB:139:PHE:CZ	2:BB:143:LEU:HD22	2.32	0.63
5:AE:36:LEU:O	5:AE:40:THR:HG23	1.98	0.63
3:BC:223:TRP:CD2	3:BC:224:ILE:HG13	2.34	0.63
4:AD:186:GLN:HB2	22:AD:402:CLA:HBC1	1.80	0.63
22:AB:602:CLA:H61	7:AH:46:LEU:HD13	1.80	0.63
2:AB:486:LEU:HD13	2:AB:486:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:150:ASP:HB3	3:BC:153:ASP:HB2	1.78	0.63
9:BJ:14:ALA:CB	26:BK:102:BCR:H393	2.28	0.63
29:AA:412:SQD:H311	22:AC:508:CLA:H71	1.81	0.63
27:AC:518:DGD:HD2	9:AJ:32:ALA:O	1.99	0.63
22:AC:511:CLA:H171	20:AZ:20:VAL:HA	1.79	0.63
10:BK:18:PHE:HD2	10:BK:18:PHE:N	1.96	0.63
3:AC:107:ASP:OD2	3:AC:110:PRO:HD3	1.99	0.63
13:BO:36:ILE:HG23	13:BO:41:LEU:HB3	1.79	0.63
1:BA:81:ALA:HB2	1:BA:175:GLY:HA3	1.80	0.63
2:AB:297:THR:OG1	2:AB:300:GLU:HG3	1.98	0.63
10:AK:18:PHE:HD2	10:AK:18:PHE:N	1.97	0.63
5:BE:79:PHE:O	5:BE:84:LYS:HB3	1.99	0.63
1:AA:190:HIS:HB3	1:AA:293:MET:HE2	1.81	0.63
13:BO:86:ARG:HD2	13:BO:86:ARG:C	2.19	0.63
5:BE:36:LEU:O	5:BE:40:THR:HG23	1.99	0.63
13:AO:230:VAL:CG1	13:AO:231:ASP:H	2.10	0.62
22:AB:605:CLA:HMB3	22:AB:606:CLA:H11	1.81	0.62
5:AE:27:ILE:HB	5:AE:28:PRO:HD3	1.80	0.62
7:BH:19:GLY:O	7:BH:21:VAL:HG13	1.98	0.62
5:AE:26:THR:O	5:AE:29:ALA:HB3	1.98	0.62
1:BA:57:PRO:HG3	1:BA:68:SER:CB	2.29	0.62
3:AC:337:LEU:HD12	13:AO:131:PRO:HG3	1.81	0.62
7:AH:19:GLY:O	7:AH:21:VAL:HG13	1.99	0.62
1:AA:29:TYR:CG	1:AA:133:LEU:HD13	2.34	0.62
20:BZ:32:ASP:HB3	20:BZ:35:ARG:NH1	2.13	0.62
2:BB:124:ARG:NE	2:BB:131:PRO:HD3	2.14	0.62
1:BA:89:ILE:HD11	1:BA:108:ASN:HB3	1.81	0.62
26:BK:102:BCR:HC8	26:BK:102:BCR:H331	1.82	0.62
26:BC:514:BCR:H312	20:BZ:9:LEU:HD11	1.80	0.62
3:AC:305:THR:HG22	3:AC:308:GLU:HB2	1.82	0.62
22:AC:505:CLA:CMD	22:AC:507:CLA:HAB	2.29	0.62
2:BB:224:ARG:HG2	7:BH:24:GLY:O	1.99	0.62
14:AT:29:ILE:N	14:AT:29:ILE:HD12	2.10	0.62
1:AA:142:TRP:HB2	4:AD:220:ASN:OD1	1.99	0.62
2:AB:356:VAL:HG22	2:AB:370:LEU:HD21	1.81	0.62
4:AD:160:TYR:HB3	4:AD:161:PRO:CD	2.30	0.62
3:BC:186:TYR:HE2	3:BC:188:THR:HG22	1.65	0.62
18:AX:11:THR:HG23	18:AX:12:ILE:HG22	1.81	0.62
2:AB:124:ARG:NE	2:AB:131:PRO:HD3	2.13	0.62
30:AD:408:LMG:HC62	11:AL:15:THR:HG21	1.82	0.62
5:AE:64:PRO:HB3	5:AE:84:LYS:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BB:605:CLA:H42	7:BH:45:ILE:HD11	1.82	0.62
1:BA:29:TYR:CG	1:BA:133:LEU:HD13	2.34	0.62
12:AM:28:GLN:HB3	12:BM:27:VAL:HG12	1.81	0.62
3:BC:310:SER:OG	3:BC:355:THR:HG23	2.00	0.62
6:BF:28:VAL:HB	6:BF:29:PRO:HD3	1.81	0.62
2:BB:222:PRO:HG3	7:BH:27:THR:H	1.63	0.62
3:AC:44:ASN:C	3:AC:45:LEU:HD12	2.20	0.62
4:AD:267:LEU:C	4:AD:267:LEU:HD23	2.20	0.62
4:AD:26:ARG:CD	6:AF:18:VAL:HG11	2.27	0.62
26:AC:514:BCR:H312	20:AZ:9:LEU:HD11	1.80	0.61
15:AU:58:ASN:ND2	15:AU:114:VAL:HG13	2.15	0.61
5:BE:64:PRO:HB3	5:BE:84:LYS:HE2	1.82	0.61
7:AH:58:VAL:O	7:AH:58:VAL:HG13	2.00	0.61
15:AU:94:ILE:O	15:AU:97:LEU:HG	2.00	0.61
1:BA:93:PHE:HZ	22:BA:407:CLA:HAA1	1.65	0.61
1:AA:93:PHE:HZ	22:AA:406:CLA:HAA1	1.64	0.61
1:AA:18:CYS:O	1:AA:22:THR:HG22	2.00	0.61
16:AV:102:MET:HE3	16:AV:141:ILE:HG21	1.81	0.61
1:BA:142:TRP:HB2	4:BD:220:ASN:OD1	2.01	0.61
15:AU:54:LYS:HB2	15:AU:113:THR:HG23	1.82	0.61
3:BC:209:ILE:HG23	26:BC:515:BCR:H382	1.81	0.61
12:AM:27:VAL:HG12	12:BM:28:GLN:HB3	1.80	0.61
1:AA:228:THR:HG22	1:AA:229:GLU:H	1.65	0.61
2:AB:192:PRO:HD2	7:AH:60:VAL:HG12	1.82	0.61
1:BA:228:THR:HG22	1:BA:229:GLU:H	1.66	0.61
1:BA:161:TYR:HB3	1:BA:162:PRO:HD3	1.82	0.61
2:AB:371:THR:HG22	2:AB:377:VAL:HA	1.81	0.61
1:BA:257:ARG:HG3	1:BA:257:ARG:HH11	1.65	0.61
3:BC:107:ASP:OD2	3:BC:110:PRO:HD3	1.99	0.61
22:AC:512:CLA:H143	22:AC:513:CLA:H162	1.82	0.61
3:AC:44:ASN:O	3:AC:45:LEU:HD12	1.99	0.61
20:BZ:55:GLY:HA2	26:BZ:101:BCR:H312	1.83	0.61
3:AC:248:GLY:O	3:AC:252:ILE:HG12	2.00	0.61
16:BV:143:GLY:O	16:BV:147:VAL:HG23	2.00	0.61
1:AA:89:ILE:HD11	1:AA:108:ASN:HB3	1.81	0.61
1:AA:343:LEU:O	1:AA:344:ALA:HB2	2.00	0.61
2:BB:471:ALA:HB2	4:BD:130:PHE:CZ	2.36	0.61
4:BD:55:VAL:HG21	4:BD:110:LEU:HD12	1.81	0.61
3:BC:318:LEU:HG	3:BC:328:VAL:HG11	1.83	0.61
16:BV:81:ARG:CZ	16:BV:157:GLY:HA3	2.30	0.61
2:BB:371:THR:HG22	2:BB:377:VAL:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:77:ILE:HD11	14:AT:6:TYR:HB3	1.82	0.61
10:BK:17:ILE:HD12	10:BK:17:ILE:N	2.16	0.61
15:AU:97:LEU:O	15:AU:102:LYS:HE2	2.01	0.61
3:AC:52:ALA:HA	22:AC:511:CLA:HMB3	1.82	0.61
2:AB:264:PRO:CG	2:AB:267:LEU:HD12	2.31	0.61
4:AD:342:PRO:O	4:AD:345:VAL:HG12	2.01	0.61
2:BB:172:TYR:O	2:BB:174:LEU:HG	2.00	0.61
16:AV:90:PRO:O	16:AV:92:ARG:HD3	2.01	0.61
3:BC:337:LEU:HD12	13:BO:131:PRO:HG3	1.83	0.61
6:AF:28:VAL:HB	6:AF:29:PRO:HD3	1.83	0.61
4:AD:209:LEU:C	4:AD:209:LEU:HD23	2.21	0.61
30:BD:408:LMG:HC62	11:BL:15:THR:HG21	1.82	0.61
5:BE:18:ARG:NH1	5:BE:18:ARG:HB3	2.14	0.61
22:AB:608:CLA:HMA1	4:AD:130:PHE:CE1	2.36	0.61
5:AE:18:ARG:O	5:AE:22:ILE:HG13	2.00	0.60
2:BB:486:LEU:O	2:BB:486:LEU:HD13	2.01	0.60
10:BK:18:PHE:N	10:BK:18:PHE:CD2	2.68	0.60
2:BB:68:ARG:HH11	2:BB:262:THR:HG23	1.67	0.60
1:BA:202:VAL:HG11	22:BA:405:CLA:OBD	1.99	0.60
3:BC:112:PHE:O	3:BC:116:VAL:HG13	2.01	0.60
10:AK:17:ILE:N	10:AK:17:ILE:HD12	2.17	0.60
29:BA:413:SQD:H311	22:BC:508:CLA:H71	1.83	0.60
18:BX:11:THR:HG23	18:BX:12:ILE:HG22	1.82	0.60
13:AO:39:THR:OG1	13:AO:41:LEU:HB2	2.01	0.60
4:AD:103:ARG:HG3	5:AE:73:LYS:HG3	1.83	0.60
13:AO:234:THR:OG1	13:AO:236:GLU:HG2	2.00	0.60
1:AA:60:ILE:HD12	1:AA:84:PRO:HD2	1.83	0.60
4:BD:250:ASN:ND2	4:BD:262:SER:HB3	2.17	0.60
3:AC:391:ARG:HD2	3:AC:395:TYR:CE2	2.36	0.60
5:BE:4:THR:HG22	5:BE:5:THR:N	2.16	0.60
3:AC:143:TYR:O	3:AC:144:SER:HB2	2.00	0.60
3:AC:461:ARG:HH11	3:AC:461:ARG:HG3	1.65	0.60
5:AE:23:HIS:HA	5:AE:26:THR:OG1	2.00	0.60
7:BH:12:ARG:HD3	7:BH:12:ARG:C	2.22	0.60
2:AB:471:ALA:HB2	4:AD:130:PHE:CZ	2.36	0.60
4:AD:199:MET:HB3	24:AD:405:PL9:H28	1.84	0.60
26:AK:102:BCR:H331	26:AK:102:BCR:HC8	1.83	0.60
3:BC:305:THR:HG22	3:BC:308:GLU:HB2	1.83	0.60
4:AD:49:LEU:O	4:AD:53:THR:HG23	2.01	0.60
20:AZ:32:ASP:CB	20:AZ:35:ARG:HG2	2.30	0.60
2:BB:222:PRO:HG3	7:BH:26:GLY:HA3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:29:TYR:CD2	1:BA:133:LEU:HD13	2.37	0.60
1:BA:214:MET:HE3	1:BA:214:MET:HA	1.82	0.60
12:AM:20:VAL:HG22	12:BM:20:VAL:HG11	1.84	0.60
2:AB:208:VAL:HG21	22:AB:602:CLA:HMC1	1.84	0.60
2:BB:208:VAL:HG21	22:BB:605:CLA:HMC1	1.83	0.60
3:BC:143:TYR:O	3:BC:144:SER:HB2	2.01	0.60
2:AB:213:GLY:O	2:AB:217:ILE:HG13	2.02	0.60
5:AE:4:THR:HG22	5:AE:5:THR:N	2.17	0.60
3:BC:52:ALA:HA	22:BC:511:CLA:HMB3	1.84	0.60
13:AO:31:LEU:HD12	13:AO:31:LEU:N	2.17	0.60
3:AC:186:TYR:CE2	3:AC:188:THR:HG22	2.37	0.60
2:AB:315:ILE:HG22	2:AB:426:PHE:HB3	1.82	0.60
1:BA:306:VAL:HG13	1:BA:314:ILE:O	2.01	0.60
2:AB:41:GLU:OE1	2:AB:63:LEU:HB2	2.02	0.60
3:AC:318:LEU:HG	3:AC:328:VAL:HG11	1.82	0.60
20:AZ:33:TRP:HD1	20:AZ:33:TRP:O	1.84	0.60
13:BO:39:THR:OG1	13:BO:41:LEU:HB2	2.02	0.60
13:BO:117:GLY:O	13:BO:159:VAL:HG12	2.01	0.60
4:BD:239:GLN:O	4:BD:240:ALA:HB3	2.02	0.60
3:AC:114:VAL:HG22	30:AC:520:LMG:H152	1.83	0.60
1:AA:153:SER:CB	22:AA:402:CLA:H11	2.32	0.60
1:AA:202:VAL:HG11	22:AA:404:CLA:OBD	2.02	0.60
16:BV:90:PRO:O	16:BV:92:ARG:HD3	2.02	0.60
4:AD:56:THR:HG21	5:AE:50:PRO:HD3	1.84	0.60
3:AC:223:TRP:CD2	3:AC:224:ILE:HG13	2.37	0.59
2:BB:213:GLY:O	2:BB:217:ILE:HG13	2.02	0.59
1:AA:306:VAL:HG13	1:AA:314:ILE:O	2.01	0.59
4:BD:267:LEU:C	4:BD:267:LEU:HD23	2.21	0.59
5:AE:79:PHE:O	5:AE:84:LYS:HB3	2.01	0.59
1:AA:214:MET:HE3	1:AA:214:MET:HA	1.83	0.59
12:AM:20:VAL:HG11	12:BM:20:VAL:HG22	1.83	0.59
5:AE:18:ARG:NH1	5:AE:18:ARG:HB3	2.17	0.59
15:BU:97:LEU:O	15:BU:102:LYS:HE2	2.02	0.59
3:BC:155:ASN:O	3:BC:158:THR:HG22	2.03	0.59
5:BE:26:THR:HB	34:BE:101:HEM:CBB	2.32	0.59
22:AD:404:CLA:HMD2	32:AD:411:LMT:H22	1.85	0.59
22:AC:502:CLA:H111	22:AC:503:CLA:HMB2	1.84	0.59
3:BC:461:ARG:HH11	3:BC:461:ARG:HG3	1.68	0.59
15:BU:113:THR:O	15:BU:114:VAL:HG23	2.02	0.59
10:AK:21:LEU:HD11	26:AK:102:BCR:HC32	1.84	0.59
10:AK:18:PHE:CD2	10:AK:18:PHE:N	2.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:AT:102:BCR:H393	22:BB:610:CLA:HAC2	1.83	0.59
1:BA:13:LEU:HD12	1:BA:13:LEU:H	1.68	0.59
10:AK:40:GLN:HA	10:AK:43:VAL:HG12	1.83	0.59
4:BD:87:HIS:CD2	4:BD:162:LEU:HD23	2.38	0.59
4:BD:209:LEU:HD23	4:BD:209:LEU:C	2.23	0.59
1:BA:153:SER:CB	22:BA:403:CLA:H11	2.33	0.59
2:AB:222:PRO:HG3	7:AH:26:GLY:HA3	1.83	0.59
16:BV:125:ASP:HA	16:BV:131:ARG:HH21	1.68	0.59
1:AA:257:ARG:HH11	1:AA:257:ARG:HG3	1.66	0.59
11:AL:7:ARG:C	11:AL:8:GLN:HE21	2.06	0.59
22:BC:502:CLA:H111	22:BC:503:CLA:HMB2	1.84	0.59
5:BE:76:VAL:O	5:BE:80:LEU:HD22	2.03	0.59
1:BA:272:HIS:CD2	4:BD:218:VAL:HG21	2.38	0.59
2:AB:68:ARG:HH11	2:AB:262:THR:HG23	1.68	0.59
3:AC:124:VAL:HB	26:AZ:101:BCR:H362	1.84	0.59
3:BC:343:ARG:NH1	3:BC:347:GLY:O	2.35	0.59
15:BU:83:ALA:CB	15:BU:84:PRO:CD	2.78	0.59
15:AU:113:THR:O	15:AU:114:VAL:HG23	2.02	0.59
22:BB:605:CLA:H61	7:BH:46:LEU:HD13	1.84	0.59
4:BD:274:VAL:HA	24:BD:405:PL9:H253	1.85	0.59
5:AE:26:THR:HB	34:AE:101:HEM:CBB	2.33	0.59
3:BC:124:VAL:HB	26:BZ:101:BCR:H362	1.84	0.59
20:BZ:32:ASP:CB	20:BZ:35:ARG:HG2	2.32	0.59
2:BB:264:PRO:CG	2:BB:267:LEU:HD12	2.32	0.59
5:AE:76:VAL:O	5:AE:80:LEU:HD22	2.03	0.59
13:BO:123:GLU:HG2	13:BO:124:GLU:N	2.17	0.59
7:BH:35:MET:HE2	26:BX:101:BCR:HC21	1.85	0.58
20:BZ:33:TRP:HD1	20:BZ:33:TRP:O	1.86	0.58
20:BZ:36:SER:OG	20:BZ:39:LEU:HD12	2.03	0.58
2:BB:192:PRO:HD2	7:BH:60:VAL:HG12	1.85	0.58
4:AD:55:VAL:HG21	4:AD:110:LEU:CD1	2.33	0.58
4:BD:18:LEU:HD22	18:BX:38:ILE:CD1	2.32	0.58
22:AB:615:CLA:H143	22:AB:616:CLA:HMA3	1.85	0.58
11:BL:7:ARG:C	11:BL:8:GLN:HE21	2.04	0.58
3:BC:248:GLY:O	3:BC:252:ILE:HG12	2.02	0.58
3:BC:318:LEU:HD23	3:BC:318:LEU:C	2.23	0.58
3:AC:305:THR:HG23	3:AC:307:PRO:CD	2.32	0.58
1:AA:13:LEU:HD12	1:AA:13:LEU:H	1.69	0.58
10:BK:40:GLN:HA	10:BK:43:VAL:HG12	1.85	0.58
3:AC:318:LEU:C	3:AC:318:LEU:HD23	2.24	0.58
3:AC:204:LEU:HD21	3:AC:238:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:123:GLU:HG2	13:AO:124:GLU:N	2.18	0.58
2:AB:212:ALA:HB2	22:AB:609:CLA:HMC3	1.85	0.58
3:AC:112:PHE:O	3:AC:116:VAL:HG13	2.03	0.58
16:BV:135:GLU:O	16:BV:139:VAL:HG23	2.03	0.58
3:AC:141:GLU:CD	3:AC:141:GLU:H	2.05	0.58
10:BK:18:PHE:CE1	20:BZ:9:LEU:HG	2.39	0.58
1:BA:82:VAL:HB	1:BA:174:LEU:HB2	1.85	0.58
6:AF:19:ARG:O	6:AF:23:VAL:HG23	2.03	0.58
2:BB:112:CYS:HB3	26:BB:622:BCR:H393	1.85	0.58
32:BB:626:LMT:H102	7:BH:35:MET:SD	2.43	0.58
3:BC:165:LEU:HD21	22:BC:506:CLA:HHC	1.85	0.58
22:AB:607:CLA:HAC2	26:AB:618:BCR:H393	1.84	0.58
1:BA:143:ILE:HD11	4:BD:217:THR:HA	1.86	0.58
2:AB:188:ASP:OD1	7:AH:58:VAL:HA	2.03	0.58
15:AU:38:GLU:HG2	15:AU:39:LEU:H	1.68	0.58
4:BD:342:PRO:O	4:BD:345:VAL:HG12	2.04	0.58
1:BA:249:VAL:HG11	2:BB:486:LEU:HD23	1.86	0.58
22:BD:404:CLA:HMD2	32:BD:411:LMT:H22	1.84	0.58
3:AC:156:LYS:O	3:AC:160:ILE:HG13	2.03	0.58
7:BH:58:VAL:HG13	7:BH:58:VAL:O	2.02	0.58
4:BD:18:LEU:O	4:BD:22:LEU:HG	2.02	0.58
3:AC:369:LEU:HD21	3:AC:384:ILE:HD13	1.85	0.58
3:AC:380:ILE:HA	3:AC:384:ILE:HD11	1.85	0.58
1:BA:49:VAL:O	1:BA:53:ILE:HG13	2.04	0.58
7:AH:12:ARG:HD3	7:AH:12:ARG:C	2.24	0.58
4:BD:160:TYR:HB3	4:BD:161:PRO:CD	2.33	0.58
22:BC:505:CLA:H92	22:BC:505:CLA:HAB	1.85	0.58
3:AC:131:TYR:HE1	3:AC:135:ARG:HD2	1.68	0.58
2:AB:329:PRO:HD3	22:AB:607:CLA:HED2	1.86	0.58
2:BB:188:ASP:OD1	7:BH:58:VAL:HA	2.04	0.58
4:AD:18:LEU:HD22	18:AX:38:ILE:CD1	2.34	0.58
4:AD:239:GLN:O	4:AD:240:ALA:HB3	2.03	0.58
1:BA:60:ILE:HD12	1:BA:84:PRO:HD2	1.86	0.58
20:AZ:16:SER:O	20:AZ:20:VAL:HG23	2.04	0.58
4:AD:87:HIS:CD2	4:AD:162:LEU:HD23	2.37	0.58
16:AV:74:THR:O	16:AV:75:ASN:HB2	2.04	0.58
3:BC:44:ASN:O	3:BC:45:LEU:HD12	2.04	0.58
15:BU:57:LEU:HD22	15:BU:79:ILE:HG21	1.86	0.58
3:AC:447:ARG:NH1	3:AC:447:ARG:HG2	2.16	0.57
5:AE:84:LYS:HB2	5:AE:84:LYS:HZ2	1.68	0.57
1:BA:190:HIS:HB3	1:BA:293:MET:HE2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:133:LEU:HB3	2:BB:138:MET:HE2	1.86	0.57
1:AA:238:LYS:O	1:AA:241:GLN:HG3	2.03	0.57
20:BZ:5:PHE:HA	20:BZ:57:LEU:CD2	2.34	0.57
2:AB:6:TYR:HA	22:AB:611:CLA:H11	1.85	0.57
10:BK:31:LEU:O	10:BK:34:ALA:HB3	2.04	0.57
2:AB:149:LEU:HG	22:AB:603:CLA:CBC	2.29	0.57
2:AB:172:TYR:O	2:AB:174:LEU:HG	2.02	0.57
16:AV:81:ARG:CZ	16:AV:157:GLY:HA3	2.34	0.57
13:BO:180:ALA:HB1	13:BO:191:ALA:HB2	1.86	0.57
4:AD:188:PHE:HE2	4:AD:329:MET:CE	2.17	0.57
1:BA:140:ARG:HH22	28:BA:412:LHG:P	2.27	0.57
4:AD:36:LEU:O	4:AD:39:PRO:HD2	2.05	0.57
11:AL:11:GLU:HG2	11:AL:12:LEU:N	2.19	0.57
20:AZ:14:ILE:O	20:AZ:18:VAL:HG23	2.04	0.57
10:AK:17:ILE:H	10:AK:17:ILE:HD12	1.69	0.57
20:BZ:16:SER:O	20:BZ:20:VAL:HG23	2.04	0.57
22:BB:618:CLA:H143	22:BB:619:CLA:HMA3	1.85	0.57
6:BF:19:ARG:O	6:BF:23:VAL:HG23	2.04	0.57
18:AX:45:LYS:N	18:AX:45:LYS:HD3	2.20	0.57
3:AC:130:VAL:O	3:AC:134:ILE:HG12	2.04	0.57
10:AK:31:LEU:O	10:AK:34:ALA:HB3	2.04	0.57
4:AD:252:PHE:O	4:AD:256:ILE:HG22	2.05	0.57
13:AO:80:GLU:O	13:AO:89:ALA:HB1	2.05	0.57
1:AA:38:ILE:O	1:AA:42:LEU:HG	2.05	0.57
4:AD:18:LEU:O	4:AD:22:LEU:HG	2.05	0.57
4:BD:36:LEU:O	4:BD:39:PRO:HD2	2.05	0.57
13:BO:118:SER:HB3	13:BO:157:PRO:HA	1.87	0.57
4:BD:188:PHE:HE2	4:BD:329:MET:CE	2.17	0.57
15:AU:57:LEU:HD22	15:AU:79:ILE:HG21	1.87	0.57
3:AC:37:ALA:HA	22:AC:508:CLA:O1A	2.04	0.57
22:AC:505:CLA:HAB	22:AC:505:CLA:H92	1.87	0.57
1:AA:11:ALA:O	1:AA:12:ASN:CB	2.53	0.57
2:AB:133:LEU:HB3	2:AB:138:MET:HE2	1.86	0.57
3:BC:44:ASN:C	3:BC:45:LEU:HD12	2.25	0.57
4:BD:346:LEU:O	4:BD:348:ARG:HG3	2.05	0.57
2:BB:248:ALA:HA	22:BB:606:CLA:H42	1.86	0.57
12:AM:29:THR:O	12:AM:32:GLN:HG3	2.05	0.57
10:AK:26:PRO:O	10:AK:29:PRO:HD2	2.05	0.57
10:AK:18:PHE:CE1	20:AZ:9:LEU:HG	2.40	0.57
5:AE:7:GLU:CD	5:AE:7:GLU:H	2.07	0.57
20:BZ:36:SER:HA	20:BZ:39:LEU:CG	2.31	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:174:LEU:HD23	2:AB:308:LYS:HG2	1.87	0.57
3:BC:130:VAL:O	3:BC:134:ILE:HG12	2.04	0.57
10:BK:26:PRO:O	10:BK:29:PRO:HD2	2.04	0.57
3:BC:37:ALA:HA	22:BC:508:CLA:O1A	2.05	0.57
4:BD:18:LEU:HD22	18:BX:38:ILE:HD13	1.85	0.57
2:AB:256:MET:HA	2:AB:263:THR:HG21	1.87	0.57
4:BD:56:THR:HG21	5:BE:50:PRO:HD3	1.86	0.57
3:AC:343:ARG:NH1	3:AC:347:GLY:O	2.38	0.57
5:AE:84:LYS:HZ3	5:AE:84:LYS:HB2	1.70	0.57
18:BX:45:LYS:N	18:BX:45:LYS:HD3	2.19	0.57
2:BB:41:GLU:OE1	2:BB:63:LEU:HB2	2.04	0.57
4:BD:199:MET:HB3	24:BD:405:PL9:H28	1.86	0.56
22:BB:608:CLA:HMB3	22:BB:609:CLA:H11	1.86	0.56
13:BO:230:VAL:CG1	13:BO:231:ASP:H	2.12	0.56
3:AC:165:LEU:HD21	22:AC:506:CLA:HHC	1.85	0.56
4:AD:266:TRP:CD1	30:AD:408:LMG:HC3	2.40	0.56
24:AD:405:PL9:H13	30:AD:408:LMG:H132	1.87	0.56
13:BO:31:LEU:HD12	13:BO:31:LEU:N	2.19	0.56
3:BC:391:ARG:HD2	3:BC:395:TYR:CE2	2.40	0.56
2:AB:191:ASN:ND2	7:AH:60:VAL:HA	2.20	0.56
3:BC:186:TYR:CE2	3:BC:188:THR:HG22	2.39	0.56
4:BD:157:PHE:CE1	4:BD:171:PRO:HG2	2.40	0.56
15:BU:100:ARG:HH11	15:BU:103:GLN:HG2	1.70	0.56
15:AU:89:GLU:H	15:AU:89:GLU:CD	2.09	0.56
2:BB:414:PRO:HB2	2:BB:415:PRO:CD	2.33	0.56
2:BB:212:ALA:HB2	22:BB:612:CLA:HMC3	1.86	0.56
2:AB:230:ARG:O	2:AB:233:ASN:HB3	2.05	0.56
3:BC:305:THR:HG22	3:BC:308:GLU:N	2.16	0.56
20:BZ:29:SER:HB2	20:BZ:31:GLN:HG3	1.88	0.56
1:AA:249:VAL:HG11	2:AB:486:LEU:HD23	1.87	0.56
6:BF:21:VAL:O	6:BF:25:THR:HG23	2.06	0.56
1:AA:272:HIS:CD2	4:AD:218:VAL:HG21	2.40	0.56
5:BE:23:HIS:HA	5:BE:26:THR:OG1	2.05	0.56
2:AB:61:PHE:CE1	22:AB:607:CLA:HMB3	2.41	0.56
2:BB:286:ARG:HG2	2:BB:286:ARG:NH1	2.17	0.56
2:BB:297:THR:OG1	2:BB:300:GLU:HG3	2.04	0.56
20:BZ:26:ALA:CB	20:BZ:40:ILE:HD11	2.36	0.56
16:AV:87:LEU:HD12	16:AV:87:LEU:N	2.20	0.56
9:BJ:14:ALA:HB3	26:BK:102:BCR:H393	1.88	0.56
10:BK:21:LEU:HD11	26:BK:102:BCR:HC32	1.87	0.56
13:BO:80:GLU:O	13:BO:89:ALA:HB1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AA:416:LMG:H112	2:BB:43:ALA:HA	1.87	0.56
3:BC:305:THR:HG23	3:BC:307:PRO:CD	2.32	0.56
20:AZ:55:GLY:HA2	26:AZ:101:BCR:H312	1.87	0.56
4:AD:274:VAL:HA	24:AD:405:PL9:H253	1.86	0.56
1:AA:265:PHE:CD1	1:AA:271:LEU:HA	2.41	0.56
26:AA:409:BCR:H321	29:AA:415:SQD:H321	1.87	0.56
22:BC:501:CLA:H42	22:BC:502:CLA:HMD1	1.88	0.56
2:AB:133:LEU:HB3	2:AB:138:MET:HE1	1.86	0.56
4:BD:85:MET:CE	5:BE:69:ARG:HA	2.35	0.56
13:BO:154:SER:O	13:BO:168:PHE:HA	2.05	0.56
20:BZ:23:VAL:O	20:BZ:26:ALA:HB3	2.06	0.56
1:BA:18:CYS:O	1:BA:22:THR:HG22	2.05	0.56
12:BM:29:THR:O	12:BM:32:GLN:HG3	2.06	0.56
16:BV:59:PHE:HA	16:BV:63:CYS:SG	2.46	0.56
10:BK:24:VAL:O	10:BK:27:VAL:HG12	2.06	0.56
30:BD:408:LMG:H111	11:BL:19:LEU:HD21	1.87	0.56
13:BO:178:ARG:HG3	13:BO:178:ARG:NH1	2.00	0.56
2:BB:12:LEU:HB2	22:BB:615:CLA:HMC2	1.88	0.56
4:AD:152:VAL:HG21	4:AD:279:LEU:CD1	2.35	0.56
7:AH:58:VAL:O	7:AH:58:VAL:CG1	2.53	0.56
1:AA:244:GLU:HG3	1:AA:246:TYR:H	1.70	0.56
3:AC:374:GLY:O	3:AC:375:LEU:C	2.44	0.56
4:BD:26:ARG:CD	6:BF:18:VAL:HG11	2.29	0.56
1:AA:140:ARG:HH22	28:AA:411:LHG:P	2.28	0.56
3:BC:239:TRP:CE3	3:BC:243:ILE:HD11	2.40	0.56
3:AC:149:TYR:HA	3:AC:156:LYS:HD3	1.88	0.56
13:BO:141:ARG:HH11	13:BO:141:ARG:HG2	1.71	0.56
3:BC:429:SER:HB3	27:BC:517:DGD:HA81	1.88	0.56
1:AA:240:GLY:HA3	14:AT:29:ILE:HG22	1.88	0.56
4:AD:199:MET:HG2	24:AD:405:PL9:H322	1.86	0.56
1:BA:265:PHE:CD1	1:BA:271:LEU:HA	2.41	0.56
2:AB:191:ASN:HD21	7:AH:60:VAL:HA	1.70	0.56
1:AA:84:PRO:HA	1:AA:112:TYR:CG	2.40	0.56
2:BB:434:THR:HG23	13:BO:204:LYS:HE3	1.86	0.56
3:BC:374:GLY:O	3:BC:375:LEU:C	2.44	0.56
2:AB:112:CYS:HB3	26:AB:620:BCR:H393	1.88	0.56
22:BB:611:CLA:H42	4:BD:127:LEU:HD11	1.86	0.56
2:AB:12:LEU:HD22	2:AB:18:ARG:HB2	1.87	0.56
18:AX:12:ILE:HG12	18:AX:16:LEU:CD1	2.31	0.56
20:AZ:29:SER:HB2	20:AZ:31:GLN:HG3	1.88	0.56
1:BA:11:ALA:O	1:BA:12:ASN:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:191:ASN:HB2	7:BH:58:VAL:CG2	2.36	0.56
13:AO:31:LEU:H	13:AO:31:LEU:HD12	1.71	0.56
2:AB:191:ASN:HB2	7:AH:58:VAL:CG2	2.36	0.56
2:BB:170:ASP:HB2	2:BB:171:PRO:CD	2.36	0.56
9:AJ:14:ALA:HB1	26:AK:102:BCR:H393	1.88	0.56
29:BA:413:SQD:H223	27:BC:518:DGD:HAE1	1.88	0.56
10:BK:17:ILE:HD12	10:BK:17:ILE:H	1.71	0.56
16:AV:125:ASP:HA	16:AV:131:ARG:HH21	1.70	0.56
1:AA:104:GLU:OE2	13:AO:99:ARG:HD3	2.06	0.56
16:BV:102:MET:HE3	16:BV:141:ILE:HG21	1.88	0.56
4:BD:60:THR:HG23	4:BD:61:HIS:HD2	1.70	0.55
20:AZ:23:VAL:O	20:AZ:26:ALA:HB3	2.07	0.55
16:BV:29:LEU:HD11	16:BV:34:LEU:HD21	1.87	0.55
3:AC:199:ILE:N	3:AC:199:ILE:HD12	2.22	0.55
8:AI:11:VAL:O	8:AI:15:PHE:HD2	1.89	0.55
24:BD:405:PL9:H13	30:BD:408:LMG:H132	1.87	0.55
14:AT:7:VAL:HG12	32:AT:101:LMT:H122	1.89	0.55
4:AD:250:ASN:ND2	4:AD:262:SER:HB3	2.21	0.55
13:BO:83:LYS:HG2	13:BO:84:ASN:N	2.20	0.55
2:AB:43:ALA:HA	30:AB:623:LMG:H112	1.87	0.55
4:AD:267:LEU:O	4:AD:267:LEU:HD23	2.06	0.55
20:BZ:5:PHE:HA	20:BZ:57:LEU:HD21	1.88	0.55
20:AZ:26:ALA:CB	20:AZ:40:ILE:HD11	2.36	0.55
3:AC:305:THR:HG22	3:AC:308:GLU:N	2.16	0.55
13:AO:83:LYS:HE2	2:BB:338:GLN:HA	1.87	0.55
4:BD:221:THR:HG23	4:BD:244:TYR:HB2	1.87	0.55
15:BU:38:GLU:HG2	15:BU:39:LEU:H	1.71	0.55
4:BD:267:LEU:HD23	4:BD:267:LEU:O	2.07	0.55
1:BA:104:GLU:OE2	13:BO:99:ARG:HD3	2.06	0.55
4:BD:53:THR:HG22	4:BD:67:TYR:CD2	2.41	0.55
13:BO:86:ARG:HH11	13:BO:87:GLN:HA	1.71	0.55
6:BF:16:PHE:CD2	29:BF:101:SQD:H262	2.41	0.55
4:BD:49:LEU:O	4:BD:53:THR:HG23	2.06	0.55
2:AB:170:ASP:HB2	2:AB:171:PRO:CD	2.36	0.55
3:AC:350:ILE:HG21	3:AC:359:TRP:HB2	1.88	0.55
3:BC:350:ILE:HG21	3:BC:359:TRP:HB2	1.89	0.55
1:BA:140:ARG:NH2	1:BA:142:TRP:HZ3	2.05	0.55
1:AA:29:TYR:CD2	1:AA:133:LEU:HD13	2.41	0.55
3:BC:107:ASP:OD2	3:BC:109:PHE:HB3	2.06	0.55
2:BB:6:TYR:HA	22:BB:614:CLA:H11	1.88	0.55
1:BA:238:LYS:O	1:BA:241:GLN:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:AD:407:LMG:O3	9:AJ:37:GLY:HA3	2.07	0.55
1:BA:244:GLU:HG3	1:BA:246:TYR:H	1.71	0.55
13:AO:66:ILE:HD12	13:AO:121:PHE:CD1	2.42	0.55
4:AD:157:PHE:CE1	4:AD:171:PRO:HG2	2.41	0.55
3:BC:346:THR:O	13:BO:40:GLY:HA2	2.07	0.55
1:BA:131:TRP:CE3	1:BA:132:GLU:N	2.74	0.55
22:AB:608:CLA:H42	4:AD:127:LEU:HD11	1.88	0.55
3:AC:95:LEU:HD13	22:AC:502:CLA:H143	1.89	0.55
18:BX:12:ILE:CG1	18:BX:16:LEU:HD12	2.36	0.55
1:AA:37:MET:HG2	1:AA:41:LEU:HD12	1.89	0.55
5:AE:55:TYR:O	5:AE:84:LYS:HE3	2.07	0.55
2:BB:174:LEU:HD23	2:BB:308:LYS:HG2	1.87	0.55
2:BB:183:PRO:HB2	2:BB:185:TRP:CH2	2.41	0.55
20:BZ:21:ILE:O	20:BZ:25:VAL:HG22	2.07	0.55
1:AA:131:TRP:CE3	1:AA:132:GLU:N	2.75	0.55
1:BA:64:ARG:NH1	13:BO:98:THR:HG21	2.22	0.55
4:BD:77:ALA:HB2	4:BD:174:GLY:HA3	1.88	0.55
3:AC:45:LEU:HD23	3:AC:48:LYS:HD2	1.89	0.55
13:BO:66:ILE:HD12	13:BO:121:PHE:CD1	2.41	0.55
20:AZ:36:SER:HA	20:AZ:39:LEU:CG	2.35	0.55
4:BD:53:THR:HG22	4:BD:67:TYR:CE2	2.42	0.55
4:AD:189:HIS:HA	4:AD:294:ARG:HD2	1.88	0.55
16:AV:59:PHE:HA	16:AV:63:CYS:SG	2.47	0.55
4:BD:152:VAL:HG21	4:BD:279:LEU:CD1	2.36	0.55
4:AD:180:ARG:CG	4:AD:180:ARG:NH1	2.70	0.55
3:BC:239:TRP:HE3	3:BC:243:ILE:HD11	1.71	0.55
3:AC:107:ASP:OD2	3:AC:109:PHE:HB3	2.06	0.55
4:BD:88:SER:HB2	5:BE:69:ARG:CZ	2.36	0.55
18:AX:32:LEU:N	18:AX:32:LEU:HD23	2.22	0.55
9:AJ:14:ALA:HB3	26:AK:102:BCR:H393	1.89	0.54
3:BC:425:TRP:CE2	22:BC:504:CLA:HBA1	2.42	0.54
1:BA:38:ILE:O	1:BA:42:LEU:HG	2.06	0.54
1:AA:217:SER:HA	1:AA:220:THR:HG22	1.88	0.54
4:BD:199:MET:HG2	24:BD:405:PL9:H322	1.89	0.54
2:BB:154:GLY:O	2:BB:159:THR:HG23	2.07	0.54
4:BD:334:GLN:N	4:BD:335:PRO:HD3	2.22	0.54
16:BV:35:THR:HG23	16:BV:46:THR:OG1	2.07	0.54
13:AO:180:ALA:HB1	13:AO:191:ALA:HB2	1.89	0.54
4:BD:180:ARG:NH1	4:BD:180:ARG:HG3	2.22	0.54
3:BC:473:ASP:HB2	14:BT:26:PRO:CB	2.33	0.54
3:BC:95:LEU:HD13	22:BC:502:CLA:H143	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:76:VAL:O	4:BD:77:ALA:HB2	2.07	0.54
3:AC:29:GLU:HB3	10:AK:46:ARG:HH11	1.70	0.54
11:BL:11:GLU:HG2	11:BL:12:LEU:N	2.22	0.54
1:AA:221:SER:HB3	4:AD:141:TYR:HB2	1.89	0.54
5:AE:8:ARG:NE	5:AE:13:ILE:HG12	2.22	0.54
20:AZ:21:ILE:O	20:AZ:25:VAL:HG22	2.07	0.54
22:BA:404:CLA:HED1	24:BD:405:PL9:H372	1.89	0.54
1:AA:64:ARG:NH1	13:AO:98:THR:HG21	2.22	0.54
3:AC:155:ASN:O	3:AC:158:THR:HG22	2.07	0.54
15:BU:66:ILE:O	15:BU:66:ILE:CG2	2.56	0.54
20:AZ:35:ARG:O	20:AZ:38:GLN:HB3	2.07	0.54
2:BB:224:ARG:NE	7:BH:25:TRP:NE1	2.55	0.54
4:AD:86:GLY:O	4:AD:166:SER:HB2	2.08	0.54
15:AU:100:ARG:O	15:AU:103:GLN:HB3	2.07	0.54
3:BC:158:THR:HG21	3:BC:254:THR:O	2.08	0.54
3:AC:425:TRP:CE2	22:AC:504:CLA:HBA1	2.42	0.54
3:BC:149:TYR:HA	3:BC:156:LYS:HD3	1.89	0.54
3:BC:135:ARG:HB2	20:BZ:27:TYR:HB3	1.90	0.54
3:AC:239:TRP:CE3	3:AC:243:ILE:HD11	2.42	0.54
4:AD:18:LEU:HD22	18:AX:38:ILE:HD13	1.89	0.54
3:BC:369:LEU:HD21	3:BC:384:ILE:HD13	1.89	0.54
13:AO:227:VAL:HG12	13:AO:228:ALA:N	2.22	0.54
2:AB:235:GLU:HG2	2:AB:235:GLU:O	2.08	0.54
13:AO:141:ARG:HH11	13:AO:141:ARG:HG2	1.71	0.54
2:AB:150:CYS:HA	22:AB:603:CLA:HBC2	1.89	0.54
2:BB:12:LEU:HD22	2:BB:18:ARG:HB2	1.89	0.54
20:BZ:32:ASP:C	20:BZ:34:ASP:N	2.60	0.54
3:AC:135:ARG:HB2	20:AZ:27:TYR:HB3	1.89	0.54
13:AO:86:ARG:C	13:AO:86:ARG:HH11	2.11	0.54
3:AC:178:LYS:HA	3:AC:182:PHE:HB2	1.90	0.54
15:AU:58:ASN:OD1	15:AU:84:PRO:HA	2.07	0.54
1:AA:82:VAL:HB	1:AA:174:LEU:HB2	1.88	0.54
1:BA:217:SER:HA	1:BA:220:THR:HG22	1.90	0.54
13:BO:271:PRO:HG2	13:BO:272:ALA:H	1.73	0.54
2:AB:487:SER:N	2:AB:488:PRO:HD2	2.23	0.54
1:AA:76:ASN:OD1	1:AA:79:THR:HG23	2.07	0.54
27:BB:602:DGD:HD3	32:BB:603:LMT:H32	1.89	0.54
3:AC:155:ASN:HA	3:AC:158:THR:CG2	2.38	0.54
5:BE:55:TYR:O	5:BE:84:LYS:HE3	2.07	0.54
13:AO:154:SER:O	13:AO:168:PHE:HA	2.07	0.54
15:BU:100:ARG:O	15:BU:103:GLN:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:453:ALA:O	8:BI:34:ARG:HB2	2.07	0.54
2:BB:487:SER:N	2:BB:488:PRO:HD2	2.22	0.54
9:BJ:15:THR:O	9:BJ:19:MET:HG3	2.08	0.54
7:AH:12:ARG:N	7:AH:13:PRO:HD2	2.23	0.54
2:BB:230:ARG:O	2:BB:233:ASN:HB3	2.08	0.54
2:BB:191:ASN:HD21	7:BH:60:VAL:HA	1.72	0.54
4:BD:239:GLN:O	4:BD:240:ALA:CB	2.56	0.54
5:BE:8:ARG:NE	5:BE:13:ILE:HG12	2.23	0.54
16:AV:35:THR:HG23	16:AV:46:THR:OG1	2.08	0.54
30:AD:408:LMG:H111	11:AL:19:LEU:HD21	1.88	0.54
20:AZ:32:ASP:CG	20:AZ:33:TRP:N	2.60	0.54
3:BC:45:LEU:HD23	3:BC:48:LYS:HD2	1.90	0.54
13:AO:190:LEU:HB2	13:AO:214:LYS:HB2	1.90	0.54
3:BC:276:LEU:HD11	3:BC:444:HIS:HD2	1.73	0.54
3:BC:36:TRP:O	22:BC:508:CLA:H11	2.08	0.53
10:BK:37:PHE:HB3	26:BK:102:BCR:C40	2.39	0.53
3:AC:276:LEU:HD11	3:AC:444:HIS:HD2	1.73	0.53
3:BC:118:HIS:CE1	30:BC:520:LMG:H192	2.42	0.53
3:BC:135:ARG:HE	20:BZ:33:TRP:HE1	1.56	0.53
20:AZ:36:SER:OG	20:AZ:39:LEU:HD12	2.07	0.53
2:BB:191:ASN:ND2	7:BH:60:VAL:HA	2.23	0.53
3:AC:30:SER:OG	4:AD:233:ARG:NH2	2.40	0.53
1:AA:81:ALA:CB	1:AA:175:GLY:HA3	2.37	0.53
4:BD:238:THR:O	4:BD:239:GLN:O	2.26	0.53
3:BC:380:ILE:HA	3:BC:384:ILE:HD11	1.88	0.53
20:BZ:14:ILE:O	20:BZ:18:VAL:HG23	2.08	0.53
16:AV:116:GLU:HG3	16:AV:116:GLU:O	2.08	0.53
3:BC:447:ARG:NH1	3:BC:447:ARG:HG2	2.16	0.53
4:BD:266:TRP:CD1	30:BD:408:LMG:HC3	2.42	0.53
6:BF:18:VAL:HG13	6:BF:19:ARG:N	2.23	0.53
1:BA:240:GLY:HA3	14:BT:29:ILE:HG22	1.90	0.53
7:BH:12:ARG:N	7:BH:13:PRO:HD2	2.23	0.53
2:BB:329:PRO:HD3	22:BB:610:CLA:HED2	1.91	0.53
13:AO:92:VAL:HG13	13:AO:93:PRO:HD2	1.90	0.53
10:BK:43:VAL:HG13	10:BK:43:VAL:O	2.08	0.53
12:AM:25:LEU:O	12:AM:28:GLN:HG3	2.08	0.53
3:AC:453:ALA:O	8:AI:34:ARG:HB2	2.08	0.53
8:BI:11:VAL:O	8:BI:15:PHE:HD2	1.91	0.53
3:AC:42:LEU:CD1	22:AC:511:CLA:HMA3	2.37	0.53
4:AD:279:LEU:HD11	22:AD:402:CLA:O1A	2.09	0.53
22:BB:610:CLA:H42	30:BB:624:LMG:H131	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:58:VAL:O	7:BH:58:VAL:CG1	2.56	0.53
4:BD:189:HIS:HA	4:BD:294:ARG:HD2	1.90	0.53
15:BU:58:ASN:OD1	15:BU:84:PRO:HA	2.07	0.53
3:BC:418:ASN:HD21	27:BC:517:DGD:HD4	1.74	0.53
13:BO:178:ARG:HD2	13:BO:182:PHE:CD1	2.43	0.53
3:AC:118:HIS:CE1	30:AC:520:LMG:H192	2.43	0.53
13:AO:83:LYS:HG2	13:AO:84:ASN:N	2.19	0.53
3:BC:30:SER:OG	4:BD:233:ARG:NH2	2.41	0.53
2:AB:434:THR:HG23	13:AO:204:LYS:HE3	1.91	0.53
3:BC:137:PRO:HB2	3:BC:139:THR:O	2.09	0.53
20:BZ:3:ILE:O	20:BZ:7:LEU:HG	2.08	0.53
16:BV:87:LEU:HD12	16:BV:87:LEU:N	2.22	0.53
2:BB:341:LYS:HD2	2:BB:429:ILE:HG22	1.90	0.53
1:BA:283:VAL:O	1:BA:286:THR:HG22	2.08	0.53
4:AD:180:ARG:NH1	4:AD:180:ARG:HG3	2.23	0.53
3:AC:473:ASP:HB2	14:AT:26:PRO:CB	2.33	0.53
3:AC:36:TRP:O	22:AC:508:CLA:H11	2.08	0.53
4:AD:239:GLN:O	4:AD:240:ALA:CB	2.55	0.53
3:BC:178:LYS:HA	3:BC:182:PHE:HB2	1.89	0.53
14:BT:29:ILE:H	14:BT:29:ILE:CD1	1.98	0.53
22:BB:612:CLA:HMC2	26:BX:101:BCR:H343	1.91	0.53
3:BC:131:TYR:HE1	3:BC:135:ARG:HD2	1.74	0.53
3:AC:174:LEU:HG	22:AC:512:CLA:H92	1.90	0.53
1:AA:143:ILE:HD11	4:AD:217:THR:HA	1.89	0.53
5:BE:28:PRO:O	5:BE:32:ILE:HG13	2.08	0.53
1:BA:322:ASN:OD1	3:BC:412:THR:HA	2.08	0.53
13:BO:227:VAL:HG12	13:BO:228:ALA:N	2.23	0.53
13:AO:178:ARG:NH1	13:AO:178:ARG:CG	2.55	0.53
5:BE:7:GLU:CD	5:BE:7:GLU:H	2.12	0.53
27:AC:517:DGD:HB62	26:AJ:102:BCR:H352	1.91	0.53
3:BC:117:VAL:HG12	30:BC:520:LMG:H191	1.91	0.53
13:BO:31:LEU:HB2	13:BO:36:ILE:CD1	2.37	0.53
3:BC:337:LEU:CD1	13:BO:131:PRO:HG3	2.38	0.53
1:BA:107:TYR:CD1	13:BO:141:ARG:NH1	2.77	0.53
1:BA:76:ASN:OD1	1:BA:79:THR:HG23	2.08	0.53
9:BJ:14:ALA:HB1	26:BK:102:BCR:H393	1.91	0.53
15:AU:66:ILE:O	15:AU:66:ILE:CG2	2.56	0.53
2:BB:235:GLU:HG2	2:BB:235:GLU:O	2.09	0.53
3:BC:33:PHE:CE1	4:BD:229:ALA:CB	2.92	0.53
4:AD:330:ALA:HB3	4:AD:331:PRO:HD3	1.91	0.53
9:AJ:15:THR:O	9:AJ:19:MET:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AK:37:PHE:HB3	26:AK:102:BCR:C40	2.39	0.53
3:BC:117:VAL:CG1	30:BC:520:LMG:H191	2.39	0.53
20:BZ:35:ARG:O	20:BZ:38:GLN:HB3	2.09	0.53
22:AC:501:CLA:H42	22:AC:502:CLA:HMD1	1.90	0.53
4:BD:161:PRO:HG3	4:BD:170:ALA:HB2	1.91	0.53
4:AD:238:THR:O	4:AD:239:GLN:O	2.27	0.53
27:AB:626:DGD:HD3	32:AB:627:LMT:H32	1.90	0.53
15:BU:89:GLU:CD	15:BU:89:GLU:H	2.11	0.53
26:AA:409:BCR:H312	8:AI:15:PHE:CE1	2.44	0.53
22:AB:608:CLA:H12	4:AD:127:LEU:HD21	1.91	0.53
20:BZ:30:PRO:C	20:BZ:32:ASP:H	2.12	0.53
13:BO:92:VAL:HG13	13:BO:93:PRO:HD2	1.92	0.53
6:AF:21:VAL:O	6:AF:25:THR:HG23	2.09	0.53
3:BC:167:VAL:HG12	22:BC:512:CLA:H2	1.89	0.52
18:BX:12:ILE:HG12	18:BX:16:LEU:CD1	2.35	0.52
20:AZ:30:PRO:C	20:AZ:32:ASP:H	2.12	0.52
3:AC:391:ARG:HH11	3:AC:391:ARG:CB	2.19	0.52
7:AH:55:LEU:O	7:AH:58:VAL:HG12	2.09	0.52
3:BC:71:GLU:OE1	3:BC:89:ILE:HG13	2.08	0.52
4:BD:55:VAL:HG21	4:BD:110:LEU:CD1	2.39	0.52
15:AU:100:ARG:HH11	15:AU:103:GLN:HG2	1.73	0.52
1:BA:43:ALA:HB1	26:BA:410:BCR:H362	1.91	0.52
1:BA:300:PHE:CZ	3:BC:404:LEU:HD23	2.45	0.52
2:AB:341:LYS:HD2	2:AB:429:ILE:HG22	1.90	0.52
15:BU:72:TYR:CB	15:BU:73:PRO:HD3	2.34	0.52
3:AC:60:ILE:HG23	22:AC:510:CLA:HMC2	1.91	0.52
4:AD:221:THR:HG23	4:AD:244:TYR:HB2	1.91	0.52
4:AD:71:CYS:HB2	4:AD:76:VAL:HG12	1.91	0.52
3:AC:80:PRO:HB2	3:AC:83:GLU:HG3	1.90	0.52
4:AD:334:GLN:N	4:AD:335:PRO:HD3	2.24	0.52
1:AA:196:PRO:HA	1:AA:199:GLN:OE1	2.09	0.52
3:AC:466:VAL:HG13	4:AD:251:ARG:HD2	1.90	0.52
1:AA:49:VAL:O	1:AA:53:ILE:HG13	2.10	0.52
13:BO:234:THR:OG1	13:BO:236:GLU:HG2	2.09	0.52
1:BA:232:SER:HB3	1:BA:235:TYR:CD1	2.44	0.52
6:AF:18:VAL:HG13	6:AF:19:ARG:N	2.25	0.52
15:AU:66:ILE:HG13	15:AU:72:TYR:CD1	2.44	0.52
4:AD:161:PRO:HG3	4:AD:170:ALA:HB2	1.91	0.52
1:AA:22:THR:HG21	8:AI:30:ARG:HD3	1.90	0.52
16:BV:74:THR:O	16:BV:75:ASN:HB2	2.09	0.52
3:AC:33:PHE:CE1	4:AD:229:ALA:CB	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BU:83:ALA:CB	15:BU:84:PRO:HD2	2.15	0.52
3:BC:269:GLU:OE1	22:BC:508:CLA:HED1	2.08	0.52
30:BD:407:LMG:O3	9:BJ:37:GLY:HA3	2.09	0.52
3:AC:429:SER:HB3	27:AC:517:DGD:HA81	1.91	0.52
2:BB:133:LEU:HB3	2:BB:138:MET:HE1	1.90	0.52
14:BT:7:VAL:HG12	32:BT:101:LMT:H122	1.91	0.52
13:AO:141:ARG:HG2	13:AO:141:ARG:NH1	2.24	0.52
3:AC:452:ALA:O	3:AC:454:GLY:N	2.42	0.52
16:AV:135:GLU:O	16:AV:139:VAL:HG23	2.08	0.52
1:AA:326:LEU:HD21	3:AC:412:THR:HB	1.91	0.52
3:AC:216:SER:HB3	3:AC:221:GLU:HB2	1.90	0.52
9:BJ:18:GLY:HA3	26:BK:102:BCR:H371	1.92	0.52
2:AB:10:THR:C	2:AB:12:LEU:H	2.12	0.52
3:BC:116:VAL:HG21	26:BZ:101:BCR:H323	1.91	0.52
3:AC:163:PHE:CD1	22:AC:512:CLA:HAB	2.45	0.52
26:AT:102:BCR:C40	2:BB:36:SER:HB2	2.40	0.52
4:AD:85:MET:HE2	5:AE:69:ARG:HA	1.90	0.52
4:BD:87:HIS:CD2	4:BD:162:LEU:HA	2.45	0.52
1:BA:81:ALA:CB	1:BA:175:GLY:HA3	2.39	0.52
2:BB:220:ARG:HB3	2:BB:221:PRO:HD2	1.92	0.52
22:BC:504:CLA:H202	27:BC:518:DGD:HAF2	1.92	0.52
27:BC:517:DGD:HB62	26:BJ:102:BCR:H352	1.91	0.52
10:AK:24:VAL:O	10:AK:27:VAL:HG12	2.10	0.52
30:AD:408:LMG:H392	26:AT:102:BCR:HC32	1.92	0.52
13:AO:178:ARG:HD2	13:AO:182:PHE:CD1	2.45	0.52
1:BA:317:TRP:CD1	4:BD:177:ALA:HB2	2.44	0.52
3:AC:269:GLU:OE1	3:AC:447:ARG:HG2	2.10	0.52
20:BZ:31:GLN:O	20:BZ:32:ASP:HB3	2.10	0.52
3:BC:29:GLU:HB3	10:BK:46:ARG:HH11	1.74	0.52
13:AO:223:ILE:HG13	13:AO:243:SER:HB3	1.92	0.52
3:AC:337:LEU:CD1	13:AO:131:PRO:HG3	2.39	0.52
3:BC:466:VAL:HG13	4:BD:251:ARG:HD2	1.92	0.52
1:AA:232:SER:HB3	1:AA:235:TYR:CD1	2.45	0.52
22:AB:604:CLA:H101	22:AB:615:CLA:H42	1.91	0.52
3:BC:155:ASN:CA	3:BC:158:THR:HG22	2.39	0.52
2:BB:10:THR:C	2:BB:12:LEU:H	2.11	0.52
3:BC:163:PHE:CD1	22:BC:512:CLA:HAB	2.44	0.52
10:AK:43:VAL:HG13	10:AK:43:VAL:O	2.09	0.52
4:AD:88:SER:HB2	5:AE:69:ARG:CZ	2.40	0.52
16:AV:147:VAL:O	16:AV:150:LYS:HB2	2.10	0.52
1:AA:78:ILE:O	1:AA:176:ILE:HB	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AZ:32:ASP:C	20:AZ:34:ASP:N	2.60	0.52
3:AC:415:ASN:O	3:AC:416:SER:CB	2.57	0.52
12:BM:25:LEU:O	12:BM:28:GLN:HG3	2.10	0.52
1:AA:322:ASN:OD1	3:AC:412:THR:HA	2.09	0.52
1:AA:232:SER:HB3	1:AA:235:TYR:HD1	1.75	0.52
3:AC:193:GLY:O	3:AC:194:GLY:C	2.49	0.52
3:AC:47:GLY:O	3:AC:50:LEU:HB3	2.10	0.52
3:BC:47:GLY:O	3:BC:50:LEU:HB3	2.10	0.52
3:BC:199:ILE:N	3:BC:199:ILE:HD12	2.25	0.52
20:AZ:17:PHE:CE2	20:AZ:21:ILE:HD11	2.45	0.52
20:BZ:17:PHE:CE2	20:BZ:21:ILE:HD11	2.45	0.52
18:AX:17:LYS:O	18:AX:21:ILE:HG13	2.10	0.52
4:AD:266:TRP:HD1	30:AD:408:LMG:HC3	1.74	0.52
4:AD:77:ALA:HB2	4:AD:174:GLY:HA3	1.91	0.52
13:BO:31:LEU:HD12	13:BO:31:LEU:H	1.75	0.52
2:AB:224:ARG:NE	7:AH:25:TRP:NE1	2.58	0.52
13:BO:59:ASP:C	13:BO:61:SER:H	2.13	0.52
1:AA:188:ALA:HB2	1:AA:328:MET:HB2	1.92	0.52
3:BC:296:VAL:HG23	3:BC:297:TYR:CD2	2.45	0.52
22:BB:607:CLA:H101	22:BB:618:CLA:H42	1.91	0.51
4:BD:252:PHE:O	4:BD:256:ILE:HG22	2.10	0.51
22:AB:603:CLA:H193	7:AH:42:LEU:HD12	1.92	0.51
22:BB:611:CLA:H12	4:BD:127:LEU:HD21	1.92	0.51
1:AA:227:THR:HA	1:AA:231:GLU:OE2	2.10	0.51
1:BA:22:THR:HG21	8:BI:30:ARG:HD3	1.91	0.51
13:BO:141:ARG:NH1	13:BO:141:ARG:HG2	2.24	0.51
4:BD:350:ASN:O	4:BD:352:LEU:N	2.42	0.51
1:AA:279:PRO:CG	4:AD:212:ALA:HB2	2.40	0.51
1:AA:43:ALA:HB1	26:AA:409:BCR:H362	1.92	0.51
13:AO:178:ARG:HG3	13:AO:178:ARG:NH1	2.01	0.51
3:AC:418:ASN:HD21	27:AC:517:DGD:HD4	1.74	0.51
28:AC:521:LHG:H162	26:AJ:102:BCR:H313	1.91	0.51
3:BC:116:VAL:CG2	26:BZ:101:BCR:H323	2.41	0.51
20:AZ:3:ILE:O	20:AZ:7:LEU:HG	2.09	0.51
4:BD:136:VAL:HG12	4:BD:136:VAL:O	2.10	0.51
10:BK:35:LEU:HA	10:BK:38:VAL:HG23	1.92	0.51
3:AC:239:TRP:HE3	3:AC:243:ILE:HD11	1.74	0.51
2:BB:61:PHE:CE1	22:BB:610:CLA:HMB3	2.45	0.51
4:AD:76:VAL:O	4:AD:77:ALA:HB2	2.10	0.51
1:BA:190:HIS:O	1:BA:298:ASN:HB3	2.11	0.51
3:BC:391:ARG:CB	3:BC:391:ARG:HH11	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:9:HIS:HB2	22:BB:614:CLA:HBA1	1.91	0.51
4:AD:85:MET:CE	5:AE:69:ARG:HA	2.41	0.51
1:AA:228:THR:HG22	1:AA:229:GLU:N	2.25	0.51
10:BK:20:PRO:O	10:BK:23:ASP:HB2	2.10	0.51
1:AA:140:ARG:NH2	1:AA:142:TRP:HZ3	2.07	0.51
20:BZ:32:ASP:CG	20:BZ:33:TRP:N	2.62	0.51
4:AD:221:THR:HG23	4:AD:221:THR:O	2.10	0.51
20:AZ:31:GLN:O	20:AZ:32:ASP:HB3	2.10	0.51
20:AZ:32:ASP:OD1	20:AZ:36:SER:HB2	2.11	0.51
4:AD:87:HIS:CD2	4:AD:162:LEU:HA	2.45	0.51
1:BA:20:TRP:O	1:BA:21:VAL:C	2.49	0.51
20:BZ:5:PHE:CE1	20:BZ:54:VAL:HG13	2.46	0.51
2:AB:293:ALA:C	2:AB:295:GLY:H	2.14	0.51
13:AO:271:PRO:HG2	13:AO:272:ALA:H	1.76	0.51
2:AB:229:LEU:O	2:AB:231:MET:N	2.43	0.51
3:AC:250:TRP:CD1	3:AC:250:TRP:C	2.84	0.51
5:AE:36:LEU:HA	5:AE:39:SER:OG	2.11	0.51
2:BB:434:THR:CG2	13:BO:204:LYS:HE3	2.40	0.51
26:BA:410:BCR:H312	8:BI:15:PHE:CE1	2.45	0.51
4:AD:136:VAL:O	4:AD:136:VAL:HG12	2.10	0.51
2:BB:150:CYS:HA	22:BB:606:CLA:HBC2	1.91	0.51
22:BB:613:CLA:H12	22:BB:613:CLA:H112	1.92	0.51
2:AB:12:LEU:CD2	2:AB:18:ARG:HB2	2.40	0.51
3:AC:62:PHE:HE2	10:AK:29:PRO:HD3	1.76	0.51
16:BV:95:ILE:O	16:BV:99:VAL:HG23	2.09	0.51
2:AB:125:ASP:OD2	2:AB:127:ARG:HB3	2.11	0.51
3:AC:117:VAL:HG12	30:AC:520:LMG:H191	1.92	0.51
2:AB:36:SER:HB2	26:AB:618:BCR:C40	2.40	0.51
7:BH:55:LEU:HB2	7:BH:58:VAL:HG12	1.93	0.51
2:AB:27:THR:HG22	2:AB:107:LEU:CD1	2.40	0.51
13:BO:223:ILE:HG12	13:BO:224:SER:N	2.25	0.51
1:BA:196:PRO:HA	1:BA:199:GLN:OE1	2.10	0.51
2:BB:55:MET:CE	2:BB:80:ILE:HD12	2.41	0.51
3:BC:72:LEU:HD11	3:BC:108:THR:HB	1.93	0.51
26:BC:514:BCR:H391	10:BK:36:ALA:HB2	1.93	0.51
22:AB:610:CLA:H112	22:AB:610:CLA:H12	1.93	0.51
20:BZ:32:ASP:OD1	20:BZ:36:SER:HB2	2.11	0.51
22:AC:513:CLA:HMC2	26:AZ:101:BCR:H372	1.93	0.51
7:AH:55:LEU:HB2	7:AH:58:VAL:HG12	1.92	0.51
3:BC:62:PHE:HE2	10:BK:29:PRO:HD3	1.75	0.51
4:AD:86:GLY:HA2	4:AD:166:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AO:240:THR:HA	13:AO:264:VAL:HA	1.91	0.51
1:AA:92:HIS:CD2	3:AC:219:GLY:HA3	2.46	0.51
3:BC:155:ASN:HA	3:BC:158:THR:CG2	2.38	0.51
32:AB:625:LMT:H102	7:AH:35:MET:SD	2.51	0.51
18:AX:16:LEU:C	18:AX:16:LEU:HD13	2.31	0.51
18:AX:12:ILE:CG1	18:AX:16:LEU:HD12	2.33	0.51
4:BD:221:THR:O	4:BD:221:THR:HG23	2.10	0.51
1:BA:306:VAL:HG11	1:BA:316:THR:HG23	1.92	0.51
4:BD:86:GLY:O	4:BD:166:SER:HB2	2.11	0.51
13:AO:118:SER:HB3	13:AO:157:PRO:HA	1.93	0.51
6:AF:16:PHE:CD2	29:AF:101:SQD:H262	2.46	0.51
3:BC:269:GLU:OE1	3:BC:447:ARG:HG2	2.11	0.51
2:BB:256:MET:HA	2:BB:263:THR:HG21	1.93	0.51
1:AA:29:TYR:OH	1:AA:132:GLU:OE2	2.25	0.51
2:AB:12:LEU:HB2	22:AB:612:CLA:HMC2	1.93	0.51
4:AD:53:THR:HG22	4:AD:67:TYR:CD2	2.46	0.51
3:BC:447:ARG:HH11	3:BC:447:ARG:CG	2.14	0.50
3:BC:42:LEU:CD1	22:BC:511:CLA:HMA3	2.38	0.50
15:AU:83:ALA:CB	15:AU:84:PRO:CD	2.77	0.50
3:BC:135:ARG:HB2	20:BZ:27:TYR:CG	2.46	0.50
3:AC:116:VAL:HG21	26:AZ:101:BCR:H323	1.92	0.50
2:AB:183:PRO:HB2	2:AB:185:TRP:CH2	2.46	0.50
24:BA:408:PL9:H301	4:BD:42:TYR:HA	1.94	0.50
8:AI:27:ASP:N	8:AI:28:PRO:CD	2.74	0.50
3:BC:80:PRO:HB2	3:BC:83:GLU:HG3	1.91	0.50
10:AK:17:ILE:H	10:AK:17:ILE:CD1	2.24	0.50
29:BA:413:SQD:H5	4:BD:232:PHE:HB3	1.93	0.50
22:BC:504:CLA:HED1	30:BC:519:LMG:O3	2.11	0.50
3:AC:158:THR:HG21	3:AC:254:THR:O	2.10	0.50
3:AC:116:VAL:CG2	26:AZ:101:BCR:H323	2.41	0.50
16:BV:147:VAL:O	16:BV:150:LYS:HB2	2.11	0.50
2:BB:63:LEU:N	2:BB:64:PRO:HD2	2.27	0.50
1:AA:149:ALA:HB3	1:AA:150:PRO:CD	2.41	0.50
20:AZ:5:PHE:HA	20:AZ:57:LEU:CD2	2.40	0.50
4:AD:346:LEU:O	4:AD:348:ARG:HG3	2.10	0.50
13:BO:190:LEU:HB2	13:BO:214:LYS:HB2	1.93	0.50
3:BC:193:GLY:O	3:BC:194:GLY:C	2.48	0.50
2:BB:149:LEU:HG	22:BB:606:CLA:CBC	2.30	0.50
18:AX:12:ILE:O	18:AX:12:ILE:CG2	2.58	0.50
3:AC:167:VAL:HG12	22:AC:512:CLA:H2	1.94	0.50
1:AA:283:VAL:O	1:AA:286:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:62:GLY:HA3	5:BE:63:ILE:HD13	1.94	0.50
13:AO:86:ARG:HH11	13:AO:87:GLN:HA	1.75	0.50
13:AO:223:ILE:HG12	13:AO:224:SER:N	2.27	0.50
10:AK:25:LEU:HB2	10:AK:26:PRO:HD3	1.93	0.50
1:BA:232:SER:HB3	1:BA:235:TYR:HD1	1.75	0.50
8:BI:27:ASP:N	8:BI:28:PRO:CD	2.74	0.50
15:AU:72:TYR:O	15:AU:73:PRO:C	2.48	0.50
22:AC:504:CLA:H202	27:AC:518:DGD:HAF2	1.94	0.50
3:AC:159:THR:HG23	3:AC:252:ILE:HD13	1.93	0.50
4:AD:53:THR:HG22	4:AD:67:TYR:CE2	2.47	0.50
5:BE:8:ARG:HB2	6:BF:13:TYR:HB3	1.92	0.50
18:BX:17:LYS:O	18:BX:21:ILE:HG13	2.11	0.50
2:AB:134:ASP:OD2	2:AB:137:LYS:HB2	2.11	0.50
22:AB:605:CLA:HBB1	22:AB:606:CLA:H51	1.92	0.50
4:BD:134:ARG:HA	4:BD:134:ARG:HE	1.76	0.50
29:AA:412:SQD:H223	27:AC:518:DGD:HAE1	1.92	0.50
3:AC:418:ASN:HB2	27:AC:518:DGD:HE2	1.92	0.50
22:AB:607:CLA:H42	30:AB:622:LMG:H131	1.92	0.50
3:BC:413:GLU:HG3	3:BC:414:ILE:N	2.27	0.50
13:BO:223:ILE:HG13	13:BO:243:SER:HB3	1.93	0.50
3:AC:81:MET:CE	3:AC:89:ILE:HG22	2.42	0.50
20:AZ:5:PHE:CE1	20:AZ:54:VAL:HG13	2.46	0.50
18:BX:32:LEU:HD23	18:BX:32:LEU:N	2.26	0.50
5:AE:34:GLY:HA2	6:AF:32:PHE:CE1	2.46	0.50
20:AZ:12:LEU:HB2	20:AZ:50:LEU:HD22	1.93	0.50
28:BA:412:LHG:HC12	22:BC:508:CLA:O1D	2.12	0.50
30:AI:101:LMG:H181	32:AI:102:LMT:H42	1.94	0.50
34:BE:101:HEM:HBC2	6:BF:27:ALA:CB	2.37	0.50
22:BB:611:CLA:H151	22:BB:612:CLA:H203	1.93	0.50
2:BB:471:ALA:HB2	4:BD:130:PHE:HZ	1.76	0.50
22:AB:612:CLA:H171	22:AB:613:CLA:HBB2	1.94	0.50
22:AB:609:CLA:HMC2	26:AH:101:BCR:H343	1.92	0.50
2:BB:12:LEU:CD2	2:BB:18:ARG:HB2	2.41	0.50
22:AA:403:CLA:HED2	4:AD:198:MET:SD	2.51	0.50
2:AB:9:HIS:HB2	22:AB:611:CLA:HBA1	1.93	0.50
20:AZ:47:TRP:O	20:AZ:50:LEU:HB2	2.11	0.50
3:BC:154:LYS:HE2	3:BC:261:ARG:HD2	1.93	0.50
1:AA:63:ILE:HB	3:AC:335:THR:HG21	1.92	0.50
18:BX:43:ILE:HG22	18:BX:43:ILE:O	2.11	0.50
29:AA:415:SQD:H2	22:BB:619:CLA:H43	1.94	0.50
22:AC:505:CLA:HMD1	22:AC:507:CLA:HAB	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:117:VAL:CG1	30:AC:520:LMG:H191	2.41	0.50
2:BB:124:ARG:NH1	2:BB:124:ARG:HG3	2.22	0.50
4:BD:217:THR:O	4:BD:221:THR:HB	2.11	0.50
3:AC:89:ILE:N	3:AC:90:PRO:CD	2.75	0.50
1:AA:20:TRP:O	1:AA:21:VAL:C	2.50	0.50
3:AC:266:TRP:HB3	3:AC:271:TYR:OH	2.11	0.50
2:AB:55:MET:CE	2:AB:80:ILE:HD12	2.42	0.50
13:AO:59:ASP:HB3	13:AO:62:GLN:HB3	1.93	0.50
27:BC:517:DGD:HBV1	28:BC:521:LHG:H151	1.93	0.50
22:AB:616:CLA:H43	29:BA:401:SQD:H2	1.94	0.50
22:BC:505:CLA:HMD1	22:BC:507:CLA:HAB	1.92	0.50
5:AE:81:GLU:C	5:AE:83:LEU:N	2.64	0.50
2:AB:286:ARG:NH1	2:AB:286:ARG:HG2	2.26	0.50
16:AV:95:ILE:O	16:AV:99:VAL:HG23	2.12	0.50
3:BC:275:SER:HB3	22:BC:509:CLA:HED3	1.94	0.50
30:AI:101:LMG:HC2	32:BB:603:LMT:H11	1.93	0.50
2:AB:141:ILE:HG23	22:AB:615:CLA:HBB1	1.92	0.50
2:BB:96:VAL:HG22	22:BB:609:CLA:HBA1	1.94	0.50
3:AC:269:GLU:OE1	22:AC:508:CLA:HED1	2.12	0.50
3:BC:250:TRP:C	3:BC:250:TRP:CD1	2.85	0.50
3:AC:265:ILE:HG12	22:AC:505:CLA:HED1	1.94	0.50
16:BV:45:ILE:HG12	16:BV:46:THR:N	2.26	0.50
32:AB:627:LMT:H11	30:BI:101:LMG:HC2	1.93	0.50
1:AA:235:TYR:C	1:AA:237:TYR:H	2.16	0.50
1:BA:221:SER:HB3	4:BD:141:TYR:HB2	1.94	0.50
4:AD:54:PHE:HB3	5:AE:47:PHE:CD2	2.46	0.50
2:BB:246:PHE:C	2:BB:246:PHE:CD1	2.85	0.50
1:BA:206:PHE:CE2	22:BD:402:CLA:HBA1	2.47	0.49
2:AB:349:LYS:HG3	2:AB:350:GLU:OE1	2.12	0.49
6:AF:11:VAL:CG1	6:AF:12:SER:H	2.25	0.49
1:BA:330:VAL:HG12	4:BD:348:ARG:HA	1.93	0.49
1:AA:107:TYR:CD1	13:AO:141:ARG:NH1	2.80	0.49
5:BE:8:ARG:HB2	6:BF:13:TYR:CB	2.42	0.49
1:BA:96:ILE:HG12	1:BA:105:TRP:CE2	2.47	0.49
1:AA:96:ILE:HG12	1:AA:105:TRP:CE2	2.47	0.49
9:AJ:18:GLY:HA3	26:AK:102:BCR:H371	1.93	0.49
3:BC:418:ASN:HB2	27:BC:518:DGD:HE2	1.93	0.49
4:BD:180:ARG:NH1	4:BD:180:ARG:CG	2.69	0.49
2:AB:471:ALA:HB2	4:AD:130:PHE:HZ	1.78	0.49
13:AO:31:LEU:HB2	13:AO:36:ILE:CD1	2.38	0.49
3:AC:391:ARG:HD2	3:AC:395:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:85:MET:HE2	5:BE:69:ARG:HA	1.94	0.49
1:BA:84:PRO:HA	1:BA:112:TYR:CG	2.47	0.49
3:BC:452:ALA:O	3:BC:454:GLY:N	2.44	0.49
18:BX:32:LEU:O	18:BX:36:VAL:HG23	2.11	0.49
3:AC:315:MET:O	3:AC:319:ILE:HG13	2.12	0.49
4:AD:350:ASN:O	4:AD:352:LEU:N	2.42	0.49
3:AC:72:LEU:HD11	3:AC:108:THR:HB	1.93	0.49
3:AC:137:PRO:HB2	3:AC:139:THR:O	2.12	0.49
18:AX:42:GLN:O	18:AX:43:ILE:HG13	2.12	0.49
22:BC:504:CLA:H151	27:BC:517:DGD:HBW1	1.93	0.49
3:AC:473:ASP:CB	14:AT:26:PRO:HB3	2.36	0.49
2:AB:462:PHE:CZ	22:AB:613:CLA:HMB3	2.47	0.49
3:AC:135:ARG:HE	20:AZ:33:TRP:HE1	1.59	0.49
4:BD:54:PHE:HB3	5:BE:47:PHE:CD2	2.47	0.49
3:AC:275:SER:HB3	22:AC:509:CLA:HED3	1.94	0.49
16:AV:29:LEU:HD11	16:AV:34:LEU:HD21	1.92	0.49
1:AA:224:ILE:O	1:AA:226:GLU:OE2	2.30	0.49
2:AB:220:ARG:HB3	2:AB:221:PRO:HD2	1.93	0.49
4:BD:279:LEU:HD11	22:BD:402:CLA:O1A	2.13	0.49
6:AF:23:VAL:O	6:AF:27:ALA:CB	2.60	0.49
14:BT:25:GLU:O	14:BT:26:PRO:C	2.50	0.49
32:BB:626:LMT:H3'	29:BD:409:SQD:H62	1.95	0.49
7:AH:35:MET:HE2	26:AH:101:BCR:H322	1.93	0.49
3:BC:116:VAL:HG23	3:BC:117:VAL:N	2.28	0.49
20:BZ:29:SER:C	20:BZ:31:GLN:H	2.16	0.49
11:AL:12:LEU:HD22	12:AM:25:LEU:HD12	1.93	0.49
4:AD:210:LEU:HA	4:AD:213:ILE:HG22	1.95	0.49
10:BK:25:LEU:HB2	10:BK:26:PRO:HD3	1.94	0.49
5:BE:34:GLY:HA2	6:BF:32:PHE:CE1	2.48	0.49
4:BD:176:ALA:HA	4:BD:179:PHE:CD2	2.47	0.49
26:AC:514:BCR:H391	10:AK:36:ALA:HB2	1.95	0.49
26:BC:514:BCR:HC22	10:BK:18:PHE:HD1	1.77	0.49
2:BB:24:LEU:HB3	2:BB:111:ALA:HB2	1.94	0.49
22:AB:608:CLA:H151	22:AB:609:CLA:H203	1.93	0.49
3:BC:174:LEU:HG	22:BC:512:CLA:H92	1.93	0.49
3:AC:109:PHE:HB3	3:AC:110:PRO:HD3	1.94	0.49
5:BE:4:THR:CG2	5:BE:5:THR:N	2.76	0.49
2:AB:173:GLY:HA3	2:AB:265:ILE:HD11	1.93	0.49
13:AO:59:ASP:C	13:AO:61:SER:H	2.14	0.49
2:BB:134:ASP:OD2	2:BB:137:LYS:HB2	2.12	0.49
4:BD:266:TRP:HD1	30:BD:408:LMG:HC3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AB:608:CLA:H51	22:AB:609:CLA:H101	1.94	0.49
3:AC:413:GLU:HG3	3:AC:414:ILE:N	2.28	0.49
13:BO:43:ASN:OD1	13:BO:103:SER:HB2	2.11	0.49
13:AO:43:ASN:OD1	13:AO:103:SER:HB2	2.12	0.49
8:BI:30:ARG:O	8:BI:31:ASN:HB3	2.13	0.49
18:AX:43:ILE:O	18:AX:43:ILE:HG22	2.12	0.49
9:BJ:34:ALA:O	9:BJ:35:GLY:O	2.31	0.49
1:BA:124:SER:O	1:BA:127:MET:HB3	2.12	0.49
2:AB:137:LYS:O	2:AB:141:ILE:HG13	2.11	0.49
22:BB:608:CLA:HMA1	22:BB:609:CLA:HBA2	1.94	0.49
3:BC:473:ASP:CB	14:BT:26:PRO:HB3	2.37	0.49
22:AD:404:CLA:C4	18:AX:26:GLY:HA3	2.34	0.49
3:AC:405:ASN:HD22	27:AC:518:DGD:C5D	2.25	0.49
24:AA:407:PL9:H301	4:AD:42:TYR:HA	1.94	0.49
1:BA:32:TRP:HA	1:BA:32:TRP:HE3	1.75	0.49
3:BC:90:PRO:O	3:BC:94:THR:HG23	2.12	0.49
3:AC:126:GLY:O	3:AC:130:VAL:HG23	2.12	0.49
3:AC:154:LYS:HE2	3:AC:261:ARG:HD2	1.94	0.49
29:BL:101:SQD:H45	14:BT:23:PHE:CD1	2.47	0.49
3:AC:155:ASN:CA	3:AC:158:THR:HG22	2.39	0.49
15:AU:72:TYR:CB	15:AU:73:PRO:HD3	2.34	0.49
3:AC:135:ARG:HB2	20:AZ:27:TYR:CG	2.48	0.49
1:AA:190:HIS:O	1:AA:298:ASN:HB3	2.13	0.49
4:BD:87:HIS:ND1	27:BH:101:DGD:HD2	2.27	0.49
13:AO:126:GLY:O	13:AO:128:ASP:N	2.45	0.49
3:AC:346:THR:O	13:AO:40:GLY:HA2	2.13	0.49
5:BE:9:PRO:HB3	30:BE:102:LMG:HC4	1.95	0.49
1:AA:300:PHE:CZ	3:AC:404:LEU:HD23	2.48	0.49
4:AD:323:GLU:HG2	13:AO:194:TYR:OH	2.12	0.49
8:AI:6:ILE:O	8:AI:10:ILE:HG12	2.13	0.49
22:BB:608:CLA:HBB1	22:BB:609:CLA:H51	1.95	0.49
3:AC:447:ARG:CG	3:AC:447:ARG:NH1	2.74	0.49
5:BE:81:GLU:C	5:BE:83:LEU:N	2.65	0.49
16:AV:45:ILE:HG12	16:AV:46:THR:N	2.28	0.49
2:AB:55:MET:HE2	2:AB:80:ILE:HD12	1.94	0.49
2:BB:293:ALA:C	2:BB:295:GLY:H	2.15	0.49
1:BA:114:LEU:C	1:BA:114:LEU:HD23	2.33	0.49
5:AE:9:PRO:HB3	30:AE:102:LMG:HC4	1.95	0.49
9:AJ:11:TRP:CG	10:AK:42:ALA:HA	2.48	0.49
10:BK:18:PHE:O	10:BK:22:VAL:HG23	2.13	0.49
1:AA:28:LEU:HD12	29:AA:415:SQD:H111	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:69:LEU:HD21	22:AB:603:CLA:HED3	1.95	0.49
5:BE:22:ILE:O	5:BE:26:THR:HG23	2.13	0.49
3:AC:405:ASN:HB2	27:AC:518:DGD:HG31	1.95	0.49
22:AA:403:CLA:HED1	24:AD:405:PL9:H372	1.95	0.49
1:AA:13:LEU:HD12	1:AA:13:LEU:N	2.28	0.49
4:BD:67:TYR:CE1	4:BD:76:VAL:HG11	2.47	0.49
13:BO:92:VAL:HG12	13:BO:93:PRO:CD	2.43	0.49
2:AB:270:PRO:HG3	2:AB:312:TYR:CD2	2.43	0.49
3:BC:94:THR:HG22	3:BC:298:PRO:HD2	1.95	0.49
3:AC:90:PRO:O	3:AC:94:THR:HG23	2.12	0.49
3:AC:347:GLY:HA3	13:AO:43:ASN:HB2	1.95	0.49
4:BD:86:GLY:HA2	4:BD:166:SER:HB3	1.94	0.49
10:AK:15:TYR:HE2	20:AZ:62:VAL:HG21	1.78	0.49
3:BC:35:TRP:CG	3:BC:36:TRP:N	2.81	0.48
1:BA:283:VAL:HG21	23:BA:406:PHO:HBC3	1.95	0.48
2:AB:69:LEU:HD12	22:AB:605:CLA:HBA1	1.95	0.48
3:BC:60:ILE:HG23	22:BC:510:CLA:HMC2	1.94	0.48
3:BC:135:ARG:NE	20:BZ:33:TRP:HE1	2.11	0.48
4:BD:71:CYS:HB2	4:BD:76:VAL:HG12	1.95	0.48
1:BA:228:THR:HG22	1:BA:229:GLU:N	2.27	0.48
13:AO:94:THR:HB	13:AO:135:GLN:O	2.12	0.48
1:BA:278:TRP:HB3	1:BA:279:PRO:CD	2.42	0.48
2:BB:35:GLY:O	2:BB:38:ALA:HB3	2.12	0.48
7:AH:30:LEU:HD11	7:AH:34:PHE:HE1	1.78	0.48
1:BA:37:MET:HG2	1:BA:41:LEU:HD12	1.94	0.48
32:AB:625:LMT:H3'	29:AD:409:SQD:H62	1.95	0.48
3:BC:159:THR:HG23	3:BC:252:ILE:HD13	1.94	0.48
22:BC:503:CLA:H172	22:BC:510:CLA:HBB2	1.94	0.48
18:BX:16:LEU:HD13	18:BX:16:LEU:C	2.33	0.48
22:AA:402:CLA:H202	22:AA:403:CLA:H93	1.96	0.48
1:BA:13:LEU:HD12	1:BA:13:LEU:N	2.27	0.48
4:BD:49:LEU:HD13	26:BD:406:BCR:C15	2.43	0.48
3:BC:89:ILE:N	3:BC:90:PRO:CD	2.74	0.48
13:AO:159:VAL:O	13:AO:159:VAL:HG13	2.12	0.48
2:BB:55:MET:HE2	2:BB:80:ILE:HD12	1.94	0.48
20:AZ:5:PHE:HA	20:AZ:57:LEU:HD21	1.95	0.48
26:AB:617:BCR:HC31	12:AM:10:ALA:HB2	1.94	0.48
2:BB:125:ASP:OD2	2:BB:127:ARG:HB3	2.13	0.48
2:AB:35:GLY:O	2:AB:38:ALA:HB3	2.13	0.48
13:BO:240:THR:HA	13:BO:264:VAL:HA	1.95	0.48
3:BC:425:TRP:CZ2	22:BC:504:CLA:HBA1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:BJ:11:TRP:CG	10:BK:42:ALA:HA	2.48	0.48
1:BA:45:THR:HG23	1:BA:46:ILE:N	2.28	0.48
2:AB:414:PRO:HB2	2:AB:415:PRO:CD	2.35	0.48
4:AD:134:ARG:HE	4:AD:134:ARG:HA	1.78	0.48
7:AH:35:MET:HE2	26:AH:101:BCR:C32	2.44	0.48
5:AE:28:PRO:O	5:AE:32:ILE:HG13	2.13	0.48
3:AC:62:PHE:CE2	10:AK:29:PRO:HD3	2.48	0.48
1:BA:326:LEU:HD21	3:BC:412:THR:HB	1.94	0.48
3:BC:33:PHE:CD1	4:BD:229:ALA:HB3	2.48	0.48
13:BO:59:ASP:HB3	13:BO:62:GLN:HB3	1.95	0.48
7:BH:30:LEU:HD11	7:BH:34:PHE:HE1	1.78	0.48
13:BO:73:PRO:HG2	13:BO:102:THR:HB	1.95	0.48
2:AB:175:THR:O	2:AB:176:GLY:O	2.31	0.48
3:BC:258:GLY:CA	3:BC:262:ARG:HH12	2.26	0.48
4:AD:201:VAL:O	4:AD:205:LEU:HB2	2.13	0.48
3:AC:425:TRP:CZ2	22:AC:504:CLA:HBA1	2.48	0.48
22:AC:504:CLA:H151	27:AC:517:DGD:HBW1	1.95	0.48
13:AO:77:LEU:HB3	13:AO:91:PHE:HB3	1.96	0.48
3:AC:413:GLU:HG3	3:AC:414:ILE:H	1.79	0.48
2:AB:256:MET:O	2:AB:448:ARG:NH1	2.42	0.48
1:AA:221:SER:HB2	4:AD:139:ARG:O	2.13	0.48
5:AE:14:ILE:CG2	9:AJ:13:VAL:HG11	2.44	0.48
2:AB:154:GLY:O	2:AB:159:THR:HG23	2.13	0.48
9:AJ:34:ALA:O	9:AJ:35:GLY:O	2.31	0.48
13:AO:226:ASN:N	13:AO:226:ASN:HD22	2.11	0.48
4:AD:193:LEU:O	4:AD:193:LEU:HG	2.14	0.48
34:AV:201:HEM:HHA	34:AV:201:HEM:HAD2	1.61	0.48
10:BK:17:ILE:CD1	10:BK:17:ILE:H	2.26	0.48
26:AA:409:BCR:H312	8:AI:15:PHE:HE1	1.79	0.48
2:BB:141:ILE:HG23	22:BB:618:CLA:HBB1	1.94	0.48
2:BB:262:THR:HG22	2:BB:263:THR:HG23	1.96	0.48
22:AC:504:CLA:HED1	30:AC:519:LMG:O3	2.13	0.48
20:BZ:35:ARG:HG3	20:BZ:36:SER:N	2.28	0.48
4:AD:62:GLY:HA3	5:AE:63:ILE:HD13	1.96	0.48
13:BO:86:ARG:HH11	13:BO:86:ARG:C	2.16	0.48
1:BA:72:LEU:HD21	32:BT:101:LMT:H31	1.96	0.48
3:AC:71:GLU:OE1	3:AC:89:ILE:HG13	2.13	0.48
1:BA:243:GLU:CD	1:BA:243:GLU:H	2.12	0.48
1:BA:63:ILE:HB	3:BC:335:THR:HG21	1.94	0.48
22:BB:606:CLA:H193	7:BH:42:LEU:HD12	1.95	0.48
10:AK:20:PRO:O	10:AK:23:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:190:HIS:HB3	1:BA:293:MET:CE	2.42	0.48
7:BH:55:LEU:O	7:BH:58:VAL:HG12	2.12	0.48
13:AO:86:ARG:O	13:AO:86:ARG:NH1	2.37	0.48
13:BO:159:VAL:O	13:BO:159:VAL:HG13	2.13	0.48
3:BC:216:SER:HB3	3:BC:221:GLU:HB2	1.95	0.48
4:AD:337:GLU:O	4:AD:338:ASN:C	2.51	0.48
20:BZ:47:TRP:O	20:BZ:50:LEU:HB2	2.13	0.48
16:BV:148:GLU:OE1	16:BV:148:GLU:HA	2.13	0.48
28:BC:521:LHG:H271	28:BC:521:LHG:H101	1.95	0.48
2:AB:137:LYS:HZ1	7:AH:17:GLU:H	1.61	0.48
15:BU:72:TYR:HB3	15:BU:73:PRO:CD	2.37	0.48
1:BA:258:LEU:HD12	4:BD:128:ARG:CD	2.42	0.48
1:BA:214:MET:HE2	1:BA:214:MET:HA	1.96	0.48
10:BK:46:ARG:NH1	10:BK:46:ARG:HB2	2.28	0.48
1:BA:343:LEU:O	1:BA:344:ALA:CB	2.60	0.48
2:AB:224:ARG:HG3	7:AH:25:TRP:CD1	2.48	0.48
3:AC:315:MET:CE	3:AC:366:LEU:HD13	2.44	0.48
3:AC:367:GLU:HB2	3:AC:368:PRO:HD3	1.95	0.48
2:BB:137:LYS:O	2:BB:141:ILE:HG13	2.14	0.48
6:BF:23:VAL:O	6:BF:27:ALA:CB	2.61	0.48
15:BU:66:ILE:HG13	15:BU:72:TYR:CD1	2.49	0.48
3:AC:48:LYS:HD2	3:AC:138:GLU:HG3	1.94	0.48
5:AE:77:GLU:HA	5:AE:80:LEU:HD23	1.95	0.48
2:AB:172:TYR:O	2:AB:173:GLY:C	2.52	0.48
5:BE:10:PHE:HB2	30:BE:102:LMG:O2	2.14	0.48
13:AO:194:TYR:CE1	13:AO:198:ILE:HD13	2.49	0.48
3:AC:296:VAL:HG23	3:AC:297:TYR:CD2	2.49	0.48
13:BO:173:ASN:ND2	13:BO:220:LYS:HD3	2.29	0.48
3:BC:308:GLU:HB2	3:BC:361:PHE:CE1	2.49	0.48
22:AC:503:CLA:H172	22:AC:510:CLA:HBB2	1.95	0.48
1:AA:13:LEU:H	1:AA:13:LEU:CD1	2.27	0.48
13:BO:36:ILE:HD12	13:BO:36:ILE:N	2.29	0.48
3:BC:126:GLY:O	3:BC:130:VAL:HG23	2.13	0.48
2:AB:434:THR:CG2	13:AO:204:LYS:HE3	2.44	0.48
13:AO:225:LEU:C	13:AO:226:ASN:HD22	2.17	0.48
11:BL:22:LEU:O	11:BL:26:VAL:HG13	2.14	0.48
11:AL:24:ILE:HD12	11:AL:24:ILE:N	2.29	0.48
1:AA:114:LEU:HD23	1:AA:114:LEU:C	2.34	0.48
10:BK:37:PHE:HB3	26:BK:102:BCR:H402	1.95	0.48
3:BC:265:ILE:HG12	22:BC:505:CLA:HED1	1.95	0.48
4:AD:126:MET:CE	4:AD:150:ILE:HG13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:AZ:32:ASP:C	20:AZ:34:ASP:H	2.17	0.48
2:AB:329:PRO:CB	22:AB:607:CLA:HED1	2.39	0.48
5:BE:15:THR:O	9:BJ:8:ILE:HD12	2.14	0.48
4:AD:87:HIS:ND1	27:AH:102:DGD:HD2	2.29	0.48
3:BC:81:MET:CE	3:BC:89:ILE:HG22	2.44	0.48
4:BD:210:LEU:HA	4:BD:213:ILE:HG22	1.96	0.48
1:AA:111:PRO:O	1:AA:115:ILE:HG13	2.14	0.48
29:BL:101:SQD:H45	14:BT:23:PHE:HD1	1.79	0.48
10:BK:15:TYR:HE2	20:BZ:62:VAL:HG21	1.77	0.48
4:BD:126:MET:CE	4:BD:150:ILE:HG13	2.44	0.47
4:BD:261:PHE:O	4:BD:262:SER:HB3	2.14	0.47
30:BD:408:LMG:O10	11:BL:18:TYR:HB3	2.13	0.47
3:AC:116:VAL:HG23	3:AC:117:VAL:N	2.28	0.47
1:BA:13:LEU:CD1	1:BA:13:LEU:H	2.26	0.47
1:AA:215:HIS:O	1:AA:216:GLY:C	2.53	0.47
16:BV:81:ARG:HH11	16:BV:81:ARG:HG2	1.78	0.47
13:BO:157:PRO:O	13:BO:158:ASN:O	2.32	0.47
3:BC:266:TRP:HB3	3:BC:271:TYR:OH	2.14	0.47
1:BA:279:PRO:CG	4:BD:212:ALA:HB2	2.44	0.47
20:BZ:12:LEU:HB2	20:BZ:50:LEU:HD22	1.96	0.47
13:AO:184:ASP:OD2	13:AO:188:ARG:HB2	2.14	0.47
13:AO:36:ILE:HD12	13:AO:36:ILE:N	2.29	0.47
2:BB:349:LYS:HG3	2:BB:350:GLU:OE1	2.14	0.47
2:BB:27:THR:HG22	2:BB:107:LEU:CD1	2.40	0.47
2:BB:224:ARG:HG3	7:BH:25:TRP:CD1	2.48	0.47
18:AX:32:LEU:O	18:AX:36:VAL:HG23	2.13	0.47
5:AE:8:ARG:HB2	6:AF:13:TYR:HB3	1.95	0.47
8:BI:6:ILE:O	8:BI:10:ILE:HG12	2.14	0.47
1:BA:188:ALA:HB2	1:BA:328:MET:HB2	1.94	0.47
5:BE:51:ARG:O	5:BE:53:ASP:N	2.47	0.47
5:AE:22:ILE:O	5:AE:26:THR:HG23	2.14	0.47
2:BB:462:PHE:CZ	22:BB:616:CLA:HMB3	2.49	0.47
3:BC:391:ARG:HD2	3:BC:395:TYR:CZ	2.49	0.47
1:BA:78:ILE:O	1:BA:176:ILE:HB	2.13	0.47
2:AB:246:PHE:CD1	2:AB:246:PHE:C	2.88	0.47
2:BB:256:MET:O	2:BB:448:ARG:NH1	2.45	0.47
28:AA:411:LHG:HC12	22:AC:508:CLA:O1D	2.13	0.47
2:BB:124:ARG:HD3	2:BB:131:PRO:N	2.30	0.47
3:BC:347:GLY:HA3	13:BO:43:ASN:HB2	1.95	0.47
2:AB:265:ILE:HG13	2:AB:266:GLU:N	2.30	0.47
2:AB:235:GLU:OE1	2:AB:472:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:33:PHE:CD1	4:AD:229:ALA:HB3	2.49	0.47
1:AA:136:ARG:NH2	8:AI:27:ASP:OD1	2.47	0.47
4:BD:93:TRP:HA	4:BD:99:GLY:H	1.80	0.47
19:AY:11:UNK:C	19:AY:13:UNK:N	2.75	0.47
19:BY:11:UNK:C	19:BY:13:UNK:N	2.76	0.47
3:BC:55:ALA:HB1	26:BC:514:BCR:C37	2.44	0.47
2:AB:24:LEU:HB3	2:AB:111:ALA:HB2	1.96	0.47
2:AB:124:ARG:HG3	2:AB:124:ARG:NH1	2.26	0.47
1:AA:10:SER:C	1:AA:12:ASN:H	2.16	0.47
1:AA:12:ASN:O	1:AA:16:ARG:HG3	2.15	0.47
3:BC:413:GLU:HG3	3:BC:414:ILE:H	1.80	0.47
20:AZ:5:PHE:HE1	20:AZ:54:VAL:HG13	1.80	0.47
5:AE:9:PRO:O	5:AE:10:PHE:C	2.53	0.47
14:AT:23:PHE:CD1	29:BB:601:SQD:H45	2.49	0.47
3:BC:367:GLU:HB2	3:BC:368:PRO:HD3	1.97	0.47
1:AA:124:SER:O	1:AA:127:MET:HB3	2.15	0.47
28:BC:521:LHG:H162	26:BJ:102:BCR:H313	1.95	0.47
2:AB:141:ILE:HG21	22:AB:615:CLA:HBB1	1.97	0.47
4:BD:263:ASN:O	4:BD:266:TRP:N	2.47	0.47
6:AF:23:VAL:O	6:AF:27:ALA:HB2	2.14	0.47
3:AC:135:ARG:NE	20:AZ:33:TRP:HE1	2.12	0.47
20:AZ:29:SER:C	20:AZ:31:GLN:H	2.17	0.47
7:BH:25:TRP:O	7:BH:26:GLY:C	2.53	0.47
8:AI:30:ARG:O	8:AI:31:ASN:HB3	2.14	0.47
3:BC:62:PHE:CE2	10:BK:29:PRO:HD3	2.49	0.47
15:BU:100:ARG:NH1	15:BU:103:GLN:HG2	2.29	0.47
2:BB:235:GLU:OE1	2:BB:472:ARG:NH1	2.48	0.47
2:AB:458:PHE:HB3	22:AB:604:CLA:HBC2	1.97	0.47
2:BB:69:LEU:HD12	22:BB:608:CLA:HBA1	1.97	0.47
5:BE:7:GLU:HB3	6:BF:19:ARG:CZ	2.45	0.47
22:BB:615:CLA:H171	22:BB:616:CLA:HBB2	1.96	0.47
22:BC:513:CLA:HMC2	26:BZ:101:BCR:H372	1.96	0.47
3:AC:250:TRP:HE1	22:AC:506:CLA:HED1	1.80	0.47
2:AB:124:ARG:HD3	2:AB:131:PRO:N	2.30	0.47
1:AA:206:PHE:CE2	22:AD:402:CLA:HBA1	2.50	0.47
3:BC:365:TRP:CB	3:BC:391:ARG:HG2	2.44	0.47
2:AB:7:ARG:NH2	30:AB:621:LMG:O3	2.46	0.47
3:AC:94:THR:HG22	3:AC:298:PRO:HD2	1.96	0.47
7:BH:18:TYR:CG	7:BH:19:GLY:N	2.83	0.47
6:AF:41:GLN:OE1	9:AJ:31:GLY:HA3	2.15	0.47
2:BB:341:LYS:HA	2:BB:405:GLU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:205:ASP:OD1	3:BC:207:ARG:HB3	2.15	0.47
4:BD:185:PHE:CE2	4:BD:289:LEU:HD12	2.49	0.47
16:AV:148:GLU:OE1	16:AV:148:GLU:HA	2.15	0.47
13:BO:194:TYR:CE1	13:BO:198:ILE:HD13	2.50	0.47
1:BA:296:ASN:HB2	3:BC:400:PRO:O	2.14	0.47
2:BB:175:THR:O	2:BB:176:GLY:O	2.33	0.47
15:AU:56:ASP:HB3	15:AU:60:THR:H	1.80	0.47
22:AB:605:CLA:HMA1	22:AB:606:CLA:HBA2	1.96	0.47
29:AA:412:SQD:H5	4:AD:232:PHE:HB3	1.96	0.47
3:BC:109:PHE:HB3	3:BC:110:PRO:HD3	1.96	0.47
4:AD:49:LEU:HD13	26:AD:406:BCR:C15	2.45	0.47
1:AA:190:HIS:HB3	1:AA:293:MET:CE	2.43	0.47
2:BB:173:GLY:HA3	2:BB:265:ILE:HD11	1.95	0.47
5:AE:4:THR:CG2	5:AE:5:THR:N	2.77	0.47
1:BA:107:TYR:HD1	13:BO:141:ARG:NH1	2.13	0.47
13:BO:135:GLN:HG2	13:BO:141:ARG:HG3	1.96	0.47
5:BE:14:ILE:CG2	9:BJ:13:VAL:HG11	2.45	0.47
16:BV:130:MET:SD	16:BV:133:LEU:HD12	2.54	0.47
16:BV:39:ASN:HD21	16:BV:43:LYS:HB3	1.79	0.47
3:AC:27:ASP:OD1	3:AC:28:GLN:HG2	2.14	0.47
14:AT:4:ILE:HD13	26:AT:102:BCR:C38	2.44	0.47
22:AB:607:CLA:H193	11:AL:27:LEU:HD11	1.95	0.47
3:AC:365:TRP:CB	3:AC:391:ARG:HG2	2.45	0.47
5:AE:15:THR:O	9:AJ:8:ILE:HD12	2.15	0.47
16:AV:98:LEU:O	16:AV:102:MET:HG3	2.15	0.47
30:BI:101:LMG:H181	32:BI:102:LMT:H42	1.97	0.47
3:AC:33:PHE:HE1	4:AD:229:ALA:CB	2.27	0.47
3:AC:229:ASN:ND2	3:AC:232:ASP:OD1	2.44	0.47
4:BD:303:ILE:CD1	12:BM:2:GLU:HG2	2.45	0.47
3:BC:34:ALA:HB2	4:BD:230:SER:CB	2.44	0.47
4:AD:176:ALA:HA	4:AD:179:PHE:CD2	2.49	0.47
3:AC:56:HIS:C	3:AC:58:GLY:N	2.68	0.47
3:BC:405:ASN:HB2	27:BC:518:DGD:HG31	1.97	0.47
1:BA:317:TRP:O	1:BA:321:ILE:HG13	2.15	0.47
15:BU:72:TYR:O	15:BU:73:PRO:C	2.51	0.47
1:BA:258:LEU:O	4:BD:128:ARG:NH1	2.48	0.47
4:AD:122:LEU:HB3	4:AD:150:ILE:CD1	2.45	0.47
4:AD:261:PHE:O	4:AD:262:SER:HB3	2.14	0.47
4:AD:274:VAL:HG13	24:AD:405:PL9:H211	1.97	0.47
1:BA:11:ALA:HB1	1:BA:15:GLU:OE1	2.15	0.47
1:BA:12:ASN:O	1:BA:16:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:306:VAL:HG11	1:AA:316:THR:HG23	1.96	0.47
3:AC:193:GLY:O	3:AC:194:GLY:O	2.33	0.47
4:AD:93:TRP:HA	4:AD:99:GLY:H	1.80	0.47
4:BD:89:LEU:HG	7:BH:50:ASN:OD1	2.15	0.47
2:BB:458:PHE:HB3	22:BB:607:CLA:HBC2	1.97	0.46
3:AC:53:HIS:HB3	22:AC:512:CLA:OBD	2.15	0.46
13:AO:92:VAL:HG12	13:AO:93:PRO:CD	2.43	0.46
4:AD:14:TRP:CE3	18:AX:38:ILE:HD12	2.50	0.46
13:BO:77:LEU:HB3	13:BO:91:PHE:HB3	1.97	0.46
1:AA:32:TRP:HA	1:AA:32:TRP:HE3	1.76	0.46
5:AE:8:ARG:HB2	6:AF:13:TYR:CB	2.45	0.46
3:BC:315:MET:HE1	3:BC:369:LEU:HD12	1.97	0.46
30:BE:102:LMG:HC71	30:BE:102:LMG:O9	2.15	0.46
1:BA:40:THR:HG23	22:BA:407:CLA:HBB1	1.96	0.46
6:BF:11:VAL:CG1	6:BF:12:SER:N	2.77	0.46
1:BA:60:ILE:HG23	1:BA:61:ASP:N	2.30	0.46
13:AO:135:GLN:HG2	13:AO:141:ARG:HG3	1.97	0.46
3:AC:258:GLY:CA	3:AC:262:ARG:HH12	2.28	0.46
13:BO:225:LEU:C	13:BO:226:ASN:HD22	2.18	0.46
4:BD:122:LEU:HB3	4:BD:150:ILE:CD1	2.46	0.46
22:AB:606:CLA:H72	26:AB:620:BCR:H311	1.97	0.46
22:BB:611:CLA:H51	22:BB:612:CLA:H101	1.97	0.46
2:AB:216:HIS:HE1	22:AB:609:CLA:C1A	2.29	0.46
13:AO:83:LYS:CG	13:AO:84:ASN:H	2.23	0.46
4:AD:60:THR:HG23	4:AD:61:HIS:HD2	1.75	0.46
3:AC:328:VAL:HG23	3:AC:329:GLY:N	2.31	0.46
16:BV:98:LEU:O	16:BV:102:MET:HG3	2.16	0.46
3:AC:452:ALA:C	3:AC:454:GLY:N	2.68	0.46
1:AA:278:TRP:HB3	1:AA:279:PRO:CD	2.46	0.46
3:BC:258:GLY:HA3	3:BC:262:ARG:HH12	1.80	0.46
13:BO:72:GLN:O	13:BO:263:GLY:HA3	2.14	0.46
26:BB:620:BCR:HC31	12:BM:10:ALA:HB2	1.97	0.46
1:BA:92:HIS:CD2	3:BC:219:GLY:HA3	2.49	0.46
16:AV:68:VAL:HG13	16:AV:68:VAL:O	2.15	0.46
27:BB:602:DGD:HE1	27:BB:602:DGD:HD5	1.66	0.46
2:AB:462:PHE:CE1	22:AB:613:CLA:HMB3	2.50	0.46
2:AB:474:LEU:O	4:AD:134:ARG:NH1	2.48	0.46
27:AC:517:DGD:HBV1	28:AC:521:LHG:H151	1.98	0.46
3:BC:114:VAL:HG13	22:BC:503:CLA:HMA3	1.97	0.46
4:AD:146:PHE:O	4:AD:150:ILE:HG12	2.14	0.46
20:AZ:36:SER:C	20:AZ:38:GLN:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:214:MET:O	1:AA:215:HIS:C	2.54	0.46
4:BD:14:TRP:CE3	18:BX:38:ILE:HD12	2.51	0.46
13:BO:94:THR:HB	13:BO:135:GLN:O	2.14	0.46
1:AA:334:ARG:NH1	13:AO:184:ASP:C	2.69	0.46
2:BB:201:HIS:HD2	2:BB:202:HIS:ND1	2.13	0.46
2:BB:422:ARG:HG2	2:BB:422:ARG:HH11	1.80	0.46
10:AK:35:LEU:HA	10:AK:38:VAL:HG23	1.96	0.46
22:BA:403:CLA:H202	22:BA:404:CLA:H93	1.98	0.46
1:AA:239:PHE:O	14:AT:29:ILE:HA	2.14	0.46
22:BD:404:CLA:C4	18:BX:26:GLY:HA3	2.36	0.46
2:BB:462:PHE:CE1	22:BB:616:CLA:HMB3	2.51	0.46
1:AA:283:VAL:HG21	23:AA:405:PHO:HBC3	1.97	0.46
5:BE:78:THR:HA	5:BE:81:GLU:HG2	1.98	0.46
13:BO:120:THR:HA	13:BO:153:ALA:O	2.15	0.46
7:AH:25:TRP:O	7:AH:26:GLY:C	2.53	0.46
2:BB:265:ILE:HG13	2:BB:266:GLU:N	2.30	0.46
2:AB:341:LYS:HA	2:AB:405:GLU:HB2	1.98	0.46
13:BO:226:ASN:HD22	13:BO:226:ASN:N	2.13	0.46
1:BA:149:ALA:HB3	1:BA:150:PRO:CD	2.45	0.46
13:BO:113:VAL:HA	13:BO:119:LEU:HD23	1.98	0.46
12:AM:24:ILE:HG12	12:BM:24:ILE:HG12	1.98	0.46
1:BA:216:GLY:O	1:BA:220:THR:HG22	2.16	0.46
5:BE:64:PRO:HD3	5:BE:84:LYS:HE2	1.97	0.46
3:BC:460:ASP:O	3:BC:461:ARG:C	2.54	0.46
3:BC:315:MET:O	3:BC:319:ILE:HG13	2.16	0.46
3:BC:33:PHE:HE1	4:BD:229:ALA:CB	2.28	0.46
13:AO:113:VAL:HA	13:AO:119:LEU:HD23	1.97	0.46
15:BU:56:ASP:HB3	15:BU:60:THR:H	1.80	0.46
4:BD:26:ARG:HD3	6:BF:18:VAL:CG1	2.34	0.46
7:BH:35:MET:HE2	26:BX:101:BCR:H322	1.96	0.46
2:AB:10:THR:O	2:AB:13:ILE:HG13	2.16	0.46
3:BC:223:TRP:CE3	3:BC:224:ILE:HG13	2.51	0.46
20:AZ:35:ARG:HG3	20:AZ:36:SER:N	2.30	0.46
1:BA:10:SER:C	1:BA:12:ASN:H	2.19	0.46
1:AA:216:GLY:O	1:AA:220:THR:HG22	2.16	0.46
5:AE:17:VAL:HG22	9:AJ:8:ILE:HD11	1.97	0.46
2:BB:7:ARG:NH2	30:BB:623:LMG:O3	2.49	0.46
3:AC:258:GLY:HA3	3:AC:262:ARG:HH12	1.81	0.46
3:AC:34:ALA:HB2	4:AD:230:SER:CB	2.46	0.46
3:BC:405:ASN:HD22	27:BC:518:DGD:C5D	2.25	0.46
2:AB:96:VAL:HG22	22:AB:606:CLA:HBA1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:229:LEU:O	2:AB:230:ARG:C	2.54	0.46
20:BZ:32:ASP:C	20:BZ:34:ASP:H	2.17	0.46
4:AD:217:THR:O	4:AD:221:THR:HB	2.15	0.46
2:AB:59:GLY:HA3	22:AB:607:CLA:HED1	1.98	0.46
3:BC:318:LEU:HD23	3:BC:318:LEU:O	2.16	0.46
3:BC:328:VAL:HG23	3:BC:329:GLY:N	2.30	0.46
20:AZ:23:VAL:HB	20:AZ:24:PRO:HD3	1.97	0.46
12:AM:18:PRO:O	12:AM:21:PHE:HB3	2.16	0.46
8:AI:24:LEU:O	8:AI:26:GLY:N	2.41	0.46
10:AK:37:PHE:HB3	26:AK:102:BCR:H402	1.97	0.46
2:BB:141:ILE:O	2:BB:144:PHE:HB3	2.16	0.46
2:BB:12:LEU:O	2:BB:14:ASN:N	2.49	0.46
1:AA:40:THR:HG23	22:AA:406:CLA:HBB1	1.98	0.46
3:BC:202:PRO:HB2	3:BC:235:GLY:HA2	1.97	0.46
2:AB:63:LEU:N	2:AB:64:PRO:HD2	2.30	0.46
1:AA:330:VAL:HG11	4:AD:348:ARG:HG2	1.98	0.46
1:BA:221:SER:HB2	4:BD:139:ARG:O	2.15	0.46
22:AC:509:CLA:H121	22:AC:509:CLA:HBD	1.97	0.46
3:BC:101:PRO:O	3:BC:104:GLU:HB2	2.16	0.46
16:BV:54:GLU:OE1	16:BV:54:GLU:HA	2.15	0.46
16:AV:54:GLU:OE1	16:AV:54:GLU:HA	2.16	0.46
2:AB:71:VAL:HG21	2:AB:96:VAL:HG21	1.98	0.46
22:BB:609:CLA:H3A	22:BB:609:CLA:HBA2	1.55	0.46
7:BH:35:MET:HE2	26:BX:101:BCR:C32	2.46	0.46
15:BU:72:TYR:CB	15:BU:73:PRO:CD	2.94	0.46
2:AB:329:PRO:HD3	22:AB:607:CLA:CED	2.46	0.46
2:AB:444:ARG:HG3	2:AB:444:ARG:HH11	1.81	0.46
3:BC:315:MET:CE	3:BC:366:LEU:HD13	2.46	0.46
14:AT:23:PHE:HD1	29:BB:601:SQD:H45	1.81	0.46
4:BD:154:VAL:O	4:BD:158:LEU:HB2	2.16	0.46
1:BA:42:LEU:HD23	29:BA:401:SQD:H192	1.98	0.45
4:BD:274:VAL:HG13	24:BD:405:PL9:H211	1.97	0.45
22:AB:608:CLA:H92	29:AD:409:SQD:H172	1.97	0.45
3:BC:163:PHE:CD1	3:BC:252:ILE:HD11	2.51	0.45
1:AA:214:MET:CE	4:AD:142:ASN:ND2	2.79	0.45
13:AO:86:ARG:HD2	13:AO:87:GLN:N	2.31	0.45
3:BC:235:GLY:O	3:BC:238:ILE:HB	2.15	0.45
7:BH:21:VAL:HG23	7:BH:22:ALA:O	2.15	0.45
18:BX:44:ASP:O	18:BX:45:LYS:HB3	2.16	0.45
3:BC:82:TYR:HA	3:BC:422:PRO:HG2	1.98	0.45
1:AA:262:TYR:O	30:AE:102:LMG:H112	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BI:24:LEU:O	8:BI:26:GLY:N	2.41	0.45
3:BC:435:PHE:O	3:BC:438:LEU:N	2.47	0.45
22:BB:609:CLA:H72	26:BB:622:BCR:H311	1.98	0.45
3:AC:114:VAL:HG13	22:AC:503:CLA:HMA3	1.97	0.45
2:AB:450:TRP:NE1	22:AB:607:CLA:HBA1	2.32	0.45
4:BD:221:THR:CG2	4:BD:244:TYR:HB2	2.45	0.45
2:BB:484:PRO:O	2:BB:485:GLU:HG2	2.16	0.45
7:AH:21:VAL:HG23	7:AH:22:ALA:O	2.16	0.45
3:AC:318:LEU:HD23	3:AC:318:LEU:O	2.16	0.45
4:BD:213:ILE:HG23	4:BD:214:HIS:N	2.32	0.45
22:BC:509:CLA:HBD	22:BC:509:CLA:H121	1.97	0.45
1:BA:334:ARG:NH1	13:BO:184:ASP:C	2.69	0.45
2:BB:444:ARG:HH11	2:BB:444:ARG:HG3	1.82	0.45
22:BA:403:CLA:HBB1	22:BD:402:CLA:NC	2.32	0.45
34:BE:101:HEM:CBC	6:BF:27:ALA:HB1	2.39	0.45
20:BZ:36:SER:C	20:BZ:38:GLN:N	2.70	0.45
3:AC:210:PHE:HZ	3:AC:243:ILE:HD11	1.81	0.45
3:AC:49:LEU:O	3:AC:53:HIS:ND1	2.43	0.45
1:AA:10:SER:C	1:AA:12:ASN:N	2.69	0.45
1:BA:214:MET:CE	4:BD:142:ASN:ND2	2.79	0.45
15:AU:99:GLU:HA	15:AU:102:LYS:HE3	1.99	0.45
13:BO:116:ASP:OD1	13:BO:157:PRO:HB3	2.16	0.45
14:BT:22:PHE:C	14:BT:23:PHE:HD2	2.20	0.45
13:BO:56:TYR:O	13:BO:161:SER:HA	2.17	0.45
11:AL:31:PHE:HB3	11:AL:35:PHE:CE1	2.51	0.45
2:BB:289:GLN:OE1	2:BB:292:LEU:HD12	2.17	0.45
2:AB:241:SER:HB3	22:AB:612:CLA:HED3	1.97	0.45
1:AA:258:LEU:HD12	4:AD:128:ARG:CD	2.42	0.45
26:AJ:102:BCR:H361	26:AJ:102:BCR:H20C	1.83	0.45
3:BC:53:HIS:HB3	22:BC:512:CLA:OBD	2.16	0.45
1:AA:45:THR:HG23	1:AA:46:ILE:N	2.31	0.45
30:AD:408:LMG:O10	11:AL:18:TYR:HB3	2.16	0.45
1:BA:10:SER:OG	1:BA:13:LEU:HD12	2.16	0.45
2:BB:270:PRO:HG3	2:BB:312:TYR:CD2	2.45	0.45
2:BB:172:TYR:O	2:BB:173:GLY:C	2.52	0.45
5:BE:77:GLU:HA	5:BE:80:LEU:HD23	1.97	0.45
26:BA:410:BCR:H312	8:BI:15:PHE:HE1	1.82	0.45
3:BC:406:SER:HA	3:BC:420:VAL:CG2	2.46	0.45
12:AM:3:VAL:HG11	14:AT:2:GLU:HG2	1.99	0.45
10:BK:21:LEU:HD11	26:BK:102:BCR:C3	2.46	0.45
2:BB:141:ILE:HG21	22:BB:618:CLA:HBB1	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:317:TRP:CD1	4:AD:177:ALA:HB2	2.52	0.45
5:AE:7:GLU:HB3	6:AF:19:ARG:CZ	2.47	0.45
13:BO:70:CYS:O	13:BO:265:PHE:HB2	2.15	0.45
13:BO:86:ARG:O	13:BO:86:ARG:HG3	2.16	0.45
13:AO:144:LEU:CD1	13:AO:259:VAL:HG11	2.45	0.45
1:BA:159:LEU:C	1:BA:162:PRO:HD2	2.37	0.45
4:AD:213:ILE:HG23	4:AD:214:HIS:N	2.30	0.45
15:AU:100:ARG:NH1	15:AU:103:GLN:HG2	2.31	0.45
1:AA:330:VAL:HG12	4:AD:348:ARG:HA	1.97	0.45
5:AE:10:PHE:HB2	30:AE:102:LMG:O2	2.16	0.45
4:BD:303:ILE:HD13	12:BM:2:GLU:HG2	1.99	0.45
13:BO:184:ASP:OD2	13:BO:188:ARG:HB2	2.16	0.45
5:BE:61:ARG:HH22	16:BV:153:GLY:HA3	1.82	0.45
4:AD:185:PHE:CE2	4:AD:289:LEU:HD12	2.52	0.45
11:BL:31:PHE:HB3	11:BL:35:PHE:CE1	2.51	0.45
16:BV:116:GLU:HG3	16:BV:116:GLU:O	2.16	0.45
4:BD:302:GLU:OE1	4:BD:302:GLU:HA	2.17	0.45
15:BU:58:ASN:HD22	15:BU:114:VAL:HG13	1.82	0.45
3:AC:284:PHE:HB3	27:AC:516:DGD:HA51	1.99	0.45
3:AC:308:GLU:HB2	3:AC:361:PHE:CE1	2.51	0.45
1:AA:202:VAL:O	1:AA:206:PHE:HB2	2.17	0.45
2:BB:59:GLY:HA3	22:BB:610:CLA:HED1	1.98	0.45
1:AA:11:ALA:HB1	1:AA:15:GLU:OE1	2.17	0.45
13:BO:120:THR:HG22	13:BO:154:SER:CB	2.47	0.45
13:AO:132:VAL:O	13:AO:144:LEU:HD23	2.17	0.45
15:AU:80:VAL:HG22	15:AU:127:ARG:NH2	2.31	0.45
13:BO:126:GLY:O	13:BO:128:ASP:N	2.50	0.45
1:AA:212:CYS:HB2	4:AD:211:CYS:HB2	1.99	0.45
13:AO:56:TYR:O	13:AO:161:SER:HA	2.17	0.45
1:BA:227:THR:HA	1:BA:231:GLU:OE2	2.17	0.45
11:BL:24:ILE:HD12	11:BL:24:ILE:N	2.31	0.45
10:AK:18:PHE:O	10:AK:22:VAL:HG23	2.16	0.45
7:AH:9:ASP:O	7:AH:12:ARG:HB3	2.17	0.45
1:AA:317:TRP:HZ3	4:AD:180:ARG:CD	2.19	0.45
2:BB:216:HIS:HE1	22:BB:612:CLA:C1A	2.30	0.45
2:BB:229:LEU:O	2:BB:231:MET:N	2.50	0.45
2:BB:474:LEU:O	4:BD:134:ARG:NH1	2.49	0.45
1:AA:258:LEU:O	4:AD:128:ARG:NH1	2.49	0.45
5:BE:17:VAL:HG22	9:BJ:8:ILE:HD11	1.98	0.45
2:BB:284:ILE:HG23	2:BB:305:ILE:CD1	2.44	0.45
30:BA:414:LMG:H421	22:BB:614:CLA:H142	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:306:PRO:HG2	2:AB:309:LEU:HB2	1.98	0.45
3:BC:176:VAL:HG11	3:BC:238:ILE:HG12	1.99	0.45
5:BE:72:ALA:O	5:BE:76:VAL:HG23	2.16	0.45
1:BA:182:PHE:O	1:BA:186:PHE:HB2	2.17	0.45
4:AD:19:ASP:O	4:AD:20:ASP:C	2.55	0.45
3:BC:457:LYS:HE3	4:BD:228:GLY:O	2.17	0.45
22:BA:404:CLA:HED2	4:BD:198:MET:SD	2.57	0.45
6:BF:23:VAL:O	6:BF:27:ALA:HB2	2.17	0.45
1:AA:72:LEU:HD21	32:AT:101:LMT:H31	1.99	0.45
2:BB:10:THR:C	2:BB:12:LEU:N	2.70	0.45
3:BC:49:LEU:O	3:BC:53:HIS:ND1	2.43	0.45
20:BZ:36:SER:HA	20:BZ:39:LEU:CD1	2.46	0.45
4:AD:67:TYR:CE1	4:AD:76:VAL:HG11	2.51	0.45
4:AD:36:LEU:C	4:AD:39:PRO:HD2	2.37	0.45
2:BB:306:PRO:HG2	2:BB:309:LEU:HB2	1.99	0.45
12:AM:28:GLN:CB	12:BM:27:VAL:HG12	2.47	0.45
3:BC:143:TYR:O	3:BC:144:SER:CB	2.65	0.45
3:AC:176:VAL:HG11	3:AC:238:ILE:HG12	1.99	0.45
20:BZ:5:PHE:HE1	20:BZ:54:VAL:HG13	1.80	0.45
3:BC:193:GLY:O	3:BC:194:GLY:O	2.34	0.45
14:BT:22:PHE:C	14:BT:23:PHE:CD2	2.89	0.45
4:BD:337:GLU:O	4:BD:338:ASN:C	2.55	0.45
4:AD:90:LEU:HD23	4:AD:90:LEU:HA	1.79	0.45
30:BC:519:LMG:H172	10:BK:27:VAL:HG11	1.99	0.45
4:BD:146:PHE:O	4:BD:150:ILE:HG12	2.17	0.45
15:AU:72:TYR:HB3	15:AU:73:PRO:CD	2.34	0.45
2:AB:474:LEU:HD11	22:AB:608:CLA:HAA1	1.98	0.45
2:BB:10:THR:O	2:BB:13:ILE:HG13	2.17	0.45
3:BC:284:PHE:HB3	27:BC:516:DGD:HA51	1.99	0.45
3:AC:245:ILE:O	3:AC:249:ILE:HG12	2.16	0.45
22:AB:607:CLA:HBA2	22:AB:607:CLA:H3A	1.68	0.45
4:BD:239:GLN:HB3	4:BD:240:ALA:H	1.34	0.45
1:BA:222:SER:O	1:BA:246:TYR:HB2	2.16	0.45
1:BA:235:TYR:C	1:BA:237:TYR:H	2.20	0.45
15:AU:80:VAL:HG22	15:AU:127:ARG:HH21	1.82	0.45
3:AC:457:LYS:HE3	4:AD:228:GLY:O	2.17	0.45
7:BH:63:LYS:O	7:BH:64:ALA:HB3	2.17	0.45
4:AD:303:ILE:HD13	12:AM:2:GLU:HG2	1.97	0.45
5:AE:51:ARG:O	5:AE:53:ASP:N	2.49	0.45
3:BC:27:ASP:OD1	3:BC:28:GLN:HG2	2.17	0.45
2:AB:141:ILE:O	2:AB:144:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:253:TRP:HB2	4:BD:260:ALA:HB2	1.99	0.45
12:BM:33:GLN:HG2	12:BM:34:LYS:N	2.30	0.45
2:BB:237:VAL:HG22	22:BB:613:CLA:HBC2	2.00	0.45
2:BB:329:PRO:HD3	22:BB:610:CLA:CED	2.46	0.45
5:BE:63:ILE:HG23	5:BE:64:PRO:HD2	1.99	0.45
5:BE:69:ARG:HG3	5:BE:70:PHE:N	2.32	0.45
13:AO:120:THR:HG22	13:AO:154:SER:CB	2.47	0.45
3:AC:435:PHE:O	3:AC:438:LEU:N	2.49	0.45
2:AB:169:SER:O	7:AH:65:LEU:HG	2.16	0.45
3:AC:225:VAL:HG13	3:AC:289:PHE:HA	1.99	0.45
16:AV:119:PRO:HG3	16:AV:127:PHE:CD1	2.52	0.45
16:AV:63:CYS:O	16:AV:64:ALA:C	2.55	0.44
3:BC:425:TRP:HE1	27:BC:517:DGD:HE62	1.82	0.44
26:BJ:102:BCR:H20C	26:BJ:102:BCR:H361	1.81	0.44
27:BB:602:DGD:HA21	32:BB:603:LMT:H121	1.98	0.44
3:AC:35:TRP:CG	3:AC:36:TRP:N	2.84	0.44
3:AC:110:PRO:O	3:AC:114:VAL:HG23	2.17	0.44
1:AA:183:MET:HG2	22:AA:403:CLA:HBC1	1.98	0.44
5:AE:64:PRO:HD3	5:AE:84:LYS:HE2	1.98	0.44
1:BA:238:LYS:HA	1:BA:238:LYS:HD3	1.86	0.44
15:BU:82:ASN:ND2	15:BU:94:ILE:HG23	2.32	0.44
3:BC:452:ALA:C	3:BC:454:GLY:N	2.68	0.44
1:BA:262:TYR:O	30:BE:102:LMG:H112	2.17	0.44
5:BE:9:PRO:O	5:BE:10:PHE:C	2.55	0.44
1:BA:210:LEU:HG	23:BD:403:PHO:NC	2.33	0.44
3:BC:243:ILE:O	22:BC:506:CLA:HMC1	2.17	0.44
22:AC:505:CLA:H42	26:AC:515:BCR:H342	1.99	0.44
5:AE:63:ILE:HG23	5:AE:64:PRO:HD2	1.99	0.44
2:BB:191:ASN:HB2	7:BH:58:VAL:HG22	1.98	0.44
2:AB:191:ASN:HB2	7:AH:58:VAL:HG22	1.98	0.44
6:BF:11:VAL:CG1	6:BF:12:SER:H	2.25	0.44
3:AC:452:ALA:O	3:AC:453:ALA:C	2.56	0.44
5:BE:51:ARG:O	5:BE:54:SER:N	2.50	0.44
4:BD:201:VAL:O	4:BD:205:LEU:HB2	2.17	0.44
13:BO:109:GLY:HA3	13:BO:122:VAL:O	2.16	0.44
8:AI:4:LEU:O	8:AI:8:VAL:HG23	2.17	0.44
16:AV:39:ASN:HD21	16:AV:43:LYS:HB3	1.82	0.44
13:AO:173:ASN:ND2	13:AO:220:LYS:HD3	2.32	0.44
3:BC:56:HIS:C	3:BC:58:GLY:N	2.70	0.44
26:BC:514:BCR:H11C	26:BK:102:BCR:H322	1.99	0.44
3:AC:276:LEU:CD1	3:AC:444:HIS:HD2	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:425:TRP:HE1	27:AC:517:DGD:HE62	1.81	0.44
30:AC:519:LMG:H172	10:AK:27:VAL:HG11	1.99	0.44
18:AX:16:LEU:HD11	18:AX:20:PHE:CE2	2.53	0.44
3:BC:210:PHE:HZ	3:BC:243:ILE:HD11	1.82	0.44
3:AC:170:ILE:HD13	22:AC:513:CLA:H201	1.98	0.44
22:AA:402:CLA:HBB1	22:AD:402:CLA:NC	2.32	0.44
2:BB:450:TRP:NE1	22:BB:610:CLA:HBA1	2.33	0.44
13:AO:218:LEU:HD22	15:AU:119:THR:CG2	2.45	0.44
13:AO:86:ARG:O	13:AO:86:ARG:HG3	2.18	0.44
13:BO:132:VAL:O	13:BO:144:LEU:HD23	2.17	0.44
18:AX:44:ASP:O	18:AX:45:LYS:HB3	2.17	0.44
3:BC:50:LEU:O	3:BC:54:VAL:HG23	2.18	0.44
1:AA:328:MET:HE1	4:AD:183:LEU:HD22	1.98	0.44
22:BB:617:CLA:H51	26:BB:620:BCR:H372	2.00	0.44
2:BB:435:GLU:O	2:BB:436:THR:C	2.56	0.44
13:AO:72:GLN:O	13:AO:263:GLY:HA3	2.17	0.44
13:BO:171:GLU:HA	13:BO:221:GLY:O	2.17	0.44
1:AA:243:GLU:CD	1:AA:243:GLU:H	2.16	0.44
2:AB:283:GLU:OE1	2:AB:283:GLU:HA	2.17	0.44
22:BC:508:CLA:H172	27:BC:517:DGD:HBW2	2.00	0.44
7:BH:53:LEU:HD21	7:BH:55:LEU:HD21	1.99	0.44
10:BK:43:VAL:O	10:BK:46:ARG:HG3	2.18	0.44
3:AC:33:PHE:CE1	4:AD:229:ALA:HB3	2.53	0.44
22:AB:614:CLA:H51	26:AB:617:BCR:H372	1.99	0.44
2:AB:15:ASP:O	2:AB:17:GLY:N	2.50	0.44
4:BD:330:ALA:HB3	4:BD:331:PRO:HD3	1.99	0.44
1:BA:224:ILE:O	1:BA:226:GLU:OE2	2.36	0.44
8:AI:11:VAL:HG22	32:AI:102:LMT:H82	2.00	0.44
2:AB:71:VAL:HG21	2:AB:96:VAL:CG2	2.47	0.44
12:BM:33:GLN:CG	12:BM:34:LYS:N	2.81	0.44
3:AC:243:ILE:O	22:AC:506:CLA:HMC1	2.18	0.44
3:AC:449:ARG:NE	22:AC:505:CLA:HED1	2.22	0.44
1:BA:214:MET:HE1	4:BD:142:ASN:ND2	2.33	0.44
1:BA:39:PRO:HB2	22:BA:407:CLA:CBB	2.48	0.44
3:AC:235:GLY:O	3:AC:238:ILE:HB	2.18	0.44
13:AO:116:ASP:OD1	13:AO:157:PRO:HB3	2.18	0.44
3:BC:363:GLY:O	3:BC:367:GLU:HG2	2.17	0.44
7:AH:28:THR:O	7:AH:31:MET:HB3	2.18	0.44
1:AA:296:ASN:HB2	3:AC:400:PRO:O	2.17	0.44
3:AC:363:GLY:O	3:AC:364:PRO:C	2.56	0.44
16:AV:59:PHE:CD1	16:AV:63:CYS:SG	3.08	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:178:ARG:HD2	13:BO:182:PHE:CG	2.53	0.44
4:BD:180:ARG:HH11	4:BD:180:ARG:HG3	1.78	0.44
4:BD:253:TRP:HA	4:BD:256:ILE:HG23	1.99	0.44
13:AO:230:VAL:CG1	13:AO:231:ASP:N	2.70	0.44
13:BO:69:LEU:HB3	13:BO:107:ILE:CB	2.36	0.44
2:AB:18:ARG:HD2	2:AB:115:TRP:CE3	2.52	0.44
2:AB:271:THR:CG2	2:AB:273:TYR:HB2	2.48	0.44
28:AC:521:LHG:H101	28:AC:521:LHG:H271	2.00	0.44
26:AJ:102:BCR:H371	26:AJ:102:BCR:H24C	1.79	0.44
3:AC:163:PHE:CD1	3:AC:252:ILE:HD11	2.52	0.44
22:BB:610:CLA:H193	11:BL:27:LEU:HD11	1.99	0.44
2:BB:329:PRO:CB	22:BB:610:CLA:HED1	2.43	0.44
1:BA:215:HIS:O	1:BA:216:GLY:C	2.56	0.44
13:BO:86:ARG:CD	13:BO:86:ARG:C	2.84	0.44
1:BA:21:VAL:HG11	1:BA:32:TRP:CE3	2.53	0.44
1:BA:77:ILE:HG12	14:BT:6:TYR:CD1	2.53	0.44
2:BB:86:ILE:C	2:BB:86:ILE:HD12	2.37	0.44
4:AD:209:LEU:O	4:AD:213:ILE:HG22	2.18	0.44
6:AF:16:PHE:O	29:AF:101:SQD:H461	2.18	0.44
2:AB:25:MET:HE2	26:AB:617:BCR:H393	1.98	0.44
2:AB:435:GLU:O	2:AB:436:THR:C	2.56	0.44
3:BC:225:VAL:HG13	3:BC:289:PHE:HA	1.99	0.44
3:AC:55:ALA:HB1	26:AC:514:BCR:C37	2.46	0.44
2:BB:145:LEU:CD1	22:BB:618:CLA:HMB2	2.47	0.44
1:BA:153:SER:HB2	22:BA:403:CLA:H43	2.00	0.44
2:BB:413:ASP:O	2:BB:414:PRO:C	2.55	0.44
5:BE:20:TRP:HD1	9:BJ:8:ILE:HD13	1.83	0.44
13:BO:86:ARG:HD2	13:BO:87:GLN:N	2.32	0.44
2:AB:27:THR:CG2	2:AB:107:LEU:HD13	2.45	0.44
4:BD:36:LEU:C	4:BD:39:PRO:HD2	2.37	0.44
2:BB:7:ARG:HG2	22:BB:614:CLA:CED	2.48	0.44
1:AA:107:TYR:HD1	13:AO:141:ARG:NH1	2.16	0.44
2:BB:25:MET:HE2	26:BB:620:BCR:H393	2.00	0.44
4:BD:101:PHE:O	4:BD:104:TRP:HB3	2.17	0.44
7:BH:39:LEU:C	7:BH:39:LEU:HD23	2.38	0.44
26:AC:514:BCR:H11C	26:AK:102:BCR:H322	2.00	0.44
3:BC:245:ILE:O	3:BC:249:ILE:HG12	2.18	0.44
1:AA:42:LEU:HA	1:AA:45:THR:HG22	2.00	0.44
2:AB:185:TRP:CE3	22:AB:601:CLA:H61	2.53	0.44
3:AC:143:TYR:O	3:AC:144:SER:CB	2.64	0.44
2:AB:263:THR:HB	2:AB:448:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:50:LEU:O	3:AC:54:VAL:HG23	2.17	0.44
5:BE:34:GLY:O	5:BE:37:PHE:HB3	2.17	0.44
10:BK:44:GLY:O	10:BK:45:PHE:C	2.56	0.44
2:AB:206:GLY:O	2:AB:210:ILE:HG13	2.18	0.44
2:AB:422:ARG:HG2	2:AB:422:ARG:HH11	1.81	0.44
4:AD:253:TRP:HB2	4:AD:260:ALA:HB2	2.00	0.44
1:AA:64:ARG:O	13:AO:178:ARG:NH2	2.51	0.44
3:AC:269:GLU:O	3:AC:272:LEU:HB3	2.18	0.44
3:AC:208:VAL:O	3:AC:209:ILE:C	2.56	0.44
2:BB:59:GLY:HA3	22:BB:610:CLA:CED	2.48	0.44
1:BA:12:ASN:O	1:BA:15:GLU:HB3	2.18	0.44
1:BA:214:MET:O	1:BA:215:HIS:C	2.54	0.44
1:AA:220:THR:O	1:AA:223:LEU:HG	2.18	0.44
3:BC:140:LEU:HB2	3:BC:148:GLY:HA2	2.00	0.44
16:AV:81:ARG:HH11	16:AV:81:ARG:HG2	1.83	0.44
30:BI:101:LMG:H132	32:BI:102:LMT:O2'	2.18	0.44
3:AC:82:TYR:HA	3:AC:422:PRO:HG2	2.00	0.44
3:BC:258:GLY:C	3:BC:262:ARG:NH1	2.71	0.44
3:BC:229:ASN:ND2	3:BC:232:ASP:OD1	2.43	0.44
1:AA:247:ASN:HB3	1:AA:250:ALA:HB3	2.00	0.44
2:AB:298:LEU:HA	2:AB:298:LEU:HD12	1.75	0.44
10:AK:17:ILE:C	10:AK:18:PHE:HD2	2.21	0.43
1:BA:183:MET:HG2	22:BA:404:CLA:HBC1	1.99	0.43
34:AE:101:HEM:HBC2	6:AF:27:ALA:CB	2.39	0.43
3:AC:472:LEU:HD12	3:AC:473:ASP:N	2.28	0.43
22:BB:611:CLA:H92	29:BD:409:SQD:H172	2.00	0.43
2:AB:118:TRP:CH2	11:AL:5:PRO:HD2	2.53	0.43
15:BU:73:PRO:HG2	16:BV:107:THR:HB	2.00	0.43
1:AA:238:LYS:HD3	1:AA:238:LYS:HA	1.86	0.43
5:BE:36:LEU:HA	5:BE:39:SER:OG	2.18	0.43
7:AH:18:TYR:CG	7:AH:19:GLY:N	2.85	0.43
20:BZ:5:PHE:CD2	20:BZ:61:VAL:HG21	2.53	0.43
8:BI:6:ILE:CD1	32:BI:102:LMT:H5'	2.48	0.43
20:AZ:5:PHE:CG	20:AZ:61:VAL:HG21	2.53	0.43
1:BA:324:ALA:O	1:BA:328:MET:HE3	2.18	0.43
2:BB:383:PHE:O	13:BO:192:SER:HA	2.18	0.43
1:AA:182:PHE:O	1:AA:186:PHE:HB2	2.18	0.43
16:AV:64:ALA:O	16:AV:65:SER:C	2.56	0.43
26:AC:514:BCR:HC22	10:AK:18:PHE:HD1	1.83	0.43
3:BC:163:PHE:CG	22:BC:512:CLA:HAB	2.52	0.43
1:AA:217:SER:O	1:AA:220:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:484:PRO:O	2:AB:485:GLU:HG2	2.18	0.43
2:BB:348:ASN:O	2:BB:349:LYS:C	2.56	0.43
3:BC:365:TRP:HB3	3:BC:391:ARG:HG2	1.99	0.43
15:BU:99:GLU:HA	15:BU:102:LYS:HE3	1.99	0.43
18:AX:32:LEU:H	18:AX:32:LEU:HD23	1.83	0.43
3:AC:386:PRO:HB3	16:AV:116:GLU:HG2	2.00	0.43
4:AD:303:ILE:CD1	12:AM:2:GLU:HG2	2.48	0.43
15:BU:64:ALA:O	15:BU:67:GLN:HG2	2.18	0.43
2:BB:243:ALA:HB2	2:BB:466:HIS:CE1	2.53	0.43
2:AB:442:ILE:HD11	13:AO:200:LEU:HD23	2.00	0.43
2:BB:343:HIS:O	2:BB:401:PHE:HA	2.18	0.43
12:BM:18:PRO:O	12:BM:21:PHE:HB3	2.18	0.43
4:AD:190:ASN:HB2	4:AD:296:TYR:CD1	2.52	0.43
12:BM:3:VAL:HG11	14:BT:2:GLU:HG2	2.00	0.43
10:AK:17:ILE:HG22	10:AK:17:ILE:O	2.17	0.43
10:BK:16:ALA:O	10:BK:19:ASP:HB2	2.18	0.43
2:BB:113:TRP:CE2	2:BB:117:TYR:CD2	3.06	0.43
15:AU:54:LYS:HD2	15:AU:113:THR:CG2	2.49	0.43
12:AM:33:GLN:HG2	12:AM:34:LYS:N	2.33	0.43
2:BB:474:LEU:HD11	22:BB:611:CLA:HAA1	1.99	0.43
7:BH:9:ASP:O	7:BH:12:ARG:HB3	2.18	0.43
2:AB:10:THR:C	2:AB:12:LEU:N	2.71	0.43
2:AB:229:LEU:HD11	22:AB:609:CLA:O1A	2.18	0.43
3:AC:362:ARG:H	27:AC:516:DGD:HE4	1.83	0.43
4:AD:152:VAL:HG12	22:AD:402:CLA:H43	2.00	0.43
26:BD:406:BCR:H363	6:BF:33:PHE:HB3	2.01	0.43
26:AB:618:BCR:C38	14:BT:4:ILE:HD13	2.48	0.43
13:BO:86:ARG:O	13:BO:86:ARG:NH1	2.44	0.43
1:AA:333:GLU:HB2	1:AA:337:HIS:HE1	1.83	0.43
2:BB:222:PRO:O	2:BB:223:GLN:C	2.56	0.43
5:AE:72:ALA:O	5:AE:76:VAL:HG23	2.18	0.43
13:BO:135:GLN:HE21	13:BO:135:GLN:HB3	1.57	0.43
2:BB:170:ASP:HB2	2:BB:171:PRO:HD2	2.01	0.43
2:AB:164:PRO:HG2	2:AB:165:GLY:H	1.82	0.43
3:BC:456:GLU:N	3:BC:456:GLU:OE1	2.52	0.43
8:AI:6:ILE:CD1	32:AI:102:LMT:H5'	2.48	0.43
15:AU:73:PRO:HG2	16:AV:107:THR:HB	2.01	0.43
22:BC:501:CLA:HMB3	26:BC:515:BCR:C40	2.44	0.43
2:AB:348:ASN:OD1	2:AB:352:GLU:HB2	2.18	0.43
1:BA:10:SER:C	1:BA:12:ASN:N	2.71	0.43
1:BA:329:GLU:O	1:BA:332:HIS:ND1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:AB:602:CLA:H162	22:AB:602:CLA:H122	1.79	0.43
2:AB:86:ILE:HD12	2:AB:86:ILE:C	2.38	0.43
5:AE:69:ARG:HG3	5:AE:70:PHE:N	2.34	0.43
4:AD:161:PRO:HB3	4:AD:170:ALA:HB2	2.01	0.43
1:AA:60:ILE:HG23	1:AA:61:ASP:N	2.32	0.43
3:AC:318:LEU:HG	3:AC:328:VAL:CG1	2.48	0.43
5:BE:49:THR:HA	5:BE:50:PRO:HD3	1.84	0.43
20:BZ:23:VAL:HB	20:BZ:24:PRO:HD3	2.00	0.43
7:AH:63:LYS:C	7:AH:65:LEU:N	2.70	0.43
6:BF:41:GLN:OE1	9:BJ:31:GLY:HA3	2.18	0.43
2:BB:368:VAL:HG21	2:BB:381:ILE:HD12	2.01	0.43
1:BA:212:CYS:HB2	4:BD:211:CYS:HB2	2.01	0.43
14:AT:25:GLU:O	14:AT:26:PRO:C	2.54	0.43
3:AC:223:TRP:CE3	3:AC:224:ILE:HG13	2.53	0.43
26:AT:102:BCR:H271	22:BB:610:CLA:HMD3	2.01	0.43
14:AT:4:ILE:HD13	26:AT:102:BCR:H381	2.00	0.43
22:AB:607:CLA:CAC	26:AB:618:BCR:H393	2.49	0.43
4:BD:244:TYR:HH	4:BD:264:LYS:HE3	1.82	0.43
5:AE:20:TRP:HD1	9:AJ:8:ILE:HD13	1.82	0.43
10:AK:46:ARG:NH1	10:AK:46:ARG:HB2	2.34	0.43
1:AA:39:PRO:HB2	22:AA:406:CLA:CBB	2.48	0.43
2:AB:284:ILE:HG23	2:AB:305:ILE:CD1	2.48	0.43
30:AA:413:LMG:H421	22:AB:611:CLA:H142	2.00	0.43
3:BC:453:ALA:HA	8:BI:34:ARG:O	2.18	0.43
18:BX:42:GLN:O	18:BX:43:ILE:HG13	2.18	0.43
4:AD:154:VAL:O	4:AD:158:LEU:HB2	2.18	0.43
2:AB:366:PHE:CD1	2:AB:367:PRO:HD2	2.53	0.43
16:BV:63:CYS:O	16:BV:64:ALA:C	2.56	0.43
10:BK:17:ILE:CD1	10:BK:17:ILE:N	2.80	0.43
19:BY:23:UNK:O	19:BY:24:UNK:C	2.67	0.43
3:AC:160:ILE:HA	3:AC:163:PHE:CD2	2.53	0.43
1:AA:198:HIS:O	1:AA:202:VAL:HG12	2.18	0.43
20:AZ:36:SER:HA	20:AZ:39:LEU:CD1	2.48	0.43
1:AA:214:MET:HA	1:AA:214:MET:HE2	1.97	0.43
1:AA:159:LEU:C	1:AA:162:PRO:HD2	2.38	0.43
3:BC:203:THR:O	3:BC:235:GLY:HA3	2.19	0.43
3:BC:452:ALA:O	3:BC:453:ALA:C	2.57	0.43
13:BO:225:LEU:HD12	13:BO:225:LEU:N	2.34	0.43
20:BZ:17:PHE:HE2	20:BZ:21:ILE:HD11	1.83	0.43
4:AD:253:TRP:HA	4:AD:256:ILE:HG23	2.01	0.43
2:BB:69:LEU:HD21	22:BB:606:CLA:HED3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BT:29:ILE:O	14:BT:31:LYS:N	2.52	0.43
2:BB:229:LEU:O	2:BB:230:ARG:C	2.56	0.43
3:BC:110:PRO:O	3:BC:114:VAL:HG23	2.19	0.43
3:AC:163:PHE:CG	22:AC:512:CLA:HAB	2.54	0.43
3:AC:162:GLY:O	3:AC:166:ILE:HG13	2.18	0.43
1:AA:153:SER:HB2	22:AA:402:CLA:H43	2.00	0.43
4:AD:126:MET:HE3	4:AD:150:ILE:HG13	2.00	0.43
4:AD:263:ASN:O	4:AD:265:ARG:N	2.52	0.43
26:AD:406:BCR:H363	6:AF:33:PHE:HB3	2.00	0.43
20:AZ:30:PRO:C	20:AZ:32:ASP:N	2.72	0.43
1:BA:220:THR:O	1:BA:223:LEU:HG	2.19	0.43
1:BA:214:MET:HE1	4:BD:142:ASN:HD21	1.84	0.43
5:AE:20:TRP:CD1	9:AJ:8:ILE:HD13	2.53	0.43
16:BV:81:ARG:NH1	16:BV:81:ARG:HG2	2.34	0.43
3:AC:460:ASP:O	3:AC:461:ARG:C	2.55	0.43
1:BA:330:VAL:HG11	4:BD:348:ARG:HG2	1.99	0.43
2:BB:472:ARG:HH11	2:BB:472:ARG:HG2	1.84	0.43
13:AO:171:GLU:HA	13:AO:221:GLY:O	2.19	0.43
4:AD:101:PHE:O	4:AD:104:TRP:HB3	2.18	0.43
15:BU:54:LYS:HD2	15:BU:113:THR:CG2	2.48	0.43
28:BA:412:LHG:HC81	3:BC:36:TRP:CZ3	2.54	0.43
28:BA:412:LHG:HC92	29:BA:413:SQD:O10	2.19	0.43
3:BC:28:GLN:HB2	22:BC:511:CLA:HED3	2.01	0.43
6:AF:24:HIS:HA	6:AF:27:ALA:HB3	2.00	0.43
1:BA:239:PHE:O	14:BT:29:ILE:HA	2.19	0.43
22:BC:505:CLA:H42	26:BC:515:BCR:H342	2.01	0.43
14:AT:21:ILE:HD12	26:AT:102:BCR:H332	2.01	0.43
2:AB:349:LYS:HG2	2:AB:395:GLN:O	2.19	0.43
2:BB:135:LEU:HD23	2:BB:138:MET:HE1	1.98	0.43
2:BB:354:LEU:HD12	2:BB:378:LYS:HB2	2.01	0.43
12:AM:31:SER:HA	30:AM:101:LMG:HC3	2.01	0.43
22:BB:605:CLA:H122	22:BB:605:CLA:H162	1.80	0.43
4:BD:323:GLU:HG2	13:BO:194:TYR:OH	2.19	0.43
16:BV:119:PRO:HG3	16:BV:127:PHE:CD1	2.53	0.43
7:AH:39:LEU:C	7:AH:39:LEU:HD23	2.39	0.43
26:BJ:102:BCR:H371	26:BJ:102:BCR:H24C	1.78	0.43
10:BK:17:ILE:C	10:BK:18:PHE:HD2	2.20	0.43
1:BA:198:HIS:O	1:BA:202:VAL:HG12	2.19	0.43
13:AO:70:CYS:O	13:AO:265:PHE:HB2	2.18	0.43
5:BE:20:TRP:CD1	9:BJ:8:ILE:HD13	2.54	0.43
10:AK:43:VAL:O	10:AK:46:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BO:168:PHE:O	13:BO:224:SER:HA	2.19	0.43
13:AO:168:PHE:O	13:AO:224:SER:HA	2.19	0.43
4:BD:188:PHE:HE2	4:BD:329:MET:HE2	1.84	0.43
1:BA:131:TRP:CE3	1:BA:132:GLU:CA	3.02	0.43
1:BA:111:PRO:O	1:BA:115:ILE:HG13	2.19	0.43
7:BH:63:LYS:C	7:BH:65:LEU:N	2.71	0.43
10:AK:44:GLY:O	10:AK:45:PHE:C	2.57	0.43
1:BA:288:LEU:O	1:BA:292:THR:HB	2.18	0.43
3:AC:464:GLU:O	3:AC:467:LEU:HB2	2.19	0.43
4:AD:203:GLY:O	4:AD:207:GLY:N	2.52	0.43
19:BY:23:UNK:O	19:BY:25:UNK:N	2.52	0.43
4:BD:204:VAL:HG22	4:BD:279:LEU:HD21	2.01	0.43
4:AD:180:ARG:HH11	4:AD:180:ARG:HG3	1.79	0.43
3:BC:165:LEU:HG	22:BC:507:CLA:HED1	2.00	0.43
22:BC:512:CLA:H162	22:BC:512:CLA:HMA2	2.01	0.43
2:BB:280:PHE:O	2:BB:284:ILE:HG13	2.19	0.43
3:BC:415:ASN:O	3:BC:416:SER:CB	2.64	0.43
1:AA:222:SER:O	1:AA:246:TYR:HB2	2.19	0.43
13:AO:227:VAL:CG1	13:AO:228:ALA:N	2.82	0.43
13:AO:225:LEU:N	13:AO:225:LEU:HD12	2.33	0.43
2:BB:289:GLN:OE1	2:BB:289:GLN:HA	2.19	0.43
3:BC:386:PRO:HB3	16:BV:116:GLU:HG2	2.00	0.43
2:BB:164:PRO:HG2	2:BB:165:GLY:H	1.83	0.43
2:AB:289:GLN:OE1	2:AB:292:LEU:HD12	2.19	0.43
3:AC:394:GLU:OE2	3:AC:398:HIS:CD2	2.71	0.43
3:AC:28:GLN:HB2	22:AC:511:CLA:HED3	2.00	0.42
10:AK:21:LEU:HD11	26:AK:102:BCR:C3	2.47	0.42
22:BB:615:CLA:H122	22:BB:615:CLA:H162	1.84	0.42
4:AD:217:THR:HG21	24:AD:405:PL9:C1	2.49	0.42
10:BK:46:ARG:HH11	10:BK:46:ARG:CB	2.32	0.42
2:BB:464:PHE:HD2	22:BB:614:CLA:HAC2	1.84	0.42
12:AM:19:SER:O	12:AM:23:ILE:HG13	2.18	0.42
7:AH:41:PHE:O	7:AH:45:ILE:HG23	2.18	0.42
2:AB:222:PRO:CG	7:AH:27:THR:H	2.28	0.42
2:BB:247:PHE:CE1	22:BB:605:CLA:H101	2.48	0.42
15:AU:82:ASN:ND2	15:AU:94:ILE:HG23	2.34	0.42
2:AB:243:ALA:HB2	2:AB:466:HIS:CE1	2.54	0.42
2:AB:275:TRP:CH2	2:AB:358:ARG:HD3	2.54	0.42
4:BD:291:LEU:O	4:BD:292:ASN:HB2	2.19	0.42
3:BC:273:SER:OG	3:BC:274:TYR:N	2.52	0.42
16:BV:68:VAL:O	16:BV:68:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:193:LEU:HG	4:BD:193:LEU:O	2.19	0.42
9:AJ:15:THR:HG23	26:AK:102:BCR:H392	2.01	0.42
22:BC:511:CLA:HMB2	26:BC:514:BCR:H382	2.01	0.42
19:BY:21:UNK:O	19:BY:22:UNK:C	2.66	0.42
1:BA:317:TRP:HZ3	4:BD:180:ARG:CD	2.20	0.42
12:AM:33:GLN:CG	12:AM:34:LYS:N	2.82	0.42
2:BB:71:VAL:HG21	2:BB:96:VAL:HG21	2.01	0.42
6:BF:24:HIS:HA	6:BF:27:ALA:HB3	2.02	0.42
1:AA:73:TYR:CE2	30:AA:416:LMG:HC61	2.53	0.42
22:AC:508:CLA:H172	27:AC:517:DGD:HBW2	2.01	0.42
3:BC:437:PHE:CZ	22:BC:510:CLA:HMB3	2.54	0.42
3:AC:437:PHE:CZ	22:AC:510:CLA:HMB3	2.55	0.42
1:AA:215:HIS:CD2	4:AD:268:HIS:HD2	2.37	0.42
1:AA:255:PHE:CE2	24:AA:407:PL9:H111	2.54	0.42
32:BT:101:LMT:H3'	32:BT:101:LMT:H1B	1.63	0.42
3:AC:48:LYS:CD	3:AC:138:GLU:HG3	2.49	0.42
2:AB:464:PHE:HD2	22:AB:611:CLA:HAC2	1.84	0.42
18:BX:45:LYS:CD	18:BX:45:LYS:N	2.82	0.42
3:BC:127:PHE:HE1	20:BZ:23:VAL:HG21	1.84	0.42
13:AO:109:GLY:HA3	13:AO:122:VAL:O	2.18	0.42
15:BU:80:VAL:HG22	15:BU:127:ARG:NH2	2.34	0.42
4:AD:291:LEU:O	4:AD:292:ASN:HB2	2.18	0.42
12:AM:5:GLN:NE2	32:AM:102:LMT:O2B	2.52	0.42
15:BU:50:ALA:HB1	15:BU:113:THR:HG21	2.01	0.42
9:AJ:12:ILE:O	9:AJ:16:VAL:HG23	2.19	0.42
26:BJ:102:BCR:H15C	26:BJ:102:BCR:H351	1.91	0.42
30:BD:408:LMG:HC2	30:BD:408:LMG:HC71	1.82	0.42
7:BH:11:LEU:C	7:BH:13:PRO:HD2	2.40	0.42
2:AB:471:ALA:HB2	4:AD:130:PHE:CE2	2.53	0.42
3:BC:170:ILE:HD13	22:BC:513:CLA:H201	2.00	0.42
22:AC:512:CLA:H162	22:AC:512:CLA:HMA2	2.01	0.42
1:AA:42:LEU:HA	1:AA:45:THR:CG2	2.49	0.42
4:AD:52:THR:HG22	4:AD:67:TYR:CE2	2.54	0.42
13:BO:218:LEU:HD22	15:BU:119:THR:CG2	2.40	0.42
10:BK:46:ARG:NH1	10:BK:46:ARG:CB	2.82	0.42
13:BO:144:LEU:CD1	13:BO:259:VAL:HG11	2.48	0.42
11:BL:12:LEU:HD22	12:BM:25:LEU:HD12	1.99	0.42
4:AD:56:THR:HB	5:AE:49:THR:HG23	2.01	0.42
20:BZ:5:PHE:CG	20:BZ:61:VAL:HG21	2.54	0.42
4:BD:294:ARG:H	4:BD:294:ARG:HG2	1.65	0.42
1:AA:92:HIS:HD2	3:AC:219:GLY:HA3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BB:617:CLA:HBC2	22:BB:617:CLA:HMC1	2.02	0.42
2:BB:234:ILE:C	2:BB:236:THR:H	2.23	0.42
3:AC:456:GLU:N	3:AC:456:GLU:OE1	2.53	0.42
3:AC:406:SER:HA	3:AC:420:VAL:CG2	2.49	0.42
5:AE:60:GLN:HG2	5:AE:62:SER:H	1.84	0.42
2:BB:393:GLU:HG2	15:BU:44:ASP:O	2.19	0.42
1:AA:160:ILE:HD12	3:AC:431:PHE:CE1	2.54	0.42
9:BJ:15:THR:HG23	26:BK:102:BCR:H392	2.01	0.42
10:BK:18:PHE:O	10:BK:19:ASP:C	2.57	0.42
2:BB:120:LEU:HD13	22:BB:619:CLA:CMD	2.40	0.42
2:AB:145:LEU:CD1	22:AB:615:CLA:HMB2	2.49	0.42
13:AO:69:LEU:HB3	13:AO:107:ILE:CB	2.35	0.42
15:AU:72:TYR:CG	15:AU:73:PRO:N	2.87	0.42
2:AB:234:ILE:C	2:AB:236:THR:H	2.23	0.42
3:AC:174:LEU:HD12	22:AC:512:CLA:H71	2.01	0.42
4:AD:221:THR:CG2	4:AD:244:TYR:HB2	2.48	0.42
4:BD:52:THR:HG22	4:BD:67:TYR:CE2	2.54	0.42
2:AB:327:THR:O	2:AB:444:ARG:NE	2.46	0.42
7:AH:55:LEU:HB2	7:AH:58:VAL:CG1	2.49	0.42
4:AD:160:TYR:CB	4:AD:161:PRO:CD	2.96	0.42
10:BK:28:ILE:O	10:BK:31:LEU:HB2	2.20	0.42
3:BC:33:PHE:CE1	4:BD:229:ALA:HB3	2.54	0.42
27:AB:626:DGD:HA21	32:AB:627:LMT:H121	2.01	0.42
5:AE:34:GLY:O	5:AE:37:PHE:HB3	2.19	0.42
15:BU:42:VAL:HG23	15:BU:43:VAL:N	2.33	0.42
3:AC:205:ASP:OD1	3:AC:207:ARG:HB3	2.19	0.42
5:AE:35:TRP:CD1	5:AE:35:TRP:C	2.93	0.42
26:AA:409:BCR:H342	29:AA:415:SQD:H342	2.02	0.42
1:BA:42:LEU:HA	1:BA:45:THR:CG2	2.50	0.42
10:AK:19:ASP:N	10:AK:20:PRO:CD	2.80	0.42
20:BZ:30:PRO:C	20:BZ:32:ASP:N	2.72	0.42
1:BA:217:SER:O	1:BA:220:THR:HG22	2.18	0.42
4:BD:35:ILE:O	4:BD:39:PRO:HG2	2.20	0.42
1:AA:228:THR:HB	1:AA:231:GLU:HB3	2.01	0.42
1:AA:77:ILE:HG12	14:AT:6:TYR:CD1	2.54	0.42
4:BD:161:PRO:HB3	4:BD:170:ALA:HB2	2.02	0.42
13:BO:59:ASP:O	13:BO:61:SER:N	2.53	0.42
20:AZ:5:PHE:CD2	20:AZ:61:VAL:HG21	2.54	0.42
1:BA:136:ARG:NH2	8:BI:27:ASP:OD1	2.49	0.42
2:BB:169:SER:O	7:BH:65:LEU:HG	2.20	0.42
4:AD:89:LEU:HG	7:AH:50:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BC:321:ASP:HA	3:BC:324:LEU:HD23	2.01	0.42
1:AA:207:GLY:O	1:AA:210:LEU:HB3	2.19	0.42
3:BC:35:TRP:CD2	3:BC:36:TRP:N	2.88	0.42
34:AE:101:HEM:HAD2	34:AE:101:HEM:HHA	1.57	0.42
22:BB:612:CLA:NB	26:BX:101:BCR:H312	2.35	0.42
3:AC:276:LEU:HD21	22:AC:508:CLA:HBB1	2.01	0.42
4:AD:263:ASN:O	4:AD:266:TRP:N	2.50	0.42
2:AB:354:LEU:HD12	2:AB:378:LYS:HB2	2.02	0.42
1:BA:255:PHE:CE2	24:BA:408:PL9:H111	2.55	0.42
9:AJ:7:ARG:HA	9:AJ:7:ARG:HE	1.83	0.42
5:AE:15:THR:CG2	9:AJ:7:ARG:HG3	2.49	0.42
16:AV:103:LYS:O	16:AV:122:ARG:HG2	2.19	0.42
16:BV:124:ALA:HB1	16:BV:131:ARG:CG	2.50	0.42
2:AB:472:ARG:HH11	2:AB:472:ARG:HG2	1.84	0.42
13:BO:192:SER:OG	13:BO:193:GLY:N	2.53	0.42
7:BH:28:THR:N	7:BH:29:PRO:HD2	2.35	0.42
2:AB:215:PHE:CD2	2:AB:215:PHE:C	2.93	0.42
34:BV:201:HEM:HHA	34:BV:201:HEM:HAD2	1.61	0.42
16:BV:59:PHE:CD1	16:BV:63:CYS:SG	3.08	0.42
2:BB:71:VAL:HG21	2:BB:96:VAL:CG2	2.50	0.42
5:BE:18:ARG:CD	5:BE:22:ILE:HD11	2.38	0.42
1:AA:73:TYR:CD2	30:AA:416:LMG:HC3	2.55	0.42
2:AB:413:ASP:O	2:AB:414:PRO:C	2.57	0.42
22:AB:612:CLA:H162	22:AB:612:CLA:H122	1.84	0.42
2:AB:237:VAL:HG12	22:AB:612:CLA:HMD1	2.02	0.42
4:AD:125:PHE:O	4:AD:128:ARG:HB3	2.19	0.42
10:AK:16:ALA:O	10:AK:19:ASP:HB2	2.20	0.42
18:BX:16:LEU:HD11	18:BX:20:PHE:CE2	2.55	0.42
4:AD:204:VAL:HG22	4:AD:279:LEU:HD21	2.01	0.42
4:BD:77:ALA:CB	4:BD:174:GLY:HA3	2.50	0.42
2:AB:59:GLY:HA3	22:AB:607:CLA:CED	2.50	0.42
2:BB:9:HIS:HB2	22:BB:614:CLA:CBA	2.49	0.42
1:AA:22:THR:HG21	8:AI:30:ARG:CD	2.50	0.42
3:BC:48:LYS:HD2	3:BC:138:GLU:HG3	1.99	0.42
6:AF:16:PHE:N	6:AF:16:PHE:CD1	2.88	0.42
14:AT:22:PHE:C	14:AT:23:PHE:CD2	2.93	0.42
12:AM:1:MET:HG2	12:AM:2:GLU:H	1.84	0.42
15:AU:91:VAL:HG13	15:AU:92:LEU:N	2.33	0.42
3:AC:321:ASP:HA	3:AC:324:LEU:HD23	2.01	0.42
5:AE:61:ARG:HH22	16:AV:153:GLY:HA3	1.85	0.42
13:BO:215:ARG:NH1	13:BO:252:GLY:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:AC:390:ARG:CZ	16:AV:126:ILE:HD13	2.50	0.42
3:BC:429:SER:HA	27:BC:517:DGD:HAT1	2.02	0.42
26:BC:514:BCR:H341	26:BK:102:BCR:H322	2.00	0.42
2:BB:263:THR:HB	2:BB:448:ARG:HH12	1.84	0.42
1:BA:42:LEU:HA	1:BA:45:THR:HG22	2.01	0.42
34:BE:101:HEM:HH A	34:BE:101:HEM:HAD2	1.57	0.42
28:AA:411:LHG:HC92	29:AA:412:SQD:O10	2.20	0.42
26:BC:515:BCR:C33	8:BI:20:VAL:HG13	2.50	0.42
12:BM:31:SER:HA	30:BM:102:LMG:HC3	2.01	0.42
5:AE:30:LEU:HD11	6:AF:28:VAL:HG13	2.02	0.42
6:AF:25:THR:O	6:AF:29:PRO:HG2	2.19	0.42
4:BD:17:ILE:HG21	18:BX:42:GLN:HG3	2.01	0.42
4:AD:17:ILE:HG21	18:AX:42:GLN:HG3	2.02	0.42
4:BD:92:LEU:HA	4:BD:104:TRP:CD1	2.55	0.42
2:BB:442:ILE:HD11	13:BO:200:LEU:HD23	2.01	0.42
2:AB:201:HIS:HD2	2:AB:202:HIS:ND1	2.16	0.42
2:BB:463:PHE:CD2	2:BB:463:PHE:C	2.92	0.42
20:AZ:17:PHE:HE2	20:AZ:21:ILE:HD11	1.83	0.42
3:BC:67:MET:HE1	22:BC:504:CLA:ND	2.35	0.42
13:BO:80:GLU:O	13:BO:89:ALA:CB	2.66	0.42
2:AB:18:ARG:HD3	2:AB:118:TRP:HB3	2.01	0.42
3:BC:249:ILE:O	3:BC:252:ILE:HB	2.20	0.42
9:BJ:7:ARG:HE	9:BJ:7:ARG:HA	1.85	0.42
2:AB:377:VAL:HG11	4:AD:342:PRO:HG2	2.01	0.42
1:BA:306:VAL:CG1	1:BA:316:THR:HG23	2.49	0.42
3:BC:276:LEU:CD1	3:BC:444:HIS:HD2	2.33	0.42
13:BO:227:VAL:CG1	13:BO:228:ALA:N	2.83	0.42
1:AA:279:PRO:HG2	4:AD:212:ALA:HB2	2.00	0.42
6:AF:15:ILE:HG22	6:AF:16:PHE:N	2.34	0.42
8:BI:27:ASP:O	8:BI:28:PRO:C	2.56	0.42
13:AO:59:ASP:O	13:AO:61:SER:N	2.53	0.42
16:AV:119:PRO:HA	16:AV:127:PHE:CD2	2.55	0.42
4:BD:203:GLY:O	4:BD:207:GLY:N	2.51	0.42
3:AC:140:LEU:HB2	3:AC:148:GLY:HA2	2.02	0.42
16:AV:130:MET:SD	16:AV:133:LEU:HD12	2.60	0.42
2:BB:275:TRP:CH2	2:BB:358:ARG:HD3	2.55	0.42
2:BB:283:GLU:OE1	2:BB:283:GLU:HA	2.19	0.42
9:AJ:11:TRP:CE2	9:AJ:12:ILE:HG12	2.55	0.42
30:AI:101:LMG:H132	32:AI:102:LMT:O2'	2.20	0.42
7:AH:13:PRO:HG2	7:AH:14:LEU:H	1.85	0.42
3:BC:335:THR:HA	13:BO:178:ARG:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BF:18:VAL:CG1	6:BF:19:ARG:N	2.82	0.42
2:AB:237:VAL:HG22	22:AB:610:CLA:HBC2	2.01	0.42
2:BB:241:SER:HB3	22:BB:615:CLA:HED3	2.01	0.42
2:AB:348:ASN:O	2:AB:349:LYS:C	2.57	0.42
1:AA:12:ASN:O	1:AA:15:GLU:HB3	2.20	0.42
1:BA:215:HIS:HA	24:BA:408:PL9:O1	2.20	0.42
22:AB:607:CLA:HMD3	26:AB:618:BCR:H271	2.02	0.42
2:BB:16:PRO:HG3	2:BB:133:LEU:HD11	2.01	0.42
3:BC:142:GLU:C	3:BC:144:SER:H	2.22	0.42
27:AB:626:DGD:HD5	27:AB:626:DGD:HE1	1.66	0.42
1:AA:96:ILE:C	1:AA:98:GLU:H	2.23	0.42
30:AE:102:LMG:HC71	30:AE:102:LMG:O9	2.19	0.42
2:AB:364:GLU:HG3	4:AD:296:TYR:CE2	2.55	0.42
2:AB:338:GLN:HB2	2:AB:431:GLU:O	2.20	0.42
5:BE:60:GLN:HG2	5:BE:62:SER:H	1.84	0.42
1:BA:339:PHE:HB3	1:BA:340:PRO:HD2	2.02	0.42
1:BA:180:PHE:O	1:BA:184:ILE:HG13	2.20	0.42
1:BA:160:ILE:HD12	3:BC:431:PHE:CE1	2.55	0.42
2:AB:330:MET:SD	2:AB:446:SER:HB3	2.59	0.42
22:AC:511:CLA:HMB2	26:AC:514:BCR:H382	2.02	0.41
3:BC:269:GLU:O	3:BC:272:LEU:HB3	2.20	0.41
9:BJ:11:TRP:CE2	9:BJ:12:ILE:HG12	2.55	0.41
15:AU:50:ALA:HB1	15:AU:113:THR:HG21	2.01	0.41
22:AB:615:CLA:H162	7:AH:7:LEU:HD21	2.02	0.41
1:BA:64:ARG:O	13:BO:178:ARG:NH2	2.53	0.41
18:AX:12:ILE:C	18:AX:12:ILE:HD13	2.40	0.41
22:BC:513:CLA:HBA2	22:BC:513:CLA:H3A	1.81	0.41
1:AA:214:MET:HE1	4:AD:142:ASN:ND2	2.35	0.41
5:BE:15:THR:O	9:BJ:8:ILE:CD1	2.68	0.41
13:AO:92:VAL:HG11	2:BB:84:THR:HG21	2.03	0.41
2:BB:349:LYS:HG2	2:BB:395:GLN:O	2.19	0.41
30:BM:102:LMG:HC72	30:BM:102:LMG:HC2	1.96	0.41
6:BF:15:ILE:HG22	6:BF:16:PHE:N	2.34	0.41
18:BX:42:GLN:HB2	18:BX:42:GLN:HE21	1.63	0.41
1:BA:339:PHE:HB3	1:BA:340:PRO:CD	2.50	0.41
2:BB:153:PHE:O	2:BB:157:HIS:HB3	2.20	0.41
4:BD:190:ASN:HB2	4:BD:296:TYR:CD1	2.55	0.41
2:BB:18:ARG:HD2	2:BB:115:TRP:CE3	2.55	0.41
22:BC:502:CLA:HBD	22:BC:503:CLA:H43	2.02	0.41
2:BB:124:ARG:NH1	2:BB:124:ARG:CG	2.82	0.41
1:AA:214:MET:HE1	4:AD:142:ASN:HD21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BH:55:LEU:HB2	7:BH:58:VAL:CG1	2.50	0.41
1:BA:333:GLU:HB2	1:BA:337:HIS:HE1	1.85	0.41
20:BZ:22:GLY:O	20:BZ:23:VAL:C	2.58	0.41
13:AO:157:PRO:O	13:AO:158:ASN:O	2.38	0.41
4:BD:185:PHE:HE2	4:BD:289:LEU:HD12	1.85	0.41
1:AA:296:ASN:HB3	3:AC:401:LEU:HA	2.01	0.41
16:BV:69:GLY:O	16:BV:156:TRP:O	2.38	0.41
16:BV:160:LYS:HA	16:BV:163:TYR:CD2	2.56	0.41
4:BD:19:ASP:O	4:BD:20:ASP:C	2.57	0.41
2:BB:225:LEU:O	2:BB:226:TYR:C	2.59	0.41
4:BD:192:THR:CG2	22:BD:402:CLA:HBC2	2.48	0.41
13:BO:55:ALA:HA	13:BO:230:VAL:HG11	2.03	0.41
2:AB:12:LEU:O	2:AB:14:ASN:N	2.53	0.41
10:BK:43:VAL:CG2	10:BK:46:ARG:HE	2.33	0.41
16:BV:103:LYS:O	16:BV:122:ARG:HG2	2.20	0.41
2:BB:7:ARG:HG2	22:BB:614:CLA:HED1	2.01	0.41
3:AC:188:THR:CG2	3:AC:298:PRO:HB3	2.51	0.41
1:AA:21:VAL:HG11	1:AA:32:TRP:CE3	2.55	0.41
3:AC:45:LEU:O	3:AC:46:SER:C	2.58	0.41
15:AU:75:LEU:O	15:AU:79:ILE:HG13	2.21	0.41
30:AD:407:LMG:O4	9:AJ:31:GLY:O	2.39	0.41
1:BA:96:ILE:C	1:BA:98:GLU:H	2.24	0.41
2:BB:239:SER:O	2:BB:466:HIS:ND1	2.49	0.41
9:AJ:36:LEU:C	9:AJ:38:SER:H	2.23	0.41
1:BA:157:VAL:HG13	1:BA:172:MET:HB3	2.01	0.41
19:BY:25:UNK:C	19:BY:27:UNK:N	2.82	0.41
26:AA:409:BCR:H342	29:AA:415:SQD:H311	2.02	0.41
13:AO:80:GLU:O	13:AO:89:ALA:CB	2.66	0.41
13:BO:81:GLU:HA	13:BO:82:PRO:HD3	1.89	0.41
1:AA:317:TRP:O	1:AA:321:ILE:HG13	2.20	0.41
32:AT:101:LMT:H3'	32:AT:101:LMT:H1B	1.64	0.41
2:AB:413:ASP:OD1	2:AB:416:THR:HB	2.20	0.41
19:AY:21:UNK:O	19:AY:22:UNK:C	2.68	0.41
3:BC:114:VAL:CG1	22:BC:503:CLA:HMA3	2.50	0.41
3:BC:250:TRP:HE1	22:BC:506:CLA:HED1	1.84	0.41
22:AC:501:CLA:HMB3	26:AC:515:BCR:C40	2.46	0.41
3:AC:365:TRP:HB3	3:AC:391:ARG:HG2	2.02	0.41
2:AB:16:PRO:HB3	2:AB:133:LEU:HD21	2.02	0.41
3:BC:29:GLU:OE2	3:BC:31:SER:N	2.31	0.41
5:BE:30:LEU:HD11	6:BF:28:VAL:HG13	2.03	0.41
1:AA:343:LEU:O	1:AA:344:ALA:CB	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BD:209:LEU:O	4:BD:213:ILE:HG22	2.20	0.41
10:BK:28:ILE:HA	10:BK:31:LEU:HD12	2.02	0.41
13:BO:180:ALA:HB2	15:BU:120:ALA:O	2.19	0.41
2:AB:448:ARG:HG3	2:AB:448:ARG:HH11	1.84	0.41
3:AC:199:ILE:N	3:AC:199:ILE:CD1	2.83	0.41
9:BJ:21:VAL:HA	9:BJ:24:ILE:HG22	2.03	0.41
13:AO:147:THR:OG1	13:AO:148:VAL:N	2.54	0.41
3:AC:189:TRP:O	3:AC:190:ALA:C	2.59	0.41
4:BD:79:SER:HA	4:BD:172:SER:HB3	2.02	0.41
3:BC:198:VAL:HG12	3:BC:200:THR:HG23	2.02	0.41
2:BB:105:GLY:O	2:BB:108:PHE:HB3	2.20	0.41
3:BC:42:LEU:HD11	22:BC:511:CLA:C1A	2.50	0.41
30:BC:519:LMG:H221	10:BK:30:VAL:CG1	2.50	0.41
2:BB:18:ARG:HD3	2:BB:118:TRP:HB3	2.01	0.41
18:BX:12:ILE:C	18:BX:12:ILE:HD13	2.40	0.41
1:AA:206:PHE:HA	1:AA:206:PHE:HD2	1.76	0.41
1:AA:45:THR:HB	23:AA:405:PHO:H93	2.02	0.41
13:BO:83:LYS:CG	13:BO:84:ASN:H	2.24	0.41
5:BE:64:PRO:HB3	5:BE:84:LYS:CD	2.50	0.41
5:BE:64:PRO:CB	5:BE:84:LYS:HE2	2.50	0.41
7:AH:53:LEU:HD21	7:AH:55:LEU:HD21	2.03	0.41
5:AE:78:THR:HA	5:AE:81:GLU:HG2	2.02	0.41
7:AH:10:ILE:H	7:AH:10:ILE:HG13	1.70	0.41
7:BH:16:SER:C	7:BH:18:TYR:H	2.23	0.41
3:AC:142:GLU:C	3:AC:144:SER:H	2.24	0.41
4:BD:107:LEU:HD21	5:BE:76:VAL:HG21	2.01	0.41
7:BH:28:THR:O	7:BH:31:MET:HB3	2.20	0.41
10:AK:11:LEU:O	10:AK:12:PRO:C	2.59	0.41
2:AB:105:GLY:O	2:AB:108:PHE:HB3	2.19	0.41
10:AK:28:ILE:O	10:AK:31:LEU:HB2	2.20	0.41
28:BC:521:LHG:HC41	28:BC:521:LHG:O9	2.20	0.41
2:BB:118:TRP:CH2	11:BL:5:PRO:HD2	2.56	0.41
1:AA:172:MET:SD	22:AA:403:CLA:HMC3	2.61	0.41
4:BD:268:HIS:CE1	33:BD:401:BCT:O3	2.73	0.41
1:AA:215:HIS:HA	24:AA:407:PL9:O1	2.21	0.41
5:AE:15:THR:O	9:AJ:8:ILE:CD1	2.69	0.41
30:AM:101:LMG:HC2	30:AM:101:LMG:HC72	1.96	0.41
3:AC:202:PRO:HB2	3:AC:235:GLY:HA2	2.01	0.41
4:BD:56:THR:HB	5:BE:49:THR:HG23	2.02	0.41
15:AU:89:GLU:N	15:AU:89:GLU:CD	2.73	0.41
11:AL:22:LEU:O	11:AL:26:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:383:PHE:O	13:AO:192:SER:HA	2.20	0.41
16:AV:83:GLU:H	16:AV:83:GLU:CD	2.23	0.41
5:AE:82:GLN:H	5:AE:82:GLN:HG3	1.54	0.41
2:AB:24:LEU:HD13	2:AB:111:ALA:N	2.36	0.41
4:AD:26:ARG:HD3	6:AF:18:VAL:CG1	2.32	0.41
27:AC:518:DGD:HG2	9:AJ:33:TYR:OH	2.21	0.41
3:BC:162:GLY:O	3:BC:166:ILE:HG13	2.21	0.41
3:AC:116:VAL:CG2	3:AC:117:VAL:N	2.84	0.41
5:BE:84:LYS:HZ3	5:BE:84:LYS:HB2	1.82	0.41
2:BB:191:ASN:ND2	7:BH:59:ASN:O	2.54	0.41
10:AK:43:VAL:CG2	10:AK:46:ARG:HE	2.33	0.41
2:AB:191:ASN:OD1	2:AB:193:TYR:N	2.52	0.41
5:BE:27:ILE:CB	5:BE:28:PRO:HD3	2.49	0.41
1:BA:21:VAL:HG11	1:BA:32:TRP:CZ3	2.56	0.41
13:AO:120:THR:HA	13:AO:153:ALA:O	2.21	0.41
3:BC:141:GLU:HA	3:BC:148:GLY:HA3	2.03	0.41
2:BB:377:VAL:HG11	4:BD:342:PRO:HG2	2.02	0.41
1:BA:249:VAL:HG11	2:BB:486:LEU:CD2	2.50	0.41
5:AE:49:THR:HA	5:AE:50:PRO:HD3	1.86	0.41
13:AO:135:GLN:HB3	13:AO:135:GLN:HE21	1.56	0.41
4:AD:190:ASN:HB2	4:AD:296:TYR:CE1	2.56	0.41
13:AO:192:SER:OG	13:AO:193:GLY:N	2.54	0.41
13:BO:229:LYS:HB2	13:BO:238:ALA:HB3	2.02	0.41
16:BV:30:THR:HB	16:BV:31:PRO:HD2	2.02	0.41
2:AB:463:PHE:C	2:AB:463:PHE:CD2	2.94	0.41
26:AC:514:BCR:H341	26:AK:102:BCR:H322	2.02	0.41
1:BA:202:VAL:O	1:BA:206:PHE:HB2	2.20	0.41
22:BA:405:CLA:H202	30:BD:407:LMG:H401	2.03	0.41
1:AA:131:TRP:CE3	1:AA:132:GLU:CA	3.03	0.41
4:BD:128:ARG:O	4:BD:129:GLN:C	2.59	0.41
20:AZ:36:SER:C	20:AZ:38:GLN:H	2.24	0.41
2:BB:331:ASN:HB3	2:BB:437:LEU:CD1	2.48	0.41
12:AM:27:VAL:HG12	12:BM:28:GLN:CB	2.47	0.41
3:AC:203:THR:O	3:AC:235:GLY:HA3	2.20	0.41
1:BA:105:TRP:CZ3	1:BA:111:PRO:HG3	2.56	0.41
1:BA:296:ASN:HB3	3:BC:401:LEU:HA	2.02	0.41
2:BB:214:LEU:O	2:BB:218:LEU:HG	2.21	0.41
1:AA:277:ALA:O	1:AA:281:VAL:HG23	2.21	0.41
2:AB:479:PHE:O	2:AB:480:SER:CB	2.68	0.41
3:AC:101:PRO:O	3:AC:104:GLU:HB2	2.19	0.41
13:AO:73:PRO:HG2	13:AO:102:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:BU:54:LYS:CB	15:BU:113:THR:HG23	2.47	0.41
10:AK:34:ALA:O	10:AK:37:PHE:HB2	2.20	0.41
19:BY:21:UNK:HA	19:BY:24:UNK:CB	2.50	0.41
3:BC:85:GLY:CA	27:BC:517:DGD:HE4	2.51	0.41
27:BC:518:DGD:HG2	9:BJ:33:TYR:OH	2.21	0.41
1:BA:45:THR:HB	23:BA:406:PHO:H93	2.02	0.41
2:BB:30:VAL:HG11	22:BB:615:CLA:H112	2.03	0.41
3:AC:307:PRO:HG3	3:AC:358:PHE:CD1	2.56	0.41
3:AC:308:GLU:HG3	3:AC:361:PHE:CZ	2.56	0.41
4:AD:128:ARG:O	4:AD:129:GLN:C	2.59	0.41
26:AJ:102:BCR:H351	26:AJ:102:BCR:H15C	1.91	0.41
19:AY:23:UNK:O	19:AY:24:UNK:C	2.68	0.41
3:BC:160:ILE:HA	3:BC:163:PHE:CD2	2.55	0.41
3:BC:116:VAL:CG2	3:BC:117:VAL:N	2.84	0.41
3:BC:449:ARG:NE	22:BC:505:CLA:HED1	2.21	0.41
3:AC:165:LEU:HG	22:AC:507:CLA:HED1	2.03	0.41
1:AA:183:MET:HB3	22:AA:402:CLA:HBC2	2.02	0.41
1:AA:215:HIS:CD2	4:AD:268:HIS:CD2	3.08	0.41
4:AD:268:HIS:CE1	33:AD:401:BCT:O3	2.74	0.41
3:AC:414:ILE:HG22	3:AC:415:ASN:N	2.35	0.41
12:BM:19:SER:O	12:BM:23:ILE:HG13	2.20	0.41
3:BC:414:ILE:HG22	3:BC:415:ASN:O	2.21	0.41
15:AU:57:LEU:HD22	15:AU:79:ILE:CG2	2.51	0.41
1:BA:22:THR:HG21	8:BI:30:ARG:CD	2.51	0.41
16:AV:124:ALA:HB1	16:AV:131:ARG:CG	2.51	0.41
13:AO:116:ASP:C	13:AO:116:ASP:OD2	2.58	0.41
3:AC:267:SER:O	3:AC:271:TYR:CD2	2.74	0.41
14:AT:22:PHE:C	14:AT:23:PHE:HD2	2.24	0.41
3:AC:258:GLY:C	3:AC:262:ARG:NH1	2.74	0.41
13:BO:184:ASP:OD1	13:BO:184:ASP:C	2.59	0.41
2:BB:364:GLU:HG3	4:BD:296:TYR:CE2	2.56	0.41
1:BA:24:THR:OG1	3:BC:469:MET:CE	2.68	0.41
1:AA:288:LEU:O	1:AA:292:THR:HB	2.21	0.41
3:BC:464:GLU:O	3:BC:467:LEU:HB2	2.20	0.41
2:AB:91:TRP:HE1	32:AB:624:LMT:H12	1.86	0.41
3:AC:198:VAL:HG12	3:AC:200:THR:HG23	2.03	0.41
2:AB:393:GLU:HG2	15:AU:44:ASP:O	2.20	0.41
2:BB:215:PHE:CD2	2:BB:215:PHE:C	2.95	0.41
22:BC:511:CLA:HBA2	26:BC:514:BCR:H271	2.03	0.41
2:AB:137:LYS:NZ	7:AH:14:LEU:O	2.54	0.41
1:BA:183:MET:HB3	22:BA:403:CLA:HBC2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:404:CLA:H62	22:BA:404:CLA:H41	1.92	0.41
4:BD:126:MET:HE3	4:BD:150:ILE:HG13	2.03	0.41
4:BD:263:ASN:O	4:BD:265:ARG:N	2.54	0.41
4:BD:283:ALA:HA	22:BD:402:CLA:HED2	2.03	0.41
1:AA:129:ARG:C	1:AA:131:TRP:H	2.23	0.41
22:AC:512:CLA:H2A	22:AC:512:CLA:HED2	2.03	0.41
22:AA:403:CLA:H62	22:AA:403:CLA:H41	1.91	0.41
1:AA:10:SER:OG	1:AA:13:LEU:HD12	2.20	0.41
1:BA:215:HIS:CD2	4:BD:268:HIS:CD2	3.09	0.41
4:BD:53:THR:CB	4:BD:67:TYR:HD2	2.34	0.41
2:BB:348:ASN:O	2:BB:350:GLU:N	2.54	0.41
15:BU:38:GLU:CG	15:BU:39:LEU:N	2.81	0.41
1:BA:20:TRP:O	1:BA:23:SER:HB3	2.20	0.41
2:AB:331:ASN:HB3	2:AB:437:LEU:CD1	2.49	0.41
16:AV:81:ARG:CG	16:AV:157:GLY:HA3	2.51	0.41
2:AB:447:PRO:O	2:AB:448:ARG:C	2.59	0.41
3:AC:80:PRO:HB3	3:AC:82:TYR:CE1	2.56	0.41
3:BC:80:PRO:HB3	3:BC:82:TYR:CE1	2.56	0.41
3:BC:261:ARG:HA	3:BC:266:TRP:HZ2	1.86	0.41
2:AB:168:VAL:O	2:AB:176:GLY:HA2	2.20	0.41
1:AA:114:LEU:HD23	1:AA:114:LEU:O	2.21	0.41
1:AA:334:ARG:NH1	13:AO:183:LEU:O	2.54	0.41
3:BC:455:PHE:C	3:BC:457:LYS:H	2.24	0.41
1:BA:247:ASN:HB3	1:BA:250:ALA:HB3	2.01	0.41
9:BJ:36:LEU:C	9:BJ:38:SER:H	2.22	0.41
8:BI:4:LEU:O	8:BI:8:VAL:HG23	2.20	0.41
16:AV:30:THR:OG1	16:AV:32:GLU:HB3	2.21	0.41
15:AU:55:ILE:HG21	15:AU:65:PHE:CE1	2.56	0.41
2:AB:113:TRP:CE2	2:AB:117:TYR:CD2	3.09	0.41
3:BC:41:ARG:NH1	22:BC:511:CLA:HMD1	2.36	0.40
2:BB:137:LYS:HZ2	7:BH:14:LEU:C	2.23	0.40
2:BB:229:LEU:HD11	22:BB:612:CLA:O1A	2.21	0.40
19:AY:23:UNK:O	19:AY:25:UNK:N	2.54	0.40
22:AA:403:CLA:HAA1	24:AD:405:PL9:C36	2.51	0.40
5:AE:64:PRO:HB3	5:AE:84:LYS:CD	2.50	0.40
2:BB:187:PRO:C	2:BB:189:GLY:H	2.24	0.40
4:BD:14:TRP:CD2	4:BD:15:PHE:N	2.89	0.40
2:AB:280:PHE:O	2:AB:284:ILE:HG13	2.20	0.40
1:BA:257:ARG:HG3	1:BA:257:ARG:NH1	2.33	0.40
4:BD:161:PRO:CB	4:BD:170:ALA:HB2	2.51	0.40
2:AB:170:ASP:HB2	2:AB:171:PRO:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BE:14:ILE:O	5:BE:14:ILE:HG22	2.21	0.40
13:BO:44:LYS:HA	13:BO:72:GLN:OE1	2.21	0.40
30:BD:408:LMG:O6	11:BL:15:THR:HG21	2.21	0.40
3:BC:155:ASN:O	3:BC:158:THR:CG2	2.69	0.40
2:AB:16:PRO:HG3	2:AB:133:LEU:HD11	2.03	0.40
3:BC:318:LEU:HG	3:BC:328:VAL:CG1	2.50	0.40
3:AC:461:ARG:NH1	3:AC:461:ARG:HG3	2.33	0.40
15:AU:75:LEU:HD21	15:AU:101:GLN:HB3	2.03	0.40
3:BC:350:ILE:CG2	3:BC:359:TRP:HB2	2.52	0.40
1:AA:105:TRP:CZ3	1:AA:111:PRO:HG3	2.55	0.40
4:BD:205:LEU:HA	4:BD:205:LEU:HD12	1.72	0.40
12:BM:5:GLN:NE2	32:BM:101:LMT:O2B	2.55	0.40
1:BA:126:TYR:O	1:BA:130:GLN:HG3	2.22	0.40
16:AV:58:LEU:HD13	16:AV:137:ASP:HB3	2.02	0.40
3:BC:394:GLU:OE2	3:BC:398:HIS:CD2	2.74	0.40
1:AA:339:PHE:HB3	1:AA:340:PRO:HD2	2.03	0.40
4:BD:48:TRP:CE2	23:BD:403:PHO:H161	2.56	0.40
32:AD:411:LMT:O3'	18:AX:21:ILE:HG21	2.21	0.40
3:BC:362:ARG:H	27:BC:516:DGD:HE4	1.87	0.40
5:BE:15:THR:CG2	9:BJ:7:ARG:HG3	2.51	0.40
30:BA:414:LMG:H292	11:BL:20:GLY:HA2	2.04	0.40
1:AA:257:ARG:NH1	1:AA:257:ARG:HG3	2.35	0.40
5:AE:14:ILE:HG22	5:AE:14:ILE:O	2.20	0.40
7:AH:63:LYS:C	7:AH:65:LEU:H	2.24	0.40
2:AB:289:GLN:OE1	2:AB:289:GLN:HA	2.21	0.40
2:BB:54:PRO:HD2	2:BB:57:ARG:HG3	2.04	0.40
16:BV:83:GLU:CD	16:BV:83:GLU:H	2.25	0.40
3:AC:42:LEU:HD11	22:AC:511:CLA:C1A	2.51	0.40
2:BB:24:LEU:HD13	2:BB:111:ALA:N	2.37	0.40
2:BB:113:TRP:CD1	22:BB:619:CLA:HBA1	2.57	0.40
22:BA:404:CLA:HAA1	24:BD:405:PL9:C36	2.51	0.40
3:BC:109:PHE:CG	30:BC:520:LMG:HC61	2.56	0.40
26:BC:515:BCR:H332	8:BI:20:VAL:HG13	2.02	0.40
22:AC:502:CLA:HBD	22:AC:503:CLA:H43	2.03	0.40
26:AC:515:BCR:C33	8:AI:20:VAL:HG13	2.52	0.40
1:BA:271:LEU:HD21	24:BA:408:PL9:HC71	2.03	0.40
4:AD:43:LEU:HA	4:AD:43:LEU:HD12	1.94	0.40
15:AU:94:ILE:HB	15:AU:97:LEU:HD11	2.03	0.40
4:BD:238:THR:O	4:BD:239:GLN:C	2.59	0.40
3:BC:461:ARG:NH1	3:BC:461:ARG:HG3	2.36	0.40
3:BC:267:SER:O	3:BC:271:TYR:CD2	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:AX:43:ILE:O	18:AX:43:ILE:CG2	2.70	0.40
3:AC:464:GLU:HA	3:AC:465:PRO:HD2	1.72	0.40
15:AU:90:ASP:HA	15:AU:93:ASN:HD22	1.87	0.40
16:AV:160:LYS:HA	16:AV:163:TYR:CD2	2.56	0.40
15:AU:88:VAL:HG13	15:AU:109:LEU:HD22	2.03	0.40
1:AA:24:THR:OG1	3:AC:469:MET:CE	2.70	0.40
4:AD:302:GLU:OE1	4:AD:302:GLU:HA	2.20	0.40
1:BA:30:VAL:HG22	1:BA:30:VAL:O	2.21	0.40
9:AJ:9:PRO:HB2	9:AJ:12:ILE:HG13	2.03	0.40
7:AH:11:LEU:C	7:AH:13:PRO:HD2	2.42	0.40
4:BD:48:TRP:CD2	23:BD:403:PHO:H161	2.56	0.40
2:AB:233:ASN:O	2:AB:236:THR:HG22	2.22	0.40
29:AA:412:SQD:H132	28:AC:521:LHG:H132	2.02	0.40
28:AC:521:LHG:HC41	28:AC:521:LHG:O9	2.21	0.40
3:AC:59:LEU:HD13	22:AC:510:CLA:HMD2	2.04	0.40
26:AT:102:BCR:H393	22:BB:610:CLA:CAC	2.48	0.40
3:AC:414:ILE:CG2	3:AC:415:ASN:N	2.84	0.40
3:BC:416:SER:OG	3:BC:417:VAL:N	2.54	0.40
3:BC:84:GLN:O	3:BC:86:LEU:HD13	2.22	0.40
2:AB:222:PRO:O	2:AB:223:GLN:C	2.59	0.40
3:AC:94:THR:CG2	3:AC:298:PRO:HD2	2.51	0.40
2:BB:385:ARG:O	2:BB:386:ALA:C	2.60	0.40
6:BF:25:THR:O	6:BF:29:PRO:HG2	2.21	0.40
4:AD:205:LEU:HA	4:AD:205:LEU:HD12	1.71	0.40
13:AO:226:ASN:N	13:AO:226:ASN:ND2	2.69	0.40
7:BH:63:LYS:C	7:BH:65:LEU:H	2.23	0.40
3:AC:451:ALA:HA	3:AC:456:GLU:CD	2.41	0.40
1:BA:291:SER:HB3	3:BC:431:PHE:CE2	2.57	0.40
8:BI:7:THR:O	8:BI:8:VAL:C	2.59	0.40
2:BB:254:GLY:O	2:BB:258:TYR:HD2	2.05	0.40
2:BB:475:PHE:HB3	2:BB:478:VAL:CG2	2.52	0.40
1:BA:116:ILE:HG13	1:BA:117:PHE:N	2.37	0.40
2:BB:380:ASP:C	2:BB:380:ASP:OD1	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	AA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	9	32
1	BA	333/344 (97%)	285 (86%)	41 (12%)	7 (2%)	9	32
2	AB	488/510 (96%)	417 (86%)	57 (12%)	14 (3%)	6	23
2	BB	488/510 (96%)	422 (86%)	52 (11%)	14 (3%)	6	23
3	AC	445/473 (94%)	371 (83%)	58 (13%)	16 (4%)	4	18
3	BC	445/473 (94%)	372 (84%)	56 (13%)	17 (4%)	4	16
4	AD	338/352 (96%)	286 (85%)	43 (13%)	9 (3%)	6	25
4	BD	338/352 (96%)	288 (85%)	42 (12%)	8 (2%)	7	29
5	AE	80/84 (95%)	71 (89%)	5 (6%)	4 (5%)	3	9
5	BE	80/84 (95%)	70 (88%)	6 (8%)	4 (5%)	3	9
6	AF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	22
6	BF	33/45 (73%)	24 (73%)	8 (24%)	1 (3%)	5	22
7	AH	63/66 (96%)	47 (75%)	10 (16%)	6 (10%)	1	2
7	BH	63/66 (96%)	48 (76%)	11 (18%)	4 (6%)	2	5
8	AI	33/38 (87%)	20 (61%)	11 (33%)	2 (6%)	2	5
8	BI	33/38 (87%)	21 (64%)	10 (30%)	2 (6%)	2	5
9	AJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	5
9	BJ	32/40 (80%)	26 (81%)	4 (12%)	2 (6%)	2	5
10	AK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	6
10	BK	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	2	6
11	AL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	BL	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	AM	32/36 (89%)	23 (72%)	9 (28%)	0	100	100
12	BM	32/36 (89%)	24 (75%)	8 (25%)	0	100	100
13	AO	241/247 (98%)	199 (83%)	30 (12%)	12 (5%)	3	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	BO	241/247 (98%)	199 (83%)	31 (13%)	11 (5%)	3	11
14	AT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	20
14	BT	30/32 (94%)	25 (83%)	4 (13%)	1 (3%)	5	20
15	AU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	13
15	BU	95/104 (91%)	79 (83%)	12 (13%)	4 (4%)	3	13
16	AV	135/137 (98%)	111 (82%)	23 (17%)	1 (1%)	26	63
16	BV	135/137 (98%)	112 (83%)	22 (16%)	1 (1%)	26	63
17	Ay	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
17	By	26/46 (56%)	14 (54%)	8 (31%)	4 (15%)	0	0
18	AX	35/50 (70%)	26 (74%)	5 (14%)	4 (11%)	0	1
18	BX	35/50 (70%)	27 (77%)	4 (11%)	4 (11%)	0	1
20	AZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	9
20	BZ	60/62 (97%)	48 (80%)	9 (15%)	3 (5%)	3	9
All	All	5138/5480 (94%)	4278 (83%)	679 (13%)	181 (4%)	4	18

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	141	PRO
1	AA	142	TRP
2	AB	176	GLY
2	AB	230	ARG
2	AB	484	PRO
2	AB	488	PRO
3	AC	144	SER
3	AC	257	PHE
3	AC	416	SER
3	AC	452	ALA
4	AD	239	GLN
4	AD	240	ALA
4	AD	262	SER
5	AE	82	GLN
7	AH	18	TYR
8	AI	25	SER
9	AJ	35	GLY
13	AO	52	ALA

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Mol	Chain	Res	Type
14	AT	30	THR
15	AU	72	TYR
15	AU	83	ALA
16	AV	75	ASN
17	Ay	43	ARG
18	AX	45	LYS
20	AZ	32	ASP
1	BA	12	ASN
1	BA	141	PRO
1	BA	142	TRP
2	BB	176	GLY
2	BB	230	ARG
2	BB	484	PRO
2	BB	488	PRO
3	BC	144	SER
3	BC	257	PHE
3	BC	416	SER
3	BC	452	ALA
4	BD	239	GLN
4	BD	240	ALA
4	BD	262	SER
7	BH	18	TYR
8	BI	25	SER
9	BJ	35	GLY
13	BO	52	ALA
14	BT	30	THR
15	BU	72	TYR
15	BU	83	ALA
17	By	43	ARG
18	BX	45	LYS
20	BZ	32	ASP
2	AB	349	LYS
3	AC	46	SER
3	AC	136	GLY
3	AC	194	GLY
3	AC	209	ILE
3	AC	456	GLU
4	AD	234	ALA
4	AD	264	LYS
7	AH	26	GLY
9	AJ	38	SER
13	AO	231	ASP

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Mol	Chain	Res	Type
15	AU	73	PRO
17	Ay	25	ILE
18	AX	43	ILE
2	BB	349	LYS
2	BB	436	THR
3	BC	136	GLY
3	BC	141	GLU
3	BC	194	GLY
4	BD	234	ALA
5	BE	82	GLN
7	BH	26	GLY
9	BJ	38	SER
13	BO	158	ASN
13	BO	231	ASP
15	BU	73	PRO
16	BV	75	ASN
18	BX	43	ILE
2	AB	127	ARG
2	AB	183	PRO
2	AB	414	PRO
2	AB	436	THR
3	AC	32	GLY
3	AC	141	GLU
3	AC	375	LEU
3	AC	453	ALA
4	AD	263	ASN
5	AE	9	PRO
7	AH	16	SER
10	AK	13	GLU
10	AK	45	PHE
13	AO	60	SER
13	AO	158	ASN
13	AO	165	SER
20	AZ	24	PRO
20	AZ	28	ALA
2	BB	13	ILE
2	BB	127	ARG
2	BB	183	PRO
2	BB	414	PRO
3	BC	32	GLY
3	BC	46	SER
3	BC	209	ILE

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Mol	Chain	Res	Type
3	BC	375	LEU
3	BC	411	ALA
3	BC	456	GLU
4	BD	263	ASN
4	BD	264	LYS
5	BE	9	PRO
7	BH	16	SER
10	BK	13	GLU
10	BK	45	PHE
13	BO	165	SER
17	By	25	ILE
20	BZ	24	PRO
20	BZ	28	ALA
2	AB	13	ILE
2	AB	173	GLY
2	AB	231	MET
2	AB	235	GLU
3	AC	154	LYS
4	AD	73	PHE
5	AE	10	PHE
13	AO	51	THR
13	AO	82	PRO
17	Ay	24	MET
18	AX	44	ASP
2	BB	235	GLU
5	BE	10	PHE
13	BO	60	SER
13	BO	82	PRO
1	AA	97	TRP
3	AC	462	GLU
6	AF	41	GLN
7	AH	6	TRP
15	AU	42	VAL
18	AX	12	ILE
2	BB	435	GLU
3	BC	453	ALA
3	BC	462	GLU
4	BD	252	PHE
6	BF	41	GLN
7	BH	6	TRP
13	BO	85	LYS
13	BO	88	GLU

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Mol	Chain	Res	Type
15	BU	42	VAL
17	By	24	MET
18	BX	44	ASP
1	AA	334	ARG
4	AD	351	ALA
7	AH	14	LEU
13	AO	88	GLU
1	BA	97	TRP
1	BA	334	ARG
2	BB	173	GLY
3	BC	382	ASN
4	BD	351	ALA
5	BE	52	PRO
13	BO	51	THR
13	BO	159	VAL
18	BX	12	ILE
1	AA	21	VAL
2	AB	16	PRO
13	AO	159	VAL
1	BA	21	VAL
17	By	35	ILE
3	AC	201	ASN
17	Ay	35	ILE
3	BC	201	ASN
5	AE	52	PRO
7	AH	60	VAL
8	AI	32	PRO
13	AO	232	GLY
2	BB	16	PRO
8	BI	32	PRO
1	AA	176	ILE
4	AD	160	TYR
13	AO	127	ILE
1	BA	39	PRO
13	AO	152	VAL
13	BO	152	VAL

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	AA	271/280 (97%)	258 (95%)	13 (5%)	31	67
1	BA	271/280 (97%)	259 (96%)	12 (4%)	35	70
2	AB	390/407 (96%)	374 (96%)	16 (4%)	37	73
2	BB	390/407 (96%)	373 (96%)	17 (4%)	35	70
3	AC	347/374 (93%)	329 (95%)	18 (5%)	29	64
3	BC	347/374 (93%)	329 (95%)	18 (5%)	29	64
4	AD	275/283 (97%)	256 (93%)	19 (7%)	19	48
4	BD	275/283 (97%)	256 (93%)	19 (7%)	19	48
5	AE	72/73 (99%)	66 (92%)	6 (8%)	14	38
5	BE	72/73 (99%)	66 (92%)	6 (8%)	14	38
6	AF	29/39 (74%)	29 (100%)	0	100	100
6	BF	29/39 (74%)	29 (100%)	0	100	100
7	AH	53/55 (96%)	50 (94%)	3 (6%)	25	59
7	BH	53/55 (96%)	50 (94%)	3 (6%)	25	59
8	AI	32/35 (91%)	31 (97%)	1 (3%)	47	82
8	BI	32/35 (91%)	31 (97%)	1 (3%)	47	82
9	AJ	24/28 (86%)	23 (96%)	1 (4%)	36	73
9	BJ	24/28 (86%)	23 (96%)	1 (4%)	36	73
10	AK	30/30 (100%)	28 (93%)	2 (7%)	20	50
10	BK	30/30 (100%)	28 (93%)	2 (7%)	20	50
11	AL	35/35 (100%)	31 (89%)	4 (11%)	7	21
11	BL	35/35 (100%)	32 (91%)	3 (9%)	13	36
12	AM	31/33 (94%)	31 (100%)	0	100	100
12	BM	31/33 (94%)	31 (100%)	0	100	100
13	AO	202/208 (97%)	195 (96%)	7 (4%)	43	78
13	BO	202/208 (97%)	194 (96%)	8 (4%)	38	74
14	AT	29/29 (100%)	28 (97%)	1 (3%)	44	79
14	BT	29/29 (100%)	28 (97%)	1 (3%)	44	79
15	AU	84/89 (94%)	80 (95%)	4 (5%)	31	67
15	BU	84/89 (94%)	80 (95%)	4 (5%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AV	116/117 (99%)	111 (96%)	5 (4%)	35	71
16	BV	116/117 (99%)	111 (96%)	5 (4%)	35	71
17	Ay	20/37 (54%)	18 (90%)	2 (10%)	9	28
17	By	20/37 (54%)	18 (90%)	2 (10%)	9	28
18	AX	30/42 (71%)	26 (87%)	4 (13%)	5	14
18	BX	30/42 (71%)	26 (87%)	4 (13%)	5	14
20	AZ	52/52 (100%)	47 (90%)	5 (10%)	10	31
20	BZ	52/52 (100%)	47 (90%)	5 (10%)	10	31
All	All	4244/4492 (94%)	4022 (95%)	222 (5%)	29	64

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	30	VAL
1	AA	32	TRP
1	AA	157	VAL
1	AA	170	ASP
1	AA	202	VAL
1	AA	206	PHE
1	AA	234	ASN
1	AA	243	GLU
1	AA	271	LEU
1	AA	286	THR
1	AA	292	THR
1	AA	298	ASN
1	AA	308	ASP
2	AB	11	VAL
2	AB	18	ARG
2	AB	84	THR
2	AB	223	GLN
2	AB	246	PHE
2	AB	262	THR
2	AB	308	LYS
2	AB	309	LEU
2	AB	362	PHE
2	AB	414	PRO
2	AB	422	ARG
2	AB	433	ASP
2	AB	483	ASP

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Mol	Chain	Res	Type
2	AB	486	LEU
2	AB	488	PRO
2	AB	490	GLN
3	AC	29	GLU
3	AC	78	GLU
3	AC	86	LEU
3	AC	104	GLU
3	AC	165	LEU
3	AC	174	LEU
3	AC	201	ASN
3	AC	207	ARG
3	AC	232	ASP
3	AC	244	CYS
3	AC	289	PHE
3	AC	305	THR
3	AC	355	THR
3	AC	382	ASN
3	AC	391	ARG
3	AC	401	LEU
3	AC	447	ARG
3	AC	472	LEU
4	AD	20	ASP
4	AD	43	LEU
4	AD	53	THR
4	AD	60	THR
4	AD	84	SER
4	AD	91	LEU
4	AD	130	PHE
4	AD	180	ARG
4	AD	201	VAL
4	AD	221	THR
4	AD	236	ASN
4	AD	241	GLU
4	AD	256	ILE
4	AD	259	ILE
4	AD	279	LEU
4	AD	291	LEU
4	AD	294	ARG
4	AD	323	GLU
4	AD	346	LEU
5	AE	5	THR
5	AE	9	PRO

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Mol	Chain	Res	Type
5	AE	18	ARG
5	AE	77	GLU
5	AE	82	GLN
5	AE	84	LYS
7	AH	27	THR
7	AH	49	TYR
7	AH	60	VAL
8	AI	33	LYS
9	AJ	7	ARG
10	AK	18	PHE
10	AK	19	ASP
11	AL	7	ARG
11	AL	8	GLN
11	AL	11	GLU
11	AL	15	THR
13	AO	31	LEU
13	AO	86	ARG
13	AO	97	VAL
13	AO	106	GLN
13	AO	141	ARG
13	AO	178	ARG
13	AO	219	THR
14	AT	29	ILE
15	AU	61	ASN
15	AU	88	VAL
15	AU	114	VAL
15	AU	132	LEU
16	AV	35	THR
16	AV	63	CYS
16	AV	92	ARG
16	AV	116	GLU
16	AV	122	ARG
17	Ay	28	ILE
17	Ay	46	LEU
18	AX	11	THR
18	AX	12	ILE
18	AX	42	GLN
18	AX	45	LYS
20	AZ	14	ILE
20	AZ	25	VAL
20	AZ	33	TRP
20	AZ	58	ASN

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Mol	Chain	Res	Type
20	AZ	62	VAL
1	BA	30	VAL
1	BA	32	TRP
1	BA	157	VAL
1	BA	170	ASP
1	BA	202	VAL
1	BA	206	PHE
1	BA	243	GLU
1	BA	271	LEU
1	BA	286	THR
1	BA	292	THR
1	BA	298	ASN
1	BA	308	ASP
2	BB	11	VAL
2	BB	18	ARG
2	BB	84	THR
2	BB	223	GLN
2	BB	246	PHE
2	BB	262	THR
2	BB	308	LYS
2	BB	309	LEU
2	BB	362	PHE
2	BB	414	PRO
2	BB	422	ARG
2	BB	433	ASP
2	BB	436	THR
2	BB	483	ASP
2	BB	486	LEU
2	BB	488	PRO
2	BB	490	GLN
3	BC	29	GLU
3	BC	78	GLU
3	BC	86	LEU
3	BC	104	GLU
3	BC	165	LEU
3	BC	174	LEU
3	BC	201	ASN
3	BC	207	ARG
3	BC	232	ASP
3	BC	244	CYS
3	BC	289	PHE
3	BC	305	THR

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Mol	Chain	Res	Type
3	BC	355	THR
3	BC	382	ASN
3	BC	391	ARG
3	BC	401	LEU
3	BC	447	ARG
3	BC	472	LEU
4	BD	20	ASP
4	BD	43	LEU
4	BD	53	THR
4	BD	60	THR
4	BD	84	SER
4	BD	91	LEU
4	BD	130	PHE
4	BD	180	ARG
4	BD	201	VAL
4	BD	221	THR
4	BD	236	ASN
4	BD	241	GLU
4	BD	256	ILE
4	BD	259	ILE
4	BD	279	LEU
4	BD	291	LEU
4	BD	294	ARG
4	BD	323	GLU
4	BD	346	LEU
5	BE	5	THR
5	BE	9	PRO
5	BE	18	ARG
5	BE	77	GLU
5	BE	82	GLN
5	BE	84	LYS
7	BH	27	THR
7	BH	49	TYR
7	BH	60	VAL
8	BI	33	LYS
9	BJ	7	ARG
10	BK	18	PHE
10	BK	19	ASP
11	BL	7	ARG
11	BL	8	GLN
11	BL	11	GLU
13	BO	31	LEU

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Mol	Chain	Res	Type
13	BO	86	ARG
13	BO	97	VAL
13	BO	106	GLN
13	BO	141	ARG
13	BO	178	ARG
13	BO	217	SER
13	BO	219	THR
14	BT	29	ILE
15	BU	61	ASN
15	BU	88	VAL
15	BU	114	VAL
15	BU	132	LEU
16	BV	35	THR
16	BV	63	CYS
16	BV	92	ARG
16	BV	116	GLU
16	BV	122	ARG
17	By	28	ILE
17	By	46	LEU
18	BX	11	THR
18	BX	12	ILE
18	BX	42	GLN
18	BX	45	LYS
20	BZ	14	ILE
20	BZ	25	VAL
20	BZ	33	TRP
20	BZ	58	ASN
20	BZ	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	12	ASN
1	AA	19	ASN
1	AA	234	ASN
1	AA	241	GLN
2	AB	201	HIS
2	AB	216	HIS
2	AB	490	GLN
3	AC	155	ASN
3	AC	398	HIS
3	AC	418	ASN

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Mol	Chain	Res	Type
3	AC	444	HIS
4	AD	98	GLN
4	AD	117	HIS
4	AD	129	GLN
4	AD	142	ASN
4	AD	239	GLN
4	AD	250	ASN
7	AH	59	ASN
11	AL	6	ASN
11	AL	8	GLN
12	AM	5	GLN
12	AM	33	GLN
13	AO	87	GLN
13	AO	106	GLN
13	AO	114	ASN
13	AO	135	GLN
13	AO	150	ASN
13	AO	173	ASN
13	AO	222	GLN
13	AO	226	ASN
15	AU	82	ASN
15	AU	93	ASN
17	Ay	21	GLN
18	AX	42	GLN
20	AZ	6	GLN
1	BA	12	ASN
1	BA	19	ASN
1	BA	234	ASN
1	BA	241	GLN
2	BB	201	HIS
2	BB	216	HIS
2	BB	490	GLN
3	BC	155	ASN
3	BC	398	HIS
3	BC	418	ASN
3	BC	444	HIS
4	BD	98	GLN
4	BD	117	HIS
4	BD	129	GLN
4	BD	142	ASN
4	BD	239	GLN
4	BD	250	ASN

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Mol	Chain	Res	Type
7	BH	59	ASN
11	BL	6	ASN
11	BL	8	GLN
12	BM	5	GLN
12	BM	33	GLN
13	BO	87	GLN
13	BO	106	GLN
13	BO	114	ASN
13	BO	135	GLN
13	BO	150	ASN
13	BO	173	ASN
13	BO	222	GLN
13	BO	226	ASN
15	BU	82	ASN
15	BU	93	ASN
18	BX	42	GLN
20	BZ	6	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 for Mogul analysis.

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
22	CLA	AA	402	1	55,73,73	0.97	4 (7%)	61,113,113	1.46	11 (18%)
22	CLA	AA	403	-	55,73,73	1.06	4 (7%)	61,113,113	1.65	11 (18%)
22	CLA	AA	404	-	55,73,73	0.95	4 (7%)	61,113,113	1.43	11 (18%)
23	PHO	AA	405	-	67,69,69	0.99	2 (2%)	84,99,99	1.33	11 (13%)
22	CLA	AA	406	1	55,73,73	0.98	3 (5%)	61,113,113	1.46	9 (14%)
24	PL9	AA	407	-	45,45,55	0.98	1 (2%)	56,57,69	1.86	16 (28%)
25	OEC	AA	408	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	BCR	AA	409	-	41,41,41	1.63	7 (17%)	56,56,56	2.13	19 (33%)
27	DGD	AA	410	-	57,57,67	1.47	12 (21%)	71,71,81	1.45	8 (11%)
28	LHG	AA	411	-	38,38,48	1.89	5 (13%)	39,44,54	1.31	3 (7%)
29	SQD	AA	412	-	50,51,54	2.38	24 (48%)	58,62,65	3.00	17 (29%)
30	LMG	AA	413	-	51,51,55	0.89	2 (3%)	59,59,63	1.00	4 (6%)
29	SQD	AA	415	-	53,54,54	2.49	28 (52%)	61,65,65	2.85	18 (29%)
30	LMG	AA	416	-	42,42,55	1.50	8 (19%)	50,50,63	1.01	3 (6%)
22	CLA	AB	601	-	55,73,73	1.05	3 (5%)	61,113,113	1.43	11 (18%)
22	CLA	AB	602	2	55,73,73	0.99	3 (5%)	61,113,113	1.42	10 (16%)
22	CLA	AB	603	2	55,73,73	1.05	5 (9%)	61,113,113	1.51	11 (18%)
22	CLA	AB	604	2	55,73,73	1.01	3 (5%)	61,113,113	1.38	9 (14%)
22	CLA	AB	605	-	55,73,73	0.95	3 (5%)	61,113,113	1.42	9 (14%)
22	CLA	AB	606	2	55,73,73	0.93	3 (5%)	61,113,113	1.38	10 (16%)
22	CLA	AB	607	-	55,73,73	1.12	5 (9%)	61,113,113	1.43	7 (11%)
22	CLA	AB	608	2	55,73,73	1.08	5 (9%)	61,113,113	1.52	12 (19%)
22	CLA	AB	609	2	55,73,73	0.99	3 (5%)	61,113,113	1.42	11 (18%)
22	CLA	AB	610	-	55,73,73	0.99	4 (7%)	61,113,113	1.51	12 (19%)
22	CLA	AB	611	2	55,73,73	1.03	4 (7%)	61,113,113	1.48	10 (16%)
22	CLA	AB	612	-	55,73,73	0.95	2 (3%)	61,113,113	1.49	10 (16%)
22	CLA	AB	613	-	55,73,73	0.94	3 (5%)	61,113,113	1.42	11 (18%)
22	CLA	AB	614	2	55,73,73	1.09	4 (7%)	61,113,113	1.57	13 (21%)
22	CLA	AB	615	-	55,73,73	0.90	4 (7%)	61,113,113	1.49	10 (16%)
22	CLA	AB	616	-	55,73,73	1.07	5 (9%)	61,113,113	1.50	11 (18%)
26	BCR	AB	617	-	41,41,41	1.70	7 (17%)	56,56,56	2.04	14 (25%)
26	BCR	AB	618	-	41,41,41	1.70	6 (14%)	56,56,56	2.25	27 (48%)
26	BCR	AB	619	-	41,41,41	1.93	8 (19%)	56,56,56	2.14	15 (26%)
26	BCR	AB	620	-	41,41,41	1.84	7 (17%)	56,56,56	2.12	17 (30%)
30	LMG	AB	621	-	49,49,55	1.01	5 (10%)	57,57,63	1.03	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LMG	AB	622	-	49,49,55	1.06	5 (10%)	57,57,63	1.06	6 (10%)
30	LMG	AB	623	-	42,42,55	1.46	7 (16%)	50,50,63	1.02	3 (6%)
32	LMT	AB	624	-	36,36,36	1.43	6 (16%)	47,47,47	1.20	3 (6%)
32	LMT	AB	625	-	36,36,36	1.37	7 (19%)	47,47,47	0.95	3 (6%)
27	DGD	AB	626	-	53,53,67	1.83	16 (30%)	67,67,81	1.65	8 (11%)
32	LMT	AB	627	-	36,36,36	1.44	5 (13%)	47,47,47	1.03	3 (6%)
22	CLA	AC	501	3	55,73,73	0.98	2 (3%)	61,113,113	1.48	11 (18%)
22	CLA	AC	502	3	55,73,73	0.98	3 (5%)	61,113,113	1.43	10 (16%)
22	CLA	AC	503	3	55,73,73	1.01	3 (5%)	61,113,113	1.40	8 (13%)
22	CLA	AC	504	-	55,73,73	1.04	4 (7%)	61,113,113	1.35	8 (13%)
22	CLA	AC	505	3	55,73,73	1.04	4 (7%)	61,113,113	1.54	12 (19%)
22	CLA	AC	506	3	55,73,73	0.97	4 (7%)	61,113,113	1.45	11 (18%)
22	CLA	AC	507	-	55,73,73	0.96	3 (5%)	61,113,113	1.49	10 (16%)
22	CLA	AC	508	3	55,73,73	0.95	4 (7%)	61,113,113	1.50	10 (16%)
22	CLA	AC	509	-	55,73,73	1.01	4 (7%)	61,113,113	1.51	10 (16%)
22	CLA	AC	510	-	55,73,73	0.98	4 (7%)	61,113,113	1.42	8 (13%)
22	CLA	AC	511	3	55,73,73	0.94	3 (5%)	61,113,113	1.43	9 (14%)
22	CLA	AC	512	-	55,73,73	1.00	3 (5%)	61,113,113	1.52	11 (18%)
22	CLA	AC	513	3	55,73,73	1.10	4 (7%)	61,113,113	1.46	10 (16%)
26	BCR	AC	514	-	41,41,41	1.75	7 (17%)	56,56,56	2.18	21 (37%)
26	BCR	AC	515	-	41,41,41	1.68	6 (14%)	56,56,56	2.21	20 (35%)
27	DGD	AC	516	-	54,54,67	1.21	8 (14%)	68,68,81	1.59	8 (11%)
27	DGD	AC	517	-	63,63,67	1.05	5 (7%)	77,77,81	1.61	8 (10%)
27	DGD	AC	518	-	67,67,67	1.02	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	AC	519	-	48,48,55	1.23	5 (10%)	56,56,63	0.87	3 (5%)
30	LMG	AC	520	-	45,45,55	1.52	8 (17%)	53,53,63	1.04	4 (7%)
28	LHG	AC	521	-	36,36,48	1.05	2 (5%)	37,42,54	1.15	3 (8%)
33	BCT	AD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	AD	402	4	55,73,73	1.05	4 (7%)	61,113,113	1.54	12 (19%)
23	PHO	AD	403	-	67,69,69	1.05	4 (5%)	84,99,99	1.35	12 (14%)
22	CLA	AD	404	-	55,73,73	1.06	3 (5%)	61,113,113	1.46	8 (13%)
24	PL9	AD	405	-	55,55,55	0.55	0	68,69,69	1.82	18 (26%)
26	BCR	AD	406	-	41,41,41	1.83	7 (17%)	56,56,56	2.36	20 (35%)
30	LMG	AD	407	-	46,46,55	0.95	4 (8%)	54,54,63	0.92	2 (3%)
30	LMG	AD	408	-	48,48,55	1.04	3 (6%)	56,56,63	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	SQD	AD	409	-	42,43,54	2.71	20 (47%)	50,54,65	3.26	14 (28%)
27	DGD	AD	410	-	64,64,67	1.79	16 (25%)	78,78,81	1.43	7 (8%)
32	LMT	AD	411	-	32,32,36	1.49	4 (12%)	43,43,47	0.99	2 (4%)
34	HEM	AE	101	5,6	30,50,50	2.37	13 (43%)	24,82,82	3.37	9 (37%)
30	LMG	AE	102	-	44,44,55	1.32	6 (13%)	52,52,63	1.12	5 (9%)
29	SQD	AF	101	-	44,45,54	2.46	21 (47%)	52,56,65	3.05	17 (32%)
26	BCR	AH	101	-	41,41,41	1.86	8 (19%)	56,56,56	2.30	21 (37%)
27	DGD	AH	102	-	59,59,67	1.24	8 (13%)	73,73,81	1.47	7 (9%)
30	LMG	AI	101	-	43,43,55	1.47	8 (18%)	51,51,63	1.08	4 (7%)
32	LMT	AI	102	-	36,36,36	1.40	4 (11%)	47,47,47	0.96	1 (2%)
24	PL9	AJ	101	-	35,35,55	1.39	4 (11%)	44,45,69	1.82	13 (29%)
26	BCR	AJ	102	-	41,41,41	2.05	8 (19%)	56,56,56	3.42	22 (39%)
26	BCR	AK	102	-	41,41,41	1.84	7 (17%)	56,56,56	2.56	25 (44%)
30	LMG	AM	101	-	42,42,55	1.59	6 (14%)	50,50,63	1.21	5 (10%)
32	LMT	AM	102	-	36,36,36	1.18	2 (5%)	47,47,47	0.94	2 (4%)
32	LMT	AT	101	-	36,36,36	1.35	5 (13%)	47,47,47	1.09	4 (8%)
26	BCR	AT	102	-	41,41,41	1.62	6 (14%)	56,56,56	2.25	25 (44%)
34	HEM	AV	201	16	30,50,50	2.31	13 (43%)	24,82,82	3.24	8 (33%)
26	BCR	AZ	101	-	41,41,41	1.83	7 (17%)	56,56,56	2.14	18 (32%)
29	SQD	BA	401	-	53,54,54	2.55	29 (54%)	61,65,65	2.91	20 (32%)
22	CLA	BA	403	1	55,73,73	1.07	5 (9%)	61,113,113	1.44	10 (16%)
22	CLA	BA	404	-	55,73,73	1.04	2 (3%)	61,113,113	1.66	11 (18%)
22	CLA	BA	405	-	55,73,73	0.90	3 (5%)	61,113,113	1.44	10 (16%)
23	PHO	BA	406	-	67,69,69	1.01	4 (5%)	84,99,99	1.31	11 (13%)
22	CLA	BA	407	1	55,73,73	0.97	3 (5%)	61,113,113	1.46	10 (16%)
24	PL9	BA	408	-	45,45,55	1.04	2 (4%)	56,57,69	1.80	14 (25%)
25	OEC	BA	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
26	BCR	BA	410	-	41,41,41	1.69	7 (17%)	56,56,56	2.12	23 (41%)
27	DGD	BA	411	-	57,57,67	1.59	13 (22%)	71,71,81	1.45	7 (9%)
28	LHG	BA	412	-	38,38,48	1.85	6 (15%)	39,44,54	1.30	3 (7%)
29	SQD	BA	413	-	50,51,54	2.40	23 (46%)	58,62,65	2.96	18 (31%)
30	LMG	BA	414	-	51,51,55	0.91	4 (7%)	59,59,63	1.02	4 (6%)
29	SQD	BB	601	-	46,47,54	2.61	23 (50%)	54,58,65	2.94	15 (27%)
27	DGD	BB	602	-	53,53,67	1.83	16 (30%)	67,67,81	1.63	9 (13%)
32	LMT	BB	603	-	36,36,36	1.42	7 (19%)	47,47,47	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	BB	604	-	55,73,73	1.09	3 (5%)	61,113,113	1.43	11 (18%)
22	CLA	BB	605	2	55,73,73	1.01	3 (5%)	61,113,113	1.44	10 (16%)
22	CLA	BB	606	2	55,73,73	1.00	3 (5%)	61,113,113	1.50	10 (16%)
22	CLA	BB	607	2	55,73,73	1.01	3 (5%)	61,113,113	1.36	9 (14%)
22	CLA	BB	608	2	55,73,73	0.92	3 (5%)	61,113,113	1.41	9 (14%)
22	CLA	BB	609	2	55,73,73	0.96	2 (3%)	61,113,113	1.41	10 (16%)
22	CLA	BB	610	-	55,73,73	1.15	6 (10%)	61,113,113	1.44	8 (13%)
22	CLA	BB	611	2	55,73,73	1.05	6 (10%)	61,113,113	1.53	12 (19%)
22	CLA	BB	612	2	55,73,73	0.98	2 (3%)	61,113,113	1.42	9 (14%)
22	CLA	BB	613	-	55,73,73	1.02	5 (9%)	61,113,113	1.50	12 (19%)
22	CLA	BB	614	2	55,73,73	0.95	3 (5%)	61,113,113	1.46	10 (16%)
22	CLA	BB	615	-	55,73,73	0.95	4 (7%)	61,113,113	1.50	11 (18%)
22	CLA	BB	616	-	55,73,73	0.96	3 (5%)	61,113,113	1.44	11 (18%)
22	CLA	BB	617	2	55,73,73	1.05	3 (5%)	61,113,113	1.55	13 (21%)
22	CLA	BB	618	-	55,73,73	0.90	3 (5%)	61,113,113	1.45	10 (16%)
22	CLA	BB	619	-	55,73,73	1.11	5 (9%)	61,113,113	1.50	12 (19%)
26	BCR	BB	620	-	41,41,41	1.56	8 (19%)	56,56,56	2.05	14 (25%)
26	BCR	BB	621	-	41,41,41	1.85	7 (17%)	56,56,56	2.18	17 (30%)
26	BCR	BB	622	-	41,41,41	1.81	7 (17%)	56,56,56	2.10	18 (32%)
30	LMG	BB	623	-	49,49,55	1.07	5 (10%)	57,57,63	1.05	4 (7%)
30	LMG	BB	624	-	49,49,55	1.04	5 (10%)	57,57,63	1.04	3 (5%)
32	LMT	BB	625	-	36,36,36	1.53	8 (22%)	47,47,47	1.23	3 (6%)
32	LMT	BB	626	-	36,36,36	1.35	5 (13%)	47,47,47	0.93	2 (4%)
22	CLA	BC	501	3	55,73,73	0.95	3 (5%)	61,113,113	1.49	10 (16%)
22	CLA	BC	502	3	55,73,73	0.96	3 (5%)	61,113,113	1.42	10 (16%)
22	CLA	BC	503	3	55,73,73	0.99	2 (3%)	61,113,113	1.40	8 (13%)
22	CLA	BC	504	-	55,73,73	1.05	4 (7%)	61,113,113	1.38	8 (13%)
22	CLA	BC	505	3	55,73,73	1.00	4 (7%)	61,113,113	1.54	12 (19%)
22	CLA	BC	506	3	55,73,73	1.04	4 (7%)	61,113,113	1.41	10 (16%)
22	CLA	BC	507	-	55,73,73	0.96	3 (5%)	61,113,113	1.49	11 (18%)
22	CLA	BC	508	3	55,73,73	0.98	4 (7%)	61,113,113	1.47	10 (16%)
22	CLA	BC	509	-	55,73,73	1.05	6 (10%)	61,113,113	1.50	11 (18%)
22	CLA	BC	510	-	55,73,73	0.92	3 (5%)	61,113,113	1.45	9 (14%)
22	CLA	BC	511	3	55,73,73	0.98	4 (7%)	61,113,113	1.43	8 (13%)
22	CLA	BC	512	-	55,73,73	0.99	2 (3%)	61,113,113	1.52	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	BC	513	3	55,73,73	1.07	4 (7%)	61,113,113	1.45	9 (14%)
26	BCR	BC	514	-	41,41,41	1.89	7 (17%)	56,56,56	2.17	21 (37%)
26	BCR	BC	515	-	41,41,41	1.81	7 (17%)	56,56,56	2.20	20 (35%)
27	DGD	BC	516	-	54,54,67	1.32	9 (16%)	68,68,81	1.55	8 (11%)
27	DGD	BC	517	-	63,63,67	1.08	6 (9%)	77,77,81	1.61	8 (10%)
27	DGD	BC	518	-	67,67,67	1.14	6 (8%)	81,81,81	1.27	4 (4%)
30	LMG	BC	519	-	48,48,55	1.26	6 (12%)	56,56,63	0.87	3 (5%)
30	LMG	BC	520	-	45,45,55	1.54	10 (22%)	53,53,63	1.06	4 (7%)
28	LHG	BC	521	-	36,36,48	1.04	2 (5%)	37,42,54	1.15	3 (8%)
33	BCT	BD	401	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	BD	402	4	55,73,73	1.04	3 (5%)	61,113,113	1.53	12 (19%)
23	PHO	BD	403	-	67,69,69	1.03	5 (7%)	84,99,99	1.36	11 (13%)
22	CLA	BD	404	-	55,73,73	1.08	5 (9%)	61,113,113	1.40	8 (13%)
24	PL9	BD	405	-	55,55,55	0.53	0	68,69,69	1.83	18 (26%)
26	BCR	BD	406	-	41,41,41	1.92	8 (19%)	56,56,56	2.35	19 (33%)
30	LMG	BD	407	-	46,46,55	1.02	4 (8%)	54,54,63	0.93	2 (3%)
30	LMG	BD	408	-	48,48,55	1.12	3 (6%)	56,56,63	1.02	3 (5%)
29	SQD	BD	409	-	42,43,54	2.68	20 (47%)	50,54,65	3.26	14 (28%)
27	DGD	BD	410	-	64,64,67	1.73	17 (26%)	78,78,81	1.43	7 (8%)
32	LMT	BD	411	-	32,32,36	1.39	4 (12%)	43,43,47	0.94	2 (4%)
34	HEM	BE	101	5,6	30,50,50	2.37	14 (46%)	24,82,82	3.36	9 (37%)
30	LMG	BE	102	-	44,44,55	1.33	6 (13%)	52,52,63	1.12	5 (9%)
29	SQD	BF	101	-	44,45,54	2.56	20 (45%)	52,56,65	3.03	16 (30%)
27	DGD	BH	101	-	59,59,67	1.20	9 (15%)	73,73,81	1.47	7 (9%)
30	LMG	BI	101	-	43,43,55	1.54	8 (18%)	51,51,63	1.10	5 (9%)
32	LMT	BI	102	-	36,36,36	1.50	4 (11%)	47,47,47	0.97	1 (2%)
24	PL9	BJ	101	-	35,35,55	1.43	5 (14%)	44,45,69	1.76	13 (29%)
26	BCR	BJ	102	-	41,41,41	2.16	8 (19%)	56,56,56	3.42	24 (42%)
26	BCR	BK	102	-	41,41,41	1.85	7 (17%)	56,56,56	2.56	27 (48%)
29	SQD	BL	101	-	46,47,54	2.72	22 (47%)	54,58,65	2.97	15 (27%)
32	LMT	BM	101	-	36,36,36	1.18	3 (8%)	47,47,47	0.96	2 (4%)
30	LMG	BM	102	-	42,42,55	1.62	8 (19%)	50,50,63	1.15	4 (8%)
32	LMT	BT	101	-	36,36,36	1.29	4 (11%)	47,47,47	1.06	3 (6%)
34	HEM	BV	201	16	30,50,50	2.34	10 (33%)	24,82,82	3.28	7 (29%)
26	BCR	BX	101	-	41,41,41	1.85	8 (19%)	56,56,56	2.31	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	BZ	101	-	41,41,41	1.94	9 (21%)	56,56,56	2.12	20 (35%)

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
22	CLA	AA	402	1	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AA	403	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AA	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PHO	AA	405	-	-	1/53/103/103	0/1/6/6
22	CLA	AA	406	1	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	AA	407	-	-	0/41/61/73	0/1/1/1
25	OEC	AA	408	1,3	-	0/0/0/54	0/0/0/5
26	BCR	AA	409	-	-	0/29/63/63	0/2/2/2
27	DGD	AA	410	-	3/3/13/13	0/45/85/95	0/2/2/2
28	LHG	AA	411	-	-	0/43/43/53	0/0/0/0
29	SQD	AA	412	-	-	0/46/66/69	0/1/1/1
30	LMG	AA	413	-	2/2/8/8	0/46/66/70	0/1/1/1
29	SQD	AA	415	-	-	0/49/69/69	0/1/1/1
30	LMG	AA	416	-	2/2/8/8	0/37/57/70	0/1/1/1
22	CLA	AB	601	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	602	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AB	603	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	604	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	606	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AB	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	608	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	609	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	611	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AB	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	614	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AB	615	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	AB	616	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	AB	617	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	618	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	619	-	-	0/29/63/63	0/2/2/2
26	BCR	AB	620	-	-	0/29/63/63	0/2/2/2
30	LMG	AB	621	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	AB	622	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	AB	623	-	2/2/8/8	0/37/57/70	0/1/1/1
32	LMT	AB	624	-	-	0/21/61/61	0/2/2/2
32	LMT	AB	625	-	-	0/21/61/61	0/2/2/2
27	DGD	AB	626	-	3/3/13/13	0/41/81/95	0/2/2/2
32	LMT	AB	627	-	-	0/21/61/61	0/2/2/2
22	CLA	AC	501	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	502	3	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AC	503	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	505	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	506	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	508	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	509	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AC	510	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	AC	511	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	AC	513	3	3/3/20/25	1/37/135/135	0/0/9/9
26	BCR	AC	514	-	-	0/29/63/63	0/2/2/2
26	BCR	AC	515	-	-	0/29/63/63	0/2/2/2
27	DGD	AC	516	-	3/3/13/13	0/42/82/95	0/2/2/2
27	DGD	AC	517	-	3/3/13/13	0/51/91/95	0/2/2/2
27	DGD	AC	518	-	3/3/13/13	0/55/95/95	0/2/2/2
30	LMG	AC	519	-	2/2/8/8	0/43/63/70	0/1/1/1
30	LMG	AC	520	-	2/2/8/8	0/40/60/70	0/1/1/1
28	LHG	AC	521	-	-	0/41/41/53	0/0/0/0
33	BCT	AD	401	21	-	0/0/0/0	0/0/0/0
22	CLA	AD	402	4	2/2/20/25	0/37/135/135	0/0/9/9
23	PHO	AD	403	-	-	0/53/103/103	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	AD	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	AD	405	-	-	0/53/73/73	0/1/1/1
26	BCR	AD	406	-	-	0/29/63/63	0/2/2/2
30	LMG	AD	407	-	2/2/8/8	0/41/61/70	0/1/1/1
30	LMG	AD	408	-	2/2/8/8	1/43/63/70	0/1/1/1
29	SQD	AD	409	-	-	2/38/58/69	0/1/1/1
27	DGD	AD	410	-	3/3/13/13	0/52/92/95	0/2/2/2
32	LMT	AD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	AE	101	5,6	-	0/10/54/54	0/0/8/8
30	LMG	AE	102	-	2/2/8/8	0/39/59/70	0/1/1/1
29	SQD	AF	101	-	-	0/40/60/69	0/1/1/1
26	BCR	AH	101	-	-	0/29/63/63	0/2/2/2
27	DGD	AH	102	-	3/3/13/13	0/47/87/95	0/2/2/2
30	LMG	AI	101	-	2/2/8/8	0/38/58/70	0/1/1/1
32	LMT	AI	102	-	-	0/21/61/61	0/2/2/2
24	PL9	AJ	101	-	-	0/29/49/73	0/1/1/1
26	BCR	AJ	102	-	-	0/29/63/63	0/2/2/2
26	BCR	AK	102	-	-	0/29/63/63	0/2/2/2
30	LMG	AM	101	-	2/2/8/8	1/37/57/70	0/1/1/1
32	LMT	AM	102	-	-	0/21/61/61	0/2/2/2
32	LMT	AT	101	-	-	0/21/61/61	0/2/2/2
26	BCR	AT	102	-	-	0/29/63/63	0/2/2/2
34	HEM	AV	201	16	-	0/10/54/54	0/0/8/8
26	BCR	AZ	101	-	-	0/29/63/63	0/2/2/2
29	SQD	BA	401	-	-	0/49/69/69	0/1/1/1
22	CLA	BA	403	1	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BA	404	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BA	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PHO	BA	406	-	-	1/53/103/103	0/1/6/6
22	CLA	BA	407	1	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	BA	408	-	-	0/41/61/73	0/1/1/1
25	OEC	BA	409	1,3	-	0/0/0/54	0/0/0/5
26	BCR	BA	410	-	-	0/29/63/63	0/2/2/2
27	DGD	BA	411	-	3/3/13/13	0/45/85/95	0/2/2/2
28	LHG	BA	412	-	-	0/43/43/53	0/0/0/0
29	SQD	BA	413	-	-	0/46/66/69	0/1/1/1
30	LMG	BA	414	-	2/2/8/8	0/46/66/70	0/1/1/1
29	SQD	BB	601	-	-	0/42/62/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	BB	602	-	3/3/13/13	0/41/81/95	0/2/2/2
32	LMT	BB	603	-	-	0/21/61/61	0/2/2/2
22	CLA	BB	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	605	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BB	606	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	607	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	608	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	609	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BB	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	611	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	612	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	614	2	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BB	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	617	2	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BB	619	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	BB	620	-	-	0/29/63/63	0/2/2/2
26	BCR	BB	621	-	-	0/29/63/63	0/2/2/2
26	BCR	BB	622	-	-	0/29/63/63	0/2/2/2
30	LMG	BB	623	-	2/2/8/8	0/44/64/70	0/1/1/1
30	LMG	BB	624	-	2/2/8/8	0/44/64/70	0/1/1/1
32	LMT	BB	625	-	-	0/21/61/61	0/2/2/2
32	LMT	BB	626	-	-	0/21/61/61	0/2/2/2
22	CLA	BC	501	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	502	3	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BC	503	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	505	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	506	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	508	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	509	-	3/3/20/25	1/37/135/135	0/0/9/9
22	CLA	BC	510	-	3/3/20/25	1/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	BC	511	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	BC	513	3	3/3/20/25	1/37/135/135	0/0/9/9
26	BCR	BC	514	-	-	0/29/63/63	0/2/2/2
26	BCR	BC	515	-	-	0/29/63/63	0/2/2/2
27	DGD	BC	516	-	3/3/13/13	0/42/82/95	0/2/2/2
27	DGD	BC	517	-	3/3/13/13	0/51/91/95	0/2/2/2
27	DGD	BC	518	-	3/3/13/13	0/55/95/95	0/2/2/2
30	LMG	BC	519	-	2/2/8/8	0/43/63/70	0/1/1/1
30	LMG	BC	520	-	2/2/8/8	0/40/60/70	0/1/1/1
28	LHG	BC	521	-	-	0/41/41/53	0/0/0/0
33	BCT	BD	401	21	-	0/0/0/0	0/0/0/0
22	CLA	BD	402	4	2/2/20/25	0/37/135/135	0/0/9/9
23	PHO	BD	403	-	-	0/53/103/103	0/1/6/6
22	CLA	BD	404	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	BD	405	-	-	0/53/73/73	0/1/1/1
26	BCR	BD	406	-	-	0/29/63/63	0/2/2/2
30	LMG	BD	407	-	2/2/8/8	0/41/61/70	0/1/1/1
30	LMG	BD	408	-	2/2/8/8	1/43/63/70	0/1/1/1
29	SQD	BD	409	-	-	2/38/58/69	0/1/1/1
27	DGD	BD	410	-	3/3/13/13	0/52/92/95	0/2/2/2
32	LMT	BD	411	-	-	0/17/57/61	0/2/2/2
34	HEM	BE	101	5,6	-	0/10/54/54	0/0/8/8
30	LMG	BE	102	-	2/2/8/8	0/39/59/70	0/1/1/1
29	SQD	BF	101	-	-	0/40/60/69	0/1/1/1
27	DGD	BH	101	-	3/3/13/13	0/47/87/95	0/2/2/2
30	LMG	BI	101	-	2/2/8/8	0/38/58/70	0/1/1/1
32	LMT	BI	102	-	-	0/21/61/61	0/2/2/2
24	PL9	BJ	101	-	-	0/29/49/73	0/1/1/1
26	BCR	BJ	102	-	-	0/29/63/63	0/2/2/2
26	BCR	BK	102	-	-	0/29/63/63	0/2/2/2
29	SQD	BL	101	-	-	0/42/62/69	0/1/1/1
32	LMT	BM	101	-	-	0/21/61/61	0/2/2/2
30	LMG	BM	102	-	2/2/8/8	1/37/57/70	0/1/1/1
32	LMT	BT	101	-	-	0/21/61/61	0/2/2/2
34	HEM	BV	201	16	-	0/10/54/54	0/0/8/8
26	BCR	BX	101	-	-	0/29/63/63	0/2/2/2
26	BCR	BZ	101	-	-	0/29/63/63	0/2/2/2

All (1087) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BV	201	HEM	C2D-C3D	-4.77	1.40	1.54
34	AE	101	HEM	C2D-C3D	-4.71	1.40	1.54
34	BE	101	HEM	C2D-C3D	-4.69	1.40	1.54
34	AV	201	HEM	C2D-C3D	-4.52	1.41	1.54
34	AV	201	HEM	C3B-C4B	-4.28	1.48	1.51
34	AE	101	HEM	CAD-C3D	-4.27	1.45	1.54
34	BV	201	HEM	CAD-C3D	-4.24	1.45	1.54
34	BE	101	HEM	C3D-C4D	-4.22	1.46	1.51
34	BE	101	HEM	CAD-C3D	-4.19	1.45	1.54
34	BV	201	HEM	C3B-C4B	-4.16	1.48	1.51
34	AE	101	HEM	C3D-C4D	-3.97	1.46	1.51
34	AV	201	HEM	CAD-C3D	-3.96	1.46	1.54
34	BV	201	HEM	C2D-C1D	-3.28	1.41	1.51
34	AV	201	HEM	C2D-C1D	-3.14	1.41	1.51
34	BV	201	HEM	C3D-C4D	-3.09	1.47	1.51
23	AD	403	PHO	CHB-C1B	-3.04	1.33	1.38
34	BE	101	HEM	C2D-C1D	-2.97	1.42	1.51
34	AE	101	HEM	C2D-C1D	-2.87	1.42	1.51
34	AV	201	HEM	C3D-C4D	-2.87	1.47	1.51
29	BD	409	SQD	C12-C11	-2.85	1.35	1.51
29	BD	409	SQD	C16-C15	-2.85	1.35	1.51
22	AA	406	CLA	C1B-CHB	-2.84	1.32	1.39
29	AA	412	SQD	C32-C31	-2.84	1.35	1.51
22	BB	605	CLA	C1B-CHB	-2.82	1.32	1.39
29	BD	409	SQD	C15-C14	-2.82	1.35	1.51
29	BB	601	SQD	C17-C16	-2.82	1.35	1.51
29	AA	415	SQD	C17-C16	-2.82	1.35	1.51
29	BA	401	SQD	C15-C14	-2.81	1.35	1.51
34	BE	101	HEM	C3B-C4B	-2.80	1.49	1.51
29	AA	415	SQD	C15-C14	-2.79	1.35	1.51
23	BD	403	PHO	CHB-C1B	-2.79	1.33	1.38
29	AA	415	SQD	C11-C10	-2.79	1.35	1.51
29	AA	412	SQD	O6-C44	-2.77	1.38	1.43
29	BA	401	SQD	C11-C10	-2.76	1.35	1.51
29	AD	409	SQD	C11-C10	-2.76	1.35	1.51
29	BB	601	SQD	C19-C18	-2.76	1.35	1.51
22	AB	602	CLA	C1B-CHB	-2.75	1.32	1.39
29	BA	401	SQD	C17-C16	-2.75	1.35	1.51
29	BL	101	SQD	C19-C18	-2.75	1.35	1.51
29	AA	412	SQD	C33-C32	-2.74	1.35	1.51
29	AA	415	SQD	C12-C11	-2.73	1.35	1.51
29	AD	409	SQD	C12-C11	-2.72	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	AE	101	HEM	C3B-C4B	-2.72	1.49	1.51
22	BB	614	CLA	C1B-CHB	-2.71	1.32	1.39
22	AB	611	CLA	C1B-CHB	-2.71	1.32	1.39
29	AD	409	SQD	C15-C14	-2.70	1.35	1.51
29	BL	101	SQD	C17-C16	-2.69	1.36	1.51
29	BL	101	SQD	C11-C10	-2.69	1.36	1.51
29	BB	601	SQD	C16-C15	-2.68	1.36	1.51
29	AD	409	SQD	C16-C15	-2.68	1.36	1.51
29	BA	413	SQD	C12-C11	-2.68	1.36	1.51
29	BB	601	SQD	C20-C19	-2.68	1.36	1.51
29	BD	409	SQD	C11-C10	-2.67	1.36	1.51
29	AA	415	SQD	C16-C15	-2.67	1.36	1.51
29	BA	413	SQD	C32-C31	-2.67	1.36	1.51
29	BB	601	SQD	C15-C14	-2.66	1.36	1.51
29	BD	409	SQD	C14-C13	-2.65	1.36	1.51
22	BA	407	CLA	C1B-CHB	-2.65	1.32	1.39
29	BL	101	SQD	C12-C11	-2.65	1.36	1.51
29	AA	412	SQD	C12-C11	-2.64	1.36	1.51
29	BL	101	SQD	C15-C14	-2.64	1.36	1.51
22	BB	606	CLA	C1B-CHB	-2.64	1.32	1.39
22	AC	504	CLA	C1B-CHB	-2.64	1.32	1.39
29	BD	409	SQD	C13-C12	-2.64	1.36	1.51
29	AA	412	SQD	C17-C16	-2.64	1.36	1.51
29	BB	601	SQD	C12-C11	-2.64	1.36	1.51
22	BA	404	CLA	C1B-CHB	-2.63	1.32	1.39
29	AA	415	SQD	C19-C18	-2.63	1.36	1.51
29	BB	601	SQD	C11-C10	-2.63	1.36	1.51
29	BF	101	SQD	C17-C16	-2.62	1.36	1.51
22	AB	603	CLA	C1B-CHB	-2.62	1.32	1.39
29	AA	412	SQD	C16-C15	-2.61	1.36	1.51
29	AA	412	SQD	C15-C14	-2.61	1.36	1.51
29	BL	101	SQD	C20-C19	-2.60	1.36	1.51
29	BL	101	SQD	C14-C13	-2.60	1.36	1.51
29	BA	413	SQD	C33-C32	-2.59	1.36	1.51
29	BL	101	SQD	C16-C15	-2.59	1.36	1.51
22	AC	507	CLA	C1B-CHB	-2.59	1.32	1.39
29	AD	409	SQD	C14-C13	-2.59	1.36	1.51
29	AF	101	SQD	C17-C16	-2.59	1.36	1.51
29	BA	413	SQD	C16-C15	-2.59	1.36	1.51
29	BA	413	SQD	C11-C10	-2.58	1.36	1.51
22	BB	610	CLA	C1B-CHB	-2.58	1.32	1.39
29	BA	413	SQD	C15-C14	-2.58	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BA	401	SQD	C12-C11	-2.57	1.36	1.51
29	AF	101	SQD	C15-C14	-2.57	1.36	1.51
29	BA	401	SQD	C19-C18	-2.57	1.36	1.51
29	AA	412	SQD	C14-C13	-2.56	1.36	1.51
29	AA	412	SQD	C11-C10	-2.56	1.36	1.51
29	BA	413	SQD	C17-C16	-2.55	1.36	1.51
29	AD	409	SQD	C13-C12	-2.53	1.36	1.51
29	BB	601	SQD	C18-C17	-2.53	1.36	1.51
29	BB	601	SQD	C14-C13	-2.53	1.36	1.51
29	BA	401	SQD	C16-C15	-2.52	1.36	1.51
29	AF	101	SQD	C16-C15	-2.52	1.37	1.51
22	BB	616	CLA	C1B-CHB	-2.51	1.32	1.39
29	BA	401	SQD	C14-C13	-2.51	1.37	1.51
22	AB	607	CLA	C1B-CHB	-2.49	1.33	1.39
29	BA	413	SQD	C19-C18	-2.48	1.37	1.51
22	BC	507	CLA	C1B-CHB	-2.48	1.33	1.39
29	BA	401	SQD	C18-C17	-2.48	1.37	1.51
29	AA	415	SQD	C20-C19	-2.48	1.37	1.51
29	AA	415	SQD	C33-C32	-2.47	1.37	1.51
29	AA	412	SQD	C20-C19	-2.47	1.37	1.51
29	BF	101	SQD	C15-C14	-2.47	1.37	1.51
29	AA	412	SQD	C19-C18	-2.47	1.37	1.51
29	BF	101	SQD	C12-C11	-2.47	1.37	1.51
22	BB	617	CLA	C1B-CHB	-2.46	1.33	1.39
29	BL	101	SQD	C18-C17	-2.46	1.37	1.51
29	AA	415	SQD	C18-C17	-2.45	1.37	1.51
22	AB	613	CLA	C1B-CHB	-2.45	1.33	1.39
22	BA	403	CLA	C1B-CHB	-2.44	1.33	1.39
29	BF	101	SQD	C11-C10	-2.44	1.37	1.51
22	AA	404	CLA	C1B-CHB	-2.44	1.33	1.39
29	BA	413	SQD	C14-C13	-2.44	1.37	1.51
29	AA	415	SQD	C32-C31	-2.44	1.37	1.51
29	BF	101	SQD	C16-C15	-2.44	1.37	1.51
29	BB	601	SQD	C13-C12	-2.44	1.37	1.51
29	BA	413	SQD	C20-C19	-2.43	1.37	1.51
22	AA	402	CLA	C1B-CHB	-2.43	1.33	1.39
29	BA	413	SQD	C13-C12	-2.41	1.37	1.51
22	BB	615	CLA	C1B-CHB	-2.40	1.33	1.39
29	AA	415	SQD	C14-C13	-2.40	1.37	1.51
22	AB	614	CLA	C1B-CHB	-2.40	1.33	1.39
22	AA	403	CLA	C1B-CHB	-2.40	1.33	1.39
29	BA	401	SQD	C32-C31	-2.40	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BA	401	SQD	C33-C32	-2.39	1.37	1.51
22	BC	504	CLA	C1B-CHB	-2.39	1.33	1.39
22	BC	506	CLA	C1B-CHB	-2.39	1.33	1.39
29	BL	101	SQD	C13-C12	-2.39	1.37	1.51
29	AF	101	SQD	C11-C10	-2.38	1.37	1.51
22	BB	619	CLA	C1B-CHB	-2.36	1.33	1.39
26	AA	409	BCR	C19-C18	-2.36	1.40	1.45
22	AB	616	CLA	C1B-CHB	-2.36	1.33	1.39
29	AA	412	SQD	C13-C12	-2.35	1.37	1.51
29	BA	401	SQD	C13-C12	-2.34	1.38	1.51
29	AA	415	SQD	C13-C12	-2.34	1.38	1.51
29	AF	101	SQD	C12-C11	-2.34	1.38	1.51
26	BZ	101	BCR	C23-C22	-2.34	1.40	1.45
29	BA	401	SQD	C20-C19	-2.33	1.38	1.51
29	BA	401	SQD	C36-C35	-2.32	1.38	1.51
29	BF	101	SQD	C14-C13	-2.29	1.38	1.51
29	AF	101	SQD	C14-C13	-2.27	1.38	1.51
26	BA	410	BCR	C19-C18	-2.27	1.40	1.45
26	BB	620	BCR	C19-C18	-2.26	1.40	1.45
22	BD	404	CLA	C1B-CHB	-2.25	1.33	1.39
29	AA	415	SQD	C36-C35	-2.24	1.38	1.51
29	BA	413	SQD	O6-C44	-2.24	1.39	1.43
29	AA	415	SQD	C34-C33	-2.24	1.38	1.51
22	BB	613	CLA	C1B-CHB	-2.22	1.33	1.39
29	AA	415	SQD	C35-C34	-2.22	1.38	1.51
22	AC	509	CLA	C1B-CHB	-2.20	1.33	1.39
22	AC	502	CLA	C1B-CHB	-2.20	1.33	1.39
29	BD	409	SQD	C17-C16	-2.20	1.35	1.51
29	BA	401	SQD	C35-C34	-2.19	1.38	1.51
26	BB	620	BCR	C23-C22	-2.19	1.41	1.45
29	BF	101	SQD	C13-C12	-2.19	1.38	1.51
22	AA	402	CLA	CAA-CBA	-2.18	1.45	1.52
22	BA	403	CLA	CAA-CBA	-2.17	1.45	1.52
29	BA	413	SQD	C18-C17	-2.16	1.39	1.51
22	BA	405	CLA	C1B-CHB	-2.16	1.33	1.39
22	AC	510	CLA	C1B-CHB	-2.16	1.33	1.39
22	AB	605	CLA	C1B-CHB	-2.15	1.33	1.39
22	AB	602	CLA	CAA-CBA	-2.14	1.45	1.52
22	BC	502	CLA	C1B-CHB	-2.14	1.33	1.39
23	BA	406	PHO	CAA-CBA	-2.14	1.45	1.52
26	AB	617	BCR	C23-C22	-2.13	1.41	1.45
28	BA	412	LHG	O8-C6	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BC	508	CLA	C1B-CHB	-2.12	1.34	1.39
22	AB	610	CLA	C1B-CHB	-2.12	1.34	1.39
22	AC	508	CLA	C1B-CHB	-2.12	1.34	1.39
29	AA	412	SQD	C18-C17	-2.11	1.39	1.51
29	BA	401	SQD	C34-C33	-2.11	1.39	1.51
22	AB	608	CLA	C1B-CHB	-2.11	1.34	1.39
22	BC	509	CLA	C1B-CHB	-2.10	1.34	1.39
22	BC	501	CLA	C1B-CHB	-2.08	1.34	1.39
22	BB	608	CLA	C1B-CHB	-2.08	1.34	1.39
22	AC	501	CLA	C1B-CHB	-2.08	1.34	1.39
29	AD	409	SQD	C17-C16	-2.08	1.36	1.51
29	AF	101	SQD	C13-C12	-2.07	1.39	1.51
26	BC	515	BCR	C19-C18	-2.07	1.41	1.45
29	BL	101	SQD	C21-C20	-2.05	1.36	1.51
22	BB	605	CLA	CAA-CBA	-2.05	1.45	1.52
22	AC	506	CLA	C1B-CHB	-2.05	1.34	1.39
29	BB	601	SQD	C21-C20	-2.04	1.36	1.51
22	AB	606	CLA	C1B-CHB	-2.04	1.34	1.39
26	BD	406	BCR	C19-C18	-2.02	1.41	1.45
22	AB	615	CLA	C1B-CHB	-2.01	1.34	1.39
23	AA	405	PHO	CAA-CBA	-2.01	1.46	1.52
22	BB	611	CLA	C1B-CHB	-2.01	1.34	1.39
22	BB	618	CLA	C1B-CHB	-2.00	1.34	1.39
27	BA	411	DGD	O6D-C5D	2.00	1.49	1.44
32	AB	624	LMT	O5B-C5B	2.00	1.49	1.44
22	BB	604	CLA	C1-C2	2.01	1.55	1.49
22	BC	501	CLA	CHC-C1C	2.01	1.41	1.35
22	BB	611	CLA	C2-C3	2.01	1.36	1.33
22	BD	404	CLA	C5-C3	2.01	1.55	1.51
22	AC	506	CLA	C4-C3	2.01	1.55	1.50
22	BA	403	CLA	C4-C3	2.01	1.55	1.50
22	BD	404	CLA	C4-C3	2.01	1.55	1.50
22	BB	614	CLA	CHC-C1C	2.01	1.41	1.35
22	AB	601	CLA	CAA-C2A	2.01	1.58	1.54
22	AB	603	CLA	C2-C3	2.01	1.36	1.33
22	AB	608	CLA	C4-C3	2.01	1.55	1.50
22	AB	601	CLA	C3C-C2C	2.01	1.41	1.36
30	BC	520	LMG	C29-C28	2.02	1.56	1.50
22	AB	603	CLA	C5-C3	2.02	1.55	1.51
30	AE	102	LMG	C4-C5	2.02	1.57	1.53
32	BB	603	LMT	C3'-C4'	2.02	1.58	1.52
26	AC	514	BCR	C38-C26	2.02	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	AH	102	DGD	C3D-C2D	2.02	1.57	1.52
22	BC	507	CLA	C4C-C3C	2.02	1.48	1.45
29	AA	412	SQD	C8-C7	2.02	1.56	1.50
30	BM	102	LMG	C11-C10	2.02	1.56	1.50
22	AC	512	CLA	CMB-C2B	2.02	1.55	1.51
27	BC	517	DGD	C4E-C3E	2.02	1.57	1.52
30	BC	519	LMG	O7-C10	2.03	1.40	1.34
22	AC	512	CLA	C1C-C2C	2.03	1.48	1.44
32	AB	624	LMT	C3B-C2B	2.03	1.57	1.52
32	BM	101	LMT	O5B-C1B	2.03	1.47	1.41
26	AJ	102	BCR	C3-C4	2.03	1.58	1.52
27	BA	411	DGD	O1G-C1A	2.04	1.39	1.33
29	AA	415	SQD	C24-C23	2.04	1.56	1.50
27	AA	410	DGD	C1G-C2G	2.04	1.56	1.50
26	BB	621	BCR	C24-C23	2.04	1.39	1.33
22	BB	611	CLA	CHC-C1C	2.04	1.41	1.35
22	BA	407	CLA	CHC-C1C	2.04	1.41	1.35
27	BB	602	DGD	C3D-C2D	2.04	1.57	1.52
22	AB	610	CLA	CAA-C2A	2.04	1.58	1.54
22	BD	402	CLA	C1C-C2C	2.05	1.48	1.44
22	AC	503	CLA	C1C-C2C	2.05	1.48	1.44
29	BB	601	SQD	C8-C7	2.05	1.56	1.50
22	BB	609	CLA	CHC-C1C	2.05	1.41	1.35
32	BB	603	LMT	C1B-C2B	2.05	1.58	1.52
22	AB	614	CLA	C1C-C2C	2.05	1.48	1.44
22	AB	611	CLA	C4-C3	2.05	1.55	1.50
22	BC	505	CLA	C1C-C2C	2.05	1.48	1.44
22	BB	610	CLA	C1-C2	2.06	1.55	1.49
22	AA	404	CLA	CHC-C1C	2.06	1.41	1.35
32	AB	625	LMT	C4'-C5'	2.06	1.58	1.52
29	AF	101	SQD	C24-C23	2.06	1.56	1.50
23	AD	403	PHO	CHC-C1C	2.07	1.42	1.38
27	AA	410	DGD	O2G-C1B	2.07	1.40	1.34
22	AB	608	CLA	CHC-C1C	2.07	1.41	1.35
27	AA	410	DGD	O6E-C5E	2.08	1.49	1.44
22	AB	613	CLA	CHC-C1C	2.08	1.41	1.35
22	BB	616	CLA	CHC-C1C	2.08	1.41	1.35
22	AB	604	CLA	C4-C3	2.08	1.55	1.50
22	BB	604	CLA	C3C-C2C	2.08	1.41	1.36
22	BB	608	CLA	CHC-C1C	2.08	1.41	1.35
30	BI	101	LMG	O1-C1	2.08	1.43	1.40
22	AB	615	CLA	C4-C3	2.08	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	AT	101	LMT	C3'-C4'	2.09	1.58	1.52
22	BC	511	CLA	C1C-C2C	2.09	1.48	1.44
22	BB	614	CLA	CAA-C2A	2.09	1.58	1.54
22	BA	405	CLA	CHC-C1C	2.09	1.41	1.35
30	AB	623	LMG	C1-C2	2.09	1.58	1.52
22	BC	506	CLA	CHC-C1C	2.09	1.41	1.35
29	AA	415	SQD	C44-C45	2.09	1.56	1.50
22	BC	511	CLA	C4-C3	2.09	1.55	1.50
27	BH	101	DGD	O6D-C1D	2.09	1.47	1.41
27	BH	101	DGD	C4E-C5E	2.10	1.57	1.53
22	AC	509	CLA	C4-C3	2.10	1.55	1.50
27	BC	516	DGD	C4E-C5E	2.10	1.57	1.53
23	BD	403	PHO	CMB-C2B	2.10	1.55	1.50
34	AV	201	HEM	CHC-C1C	2.10	1.41	1.36
22	AA	404	CLA	C4-C3	2.10	1.55	1.50
22	AB	611	CLA	CHC-C1C	2.11	1.41	1.35
27	BB	602	DGD	C1D-C2D	2.11	1.58	1.52
26	BX	101	BCR	C14-C13	2.11	1.38	1.35
22	AC	510	CLA	C1C-C2C	2.11	1.48	1.44
32	AB	625	LMT	O5B-C5B	2.11	1.49	1.44
32	BB	626	LMT	O1B-C1B	2.11	1.47	1.41
22	AB	609	CLA	C1C-C2C	2.11	1.48	1.44
22	AC	504	CLA	C4-C3	2.11	1.55	1.50
29	BA	401	SQD	C8-C7	2.12	1.57	1.50
27	BC	518	DGD	C4E-C3E	2.12	1.58	1.52
27	BD	410	DGD	C1G-C2G	2.12	1.56	1.50
32	AI	102	LMT	C4B-C5B	2.12	1.57	1.53
22	AA	403	CLA	CHC-C1C	2.12	1.41	1.35
30	BM	102	LMG	C4-C3	2.12	1.58	1.52
32	BB	603	LMT	O1B-C4'	2.12	1.49	1.43
22	BC	506	CLA	C4-C3	2.13	1.55	1.50
22	AB	616	CLA	CHC-C1C	2.13	1.41	1.35
30	AE	102	LMG	C7-C8	2.13	1.56	1.50
22	AC	508	CLA	CAA-C2A	2.13	1.58	1.54
22	AB	608	CLA	C5-C3	2.13	1.56	1.51
22	AC	511	CLA	C4-C3	2.13	1.55	1.50
26	AZ	101	BCR	C38-C26	2.13	1.54	1.51
32	AB	625	LMT	O1B-C1B	2.13	1.47	1.41
29	AA	415	SQD	C6-S	2.13	1.81	1.77
26	BZ	101	BCR	C35-C13	2.13	1.55	1.50
32	BI	102	LMT	C4B-C5B	2.13	1.57	1.53
22	AD	404	CLA	C4C-C3C	2.14	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BE	102	LMG	C1-C2	2.14	1.58	1.52
22	BC	511	CLA	CHC-C1C	2.14	1.42	1.35
22	BC	509	CLA	C5-C3	2.14	1.56	1.51
22	BB	613	CLA	C4-C3	2.14	1.55	1.50
22	BB	610	CLA	C1C-C2C	2.14	1.48	1.44
27	BC	517	DGD	C6D-C5D	2.14	1.58	1.51
27	AC	516	DGD	C4D-C3D	2.14	1.58	1.52
27	AC	517	DGD	O3G-C1D	2.15	1.44	1.40
22	BB	615	CLA	C4-C3	2.15	1.55	1.50
22	AC	506	CLA	CHC-C1C	2.15	1.42	1.35
22	AB	606	CLA	CHC-C1C	2.15	1.42	1.35
22	AB	613	CLA	CAA-C2A	2.15	1.58	1.54
27	BH	101	DGD	O6D-C5D	2.15	1.49	1.44
30	AA	416	LMG	C9-C8	2.15	1.56	1.50
30	AI	101	LMG	O1-C1	2.16	1.44	1.40
34	BV	201	HEM	C2A-C3A	2.16	1.44	1.37
22	BC	505	CLA	C4C-C3C	2.16	1.48	1.45
22	BB	613	CLA	CHC-C1C	2.16	1.42	1.35
30	BA	414	LMG	C4-C3	2.16	1.58	1.52
26	BC	514	BCR	C38-C26	2.16	1.54	1.51
22	BB	619	CLA	CHC-C1C	2.16	1.42	1.35
27	AC	516	DGD	O3G-C1D	2.17	1.44	1.40
22	AC	513	CLA	C1C-C2C	2.17	1.48	1.44
22	BC	509	CLA	C4-C3	2.17	1.56	1.50
26	BZ	101	BCR	C38-C26	2.17	1.54	1.51
27	BD	410	DGD	O1G-C1A	2.17	1.39	1.33
23	BA	406	PHO	CHD-C1D	2.17	1.43	1.38
27	AB	626	DGD	C1E-C2E	2.17	1.59	1.52
22	BB	610	CLA	C2-C3	2.17	1.37	1.33
32	BM	101	LMT	O5'-C1'	2.18	1.47	1.41
30	AI	101	LMG	C1-C2	2.18	1.59	1.52
34	AV	201	HEM	FE-NB	2.18	2.09	1.97
29	AD	409	SQD	C8-C7	2.18	1.57	1.50
22	AC	507	CLA	CHC-C1C	2.18	1.42	1.35
32	AM	102	LMT	O5'-C1'	2.18	1.47	1.41
30	AB	622	LMG	C4-C3	2.18	1.58	1.52
22	AB	609	CLA	CHC-C1C	2.18	1.42	1.35
22	BC	512	CLA	C4-C3	2.19	1.56	1.50
23	BD	403	PHO	C4-C3	2.19	1.56	1.50
32	BT	101	LMT	O1B-C4'	2.19	1.49	1.43
27	BB	602	DGD	O1G-C1A	2.19	1.39	1.33
27	AC	517	DGD	C6D-C5D	2.19	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BB	616	CLA	CAA-C2A	2.19	1.58	1.54
22	AC	507	CLA	C4-C3	2.19	1.56	1.50
22	AB	616	CLA	C4-C3	2.19	1.56	1.50
29	BA	401	SQD	C44-C45	2.19	1.56	1.50
22	BC	503	CLA	CHC-C1C	2.19	1.42	1.35
22	BC	509	CLA	CHC-C1C	2.19	1.42	1.35
22	AC	511	CLA	CHC-C1C	2.19	1.42	1.35
23	BD	403	PHO	CHC-C1C	2.20	1.43	1.38
27	AB	626	DGD	C3E-C2E	2.20	1.58	1.52
22	BC	507	CLA	CHC-C1C	2.20	1.42	1.35
22	AB	612	CLA	CAA-C2A	2.20	1.58	1.54
27	AC	516	DGD	C4D-C5D	2.20	1.57	1.53
22	BC	509	CLA	C4C-C3C	2.20	1.49	1.45
32	AB	624	LMT	C4B-C5B	2.20	1.57	1.53
32	BB	603	LMT	C4B-C5B	2.20	1.57	1.53
29	BA	413	SQD	C6-S	2.20	1.81	1.77
32	BB	625	LMT	C3B-C2B	2.20	1.58	1.52
22	BB	613	CLA	C4C-C3C	2.20	1.49	1.45
22	BB	604	CLA	C4-C3	2.21	1.56	1.50
30	BA	414	LMG	O6-C5	2.21	1.49	1.44
22	AC	510	CLA	CHC-C1C	2.21	1.42	1.35
27	BB	602	DGD	O5D-C6D	2.21	1.47	1.43
24	BJ	101	PL9	C3-C4	2.21	1.53	1.49
27	BD	410	DGD	C3E-C2E	2.21	1.58	1.52
32	BB	626	LMT	C4B-C5B	2.21	1.57	1.53
30	AB	621	LMG	O6-C5	2.22	1.49	1.44
27	AA	410	DGD	C1E-C2E	2.22	1.59	1.52
22	BC	510	CLA	C4-C3	2.22	1.56	1.50
22	AC	510	CLA	CAA-C2A	2.22	1.58	1.54
22	BB	607	CLA	C4-C3	2.23	1.56	1.50
22	BC	510	CLA	CAA-C2A	2.23	1.58	1.54
22	AB	605	CLA	CHC-C1C	2.23	1.42	1.35
30	AD	407	LMG	O6-C5	2.23	1.49	1.44
22	AC	503	CLA	CHC-C1C	2.23	1.42	1.35
22	AB	607	CLA	C1C-C2C	2.23	1.49	1.44
34	AE	101	HEM	FE-NB	2.23	2.09	1.97
22	AB	610	CLA	C4C-C3C	2.24	1.49	1.45
26	AD	406	BCR	C38-C26	2.24	1.54	1.51
34	BE	101	HEM	CAD-CBD	2.24	1.63	1.52
27	BH	101	DGD	C3D-C2D	2.25	1.58	1.52
22	BC	513	CLA	C4-C3	2.25	1.56	1.50
27	BC	516	DGD	C4D-C5D	2.25	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AE	102	LMG	O7-C10	2.25	1.41	1.34
22	AA	406	CLA	CHC-C1C	2.26	1.42	1.35
26	AB	619	BCR	C24-C23	2.26	1.39	1.33
30	BB	624	LMG	C4-C3	2.26	1.58	1.52
26	BJ	102	BCR	C3-C4	2.26	1.59	1.52
27	BA	411	DGD	C3E-C2E	2.26	1.58	1.52
32	AT	101	LMT	O1B-C4'	2.26	1.49	1.43
32	BT	101	LMT	O1B-C1B	2.27	1.47	1.41
27	AD	410	DGD	O6E-C5E	2.27	1.50	1.44
27	AC	518	DGD	O6E-C1E	2.27	1.47	1.41
22	BB	615	CLA	CAA-C2A	2.27	1.58	1.54
22	BC	508	CLA	CAA-C2A	2.28	1.58	1.54
27	AC	516	DGD	O6E-C1E	2.28	1.47	1.41
27	AH	102	DGD	O6E-C1E	2.29	1.47	1.41
24	BA	408	PL9	C2-C1	2.29	1.51	1.44
22	AB	615	CLA	CHC-C1C	2.29	1.42	1.35
22	AB	615	CLA	CAA-C2A	2.29	1.58	1.54
32	BD	411	LMT	C4B-C5B	2.29	1.57	1.53
27	AB	626	DGD	O5D-C6D	2.30	1.47	1.43
27	BC	516	DGD	O6E-C1E	2.30	1.47	1.41
27	AD	410	DGD	C1E-C2E	2.30	1.59	1.52
22	BC	513	CLA	C1C-C2C	2.30	1.49	1.44
22	AC	509	CLA	CHC-C1C	2.31	1.42	1.35
22	BB	611	CLA	C5-C3	2.31	1.56	1.51
22	BC	513	CLA	CHC-C1C	2.32	1.42	1.35
34	BE	101	HEM	FE-NB	2.32	2.09	1.97
23	AA	405	PHO	C3B-C4B	2.32	1.48	1.43
32	BB	625	LMT	C1B-C2B	2.32	1.59	1.52
32	BB	625	LMT	O1'-C1'	2.32	1.44	1.40
22	AC	505	CLA	C4C-C3C	2.33	1.49	1.45
22	BC	510	CLA	CHC-C1C	2.33	1.42	1.35
22	AB	601	CLA	C4-C3	2.33	1.56	1.50
30	BB	623	LMG	O1-C1	2.33	1.44	1.40
22	AC	502	CLA	CHC-C1C	2.33	1.42	1.35
27	AH	102	DGD	O6D-C1D	2.33	1.47	1.41
27	AB	626	DGD	C4D-C3D	2.33	1.58	1.52
27	BC	518	DGD	O6E-C1E	2.33	1.47	1.41
29	AA	412	SQD	O5-C1	2.33	1.47	1.41
22	BB	618	CLA	CAA-C2A	2.34	1.58	1.54
22	AA	402	CLA	CHC-C1C	2.34	1.42	1.35
22	AD	404	CLA	CHC-C1C	2.34	1.42	1.35
32	BB	625	LMT	O5B-C5B	2.34	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	625	LMT	C4B-C3B	2.35	1.58	1.52
32	AB	625	LMT	C4B-C5B	2.35	1.58	1.53
32	AB	627	LMT	O1B-C4'	2.35	1.49	1.43
30	BC	520	LMG	C3-C2	2.36	1.58	1.52
27	BA	411	DGD	O6E-C5E	2.36	1.50	1.44
30	BC	520	LMG	O8-C28	2.36	1.40	1.33
30	BC	520	LMG	O1-C1	2.36	1.44	1.40
27	BD	410	DGD	O6E-C5E	2.36	1.50	1.44
29	BA	401	SQD	C24-C23	2.37	1.57	1.50
29	BD	409	SQD	C44-C45	2.37	1.57	1.50
32	AB	624	LMT	O1'-C1'	2.37	1.44	1.40
30	BD	407	LMG	O6-C5	2.37	1.50	1.44
24	AJ	101	PL9	C3-C4	2.37	1.53	1.49
26	BX	101	BCR	C5-C6	2.37	1.38	1.34
30	AC	519	LMG	C4-C3	2.38	1.58	1.52
22	BD	402	CLA	CHC-C1C	2.38	1.42	1.35
30	AD	407	LMG	O1-C1	2.38	1.44	1.40
27	AH	102	DGD	C4E-C3E	2.38	1.58	1.52
27	BD	410	DGD	C4D-C5D	2.38	1.58	1.53
30	BC	519	LMG	C4-C3	2.39	1.58	1.52
30	BA	414	LMG	O1-C1	2.39	1.44	1.40
30	BD	407	LMG	O1-C1	2.39	1.44	1.40
23	BA	406	PHO	CHC-C1C	2.40	1.43	1.38
23	BD	403	PHO	C3B-C4B	2.40	1.48	1.43
30	AB	621	LMG	O7-C10	2.40	1.41	1.34
30	AB	621	LMG	C4-C3	2.40	1.58	1.52
22	BB	615	CLA	CHC-C1C	2.40	1.42	1.35
29	BD	409	SQD	C8-C7	2.40	1.57	1.50
27	BD	410	DGD	C1E-C2E	2.40	1.59	1.52
22	BB	606	CLA	C4-C3	2.40	1.56	1.50
30	BB	624	LMG	O6-C5	2.41	1.50	1.44
22	AD	402	CLA	C4C-C3C	2.41	1.49	1.45
27	BD	410	DGD	C3D-C2D	2.41	1.58	1.52
22	AD	402	CLA	C1C-C2C	2.41	1.49	1.44
32	AB	625	LMT	O5B-C1B	2.41	1.48	1.41
22	BB	611	CLA	C4-C3	2.41	1.56	1.50
22	AC	508	CLA	C4-C3	2.41	1.56	1.50
30	AA	416	LMG	C4-C3	2.41	1.58	1.52
30	BE	102	LMG	O7-C10	2.42	1.41	1.34
22	BC	502	CLA	CHC-C1C	2.42	1.42	1.35
22	BC	504	CLA	C4-C3	2.42	1.56	1.50
22	BB	610	CLA	CHC-C1C	2.42	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AA	416	LMG	O8-C28	2.42	1.40	1.33
23	AD	403	PHO	C4-C3	2.42	1.56	1.50
32	BB	626	LMT	O5'-C1'	2.42	1.48	1.41
27	BH	101	DGD	C1E-C2E	2.42	1.59	1.52
24	AJ	101	PL9	C2-C1	2.42	1.51	1.44
30	AC	520	LMG	C3-C2	2.42	1.58	1.52
26	AB	620	BCR	C14-C13	2.43	1.39	1.35
27	AC	518	DGD	O5D-C1E	2.43	1.44	1.40
29	AD	409	SQD	C44-C45	2.43	1.57	1.50
22	BB	613	CLA	CAA-C2A	2.43	1.59	1.54
30	BE	102	LMG	C4-C5	2.43	1.58	1.53
27	AD	410	DGD	O1G-C1A	2.43	1.40	1.33
22	BB	612	CLA	CHC-C1C	2.43	1.42	1.35
27	AB	626	DGD	C1D-C2D	2.43	1.59	1.52
22	AB	607	CLA	CHC-C1C	2.43	1.42	1.35
22	AB	610	CLA	C4-C3	2.44	1.56	1.50
22	BB	618	CLA	CHC-C1C	2.44	1.42	1.35
27	BC	517	DGD	C4D-C5D	2.44	1.58	1.53
30	AA	413	LMG	O1-C1	2.44	1.44	1.40
22	BC	508	CLA	C4-C3	2.44	1.56	1.50
22	AB	607	CLA	C2-C3	2.44	1.37	1.33
22	BD	404	CLA	CHC-C1C	2.45	1.43	1.35
32	BB	626	LMT	O5B-C1B	2.46	1.48	1.41
27	BA	411	DGD	C1E-C2E	2.46	1.59	1.52
27	AH	102	DGD	O3G-C1D	2.46	1.44	1.40
22	AB	612	CLA	CHC-C1C	2.46	1.43	1.35
22	AA	403	CLA	C5-C3	2.46	1.56	1.51
30	AC	520	LMG	O8-C28	2.46	1.40	1.33
27	BH	101	DGD	C4E-C3E	2.46	1.58	1.52
30	BM	102	LMG	C4-C5	2.46	1.58	1.53
27	BC	516	DGD	C4D-C3D	2.47	1.58	1.52
22	BB	619	CLA	C4-C3	2.47	1.56	1.50
22	AB	603	CLA	C4-C3	2.47	1.56	1.50
30	AD	407	LMG	C4-C3	2.47	1.58	1.52
30	BE	102	LMG	O6-C5	2.47	1.50	1.44
34	AV	201	HEM	C2A-C3A	2.47	1.45	1.37
30	AD	407	LMG	O6-C1	2.48	1.48	1.41
27	BB	602	DGD	C3E-C2E	2.48	1.58	1.52
32	AB	627	LMT	O1'-C1'	2.48	1.44	1.40
24	BJ	101	PL9	C7-C8	2.48	1.54	1.50
27	BH	101	DGD	O6E-C1E	2.48	1.48	1.41
27	BC	518	DGD	O6D-C5D	2.49	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	602	DGD	O6E-C5E	2.49	1.50	1.44
29	BL	101	SQD	O6-C1	2.49	1.44	1.40
27	BA	411	DGD	O2G-C1B	2.49	1.41	1.34
27	BC	517	DGD	O6D-C5D	2.49	1.50	1.44
30	BB	623	LMG	O6-C5	2.49	1.50	1.44
30	AE	102	LMG	O6-C5	2.50	1.50	1.44
30	BC	519	LMG	C4-C5	2.50	1.58	1.53
22	AD	402	CLA	CHC-C1C	2.50	1.43	1.35
27	AD	410	DGD	C3E-C2E	2.50	1.59	1.52
27	BB	602	DGD	O6D-C1D	2.50	1.48	1.41
27	AB	626	DGD	O6E-C5E	2.50	1.50	1.44
27	BH	101	DGD	O3G-C1D	2.50	1.44	1.40
27	AC	516	DGD	C4E-C3E	2.50	1.59	1.52
22	BA	407	CLA	C4-C3	2.50	1.56	1.50
30	BC	520	LMG	C9-C8	2.51	1.57	1.50
27	AD	410	DGD	C4D-C5D	2.51	1.58	1.53
22	AC	513	CLA	C4-C3	2.51	1.56	1.50
30	AB	623	LMG	C4-C3	2.51	1.59	1.52
30	AB	621	LMG	O1-C1	2.51	1.44	1.40
22	BB	606	CLA	CAA-C2A	2.51	1.59	1.54
22	BC	512	CLA	CHC-C1C	2.51	1.43	1.35
22	AB	602	CLA	CHC-C1C	2.52	1.43	1.35
29	BA	413	SQD	O5-C1	2.52	1.48	1.41
22	BC	508	CLA	CHC-C1C	2.52	1.43	1.35
22	AC	513	CLA	CHC-C1C	2.52	1.43	1.35
22	BB	605	CLA	CHC-C1C	2.52	1.43	1.35
22	AC	512	CLA	CHC-C1C	2.53	1.43	1.35
30	AC	520	LMG	O7-C10	2.53	1.41	1.34
34	BE	101	HEM	CHC-C1C	2.53	1.42	1.36
27	BD	410	DGD	C4D-C3D	2.53	1.59	1.52
30	AD	408	LMG	O6-C5	2.53	1.50	1.44
22	AC	504	CLA	CHC-C1C	2.54	1.43	1.35
27	BD	410	DGD	C1D-C2D	2.54	1.60	1.52
22	BB	607	CLA	CHC-C1C	2.54	1.43	1.35
30	AB	623	LMG	O6-C5	2.54	1.50	1.44
30	AC	520	LMG	C9-C8	2.54	1.57	1.50
22	AB	604	CLA	CHC-C1C	2.54	1.43	1.35
22	AB	616	CLA	C2-C3	2.55	1.38	1.33
27	AC	518	DGD	C4E-C3E	2.55	1.59	1.52
27	AC	516	DGD	O6D-C1D	2.55	1.48	1.41
27	AC	517	DGD	C4D-C5D	2.55	1.58	1.53
29	AF	101	SQD	C6-S	2.56	1.81	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BI	101	LMG	C1-C2	2.56	1.60	1.52
32	AT	101	LMT	O1'-C1'	2.57	1.44	1.40
26	BB	622	BCR	C14-C13	2.57	1.39	1.35
27	AD	410	DGD	C4D-C3D	2.57	1.59	1.52
32	BB	625	LMT	C4B-C5B	2.58	1.58	1.53
30	AI	101	LMG	O7-C10	2.58	1.42	1.34
27	BA	411	DGD	O6E-C1E	2.58	1.48	1.41
27	AD	410	DGD	O2G-C1B	2.58	1.42	1.34
27	BC	516	DGD	O6D-C5D	2.58	1.50	1.44
26	AH	101	BCR	C5-C6	2.58	1.38	1.34
27	AC	517	DGD	O6D-C5D	2.59	1.50	1.44
30	AB	622	LMG	O6-C5	2.59	1.50	1.44
22	BC	504	CLA	CHC-C1C	2.59	1.43	1.35
27	AC	516	DGD	O6D-C5D	2.59	1.50	1.44
26	BD	406	BCR	C38-C26	2.59	1.55	1.51
29	BD	409	SQD	O5-C1	2.60	1.48	1.41
26	AB	619	BCR	C14-C13	2.60	1.39	1.35
22	AB	614	CLA	CHC-C1C	2.60	1.43	1.35
34	BE	101	HEM	C2A-C3A	2.60	1.45	1.37
26	BX	101	BCR	C38-C26	2.61	1.55	1.51
30	BI	101	LMG	O7-C10	2.61	1.42	1.34
30	BD	408	LMG	O6-C5	2.61	1.50	1.44
30	AB	623	LMG	C3-C2	2.61	1.59	1.52
22	AC	505	CLA	C1C-C2C	2.61	1.49	1.44
26	AH	101	BCR	C38-C26	2.61	1.55	1.51
23	BA	406	PHO	C4-C3	2.62	1.57	1.50
22	AC	509	CLA	CAA-C2A	2.62	1.59	1.54
22	BC	509	CLA	CAA-C2A	2.62	1.59	1.54
26	BJ	102	BCR	C14-C13	2.63	1.39	1.35
22	BA	403	CLA	CHC-C1C	2.64	1.43	1.35
34	BE	101	HEM	C4C-NC	2.64	1.39	1.36
27	AA	410	DGD	C3E-C2E	2.64	1.59	1.52
27	BD	410	DGD	O2G-C1B	2.64	1.42	1.34
22	AA	406	CLA	C4-C3	2.65	1.57	1.50
32	AI	102	LMT	O5'-C1'	2.65	1.48	1.41
29	BB	601	SQD	O6-C1	2.65	1.44	1.40
24	BJ	101	PL9	C2-C1	2.65	1.52	1.44
30	BB	624	LMG	C4-C5	2.66	1.58	1.53
30	AB	621	LMG	O6-C1	2.66	1.48	1.41
27	AH	102	DGD	C4E-C5E	2.66	1.58	1.53
27	AC	518	DGD	O6D-C5D	2.66	1.51	1.44
34	AE	101	HEM	CHC-C1C	2.66	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AC	519	LMG	C4-C5	2.66	1.58	1.53
26	AC	514	BCR	C2-C1	2.67	1.60	1.54
29	AF	101	SQD	O5-C1	2.67	1.48	1.41
22	BC	505	CLA	CHC-C1C	2.67	1.43	1.35
30	AB	622	LMG	O1-C1	2.68	1.45	1.40
27	AB	626	DGD	C3D-C2D	2.68	1.59	1.52
26	AJ	102	BCR	C14-C13	2.68	1.39	1.35
34	BE	101	HEM	CMA-C3A	2.68	1.57	1.51
27	BC	516	DGD	C4E-C3E	2.68	1.59	1.52
30	BB	623	LMG	C4-C3	2.69	1.59	1.52
30	AB	622	LMG	C4-C5	2.70	1.58	1.53
32	AB	627	LMT	O5'-C1'	2.71	1.48	1.41
32	BT	101	LMT	O1'-C1'	2.71	1.45	1.40
27	AH	102	DGD	C1E-C2E	2.71	1.60	1.52
23	AD	403	PHO	C3B-C4B	2.71	1.49	1.43
26	AK	102	BCR	C14-C13	2.71	1.39	1.35
30	AM	101	LMG	C4-C5	2.71	1.58	1.53
26	AJ	102	BCR	C2-C1	2.72	1.60	1.54
27	AC	518	DGD	O3G-C1D	2.72	1.45	1.40
30	AA	416	LMG	C3-C2	2.73	1.59	1.52
30	BC	520	LMG	O7-C10	2.73	1.42	1.34
30	BB	623	LMG	O7-C10	2.73	1.42	1.34
22	AB	606	CLA	CAA-C2A	2.74	1.59	1.54
22	BB	617	CLA	CHC-C1C	2.74	1.43	1.35
32	AB	625	LMT	O5'-C1'	2.74	1.48	1.41
29	BA	413	SQD	O3-C3	2.74	1.49	1.43
29	BA	401	SQD	O5-C1	2.74	1.48	1.41
30	BC	519	LMG	O6-C5	2.74	1.51	1.44
27	AB	626	DGD	O2G-C1B	2.75	1.42	1.34
22	AB	603	CLA	CAA-C2A	2.75	1.59	1.54
22	AC	508	CLA	CHC-C1C	2.75	1.43	1.35
22	AC	502	CLA	CAA-C2A	2.75	1.59	1.54
32	AT	101	LMT	O1B-C1B	2.76	1.49	1.41
22	AB	611	CLA	CAA-C2A	2.76	1.59	1.54
32	AI	102	LMT	O5B-C1B	2.77	1.48	1.41
32	BI	102	LMT	O5B-C1B	2.77	1.48	1.41
26	AH	101	BCR	C14-C13	2.77	1.39	1.35
26	BB	622	BCR	C26-C25	2.77	1.38	1.34
34	AE	101	HEM	CMA-C3A	2.77	1.57	1.51
32	BB	603	LMT	O5'-C1'	2.78	1.48	1.41
27	BC	516	DGD	O3G-C1D	2.78	1.45	1.40
27	AA	410	DGD	C4E-C5E	2.78	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	AC	519	LMG	O6-C5	2.78	1.51	1.44
32	AD	411	LMT	C4B-C5B	2.78	1.59	1.53
29	BF	101	SQD	C44-C45	2.78	1.58	1.50
22	BB	609	CLA	CAA-C2A	2.79	1.59	1.54
30	BD	407	LMG	O6-C1	2.79	1.49	1.41
30	BD	407	LMG	C4-C3	2.79	1.59	1.52
30	BI	101	LMG	C3-C2	2.79	1.59	1.52
26	AK	102	BCR	C26-C25	2.80	1.38	1.34
30	BM	102	LMG	C3-C2	2.80	1.59	1.52
27	BC	517	DGD	O3G-C1D	2.80	1.45	1.40
26	BA	410	BCR	C29-C30	2.81	1.60	1.54
22	AC	505	CLA	CHC-C1C	2.81	1.44	1.35
22	AA	402	CLA	CAA-C2A	2.82	1.59	1.54
34	AE	101	HEM	C2A-C3A	2.82	1.46	1.37
29	AA	412	SQD	C6-S	2.82	1.82	1.77
32	AD	411	LMT	O5B-C1B	2.82	1.49	1.41
27	AD	410	DGD	C3D-C2D	2.83	1.59	1.52
30	BB	624	LMG	O1-C1	2.83	1.45	1.40
22	AC	511	CLA	CAA-C2A	2.84	1.59	1.54
26	AT	102	BCR	C26-C25	2.84	1.38	1.34
27	AD	410	DGD	C4E-C3E	2.84	1.59	1.52
34	AV	201	HEM	CMA-C3A	2.84	1.57	1.51
29	AF	101	SQD	C44-C45	2.84	1.58	1.50
27	AD	410	DGD	C1D-C2D	2.85	1.61	1.52
32	AB	624	LMT	O5B-C1B	2.85	1.49	1.41
26	AC	515	BCR	C29-C30	2.86	1.61	1.54
22	AC	506	CLA	CAA-C2A	2.86	1.59	1.54
32	AD	411	LMT	O5'-C1'	2.86	1.49	1.41
26	AT	102	BCR	C29-C30	2.86	1.61	1.54
27	AC	518	DGD	O6D-C1D	2.86	1.49	1.41
32	BD	411	LMT	O5B-C1B	2.86	1.49	1.41
29	AA	415	SQD	O5-C1	2.87	1.49	1.41
30	AM	101	LMG	C3-C2	2.87	1.59	1.52
32	BI	102	LMT	O5'-C1'	2.87	1.49	1.41
29	AF	101	SQD	O3-C3	2.87	1.49	1.43
22	BB	619	CLA	C2-C3	2.88	1.38	1.33
27	BB	602	DGD	C4D-C3D	2.88	1.59	1.52
26	BK	102	BCR	C14-C13	2.88	1.39	1.35
30	AA	416	LMG	O6-C5	2.89	1.51	1.44
28	AA	411	LHG	O8-C23	2.89	1.42	1.33
27	AA	410	DGD	O6E-C1E	2.89	1.49	1.41
30	AI	101	LMG	C3-C2	2.89	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BB	601	SQD	O3-C3	2.89	1.49	1.43
32	AB	627	LMT	O5B-C1B	2.90	1.49	1.41
29	AF	101	SQD	C8-C7	2.90	1.59	1.50
30	BB	624	LMG	O6-C1	2.92	1.49	1.41
29	BA	401	SQD	O6-C1	2.92	1.45	1.40
27	AB	626	DGD	O6D-C1D	2.92	1.49	1.41
26	AC	514	BCR	C5-C6	2.92	1.39	1.34
28	BA	412	LHG	O8-C23	2.93	1.42	1.33
30	AA	416	LMG	O1-C1	2.93	1.45	1.40
29	BF	101	SQD	O5-C1	2.93	1.49	1.41
22	BB	617	CLA	CAA-C2A	2.93	1.60	1.54
22	AC	505	CLA	CAA-C2A	2.93	1.60	1.54
30	BE	102	LMG	O6-C1	2.94	1.49	1.41
27	BD	410	DGD	C4E-C3E	2.94	1.60	1.52
27	BD	410	DGD	C4E-C5E	2.94	1.59	1.53
30	BB	623	LMG	O6-C1	2.94	1.49	1.41
22	AB	607	CLA	CAA-C2A	2.94	1.60	1.54
22	AB	616	CLA	CAA-C2A	2.95	1.60	1.54
22	BD	404	CLA	CAA-C2A	2.95	1.60	1.54
22	BC	504	CLA	CAA-C2A	2.96	1.60	1.54
32	BD	411	LMT	O5'-C1'	2.96	1.49	1.41
29	BL	101	SQD	O5-C1	2.96	1.49	1.41
27	AC	517	DGD	O6D-C1D	2.97	1.49	1.41
22	BB	619	CLA	CAA-C2A	2.98	1.60	1.54
27	AA	410	DGD	C4E-C3E	2.98	1.60	1.52
26	BK	102	BCR	C2-C1	2.98	1.61	1.54
22	BB	612	CLA	CAA-C2A	2.99	1.60	1.54
32	BB	625	LMT	O5B-C1B	2.99	1.49	1.41
34	BE	101	HEM	FE-NC	2.99	2.07	1.95
29	AD	409	SQD	C6-S	2.99	1.82	1.77
30	AB	622	LMG	O6-C1	2.99	1.49	1.41
29	BF	101	SQD	O3-C3	3.00	1.50	1.43
26	AD	406	BCR	C2-C1	3.00	1.61	1.54
29	BF	101	SQD	C6-S	3.00	1.82	1.77
29	BF	101	SQD	C8-C7	3.00	1.59	1.50
24	BJ	101	PL9	C6-C1	3.01	1.54	1.48
32	AB	625	LMT	O1'-C1'	3.01	1.45	1.40
22	BD	402	CLA	CAA-C2A	3.01	1.60	1.54
32	BT	101	LMT	O5B-C1B	3.01	1.49	1.41
30	AE	102	LMG	O1-C1	3.01	1.45	1.40
32	BB	603	LMT	O5B-C1B	3.02	1.49	1.41
24	AJ	101	PL9	C6-C1	3.02	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AB	605	CLA	CAA-C2A	3.02	1.60	1.54
22	BA	403	CLA	CAA-C2A	3.02	1.60	1.54
26	AB	618	BCR	C26-C25	3.02	1.39	1.34
26	AA	409	BCR	C29-C30	3.03	1.61	1.54
26	AH	101	BCR	C2-C1	3.03	1.61	1.54
26	BK	102	BCR	C26-C25	3.03	1.39	1.34
32	BB	626	LMT	O1'-C1'	3.03	1.45	1.40
26	AK	102	BCR	C2-C1	3.03	1.61	1.54
22	AB	609	CLA	CAA-C2A	3.03	1.60	1.54
22	BB	608	CLA	CAA-C2A	3.04	1.60	1.54
34	AV	201	HEM	C4C-NC	3.04	1.39	1.36
26	AB	619	BCR	C2-C1	3.05	1.61	1.54
26	BB	621	BCR	C2-C1	3.05	1.61	1.54
26	BB	620	BCR	C2-C1	3.05	1.61	1.54
26	AC	515	BCR	C26-C25	3.05	1.39	1.34
22	AD	402	CLA	CAA-C2A	3.05	1.60	1.54
30	BC	520	LMG	O6-C5	3.05	1.52	1.44
22	BA	405	CLA	CAA-C2A	3.05	1.60	1.54
30	AI	101	LMG	O6-C5	3.06	1.52	1.44
29	AA	412	SQD	O3-C3	3.06	1.50	1.43
27	BA	411	DGD	C4E-C3E	3.06	1.60	1.52
26	BC	514	BCR	C5-C6	3.06	1.39	1.34
22	BC	506	CLA	CAA-C2A	3.07	1.60	1.54
27	BB	602	DGD	O2G-C1B	3.07	1.43	1.34
27	AA	410	DGD	O6D-C1D	3.07	1.49	1.41
26	AZ	101	BCR	C5-C6	3.08	1.39	1.34
30	AM	101	LMG	O6-C5	3.08	1.52	1.44
29	BA	401	SQD	C6-S	3.09	1.82	1.77
26	BB	620	BCR	C29-C30	3.09	1.61	1.54
27	BA	411	DGD	C4E-C5E	3.09	1.59	1.53
22	AB	604	CLA	CAA-C2A	3.09	1.60	1.54
30	AI	101	LMG	C4-C5	3.10	1.59	1.53
22	BC	505	CLA	CAA-C2A	3.10	1.60	1.54
30	AC	519	LMG	O6-C1	3.11	1.49	1.41
29	BB	601	SQD	O5-C1	3.11	1.49	1.41
24	AJ	101	PL9	C7-C3	3.11	1.53	1.51
29	BD	409	SQD	C6-S	3.11	1.82	1.77
26	AZ	101	BCR	C2-C1	3.11	1.61	1.54
26	BB	620	BCR	C5-C6	3.11	1.39	1.34
22	AC	504	CLA	CAA-C2A	3.11	1.60	1.54
26	AC	515	BCR	C2-C1	3.11	1.61	1.54
26	AB	617	BCR	C2-C1	3.12	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BB	602	DGD	O6D-C5D	3.12	1.52	1.44
26	BC	515	BCR	C29-C30	3.12	1.61	1.54
29	BA	401	SQD	O3-C3	3.12	1.50	1.43
29	AD	409	SQD	O5-C1	3.12	1.49	1.41
29	AA	415	SQD	O3-C3	3.13	1.50	1.43
30	BI	101	LMG	C4-C5	3.13	1.59	1.53
26	BZ	101	BCR	C5-C6	3.13	1.39	1.34
26	BA	410	BCR	C2-C1	3.13	1.61	1.54
30	BE	102	LMG	O1-C1	3.14	1.45	1.40
22	BB	607	CLA	CAA-C2A	3.14	1.60	1.54
27	AA	410	DGD	C4D-C5D	3.14	1.59	1.53
34	AV	201	HEM	CAA-C2A	3.15	1.57	1.52
24	BJ	101	PL9	C7-C3	3.15	1.53	1.51
26	AB	618	BCR	C29-C30	3.15	1.61	1.54
30	AB	623	LMG	O1-C1	3.15	1.45	1.40
27	BA	411	DGD	O3G-C1D	3.16	1.45	1.40
26	BJ	102	BCR	C2-C1	3.16	1.61	1.54
32	AT	101	LMT	O5B-C1B	3.16	1.49	1.41
27	AA	410	DGD	O3G-C1D	3.16	1.45	1.40
34	AE	101	HEM	FE-NC	3.17	2.08	1.95
27	BC	516	DGD	O6D-C1D	3.17	1.50	1.41
26	AC	514	BCR	C29-C30	3.17	1.61	1.54
32	BB	603	LMT	O1B-C1B	3.17	1.50	1.41
30	AC	520	LMG	C4-C5	3.18	1.59	1.53
30	BC	519	LMG	O1-C1	3.19	1.45	1.40
27	BB	602	DGD	O5D-C1E	3.20	1.45	1.40
22	AB	614	CLA	CAA-C2A	3.20	1.60	1.54
28	BA	412	LHG	O7-C7	3.20	1.43	1.34
27	AB	626	DGD	C4E-C5E	3.20	1.59	1.53
27	AD	410	DGD	C4E-C5E	3.20	1.59	1.53
26	AB	617	BCR	C29-C30	3.21	1.61	1.54
34	AV	201	HEM	FE-NC	3.21	2.08	1.95
26	BD	406	BCR	C2-C1	3.21	1.61	1.54
34	BV	201	HEM	CAA-C2A	3.21	1.57	1.52
26	BK	102	BCR	C29-C30	3.21	1.61	1.54
29	AA	412	SQD	O5-C5	3.22	1.52	1.44
28	BA	412	LHG	P-O6	3.22	1.73	1.59
27	AB	626	DGD	O3G-C1D	3.22	1.46	1.40
26	AA	409	BCR	C5-C6	3.22	1.39	1.34
30	AC	520	LMG	O6-C5	3.23	1.52	1.44
29	BL	101	SQD	O3-C3	3.23	1.50	1.43
30	AA	416	LMG	C4-C5	3.23	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	BD	410	DGD	O5D-C1E	3.24	1.46	1.40
27	BD	410	DGD	O6E-C1E	3.24	1.50	1.41
22	AA	404	CLA	CAA-C2A	3.24	1.60	1.54
30	BC	519	LMG	O6-C1	3.25	1.50	1.41
34	AE	101	HEM	C4C-NC	3.25	1.40	1.36
30	BA	414	LMG	O6-C1	3.26	1.50	1.41
30	AC	519	LMG	O1-C1	3.26	1.46	1.40
30	AD	408	LMG	O6-C1	3.26	1.50	1.41
29	BA	413	SQD	O48-C23	3.26	1.43	1.33
27	AB	626	DGD	O6E-C1E	3.27	1.50	1.41
26	BB	622	BCR	C2-C1	3.27	1.62	1.54
24	AA	407	PL9	C7-C3	3.28	1.54	1.51
26	BC	514	BCR	C2-C1	3.28	1.62	1.54
22	BC	511	CLA	CAA-C2A	3.28	1.60	1.54
26	AT	102	BCR	C2-C1	3.28	1.62	1.54
26	BC	514	BCR	C29-C30	3.28	1.62	1.54
29	AF	101	SQD	C1-C2	3.28	1.62	1.52
22	AD	404	CLA	CAA-C2A	3.29	1.60	1.54
34	BV	201	HEM	FE-NC	3.29	2.08	1.95
22	AA	403	CLA	CAA-C2A	3.30	1.60	1.54
26	AK	102	BCR	C29-C30	3.30	1.62	1.54
30	AA	413	LMG	O6-C1	3.30	1.50	1.41
27	BC	518	DGD	O6D-C1D	3.30	1.50	1.41
30	BI	101	LMG	O6-C5	3.31	1.52	1.44
32	AB	627	LMT	O1B-C1B	3.32	1.50	1.41
26	AB	620	BCR	C2-C1	3.32	1.62	1.54
29	BD	409	SQD	O3-C3	3.32	1.50	1.43
27	BA	411	DGD	O6D-C1D	3.32	1.50	1.41
26	AB	618	BCR	C2-C1	3.32	1.62	1.54
22	BC	502	CLA	CAA-C2A	3.33	1.60	1.54
27	BC	518	DGD	O3G-C1D	3.33	1.46	1.40
27	BB	602	DGD	O3G-C1D	3.34	1.46	1.40
27	BC	518	DGD	O5D-C1E	3.34	1.46	1.40
22	BC	513	CLA	CAA-C2A	3.34	1.60	1.54
27	BB	602	DGD	C4D-C5D	3.34	1.60	1.53
30	BM	102	LMG	O6-C5	3.36	1.52	1.44
26	AA	409	BCR	C2-C1	3.37	1.62	1.54
26	BX	101	BCR	C2-C1	3.38	1.62	1.54
29	AF	101	SQD	O6-C1	3.38	1.46	1.40
32	BM	101	LMT	O1'-C1'	3.39	1.46	1.40
27	BD	410	DGD	O6D-C5D	3.39	1.52	1.44
22	BC	501	CLA	CAA-C2A	3.39	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BC	515	BCR	C2-C1	3.39	1.62	1.54
22	AC	501	CLA	CAA-C2A	3.39	1.60	1.54
26	BB	622	BCR	C29-C30	3.39	1.62	1.54
26	BB	620	BCR	C26-C25	3.39	1.39	1.34
27	BC	517	DGD	O6D-C1D	3.40	1.50	1.41
29	BF	101	SQD	O6-C1	3.41	1.46	1.40
26	AB	620	BCR	C29-C30	3.41	1.62	1.54
26	BB	621	BCR	C29-C30	3.41	1.62	1.54
29	AA	415	SQD	O48-C23	3.41	1.43	1.33
30	AB	623	LMG	C4-C5	3.42	1.60	1.53
26	AA	409	BCR	C26-C25	3.42	1.39	1.34
29	AA	415	SQD	O6-C1	3.42	1.46	1.40
22	BB	611	CLA	CAA-C2A	3.45	1.61	1.54
30	AI	101	LMG	C4-C3	3.45	1.61	1.52
30	BD	408	LMG	O6-C1	3.46	1.50	1.41
27	BH	101	DGD	O5D-C1E	3.46	1.46	1.40
26	BZ	101	BCR	C29-C30	3.47	1.62	1.54
26	AZ	101	BCR	C29-C30	3.47	1.62	1.54
28	AA	411	LHG	P-O6	3.48	1.74	1.59
26	BX	101	BCR	C29-C30	3.48	1.62	1.54
27	AB	626	DGD	O6D-C5D	3.48	1.53	1.44
30	BC	520	LMG	O6-C1	3.49	1.50	1.41
29	AD	409	SQD	O3-C3	3.49	1.51	1.43
27	AB	626	DGD	O5D-C1E	3.49	1.46	1.40
30	AM	101	LMG	O6-C1	3.50	1.50	1.41
30	AC	520	LMG	O6-C1	3.50	1.50	1.41
28	AA	411	LHG	O7-C7	3.50	1.44	1.34
30	BC	520	LMG	C4-C3	3.50	1.61	1.52
34	BV	201	HEM	C4C-NC	3.51	1.40	1.36
30	AD	408	LMG	O1-C1	3.51	1.46	1.40
26	AB	619	BCR	C29-C30	3.51	1.62	1.54
29	AA	412	SQD	O7-S	3.51	1.56	1.45
32	BD	411	LMT	O1'-C1'	3.52	1.46	1.40
26	BA	410	BCR	C26-C25	3.53	1.39	1.34
29	BD	409	SQD	O6-C1	3.53	1.46	1.40
30	BC	520	LMG	C4-C5	3.53	1.60	1.53
29	AA	412	SQD	O48-C23	3.53	1.44	1.33
26	BB	620	BCR	C1-C6	3.54	1.58	1.53
27	BB	602	DGD	O6E-C1E	3.55	1.50	1.41
27	BD	410	DGD	O6D-C1D	3.55	1.50	1.41
22	AC	513	CLA	CAA-C2A	3.56	1.61	1.54
26	AT	102	BCR	C30-C25	3.56	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AB	620	BCR	C26-C25	3.57	1.40	1.34
30	AA	416	LMG	O6-C1	3.57	1.51	1.41
26	BZ	101	BCR	C2-C1	3.58	1.62	1.54
29	BB	601	SQD	O47-C7	3.59	1.45	1.34
30	BM	102	LMG	O7-C10	3.59	1.45	1.34
22	AB	608	CLA	CAA-C2A	3.59	1.61	1.54
30	AE	102	LMG	O6-C1	3.60	1.51	1.41
32	AD	411	LMT	O1'-C1'	3.60	1.46	1.40
26	AD	406	BCR	C29-C30	3.61	1.62	1.54
29	BA	413	SQD	O5-C5	3.62	1.53	1.44
27	AB	626	DGD	C4D-C5D	3.62	1.60	1.53
29	BB	601	SQD	O48-C23	3.63	1.44	1.33
30	BM	102	LMG	O6-C1	3.64	1.51	1.41
32	AM	102	LMT	O1'-C1'	3.64	1.46	1.40
22	BB	610	CLA	CAA-C2A	3.65	1.61	1.54
32	AB	624	LMT	O5'-C1'	3.66	1.51	1.41
27	AC	516	DGD	O5D-C1E	3.66	1.46	1.40
22	BC	503	CLA	CAA-C2A	3.66	1.61	1.54
27	BC	516	DGD	O5D-C1E	3.67	1.46	1.40
30	AI	101	LMG	O6-C1	3.67	1.51	1.41
27	BA	411	DGD	C4D-C5D	3.67	1.60	1.53
27	AD	410	DGD	O6E-C1E	3.68	1.51	1.41
26	BC	515	BCR	C26-C25	3.68	1.40	1.34
27	AD	410	DGD	O6D-C1D	3.69	1.51	1.41
29	AA	412	SQD	C1-C2	3.70	1.63	1.52
26	BA	410	BCR	C5-C6	3.70	1.40	1.34
27	AH	102	DGD	O5D-C1E	3.71	1.46	1.40
26	BD	406	BCR	C29-C30	3.72	1.63	1.54
29	BF	101	SQD	C1-C2	3.72	1.63	1.52
29	BL	101	SQD	O48-C23	3.73	1.44	1.33
30	AM	101	LMG	O7-C10	3.74	1.45	1.34
29	AA	415	SQD	C1-C2	3.75	1.63	1.52
30	AB	623	LMG	O6-C1	3.76	1.51	1.41
22	AC	503	CLA	CAA-C2A	3.76	1.61	1.54
29	BL	101	SQD	O47-C7	3.76	1.45	1.34
26	AC	514	BCR	C26-C25	3.76	1.40	1.34
26	AB	617	BCR	C1-C6	3.77	1.59	1.53
26	AH	101	BCR	C29-C30	3.77	1.63	1.54
30	BI	101	LMG	C4-C3	3.79	1.62	1.52
26	AJ	102	BCR	C29-C30	3.80	1.63	1.54
29	BA	413	SQD	C1-C2	3.80	1.63	1.52
32	BI	102	LMT	O1'-C1'	3.81	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	BB	625	LMT	O5'-C1'	3.81	1.51	1.41
26	BB	622	BCR	C5-C6	3.82	1.40	1.34
27	BB	602	DGD	C4E-C5E	3.82	1.61	1.53
27	AD	410	DGD	O6D-C5D	3.83	1.53	1.44
30	BD	408	LMG	O1-C1	3.83	1.47	1.40
30	AC	520	LMG	C4-C3	3.85	1.62	1.52
32	AI	102	LMT	O1'-C1'	3.85	1.47	1.40
26	AB	617	BCR	C5-C6	3.86	1.40	1.34
26	BJ	102	BCR	C29-C30	3.87	1.63	1.54
26	BB	621	BCR	C5-C6	3.87	1.40	1.34
28	BC	521	LHG	O7-C7	3.87	1.45	1.34
28	AC	521	LHG	O7-C7	3.88	1.45	1.34
26	BC	514	BCR	C26-C25	3.88	1.40	1.34
26	AC	515	BCR	C5-C6	3.89	1.40	1.34
26	AD	406	BCR	C1-C6	3.89	1.59	1.53
29	AA	415	SQD	O47-C7	3.90	1.46	1.34
29	AA	415	SQD	O7-S	3.92	1.57	1.45
29	AA	415	SQD	O5-C5	3.92	1.54	1.44
29	AD	409	SQD	O47-C7	3.92	1.46	1.34
26	BD	406	BCR	C5-C6	3.93	1.40	1.34
29	BF	101	SQD	O7-S	3.94	1.57	1.45
34	AE	101	HEM	CAA-C2A	3.94	1.58	1.52
29	BB	601	SQD	C1-C2	3.96	1.64	1.52
27	AA	410	DGD	O5D-C1E	3.96	1.47	1.40
27	BB	602	DGD	C4E-C3E	3.96	1.62	1.52
30	BI	101	LMG	O6-C1	3.97	1.52	1.41
29	BD	409	SQD	O48-C23	3.98	1.45	1.33
29	BA	401	SQD	O48-C23	3.98	1.45	1.33
29	AF	101	SQD	O7-S	4.00	1.57	1.45
29	AD	409	SQD	O6-C1	4.01	1.47	1.40
29	AF	101	SQD	O5-C5	4.01	1.54	1.44
22	BA	404	CLA	CAA-C2A	4.01	1.62	1.54
34	AE	101	HEM	CBC-CAC	4.01	1.52	1.29
26	AB	619	BCR	C5-C6	4.01	1.40	1.34
29	BA	401	SQD	O7-S	4.04	1.57	1.45
29	AA	412	SQD	O47-C7	4.05	1.46	1.34
24	BA	408	PL9	C7-C3	4.06	1.54	1.51
29	AA	412	SQD	O8-S	4.07	1.56	1.46
27	AD	410	DGD	O5D-C1E	4.09	1.47	1.40
26	AT	102	BCR	C5-C6	4.09	1.40	1.34
26	BK	102	BCR	C1-C6	4.10	1.59	1.53
26	BX	101	BCR	C1-C6	4.11	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AB	620	BCR	C5-C6	4.11	1.40	1.34
26	AB	618	BCR	C1-C6	4.13	1.59	1.53
29	BB	601	SQD	C6-S	4.13	1.84	1.77
26	AB	617	BCR	C30-C25	4.14	1.59	1.53
28	BC	521	LHG	O8-C23	4.14	1.45	1.33
26	AA	409	BCR	C30-C25	4.15	1.59	1.53
29	BL	101	SQD	C1-C2	4.16	1.65	1.52
26	AK	102	BCR	C1-C6	4.16	1.59	1.53
34	BE	101	HEM	CBC-CAC	4.16	1.53	1.29
27	AB	626	DGD	C4E-C3E	4.17	1.63	1.52
28	AC	521	LHG	O8-C23	4.17	1.45	1.33
29	BA	413	SQD	O47-C7	4.17	1.46	1.34
29	BA	401	SQD	C1-C2	4.18	1.65	1.52
29	BA	401	SQD	O5-C5	4.19	1.54	1.44
34	BE	101	HEM	CAA-C2A	4.20	1.59	1.52
26	BZ	101	BCR	C26-C25	4.21	1.41	1.34
26	BB	620	BCR	C30-C25	4.22	1.59	1.53
29	BD	409	SQD	O47-C7	4.24	1.47	1.34
28	AA	411	LHG	P-O3	4.27	1.78	1.59
29	AF	101	SQD	O48-C23	4.27	1.46	1.33
34	AV	201	HEM	CBC-CAC	4.27	1.54	1.29
34	BV	201	HEM	CBC-CAC	4.28	1.54	1.29
29	AF	101	SQD	O8-S	4.28	1.57	1.46
26	AD	406	BCR	C5-C6	4.28	1.41	1.34
29	AF	101	SQD	O47-C7	4.29	1.47	1.34
29	BF	101	SQD	O47-C7	4.30	1.47	1.34
29	AD	409	SQD	O7-S	4.30	1.58	1.45
29	BD	409	SQD	C1-C2	4.31	1.65	1.52
29	BA	401	SQD	O47-C7	4.33	1.47	1.34
26	BC	515	BCR	C5-C6	4.34	1.41	1.34
26	AZ	101	BCR	C26-C25	4.35	1.41	1.34
29	BB	601	SQD	O5-C5	4.35	1.55	1.44
29	BA	413	SQD	O7-S	4.36	1.58	1.45
26	BD	406	BCR	C30-C25	4.36	1.60	1.53
29	BL	101	SQD	O7-S	4.37	1.58	1.45
26	AT	102	BCR	C1-C6	4.38	1.60	1.53
26	AC	515	BCR	C1-C6	4.40	1.60	1.53
26	AB	617	BCR	C26-C25	4.41	1.41	1.34
26	AH	101	BCR	C1-C6	4.42	1.60	1.53
28	BA	412	LHG	P-O3	4.42	1.79	1.59
26	AC	515	BCR	C30-C25	4.44	1.60	1.53
29	BF	101	SQD	O48-C23	4.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BL	101	SQD	O5-C5	4.46	1.55	1.44
26	BC	515	BCR	C30-C25	4.48	1.60	1.53
29	BA	413	SQD	O8-S	4.48	1.58	1.46
26	AH	101	BCR	C30-C25	4.50	1.60	1.53
26	AB	618	BCR	C30-C25	4.50	1.60	1.53
26	BB	621	BCR	C1-C6	4.50	1.60	1.53
29	BB	601	SQD	O7-S	4.51	1.59	1.45
30	BM	102	LMG	O1-C1	4.52	1.48	1.40
29	BF	101	SQD	O5-C5	4.52	1.55	1.44
26	AB	618	BCR	C5-C6	4.52	1.41	1.34
30	AM	101	LMG	O1-C1	4.55	1.48	1.40
26	BJ	102	BCR	C1-C6	4.56	1.60	1.53
29	AD	409	SQD	O48-C23	4.57	1.47	1.33
26	AJ	102	BCR	C1-C6	4.61	1.60	1.53
26	BB	622	BCR	C1-C6	4.62	1.60	1.53
26	BA	410	BCR	C30-C25	4.62	1.60	1.53
29	BD	409	SQD	O7-S	4.62	1.59	1.45
26	BA	410	BCR	C1-C6	4.63	1.60	1.53
29	AD	409	SQD	O5-C5	4.64	1.56	1.44
26	BB	621	BCR	C26-C25	4.66	1.41	1.34
26	BX	101	BCR	C30-C25	4.68	1.60	1.53
27	BA	411	DGD	O5D-C1E	4.69	1.48	1.40
26	AD	406	BCR	C30-C25	4.71	1.60	1.53
26	AA	409	BCR	C1-C6	4.72	1.60	1.53
26	AB	619	BCR	C26-C25	4.75	1.41	1.34
29	BF	101	SQD	O8-S	4.78	1.58	1.46
26	BD	406	BCR	C1-C6	4.79	1.60	1.53
29	BD	409	SQD	O5-C5	4.80	1.56	1.44
29	AD	409	SQD	C1-C2	4.81	1.66	1.52
26	AJ	102	BCR	C26-C25	4.83	1.42	1.34
26	AJ	102	BCR	C30-C25	4.84	1.60	1.53
26	AZ	101	BCR	C30-C25	4.93	1.60	1.53
26	AB	620	BCR	C1-C6	5.01	1.60	1.53
29	AA	415	SQD	O8-S	5.02	1.59	1.46
26	AB	619	BCR	C1-C6	5.03	1.60	1.53
26	AC	514	BCR	C30-C25	5.04	1.60	1.53
26	AD	406	BCR	C26-C25	5.04	1.42	1.34
26	BC	515	BCR	C1-C6	5.07	1.61	1.53
29	BD	409	SQD	O8-S	5.11	1.59	1.46
29	BA	401	SQD	O8-S	5.11	1.59	1.46
26	AB	620	BCR	C30-C25	5.12	1.61	1.53
29	AD	409	SQD	O8-S	5.17	1.59	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BB	601	SQD	O8-S	5.20	1.59	1.46
26	AZ	101	BCR	C1-C6	5.22	1.61	1.53
26	BB	621	BCR	C30-C25	5.26	1.61	1.53
26	BK	102	BCR	C5-C6	5.27	1.42	1.34
26	BK	102	BCR	C30-C25	5.29	1.61	1.53
26	AK	102	BCR	C30-C25	5.30	1.61	1.53
26	AC	514	BCR	C1-C6	5.33	1.61	1.53
26	BZ	101	BCR	C30-C25	5.35	1.61	1.53
26	AK	102	BCR	C5-C6	5.44	1.43	1.34
29	BL	101	SQD	O8-S	5.46	1.60	1.46
27	AD	410	DGD	O3G-C1D	5.50	1.50	1.40
26	AB	619	BCR	C30-C25	5.52	1.61	1.53
26	BJ	102	BCR	C26-C25	5.54	1.43	1.34
26	BB	622	BCR	C30-C25	5.56	1.61	1.53
26	BC	514	BCR	C30-C25	5.58	1.61	1.53
26	BD	406	BCR	C26-C25	5.60	1.43	1.34
26	BJ	102	BCR	C30-C25	5.66	1.61	1.53
29	BL	101	SQD	C6-S	5.70	1.86	1.77
26	BJ	102	BCR	C5-C6	5.71	1.43	1.34
26	AH	101	BCR	C26-C25	5.86	1.43	1.34
26	BZ	101	BCR	C1-C6	5.87	1.62	1.53
27	BD	410	DGD	O3G-C1D	5.88	1.50	1.40
26	AJ	102	BCR	C5-C6	5.98	1.43	1.34
26	BC	514	BCR	C1-C6	6.18	1.62	1.53
26	BX	101	BCR	C26-C25	6.19	1.44	1.34
29	AF	101	SQD	C4-C3	6.81	1.70	1.52
29	BF	101	SQD	C4-C3	6.95	1.70	1.52
29	BD	409	SQD	C4-C3	7.22	1.71	1.52
29	AD	409	SQD	C4-C3	7.48	1.72	1.52
28	BA	412	LHG	P-O5	7.56	1.78	1.51
29	AA	415	SQD	C4-C3	7.57	1.72	1.52
29	BA	401	SQD	C4-C3	7.65	1.72	1.52
29	BA	413	SQD	C4-C3	7.68	1.72	1.52
29	AA	412	SQD	C4-C3	7.71	1.72	1.52
29	BB	601	SQD	C4-C3	7.76	1.72	1.52
28	AA	411	LHG	P-O5	7.86	1.79	1.51
29	BL	101	SQD	C4-C3	8.29	1.74	1.52

All (1765) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AJ	102	BCR	C32-C1-C6	-10.35	94.07	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BJ	102	BCR	C32-C1-C6	-10.19	94.32	110.30
26	BJ	102	BCR	C32-C1-C31	-9.18	78.96	108.37
26	AJ	102	BCR	C32-C1-C31	-8.87	79.94	108.37
34	BV	201	HEM	C3C-CAC-CBC	-8.33	111.69	124.46
34	AV	201	HEM	C3C-CAC-CBC	-7.95	112.27	124.46
26	AJ	102	BCR	C32-C1-C2	-7.85	80.67	108.79
34	AE	101	HEM	C3C-CAC-CBC	-7.85	112.42	124.46
26	BJ	102	BCR	C32-C1-C2	-7.77	80.97	108.79
34	BE	101	HEM	C3C-CAC-CBC	-7.61	112.79	124.46
24	BD	405	PL9	C7-C3-C2	-5.96	118.48	123.42
29	BL	101	SQD	O9-S-C6	-5.83	102.02	106.94
24	AD	405	PL9	C7-C3-C2	-5.82	118.59	123.42
29	BD	409	SQD	O9-S-C6	-5.68	102.15	106.94
29	BA	413	SQD	O9-S-C6	-5.65	102.18	106.94
32	BB	625	LMT	C1-O1'-C1'	-5.59	104.17	113.94
32	AB	624	LMT	C1-O1'-C1'	-5.47	104.38	113.94
29	BA	401	SQD	O9-S-C6	-5.46	102.34	106.94
29	BF	101	SQD	O9-S-C6	-5.29	102.48	106.94
24	AJ	101	PL9	C7-C3-C2	-5.19	119.11	123.42
29	BB	601	SQD	O9-S-C6	-5.18	102.58	106.94
29	AD	409	SQD	O9-S-C6	-5.01	102.72	106.94
29	AF	101	SQD	O9-S-C6	-4.92	102.80	106.94
29	AA	412	SQD	O9-S-C6	-4.83	102.87	106.94
24	BJ	101	PL9	C7-C3-C2	-4.72	119.51	123.42
26	AJ	102	BCR	C38-C26-C27	-4.58	104.74	113.43
26	BJ	102	BCR	C38-C26-C27	-4.58	104.75	113.43
27	BC	517	DGD	C3G-O3G-C1D	-4.47	104.44	113.82
27	AC	517	DGD	C3G-O3G-C1D	-4.45	104.47	113.82
29	AA	415	SQD	O9-S-C6	-4.43	103.21	106.94
22	AA	403	CLA	CAA-C2A-C3A	-4.33	100.76	113.22
26	AK	102	BCR	C33-C5-C4	-4.30	105.28	113.43
26	AD	406	BCR	C38-C26-C27	-4.28	105.32	113.43
26	BD	406	BCR	C38-C26-C27	-4.24	105.38	113.43
26	BK	102	BCR	C33-C5-C4	-4.19	105.48	113.43
22	BA	404	CLA	CAA-C2A-C3A	-4.17	101.22	113.22
26	BB	621	BCR	C38-C26-C27	-4.16	105.54	113.43
34	BE	101	HEM	CBD-CAD-C3D	-4.14	101.50	113.55
24	AA	407	PL9	C7-C8-C9	-4.12	119.71	126.70
26	BX	101	BCR	C38-C26-C27	-4.12	105.61	113.43
26	AD	406	BCR	C33-C5-C4	-4.12	105.62	113.43
26	AH	101	BCR	C38-C26-C27	-4.11	105.63	113.43
26	AB	619	BCR	C38-C26-C27	-4.11	105.63	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AT	102	BCR	C38-C26-C27	-4.09	105.68	113.43
26	AJ	102	BCR	C1-C6-C5	-4.05	116.71	122.66
34	AE	101	HEM	CBD-CAD-C3D	-4.02	101.85	113.55
26	AB	618	BCR	C33-C5-C4	-3.93	105.97	113.43
26	AC	515	BCR	C38-C26-C27	-3.93	105.97	113.43
26	BJ	102	BCR	C33-C5-C4	-3.92	105.99	113.43
26	AC	514	BCR	C33-C5-C4	-3.92	106.00	113.43
26	AB	620	BCR	C38-C26-C27	-3.89	106.05	113.43
26	BK	102	BCR	C8-C9-C10	-3.87	112.74	118.98
26	AB	618	BCR	C38-C26-C27	-3.87	106.09	113.43
24	BA	408	PL9	C3-C2-C1	-3.87	120.61	122.97
24	AD	405	PL9	C3-C2-C1	-3.86	120.62	122.97
26	BC	515	BCR	C38-C26-C27	-3.85	106.12	113.43
26	AT	102	BCR	C33-C5-C4	-3.85	106.14	113.43
26	BD	406	BCR	C33-C5-C4	-3.82	106.18	113.43
26	BB	620	BCR	C38-C26-C27	-3.81	106.21	113.43
26	BJ	102	BCR	C1-C6-C5	-3.81	117.07	122.66
24	BA	408	PL9	C7-C8-C9	-3.80	120.26	126.70
23	BA	406	PHO	CBD-CHA-C4D	-3.78	104.22	108.46
26	AB	619	BCR	C33-C5-C4	-3.78	106.27	113.43
26	BC	515	BCR	C33-C5-C4	-3.76	106.29	113.43
26	BB	620	BCR	C33-C5-C4	-3.76	106.30	113.43
26	AK	102	BCR	C8-C9-C10	-3.76	112.93	118.98
26	BB	621	BCR	C33-C5-C4	-3.75	106.31	113.43
26	AB	620	BCR	C33-C5-C4	-3.75	106.33	113.43
26	AC	515	BCR	C33-C5-C4	-3.73	106.36	113.43
26	BC	514	BCR	C38-C26-C27	-3.73	106.36	113.43
23	BD	403	PHO	CBD-CHA-C4D	-3.71	104.30	108.46
32	AT	101	LMT	C1-O1'-C1'	-3.71	107.45	113.94
26	BC	514	BCR	C33-C5-C4	-3.71	106.39	113.43
34	BV	201	HEM	CBD-CAD-C3D	-3.71	102.76	113.55
26	AZ	101	BCR	C38-C26-C27	-3.70	106.41	113.43
26	AC	514	BCR	C38-C26-C27	-3.70	106.41	113.43
32	AI	102	LMT	C1-O1'-C1'	-3.69	107.49	113.94
26	AA	409	BCR	C38-C26-C27	-3.69	106.43	113.43
24	BD	405	PL9	C3-C2-C1	-3.69	120.72	122.97
26	AB	617	BCR	C38-C26-C27	-3.66	106.49	113.43
26	AA	409	BCR	C33-C5-C4	-3.64	106.52	113.43
26	AB	619	BCR	C30-C25-C26	-3.64	117.31	122.66
26	AJ	102	BCR	C33-C5-C4	-3.64	106.53	113.43
32	BI	102	LMT	C1-O1'-C1'	-3.63	107.59	113.94
24	AA	407	PL9	C3-C2-C1	-3.63	120.76	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BK	102	BCR	C38-C26-C27	-3.63	106.54	113.43
26	BB	622	BCR	C33-C5-C4	-3.62	106.57	113.43
26	BZ	101	BCR	C38-C26-C27	-3.61	106.59	113.43
26	AB	617	BCR	C33-C5-C4	-3.60	106.60	113.43
26	BB	622	BCR	C38-C26-C27	-3.59	106.61	113.43
24	AA	407	PL9	C27-C28-C29	-3.58	119.97	127.76
24	AJ	101	PL9	C7-C8-C9	-3.58	120.63	126.70
34	AV	201	HEM	CBD-CAD-C3D	-3.56	103.18	113.55
24	BA	408	PL9	C27-C28-C29	-3.56	120.01	127.76
26	BA	410	BCR	C38-C26-C27	-3.56	106.68	113.43
24	AA	407	PL9	C17-C18-C19	-3.56	120.03	127.76
26	BB	621	BCR	C30-C25-C26	-3.54	117.45	122.66
22	AD	402	CLA	OBD-CAD-CBD	-3.54	120.59	125.94
23	AD	403	PHO	CBD-CHA-C4D	-3.54	104.49	108.46
22	BB	619	CLA	CAA-C2A-C3A	-3.54	103.04	113.22
26	AK	102	BCR	C1-C6-C5	-3.52	117.49	122.66
22	AA	406	CLA	OBD-CAD-CBD	-3.50	120.65	125.94
26	BK	102	BCR	C1-C6-C5	-3.50	117.53	122.66
23	AA	405	PHO	CBD-CHA-C4D	-3.50	104.54	108.46
22	AB	616	CLA	CAA-C2A-C3A	-3.49	103.18	113.22
26	AK	102	BCR	C38-C26-C27	-3.49	106.81	113.43
26	BA	410	BCR	C33-C5-C4	-3.48	106.83	113.43
26	BD	406	BCR	C30-C25-C26	-3.47	117.56	122.66
24	AA	407	PL9	C22-C23-C24	-3.47	120.22	127.76
26	AD	406	BCR	C30-C25-C26	-3.45	117.60	122.66
26	AH	101	BCR	C30-C25-C26	-3.45	117.60	122.66
26	BC	515	BCR	C30-C25-C26	-3.43	117.62	122.66
32	BT	101	LMT	C1-O1'-C1'	-3.43	107.95	113.94
26	BX	101	BCR	C30-C25-C26	-3.42	117.64	122.66
26	AH	101	BCR	C33-C5-C4	-3.41	106.96	113.43
22	AC	505	CLA	OBD-CAD-CBD	-3.40	120.80	125.94
26	BX	101	BCR	C33-C5-C4	-3.39	107.01	113.43
24	BA	408	PL9	C22-C23-C24	-3.38	120.42	127.76
24	AA	407	PL9	C12-C13-C14	-3.37	120.42	127.76
26	BZ	101	BCR	C33-C5-C4	-3.37	107.03	113.43
24	BA	408	PL9	C17-C18-C19	-3.37	120.44	127.76
22	AB	607	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
26	AC	515	BCR	C30-C25-C26	-3.36	117.73	122.66
22	AB	603	CLA	CAA-C2A-C3A	-3.35	103.58	113.22
26	BB	622	BCR	C30-C25-C26	-3.35	117.74	122.66
26	AK	102	BCR	C30-C25-C26	-3.35	117.74	122.66
22	BC	505	CLA	OBD-CAD-CBD	-3.35	120.89	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AD	403	PHO	C7-C6-C5	-3.34	103.19	113.06
26	AD	406	BCR	C1-C6-C5	-3.32	117.78	122.66
29	AA	415	SQD	C3-C4-C5	-3.32	104.41	110.20
22	AB	611	CLA	OBD-CAD-CBD	-3.32	120.93	125.94
22	BB	614	CLA	OBD-CAD-CBD	-3.32	120.93	125.94
22	BB	606	CLA	CAA-C2A-C3A	-3.31	103.71	113.22
24	BD	405	PL9	C17-C18-C19	-3.29	120.60	127.76
26	AZ	101	BCR	C33-C5-C4	-3.29	107.18	113.43
26	AB	618	BCR	C30-C25-C26	-3.29	117.82	122.66
26	AA	409	BCR	C30-C25-C26	-3.29	117.83	122.66
24	BA	408	PL9	C12-C13-C14	-3.29	120.62	127.76
26	AB	620	BCR	C30-C25-C26	-3.27	117.85	122.66
22	BB	611	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
26	BD	406	BCR	C1-C6-C5	-3.27	117.86	122.66
29	BA	401	SQD	C3-C4-C5	-3.27	104.50	110.20
26	AT	102	BCR	C30-C25-C26	-3.26	117.87	122.66
26	AJ	102	BCR	C30-C25-C26	-3.22	117.93	122.66
22	AC	505	CLA	CAA-C2A-C3A	-3.21	103.98	113.22
22	AA	404	CLA	OBD-CAD-CBD	-3.21	121.10	125.94
24	AJ	101	PL9	C3-C2-C1	-3.21	121.02	122.97
24	AD	405	PL9	C17-C18-C19	-3.21	120.79	127.76
22	AB	610	CLA	OBD-CAD-CBD	-3.20	121.11	125.94
26	BK	102	BCR	C30-C25-C26	-3.19	117.98	122.66
22	AC	509	CLA	OBD-CAD-CBD	-3.19	121.13	125.94
30	BI	101	LMG	C7-O1-C1	-3.18	107.14	113.82
22	BB	619	CLA	OBD-CAD-CBD	-3.18	121.14	125.94
22	BC	509	CLA	OBD-CAD-CBD	-3.17	121.15	125.94
22	AA	404	CLA	CAA-C2A-C3A	-3.16	104.12	113.22
23	BD	403	PHO	C7-C6-C5	-3.16	103.74	113.06
22	AC	507	CLA	C7-C6-C5	-3.15	103.76	113.06
26	BJ	102	BCR	C30-C25-C26	-3.15	118.04	122.66
22	BC	505	CLA	CAA-C2A-C3A	-3.14	104.18	113.22
26	AH	101	BCR	C12-C13-C14	-3.13	113.94	118.98
22	BB	605	CLA	C7-C6-C5	-3.13	103.82	113.06
24	BJ	101	PL9	C3-C2-C1	-3.13	121.06	122.97
24	BJ	101	PL9	C7-C8-C9	-3.13	121.40	126.70
22	AB	611	CLA	C7-C6-C5	-3.12	103.86	113.06
24	AJ	101	PL9	C22-C23-C24	-3.11	120.99	127.76
26	BX	101	BCR	C12-C13-C14	-3.11	113.97	118.98
30	AB	622	LMG	C7-O1-C1	-3.11	107.29	113.82
26	BA	410	BCR	C30-C25-C26	-3.11	118.10	122.66
22	BB	610	CLA	OBD-CAD-CBD	-3.10	121.26	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AC	514	BCR	C1-C6-C5	-3.09	118.11	122.66
22	BB	607	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
24	AD	405	PL9	C37-C38-C39	-3.09	121.04	127.76
22	BA	405	CLA	CAA-C2A-C3A	-3.09	104.33	113.22
22	AB	616	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
22	BA	407	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
30	BB	623	LMG	C7-O1-C1	-3.07	107.36	113.82
22	AB	614	CLA	OBD-CAD-CBD	-3.07	121.30	125.94
22	BB	616	CLA	OBD-CAD-CBD	-3.07	121.31	125.94
24	AD	405	PL9	C42-C43-C44	-3.07	121.09	127.76
22	BB	614	CLA	C7-C6-C5	-3.07	104.00	113.06
32	BD	411	LMT	C1-O1'-C1'	-3.06	108.59	113.94
26	BC	514	BCR	C1-C6-C5	-3.06	118.17	122.66
24	BJ	101	PL9	C22-C23-C24	-3.05	121.13	127.76
30	BB	624	LMG	C7-O1-C1	-3.05	107.41	113.82
32	AD	411	LMT	C1-O1'-C1'	-3.05	108.61	113.94
22	BC	504	CLA	OBD-CAD-CBD	-3.04	121.35	125.94
29	AF	101	SQD	C3-C4-C5	-3.03	104.91	110.20
22	AB	609	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
22	BB	612	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
22	BB	617	CLA	OBD-CAD-CBD	-3.02	121.39	125.94
22	AC	501	CLA	CAA-C2A-C3A	-3.01	104.55	113.22
22	BB	605	CLA	CAA-C2A-C3A	-3.01	104.56	113.22
32	AM	102	LMT	C1B-O1B-C4'	-3.01	110.15	118.01
22	AB	608	CLA	OBD-CAD-CBD	-3.01	121.40	125.94
22	BB	609	CLA	OBD-CAD-CBD	-3.00	121.40	125.94
26	BB	621	BCR	C1-C6-C5	-3.00	118.25	122.66
22	BA	405	CLA	OBD-CAD-CBD	-3.00	121.41	125.94
22	AC	502	CLA	OBD-CAD-CBD	-3.00	121.41	125.94
24	BD	405	PL9	C37-C38-C39	-3.00	121.25	127.76
24	AD	405	PL9	C7-C8-C9	-3.00	121.62	126.70
24	BD	405	PL9	C42-C43-C44	-3.00	121.25	127.76
22	BC	507	CLA	C7-C6-C5	-2.99	104.22	113.06
26	AB	617	BCR	C30-C25-C26	-2.99	118.28	122.66
22	AB	603	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
22	AB	615	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
22	AC	508	CLA	OBD-CAD-CBD	-2.98	121.44	125.94
22	AA	406	CLA	C7-C6-C5	-2.98	104.27	113.06
23	AA	405	PHO	CAB-C3B-C2B	-2.98	118.44	128.41
22	AB	602	CLA	CAA-C2A-C3A	-2.97	104.67	113.22
22	AD	404	CLA	CAA-C2A-C3A	-2.97	104.68	113.22
22	AC	513	CLA	OBD-CAD-CBD	-2.97	121.46	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	602	CLA	C7-C6-C5	-2.96	104.30	113.06
26	AC	515	BCR	C1-C6-C5	-2.96	118.31	122.66
32	BM	101	LMT	C1-O1'-C1'	-2.96	108.78	113.94
26	BC	515	BCR	C40-C30-C29	-2.95	98.20	108.79
23	AD	403	PHO	CAA-C2A-C3A	-2.95	104.72	113.22
26	BB	620	BCR	C30-C25-C26	-2.95	118.33	122.66
29	BD	409	SQD	C3-C4-C5	-2.95	105.06	110.20
22	BB	615	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
26	AC	515	BCR	C40-C30-C29	-2.93	98.28	108.79
23	BD	403	PHO	CAA-C2A-C3A	-2.93	104.78	113.22
22	AC	506	CLA	OBD-CAD-CBD	-2.93	121.51	125.94
24	BD	405	PL9	C7-C8-C9	-2.92	121.74	126.70
32	BM	101	LMT	C1B-O1B-C4'	-2.92	110.38	118.01
22	BA	404	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
30	AB	621	LMG	C7-O1-C1	-2.91	107.71	113.82
22	BD	402	CLA	OBD-CAD-CBD	-2.91	121.55	125.94
30	AI	101	LMG	C7-O1-C1	-2.90	107.72	113.82
22	BB	613	CLA	OBD-CAD-CBD	-2.90	121.56	125.94
22	BC	508	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
22	AC	501	CLA	OBD-CAD-CBD	-2.89	121.57	125.94
26	AC	514	BCR	C30-C25-C26	-2.88	118.43	122.66
22	AA	406	CLA	CAA-C2A-C3A	-2.87	104.96	113.22
22	BB	606	CLA	OBD-CAD-CBD	-2.87	121.60	125.94
22	AB	604	CLA	OBD-CAD-CBD	-2.87	121.61	125.94
24	BJ	101	PL9	C17-C18-C19	-2.87	121.53	127.76
23	BA	406	PHO	CAB-C3B-C2B	-2.87	118.80	128.41
22	AC	504	CLA	OBD-CAD-CBD	-2.86	121.61	125.94
27	BC	517	DGD	C3G-C2G-C1G	-2.86	105.37	112.07
22	BA	407	CLA	CAA-C2A-C3A	-2.86	105.00	113.22
24	AD	405	PL9	C12-C13-C14	-2.86	121.55	127.76
26	BB	622	BCR	C1-C6-C5	-2.85	118.47	122.66
22	AB	605	CLA	OBD-CAD-CBD	-2.85	121.63	125.94
26	BC	514	BCR	C30-C25-C26	-2.85	118.48	122.66
27	AC	517	DGD	C3G-C2G-C1G	-2.85	105.41	112.07
22	BC	501	CLA	OBD-CAD-CBD	-2.85	121.64	125.94
26	BK	102	BCR	C12-C13-C14	-2.84	114.41	118.98
22	BC	501	CLA	CAA-C2A-C3A	-2.84	105.05	113.22
29	BF	101	SQD	C3-C4-C5	-2.84	105.25	110.20
22	BA	407	CLA	C7-C6-C5	-2.84	104.68	113.06
26	BC	515	BCR	C1-C6-C5	-2.84	118.50	122.66
32	BB	626	LMT	C1B-O1B-C4'	-2.84	110.60	118.01
22	BA	404	CLA	O1D-CGD-CBD	-2.84	120.56	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	608	CLA	CAA-C2A-C3A	-2.83	105.07	113.22
26	BB	620	BCR	C1-C6-C5	-2.83	118.50	122.66
23	BA	406	PHO	C7-C6-C5	-2.83	104.71	113.06
22	AB	612	CLA	OBD-CAD-CBD	-2.82	121.68	125.94
26	AA	409	BCR	C1-C6-C5	-2.82	118.52	122.66
29	AA	412	SQD	C3-C4-C5	-2.82	105.28	110.20
23	BD	403	PHO	C2A-C1A-NA	-2.82	108.47	112.08
22	BA	405	CLA	C7-C6-C5	-2.81	104.75	113.06
22	AB	615	CLA	C7-C6-C5	-2.81	104.76	113.06
26	AK	102	BCR	C32-C1-C2	-2.81	98.74	108.79
22	BC	506	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
22	AB	616	CLA	C7-C6-C5	-2.80	104.80	113.06
30	AA	416	LMG	C7-O1-C1	-2.80	107.94	113.82
23	AD	403	PHO	CAB-C3B-C2B	-2.79	119.05	128.41
26	AB	619	BCR	C1-C6-C5	-2.79	118.56	122.66
22	BB	608	CLA	CAA-C2A-C3A	-2.78	105.22	113.22
26	BD	406	BCR	C12-C13-C14	-2.78	114.51	118.98
22	AC	512	CLA	OBD-CAD-CBD	-2.78	121.75	125.94
22	AA	403	CLA	O1D-CGD-CBD	-2.77	120.65	124.62
22	AC	503	CLA	OBD-CAD-CBD	-2.77	121.76	125.94
22	BC	503	CLA	OBD-CAD-CBD	-2.77	121.76	125.94
22	BB	618	CLA	C7-C6-C5	-2.77	104.89	113.06
22	BB	619	CLA	C7-C6-C5	-2.76	104.91	113.06
26	BD	406	BCR	C23-C22-C21	-2.76	114.54	118.98
24	BD	405	PL9	C27-C28-C29	-2.76	121.76	127.76
32	BB	603	LMT	C1B-O1B-C4'	-2.76	110.80	118.01
32	AB	625	LMT	C1B-O1B-C4'	-2.76	110.81	118.01
22	AA	402	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
22	BC	502	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
22	AB	606	CLA	OBD-CAD-CBD	-2.75	121.80	125.94
22	BC	512	CLA	C7-C6-C5	-2.74	104.96	113.06
22	BC	506	CLA	C7-C6-C5	-2.74	104.96	113.06
22	AB	605	CLA	CAA-C2A-C3A	-2.74	105.34	113.22
22	BB	618	CLA	OBD-CAD-CBD	-2.74	121.81	125.94
22	AB	609	CLA	C7-C6-C5	-2.73	104.99	113.06
22	BC	508	CLA	CAA-C2A-C3A	-2.73	105.37	113.22
32	AB	627	LMT	C1B-O1B-C4'	-2.73	110.88	118.01
29	BA	413	SQD	C3-C4-C5	-2.72	105.45	110.20
26	AB	618	BCR	C1-C6-C5	-2.72	118.66	122.66
22	BC	510	CLA	C7-C6-C5	-2.72	105.03	113.06
22	BB	605	CLA	OBD-CAD-CBD	-2.72	121.83	125.94
22	BD	402	CLA	CMB-C2B-C1B	-2.72	123.87	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AT	102	BCR	C1-C6-C5	-2.71	118.67	122.66
22	BC	501	CLA	C7-C6-C5	-2.71	105.04	113.06
26	BX	101	BCR	C1-C6-C5	-2.71	118.67	122.66
22	BC	511	CLA	C7-C6-C5	-2.71	105.07	113.06
22	BB	610	CLA	CAA-C2A-C3A	-2.71	105.44	113.22
26	AB	617	BCR	C1-C6-C5	-2.71	118.69	122.66
32	AM	102	LMT	C1-O1'-C1'	-2.71	109.21	113.94
32	BB	603	LMT	C1-O1'-C1'	-2.71	109.22	113.94
22	AB	607	CLA	CAA-C2A-C3A	-2.71	105.44	113.22
24	BD	405	PL9	C12-C13-C14	-2.70	121.88	127.76
22	AB	613	CLA	C7-C6-C5	-2.70	105.08	113.06
22	BD	404	CLA	CAA-C2A-C3A	-2.70	105.45	113.22
22	AB	601	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
22	AC	506	CLA	CAA-C2A-C3A	-2.70	105.45	113.22
22	AA	404	CLA	C7-C6-C5	-2.70	105.09	113.06
23	BD	403	PHO	CAB-C3B-C2B	-2.69	119.38	128.41
26	AK	102	BCR	C12-C13-C14	-2.69	114.65	118.98
22	AC	512	CLA	C7-C6-C5	-2.69	105.12	113.06
22	BB	604	CLA	OBD-CAD-CBD	-2.69	121.88	125.94
22	AC	512	CLA	O1D-CGD-CBD	-2.69	120.77	124.62
22	AC	510	CLA	C7-C6-C5	-2.68	105.14	113.06
22	AD	404	CLA	OBD-CAD-CBD	-2.68	121.89	125.94
24	AD	405	PL9	C27-C28-C29	-2.68	121.94	127.76
26	BK	102	BCR	C32-C1-C2	-2.68	99.20	108.79
22	BB	612	CLA	C7-C6-C5	-2.68	105.16	113.06
26	BA	410	BCR	C1-C6-C5	-2.67	118.73	122.66
26	AB	620	BCR	C1-C6-C5	-2.67	118.74	122.66
23	AD	403	PHO	O1D-CGD-CBD	-2.66	120.80	124.62
26	AD	406	BCR	C23-C22-C21	-2.65	114.71	118.98
22	AC	508	CLA	CAA-C2A-C3A	-2.65	105.60	113.22
26	AD	406	BCR	C12-C13-C14	-2.65	114.72	118.98
22	BC	502	CLA	C7-C6-C5	-2.64	105.25	113.06
22	AA	403	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
22	BC	513	CLA	C7-C6-C5	-2.64	105.26	113.06
22	BC	513	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
32	AD	411	LMT	C1B-O1B-C4'	-2.64	111.11	118.01
22	BC	510	CLA	OBD-CAD-CBD	-2.64	121.96	125.94
30	AB	623	LMG	C7-O1-C1	-2.64	108.28	113.82
22	AC	506	CLA	C7-C6-C5	-2.64	105.28	113.06
23	AA	405	PHO	O1D-CGD-CBD	-2.63	120.85	124.62
22	AC	502	CLA	O1D-CGD-CBD	-2.63	120.85	124.62
22	BB	617	CLA	O1D-CGD-CBD	-2.63	120.85	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	613	CLA	OBD-CAD-CBD	-2.63	121.97	125.94
26	AZ	101	BCR	C1-C6-C5	-2.62	118.81	122.66
22	AB	601	CLA	C7-C6-C5	-2.61	105.34	113.06
22	BC	504	CLA	CAA-C2A-C3A	-2.61	105.71	113.22
22	AC	511	CLA	C7-C6-C5	-2.61	105.35	113.06
22	BD	404	CLA	OBD-CAD-CBD	-2.60	122.01	125.94
22	BB	616	CLA	C7-C6-C5	-2.60	105.37	113.06
26	AT	102	BCR	C40-C30-C29	-2.60	99.47	108.79
26	AH	101	BCR	C1-C6-C5	-2.60	118.84	122.66
22	AD	402	CLA	CMB-C2B-C1B	-2.60	124.06	128.36
22	AC	505	CLA	C7-C6-C5	-2.60	105.38	113.06
23	AA	405	PHO	C7-C6-C5	-2.59	105.40	113.06
22	BC	512	CLA	CAA-C2A-C3A	-2.58	105.79	113.22
22	AB	614	CLA	O1D-CGD-CBD	-2.58	120.93	124.62
22	AB	605	CLA	C7-C6-C5	-2.57	105.46	113.06
22	AC	502	CLA	C7-C6-C5	-2.57	105.46	113.06
22	BB	611	CLA	CAA-C2A-C3A	-2.57	105.82	113.22
29	AD	409	SQD	C3-C4-C5	-2.57	105.71	110.20
26	BZ	101	BCR	C1-C6-C5	-2.57	118.89	122.66
22	BB	616	CLA	CMB-C2B-C1B	-2.57	124.11	128.36
22	BB	604	CLA	C7-C6-C5	-2.57	105.48	113.06
22	AC	508	CLA	C7-C6-C5	-2.56	105.50	113.06
22	BD	402	CLA	C7-C6-C5	-2.56	105.51	113.06
29	AA	412	SQD	O8-S-O9	-2.56	105.66	111.61
26	BZ	101	BCR	C30-C25-C26	-2.55	118.91	122.66
22	BC	506	CLA	CAA-C2A-C3A	-2.55	105.88	113.22
22	BB	614	CLA	O1D-CGD-CBD	-2.55	120.97	124.62
28	BC	521	LHG	C5-O7-C7	-2.54	111.79	117.89
28	AC	521	LHG	C5-O7-C7	-2.54	111.79	117.89
22	BC	512	CLA	OBD-CAD-CBD	-2.54	122.10	125.94
24	AJ	101	PL9	C17-C18-C19	-2.54	122.24	127.76
22	AC	501	CLA	C7-C6-C5	-2.54	105.56	113.06
22	AC	510	CLA	OBD-CAD-CBD	-2.54	122.11	125.94
22	AB	609	CLA	CAA-C2A-C3A	-2.54	105.92	113.22
22	AB	610	CLA	CAA-C2A-C3A	-2.54	105.93	113.22
22	AC	504	CLA	CAA-C2A-C3A	-2.53	105.93	113.22
32	AB	627	LMT	C1-O1'-C1'	-2.53	109.52	113.94
26	AZ	101	BCR	C30-C25-C26	-2.53	118.94	122.66
22	BC	505	CLA	C7-C6-C5	-2.52	105.61	113.06
22	AB	602	CLA	OBD-CAD-CBD	-2.52	122.14	125.94
24	BJ	101	PL9	C12-C13-C14	-2.52	122.29	127.76
22	AC	513	CLA	C7-C6-C5	-2.51	105.64	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BB	608	CLA	OBD-CAD-CBD	-2.51	122.15	125.94
22	BC	508	CLA	O1D-CGD-CBD	-2.51	121.03	124.62
22	BB	612	CLA	CAA-C2A-C3A	-2.50	106.02	113.22
22	BC	508	CLA	C7-C6-C5	-2.50	105.68	113.06
26	AJ	102	BCR	C15-C16-C17	-2.50	117.87	123.39
24	BD	405	PL9	C22-C23-C24	-2.50	122.33	127.76
26	AB	618	BCR	C40-C30-C29	-2.50	99.85	108.79
24	AD	405	PL9	C22-C23-C24	-2.50	122.33	127.76
30	BB	623	LMG	C9-C8-C7	-2.50	106.23	112.07
22	AB	606	CLA	C7-C6-C5	-2.49	105.71	113.06
26	AJ	102	BCR	C20-C21-C22	-2.49	123.60	127.20
27	BB	602	DGD	C3G-O3G-C1D	-2.49	108.60	113.82
29	BB	601	SQD	C3-C4-C5	-2.49	105.86	110.20
22	AB	611	CLA	O1D-CGD-CBD	-2.48	121.07	124.62
30	BA	414	LMG	C7-O1-C1	-2.48	108.61	113.82
22	AC	503	CLA	C7-C6-C5	-2.48	105.75	113.06
22	BC	502	CLA	O1D-CGD-CBD	-2.47	121.08	124.62
22	BC	503	CLA	C7-C6-C5	-2.47	105.77	113.06
23	BD	403	PHO	O1D-CGD-CBD	-2.45	121.10	124.62
22	AC	512	CLA	CAA-C2A-C3A	-2.45	106.17	113.22
22	BB	608	CLA	C7-C6-C5	-2.45	105.84	113.06
22	AC	508	CLA	O1D-CGD-CBD	-2.45	121.12	124.62
22	AB	614	CLA	CMB-C2B-C1B	-2.44	124.32	128.36
22	AB	604	CLA	C7-C6-C5	-2.44	105.85	113.06
22	BB	609	CLA	C7-C6-C5	-2.44	105.86	113.06
26	AT	102	BCR	C23-C22-C21	-2.44	115.06	118.98
26	AZ	101	BCR	C19-C18-C17	-2.43	115.07	118.98
22	AB	602	CLA	CMB-C2B-C1B	-2.42	124.36	128.36
22	BC	502	CLA	CAA-C2A-C3A	-2.42	106.25	113.22
26	AB	618	BCR	C23-C22-C21	-2.42	115.08	118.98
26	AC	514	BCR	C12-C13-C14	-2.42	115.09	118.98
24	AJ	101	PL9	C12-C13-C14	-2.41	122.52	127.76
29	BL	101	SQD	C3-C4-C5	-2.41	106.00	110.20
26	BJ	102	BCR	C20-C21-C22	-2.41	123.72	127.20
26	BZ	101	BCR	C12-C13-C14	-2.41	115.11	118.98
29	BA	413	SQD	O8-S-O9	-2.40	106.02	111.61
32	BD	411	LMT	C1B-O1B-C4'	-2.40	111.73	118.01
22	AB	608	CLA	C7-C6-C5	-2.40	105.97	113.06
22	BB	606	CLA	CMB-C2B-C1B	-2.40	124.39	128.36
22	BA	403	CLA	OBD-CAD-CBD	-2.40	122.32	125.94
22	BA	403	CLA	C7-C6-C5	-2.40	105.98	113.06
30	AA	413	LMG	C7-O1-C1	-2.39	108.79	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AB	618	BCR	C8-C9-C10	-2.39	115.13	118.98
22	BB	604	CLA	CAA-C2A-C3A	-2.39	106.35	113.22
22	BC	507	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
26	AC	514	BCR	C23-C22-C21	-2.39	115.14	118.98
26	BA	410	BCR	C8-C9-C10	-2.39	115.14	118.98
22	BB	614	CLA	CAA-C2A-C3A	-2.38	106.37	113.22
24	BD	405	PL9	C32-C33-C34	-2.38	122.59	127.76
30	AB	621	LMG	C9-C8-C7	-2.38	106.51	112.07
22	AD	402	CLA	C7-C6-C5	-2.38	106.04	113.06
22	BC	512	CLA	O1D-CGD-CBD	-2.38	121.22	124.62
22	AA	402	CLA	C7-C6-C5	-2.38	106.04	113.06
23	AD	403	PHO	C2A-C1A-NA	-2.37	109.04	112.08
22	BB	613	CLA	CMB-C2B-C1B	-2.37	124.44	128.36
26	BC	514	BCR	C12-C13-C14	-2.37	115.17	118.98
22	BB	613	CLA	CAA-C2A-C3A	-2.37	106.41	113.22
22	AB	610	CLA	CMB-C2B-C1B	-2.36	124.45	128.36
22	AC	511	CLA	OBD-CAD-CBD	-2.35	122.39	125.94
22	AB	613	CLA	CMB-C2B-C1B	-2.35	124.48	128.36
22	AC	507	CLA	OBD-CAD-CBD	-2.34	122.40	125.94
22	BC	511	CLA	OBD-CAD-CBD	-2.34	122.40	125.94
22	AB	614	CLA	CAA-C2A-C3A	-2.34	106.48	113.22
22	BA	404	CLA	CMB-C2B-C1B	-2.34	124.49	128.36
26	BJ	102	BCR	C8-C9-C10	-2.34	115.21	118.98
22	BB	605	CLA	CMB-C2B-C1B	-2.34	124.50	128.36
24	AA	407	PL9	C32-C33-C34	-2.34	122.68	127.76
24	BA	408	PL9	C32-C33-C34	-2.34	122.69	127.76
22	AC	509	CLA	C7-C6-C5	-2.33	106.17	113.06
30	BC	520	LMG	C7-O1-C1	-2.33	108.92	113.82
22	AC	504	CLA	C7-C6-C5	-2.33	106.17	113.06
26	AB	617	BCR	C12-C13-C14	-2.33	115.23	118.98
26	AZ	101	BCR	C12-C13-C14	-2.33	115.24	118.98
26	BJ	102	BCR	C15-C16-C17	-2.32	118.25	123.39
30	AE	102	LMG	C9-C8-C7	-2.32	106.63	112.07
22	BC	504	CLA	C7-C6-C5	-2.32	106.20	113.06
30	AM	101	LMG	O8-C9-C8	-2.32	102.44	108.69
27	AA	410	DGD	C3G-C2G-C1G	-2.32	106.64	112.07
22	BC	510	CLA	CAA-C2A-C3A	-2.32	106.55	113.22
22	BB	611	CLA	CMB-C2B-C1B	-2.31	124.53	128.36
24	AD	405	PL9	C32-C33-C34	-2.31	122.73	127.76
22	BB	613	CLA	C7-C6-C5	-2.31	106.23	113.06
26	BC	514	BCR	C23-C22-C21	-2.31	115.26	118.98
22	BC	504	CLA	CMB-C2B-C1B	-2.30	124.56	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AB	626	DGD	C3G-O3G-C1D	-2.30	108.98	113.82
22	AC	502	CLA	CAA-C2A-C3A	-2.30	106.60	113.22
22	AB	603	CLA	CMB-C2B-C1B	-2.30	124.56	128.36
22	BB	607	CLA	C7-C6-C5	-2.29	106.29	113.06
22	BB	611	CLA	C7-C6-C5	-2.29	106.29	113.06
26	BB	620	BCR	C12-C13-C14	-2.28	115.31	118.98
22	BB	617	CLA	CMB-C2B-C1B	-2.28	124.60	128.36
22	AB	610	CLA	C7-C6-C5	-2.27	106.34	113.06
22	AB	601	CLA	CAA-C2A-C3A	-2.27	106.68	113.22
30	BM	102	LMG	O8-C9-C8	-2.27	102.59	108.69
22	AC	511	CLA	CMB-C2B-C1B	-2.26	124.62	128.36
22	AA	403	CLA	CMB-C2B-C1B	-2.25	124.64	128.36
26	AC	514	BCR	C32-C1-C2	-2.25	100.73	108.79
22	BC	510	CLA	O1D-CGD-CBD	-2.25	121.40	124.62
26	BZ	101	BCR	C19-C18-C17	-2.25	115.36	118.98
22	AC	505	CLA	CMB-C2B-C1B	-2.25	124.65	128.36
22	BB	604	CLA	CMB-C2B-C1B	-2.24	124.65	128.36
26	AH	101	BCR	C23-C22-C21	-2.24	115.38	118.98
23	BA	406	PHO	O1D-CGD-CBD	-2.24	121.41	124.62
30	AM	101	LMG	C7-O1-C1	-2.24	109.12	113.82
22	AB	613	CLA	CAA-C2A-C3A	-2.24	106.78	113.22
22	AB	603	CLA	O1D-CGD-CBD	-2.23	121.42	124.62
22	AB	604	CLA	CAA-C2A-C3A	-2.23	106.80	113.22
22	AC	513	CLA	CMB-C2B-C1B	-2.23	124.68	128.36
22	BC	507	CLA	CAA-C2A-C3A	-2.23	106.81	113.22
24	AJ	101	PL9	C10-C9-C8	-2.22	119.14	123.50
22	AB	611	CLA	CAA-C2A-C3A	-2.22	106.84	113.22
26	AB	618	BCR	C12-C13-C14	-2.21	115.42	118.98
22	AB	612	CLA	CMB-C2B-C1B	-2.21	124.70	128.36
22	AC	504	CLA	CMB-C2B-C1B	-2.21	124.70	128.36
26	BX	101	BCR	C23-C22-C21	-2.20	115.44	118.98
26	BC	514	BCR	C32-C1-C2	-2.19	100.93	108.79
26	AT	102	BCR	C8-C9-C10	-2.19	115.46	118.98
22	BA	403	CLA	CMB-C2B-C1B	-2.18	124.75	128.36
22	AA	402	CLA	CMB-C2B-C1B	-2.18	124.75	128.36
22	BA	407	CLA	CMB-C2B-C1B	-2.18	124.75	128.36
26	AC	515	BCR	C12-C13-C14	-2.18	115.47	118.98
27	BA	411	DGD	C3G-C2G-C1G	-2.18	106.97	112.07
22	BB	617	CLA	CAA-C2A-C3A	-2.18	106.95	113.22
30	BA	414	LMG	C9-C8-C7	-2.18	106.98	112.07
22	AB	612	CLA	C7-C6-C5	-2.17	106.64	113.06
24	BJ	101	PL9	C10-C9-C8	-2.17	119.23	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BK	102	BCR	C40-C30-C29	-2.17	101.01	108.79
22	BC	513	CLA	CMB-C2B-C1B	-2.17	124.77	128.36
22	AB	603	CLA	C7-C6-C5	-2.17	106.66	113.06
22	AB	608	CLA	CMB-C2B-C1B	-2.17	124.78	128.36
26	BK	102	BCR	C23-C22-C21	-2.17	115.49	118.98
22	AB	601	CLA	CMB-C2B-C1B	-2.17	124.78	128.36
24	AJ	101	PL9	C25-C24-C23	-2.16	119.26	123.50
24	AA	407	PL9	C30-C29-C28	-2.16	119.27	123.50
22	AC	509	CLA	CMB-C2B-C1B	-2.15	124.80	128.36
22	BB	608	CLA	CMB-C2B-C1B	-2.15	124.81	128.36
26	AT	102	BCR	C12-C13-C14	-2.15	115.52	118.98
22	AB	612	CLA	CAA-C2A-C3A	-2.14	107.05	113.22
30	AA	413	LMG	C9-C8-C7	-2.14	107.05	112.07
32	BB	625	LMT	C1'-O5'-C5'	-2.14	109.58	113.75
22	BC	509	CLA	C7-C6-C5	-2.14	106.73	113.06
27	BH	101	DGD	C3G-O3G-C1D	-2.14	109.33	113.82
22	BB	619	CLA	CMB-C2B-C1B	-2.14	124.83	128.36
26	AB	619	BCR	C32-C1-C2	-2.13	101.14	108.79
27	BC	516	DGD	C3G-C2G-C1G	-2.13	107.08	112.07
32	AB	624	LMT	C1'-O5'-C5'	-2.13	109.60	113.75
26	AK	102	BCR	C40-C30-C29	-2.13	101.15	108.79
26	AT	102	BCR	C19-C18-C17	-2.13	115.55	118.98
22	BB	609	CLA	CMB-C2B-C1B	-2.13	124.84	128.36
22	BB	607	CLA	CAA-C2A-C3A	-2.13	107.09	113.22
26	BA	410	BCR	C23-C22-C21	-2.13	115.56	118.98
22	AC	508	CLA	CMB-C2B-C1B	-2.13	124.85	128.36
22	BC	509	CLA	O1D-CGD-CBD	-2.12	121.58	124.62
22	AB	616	CLA	CMB-C2B-C1B	-2.12	124.85	128.36
22	BC	512	CLA	CMB-C2B-C1B	-2.12	124.86	128.36
22	BC	505	CLA	CMB-C2B-C1B	-2.12	124.86	128.36
22	AB	615	CLA	CMB-C2B-C1B	-2.11	124.87	128.36
24	BA	408	PL9	C30-C29-C28	-2.11	119.36	123.50
22	BC	511	CLA	CMB-C2B-C1B	-2.11	124.88	128.36
22	AD	404	CLA	CMB-C2B-C1B	-2.11	124.88	128.36
26	BK	102	BCR	C19-C18-C17	-2.10	115.59	118.98
26	BC	515	BCR	C12-C13-C14	-2.10	115.59	118.98
26	BB	621	BCR	C32-C1-C2	-2.10	101.25	108.79
22	AC	506	CLA	O1D-CGD-CBD	-2.10	121.61	124.62
22	BA	405	CLA	CMB-C2B-C1B	-2.10	124.89	128.36
27	AH	102	DGD	C3G-O3G-C1D	-2.10	109.41	113.82
22	BB	615	CLA	CAA-C2A-C3A	-2.10	107.18	113.22
32	AB	625	LMT	C1-O1'-C1'	-2.10	110.28	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AA	409	BCR	C8-C9-C10	-2.10	115.60	118.98
27	AC	516	DGD	O3E-C3E-C2E	-2.10	105.62	110.34
22	AC	506	CLA	CMB-C2B-C1B	-2.10	124.89	128.36
27	BA	411	DGD	C3G-O3G-C1D	-2.09	109.42	113.82
22	BB	615	CLA	O1D-CGD-CBD	-2.09	121.62	124.62
22	BC	509	CLA	CMB-C2B-C1B	-2.09	124.90	128.36
22	AB	607	CLA	C7-C6-C5	-2.09	106.88	113.06
32	BB	625	LMT	C6'-C5'-C4'	-2.09	107.17	113.25
22	AC	507	CLA	CAA-C2A-C3A	-2.09	107.21	113.22
29	BA	413	SQD	O3-C3-C2	-2.09	105.64	110.34
22	BB	606	CLA	C7-C6-C5	-2.08	106.91	113.06
22	BB	613	CLA	O1D-CGD-CBD	-2.08	121.65	124.62
22	AC	509	CLA	O1D-CGD-CBD	-2.08	121.65	124.62
22	BC	506	CLA	CMB-C2B-C1B	-2.07	124.94	128.36
26	AK	102	BCR	C19-C18-C17	-2.07	115.65	118.98
22	BB	610	CLA	C7-C6-C5	-2.07	106.95	113.06
27	AA	410	DGD	C3G-O3G-C1D	-2.06	109.48	113.82
22	BB	617	CLA	C7-C6-C5	-2.06	106.97	113.06
24	BJ	101	PL9	C25-C24-C23	-2.06	119.45	123.50
22	AC	502	CLA	CMB-C2B-C1B	-2.06	124.95	128.36
22	AA	404	CLA	CMB-C2B-C1B	-2.06	124.96	128.36
22	AB	614	CLA	C7-C6-C5	-2.06	106.98	113.06
22	AA	404	CLA	O1D-CGD-CBD	-2.06	121.68	124.62
24	AA	407	PL9	C15-C14-C13	-2.05	119.47	123.50
22	BC	507	CLA	CMB-C2B-C1B	-2.05	124.97	128.36
32	AB	624	LMT	C6'-C5'-C4'	-2.05	107.28	113.25
22	BB	616	CLA	CAA-C2A-C3A	-2.05	107.32	113.22
29	BA	401	SQD	O48-C23-O10	-2.05	118.20	123.49
22	AC	510	CLA	CMA-C3A-C2A	-2.05	105.29	114.35
29	BL	101	SQD	O3-C3-C2	-2.04	105.74	110.34
30	AB	622	LMG	C9-C8-C7	-2.04	107.30	112.07
22	AB	605	CLA	CMB-C2B-C1B	-2.04	124.99	128.36
22	BB	615	CLA	C7-C6-C5	-2.04	107.05	113.06
22	BC	502	CLA	CMB-C2B-C1B	-2.03	125.00	128.36
26	BA	410	BCR	C12-C13-C14	-2.03	115.71	118.98
22	BB	618	CLA	CMB-C2B-C1B	-2.03	125.00	128.36
30	AB	622	LMG	O8-C9-C8	-2.03	103.23	108.69
26	AD	406	BCR	C40-C30-C29	-2.02	101.53	108.79
22	AB	615	CLA	O1D-CGD-CBD	-2.02	121.72	124.62
30	AC	520	LMG	C7-O1-C1	-2.02	109.58	113.82
22	AC	503	CLA	CMB-C2B-C1B	-2.02	125.03	128.36
22	BB	613	CLA	C12-C11-C10	-2.02	102.98	112.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	BC	517	DGD	C6E-C5E-C4E	-2.02	108.04	113.02
32	AT	101	LMT	C1B-O1B-C4'	-2.02	112.74	118.01
22	AB	606	CLA	CMB-C2B-C1B	-2.01	125.03	128.36
26	BC	515	BCR	C23-C22-C21	-2.01	115.74	118.98
22	BC	509	CLA	C12-C11-C10	-2.01	103.01	112.99
22	AB	609	CLA	O1D-CGD-CBD	-2.01	121.74	124.62
26	BB	622	BCR	C40-C30-C29	-2.01	101.59	108.79
22	BC	508	CLA	CMB-C2B-C1B	-2.01	125.04	128.36
29	BB	601	SQD	O3-C3-C2	-2.01	105.82	110.34
26	AB	618	BCR	C19-C18-C17	-2.01	115.75	118.98
26	BB	620	BCR	C19-C18-C17	-2.01	115.75	118.98
26	AC	515	BCR	C32-C1-C2	-2.01	101.61	108.79
30	AD	408	LMG	O8-C9-C8	-2.00	103.30	108.69
22	AB	609	CLA	CMA-C3A-C2A	-2.00	105.48	114.35
27	AC	517	DGD	C6E-C5E-C4E	-2.00	108.07	113.02
27	BB	602	DGD	C3G-C2G-C1G	-2.00	107.39	112.07
24	AA	407	PL9	C53-C6-C1	2.00	119.72	114.94
22	AB	613	CLA	CMB-C2B-C3B	2.00	129.00	125.09
29	AF	101	SQD	O5-C5-C4	2.00	113.44	109.68
26	BX	101	BCR	C34-C9-C8	2.00	121.43	118.10
29	AA	415	SQD	O5-C5-C4	2.00	113.44	109.68
22	BC	503	CLA	C6-C5-C3	2.01	116.89	112.48
22	BC	505	CLA	O2D-CGD-CBD	2.01	114.05	111.30
22	BD	404	CLA	C6-C5-C3	2.01	116.89	112.48
29	BA	401	SQD	C13-C12-C11	2.01	124.90	114.53
22	BB	605	CLA	C6-C5-C3	2.01	116.89	112.48
29	BF	101	SQD	O47-C7-C8	2.01	115.89	111.53
29	BB	601	SQD	C17-C16-C15	2.01	124.91	114.53
26	BB	621	BCR	C21-C20-C19	2.01	129.25	123.13
22	AC	501	CLA	C2A-C1A-CHA	2.01	127.59	123.89
26	AZ	101	BCR	C7-C8-C9	2.01	129.29	126.22
23	AD	403	PHO	C6-C5-C3	2.02	116.91	112.48
27	AA	410	DGD	C6D-C5D-C4D	2.02	116.60	112.03
26	BA	410	BCR	C1-C6-C7	2.02	121.47	115.82
26	BZ	101	BCR	C7-C8-C9	2.02	129.29	126.22
22	AB	606	CLA	C2A-C1A-CHA	2.02	127.61	123.89
26	AK	102	BCR	C28-C27-C26	2.02	117.08	113.87
22	BB	619	CLA	C2A-C1A-CHA	2.02	127.61	123.89
30	AB	622	LMG	O1-C1-C2	2.02	110.59	108.04
22	BB	618	CLA	C6-C5-C3	2.02	116.93	112.48
26	BA	410	BCR	C36-C18-C19	2.02	121.47	118.10
26	AB	619	BCR	C21-C20-C19	2.03	129.31	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AI	101	LMG	O6-C1-C2	2.03	114.44	110.28
26	AD	406	BCR	C40-C30-C25	2.03	113.48	110.30
22	BB	617	CLA	CBA-CAA-C2A	2.03	119.46	113.73
24	AJ	101	PL9	C31-C29-C30	2.03	119.63	114.64
26	BZ	101	BCR	C32-C1-C6	2.03	113.49	110.30
29	AF	101	SQD	C13-C12-C11	2.03	125.02	114.53
22	BB	607	CLA	C2A-C1A-CHA	2.03	127.63	123.89
26	AB	618	BCR	C34-C9-C8	2.03	121.48	118.10
32	AB	625	LMT	O1B-C1B-C2B	2.04	113.06	108.10
24	BJ	101	PL9	C31-C29-C30	2.04	119.65	114.64
22	AB	602	CLA	CMB-C2B-C3B	2.04	129.07	125.09
26	AA	409	BCR	C32-C1-C6	2.04	113.50	110.30
26	AC	515	BCR	C36-C18-C19	2.04	121.49	118.10
29	BL	101	SQD	C17-C16-C15	2.04	125.08	114.53
26	AT	102	BCR	C16-C17-C18	2.04	130.15	127.20
29	BF	101	SQD	C17-C16-C15	2.05	125.12	114.53
34	AE	101	HEM	C2D-C3D-C4D	2.05	104.98	101.50
29	BA	401	SQD	O47-C45-C44	2.06	115.60	108.36
26	BB	621	BCR	C35-C13-C12	2.06	121.52	118.10
26	BK	102	BCR	C36-C18-C19	2.06	121.52	118.10
26	AD	406	BCR	C20-C21-C22	2.06	130.17	127.20
26	BC	515	BCR	C32-C1-C6	2.06	113.53	110.30
22	AB	610	CLA	C16-C15-C13	2.06	122.33	115.49
26	AT	102	BCR	C37-C22-C23	2.06	121.53	118.10
29	AF	101	SQD	O47-C7-C8	2.06	116.01	111.53
22	BB	610	CLA	C6-C5-C3	2.06	117.02	112.48
22	BB	616	CLA	CMB-C2B-C3B	2.07	129.13	125.09
26	BC	515	BCR	C36-C18-C19	2.07	121.54	118.10
26	BA	410	BCR	C32-C1-C6	2.07	113.55	110.30
29	BF	101	SQD	C32-C31-C30	2.07	129.71	113.44
26	BB	622	BCR	C16-C17-C18	2.07	130.19	127.20
26	BJ	102	BCR	C34-C9-C8	2.07	121.55	118.10
26	BA	410	BCR	C40-C30-C25	2.08	113.56	110.30
22	AB	604	CLA	C2A-C1A-CHA	2.08	127.71	123.89
23	BA	406	PHO	CMD-C2D-C1D	2.08	128.44	125.06
26	BK	102	BCR	C28-C27-C26	2.08	117.17	113.87
22	BB	618	CLA	C2A-C1A-CHA	2.08	127.72	123.89
22	BB	607	CLA	C6-C5-C3	2.08	117.06	112.48
26	BJ	102	BCR	C3-C4-C5	2.09	117.18	113.87
26	AB	617	BCR	C16-C17-C18	2.09	130.21	127.20
26	BD	406	BCR	C7-C8-C9	2.09	129.40	126.22
30	BI	101	LMG	O1-C1-C2	2.09	110.68	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AB	620	BCR	C1-C6-C7	2.09	121.67	115.82
29	AF	101	SQD	C32-C31-C30	2.09	129.86	113.44
22	BB	609	CLA	C2A-C1A-CHA	2.09	127.74	123.89
26	BZ	101	BCR	C34-C9-C8	2.09	121.58	118.10
23	AA	405	PHO	CMD-C2D-C1D	2.09	128.47	125.06
26	AB	618	BCR	C28-C27-C26	2.10	117.19	113.87
34	BE	101	HEM	C2D-C3D-C4D	2.10	105.05	101.50
34	AV	201	HEM	C3B-C4B-CHC	2.10	126.12	123.16
32	BB	626	LMT	O1B-C1B-C2B	2.10	113.21	108.10
26	AD	406	BCR	C16-C17-C18	2.10	130.23	127.20
26	AH	101	BCR	C36-C18-C19	2.10	121.59	118.10
22	AB	610	CLA	CMB-C2B-C3B	2.11	129.21	125.09
26	AC	515	BCR	C32-C1-C6	2.11	113.62	110.30
26	BB	621	BCR	C7-C8-C9	2.12	129.44	126.22
22	AA	402	CLA	C16-C15-C13	2.12	122.50	115.49
26	AZ	101	BCR	C28-C27-C26	2.12	117.22	113.87
26	BB	621	BCR	C1-C6-C7	2.12	121.75	115.82
26	AC	515	BCR	C37-C22-C23	2.12	121.62	118.10
22	AB	601	CLA	C2A-C1A-CHA	2.12	127.79	123.89
29	AD	409	SQD	C15-C14-C13	2.12	125.48	114.53
26	AB	620	BCR	C40-C30-C25	2.12	113.63	110.30
22	BC	501	CLA	C6-C5-C3	2.12	117.14	112.48
26	AA	409	BCR	C34-C9-C8	2.13	121.63	118.10
22	AC	504	CLA	CED-O2D-CGD	2.13	120.97	115.99
22	AD	402	CLA	CMB-C2B-C3B	2.13	129.25	125.09
26	AB	620	BCR	C30-C25-C24	2.13	121.77	115.82
22	BB	604	CLA	C2A-C1A-CHA	2.13	127.80	123.89
30	BD	408	LMG	O1-C1-C2	2.13	110.73	108.04
22	BB	619	CLA	O2D-CGD-CBD	2.13	114.22	111.30
34	AV	201	HEM	C2D-C3D-C4D	2.13	105.11	101.50
26	AK	102	BCR	C8-C7-C6	2.13	133.72	127.32
26	BA	410	BCR	C35-C13-C12	2.13	121.65	118.10
29	AF	101	SQD	O48-C46-C45	2.14	114.44	108.69
22	AB	614	CLA	CBA-CAA-C2A	2.14	119.76	113.73
26	BK	102	BCR	C8-C7-C6	2.14	133.74	127.32
26	AC	514	BCR	C11-C10-C9	2.14	130.29	127.20
22	BB	615	CLA	CBA-CAA-C2A	2.14	119.78	113.73
22	AB	615	CLA	C2A-C1A-CHA	2.14	127.83	123.89
26	BC	515	BCR	C35-C13-C12	2.14	121.67	118.10
22	AA	406	CLA	C6-C5-C3	2.15	117.20	112.48
26	AB	617	BCR	C36-C18-C19	2.15	121.67	118.10
22	BB	617	CLA	C16-C15-C13	2.15	122.62	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AA	409	BCR	C1-C6-C7	2.15	121.84	115.82
26	AB	618	BCR	C35-C13-C12	2.15	121.68	118.10
26	BD	406	BCR	C16-C17-C18	2.15	130.31	127.20
26	BD	406	BCR	C32-C1-C6	2.15	113.68	110.30
30	AB	623	LMG	O6-C5-C6	2.15	111.80	106.36
26	AB	619	BCR	C1-C6-C7	2.16	121.86	115.82
22	AB	604	CLA	CED-O2D-CGD	2.16	121.05	115.99
29	BF	101	SQD	O48-C46-C45	2.16	114.50	108.69
22	AC	501	CLA	CBA-CAA-C2A	2.16	119.83	113.73
26	BX	101	BCR	C32-C1-C6	2.16	113.69	110.30
26	AH	101	BCR	C37-C22-C23	2.16	121.69	118.10
26	AT	102	BCR	C20-C21-C22	2.16	130.32	127.20
29	BD	409	SQD	C15-C14-C13	2.17	125.71	114.53
26	BZ	101	BCR	C1-C6-C7	2.17	121.89	115.82
26	BB	622	BCR	C1-C6-C7	2.17	121.89	115.82
22	AB	607	CLA	O2D-CGD-CBD	2.17	114.27	111.30
22	BA	403	CLA	O2D-CGD-CBD	2.17	114.28	111.30
34	BV	201	HEM	C2D-C3D-C4D	2.17	105.18	101.50
26	BB	622	BCR	C28-C27-C26	2.17	117.31	113.87
26	AB	618	BCR	C37-C22-C23	2.18	121.72	118.10
26	BB	622	BCR	C8-C7-C6	2.18	133.86	127.32
26	AB	618	BCR	C16-C17-C18	2.18	130.35	127.20
26	BC	514	BCR	C11-C10-C9	2.19	130.36	127.20
29	BL	101	SQD	C15-C14-C13	2.19	125.84	114.53
22	AC	512	CLA	C2A-C1A-CHA	2.19	127.92	123.89
26	AC	514	BCR	C30-C25-C24	2.19	121.95	115.82
26	AT	102	BCR	C30-C25-C24	2.19	121.96	115.82
26	AB	620	BCR	C16-C17-C18	2.19	130.36	127.20
26	AK	102	BCR	C40-C30-C25	2.19	113.74	110.30
29	BA	413	SQD	C17-C16-C15	2.19	125.86	114.53
26	BX	101	BCR	C37-C22-C23	2.20	121.75	118.10
29	AA	415	SQD	O8-S-O7	2.20	116.73	111.61
26	AT	102	BCR	C35-C13-C12	2.20	121.76	118.10
30	BE	102	LMG	C8-O7-C10	2.20	123.18	117.89
22	AB	616	CLA	CBA-CAA-C2A	2.21	119.95	113.73
30	BI	101	LMG	O6-C1-C2	2.21	114.81	110.28
22	AC	501	CLA	C6-C5-C3	2.21	117.33	112.48
26	BX	101	BCR	C36-C18-C19	2.21	121.78	118.10
26	BB	622	BCR	C30-C25-C24	2.21	122.01	115.82
22	AB	614	CLA	C16-C15-C13	2.21	122.83	115.49
22	BB	611	CLA	C6-C7-C8	2.21	122.83	115.49
26	BA	410	BCR	C34-C9-C8	2.22	121.79	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AC	514	BCR	C37-C22-C23	2.23	121.80	118.10
29	AF	101	SQD	C15-C14-C13	2.23	126.04	114.53
22	AC	505	CLA	C2A-C1A-CHA	2.23	127.99	123.89
22	AD	402	CLA	C6-C5-C3	2.23	117.38	112.48
29	AA	412	SQD	C17-C16-C15	2.23	126.04	114.53
32	AB	627	LMT	O1B-C1B-C2B	2.23	113.53	108.10
26	AC	514	BCR	C40-C30-C25	2.23	113.80	110.30
27	BC	517	DGD	O6D-C5D-C6D	2.24	111.18	106.61
22	BB	612	CLA	O2D-CGD-CBD	2.24	114.37	111.30
26	AZ	101	BCR	C1-C6-C7	2.24	122.09	115.82
32	BT	101	LMT	O1B-C4'-C3'	2.24	112.96	107.17
29	BA	401	SQD	O5-C5-C4	2.25	113.90	109.68
22	BC	501	CLA	CBA-CAA-C2A	2.25	120.08	113.73
22	AC	513	CLA	CBA-CAA-C2A	2.25	120.08	113.73
26	AT	102	BCR	C36-C18-C19	2.25	121.84	118.10
24	BJ	101	PL9	C15-C14-C16	2.25	118.84	115.41
26	BZ	101	BCR	C28-C27-C26	2.25	117.44	113.87
23	BA	406	PHO	O2A-CGA-CBA	2.25	118.76	111.90
22	AD	402	CLA	C2A-C1A-CHA	2.25	128.03	123.89
26	AT	102	BCR	C32-C1-C6	2.25	113.83	110.30
26	AK	102	BCR	C37-C22-C23	2.25	121.84	118.10
22	BB	607	CLA	CED-O2D-CGD	2.25	121.27	115.99
22	AC	505	CLA	O2D-CGD-CBD	2.25	114.39	111.30
26	AA	409	BCR	C35-C13-C12	2.26	121.85	118.10
26	AB	620	BCR	C8-C7-C6	2.26	134.10	127.32
29	BF	101	SQD	C15-C14-C13	2.26	126.21	114.53
27	BD	410	DGD	O6D-C5D-C4D	2.26	113.93	109.68
22	AB	601	CLA	C6-C5-C3	2.27	117.45	112.48
29	BD	409	SQD	O8-S-O7	2.27	116.88	111.61
22	AB	604	CLA	C6-C5-C3	2.27	117.46	112.48
22	AB	609	CLA	O2D-CGD-CBD	2.27	114.41	111.30
22	AB	602	CLA	O2D-CGD-CBD	2.27	114.41	111.30
26	AZ	101	BCR	C36-C18-C19	2.27	121.88	118.10
22	BD	402	CLA	CMB-C2B-C3B	2.27	129.54	125.09
26	BK	102	BCR	C37-C22-C23	2.27	121.88	118.10
27	BC	516	DGD	O3G-C1D-C2D	2.27	110.91	108.04
29	BA	401	SQD	C34-C33-C32	2.28	126.30	114.53
26	BD	406	BCR	C35-C13-C12	2.28	121.89	118.10
26	BK	102	BCR	C40-C30-C25	2.28	113.88	110.30
26	BC	515	BCR	C37-C22-C23	2.28	121.90	118.10
22	AB	613	CLA	O2D-CGD-CBD	2.28	114.43	111.30
27	BD	410	DGD	C2G-O2G-C1B	2.29	123.38	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	512	CLA	C6-C5-C3	2.29	117.51	112.48
22	BC	512	CLA	C2A-C1A-CHA	2.29	128.10	123.89
29	AD	409	SQD	O8-S-O7	2.29	116.95	111.61
22	AA	402	CLA	O2D-CGD-CBD	2.29	114.44	111.30
26	AB	618	BCR	C36-C18-C19	2.29	121.91	118.10
22	AB	608	CLA	O2D-CGD-CBD	2.30	114.45	111.30
26	BC	514	BCR	C30-C25-C24	2.30	122.25	115.82
29	AA	415	SQD	C15-C14-C13	2.30	126.39	114.53
22	BC	512	CLA	C6-C5-C3	2.30	117.53	112.48
26	BC	514	BCR	C7-C8-C9	2.30	129.72	126.22
22	BB	616	CLA	O2D-CGD-CBD	2.30	114.45	111.30
26	BX	101	BCR	C1-C6-C7	2.30	122.26	115.82
22	BD	402	CLA	C2A-C1A-CHA	2.31	128.14	123.89
26	AC	514	BCR	C1-C6-C7	2.32	122.31	115.82
22	BC	505	CLA	C2A-C1A-CHA	2.32	128.16	123.89
29	BB	601	SQD	C15-C14-C13	2.32	126.52	114.53
26	AB	618	BCR	C20-C21-C22	2.32	130.55	127.20
22	BB	619	CLA	CBA-CAA-C2A	2.32	120.29	113.73
26	BB	620	BCR	C35-C13-C12	2.32	121.96	118.10
26	BC	514	BCR	C37-C22-C23	2.32	121.96	118.10
26	AH	101	BCR	C32-C1-C6	2.33	113.95	110.30
29	BA	401	SQD	C15-C14-C13	2.33	126.55	114.53
22	AC	511	CLA	O2D-CGD-CBD	2.33	114.50	111.30
27	AB	626	DGD	O6D-C5D-C6D	2.34	111.38	106.61
26	AB	618	BCR	C30-C25-C24	2.34	122.36	115.82
26	BZ	101	BCR	C36-C18-C19	2.34	121.98	118.10
27	AC	517	DGD	O6D-C5D-C6D	2.34	111.38	106.61
22	BB	613	CLA	CED-O2D-CGD	2.34	121.47	115.99
26	BB	622	BCR	C32-C1-C6	2.34	113.97	110.30
26	AT	102	BCR	C7-C8-C9	2.34	129.78	126.22
29	BL	101	SQD	O47-C7-C8	2.34	116.62	111.53
23	AA	405	PHO	O2A-CGA-CBA	2.35	119.05	111.90
26	AA	409	BCR	C30-C25-C24	2.35	122.39	115.82
22	AD	402	CLA	O2D-CGD-CBD	2.35	114.52	111.30
22	AC	511	CLA	C2A-C1A-CHA	2.35	128.22	123.89
22	AB	608	CLA	C6-C7-C8	2.35	123.29	115.49
26	AB	620	BCR	C32-C1-C6	2.36	114.00	110.30
30	BE	102	LMG	O7-C8-C7	2.37	116.70	108.36
24	AJ	101	PL9	C15-C14-C16	2.37	119.02	115.41
22	BD	402	CLA	C6-C5-C3	2.37	117.69	112.48
26	AT	102	BCR	C11-C10-C9	2.37	130.62	127.20
26	AD	406	BCR	C35-C13-C12	2.38	122.05	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	511	CLA	C2A-C1A-CHA	2.38	128.26	123.89
22	BC	506	CLA	C6-C5-C3	2.38	117.70	112.48
32	AT	101	LMT	O1B-C4'-C3'	2.38	113.31	107.17
27	AD	410	DGD	C2G-O2G-C1B	2.38	123.60	117.89
22	AB	610	CLA	CED-O2D-CGD	2.38	121.58	115.99
26	BC	514	BCR	C1-C6-C7	2.38	122.50	115.82
26	AC	515	BCR	C35-C13-C12	2.39	122.07	118.10
26	BA	410	BCR	C16-C17-C18	2.39	130.64	127.20
22	AB	608	CLA	CBA-CAA-C2A	2.39	120.47	113.73
26	BJ	102	BCR	C28-C27-C26	2.39	117.66	113.87
22	AB	613	CLA	CED-O2D-CGD	2.39	121.59	115.99
29	BA	413	SQD	C44-O6-C1	2.39	118.84	113.82
26	AH	101	BCR	C1-C6-C7	2.39	122.52	115.82
22	BA	407	CLA	C6-C5-C3	2.39	117.73	112.48
34	AE	101	HEM	C3B-C4B-CHC	2.39	126.53	123.16
22	AA	406	CLA	O2D-CGD-CBD	2.39	114.58	111.30
29	BA	401	SQD	C36-C35-C34	2.39	126.90	114.53
29	AA	415	SQD	C45-O47-C7	2.40	123.64	117.89
22	BB	610	CLA	O2D-CGD-CBD	2.40	114.59	111.30
29	BB	601	SQD	C44-O6-C1	2.40	118.86	113.82
29	AA	415	SQD	C34-C33-C32	2.40	126.93	114.53
22	BC	504	CLA	O2D-CGD-CBD	2.40	114.59	111.30
22	AB	609	CLA	O2A-CGA-CBA	2.40	119.22	111.90
27	AD	410	DGD	O6D-C5D-C6D	2.40	111.52	106.61
22	BC	507	CLA	C6-C5-C3	2.40	117.76	112.48
27	AC	516	DGD	O3G-C1D-C2D	2.40	111.08	108.04
22	BA	405	CLA	O2A-CGA-CBA	2.41	119.23	111.90
22	BC	513	CLA	C6-C5-C3	2.41	117.77	112.48
30	AC	520	LMG	O8-C28-C29	2.41	119.24	111.90
26	BB	620	BCR	C16-C17-C18	2.41	130.68	127.20
34	BE	101	HEM	C3B-C4B-CHC	2.41	126.56	123.16
22	BB	609	CLA	CBA-CAA-C2A	2.41	120.54	113.73
22	BB	612	CLA	O2A-CGA-CBA	2.41	119.25	111.90
30	AA	416	LMG	O6-C5-C6	2.41	112.46	106.36
22	AB	606	CLA	CBA-CAA-C2A	2.42	120.56	113.73
29	BL	101	SQD	C31-C30-C29	2.42	132.47	113.44
29	BA	413	SQD	O47-C7-C8	2.42	116.79	111.53
30	BC	519	LMG	O1-C1-C2	2.42	111.10	108.04
22	AA	404	CLA	O2A-CGA-CBA	2.43	119.29	111.90
22	BB	604	CLA	C6-C5-C3	2.43	117.82	112.48
22	BB	616	CLA	CED-O2D-CGD	2.43	121.69	115.99
22	BC	507	CLA	C2A-C1A-CHA	2.43	128.36	123.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BA	413	SQD	O8-S-O7	2.43	117.27	111.61
32	BB	603	LMT	O1B-C1B-C2B	2.43	114.02	108.10
22	AC	507	CLA	C2A-C1A-CHA	2.44	128.37	123.89
26	BB	622	BCR	C23-C24-C25	2.44	134.64	127.32
26	AB	618	BCR	C7-C8-C9	2.44	129.93	126.22
29	BB	601	SQD	C31-C30-C29	2.44	132.62	113.44
26	AB	618	BCR	C11-C10-C9	2.44	130.72	127.20
29	BD	409	SQD	C31-C30-C29	2.44	132.63	113.44
29	AA	412	SQD	C15-C14-C13	2.44	127.14	114.53
26	BC	515	BCR	C24-C23-C22	2.44	129.94	126.22
29	AA	415	SQD	C36-C35-C34	2.45	127.18	114.53
22	BC	512	CLA	CED-O2D-CGD	2.45	121.74	115.99
22	BB	609	CLA	CED-O2D-CGD	2.45	121.74	115.99
27	BD	410	DGD	O6D-C5D-C6D	2.46	111.63	106.61
27	AD	410	DGD	O6D-C5D-C4D	2.46	114.30	109.68
26	AZ	101	BCR	C35-C13-C12	2.46	122.19	118.10
30	BB	624	LMG	O6-C5-C6	2.46	112.58	106.36
27	BH	101	DGD	O3G-C1D-C2D	2.47	111.16	108.04
22	AB	606	CLA	O2D-CGD-CBD	2.47	114.69	111.30
22	BB	611	CLA	CBA-CAA-C2A	2.47	120.71	113.73
29	BA	413	SQD	C15-C14-C13	2.47	127.30	114.53
22	AC	513	CLA	C6-C5-C3	2.48	117.92	112.48
29	BB	601	SQD	O47-C7-C8	2.48	116.92	111.53
29	AD	409	SQD	C31-C30-C29	2.49	132.96	113.44
22	BB	604	CLA	C1D-CHD-C4C	2.49	126.36	122.60
26	AB	617	BCR	C35-C13-C12	2.49	122.23	118.10
26	AC	515	BCR	C30-C25-C24	2.49	122.78	115.82
22	BC	506	CLA	O2D-CGD-CBD	2.49	114.71	111.30
28	AA	411	LHG	O7-C7-C8	2.49	116.93	111.53
26	AC	514	BCR	C7-C8-C9	2.49	130.01	126.22
22	AB	613	CLA	C6-C5-C3	2.49	117.95	112.48
26	BA	410	BCR	C30-C25-C24	2.49	122.80	115.82
22	AB	616	CLA	O2D-CGD-CBD	2.50	114.72	111.30
22	AA	404	CLA	CAA-CBA-CGA	2.50	120.62	113.32
29	AF	101	SQD	C45-O47-C7	2.50	123.88	117.89
26	AH	101	BCR	C35-C13-C12	2.50	122.25	118.10
26	AJ	102	BCR	C28-C27-C26	2.50	117.83	113.87
26	AB	620	BCR	C23-C24-C25	2.50	134.84	127.32
30	AB	622	LMG	O6-C5-C6	2.50	112.69	106.36
30	BC	520	LMG	O8-C28-C29	2.50	119.53	111.90
22	BC	505	CLA	C6-C5-C3	2.51	117.98	112.48
26	AA	409	BCR	C37-C22-C23	2.51	122.27	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AB	618	BCR	C32-C1-C6	2.51	114.23	110.30
22	AC	507	CLA	C6-C5-C3	2.51	117.99	112.48
26	AB	619	BCR	C32-C1-C6	2.51	114.24	110.30
29	AA	412	SQD	O8-S-O7	2.51	117.45	111.61
28	BA	412	LHG	O7-C7-C8	2.51	116.98	111.53
29	BF	101	SQD	C45-O47-C7	2.51	123.92	117.89
26	BD	406	BCR	C23-C24-C25	2.52	134.88	127.32
22	BB	609	CLA	O2D-CGD-CBD	2.52	114.75	111.30
22	AA	403	CLA	CED-O2D-CGD	2.52	121.90	115.99
22	BB	605	CLA	O2D-CGD-CBD	2.52	114.76	111.30
24	AD	405	PL9	C10-C9-C11	2.53	119.27	115.41
26	BD	406	BCR	C15-C14-C13	2.53	130.85	127.20
26	BK	102	BCR	C30-C25-C24	2.53	122.92	115.82
26	AZ	101	BCR	C8-C7-C6	2.54	134.94	127.32
22	AA	402	CLA	CBA-CAA-C2A	2.54	120.90	113.73
22	AB	606	CLA	CED-O2D-CGD	2.54	121.95	115.99
26	BC	515	BCR	C30-C25-C24	2.54	122.94	115.82
22	BB	616	CLA	C6-C5-C3	2.54	118.06	112.48
26	AC	515	BCR	C24-C23-C22	2.54	130.09	126.22
26	AH	101	BCR	C23-C24-C25	2.54	134.96	127.32
26	AB	620	BCR	C7-C8-C9	2.54	130.09	126.22
22	BA	405	CLA	CAA-CBA-CGA	2.55	120.77	113.32
30	AI	101	LMG	O6-C5-C6	2.55	112.79	106.36
26	AJ	102	BCR	C3-C4-C5	2.55	117.91	113.87
32	BT	101	LMT	O1B-C1B-C2B	2.55	114.31	108.10
26	AK	102	BCR	C35-C13-C12	2.56	122.35	118.10
26	AA	409	BCR	C16-C17-C18	2.56	130.89	127.20
22	BA	403	CLA	CBA-CAA-C2A	2.56	120.95	113.73
22	AA	403	CLA	C1D-CHD-C4C	2.56	126.47	122.60
26	BB	621	BCR	C32-C1-C6	2.56	114.31	110.30
29	BL	101	SQD	C44-O6-C1	2.56	119.20	113.82
22	BC	506	CLA	O2A-CGA-CBA	2.56	119.70	111.90
22	AB	616	CLA	C1D-CHD-C4C	2.56	126.48	122.60
26	AD	406	BCR	C15-C14-C13	2.56	130.90	127.20
22	BC	513	CLA	O2D-CGD-CBD	2.57	114.82	111.30
30	AC	519	LMG	O1-C1-C2	2.57	111.28	108.04
30	AE	102	LMG	O7-C8-C7	2.57	117.42	108.36
23	AA	405	PHO	CBD-CHA-C1A	2.57	132.41	126.36
27	BA	411	DGD	O6D-C5D-C6D	2.57	111.87	106.61
22	AB	601	CLA	C1D-CHD-C4C	2.57	126.50	122.60
26	AJ	102	BCR	C16-C17-C18	2.57	130.91	127.20
22	AC	506	CLA	C6-C5-C3	2.57	118.14	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	502	CLA	O2A-CGA-CBA	2.58	119.75	111.90
26	BZ	101	BCR	C8-C7-C6	2.58	135.05	127.32
24	AD	405	PL9	C35-C34-C36	2.58	119.34	115.41
22	AC	505	CLA	C6-C5-C3	2.58	118.14	112.48
26	BX	101	BCR	C23-C24-C25	2.58	135.07	127.32
24	BD	405	PL9	C10-C9-C11	2.59	119.36	115.41
29	AA	412	SQD	O47-C7-C8	2.59	117.16	111.53
27	BB	602	DGD	O6D-C5D-C6D	2.59	111.90	106.61
22	BB	608	CLA	O2D-CGD-CBD	2.61	114.88	111.30
22	BB	619	CLA	C1D-CHD-C4C	2.61	126.55	122.60
22	AC	508	CLA	CED-O2D-CGD	2.62	122.12	115.99
26	BC	514	BCR	C23-C24-C25	2.62	135.17	127.32
22	AC	506	CLA	O2A-CGA-CBA	2.62	119.88	111.90
22	AC	513	CLA	O2D-CGD-CBD	2.62	114.89	111.30
22	BC	504	CLA	O2A-CGA-CBA	2.62	119.89	111.90
26	AC	514	BCR	C23-C24-C25	2.62	135.20	127.32
27	AA	410	DGD	O6D-C5D-C6D	2.63	111.98	106.61
26	AJ	102	BCR	C31-C1-C2	2.63	118.20	108.79
22	BA	404	CLA	CED-O2D-CGD	2.63	122.16	115.99
22	BC	510	CLA	CED-O2D-CGD	2.63	122.17	115.99
22	AC	502	CLA	O2A-CGA-CBA	2.64	119.94	111.90
23	BA	406	PHO	CED-O2D-CGD	2.64	122.18	115.99
30	AA	413	LMG	O7-C10-C11	2.64	117.26	111.53
26	BJ	102	BCR	C31-C1-C2	2.64	118.23	108.79
26	AD	406	BCR	C23-C24-C25	2.64	135.24	127.32
22	AC	504	CLA	O2A-CGA-CBA	2.64	119.95	111.90
26	BK	102	BCR	C35-C13-C12	2.64	122.50	118.10
29	BA	401	SQD	C45-O47-C7	2.65	124.24	117.89
22	BC	503	CLA	CED-O2D-CGD	2.65	122.19	115.99
30	BC	519	LMG	O7-C10-C11	2.65	117.28	111.53
30	BI	101	LMG	O6-C5-C6	2.65	113.06	106.36
22	BB	616	CLA	O2A-CGA-CBA	2.65	119.98	111.90
34	AV	201	HEM	CMD-C2D-C3D	2.66	126.10	114.35
22	BB	606	CLA	C6-C5-C3	2.66	118.31	112.48
30	BD	407	LMG	O6-C5-C6	2.66	113.07	106.36
34	BE	101	HEM	CMD-C2D-C3D	2.66	126.11	114.35
26	AA	409	BCR	C23-C24-C25	2.66	135.30	127.32
30	AC	519	LMG	O6-C5-C6	2.66	113.08	106.36
22	AD	402	CLA	CED-O2D-CGD	2.66	122.23	115.99
34	AE	101	HEM	CMD-C2D-C3D	2.67	126.14	114.35
26	BX	101	BCR	C35-C13-C12	2.67	122.54	118.10
22	AC	512	CLA	CED-O2D-CGD	2.67	122.25	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	612	CLA	CED-O2D-CGD	2.67	122.26	115.99
26	AK	102	BCR	C30-C25-C24	2.68	123.31	115.82
22	AB	610	CLA	O2A-CGA-CBA	2.68	120.06	111.90
23	BA	406	PHO	CBD-CHA-C1A	2.68	132.66	126.36
22	AB	611	CLA	O2A-CGA-CBA	2.68	120.06	111.90
23	AD	403	PHO	CBD-CHA-C1A	2.68	132.67	126.36
22	BB	619	CLA	C6-C5-C3	2.68	118.36	112.48
22	AB	607	CLA	C1D-CHD-C4C	2.68	126.66	122.60
22	BA	403	CLA	C1D-CHD-C4C	2.68	126.66	122.60
24	BD	405	PL9	C40-C39-C41	2.69	119.51	115.41
26	BA	410	BCR	C23-C24-C25	2.69	135.38	127.32
22	AB	613	CLA	O2A-CGA-CBA	2.69	120.09	111.90
26	BB	622	BCR	C7-C8-C9	2.69	130.32	126.22
24	BJ	101	PL9	C20-C19-C21	2.69	119.52	115.41
23	AD	403	PHO	O2A-CGA-CBA	2.69	120.11	111.90
22	BC	503	CLA	O2A-CGA-CBA	2.70	120.11	111.90
30	BC	520	LMG	O6-C5-C6	2.70	113.17	106.36
23	BD	403	PHO	CBD-CHA-C1A	2.70	132.72	126.36
22	BC	511	CLA	O2A-CGA-CBA	2.70	120.13	111.90
26	AC	515	BCR	C16-C17-C18	2.71	131.10	127.20
22	BA	405	CLA	CED-O2D-CGD	2.71	122.34	115.99
22	BD	402	CLA	O2D-CGD-CBD	2.71	115.01	111.30
26	BC	515	BCR	C16-C17-C18	2.71	131.11	127.20
22	AB	603	CLA	C6-C5-C3	2.71	118.43	112.48
26	AD	406	BCR	C37-C22-C23	2.71	122.61	118.10
28	BC	521	LHG	O8-C23-C24	2.71	120.16	111.90
23	BD	403	PHO	O2A-CGA-CBA	2.71	120.16	111.90
28	AC	521	LHG	O8-C23-C24	2.71	120.17	111.90
24	BA	408	PL9	C20-C19-C21	2.71	119.55	115.41
22	BD	404	CLA	CED-O2D-CGD	2.71	122.35	115.99
34	BV	201	HEM	CMD-C2D-C3D	2.72	126.37	114.35
22	BB	608	CLA	O2A-CGA-CBA	2.72	120.19	111.90
22	AC	503	CLA	CED-O2D-CGD	2.72	122.37	115.99
22	BC	513	CLA	O2A-CGA-CBA	2.72	120.19	111.90
22	AC	501	CLA	CED-O2D-CGD	2.72	122.37	115.99
22	BB	611	CLA	O2D-CGD-CBD	2.72	115.03	111.30
27	AB	626	DGD	O5D-C6D-C5D	2.72	114.01	109.08
23	BA	406	PHO	C6-C5-C3	2.72	118.46	112.48
24	AD	405	PL9	C30-C29-C31	2.72	119.57	115.41
27	AH	102	DGD	O3G-C1D-C2D	2.73	111.48	108.04
26	BA	410	BCR	C37-C22-C23	2.73	122.64	118.10
30	BM	102	LMG	O1-C1-C2	2.73	111.49	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BZ	101	BCR	C35-C13-C12	2.73	122.65	118.10
22	AA	402	CLA	C1D-CHD-C4C	2.75	126.76	122.60
32	AT	101	LMT	O1B-C1B-C2B	2.75	114.79	108.10
22	BB	618	CLA	CED-O2D-CGD	2.75	122.45	115.99
22	AB	605	CLA	C1D-CHD-C4C	2.76	126.78	122.60
26	BX	101	BCR	C11-C10-C9	2.76	131.18	127.20
26	BC	514	BCR	C40-C30-C25	2.76	114.63	110.30
26	BD	406	BCR	C37-C22-C23	2.76	122.69	118.10
22	AC	510	CLA	CED-O2D-CGD	2.76	122.46	115.99
22	BD	402	CLA	CED-O2D-CGD	2.76	122.47	115.99
22	AC	503	CLA	O2A-CGA-CBA	2.77	120.33	111.90
22	AC	513	CLA	O2A-CGA-CBA	2.77	120.33	111.90
22	AC	506	CLA	O2D-CGD-CBD	2.77	115.10	111.30
22	BC	506	CLA	C1D-CHD-C4C	2.77	126.80	122.60
27	AC	517	DGD	C1E-O6E-C5E	2.78	119.14	113.75
22	BB	611	CLA	CED-O2D-CGD	2.78	122.52	115.99
22	AB	602	CLA	C1D-CHD-C4C	2.79	126.82	122.60
22	BB	610	CLA	C1D-CHD-C4C	2.79	126.82	122.60
22	AB	606	CLA	C1D-CHD-C4C	2.79	126.82	122.60
29	BD	409	SQD	O47-C7-C8	2.79	117.59	111.53
22	BA	407	CLA	O2D-CGD-CBD	2.79	115.13	111.30
22	BB	617	CLA	O2A-CGA-CBA	2.79	120.41	111.90
30	BC	519	LMG	O6-C5-C6	2.79	113.42	106.36
26	AB	619	BCR	C8-C7-C6	2.79	135.71	127.32
26	AB	619	BCR	C23-C24-C25	2.79	135.71	127.32
24	BA	408	PL9	C10-C9-C11	2.79	119.68	115.41
22	AB	614	CLA	O2A-CGA-CBA	2.80	120.42	111.90
22	BC	501	CLA	CED-O2D-CGD	2.80	122.56	115.99
22	BC	508	CLA	CED-O2D-CGD	2.80	122.56	115.99
22	AA	406	CLA	O2A-CGA-CBA	2.80	120.44	111.90
22	AC	507	CLA	CED-O2D-CGD	2.80	122.56	115.99
22	AB	608	CLA	CED-O2D-CGD	2.80	122.56	115.99
26	AB	618	BCR	C23-C24-C25	2.80	135.74	127.32
22	AB	611	CLA	C1D-CHD-C4C	2.81	126.85	122.60
30	AD	407	LMG	O6-C5-C6	2.81	113.45	106.36
22	BB	612	CLA	C6-C5-C3	2.81	118.64	112.48
22	AB	612	CLA	O2A-CGA-CBA	2.81	120.45	111.90
26	BC	514	BCR	C32-C1-C6	2.81	114.71	110.30
22	BB	614	CLA	CED-O2D-CGD	2.81	122.58	115.99
22	BB	606	CLA	CED-O2D-CGD	2.81	122.58	115.99
22	BB	605	CLA	C1D-CHD-C4C	2.81	126.86	122.60
22	BB	614	CLA	C6-C5-C3	2.81	118.66	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	407	CLA	O2A-CGA-CBA	2.81	120.47	111.90
22	BB	604	CLA	CED-O2D-CGD	2.81	122.59	115.99
29	AD	409	SQD	O47-C7-C8	2.82	117.65	111.53
24	BD	405	PL9	C35-C34-C36	2.82	119.71	115.41
22	BD	404	CLA	O2A-CGA-CBA	2.82	120.49	111.90
26	AK	102	BCR	C34-C9-C8	2.82	122.79	118.10
22	AC	506	CLA	C1D-CHD-C4C	2.82	126.87	122.60
22	AB	616	CLA	O2A-CGA-CBA	2.82	120.50	111.90
22	BB	614	CLA	C1D-CHD-C4C	2.82	126.88	122.60
22	BB	607	CLA	O2A-CGA-CBA	2.83	120.51	111.90
22	AD	404	CLA	O2A-CGA-CBA	2.83	120.52	111.90
22	BA	404	CLA	C1D-CHD-C4C	2.83	126.88	122.60
24	BD	405	PL9	C30-C29-C31	2.83	119.73	115.41
22	AA	406	CLA	CED-O2D-CGD	2.83	122.63	115.99
24	BD	405	PL9	C45-C44-C46	2.84	119.74	115.41
22	BB	613	CLA	O2A-CGA-CBA	2.84	120.56	111.90
24	AD	405	PL9	C40-C39-C41	2.84	119.75	115.41
30	AC	519	LMG	O7-C10-C11	2.85	117.71	111.53
22	BB	615	CLA	O2A-CGA-CBA	2.85	120.57	111.90
22	BB	614	CLA	O2A-CGA-CBA	2.85	120.57	111.90
22	AD	404	CLA	CED-O2D-CGD	2.85	122.68	115.99
22	AB	604	CLA	O2A-CGA-CBA	2.86	120.61	111.90
22	BC	508	CLA	O2A-CGA-CBA	2.86	120.61	111.90
22	AC	508	CLA	O2A-CGA-CBA	2.86	120.62	111.90
26	AC	514	BCR	C35-C13-C12	2.86	122.86	118.10
22	BC	504	CLA	C1D-CHD-C4C	2.86	126.93	122.60
26	BB	621	BCR	C8-C7-C6	2.86	135.92	127.32
22	BB	608	CLA	C1D-CHD-C4C	2.86	126.94	122.60
26	AT	102	BCR	C23-C24-C25	2.86	135.92	127.32
27	AC	516	DGD	O2G-C1B-C2B	2.87	117.75	111.53
22	BC	510	CLA	O2A-CGA-CBA	2.87	120.64	111.90
22	AC	501	CLA	C1D-CHD-C4C	2.87	126.94	122.60
22	BB	617	CLA	CED-O2D-CGD	2.87	122.72	115.99
22	BB	618	CLA	O2A-CGA-CBA	2.87	120.64	111.90
22	BA	407	CLA	C1D-CHD-C4C	2.87	126.95	122.60
27	BC	517	DGD	C1E-O6E-C5E	2.87	119.32	113.75
22	BB	612	CLA	C1D-CHD-C4C	2.87	126.95	122.60
22	AC	511	CLA	O2A-CGA-CBA	2.88	120.66	111.90
22	BB	609	CLA	C1D-CHD-C4C	2.88	126.96	122.60
26	BA	410	BCR	C2-C1-C6	2.88	114.92	110.36
22	AB	609	CLA	C6-C5-C3	2.88	118.80	112.48
22	BB	619	CLA	O2A-CGA-CBA	2.88	120.68	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AC	520	LMG	O6-C5-C6	2.88	113.64	106.36
22	AB	603	CLA	C1D-CHD-C4C	2.89	126.97	122.60
22	AA	404	CLA	O2D-CGD-CBD	2.89	115.26	111.30
22	BC	503	CLA	C1D-CHD-C4C	2.89	126.97	122.60
22	AB	614	CLA	CED-O2D-CGD	2.89	122.76	115.99
22	AC	511	CLA	CED-O2D-CGD	2.89	122.77	115.99
26	BC	514	BCR	C35-C13-C12	2.89	122.91	118.10
24	AJ	101	PL9	C20-C19-C21	2.89	119.82	115.41
22	AB	610	CLA	C6-C5-C3	2.89	118.83	112.48
22	BB	617	CLA	C6-C5-C3	2.89	118.83	112.48
22	AA	404	CLA	CED-O2D-CGD	2.89	122.77	115.99
22	AB	605	CLA	O2A-CGA-CBA	2.89	120.71	111.90
22	BA	403	CLA	CED-O2D-CGD	2.89	122.77	115.99
24	AA	407	PL9	C20-C19-C21	2.89	119.83	115.41
22	BB	604	CLA	O2D-CGD-CBD	2.89	115.27	111.30
24	AA	407	PL9	C15-C14-C16	2.89	119.83	115.41
24	BD	405	PL9	C25-C24-C26	2.90	119.83	115.41
22	AB	604	CLA	C1D-CHD-C4C	2.90	126.99	122.60
22	AB	615	CLA	CED-O2D-CGD	2.90	122.79	115.99
22	AA	406	CLA	C1D-CHD-C4C	2.90	126.99	122.60
22	AA	404	CLA	C1D-CHD-C4C	2.90	126.99	122.60
22	AC	507	CLA	C1D-CHD-C4C	2.90	127.00	122.60
30	AM	101	LMG	O6-C5-C6	2.91	113.70	106.36
22	BB	617	CLA	C1D-CHD-C4C	2.91	127.00	122.60
22	BC	501	CLA	C1D-CHD-C4C	2.91	127.00	122.60
26	BK	102	BCR	C34-C9-C8	2.91	122.94	118.10
22	AA	402	CLA	CED-O2D-CGD	2.91	122.81	115.99
22	AB	615	CLA	O2A-CGA-CBA	2.91	120.77	111.90
26	BB	621	BCR	C23-C24-C25	2.91	136.07	127.32
26	BX	101	BCR	C16-C17-C18	2.91	131.41	127.20
22	BC	502	CLA	C1D-CHD-C4C	2.92	127.01	122.60
22	AC	503	CLA	O2D-CGD-CBD	2.92	115.30	111.30
23	AA	405	PHO	CED-O2D-CGD	2.92	122.83	115.99
22	BB	605	CLA	CED-O2D-CGD	2.92	122.83	115.99
26	BB	620	BCR	C23-C24-C25	2.92	136.08	127.32
29	AA	412	SQD	C44-O6-C1	2.92	119.95	113.82
22	AB	605	CLA	CED-O2D-CGD	2.92	122.84	115.99
23	BD	403	PHO	CED-O2D-CGD	2.92	122.84	115.99
22	AB	603	CLA	CED-O2D-CGD	2.92	122.85	115.99
30	BE	102	LMG	O7-C10-C11	2.92	117.88	111.53
22	AA	403	CLA	C6-C5-C3	2.93	118.91	112.48
22	AB	616	CLA	C6-C5-C3	2.93	118.91	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	614	CLA	C6-C5-C3	2.93	118.91	112.48
22	AB	601	CLA	CED-O2D-CGD	2.93	122.86	115.99
29	BA	401	SQD	C32-C31-C30	2.93	129.66	114.53
26	AB	618	BCR	C24-C23-C22	2.93	130.68	126.22
22	AB	609	CLA	C1D-CHD-C4C	2.93	127.04	122.60
26	AB	617	BCR	C23-C24-C25	2.94	136.14	127.32
22	BC	507	CLA	O2D-CGD-CBD	2.94	115.33	111.30
30	BA	414	LMG	O7-C10-C11	2.94	117.91	111.53
22	BD	404	CLA	C1D-CHD-C4C	2.94	127.05	122.60
30	BE	102	LMG	O6-C5-C6	2.94	113.78	106.36
26	AT	102	BCR	C24-C23-C22	2.94	130.70	126.22
26	BJ	102	BCR	C16-C17-C18	2.94	131.45	127.20
22	AC	505	CLA	CED-O2D-CGD	2.94	122.89	115.99
22	BC	502	CLA	O2D-CGD-CBD	2.94	115.34	111.30
22	AB	601	CLA	O2D-CGD-CBD	2.95	115.34	111.30
30	BM	102	LMG	O6-C5-C6	2.95	113.81	106.36
27	BD	410	DGD	O2G-C1B-C2B	2.95	117.94	111.53
22	BB	606	CLA	O2D-CGD-CBD	2.95	115.35	111.30
26	BB	620	BCR	C8-C7-C6	2.95	136.19	127.32
27	AD	410	DGD	O2G-C1B-C2B	2.95	117.95	111.53
29	AA	415	SQD	C32-C31-C30	2.96	129.80	114.53
22	AC	505	CLA	CBA-CAA-C2A	2.96	122.08	113.73
22	BB	607	CLA	C1D-CHD-C4C	2.96	127.08	122.60
24	AD	405	PL9	C45-C44-C46	2.96	119.93	115.41
22	BB	604	CLA	O2A-CGA-CBA	2.96	120.93	111.90
22	BA	405	CLA	O2D-CGD-CBD	2.96	115.36	111.30
22	BC	507	CLA	C1D-CHD-C4C	2.97	127.09	122.60
22	AC	509	CLA	CED-O2D-CGD	2.97	122.94	115.99
26	AB	617	BCR	C8-C7-C6	2.97	136.23	127.32
30	BB	624	LMG	O7-C10-C11	2.97	117.98	111.53
22	AB	611	CLA	CED-O2D-CGD	2.97	122.96	115.99
30	AE	102	LMG	O6-C5-C6	2.97	113.87	106.36
22	AB	614	CLA	C1D-CHD-C4C	2.98	127.11	122.60
22	BA	405	CLA	C1D-CHD-C4C	2.98	127.11	122.60
22	AB	606	CLA	O2A-CGA-CBA	2.98	120.98	111.90
24	AA	407	PL9	C10-C9-C11	2.98	119.97	115.41
22	BC	505	CLA	CED-O2D-CGD	2.99	122.99	115.99
22	AC	502	CLA	O2D-CGD-CBD	2.99	115.40	111.30
30	AA	416	LMG	O7-C10-C11	2.99	118.02	111.53
22	AB	601	CLA	O2A-CGA-CBA	2.99	121.01	111.90
22	AB	602	CLA	O2A-CGA-CBA	2.99	121.01	111.90
26	AB	619	BCR	C2-C1-C6	3.00	115.11	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AH	101	BCR	C8-C7-C6	3.00	136.33	127.32
22	AC	503	CLA	C1D-CHD-C4C	3.01	127.15	122.60
26	BX	101	BCR	C8-C7-C6	3.01	136.36	127.32
24	AD	405	PL9	C15-C14-C16	3.01	120.01	115.41
22	AC	504	CLA	C1D-CHD-C4C	3.01	127.16	122.60
26	AA	409	BCR	C2-C1-C6	3.02	115.14	110.36
22	BB	609	CLA	O2A-CGA-CBA	3.02	121.09	111.90
26	AH	101	BCR	C16-C17-C18	3.02	131.55	127.20
22	BB	615	CLA	CED-O2D-CGD	3.02	123.06	115.99
22	AB	605	CLA	O2D-CGD-CBD	3.02	115.44	111.30
22	BA	404	CLA	C6-C5-C3	3.02	119.11	112.48
22	AC	510	CLA	O2A-CGA-CBA	3.02	121.10	111.90
29	AA	412	SQD	C32-C31-C30	3.02	130.13	114.53
22	BB	619	CLA	CED-O2D-CGD	3.02	123.08	115.99
22	BB	605	CLA	O2A-CGA-CBA	3.02	121.11	111.90
22	BD	404	CLA	O2D-CGD-CBD	3.02	115.44	111.30
22	AC	502	CLA	CED-O2D-CGD	3.02	123.08	115.99
22	AC	509	CLA	O2D-CGD-CBD	3.02	115.45	111.30
22	BB	613	CLA	C6-C5-C3	3.03	119.12	112.48
22	AB	611	CLA	C6-C5-C3	3.03	119.14	112.48
24	BA	408	PL9	C15-C14-C16	3.03	120.04	115.41
24	BD	405	PL9	C15-C14-C16	3.04	120.04	115.41
26	AB	620	BCR	C2-C1-C6	3.04	115.17	110.36
24	BA	408	PL9	C25-C24-C26	3.04	120.05	115.41
22	BC	512	CLA	C1D-CHD-C4C	3.04	127.20	122.60
29	BA	413	SQD	C32-C31-C30	3.04	130.25	114.53
22	AC	502	CLA	C1D-CHD-C4C	3.04	127.21	122.60
26	BX	101	BCR	C15-C14-C13	3.04	131.59	127.20
27	BC	516	DGD	O2G-C1B-C2B	3.05	118.15	111.53
26	AT	102	BCR	C2-C1-C6	3.05	115.19	110.36
22	AD	404	CLA	C1D-CHD-C4C	3.05	127.21	122.60
22	BC	508	CLA	C1D-CHD-C4C	3.05	127.22	122.60
22	AC	513	CLA	C1D-CHD-C4C	3.05	127.22	122.60
22	BB	606	CLA	C1D-CHD-C4C	3.05	127.22	122.60
30	AE	102	LMG	O1-C1-C2	3.05	111.89	108.04
27	BA	411	DGD	O2G-C1B-C2B	3.05	118.16	111.53
26	BC	514	BCR	C29-C30-C25	3.05	115.20	110.36
22	BB	608	CLA	CED-O2D-CGD	3.05	123.15	115.99
30	AM	101	LMG	O1-C1-C2	3.06	111.90	108.04
27	BB	602	DGD	O5D-C6D-C5D	3.06	114.62	109.08
22	AB	607	CLA	O2A-CGA-CBA	3.06	121.22	111.90
22	BC	507	CLA	CED-O2D-CGD	3.06	123.18	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BC	505	CLA	CBA-CAA-C2A	3.07	122.38	113.73
22	BC	513	CLA	C1D-CHD-C4C	3.07	127.25	122.60
22	AC	509	CLA	O2A-CGA-CBA	3.07	121.26	111.90
22	BC	509	CLA	C1D-CHD-C4C	3.07	127.25	122.60
22	AC	512	CLA	C1D-CHD-C4C	3.07	127.25	122.60
30	AE	102	LMG	O7-C10-C11	3.07	118.21	111.53
22	BB	611	CLA	C1D-CHD-C4C	3.08	127.26	122.60
30	AD	407	LMG	O7-C10-C11	3.08	118.22	111.53
22	BB	610	CLA	O2A-CGA-CBA	3.08	121.28	111.90
22	BC	505	CLA	O2A-CGA-CBA	3.08	121.28	111.90
27	BC	516	DGD	O5D-C6D-C5D	3.08	114.66	109.08
30	AB	622	LMG	O7-C10-C11	3.08	118.22	111.53
26	AB	617	BCR	C2-C1-C6	3.08	115.24	110.36
23	AA	405	PHO	C6-C5-C3	3.08	119.24	112.48
24	AD	405	PL9	C25-C24-C26	3.08	120.11	115.41
22	AB	608	CLA	C1D-CHD-C4C	3.08	127.26	122.60
22	BC	509	CLA	O2A-CGA-CBA	3.08	121.29	111.90
22	BB	613	CLA	C1D-CHD-C4C	3.08	127.27	122.60
26	BB	621	BCR	C2-C1-C6	3.09	115.25	110.36
22	AC	505	CLA	C1D-CHD-C4C	3.09	127.28	122.60
27	AB	626	DGD	O3G-C1D-C2D	3.09	111.95	108.04
22	AB	610	CLA	C1D-CHD-C4C	3.09	127.28	122.60
22	AB	602	CLA	CED-O2D-CGD	3.10	123.25	115.99
26	AH	101	BCR	C11-C10-C9	3.10	131.67	127.20
27	BB	602	DGD	O3G-C1D-C2D	3.10	111.95	108.04
23	BA	406	PHO	O2D-CGD-CBD	3.10	115.55	111.30
24	AA	407	PL9	C25-C24-C26	3.10	120.14	115.41
22	AB	603	CLA	O2D-CGD-CBD	3.10	115.56	111.30
22	AC	509	CLA	C6-C5-C3	3.11	119.30	112.48
22	BB	611	CLA	C6-C5-C3	3.11	119.31	112.48
22	BC	503	CLA	O2D-CGD-CBD	3.11	115.56	111.30
30	BB	623	LMG	O7-C10-C11	3.11	118.29	111.53
22	BC	502	CLA	CED-O2D-CGD	3.11	123.30	115.99
22	BC	509	CLA	C6-C5-C3	3.12	119.32	112.48
26	AC	514	BCR	C32-C1-C6	3.12	115.19	110.30
22	AB	612	CLA	C1D-CHD-C4C	3.12	127.32	122.60
22	AC	513	CLA	CED-O2D-CGD	3.12	123.31	115.99
27	BC	518	DGD	O2G-C1B-C2B	3.12	118.32	111.53
22	BA	407	CLA	CED-O2D-CGD	3.13	123.32	115.99
26	AB	618	BCR	C2-C1-C6	3.13	115.31	110.36
27	AA	410	DGD	O2G-C1B-C2B	3.13	118.34	111.53
22	BC	509	CLA	CED-O2D-CGD	3.14	123.35	115.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	518	DGD	O2G-C1B-C2B	3.14	118.36	111.53
26	AC	514	BCR	C29-C30-C25	3.14	115.34	110.36
22	BC	513	CLA	CED-O2D-CGD	3.15	123.37	115.99
22	BB	614	CLA	O2D-CGD-CBD	3.15	115.62	111.30
26	BD	406	BCR	C8-C7-C6	3.15	136.77	127.32
26	BC	515	BCR	C8-C7-C6	3.15	136.78	127.32
34	BE	101	HEM	CAA-CBA-CGA	3.15	118.52	112.75
22	BB	618	CLA	C1D-CHD-C4C	3.15	127.37	122.60
26	AT	102	BCR	C8-C7-C6	3.16	136.80	127.32
26	BK	102	BCR	C24-C23-C22	3.16	131.03	126.22
26	BB	620	BCR	C29-C30-C25	3.16	115.36	110.36
22	AB	608	CLA	C6-C5-C3	3.16	119.42	112.48
23	AD	403	PHO	CED-O2D-CGD	3.16	123.40	115.99
26	AB	620	BCR	C24-C23-C22	3.16	131.03	126.22
22	AC	501	CLA	O2A-CGA-CBA	3.16	121.53	111.90
22	AB	611	CLA	O2D-CGD-CBD	3.16	115.64	111.30
22	BC	509	CLA	O2D-CGD-CBD	3.17	115.64	111.30
22	AC	508	CLA	C1D-CHD-C4C	3.17	127.39	122.60
26	AD	406	BCR	C8-C7-C6	3.17	136.83	127.32
22	BC	510	CLA	O2D-CGD-CBD	3.17	115.65	111.30
24	AD	405	PL9	C20-C19-C21	3.17	120.25	115.41
22	BC	510	CLA	C1D-CHD-C4C	3.17	127.41	122.60
26	AB	618	BCR	C8-C7-C6	3.18	136.87	127.32
24	BA	408	PL9	C35-C34-C36	3.18	120.27	115.41
26	AK	102	BCR	C23-C24-C25	3.18	136.88	127.32
23	BD	403	PHO	O2D-CGD-CBD	3.18	115.67	111.30
26	BC	515	BCR	C23-C24-C25	3.18	136.88	127.32
22	AA	402	CLA	C6-C5-C3	3.19	119.48	112.48
30	AB	621	LMG	O7-C10-C11	3.19	118.46	111.53
28	BA	412	LHG	O8-C23-C24	3.19	121.61	111.90
26	AK	102	BCR	C24-C23-C22	3.19	131.08	126.22
34	AE	101	HEM	CAA-CBA-CGA	3.19	118.60	112.75
22	AC	507	CLA	O2D-CGD-CBD	3.19	115.68	111.30
26	BK	102	BCR	C23-C24-C25	3.20	136.92	127.32
26	BJ	102	BCR	C21-C20-C19	3.20	132.89	123.13
22	AC	512	CLA	O2D-CGD-CBD	3.20	115.69	111.30
30	BD	407	LMG	O7-C10-C11	3.20	118.49	111.53
26	AC	515	BCR	C8-C7-C6	3.21	136.95	127.32
22	BC	505	CLA	C1D-CHD-C4C	3.21	127.46	122.60
26	AC	514	BCR	C24-C23-C22	3.21	131.11	126.22
22	BD	402	CLA	CBA-CAA-C2A	3.21	122.79	113.73
22	BA	403	CLA	C6-C5-C3	3.21	119.53	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	AI	101	LMG	O7-C10-C11	3.22	118.52	111.53
22	AB	613	CLA	C1D-CHD-C4C	3.22	127.47	122.60
22	BC	501	CLA	O2A-CGA-CBA	3.22	121.72	111.90
22	BC	511	CLA	C1D-CHD-C4C	3.22	127.48	122.60
26	BZ	101	BCR	C2-C1-C6	3.22	115.47	110.36
22	BC	511	CLA	CED-O2D-CGD	3.23	123.56	115.99
22	AC	510	CLA	O2D-CGD-CBD	3.23	115.73	111.30
27	BA	411	DGD	C1E-O6E-C5E	3.23	120.01	113.75
22	AD	402	CLA	C1D-CHD-C4C	3.23	127.49	122.60
22	AB	615	CLA	O2D-CGD-CBD	3.23	115.73	111.30
22	AC	511	CLA	C1D-CHD-C4C	3.23	127.49	122.60
27	AH	102	DGD	C1E-O6E-C5E	3.23	120.02	113.75
22	AB	616	CLA	CED-O2D-CGD	3.24	123.58	115.99
26	AK	102	BCR	C16-C17-C18	3.24	131.87	127.20
26	BB	622	BCR	C24-C23-C22	3.24	131.16	126.22
30	AB	623	LMG	O7-C10-C11	3.24	118.58	111.53
26	BC	514	BCR	C24-C23-C22	3.24	131.16	126.22
22	BD	402	CLA	C1D-CHD-C4C	3.25	127.52	122.60
26	AC	514	BCR	C2-C1-C6	3.25	115.51	110.36
26	AC	515	BCR	C23-C24-C25	3.25	137.08	127.32
22	BC	508	CLA	O2D-CGD-CBD	3.25	115.76	111.30
22	AC	505	CLA	O2A-CGA-CBA	3.25	121.81	111.90
26	AH	101	BCR	C15-C14-C13	3.26	131.90	127.20
26	BA	410	BCR	C7-C8-C9	3.26	131.18	126.22
22	BB	618	CLA	O2D-CGD-CBD	3.26	115.77	111.30
22	BB	615	CLA	C1D-CHD-C4C	3.26	127.54	122.60
22	BB	615	CLA	O2D-CGD-CBD	3.27	115.78	111.30
26	AJ	102	BCR	C21-C20-C19	3.27	133.08	123.13
22	AD	402	CLA	O2A-CGA-CBA	3.27	121.87	111.90
26	AH	101	BCR	C2-C1-C6	3.27	115.54	110.36
30	BI	101	LMG	O7-C10-C11	3.28	118.65	111.53
24	BA	408	PL9	C30-C29-C31	3.28	120.41	115.41
24	AJ	101	PL9	C25-C24-C26	3.28	120.42	115.41
26	BX	101	BCR	C2-C1-C6	3.29	115.58	110.36
23	AD	403	PHO	O2D-CGD-CBD	3.30	115.82	111.30
29	AA	412	SQD	O48-C23-C24	3.30	121.95	111.90
27	AA	410	DGD	C1E-O6E-C5E	3.30	120.15	113.75
22	BB	606	CLA	O2A-CGA-CBA	3.30	121.95	111.90
22	AB	603	CLA	O2A-CGA-CBA	3.30	121.97	111.90
22	AA	402	CLA	O2A-CGA-CBA	3.31	121.97	111.90
22	AC	509	CLA	C1D-CHD-C4C	3.31	127.61	122.60
26	BZ	101	BCR	C16-C17-C18	3.31	131.98	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	506	CLA	CED-O2D-CGD	3.31	123.75	115.99
27	AD	410	DGD	C1E-O6E-C5E	3.31	120.17	113.75
26	AB	617	BCR	C29-C30-C25	3.31	115.61	110.36
27	BC	516	DGD	C1E-O6E-C5E	3.32	120.18	113.75
26	AB	619	BCR	C29-C30-C25	3.32	115.61	110.36
26	BD	406	BCR	C2-C1-C6	3.32	115.61	110.36
22	AC	501	CLA	O2D-CGD-CBD	3.32	115.85	111.30
27	BC	516	DGD	O6D-C5D-C6D	3.33	113.41	106.61
27	AC	516	DGD	O5D-C6D-C5D	3.33	115.11	109.08
29	BA	413	SQD	O48-C23-C24	3.33	122.05	111.90
24	AA	407	PL9	C30-C29-C31	3.34	120.50	115.41
27	BH	101	DGD	C1E-O6E-C5E	3.34	120.23	113.75
29	BF	101	SQD	O48-C23-C24	3.35	122.09	111.90
22	BD	402	CLA	O2A-CGA-CBA	3.35	122.09	111.90
26	AD	406	BCR	C2-C1-C6	3.35	115.66	110.36
26	BA	410	BCR	C29-C30-C25	3.35	115.67	110.36
22	BC	506	CLA	CED-O2D-CGD	3.35	123.85	115.99
22	AB	615	CLA	C1D-CHD-C4C	3.35	127.68	122.60
26	AA	409	BCR	C29-C30-C25	3.36	115.68	110.36
30	AA	413	LMG	O6-C5-C6	3.36	114.84	106.36
27	AC	516	DGD	O6D-C5D-C6D	3.37	113.49	106.61
30	AB	621	LMG	O6-C5-C6	3.37	114.86	106.36
30	BC	520	LMG	O7-C10-C11	3.37	118.85	111.53
26	BA	410	BCR	C24-C23-C22	3.37	131.36	126.22
22	AB	610	CLA	O2D-CGD-CBD	3.38	115.94	111.30
22	BA	403	CLA	O2A-CGA-CBA	3.39	122.22	111.90
30	AC	520	LMG	O7-C10-C11	3.39	118.89	111.53
24	BJ	101	PL9	C25-C24-C26	3.39	120.58	115.41
22	BC	501	CLA	O2D-CGD-CBD	3.39	115.95	111.30
22	AC	510	CLA	C1D-CHD-C4C	3.39	127.74	122.60
27	BC	518	DGD	C1E-O6E-C5E	3.39	120.33	113.75
27	AH	102	DGD	O2G-C1B-C2B	3.40	118.91	111.53
30	BD	408	LMG	O7-C10-C11	3.40	118.91	111.53
28	AA	411	LHG	O8-C23-C24	3.41	122.28	111.90
27	AH	102	DGD	O6D-C5D-C6D	3.41	113.58	106.61
27	BD	410	DGD	C1E-O6E-C5E	3.41	120.36	113.75
26	AZ	101	BCR	C2-C1-C6	3.41	115.76	110.36
22	AB	609	CLA	CED-O2D-CGD	3.41	123.99	115.99
26	BB	621	BCR	C24-C23-C22	3.41	131.42	126.22
29	AF	101	SQD	O48-C23-C24	3.42	122.31	111.90
30	BD	408	LMG	O6-C5-C6	3.42	114.99	106.36
26	BC	514	BCR	C2-C1-C6	3.42	115.78	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	BB	623	LMG	O6-C5-C6	3.42	115.01	106.36
22	AC	507	CLA	O2A-CGA-CBA	3.43	122.36	111.90
24	BD	405	PL9	C20-C19-C21	3.43	120.65	115.41
22	AD	402	CLA	CBA-CAA-C2A	3.43	123.42	113.73
26	AA	409	BCR	C7-C8-C9	3.44	131.46	126.22
30	AD	408	LMG	O7-C10-C11	3.45	119.03	111.53
30	BA	414	LMG	O6-C5-C6	3.46	115.10	106.36
26	BB	620	BCR	C2-C1-C6	3.46	115.84	110.36
24	AA	407	PL9	C35-C34-C36	3.46	120.69	115.41
22	BB	616	CLA	C1D-CHD-C4C	3.47	127.84	122.60
23	AA	405	PHO	O2D-CGD-CBD	3.47	116.06	111.30
26	AZ	101	BCR	C16-C17-C18	3.48	132.22	127.20
29	BF	101	SQD	C11-C10-C9	3.48	132.49	114.53
22	BC	507	CLA	O2A-CGA-CBA	3.48	122.50	111.90
22	BC	512	CLA	O2A-CGA-CBA	3.48	122.51	111.90
22	BB	615	CLA	C6-C5-C3	3.48	120.13	112.48
22	BA	404	CLA	O2D-CGD-CBD	3.49	116.08	111.30
29	BA	401	SQD	C31-C30-C29	3.50	132.58	114.53
26	BC	515	BCR	C2-C1-C6	3.50	115.90	110.36
30	BE	102	LMG	O1-C1-C2	3.50	112.45	108.04
22	BC	512	CLA	O2D-CGD-CBD	3.50	116.10	111.30
22	AB	608	CLA	O2A-CGA-CBA	3.50	122.56	111.90
27	BH	101	DGD	O2G-C1B-C2B	3.50	119.14	111.53
22	AB	612	CLA	O2D-CGD-CBD	3.51	116.11	111.30
29	BL	101	SQD	C11-C10-C9	3.51	132.66	114.53
22	AC	512	CLA	O2A-CGA-CBA	3.51	122.60	111.90
29	AA	415	SQD	C11-C10-C9	3.52	132.69	114.53
26	AB	619	BCR	C24-C23-C22	3.52	131.58	126.22
26	BB	621	BCR	C29-C30-C25	3.53	115.96	110.36
29	BB	601	SQD	C11-C10-C9	3.54	132.81	114.53
26	BB	622	BCR	C2-C1-C6	3.54	115.97	110.36
29	AF	101	SQD	C11-C10-C9	3.55	132.85	114.53
29	BA	401	SQD	C11-C10-C9	3.55	132.86	114.53
29	AD	409	SQD	C11-C10-C9	3.55	132.86	114.53
27	BH	101	DGD	O6D-C5D-C6D	3.55	113.87	106.61
26	AA	409	BCR	C24-C23-C22	3.55	131.63	126.22
22	AA	403	CLA	O2A-CGA-CBA	3.55	122.73	111.90
22	AB	612	CLA	C6-C5-C3	3.56	120.29	112.48
26	BZ	101	BCR	C23-C24-C25	3.56	138.02	127.32
26	BK	102	BCR	C16-C17-C18	3.56	132.34	127.20
22	BB	612	CLA	CED-O2D-CGD	3.57	124.36	115.99
26	AJ	102	BCR	C16-C15-C14	3.57	131.28	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	AC	518	DGD	C1E-O6E-C5E	3.57	120.68	113.75
29	BD	409	SQD	O48-C23-C24	3.58	122.80	111.90
26	AZ	101	BCR	C29-C30-C25	3.58	116.03	110.36
26	AB	620	BCR	C29-C30-C25	3.58	116.04	110.36
22	AC	508	CLA	O2D-CGD-CBD	3.59	116.22	111.30
22	AD	404	CLA	O2D-CGD-CBD	3.60	116.23	111.30
30	AD	408	LMG	O6-C5-C6	3.61	115.47	106.36
29	BD	409	SQD	C11-C10-C9	3.61	133.17	114.53
22	BB	611	CLA	O2A-CGA-CBA	3.61	122.90	111.90
29	AA	415	SQD	C31-C30-C29	3.61	133.18	114.53
26	BZ	101	BCR	C29-C30-C25	3.61	116.08	110.36
26	AK	102	BCR	C29-C30-C25	3.62	116.09	110.36
29	AA	412	SQD	C31-C30-C29	3.63	133.27	114.53
29	BA	413	SQD	C31-C30-C29	3.64	133.32	114.53
22	BB	605	CLA	C4A-NA-C1A	3.65	111.07	106.36
22	BA	404	CLA	O2A-CGA-CBA	3.65	123.02	111.90
26	BJ	102	BCR	C16-C15-C14	3.65	131.46	123.39
26	BX	101	BCR	C29-C30-C25	3.66	116.16	110.36
22	AA	403	CLA	O2D-CGD-CBD	3.66	116.32	111.30
26	AH	101	BCR	C29-C30-C25	3.66	116.16	110.36
26	BJ	102	BCR	C29-C30-C25	3.66	116.16	110.36
29	AD	409	SQD	O48-C23-C24	3.67	123.07	111.90
26	AZ	101	BCR	C23-C24-C25	3.67	138.34	127.32
24	BJ	101	PL9	C10-C9-C11	3.68	121.02	115.41
26	BK	102	BCR	C29-C30-C25	3.68	116.19	110.36
27	AC	516	DGD	C1E-O6E-C5E	3.69	120.91	113.75
26	AD	406	BCR	C24-C23-C22	3.69	131.84	126.22
29	BA	413	SQD	C11-C10-C9	3.69	133.61	114.53
22	AA	403	CLA	C4A-NA-C1A	3.70	111.14	106.36
22	AB	602	CLA	C4A-NA-C1A	3.71	111.16	106.36
29	AA	412	SQD	C11-C10-C9	3.72	133.75	114.53
23	AD	403	PHO	C4A-NA-C1A	3.73	111.54	108.21
27	BC	518	DGD	O6D-C5D-C6D	3.73	114.23	106.61
27	AB	626	DGD	C1E-O6E-C5E	3.73	120.98	113.75
27	BB	602	DGD	C1E-O6E-C5E	3.73	120.99	113.75
27	BB	602	DGD	O2G-C1B-C2B	3.77	119.71	111.53
26	AC	515	BCR	C2-C1-C6	3.77	116.34	110.36
22	BB	613	CLA	O2D-CGD-CBD	3.80	116.52	111.30
26	AH	101	BCR	C24-C23-C22	3.83	132.04	126.22
22	BA	404	CLA	CBA-CAA-C2A	3.84	124.57	113.73
26	AJ	102	BCR	C29-C30-C25	3.86	116.47	110.36
24	AJ	101	PL9	C10-C9-C11	3.86	121.30	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	622	BCR	C29-C30-C25	3.86	116.47	110.36
26	AD	406	BCR	C29-C30-C25	3.88	116.50	110.36
27	AC	518	DGD	O6D-C5D-C6D	3.90	114.57	106.61
26	AB	618	BCR	C29-C30-C25	3.90	116.53	110.36
22	BB	614	CLA	C4A-NA-C1A	3.90	111.40	106.36
22	BA	407	CLA	C4A-NA-C1A	3.91	111.41	106.36
27	AB	626	DGD	O2G-C1B-C2B	3.91	120.02	111.53
26	AC	515	BCR	C29-C30-C25	3.91	116.56	110.36
29	BL	101	SQD	O48-C23-C24	3.92	123.84	111.90
22	AB	614	CLA	O2D-CGD-CBD	3.92	116.68	111.30
26	BX	101	BCR	C24-C23-C22	3.92	132.19	126.22
26	BD	406	BCR	C29-C30-C25	3.94	116.60	110.36
22	AC	510	CLA	C4A-NA-C1A	3.94	111.45	106.36
27	AC	517	DGD	O2G-C1B-C2B	3.97	120.15	111.53
30	BM	102	LMG	O7-C10-C11	3.97	120.15	111.53
29	AA	415	SQD	O48-C23-C24	3.97	124.00	111.90
28	AC	521	LHG	O7-C7-C8	3.98	120.17	111.53
29	AA	415	SQD	C44-O6-C1	3.98	122.17	113.82
26	BC	515	BCR	C29-C30-C25	3.98	116.67	110.36
28	BC	521	LHG	O7-C7-C8	3.99	120.21	111.53
22	BB	611	CLA	C4A-NA-C1A	4.00	111.53	106.36
29	BB	601	SQD	O48-C23-C24	4.01	124.10	111.90
22	BA	404	CLA	C4A-NA-C1A	4.01	111.54	106.36
29	AD	409	SQD	C44-O6-C1	4.01	122.25	113.82
22	AA	403	CLA	CBA-CAA-C2A	4.01	125.05	113.73
29	BA	401	SQD	C44-O6-C1	4.01	122.25	113.82
22	AA	406	CLA	C4A-NA-C1A	4.02	111.55	106.36
22	BB	606	CLA	C4A-NA-C1A	4.02	111.55	106.36
26	BD	406	BCR	C24-C23-C22	4.02	132.34	126.22
23	BA	406	PHO	C4A-NA-C1A	4.02	111.80	108.21
26	AT	102	BCR	C29-C30-C25	4.02	116.73	110.36
29	BA	401	SQD	O48-C23-C24	4.02	124.16	111.90
30	AM	101	LMG	O7-C10-C11	4.03	120.28	111.53
22	AB	609	CLA	C4A-NA-C1A	4.04	111.58	106.36
23	AA	405	PHO	C4A-NA-C1A	4.05	111.83	108.21
22	AB	608	CLA	C4A-NA-C1A	4.08	111.64	106.36
22	BC	510	CLA	C4A-NA-C1A	4.09	111.64	106.36
22	AB	603	CLA	C4A-NA-C1A	4.09	111.65	106.36
22	AC	504	CLA	C4A-NA-C1A	4.10	111.66	106.36
22	BB	617	CLA	O2D-CGD-CBD	4.10	116.92	111.30
22	AB	611	CLA	C4A-NA-C1A	4.10	111.66	106.36
27	BC	517	DGD	O2G-C1B-C2B	4.11	120.46	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AB	605	CLA	C4A-NA-C1A	4.11	111.68	106.36
22	BB	616	CLA	C4A-NA-C1A	4.12	111.69	106.36
22	AC	509	CLA	C4A-NA-C1A	4.12	111.69	106.36
22	AA	404	CLA	C4A-NA-C1A	4.13	111.71	106.36
22	BA	403	CLA	C4A-NA-C1A	4.14	111.71	106.36
22	AB	612	CLA	C4A-NA-C1A	4.14	111.72	106.36
22	BB	608	CLA	C4A-NA-C1A	4.15	111.73	106.36
22	AA	402	CLA	C4A-NA-C1A	4.16	111.74	106.36
22	AB	616	CLA	C4A-NA-C1A	4.17	111.75	106.36
22	BC	504	CLA	C4A-NA-C1A	4.18	111.76	106.36
26	BK	102	BCR	C2-C1-C6	4.20	117.01	110.36
22	BB	612	CLA	C4A-NA-C1A	4.20	111.78	106.36
27	AA	410	DGD	O5D-C6D-C5D	4.20	116.69	109.08
34	AV	201	HEM	CMC-C2C-C3C	4.23	127.08	116.53
22	BB	613	CLA	C4A-NA-C1A	4.23	111.83	106.36
22	AB	606	CLA	C4A-NA-C1A	4.25	111.85	106.36
22	AB	613	CLA	C4A-NA-C1A	4.25	111.86	106.36
22	BC	509	CLA	C4A-NA-C1A	4.26	111.87	106.36
22	BB	615	CLA	C4A-NA-C1A	4.26	111.87	106.36
23	BD	403	PHO	C4A-NA-C1A	4.27	112.02	108.21
22	AC	502	CLA	C4A-NA-C1A	4.27	111.89	106.36
22	BA	405	CLA	C4A-NA-C1A	4.28	111.89	106.36
34	AE	101	HEM	CMC-C2C-C3C	4.28	127.22	116.53
22	AB	610	CLA	C4A-NA-C1A	4.28	111.90	106.36
34	BV	201	HEM	CMC-C2C-C3C	4.29	127.24	116.53
22	BB	617	CLA	C4A-NA-C1A	4.30	111.92	106.36
22	AC	501	CLA	C4A-NA-C1A	4.30	111.92	106.36
29	BD	409	SQD	C44-O6-C1	4.33	122.92	113.82
22	BC	507	CLA	C4A-NA-C1A	4.33	111.96	106.36
22	BC	506	CLA	C4A-NA-C1A	4.34	111.97	106.36
22	AB	607	CLA	C4A-NA-C1A	4.34	111.97	106.36
22	AD	404	CLA	C4A-NA-C1A	4.35	111.98	106.36
22	AC	505	CLA	C4A-NA-C1A	4.36	112.00	106.36
22	BD	404	CLA	C4A-NA-C1A	4.36	112.00	106.36
22	BB	609	CLA	C4A-NA-C1A	4.37	112.00	106.36
34	BE	101	HEM	CMC-C2C-C3C	4.37	127.44	116.53
27	BA	411	DGD	O5D-C6D-C5D	4.37	117.00	109.08
22	BC	501	CLA	C4A-NA-C1A	4.38	112.02	106.36
22	AC	507	CLA	C4A-NA-C1A	4.38	112.02	106.36
22	BB	619	CLA	C4A-NA-C1A	4.38	112.03	106.36
22	AC	512	CLA	C4A-NA-C1A	4.40	112.05	106.36
22	AB	614	CLA	C4A-NA-C1A	4.41	112.06	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AC	506	CLA	C4A-NA-C1A	4.42	112.08	106.36
22	AC	513	CLA	C4A-NA-C1A	4.43	112.09	106.36
26	AK	102	BCR	C2-C1-C6	4.43	117.38	110.36
22	BD	402	CLA	C4A-NA-C1A	4.44	112.11	106.36
22	BB	610	CLA	C4A-NA-C1A	4.46	112.13	106.36
22	AD	402	CLA	C4A-NA-C1A	4.46	112.13	106.36
22	BC	513	CLA	C4A-NA-C1A	4.47	112.14	106.36
26	BJ	102	BCR	C8-C7-C6	4.47	140.74	127.32
22	BC	502	CLA	C4A-NA-C1A	4.48	112.15	106.36
22	BC	512	CLA	C4A-NA-C1A	4.50	112.18	106.36
34	BE	101	HEM	CMB-C2B-C3B	4.53	127.83	116.53
22	BC	503	CLA	C4A-NA-C1A	4.56	112.26	106.36
26	AJ	102	BCR	C8-C7-C6	4.56	141.01	127.32
22	BC	508	CLA	C4A-NA-C1A	4.56	112.26	106.36
22	BC	505	CLA	C4A-NA-C1A	4.58	112.28	106.36
22	BB	618	CLA	C4A-NA-C1A	4.59	112.29	106.36
22	BB	604	CLA	C4A-NA-C1A	4.59	112.29	106.36
22	AB	601	CLA	C4A-NA-C1A	4.59	112.30	106.36
22	AB	615	CLA	C4A-NA-C1A	4.59	112.30	106.36
34	AE	101	HEM	CMB-C2B-C3B	4.64	128.11	116.53
27	BH	101	DGD	O5D-C1E-C2E	4.69	113.96	108.04
22	AC	511	CLA	C4A-NA-C1A	4.69	112.43	106.36
22	AC	503	CLA	C4A-NA-C1A	4.73	112.47	106.36
22	BC	511	CLA	C4A-NA-C1A	4.75	112.50	106.36
29	AF	101	SQD	C44-O6-C1	4.77	123.83	113.82
22	AC	508	CLA	C4A-NA-C1A	4.80	112.56	106.36
27	AH	102	DGD	O5D-C1E-C2E	4.81	114.11	108.04
22	BB	607	CLA	C4A-NA-C1A	4.83	112.61	106.36
29	BF	101	SQD	C44-O6-C1	4.85	124.00	113.82
26	BJ	102	BCR	C23-C24-C25	4.85	141.90	127.32
22	AB	604	CLA	C4A-NA-C1A	4.88	112.67	106.36
34	AV	201	HEM	CMB-C2B-C3B	4.93	128.83	116.53
26	AJ	102	BCR	C23-C24-C25	4.94	142.16	127.32
26	AJ	102	BCR	C31-C1-C6	5.00	118.14	110.30
27	BC	516	DGD	O5D-C1E-C2E	5.01	114.37	108.04
34	BV	201	HEM	CMB-C2B-C3B	5.03	129.09	116.53
29	BD	409	SQD	C25-C24-C23	5.08	133.58	113.59
26	BJ	102	BCR	C31-C1-C6	5.10	118.29	110.30
29	AD	409	SQD	C25-C24-C23	5.13	133.76	113.59
26	BK	102	BCR	C11-C10-C9	5.14	134.63	127.20
26	AK	102	BCR	C11-C10-C9	5.17	134.66	127.20
26	AH	101	BCR	C33-C5-C6	5.18	129.69	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BX	101	BCR	C33-C5-C6	5.18	129.70	124.61
29	AF	101	SQD	C25-C24-C23	5.20	134.03	113.59
29	BB	601	SQD	C25-C24-C23	5.20	134.05	113.59
26	AK	102	BCR	C38-C26-C25	5.21	129.72	124.61
29	BL	101	SQD	C25-C24-C23	5.23	134.16	113.59
29	AA	412	SQD	C25-C24-C23	5.31	134.46	113.59
29	BA	413	SQD	C25-C24-C23	5.37	134.72	113.59
26	BK	102	BCR	C7-C8-C9	5.38	134.41	126.22
29	BF	101	SQD	C25-C24-C23	5.38	134.74	113.59
26	AK	102	BCR	C7-C8-C9	5.41	134.46	126.22
29	AA	415	SQD	C25-C24-C23	5.41	134.88	113.59
26	BZ	101	BCR	C33-C5-C6	5.44	129.95	124.61
29	BA	401	SQD	C25-C24-C23	5.45	135.03	113.59
27	BB	602	DGD	O5D-C1E-C2E	5.47	114.95	108.04
26	BK	102	BCR	C38-C26-C25	5.56	130.06	124.61
27	AC	516	DGD	O5D-C1E-C2E	5.67	115.20	108.04
26	BC	514	BCR	C33-C5-C6	5.69	130.20	124.61
26	AZ	101	BCR	C33-C5-C6	5.72	130.22	124.61
26	AA	409	BCR	C38-C26-C25	5.73	130.23	124.61
28	AA	411	LHG	C25-C24-C23	5.78	136.33	113.59
28	BA	412	LHG	C25-C24-C23	5.79	136.36	113.59
29	BA	401	SQD	C10-C9-C8	5.80	134.57	113.29
26	BA	410	BCR	C33-C5-C6	5.84	130.34	124.61
26	BA	410	BCR	C38-C26-C25	5.84	130.34	124.61
27	BC	517	DGD	O5D-C6D-C5D	5.87	119.71	109.08
29	BD	409	SQD	C10-C9-C8	5.91	134.96	113.29
29	AA	415	SQD	C10-C9-C8	5.91	134.98	113.29
26	AA	409	BCR	C33-C5-C6	5.94	130.43	124.61
26	AC	514	BCR	C33-C5-C6	5.94	130.44	124.61
29	BL	101	SQD	C10-C9-C8	5.94	135.09	113.29
29	AD	409	SQD	C10-C9-C8	5.95	135.12	113.29
27	AC	517	DGD	O5D-C6D-C5D	5.97	119.90	109.08
26	BB	621	BCR	C33-C5-C6	5.97	130.47	124.61
26	BB	622	BCR	C38-C26-C25	6.02	130.51	124.61
26	BB	622	BCR	C33-C5-C6	6.05	130.54	124.61
27	AB	626	DGD	O5D-C1E-C2E	6.05	115.68	108.04
27	BD	410	DGD	O3G-C1D-C2D	6.05	115.68	108.04
27	AD	410	DGD	O3G-C1D-C2D	6.05	115.68	108.04
26	AB	620	BCR	C33-C5-C6	6.06	130.56	124.61
26	AB	619	BCR	C33-C5-C6	6.07	130.57	124.61
29	BB	601	SQD	C10-C9-C8	6.09	135.62	113.29
26	AC	514	BCR	C38-C26-C25	6.11	130.61	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AB	617	BCR	C33-C5-C6	6.16	130.66	124.61
29	BA	413	SQD	C10-C9-C8	6.21	136.06	113.29
26	BC	514	BCR	C38-C26-C25	6.21	130.71	124.61
29	AA	412	SQD	C10-C9-C8	6.25	136.20	113.29
26	BB	620	BCR	C38-C26-C25	6.25	130.74	124.61
29	AF	101	SQD	C10-C9-C8	6.26	136.26	113.29
29	BF	101	SQD	C10-C9-C8	6.28	136.31	113.29
26	BC	515	BCR	C38-C26-C25	6.28	130.77	124.61
26	BB	620	BCR	C33-C5-C6	6.29	130.78	124.61
26	AB	618	BCR	C38-C26-C25	6.33	130.82	124.61
26	AC	515	BCR	C38-C26-C25	6.37	130.86	124.61
26	AB	618	BCR	C33-C5-C6	6.38	130.87	124.61
26	AC	515	BCR	C33-C5-C6	6.42	130.91	124.61
26	AB	620	BCR	C38-C26-C25	6.46	130.95	124.61
26	AT	102	BCR	C33-C5-C6	6.51	131.00	124.61
26	BZ	101	BCR	C38-C26-C25	6.52	131.01	124.61
26	BC	515	BCR	C33-C5-C6	6.58	131.06	124.61
26	AB	617	BCR	C38-C26-C25	6.62	131.10	124.61
27	AC	516	DGD	O6E-C5E-C4E	6.63	122.12	109.68
26	BD	406	BCR	C33-C5-C6	6.64	131.13	124.61
26	AT	102	BCR	C38-C26-C25	6.64	131.13	124.61
26	AZ	101	BCR	C38-C26-C25	6.70	131.18	124.61
26	BJ	102	BCR	C2-C1-C6	6.71	120.99	110.36
27	AC	518	DGD	O6E-C5E-C4E	6.75	122.36	109.68
27	BB	602	DGD	O6E-C5E-C4E	6.80	122.44	109.68
26	AB	619	BCR	C38-C26-C25	6.88	131.36	124.61
27	AD	410	DGD	O6E-C5E-C4E	6.88	122.59	109.68
27	AB	626	DGD	O6E-C5E-C4E	6.89	122.61	109.68
27	BC	518	DGD	O6E-C5E-C4E	6.91	122.65	109.68
27	BD	410	DGD	O6E-C5E-C4E	6.91	122.66	109.68
27	BC	516	DGD	O6E-C5E-C4E	6.92	122.67	109.68
26	AJ	102	BCR	C2-C1-C6	6.92	121.32	110.36
27	BH	101	DGD	O6E-C5E-C4E	7.03	122.88	109.68
26	BK	102	BCR	C33-C5-C6	7.07	131.55	124.61
26	AD	406	BCR	C33-C5-C6	7.12	131.60	124.61
27	AH	102	DGD	O6E-C5E-C4E	7.19	123.17	109.68
27	AA	410	DGD	O6E-C5E-C4E	7.22	123.23	109.68
26	BB	621	BCR	C38-C26-C25	7.22	131.69	124.61
27	BA	411	DGD	O6E-C5E-C4E	7.23	123.25	109.68
27	AC	517	DGD	O6E-C5E-C4E	7.27	123.33	109.68
27	BC	517	DGD	O6E-C5E-C4E	7.28	123.34	109.68
26	AD	406	BCR	C38-C26-C25	7.41	131.88	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AK	102	BCR	C33-C5-C6	7.47	131.94	124.61
26	AJ	102	BCR	C33-C5-C6	7.50	131.97	124.61
26	BD	406	BCR	C38-C26-C25	7.53	132.00	124.61
26	AH	101	BCR	C38-C26-C25	7.58	132.05	124.61
26	BJ	102	BCR	C33-C5-C6	7.64	132.11	124.61
26	BJ	102	BCR	C38-C26-C25	7.66	132.13	124.61
26	AJ	102	BCR	C38-C26-C25	7.69	132.16	124.61
29	BL	101	SQD	O5-C1-O6	7.74	128.68	110.05
29	BB	601	SQD	O5-C1-O6	7.78	128.79	110.05
26	BX	101	BCR	C38-C26-C25	7.86	132.32	124.61
29	BA	401	SQD	O5-C1-O6	8.19	129.78	110.05
29	BA	413	SQD	O5-C1-O6	8.20	129.80	110.05
29	BF	101	SQD	O6-C1-C2	8.22	118.42	108.04
29	AA	412	SQD	O5-C1-O6	8.26	129.94	110.05
29	BD	409	SQD	O5-C1-O6	8.28	129.98	110.05
29	AF	101	SQD	O6-C1-C2	8.33	118.56	108.04
29	AD	409	SQD	O5-C1-O6	8.36	130.18	110.05
29	AA	415	SQD	O5-C1-O6	8.39	130.25	110.05
29	AA	412	SQD	O6-C1-C2	8.74	119.08	108.04
29	BA	413	SQD	O6-C1-C2	8.75	119.08	108.04
29	AA	415	SQD	O6-C1-C2	8.77	119.12	108.04
29	BF	101	SQD	O5-C1-O6	8.95	131.61	110.05
29	BA	401	SQD	O6-C1-C2	8.98	119.39	108.04
29	AF	101	SQD	O5-C1-O6	9.03	131.79	110.05
29	BL	101	SQD	O6-C1-C2	9.31	119.80	108.04
29	BB	601	SQD	O6-C1-C2	9.64	120.21	108.04
29	BD	409	SQD	O6-C1-C2	9.66	120.24	108.04
29	AD	409	SQD	O6-C1-C2	9.80	120.42	108.04
34	BV	201	HEM	CAD-C3D-C2D	9.90	141.69	113.22
34	AV	201	HEM	CAD-C3D-C2D	9.96	141.84	113.22
29	AA	415	SQD	O7-S-C6	10.01	115.38	106.94
29	BF	101	SQD	O7-S-C6	10.27	115.60	106.94
29	BA	401	SQD	O7-S-C6	10.37	115.68	106.94
29	AF	101	SQD	O7-S-C6	10.64	115.91	106.94
34	AE	101	HEM	CAD-C3D-C2D	10.64	143.81	113.22
34	BE	101	HEM	CAD-C3D-C2D	10.70	143.98	113.22
29	BB	601	SQD	O7-S-C6	10.75	116.00	106.94
29	BL	101	SQD	O7-S-C6	11.19	116.37	106.94
29	BA	413	SQD	O7-S-C6	11.22	116.40	106.94
29	AA	412	SQD	O7-S-C6	11.85	116.93	106.94
29	BD	409	SQD	O7-S-C6	12.68	117.63	106.94
29	AD	409	SQD	O7-S-C6	12.87	117.79	106.94

All (294) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AB	614	CLA	NC
22	AB	614	CLA	ND
22	AB	614	CLA	NA
22	BB	617	CLA	NC
22	BB	617	CLA	ND
22	BB	617	CLA	NA
22	BC	501	CLA	NC
22	BC	501	CLA	ND
22	BC	501	CLA	NA
22	AC	510	CLA	NC
22	AC	510	CLA	ND
22	AC	510	CLA	NA
22	AA	403	CLA	NC
22	AA	403	CLA	ND
22	AA	403	CLA	NA
22	BB	615	CLA	NC
22	BB	615	CLA	ND
22	BB	615	CLA	NA
22	AB	613	CLA	NC
22	AB	613	CLA	ND
22	AB	613	CLA	NA
30	AC	520	LMG	C2
30	AC	520	LMG	C5
27	AB	626	DGD	C2D
27	AB	626	DGD	C5D
27	AB	626	DGD	C5E
27	AH	102	DGD	C2D
27	AH	102	DGD	C5D
27	AH	102	DGD	C5E
22	BB	611	CLA	NC
22	BB	611	CLA	ND
22	BB	611	CLA	NA
22	BA	407	CLA	NC
22	BA	407	CLA	ND
22	BA	407	CLA	NA
30	AB	623	LMG	C2
30	AB	623	LMG	C5
30	AM	101	LMG	C2
30	AM	101	LMG	C5
22	AD	404	CLA	NC
22	AD	404	CLA	ND
22	AD	404	CLA	NA

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Mol	Chain	Res	Type	Atom
22	BB	608	CLA	NC
22	BB	608	CLA	ND
22	BB	608	CLA	NA
22	BC	512	CLA	NC
22	BC	512	CLA	ND
22	BC	512	CLA	NA
30	AE	102	LMG	C2
30	AE	102	LMG	C5
27	AC	517	DGD	C2D
27	AC	517	DGD	C5D
27	AC	517	DGD	C5E
22	AB	605	CLA	NC
22	AB	605	CLA	ND
22	AB	605	CLA	NA
22	AC	503	CLA	NC
22	AC	503	CLA	ND
22	AC	503	CLA	NA
30	AB	622	LMG	C2
30	AB	622	LMG	C5
27	BC	518	DGD	C2D
27	BC	518	DGD	C5D
27	BC	518	DGD	C5E
22	AB	611	CLA	NC
22	AB	611	CLA	ND
22	AB	611	CLA	NA
30	BA	414	LMG	C2
30	BA	414	LMG	C5
22	AB	606	CLA	NC
22	AB	606	CLA	ND
22	AB	606	CLA	NA
22	AB	603	CLA	NC
22	AB	603	CLA	ND
22	AB	603	CLA	NA
22	BC	504	CLA	NC
22	BC	504	CLA	ND
22	BC	504	CLA	NA
22	BB	612	CLA	NC
22	BB	612	CLA	ND
22	BB	612	CLA	NA
22	BB	618	CLA	NC
22	BB	618	CLA	ND
22	BB	618	CLA	NA

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Mol	Chain	Res	Type	Atom
30	BE	102	LMG	C2
30	BE	102	LMG	C5
22	BA	404	CLA	NC
22	BA	404	CLA	ND
22	BA	404	CLA	NA
27	AA	410	DGD	C2D
27	AA	410	DGD	C5D
27	AA	410	DGD	C5E
22	BB	605	CLA	NC
22	BB	605	CLA	ND
22	BB	605	CLA	NA
27	AC	518	DGD	C2D
27	AC	518	DGD	C5D
27	AC	518	DGD	C5E
22	BC	508	CLA	NC
22	BC	508	CLA	ND
22	BC	508	CLA	NA
22	BA	405	CLA	NC
22	BA	405	CLA	ND
22	BA	405	CLA	NA
22	AC	506	CLA	NC
22	AC	506	CLA	ND
22	AC	506	CLA	NA
30	BB	623	LMG	C2
30	BB	623	LMG	C5
22	BB	604	CLA	NC
22	BB	604	CLA	ND
22	BB	604	CLA	NA
22	BB	607	CLA	NC
22	BB	607	CLA	ND
22	BB	607	CLA	NA
22	BB	613	CLA	NC
22	BB	613	CLA	ND
22	BB	613	CLA	NA
22	AC	509	CLA	NC
22	AC	509	CLA	ND
22	AC	509	CLA	NA
27	BD	410	DGD	C2D
27	BD	410	DGD	C5D
27	BD	410	DGD	C5E
27	BC	516	DGD	C2D
27	BC	516	DGD	C5D

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Mol	Chain	Res	Type	Atom
27	BC	516	DGD	C5E
30	BI	101	LMG	C2
30	BI	101	LMG	C5
22	AB	601	CLA	NC
22	AB	601	CLA	ND
22	AB	601	CLA	NA
27	BC	517	DGD	C2D
27	BC	517	DGD	C5D
27	BC	517	DGD	C5E
22	BB	610	CLA	NC
22	BB	610	CLA	ND
22	BB	610	CLA	NA
22	BC	505	CLA	NC
22	BC	505	CLA	ND
22	BC	505	CLA	NA
27	BA	411	DGD	C2D
27	BA	411	DGD	C5D
27	BA	411	DGD	C5E
22	BC	506	CLA	NC
22	BC	506	CLA	ND
22	BC	506	CLA	NA
30	AA	413	LMG	C2
30	AA	413	LMG	C5
27	BH	101	DGD	C2D
27	BH	101	DGD	C5D
27	BH	101	DGD	C5E
22	AB	615	CLA	NC
22	AB	615	CLA	ND
22	AB	615	CLA	NA
30	BD	408	LMG	C2
30	BD	408	LMG	C5
22	AA	406	CLA	NC
22	AA	406	CLA	ND
22	AA	406	CLA	NA
22	BB	609	CLA	NC
22	BB	609	CLA	ND
22	BB	609	CLA	NA
22	AB	609	CLA	NC
22	AB	609	CLA	ND
22	AB	609	CLA	NA
22	BB	614	CLA	NC
22	BB	614	CLA	ND

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Mol	Chain	Res	Type	Atom
22	BB	614	CLA	NA
22	AB	604	CLA	NC
22	AB	604	CLA	ND
22	AB	604	CLA	NA
30	AB	621	LMG	C2
30	AB	621	LMG	C5
22	AC	513	CLA	NC
22	AC	513	CLA	ND
22	AC	513	CLA	NA
30	BC	520	LMG	C2
30	BC	520	LMG	C5
22	BB	606	CLA	NC
22	BB	606	CLA	ND
22	BB	606	CLA	NA
22	BC	503	CLA	NC
22	BC	503	CLA	ND
22	BC	503	CLA	NA
22	BC	513	CLA	NC
22	BC	513	CLA	ND
22	BC	513	CLA	NA
30	AC	519	LMG	C2
30	AC	519	LMG	C5
30	BB	624	LMG	C2
30	BB	624	LMG	C5
22	BC	510	CLA	NC
22	BC	510	CLA	ND
22	BC	510	CLA	NA
27	AC	516	DGD	C2D
27	AC	516	DGD	C5D
27	AC	516	DGD	C5E
22	AB	608	CLA	NC
22	AB	608	CLA	ND
22	AB	608	CLA	NA
22	BC	502	CLA	NC
22	BC	502	CLA	ND
22	BC	502	CLA	NA
30	AA	416	LMG	C2
30	AA	416	LMG	C5
22	AC	505	CLA	NC
22	AC	505	CLA	ND
22	AC	505	CLA	NA
22	AB	602	CLA	NC

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Mol	Chain	Res	Type	Atom
22	AB	602	CLA	ND
22	AB	602	CLA	NA
22	AA	404	CLA	NC
22	AA	404	CLA	ND
22	AA	404	CLA	NA
22	AD	402	CLA	NC
22	AD	402	CLA	ND
27	AD	410	DGD	C2D
27	AD	410	DGD	C5D
27	AD	410	DGD	C5E
22	AA	402	CLA	NC
22	AA	402	CLA	ND
22	AA	402	CLA	NA
22	BC	509	CLA	NC
22	BC	509	CLA	ND
22	BC	509	CLA	NA
22	AC	502	CLA	NC
22	AC	502	CLA	ND
22	AC	502	CLA	NA
22	AC	512	CLA	NC
22	AC	512	CLA	ND
22	AC	512	CLA	NA
22	AB	612	CLA	NC
22	AB	612	CLA	ND
22	AB	612	CLA	NA
30	BD	407	LMG	C2
30	BD	407	LMG	C5
22	BD	404	CLA	NC
22	BD	404	CLA	ND
22	BD	404	CLA	NA
22	AB	610	CLA	NC
22	AB	610	CLA	ND
22	AB	610	CLA	NA
22	BC	511	CLA	NC
22	BC	511	CLA	ND
22	BC	511	CLA	NA
30	BM	102	LMG	C2
30	BM	102	LMG	C5
22	AC	508	CLA	NC
22	AC	508	CLA	ND
22	AC	508	CLA	NA
30	AD	408	LMG	C2

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Mol	Chain	Res	Type	Atom
30	AD	408	LMG	C5
30	BC	519	LMG	C2
30	BC	519	LMG	C5
22	BC	507	CLA	NC
22	BC	507	CLA	ND
22	BC	507	CLA	NA
27	BB	602	DGD	C2D
27	BB	602	DGD	C5D
27	BB	602	DGD	C5E
22	BB	616	CLA	NC
22	BB	616	CLA	ND
22	BB	616	CLA	NA
22	AB	616	CLA	NC
22	AB	616	CLA	ND
22	AB	616	CLA	NA
22	BD	402	CLA	NC
22	BD	402	CLA	ND
22	AC	507	CLA	NC
22	AC	507	CLA	ND
22	AC	507	CLA	NA
30	AI	101	LMG	C2
30	AI	101	LMG	C5
22	AC	511	CLA	NC
22	AC	511	CLA	ND
22	AC	511	CLA	NA
22	AB	607	CLA	NC
22	AB	607	CLA	ND
22	AB	607	CLA	NA
30	AD	407	LMG	C2
30	AD	407	LMG	C5
22	AC	504	CLA	NC
22	AC	504	CLA	ND
22	AC	504	CLA	NA
22	AC	501	CLA	NC
22	AC	501	CLA	ND
22	AC	501	CLA	NA
22	BA	403	CLA	NC
22	BA	403	CLA	ND
22	BA	403	CLA	NA
22	BB	619	CLA	NC
22	BB	619	CLA	ND
22	BB	619	CLA	NA

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	AB	611	CLA	C1-C2-C3-C4
22	BB	614	CLA	C1-C2-C3-C4
22	AC	513	CLA	C1-C2-C3-C4
22	BC	513	CLA	C1-C2-C3-C4
22	BC	510	CLA	C1-C2-C3-C4
22	AC	510	CLA	C1-C2-C3-C4
23	BA	406	PHO	C1-C2-C3-C4
23	AA	405	PHO	C1-C2-C3-C4
22	BB	609	CLA	C1-C2-C3-C4
22	AB	606	CLA	C1-C2-C3-C4
22	AB	602	CLA	C1-C2-C3-C4
22	AA	403	CLA	C1-C2-C3-C4
22	BA	404	CLA	C1-C2-C3-C4
22	BB	605	CLA	C1-C2-C3-C4
22	BC	509	CLA	C1-C2-C3-C4
30	AD	408	LMG	C7-O1-C1-O6
22	AC	509	CLA	C1-C2-C3-C4
30	BD	408	LMG	C7-O1-C1-O6
22	BC	502	CLA	C1-C2-C3-C4
22	AC	502	CLA	C1-C2-C3-C4
30	AM	101	LMG	C8-O7-C10-C11
30	BM	102	LMG	C8-O7-C10-C11
29	BD	409	SQD	C45-O47-C7-O49
29	AD	409	SQD	C45-O47-C7-O49
29	BD	409	SQD	C45-O47-C7-C8
29	AD	409	SQD	C45-O47-C7-C8

There are no ring outliers.

165 monomers are involved in 627 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AA	402	CLA	7	0
22	AA	403	CLA	7	0
22	AA	404	CLA	2	0
23	AA	405	PHO	5	0
22	AA	406	CLA	3	0
24	AA	407	PL9	5	0
26	AA	409	BCR	6	0
28	AA	411	LHG	3	0
29	AA	412	SQD	5	0
30	AA	413	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	AA	415	SQD	5	0
30	AA	416	LMG	4	0
22	AB	601	CLA	2	0
22	AB	602	CLA	5	0
22	AB	603	CLA	7	0
22	AB	604	CLA	5	0
22	AB	605	CLA	5	0
22	AB	606	CLA	5	0
22	AB	607	CLA	15	0
22	AB	608	CLA	9	0
22	AB	609	CLA	6	0
22	AB	610	CLA	3	0
22	AB	611	CLA	4	0
22	AB	612	CLA	5	0
22	AB	613	CLA	3	0
22	AB	614	CLA	1	0
22	AB	615	CLA	7	0
22	AB	616	CLA	4	0
26	AB	617	BCR	3	0
26	AB	618	BCR	5	0
26	AB	620	BCR	2	0
30	AB	621	LMG	1	0
30	AB	622	LMG	1	0
30	AB	623	LMG	2	0
32	AB	624	LMT	1	0
32	AB	625	LMT	2	0
27	AB	626	DGD	3	0
32	AB	627	LMT	3	0
22	AC	501	CLA	3	0
22	AC	502	CLA	4	0
22	AC	503	CLA	4	0
22	AC	504	CLA	5	0
22	AC	505	CLA	10	0
22	AC	506	CLA	3	0
22	AC	507	CLA	4	0
22	AC	508	CLA	8	0
22	AC	509	CLA	2	0
22	AC	510	CLA	4	0
22	AC	511	CLA	9	0
22	AC	512	CLA	9	0
22	AC	513	CLA	3	0
26	AC	514	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	AC	515	BCR	6	0
27	AC	516	DGD	3	0
27	AC	517	DGD	8	0
27	AC	518	DGD	8	0
30	AC	519	LMG	2	0
30	AC	520	LMG	4	0
28	AC	521	LHG	5	0
33	AD	401	BCT	1	0
22	AD	402	CLA	7	0
23	AD	403	PHO	2	0
22	AD	404	CLA	4	0
24	AD	405	PL9	9	0
26	AD	406	BCR	3	0
30	AD	407	LMG	2	0
30	AD	408	LMG	7	0
29	AD	409	SQD	2	0
32	AD	411	LMT	2	0
34	AE	101	HEM	5	0
30	AE	102	LMG	4	0
29	AF	101	SQD	2	0
26	AH	101	BCR	5	0
27	AH	102	DGD	1	0
30	AI	101	LMG	3	0
32	AI	102	LMT	4	0
26	AJ	102	BCR	5	0
26	AK	102	BCR	13	0
30	AM	101	LMG	4	0
32	AM	102	LMT	1	0
32	AT	101	LMT	3	0
26	AT	102	BCR	8	0
34	AV	201	HEM	3	0
26	AZ	101	BCR	5	0
29	BA	401	SQD	2	0
22	BA	403	CLA	7	0
22	BA	404	CLA	6	0
22	BA	405	CLA	3	0
23	BA	406	PHO	5	0
22	BA	407	CLA	3	0
24	BA	408	PL9	6	0
26	BA	410	BCR	3	0
28	BA	412	LHG	4	0
29	BA	413	SQD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	BA	414	LMG	2	0
29	BB	601	SQD	2	0
27	BB	602	DGD	3	0
32	BB	603	LMT	3	0
22	BB	604	CLA	1	0
22	BB	605	CLA	6	0
22	BB	606	CLA	7	0
22	BB	607	CLA	5	0
22	BB	608	CLA	5	0
22	BB	609	CLA	6	0
22	BB	610	CLA	14	0
22	BB	611	CLA	9	0
22	BB	612	CLA	7	0
22	BB	613	CLA	3	0
22	BB	614	CLA	7	0
22	BB	615	CLA	5	0
22	BB	616	CLA	3	0
22	BB	617	CLA	2	0
22	BB	618	CLA	6	0
22	BB	619	CLA	6	0
26	BB	620	BCR	3	0
26	BB	622	BCR	2	0
30	BB	623	LMG	1	0
30	BB	624	LMG	1	0
32	BB	626	LMT	2	0
22	BC	501	CLA	3	0
22	BC	502	CLA	4	0
22	BC	503	CLA	5	0
22	BC	504	CLA	6	0
22	BC	505	CLA	10	0
22	BC	506	CLA	3	0
22	BC	507	CLA	4	0
22	BC	508	CLA	7	0
22	BC	509	CLA	2	0
22	BC	510	CLA	3	0
22	BC	511	CLA	11	0
22	BC	512	CLA	7	0
22	BC	513	CLA	4	0
26	BC	514	BCR	10	0
26	BC	515	BCR	7	0
27	BC	516	DGD	3	0
27	BC	517	DGD	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	BC	518	DGD	8	0
30	BC	519	LMG	3	0
30	BC	520	LMG	5	0
28	BC	521	LHG	4	0
33	BD	401	BCT	1	0
22	BD	402	CLA	8	0
23	BD	403	PHO	5	0
22	BD	404	CLA	4	0
24	BD	405	PL9	8	0
26	BD	406	BCR	3	0
30	BD	407	LMG	2	0
30	BD	408	LMG	8	0
29	BD	409	SQD	2	0
32	BD	411	LMT	1	0
34	BE	101	HEM	6	0
30	BE	102	LMG	4	0
29	BF	101	SQD	1	0
27	BH	101	DGD	1	0
30	BI	101	LMG	3	0
32	BI	102	LMT	3	0
26	BJ	102	BCR	5	0
26	BK	102	BCR	13	0
29	BL	101	SQD	2	0
32	BM	101	LMT	1	0
30	BM	102	LMG	4	0
32	BT	101	LMT	3	0
34	BV	201	HEM	3	0
26	BX	101	BCR	6	0
26	BZ	101	BCR	5	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	AA	335/344 (97%)	-0.44	8 (2%) 62 57	23, 59, 88, 103	0
1	BA	335/344 (97%)	-0.24	5 (1%) 76 74	47, 70, 89, 103	0
2	AB	490/510 (96%)	-0.23	9 (1%) 71 68	37, 63, 86, 99	0
2	BB	490/510 (96%)	-0.24	11 (2%) 65 60	41, 64, 87, 103	0
3	AC	447/473 (94%)	-0.19	12 (2%) 58 52	43, 72, 87, 102	0
3	BC	447/473 (94%)	0.06	18 (4%) 42 35	54, 83, 95, 101	0
4	AD	340/352 (96%)	-0.43	3 (0%) 85 84	29, 59, 84, 95	0
4	BD	340/352 (96%)	-0.32	5 (1%) 76 74	40, 69, 91, 101	0
5	AE	82/84 (97%)	0.10	6 (7%) 18 12	54, 75, 93, 99	0
5	BE	82/84 (97%)	0.51	8 (9%) 10 6	71, 85, 98, 104	0
6	AF	35/45 (77%)	-0.13	2 (5%) 27 21	56, 73, 94, 97	0
6	BF	35/45 (77%)	0.39	5 (14%) 4 2	75, 82, 97, 99	0
7	AH	65/66 (98%)	0.16	4 (6%) 24 17	57, 76, 92, 97	0
7	BH	65/66 (98%)	0.30	8 (12%) 5 3	62, 80, 91, 103	0
8	AI	35/38 (92%)	-0.07	3 (8%) 13 8	57, 70, 87, 94	0
8	BI	35/38 (92%)	-0.03	0 100 100	69, 80, 92, 95	0
9	AJ	34/40 (85%)	-0.41	0 100 100	65, 74, 83, 89	0
9	BJ	34/40 (85%)	-0.20	1 (2%) 55 49	73, 81, 93, 98	0
10	AK	37/37 (100%)	-0.35	1 (2%) 58 52	67, 75, 87, 93	0
10	BK	37/37 (100%)	0.01	2 (5%) 29 23	84, 90, 96, 101	0
11	AL	37/37 (100%)	0.19	6 (16%) 3 1	45, 60, 98, 107	0
11	BL	37/37 (100%)	0.26	5 (13%) 4 2	46, 62, 94, 102	0
12	AM	34/36 (94%)	-0.05	2 (5%) 26 19	51, 65, 94, 100	0
12	BM	34/36 (94%)	-0.16	2 (5%) 26 19	55, 61, 76, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AO	243/247 (98%)	0.11	15 (6%) 24 17	39, 70, 93, 107	0
13	BO	243/247 (98%)	0.24	18 (7%) 17 11	48, 76, 97, 107	0
14	AT	32/32 (100%)	0.10	3 (9%) 11 6	53, 63, 102, 104	0
14	BT	32/32 (100%)	-0.12	2 (6%) 23 17	57, 67, 93, 103	0
15	AU	97/104 (93%)	-0.05	1 (1%) 84 82	43, 63, 78, 86	0
15	BU	97/104 (93%)	-0.20	1 (1%) 84 82	55, 67, 77, 87	0
16	AV	137/137 (100%)	-0.19	1 (0%) 89 88	49, 66, 76, 79	0
16	BV	137/137 (100%)	0.15	7 (5%) 32 25	64, 79, 95, 102	0
17	Ay	28/46 (60%)	0.40	4 (14%) 4 2	79, 91, 97, 99	0
17	By	28/46 (60%)	0.43	3 (10%) 8 4	89, 98, 102, 106	0
18	AX	37/50 (74%)	-0.17	2 (5%) 29 23	70, 79, 93, 95	0
18	BX	37/50 (74%)	0.35	6 (16%) 3 1	75, 82, 91, 94	0
19	AY	0/28	-	-	-	-
19	BY	0/28	-	-	-	-
20	AZ	62/62 (100%)	0.33	10 (16%) 3 1	76, 85, 103, 110	0
20	BZ	62/62 (100%)	0.69	12 (19%) 1 1	86, 96, 105, 110	0
All	All	5214/5536 (94%)	-0.11	211 (4%) 42 35	23, 71, 94, 110	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	BH	65	LEU	8.7
12	AM	33	GLN	6.9
3	BC	473	ASP	6.3
11	BL	1	MET	6.3
14	AT	30	THR	6.3
1	BA	10	SER	6.3
20	BZ	62	VAL	5.9
7	BH	66	GLY	5.8
5	BE	84	LYS	5.7
20	BZ	1	MET	5.5
5	BE	4	THR	5.5
20	AZ	1	MET	5.3
2	BB	128	THR	5.3
11	BL	2	GLU	5.2
14	AT	32	LYS	5.2
6	BF	11	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
20	AZ	34	ASP	5.1
13	BO	49	ASP	5.1
1	BA	12	ASN	5.1
6	AF	12	SER	5.0
20	AZ	33	TRP	5.0
3	BC	253	LEU	4.9
5	AE	84	LYS	4.9
1	BA	11	ALA	4.9
13	BO	50	ASP	4.8
4	BD	227	GLU	4.8
14	AT	31	LYS	4.6
14	BT	32	LYS	4.5
18	BX	46	VAL	4.5
4	BD	239	GLN	4.5
5	AE	6	GLY	4.3
20	BZ	61	VAL	4.2
13	AO	84	ASN	4.2
20	BZ	60	PHE	4.2
18	BX	47	GLN	4.2
6	BF	13	TYR	4.2
2	BB	85	GLY	4.2
12	BM	33	GLN	4.1
3	AC	192	GLY	4.1
20	BZ	31	GLN	4.1
20	BZ	34	ASP	4.1
13	BO	51	THR	4.1
13	AO	87	GLN	4.1
18	BX	12	ILE	4.0
5	AE	17	VAL	4.0
11	BL	3	PRO	3.9
13	BO	232	GLY	3.8
13	BO	84	ASN	3.8
20	AZ	62	VAL	3.7
7	BH	64	ALA	3.7
4	AD	227	GLU	3.6
5	BE	61	ARG	3.6
13	BO	61	SER	3.6
20	AZ	38	GLN	3.6
1	AA	10	SER	3.6
5	BE	60	GLN	3.6
13	BO	87	GLN	3.6
13	BO	52	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
13	BO	48	LEU	3.5
11	AL	2	GLU	3.5
18	AX	47	GLN	3.4
13	BO	60	SER	3.4
5	BE	6	GLY	3.4
17	Ay	45	ASN	3.4
3	BC	142	GLU	3.4
13	AO	272	ALA	3.4
18	AX	46	VAL	3.4
1	BA	15	GLU	3.3
3	BC	30	SER	3.3
17	Ay	41	VAL	3.3
2	BB	488	PRO	3.3
18	BX	11	THR	3.3
20	AZ	30	PRO	3.3
1	AA	12	ASN	3.3
3	BC	472	LEU	3.3
2	AB	85	GLY	3.3
3	AC	182	PHE	3.2
16	BV	39	ASN	3.2
20	BZ	4	LEU	3.2
3	AC	214	LEU	3.2
3	AC	143	TYR	3.2
4	AD	13	GLY	3.2
4	BD	226	GLY	3.2
11	BL	7	ARG	3.2
5	BE	17	VAL	3.1
1	AA	11	ALA	3.1
16	BV	43	LYS	3.1
15	BU	53	GLU	3.1
11	AL	1	MET	3.1
7	BH	6	TRP	3.0
20	AZ	60	PHE	3.0
5	AE	5	THR	3.0
3	AC	27	ASP	3.0
13	AO	88	GLU	3.0
20	AZ	4	LEU	3.0
5	AE	83	LEU	2.9
2	AB	127	ARG	2.9
9	BJ	7	ARG	2.9
6	BF	12	SER	2.9
13	AO	115	SER	2.9

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Mol	Chain	Res	Type	RSRZ
13	AO	114	ASN	2.9
16	BV	50	LYS	2.9
3	BC	471	SER	2.9
13	BO	88	GLU	2.9
2	AB	128	THR	2.9
13	AO	271	PRO	2.8
13	BO	35	ASP	2.8
3	BC	204	LEU	2.8
20	BZ	3	ILE	2.8
3	BC	252	ILE	2.8
8	AI	34	ARG	2.7
10	BK	10	LYS	2.7
13	AO	59	ASP	2.7
12	BM	34	LYS	2.7
1	AA	243	GLU	2.7
18	BX	13	THR	2.7
3	BC	214	LEU	2.7
5	BE	3	GLY	2.7
2	AB	130	GLU	2.7
7	AH	66	GLY	2.7
17	By	19	ILE	2.6
5	AE	12	ASP	2.6
4	BD	241	GLU	2.6
16	BV	116	GLU	2.6
20	BZ	35	ARG	2.6
7	BH	23	PRO	2.6
11	BL	5	PRO	2.6
16	BV	42	GLY	2.6
3	BC	207	ARG	2.6
13	AO	51	THR	2.6
12	AM	34	LYS	2.6
7	AH	6	TRP	2.6
6	AF	11	VAL	2.6
17	By	22	LEU	2.5
5	BE	71	GLU	2.5
3	AC	102	GLY	2.5
6	BF	44	GLN	2.5
3	BC	145	SER	2.5
13	AO	35	ASP	2.5
11	AL	3	PRO	2.5
1	AA	16	ARG	2.5
7	AH	4	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
20	BZ	38	GLN	2.5
15	AU	38	GLU	2.5
1	BA	16	ARG	2.5
11	AL	5	PRO	2.5
20	AZ	35	ARG	2.5
13	AO	62	GLN	2.5
3	BC	208	VAL	2.4
3	AC	191	PRO	2.4
13	AO	124	GLU	2.4
8	AI	33	LYS	2.4
14	BT	31	LYS	2.4
10	BK	46	ARG	2.4
20	AZ	3	ILE	2.4
3	BC	32	GLY	2.4
2	AB	490	GLN	2.4
17	By	41	VAL	2.4
13	BO	32	THR	2.4
13	BO	63	THR	2.4
11	AL	7	ARG	2.4
3	BC	146	PHE	2.4
3	BC	182	PHE	2.4
17	Ay	21	GLN	2.4
2	BB	130	GLU	2.4
16	BV	132	ASN	2.4
2	AB	129	GLY	2.3
2	BB	127	ARG	2.3
1	AA	227	THR	2.3
2	BB	490	GLN	2.3
11	AL	4	ASN	2.3
13	AO	31	LEU	2.3
8	AI	35	LYS	2.3
2	BB	294	SER	2.3
2	BB	350	GLU	2.3
2	BB	161	LEU	2.3
2	AB	487	SER	2.3
7	AH	9	ASP	2.2
3	BC	255	THR	2.2
7	BH	59	ASN	2.2
3	AC	460	ASP	2.2
17	Ay	19	ILE	2.2
2	BB	293	ALA	2.2
10	AK	10	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
13	BO	54	GLY	2.2
3	AC	471	SER	2.2
16	AV	40	SER	2.2
6	BF	42	PHE	2.2
20	BZ	37	LYS	2.2
4	AD	228	GLY	2.2
18	BX	45	LYS	2.2
7	BH	7	LEU	2.2
20	BZ	33	TRP	2.2
13	AO	222	GLN	2.1
7	BH	18	TYR	2.1
16	BV	115	ALA	2.1
13	BO	112	LYS	2.1
13	BO	89	ALA	2.1
2	BB	413	ASP	2.1
13	AO	158	ASN	2.1
3	AC	207	ARG	2.1
1	AA	225	ARG	2.1
3	BC	144	SER	2.1
3	BC	53	HIS	2.1
2	AB	488	PRO	2.1
1	AA	31	GLY	2.0
3	AC	236	GLY	2.0
4	BD	17	ILE	2.0
2	AB	125	ASP	2.0
3	AC	181	PHE	2.0
13	BO	90	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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
31	CL	AA	414	1/1	0.94	0.62	21.13	73,73,73,73	0
27	DGD	AD	410	63/66	0.63	0.53	10.64	91,97,107,108	0
26	BCR	BJ	102	40/40	0.68	0.49	9.03	93,98,101,102	0
24	PL9	AJ	101	35/55	0.60	0.56	8.38	93,101,107,109	0
27	DGD	BD	410	63/66	0.64	0.51	7.79	84,100,105,105	0
24	PL9	BJ	101	35/55	0.71	0.44	7.20	78,99,111,112	0
30	LMG	AA	416	42/55	0.72	0.37	6.04	67,92,96,99	0
32	LMT	BI	102	35/35	0.62	0.57	6.03	90,104,106,106	0
32	LMT	AI	102	35/35	0.78	0.49	5.79	74,92,95,95	0
22	CLA	AD	404	65/65	0.83	0.32	5.62	80,83,102,103	0
26	BCR	AJ	102	40/40	0.71	0.41	5.54	85,91,101,102	0
22	CLA	BA	407	65/65	0.75	0.35	5.50	72,76,103,104	0
30	LMG	AB	623	42/55	0.71	0.36	5.29	70,89,92,93	0
27	DGD	AB	626	52/66	0.79	0.29	4.84	79,94,105,107	0
24	PL9	AA	407	45/55	0.85	0.32	4.81	83,87,94,95	0
22	CLA	AB	601	65/65	0.74	0.39	4.80	88,97,102,105	0
32	LMT	AD	411	31/35	0.74	0.46	4.77	52,96,104,104	0
30	LMG	BC	520	45/55	0.71	0.48	4.69	86,93,101,102	0
30	LMG	AC	520	45/55	0.65	0.42	4.48	75,92,97,98	0
22	CLA	AA	406	65/65	0.79	0.31	4.39	54,60,89,90	0
24	PL9	BA	408	45/55	0.86	0.30	4.26	82,88,90,92	0
32	LMT	AT	101	35/35	0.70	0.34	4.21	72,91,97,98	0
29	SQD	BA	401	54/54	0.75	0.34	4.13	82,91,107,108	0
28	LHG	AC	521	37/49	0.68	0.44	3.88	78,99,109,109	0
32	LMT	AB	625	35/35	0.74	0.43	3.76	82,98,100,101	0
27	DGD	BB	602	52/66	0.72	0.31	3.73	71,85,104,105	0
28	LHG	BC	521	37/49	0.68	0.49	3.59	90,100,113,114	0
26	BCR	AK	102	40/40	0.85	0.31	3.54	73,77,81,81	0
32	LMT	BD	411	31/35	0.65	0.50	3.46	67,91,99,100	0
22	CLA	AB	604	65/65	0.89	0.25	3.43	67,73,91,91	0
30	LMG	BD	408	48/55	0.85	0.26	3.40	68,75,85,87	0
29	SQD	AA	415	54/54	0.83	0.27	3.39	71,87,105,105	0
26	BCR	AZ	101	40/40	0.79	0.32	3.16	75,82,90,91	0
26	BCR	BK	102	40/40	0.84	0.35	3.14	76,81,85,85	0
30	LMG	BD	407	46/55	0.88	0.24	3.05	70,80,92,94	0
22	CLA	AC	512	65/65	0.81	0.32	2.98	91,95,106,106	0
32	LMT	AB	627	35/35	0.47	0.54	2.92	73,103,106,107	0
31	CL	BA	415	1/1	0.93	0.29	2.87	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	LMG	BE	102	44/55	0.81	0.37	2.84	75,92,98,99	0
22	CLA	BB	612	65/65	0.88	0.28	2.77	82,89,92,95	0
22	CLA	AC	504	65/65	0.90	0.23	2.66	78,86,107,107	0
29	SQD	AF	101	45/54	0.72	0.35	2.63	82,97,102,103	0
23	PHO	BD	403	64/64	0.93	0.23	2.61	77,88,92,93	0
30	LMG	AD	408	48/55	0.90	0.23	2.46	63,68,74,80	0
29	SQD	BF	101	45/54	0.66	0.38	2.40	95,98,103,104	0
22	CLA	AC	507	65/65	0.87	0.27	2.33	83,90,95,97	0
22	CLA	AD	402	65/65	0.94	0.21	2.24	47,58,69,71	0
22	CLA	BA	405	65/65	0.94	0.20	2.23	72,76,104,105	0
26	BCR	AH	101	40/40	0.78	0.32	2.19	76,88,95,95	0
27	DGD	AC	517	62/66	0.89	0.22	2.17	70,78,91,92	0
22	CLA	AC	503	65/65	0.94	0.21	2.14	78,86,92,95	0
22	CLA	AB	609	65/65	0.88	0.26	2.12	76,87,91,92	0
22	CLA	BC	513	65/65	0.82	0.34	2.08	96,99,106,107	0
27	DGD	BA	411	56/66	0.76	0.35	2.07	76,85,103,104	0
32	LMT	BT	101	35/35	0.78	0.34	2.02	77,91,94,95	0
33	BCT	BD	401	4/4	0.95	0.20	1.96	84,86,87,88	0
26	BCR	BC	514	40/40	0.90	0.24	1.94	81,83,87,87	0
26	BCR	AC	514	40/40	0.90	0.23	1.93	56,66,73,74	0
32	LMT	BB	626	35/35	0.77	0.31	1.93	76,93,101,102	0
30	LMG	AC	519	48/55	0.79	0.31	1.92	75,84,89,90	0
26	BCR	BZ	101	40/40	0.81	0.27	1.91	81,90,93,94	0
32	LMT	BM	101	35/35	0.79	0.31	1.89	70,88,97,101	0
22	CLA	AC	513	65/65	0.77	0.35	1.86	92,98,104,106	0
22	CLA	AB	614	65/65	0.91	0.23	1.83	78,85,98,99	0
26	BCR	AT	102	40/40	0.92	0.21	1.83	72,79,91,91	0
26	BCR	AB	618	40/40	0.90	0.20	1.79	75,78,82,83	0
24	PL9	BD	405	55/55	0.93	0.21	1.78	63,70,76,78	0
30	LMG	AE	102	44/55	0.77	0.34	1.76	81,91,96,96	0
26	BCR	BB	622	40/40	0.92	0.25	1.72	67,71,79,80	0
22	CLA	BC	510	65/65	0.92	0.22	1.68	79,83,92,92	0
22	CLA	BD	404	65/65	0.83	0.26	1.68	89,92,101,102	0
26	BCR	AB	620	40/40	0.87	0.24	1.67	75,77,83,84	0
30	LMG	BB	623	49/55	0.88	0.23	1.66	70,78,88,91	0
34	HEM	AE	101	43/43	0.93	0.29	1.65	85,92,103,106	0
22	CLA	AA	404	65/65	0.93	0.20	1.63	63,72,97,99	0
30	LMG	BC	519	48/55	0.86	0.31	1.61	83,90,94,95	0
24	PL9	AD	405	55/55	0.93	0.20	1.61	52,67,71,73	0
22	CLA	AC	505	65/65	0.93	0.20	1.60	69,73,77,79	0
26	BCR	BC	515	40/40	0.79	0.30	1.60	74,80,91,92	0
27	DGD	AC	516	53/66	0.89	0.23	1.59	57,72,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	BB	609	65/65	0.83	0.26	1.58	72,80,96,96	0
26	BCR	BD	406	40/40	0.88	0.23	1.56	66,78,92,92	0
26	BCR	BB	620	40/40	0.92	0.20	1.56	66,69,72,73	0
27	DGD	BC	517	62/66	0.86	0.22	1.52	78,82,100,101	0
27	DGD	AA	410	56/66	0.76	0.32	1.48	78,86,91,92	0
27	DGD	BC	516	53/66	0.90	0.23	1.48	69,77,96,97	0
28	LHG	AA	411	39/49	0.90	0.22	1.43	63,68,76,78	0
22	CLA	AB	602	65/65	0.94	0.22	1.42	81,85,88,90	0
26	BCR	AB	619	40/40	0.91	0.19	1.38	62,70,82,83	0
30	LMG	AA	413	51/55	0.88	0.24	1.33	70,74,77,79	0
22	CLA	AB	606	65/65	0.85	0.25	1.31	73,87,96,96	0
34	HEM	BE	101	43/43	0.92	0.28	1.30	93,95,104,107	0
22	CLA	BB	617	65/65	0.92	0.22	1.29	75,79,99,100	0
27	DGD	BC	518	66/66	0.86	0.24	1.29	71,78,89,90	0
30	LMG	AD	407	46/55	0.92	0.20	1.27	63,71,90,92	0
22	CLA	BB	613	65/65	0.92	0.22	1.26	69,77,82,84	0
30	LMG	AB	621	49/55	0.87	0.23	1.26	62,75,80,83	0
22	CLA	BC	507	65/65	0.89	0.24	1.24	84,92,96,97	0
27	DGD	AC	518	66/66	0.89	0.22	1.23	62,68,84,86	0
32	LMT	AM	102	35/35	0.83	0.30	1.20	67,89,93,96	0
26	BCR	AA	409	40/40	0.92	0.21	1.20	59,67,70,71	0
22	CLA	AB	605	65/65	0.94	0.20	1.19	68,76,84,85	0
22	CLA	AA	402	65/65	0.96	0.17	1.16	51,58,66,69	0
23	PHO	AD	403	64/64	0.93	0.18	1.16	39,56,70,72	0
22	CLA	BB	605	65/65	0.94	0.20	1.16	77,82,86,89	0
29	SQD	AD	409	43/54	0.82	0.24	1.14	68,92,108,111	0
22	CLA	BC	512	65/65	0.81	0.31	1.13	95,99,109,110	0
22	CLA	AB	608	65/65	0.93	0.19	1.10	72,79,87,91	0
22	CLA	AB	616	65/65	0.80	0.27	1.10	73,85,105,106	0
27	DGD	BH	101	58/66	0.91	0.19	1.10	66,73,80,81	0
29	SQD	BA	413	51/54	0.81	0.25	1.07	73,90,103,104	0
30	LMG	BM	102	42/55	0.79	0.31	1.06	72,90,95,98	0
22	CLA	AA	403	65/65	0.95	0.16	1.06	41,48,56,60	0
22	CLA	BC	505	65/65	0.90	0.22	1.04	88,93,94,95	0
34	HEM	AV	201	43/43	0.96	0.20	1.03	60,63,66,67	0
22	CLA	AC	508	65/65	0.91	0.20	1.02	80,86,99,101	0
26	BCR	BB	621	40/40	0.92	0.19	1.02	57,69,82,83	0
22	CLA	BB	604	65/65	0.71	0.34	1.00	86,98,107,109	0
29	SQD	AA	412	51/54	0.83	0.23	0.97	73,83,98,99	0
22	CLA	BB	606	65/65	0.93	0.19	0.97	58,61,74,76	0
32	LMT	BB	603	35/35	0.67	0.35	0.94	68,86,95,96	0
30	LMG	AB	622	49/55	0.89	0.19	0.93	64,73,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	AB	612	65/65	0.93	0.21	0.91	63,75,81,83	0
22	CLA	AB	610	65/65	0.91	0.21	0.89	60,67,79,80	0
22	CLA	BC	508	65/65	0.89	0.23	0.88	92,97,101,106	0
22	CLA	BD	402	65/65	0.96	0.17	0.88	50,57,79,83	0
22	CLA	BB	607	65/65	0.93	0.19	0.86	53,64,86,87	0
22	CLA	BB	608	65/65	0.95	0.18	0.85	45,53,76,78	0
22	CLA	AC	501	65/65	0.95	0.20	0.80	78,83,85,86	0
22	CLA	BB	619	65/65	0.74	0.29	0.78	75,81,93,95	0
26	BCR	BX	101	40/40	0.80	0.30	0.74	76,79,89,90	0
29	SQD	BD	409	43/54	0.80	0.25	0.71	73,88,110,111	0
30	LMG	BB	624	49/55	0.91	0.18	0.70	68,72,78,79	0
22	CLA	AC	511	65/65	0.89	0.25	0.70	77,85,89,90	0
23	PHO	AA	405	64/64	0.95	0.16	0.70	40,64,67,69	0
26	BCR	BA	410	40/40	0.92	0.20	0.67	61,74,82,83	0
26	BCR	AD	406	40/40	0.94	0.16	0.66	64,72,85,85	0
28	LHG	BA	412	39/49	0.91	0.23	0.65	72,77,80,81	0
22	CLA	BB	615	65/65	0.94	0.18	0.64	60,72,77,81	0
22	CLA	BB	610	65/65	0.95	0.17	0.61	60,70,77,81	0
22	CLA	AC	506	65/65	0.86	0.22	0.61	83,87,101,102	0
30	LMG	BA	414	51/55	0.90	0.20	0.58	62,71,78,80	0
29	SQD	BB	601	47/54	0.88	0.23	0.57	74,87,109,111	0
22	CLA	AB	613	65/65	0.95	0.17	0.53	65,69,84,87	0
34	HEM	BV	201	43/43	0.96	0.19	0.52	58,67,76,79	0
22	CLA	BC	504	65/65	0.92	0.19	0.52	87,92,102,102	0
27	DGD	AH	102	58/66	0.92	0.19	0.51	57,72,85,86	0
22	CLA	AB	611	65/65	0.94	0.19	0.51	62,68,71,73	0
22	CLA	BC	502	65/65	0.91	0.21	0.49	81,85,101,103	0
22	CLA	BC	511	65/65	0.89	0.25	0.45	91,99,104,105	0
29	SQD	BL	101	47/54	0.84	0.24	0.44	75,91,115,116	0
30	LMG	AM	101	42/55	0.80	0.29	0.41	68,86,93,95	0
22	CLA	AC	509	65/65	0.95	0.20	0.37	59,74,86,89	0
22	CLA	AB	603	65/65	0.94	0.17	0.33	54,60,72,74	0
22	CLA	AB	615	65/65	0.92	0.20	0.33	83,93,97,99	0
22	CLA	BC	506	65/65	0.86	0.24	0.33	81,85,97,99	0
33	BCT	AD	401	4/4	0.97	0.18	0.33	90,91,91,92	0
22	CLA	BC	509	65/65	0.92	0.21	0.32	73,83,93,94	0
26	BCR	AC	515	40/40	0.89	0.22	0.29	69,75,80,81	0
22	CLA	BC	501	65/65	0.93	0.19	0.28	76,80,87,88	0
23	PHO	BA	406	64/64	0.95	0.16	0.24	54,61,70,74	0
22	CLA	BC	503	65/65	0.91	0.20	0.15	82,97,100,101	0
22	CLA	BB	618	65/65	0.91	0.21	0.12	69,84,87,88	0
22	CLA	BA	404	65/65	0.95	0.16	0.10	55,60,68,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
22	CLA	BB	616	65/65	0.95	0.15	0.04	49,54,79,82	0
22	CLA	AB	607	65/65	0.95	0.15	0.02	50,55,74,74	0
22	CLA	BA	403	65/65	0.95	0.17	-0.06	57,64,71,75	0
26	BCR	AB	617	40/40	0.93	0.17	-0.07	56,67,75,76	0
22	CLA	AC	502	65/65	0.95	0.16	-0.07	50,58,81,84	0
22	CLA	BB	611	65/65	0.95	0.17	-0.07	67,74,81,85	0
22	CLA	BB	614	65/65	0.95	0.16	-0.25	59,68,75,77	0
25	OEC	BA	409	5/9	0.71	0.14	-0.51	30,74,79,92	0
25	OEC	AA	408	5/9	0.93	0.13	-0.71	56,62,67,75	0
22	CLA	AC	510	65/65	0.95	0.14	-0.79	48,56,70,72	0
21	FE2	AA	401	1/1	0.98	0.12	-1.91	69,69,69,69	0
21	FE2	BA	402	1/1	0.98	0.12	-2.36	81,81,81,81	0
32	LMT	AB	624	35/35	0.51	0.63	-	71,100,106,107	0
30	LMG	AI	101	43/55	0.63	0.46	-	83,92,97,98	0
35	CA	AO	301	1/1	0.91	0.23	-	87,87,87,87	0
35	CA	BO	301	1/1	0.76	0.34	-	100,100,100,100	0
32	LMT	BB	625	35/35	0.72	0.42	-	66,103,111,111	0
35	CA	BK	101	1/1	0.84	0.13	-	90,90,90,90	0
35	CA	AK	101	1/1	0.79	0.09	-	95,95,95,95	0
30	LMG	BI	101	43/55	0.73	0.37	-	84,90,99,100	0

6.5 Other polymers

There are no such residues in this entry.