



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2017 – 03:46 PM EST

PDB ID : 5E79
Title : Macromolecular diffractive imaging using imperfect crystals
Authors : Ayer, K.; Yefanov, O.; Oberthur, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffer, A.; Dorner, K.; James, D.; Kupitz, C.; Metz, M.; Nelson, G.; Xavier, P.L.; Beyerlein, K.R.; Schmidt, M.; Sarrou, I.; Spence, J.C.H.; Weierstall, U.; White, T.A.; Yang, J.-H.; Zhao, Y.; Liang, M.; Aquila, A.; Hunter, M.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 3.50 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

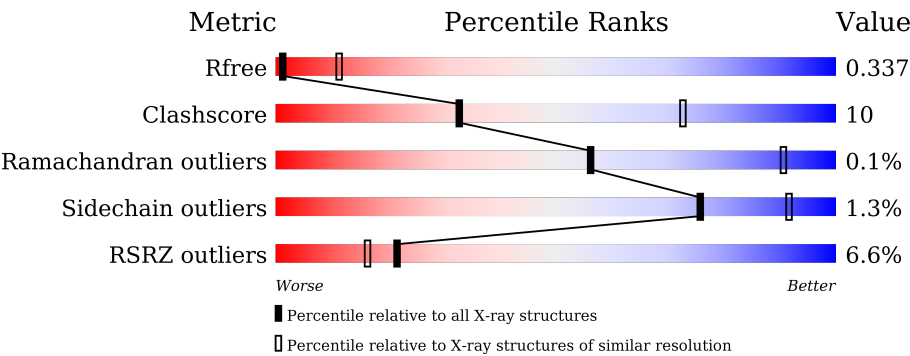
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div><div>6%</div><div>69%</div><div>31%</div></div>
1	a	334	<div><div>7%</div><div>100%</div></div>
2	B	504	<div><div>3%</div><div>70%</div><div>29%</div><div>.</div></div>
2	b	504	<div><div>9%</div><div>99%</div><div>.</div></div>
3	C	451	<div><div>6%</div><div>75%</div><div>24%</div></div>
3	c	451	<div><div>9%</div><div>99%</div><div>.</div></div>

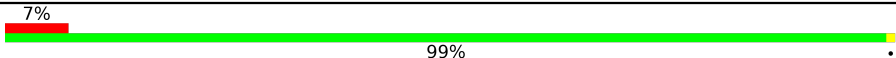
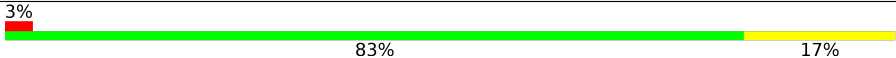

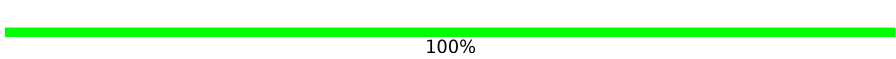
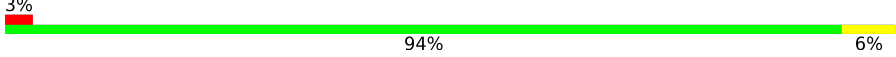
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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	38	
9	j	38	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	243	
13	o	243	
14	T	30	
14	t	30	
15	U	97	
15	u	97	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	29	
17	y	29	
18	X	39	
18	x	39	
19	Z	62	
19	z	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	CL	A	603	-	-	-	X
22	CL	A	604	-	-	-	X
23	BCT	A	605	-	-	-	X
23	BCT	a	605	-	-	-	X
24	CLA	A	606	X	-	-	X
24	CLA	A	607	X	-	-	X
24	CLA	A	609	X	-	-	X
24	CLA	B	602	X	-	-	X
24	CLA	B	603	X	-	-	X
24	CLA	B	604	X	-	-	X
24	CLA	B	605	X	-	-	X
24	CLA	B	606	X	-	-	X
24	CLA	B	607[A]	X	-	-	X
24	CLA	B	607[B]	X	-	-	X
24	CLA	B	608	X	-	-	X
24	CLA	B	609	X	-	-	X
24	CLA	B	610	X	-	-	X
24	CLA	B	611	X	-	-	X
24	CLA	B	612	X	-	-	X
24	CLA	B	613	X	-	-	X
24	CLA	B	614	X	-	-	X
24	CLA	B	615	X	-	-	X
24	CLA	B	616	X	-	-	X
24	CLA	B	617	X	-	-	X
24	CLA	C	501	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	502	X	-	-	X
24	CLA	C	503	X	-	-	X
24	CLA	C	504	X	-	-	X
24	CLA	C	505	X	-	-	X
24	CLA	C	506	X	-	-	X
24	CLA	C	507	X	-	-	X
24	CLA	C	508	X	-	-	X
24	CLA	C	509	X	-	-	X
24	CLA	C	510	X	-	-	X
24	CLA	C	511	X	-	-	X
24	CLA	C	512	X	-	-	X
24	CLA	C	513	X	-	-	X
24	CLA	D	402	X	-	-	X
24	CLA	D	403	X	-	-	X
24	CLA	D	404	X	-	-	X
24	CLA	a	606	X	-	-	X
24	CLA	a	607	X	-	-	X
24	CLA	a	609	X	-	-	X
24	CLA	a	615	X	-	-	X
24	CLA	b	603	X	-	-	X
24	CLA	b	604	X	-	-	X
24	CLA	b	605	X	-	-	X
24	CLA	b	606	X	-	-	X
24	CLA	b	607	X	-	-	X
24	CLA	b	608[A]	X	-	-	X
24	CLA	b	608[B]	X	-	-	X
24	CLA	b	609	X	-	-	X
24	CLA	b	610	X	-	-	X
24	CLA	b	611	X	-	-	X
24	CLA	b	612	X	-	-	X
24	CLA	b	613	X	-	-	X
24	CLA	b	614	X	-	-	X
24	CLA	b	615	X	-	-	X
24	CLA	b	616	X	-	-	X
24	CLA	b	617	X	-	-	X
24	CLA	b	618	X	-	-	X
24	CLA	c	501	X	-	-	X
24	CLA	c	502	X	-	-	X
24	CLA	c	503	X	-	-	X
24	CLA	c	504	X	-	-	X
24	CLA	c	505	X	-	-	X
24	CLA	c	506	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	507	X	-	-	X
24	CLA	c	508	X	-	-	X
24	CLA	c	509	X	-	-	X
24	CLA	c	510	X	-	-	X
24	CLA	c	511	X	-	-	X
24	CLA	c	512	X	-	-	X
24	CLA	c	513	X	-	-	X
24	CLA	d	402	X	-	-	X
24	CLA	d	403	X	-	-	-
25	PHO	A	608	-	-	-	X
25	PHO	D	401	-	-	-	X
25	PHO	a	608	-	-	-	X
25	PHO	d	401	-	-	-	X
26	BCR	A	610	-	-	-	X
26	BCR	B	618	-	-	X	X
26	BCR	B	619	-	-	X	X
26	BCR	B	620	-	-	X	X
26	BCR	C	514	-	-	X	X
26	BCR	F	101	-	-	X	X
26	BCR	H	101	-	-	X	X
26	BCR	I	101	-	-	-	X
26	BCR	K	101	-	-	X	X
26	BCR	K	102	-	-	-	X
26	BCR	T	101	-	-	X	X
26	BCR	a	610	-	-	-	X
26	BCR	b	619	-	-	-	X
26	BCR	b	620	-	-	-	X
26	BCR	b	621	-	-	-	X
26	BCR	c	514	-	X	-	X
26	BCR	c	515	-	-	-	X
26	BCR	c	521	-	-	-	X
26	BCR	f	101	-	-	-	X
26	BCR	h	101	-	X	-	X
26	BCR	k	101	-	-	-	X
26	BCR	t	101	-	-	-	X
27	PL9	A	611	-	-	-	X
27	PL9	D	405	-	-	-	X
27	PL9	a	611	-	-	-	X
27	PL9	d	404	-	-	-	X
28	SQD	A	612	-	-	-	X
28	SQD	A	614	-	-	-	X
28	SQD	B	622	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	SQD	L	102	-	-	-	X
28	SQD	X	101	-	-	-	X
28	SQD	a	612	-	-	-	X
28	SQD	a	614	-	-	-	X
28	SQD	b	601	-	-	-	X
28	SQD	l	101	-	-	-	X
28	SQD	x	101	-	-	-	X
29	LMG	A	613	-	-	-	X
29	LMG	B	621	-	-	-	X
29	LMG	C	518	-	-	-	X
29	LMG	C	519	-	-	-	X
29	LMG	D	408	-	-	-	X
29	LMG	Z	101	-	-	-	X
29	LMG	a	613	-	-	-	X
29	LMG	b	622	-	-	-	X
29	LMG	c	519	-	-	-	X
29	LMG	c	520	-	-	-	X
29	LMG	j	101	-	-	-	X
29	LMG	z	101	-	-	-	X
30	LHG	A	615	-	-	-	X
30	LHG	D	406	-	-	-	X
30	LHG	D	407	-	-	-	X
30	LHG	E	102	-	-	-	X
30	LHG	L	101	-	-	-	X
30	LHG	a	616	-	-	-	X
30	LHG	d	406	-	-	-	X
30	LHG	d	407	-	-	-	X
30	LHG	e	101	-	-	-	X
30	LHG	l	102	-	-	-	X
31	CA	o	301	-	-	-	X
32	DGD	C	515	-	-	-	X
32	DGD	C	516	-	-	-	X
32	DGD	C	517	-	-	-	X
32	DGD	E	101	-	-	-	X
32	DGD	H	102	-	-	-	X
32	DGD	c	516	-	-	-	X
32	DGD	c	517	-	-	-	X
32	DGD	c	518	-	-	-	X
32	DGD	d	405	-	-	-	X
32	DGD	h	102	-	-	-	X
33	HEM	E	103	-	-	-	X
33	HEM	V	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	HEM	e	102	-	-	-	X
33	HEM	v	201	-	-	-	X
34	MG	j	102	-	-	-	X

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 50074 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 II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2637	1730	432	460	15			
1	a	334	Total	C	N	O	S	3	4	0
			2637	1730	432	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	conflict	UNP P0A444
a	286	ALA	THR	conflict	UNP P0A444

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			
2	b	504	Total	C	N	O	S	0	10	0
			4024	2641	668	702	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			
3	c	451	Total	C	N	O	S	0	5	0
			3506	2296	584	613	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O		0	2	0
			668	436	107	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			
8	i	38	Total	C	N	O	S	0	1	0
			320	215	49	54	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	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	L	37	Total	C	N	O	S	5	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			
12	m	34	Total	C	N	O	S	0	1	0
			272	183	40	48	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			
13	o	243	Total	C	N	O	S	0	4	0
			1883	1178	315	385	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			
14	t	30	Total	C	N	O	S	0	2	0
			270	189	37	41	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	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	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

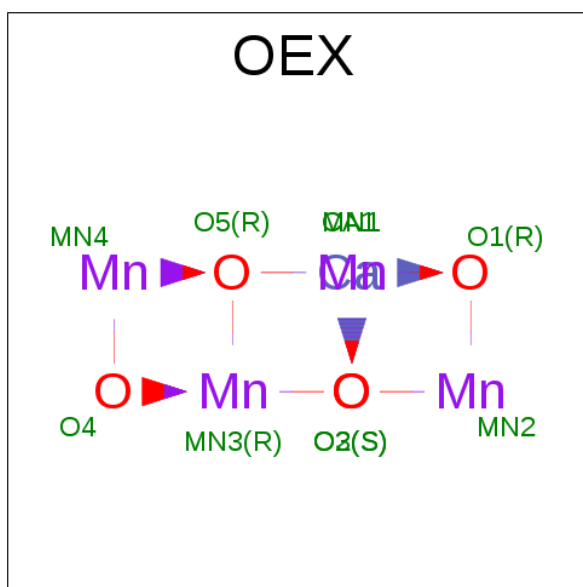
- Molecule 18 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	1	0
			292	196	46	50			
18	x	39	Total	C	N	O	0	1	0
			292	196	46	50			

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

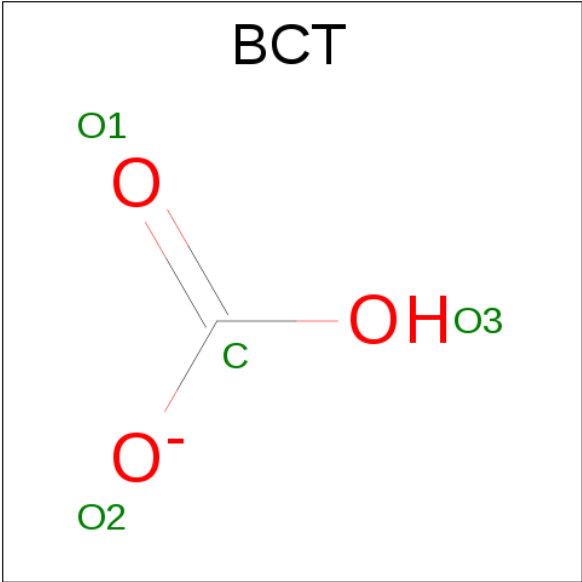
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

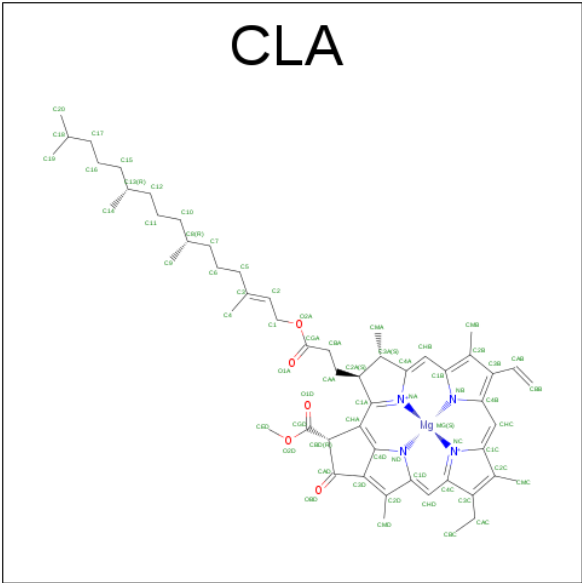
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	u	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	U	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	O		0	0
			4	1	3			
23	a	1	Total	C	O		0	0
			4	1	3			

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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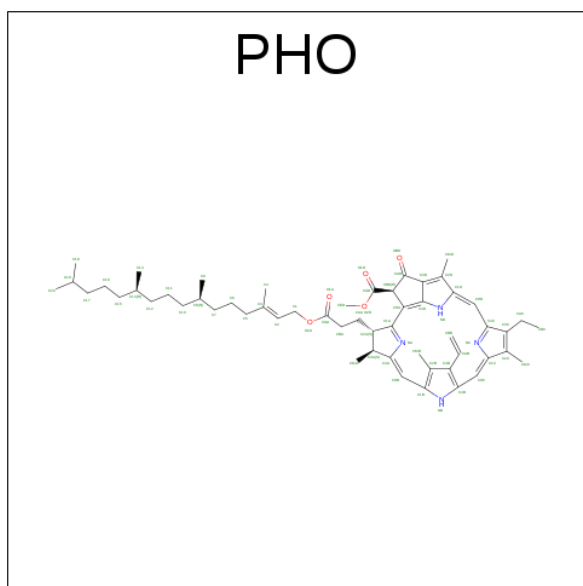
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	b	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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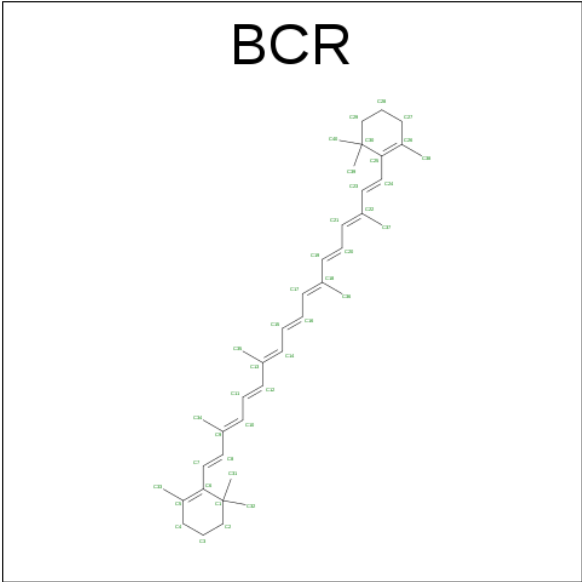
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



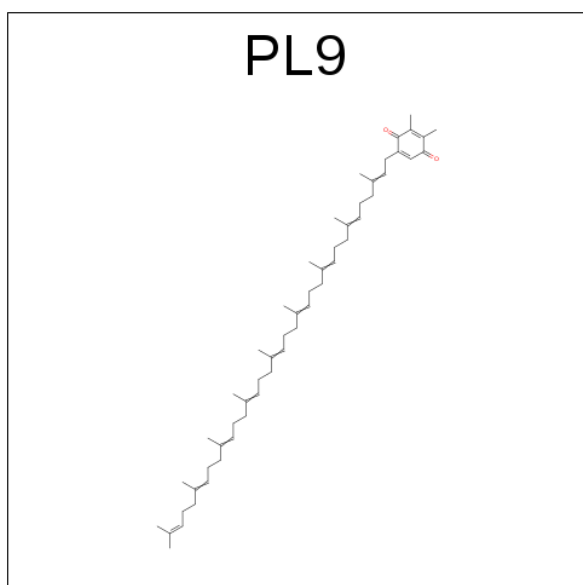
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	F	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	I	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0

- Molecule 27 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: $C_{53}H_{80}O_2$).



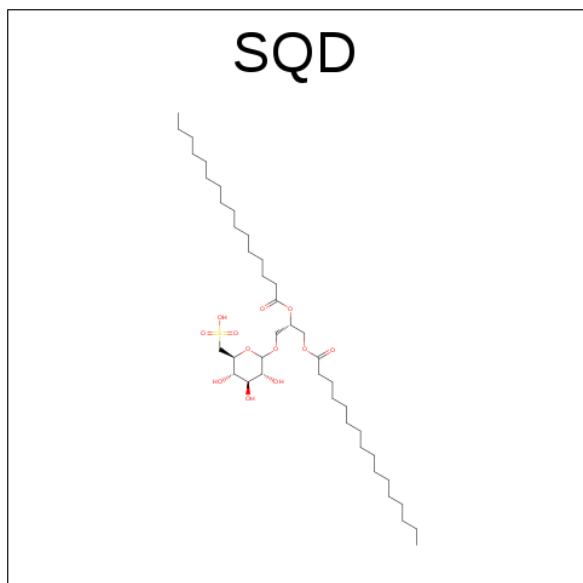
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



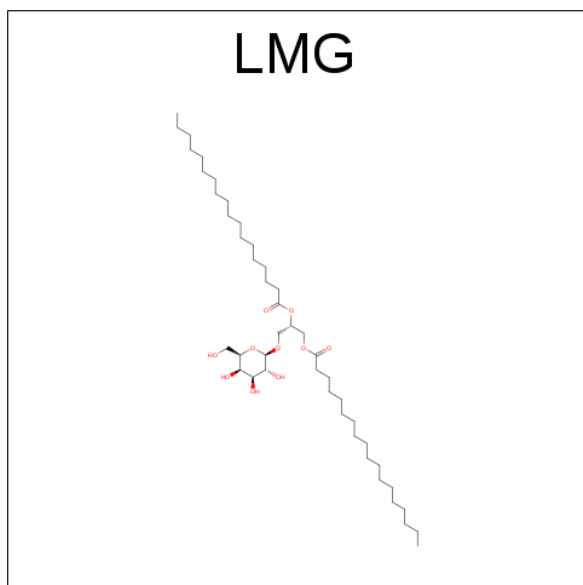
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	0
			54	41	12	1		
28	L	1	Total	C	O	S	0	0
			54	41	12	1		
28	X	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	0
			54	41	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	x	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



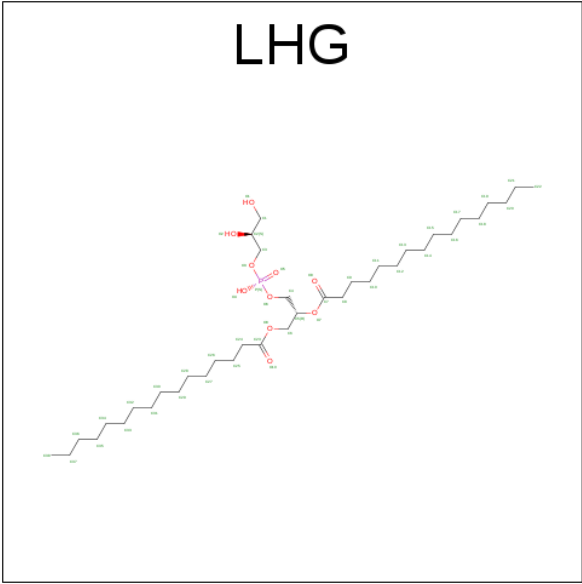
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O		0	0
			51	41	10			
29	B	1	Total	C	O		0	0
			51	41	10			
29	C	1	Total	C	O		0	0
			51	41	10			
29	C	1	Total	C	O		0	0
			51	41	10			
29	D	1	Total	C	O		0	0
			51	41	10			
29	Z	1	Total	C	O		0	0
			37	27	10			
29	a	1	Total	C	O		0	0
			51	41	10			
29	b	1	Total	C	O		0	0
			51	41	10			
29	c	1	Total	C	O		0	0
			51	41	10			
29	c	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	j	1	Total	C	O	0	0
			51	41	10		
29	z	1	Total	C	O	0	0
			37	27	10		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	D	1	Total	C	O	P	0	0
			49	38	10	1		
30	E	1	Total	C	O	P	0	0
			42	31	10	1		
30	L	1	Total	C	O	P	0	0
			49	38	10	1		
30	a	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	d	1	Total	C	O	P	0	0
			49	38	10	1		
30	e	1	Total	C	O	P	0	0
			42	31	10	1		

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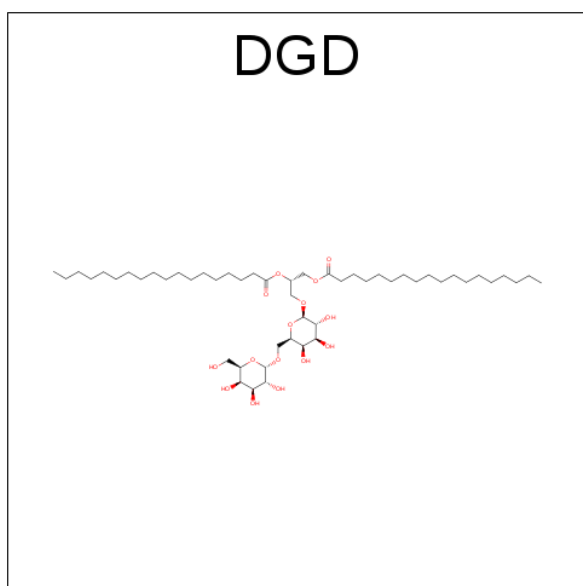
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 31 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	B	1	Total	Ca	0	0
			1	1		
31	F	1	Total	Ca	0	0
			1	1		
31	o	1	Total	Ca	0	0
			1	1		
31	O	1	Total	Ca	0	0
			1	1		
31	b	1	Total	Ca	0	0
			1	1		
31	f	1	Total	Ca	0	0
			1	1		

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



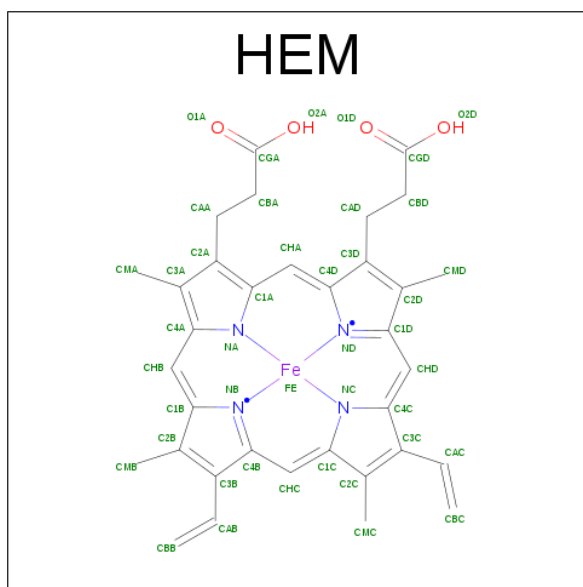
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	C	1	Total C O 62 47 15	0	0
32	E	1	Total C O 62 47 15	0	0
32	H	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	c	1	Total C O 62 47 15	0	0
32	d	1	Total C O 62 47 15	0	0
32	h	1	Total C O 62 47 15	0	0

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
33	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
33	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

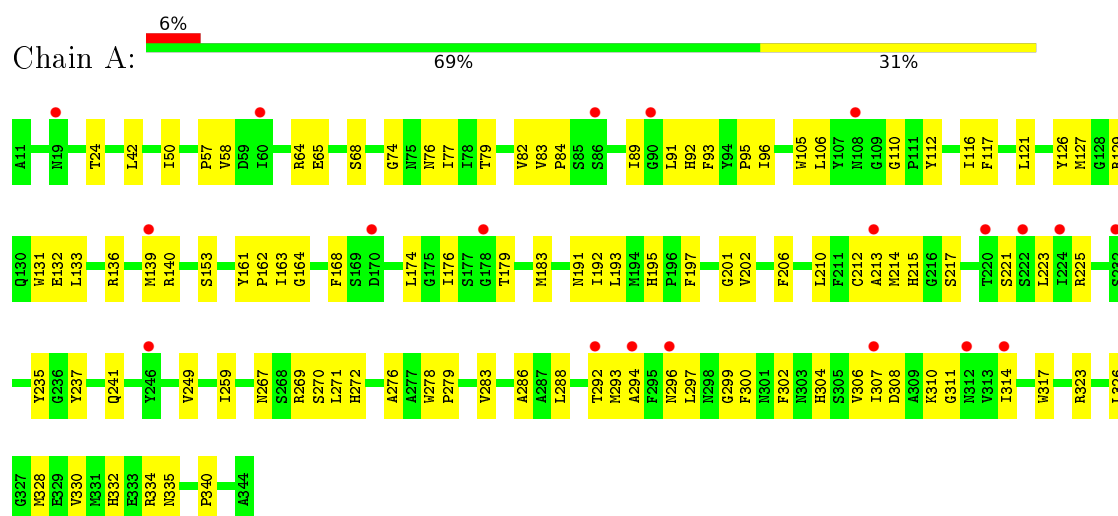
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

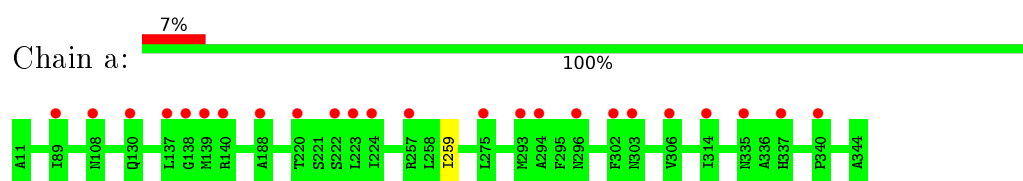
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

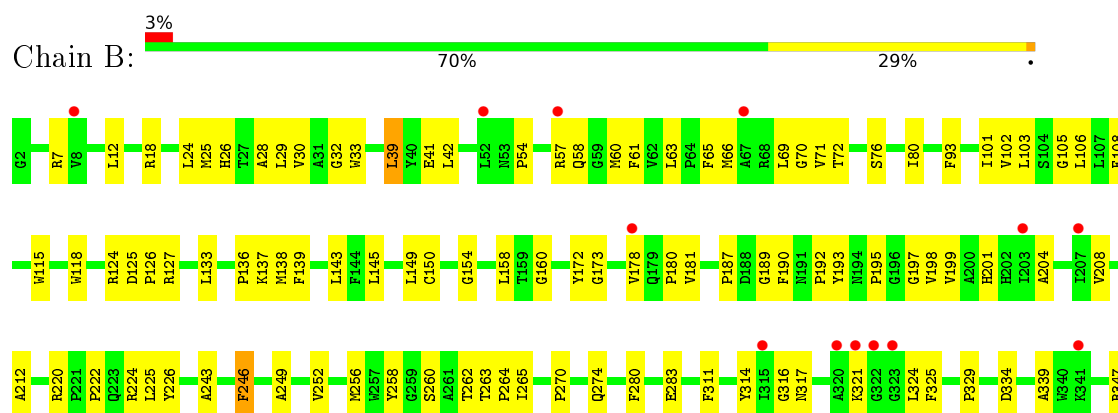
• Molecule 1: Photosystem II protein D1 1

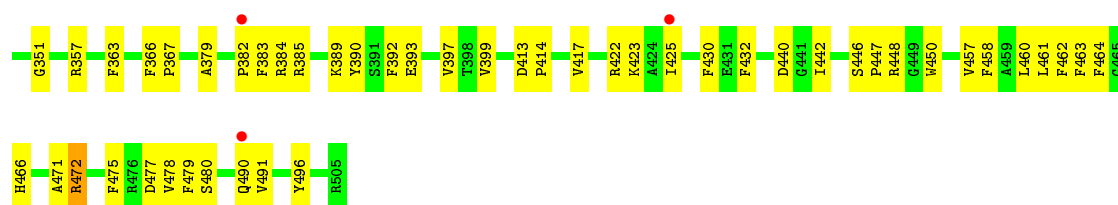


• Molecule 1: Photosystem II protein D1 1

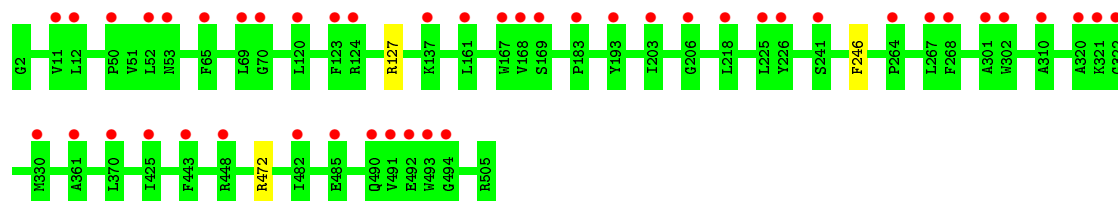


• Molecule 2: Photosystem II CP47 reaction center protein

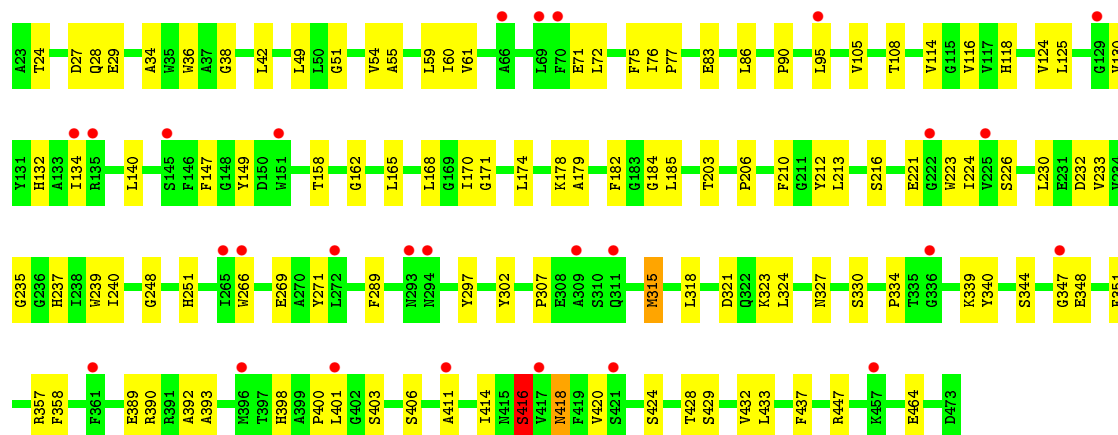
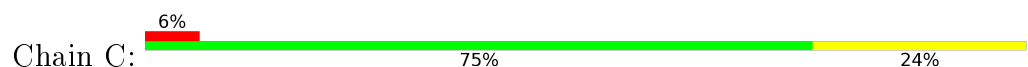




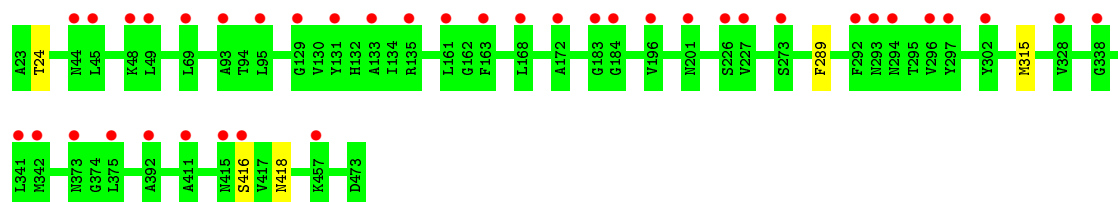
• Molecule 2: Photosystem II CP47 reaction center protein



• Molecule 3: Photosystem II CP43 reaction center protein

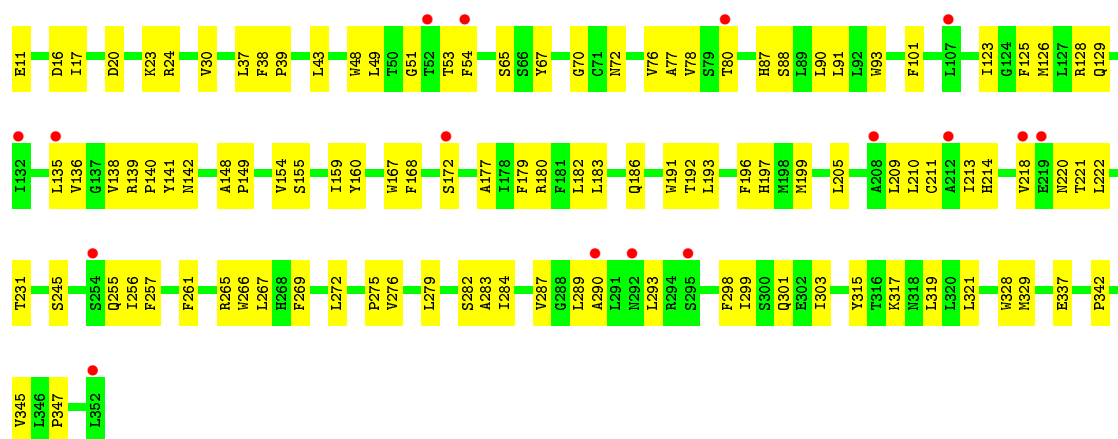


• Molecule 3: Photosystem II CP43 reaction center protein

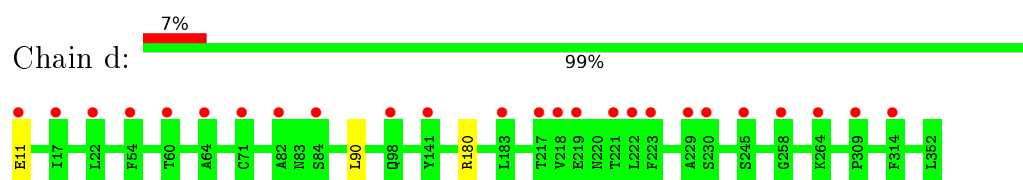


• Molecule 4: Photosystem II D2 protein

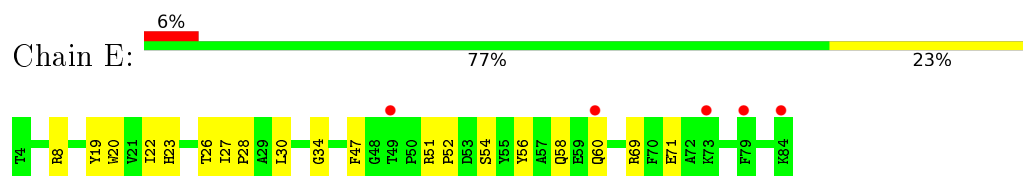




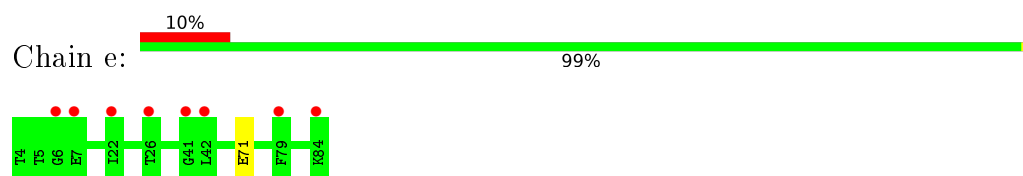
• Molecule 4: Photosystem II D2 protein



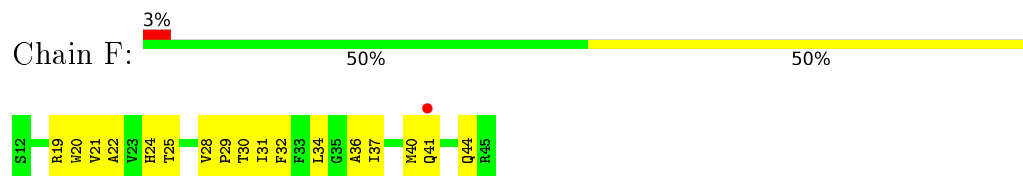
• Molecule 5: Cytochrome b559 subunit alpha



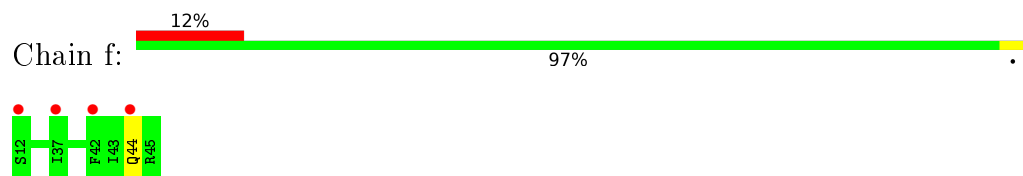
• Molecule 5: Cytochrome b559 subunit alpha



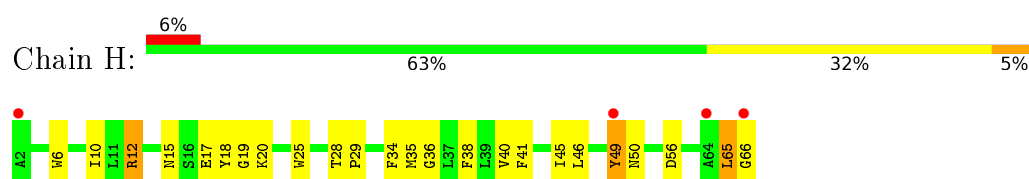
• Molecule 6: Cytochrome b559 subunit beta



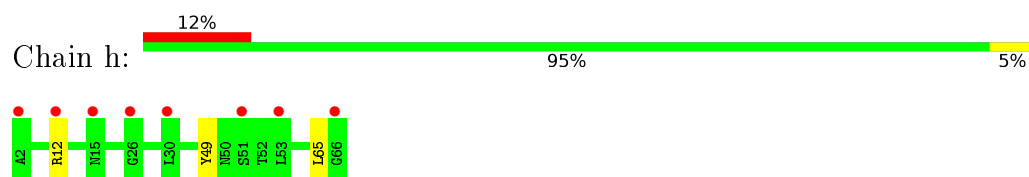
• Molecule 6: Cytochrome b559 subunit beta



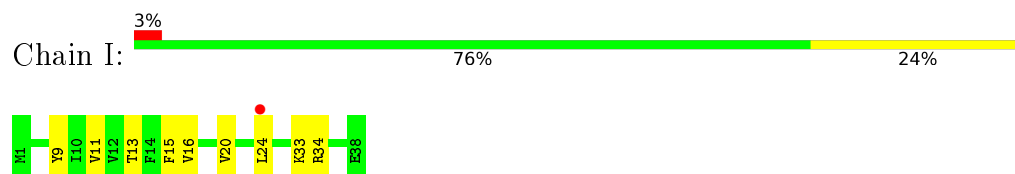
• Molecule 7: Photosystem II reaction center protein H



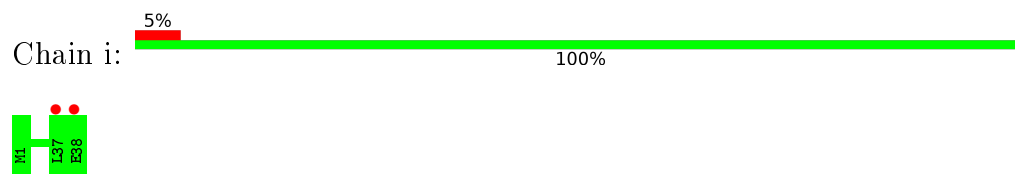
- Molecule 7: Photosystem II reaction center protein H



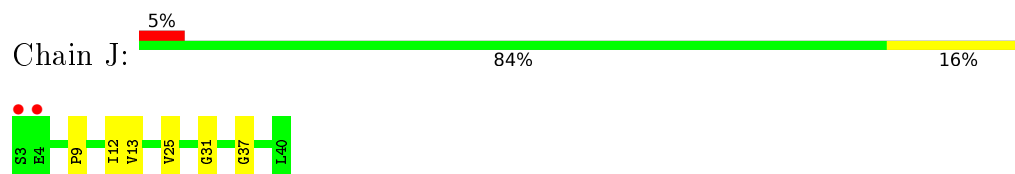
- Molecule 8: Photosystem II reaction center protein I



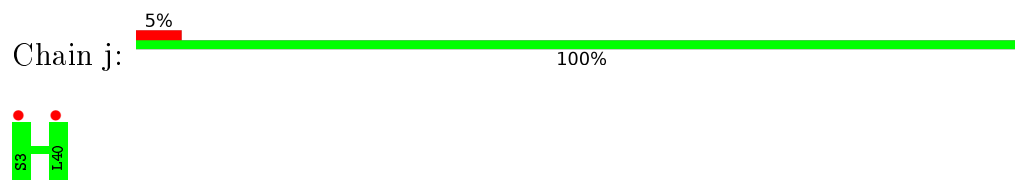
- Molecule 8: Photosystem II reaction center protein I



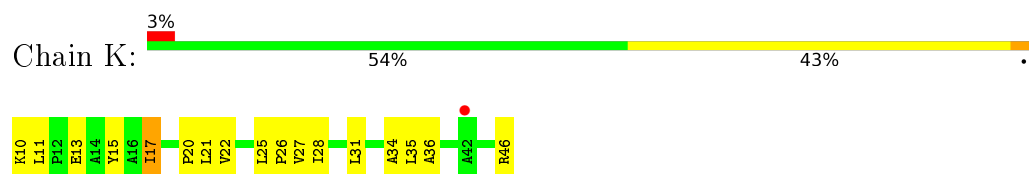
- Molecule 9: Photosystem II reaction center protein J



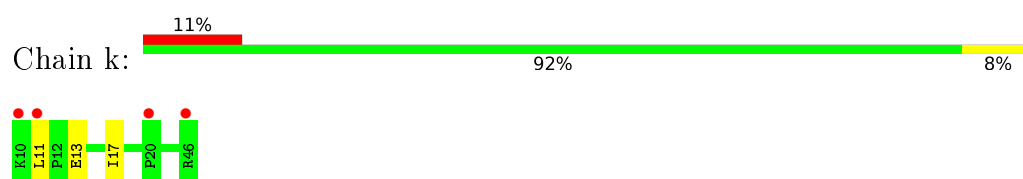
- Molecule 9: Photosystem II reaction center protein J



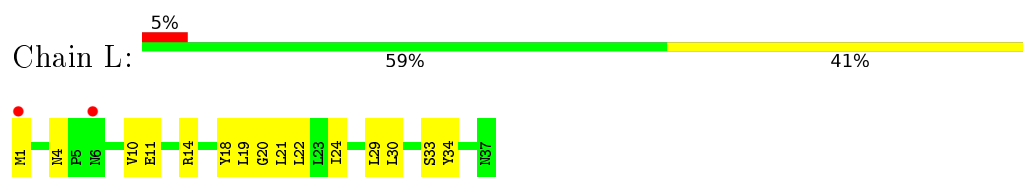
- Molecule 10: Photosystem II reaction center protein K



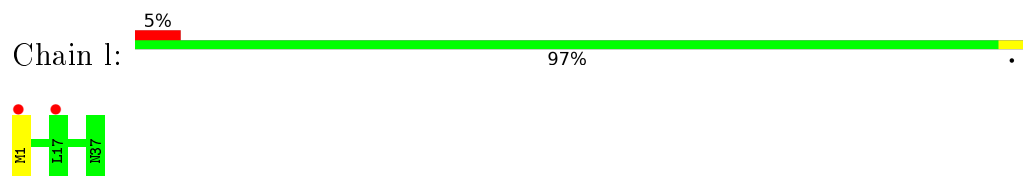
- Molecule 10: Photosystem II reaction center protein K



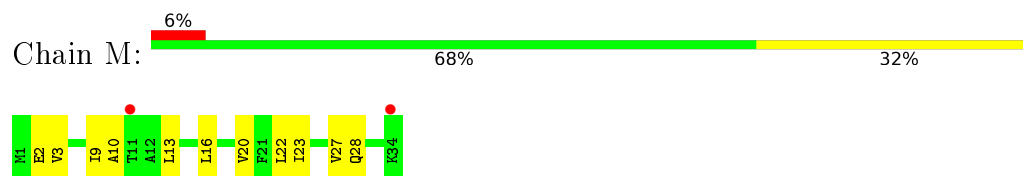
- Molecule 11: Photosystem II reaction center protein L



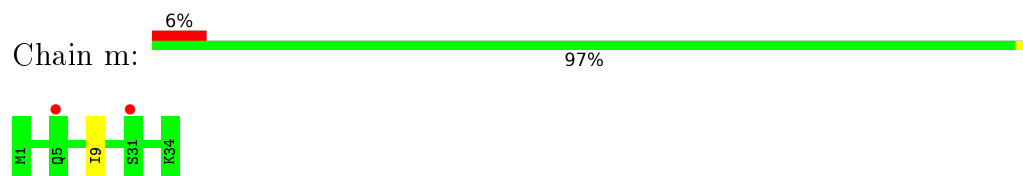
- Molecule 11: Photosystem II reaction center protein L



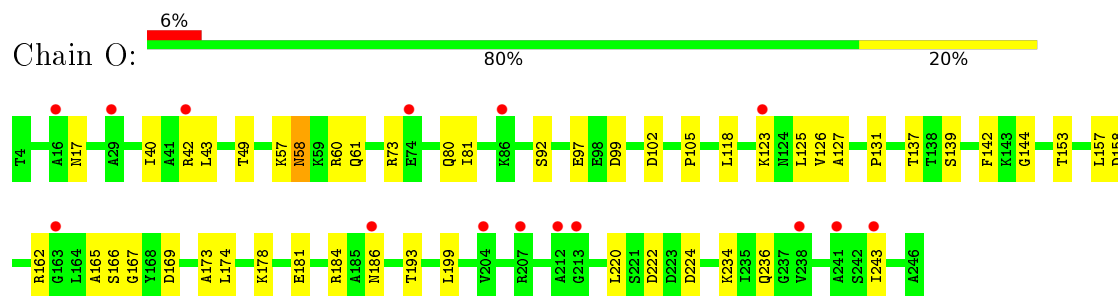
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

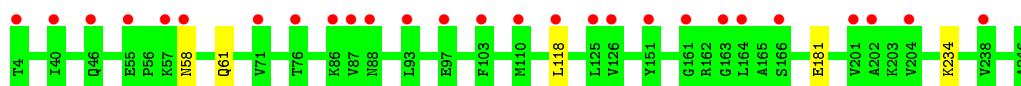


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





- Molecule 14: Photosystem II reaction center protein T

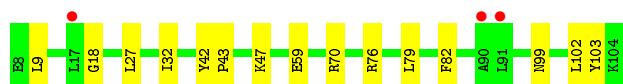
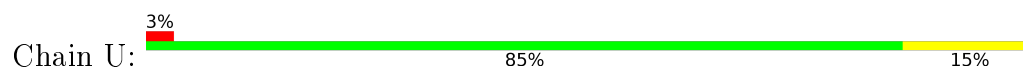


- Molecule 14: Photosystem II reaction center protein T

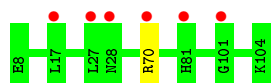


There are no outlier residues recorded for this chain.

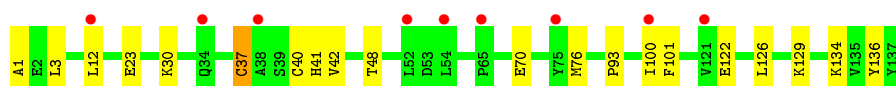
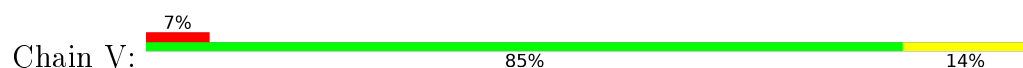
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



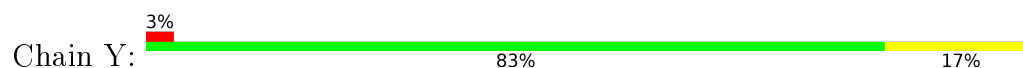
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550

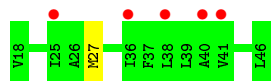


- Molecule 17: Photosystem II reaction center protein Ycf12

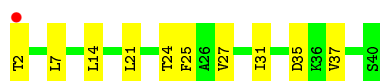




- Molecule 17: Photosystem II reaction center protein Ycf12



- Molecule 18: Photosystem II reaction center X protein

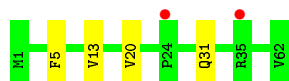
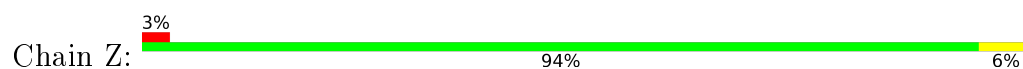


- Molecule 18: Photosystem II reaction center X protein

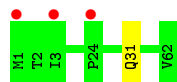


There are no outlier residues recorded for this chain.

- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	250.80 Å 250.80 Å 250.80 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.50 250.80 – 3.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.98-3.50) 100.0 (250.80-3.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.324 , 0.331 0.332 , 0.337	Depositor DCC
R_{free} test set	37670 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 1.5	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	50074	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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, MG, OEX, PHO, DGD, CL, CA, CLA, PL9, FE2, BCT, 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	A	0.56	0/2734	0.68	0/3727
1	a	0.49	0/2734	0.64	0/3727
2	B	0.51	0/4194	0.65	1/5713 (0.0%)
2	b	0.48	0/4194	0.63	1/5713 (0.0%)
3	C	0.51	0/3634	0.64	0/4947
3	c	0.47	0/3634	0.60	0/4947
4	D	0.53	0/2821	0.65	0/3844
4	d	0.48	0/2821	0.60	0/3844
5	E	0.46	0/693	0.63	0/944
5	e	0.43	0/693	0.58	0/944
6	F	0.51	0/284	0.61	0/387
6	f	0.41	0/284	0.56	0/387
7	H	0.47	0/544	0.64	0/739
7	h	0.46	0/544	0.66	0/739
8	I	0.52	0/327	0.68	0/439
8	i	0.46	0/327	0.60	0/439
9	J	0.46	0/278	0.59	0/376
9	j	0.43	0/278	0.53	0/376
10	K	0.48	0/303	0.70	0/416
10	k	0.55	0/303	0.79	0/416
11	L	0.55	0/319	0.70	0/433
11	l	0.48	0/319	0.62	0/433
12	M	0.52	0/278	0.74	0/378
12	m	0.49	0/278	0.69	0/378
13	O	0.46	0/1926	0.65	0/2611
13	o	0.41	0/1926	0.61	0/2611
14	T	0.60	0/282	0.68	0/382
14	t	0.49	0/282	0.60	0/382
15	U	0.48	0/785	0.64	0/1064
15	u	0.46	0/785	0.63	0/1064
16	V	0.52	1/1096 (0.1%)	0.66	0/1487
16	v	0.42	0/1096	0.62	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.44	0/216	0.61	0/289
17	y	0.44	0/216	0.59	0/289
18	X	0.43	0/298	0.53	0/403
18	x	0.44	0/298	0.54	0/403
19	Z	0.44	0/490	0.58	0/669
19	z	0.46	0/490	0.56	0/669
All	All	0.49	1/43004 (0.0%)	0.63	2/58496 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	37	CYS	CB-SG	-5.25	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	127	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	B	39	LEU	CA-CB-CG	-5.25	103.23	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2637	0	2551	104	0
1	a	2637	0	2551	0	0
2	B	4024	0	3901	160	0
2	b	4024	0	3901	0	0
3	C	3506	0	3439	96	0
3	c	3506	0	3439	0	0
4	D	2726	0	2627	107	0
4	d	2726	0	2627	0	0
5	E	668	0	658	17	0
5	e	668	0	658	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	275	0	282	17	0
6	f	275	0	282	0	0
7	H	525	0	558	26	0
7	h	525	0	558	0	0
8	I	320	0	339	7	0
8	i	320	0	339	0	0
9	J	272	0	279	5	0
9	j	272	0	279	0	0
10	K	293	0	305	19	0
10	k	293	0	305	0	0
11	L	309	0	327	19	0
11	l	309	0	327	0	0
12	M	272	0	300	12	0
12	m	272	0	300	0	0
13	O	1883	0	1865	35	0
13	o	1883	0	1865	0	0
14	T	270	0	278	18	0
14	t	270	0	278	0	0
15	U	774	0	773	12	0
15	u	774	0	773	0	0
16	V	1072	0	1088	17	0
16	v	1072	0	1088	0	0
17	Y	215	0	246	8	0
17	y	215	0	246	0	0
18	X	292	0	328	13	0
18	x	292	0	328	0	0
19	Z	479	0	516	3	0
19	z	479	0	516	0	0
20	A	10	0	0	1	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	1	0
22	U	1	0	0	0	0
22	a	2	0	0	0	0
22	u	1	0	0	0	0
23	A	4	0	1	0	0
23	a	4	0	1	0	0
24	A	195	0	216	29	0
24	B	1105	0	1224	115	0
24	C	845	0	936	74	0
24	D	195	0	216	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	260	0	288	0	0
24	b	1105	0	1224	0	0
24	c	845	0	936	0	0
24	d	130	0	144	0	0
25	A	64	0	74	4	0
25	D	64	0	74	12	0
25	a	64	0	74	0	0
25	d	64	0	74	0	0
26	A	40	0	55	19	0
26	B	120	0	165	82	0
26	C	40	0	55	21	0
26	F	40	0	55	28	0
26	H	40	0	55	25	0
26	I	40	0	55	18	0
26	K	80	0	110	36	0
26	T	40	0	55	29	0
26	a	40	0	55	0	0
26	b	120	0	166	0	0
26	c	120	0	165	0	0
26	f	40	0	55	0	0
26	h	40	0	55	0	0
26	k	40	0	55	0	0
26	t	40	0	55	0	0
27	A	55	0	80	17	0
27	D	55	0	80	14	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	108	0	156	4	0
28	B	54	0	30	6	0
28	L	54	0	26	6	0
28	X	43	0	53	4	0
28	a	108	0	156	0	0
28	b	54	0	30	0	0
28	l	54	0	29	0	0
28	x	43	0	53	0	0
29	A	51	0	72	3	0
29	B	51	0	72	2	0
29	C	102	0	144	6	0
29	D	51	0	72	7	0
29	Z	37	0	44	1	0
29	a	51	0	72	0	0
29	b	51	0	72	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	102	0	144	0	0
29	j	51	0	72	0	0
29	z	37	0	44	0	0
30	A	49	0	74	10	0
30	D	98	0	148	10	0
30	E	42	0	57	0	0
30	L	49	0	74	6	0
30	a	49	0	74	0	0
30	d	98	0	148	0	0
30	e	42	0	57	0	0
30	l	49	0	74	0	0
31	B	1	0	0	0	0
31	F	1	0	0	0	0
31	O	1	0	0	0	0
31	b	1	0	0	0	0
31	f	1	0	0	0	0
31	o	1	0	0	0	0
32	C	186	0	246	10	0
32	E	62	0	82	1	0
32	H	62	0	82	11	0
32	c	186	0	246	0	0
32	d	62	0	82	0	0
32	h	62	0	82	0	0
33	E	43	0	30	6	0
33	V	43	0	30	10	0
33	e	43	0	30	0	0
33	v	43	0	30	0	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	50074	0	51320	924	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 10.

All (924) 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)
26:T:101:BCR:C37	26:T:101:BCR:C22	1.74	1.65
26:B:619:BCR:C19	26:B:619:BCR:C20	1.76	1.64
26:B:620:BCR:C22	26:B:620:BCR:C37	1.76	1.64
26:C:514:BCR:C19	26:C:514:BCR:C20	1.73	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:619:BCR:C37	26:B:619:BCR:C22	1.74	1.62
26:T:101:BCR:C19	26:T:101:BCR:C20	1.75	1.62
26:B:619:BCR:C18	26:B:619:BCR:C36	1.76	1.61
26:F:101:BCR:C22	26:F:101:BCR:C37	1.74	1.61
26:B:618:BCR:C36	26:B:618:BCR:C18	1.77	1.61
26:T:101:BCR:C18	26:T:101:BCR:C36	1.79	1.61
26:T:101:BCR:C21	26:T:101:BCR:C20	1.78	1.61
26:C:514:BCR:C21	26:C:514:BCR:C20	1.78	1.61
26:K:101:BCR:C37	26:K:101:BCR:C22	1.75	1.61
26:B:618:BCR:C19	26:B:618:BCR:C20	1.75	1.61
26:H:101:BCR:C18	26:H:101:BCR:C36	1.79	1.60
26:K:102:BCR:C21	26:K:102:BCR:C20	1.79	1.59
26:B:620:BCR:C18	26:B:620:BCR:C36	1.80	1.59
26:B:618:BCR:C22	26:B:618:BCR:C37	1.75	1.59
26:A:610:BCR:C36	26:A:610:BCR:C18	1.79	1.59
26:F:101:BCR:C20	26:F:101:BCR:C21	1.80	1.59
26:F:101:BCR:C36	26:F:101:BCR:C18	1.77	1.59
26:K:101:BCR:C20	26:K:101:BCR:C21	1.78	1.59
26:C:514:BCR:C36	26:C:514:BCR:C18	1.80	1.58
26:B:619:BCR:C21	26:B:619:BCR:C20	1.80	1.58
26:C:514:BCR:C22	26:C:514:BCR:C37	1.76	1.58
26:A:610:BCR:C21	26:A:610:BCR:C20	1.77	1.57
26:F:101:BCR:C20	26:F:101:BCR:C19	1.74	1.57
26:B:618:BCR:C20	26:B:618:BCR:C21	1.80	1.57
26:H:101:BCR:C20	26:H:101:BCR:C19	1.71	1.57
26:A:610:BCR:C37	26:A:610:BCR:C22	1.75	1.56
26:I:101:BCR:C21	26:I:101:BCR:C20	1.78	1.56
26:B:620:BCR:C20	26:B:620:BCR:C21	1.78	1.56
26:K:102:BCR:C37	26:K:102:BCR:C22	1.76	1.56
26:K:102:BCR:C36	26:K:102:BCR:C18	1.80	1.56
26:H:101:BCR:C20	26:H:101:BCR:C21	1.76	1.55
26:K:101:BCR:C36	26:K:101:BCR:C18	1.78	1.55
26:I:101:BCR:C36	26:I:101:BCR:C18	1.79	1.53
3:C:165:LEU:HD21	24:C:506:CLA:HAB	1.85	1.01
26:B:618:BCR:C37	26:B:618:BCR:C21	2.42	0.97
26:T:101:BCR:C21	26:T:101:BCR:C37	2.43	0.96
26:B:618:BCR:H12C	26:B:619:BCR:H10C	1.48	0.94
2:B:106:LEU:HB3	26:B:620:BCR:H15C	1.49	0.94
26:K:101:BCR:C37	26:K:101:BCR:C21	2.45	0.93
26:B:619:BCR:C36	26:B:619:BCR:C19	2.47	0.93
26:C:514:BCR:C20	26:C:514:BCR:C22	2.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:619:BCR:C37	26:B:619:BCR:C21	2.45	0.92
26:K:102:BCR:C20	26:K:102:BCR:C22	2.46	0.92
3:C:124:VAL:HG11	26:C:514:BCR:H17C	1.48	0.92
26:B:619:BCR:H20C	26:B:619:BCR:C19	2.05	0.90
26:A:610:BCR:C21	26:A:610:BCR:C37	2.48	0.90
26:H:101:BCR:H20C	26:H:101:BCR:C19	2.06	0.89
24:B:615:CLA:H43	28:B:622:SQD:H121	1.54	0.89
26:K:102:BCR:C21	26:K:102:BCR:C37	2.49	0.89
26:C:514:BCR:C19	26:C:514:BCR:H20C	2.01	0.88
26:B:620:BCR:C21	26:B:620:BCR:C37	2.46	0.88
26:T:101:BCR:C19	26:T:101:BCR:H20C	2.01	0.87
26:B:620:BCR:C20	26:B:620:BCR:C22	2.51	0.87
26:B:619:BCR:C21	26:B:619:BCR:H20C	2.09	0.87
26:T:101:BCR:C22	26:T:101:BCR:C20	2.50	0.87
26:C:514:BCR:C21	26:C:514:BCR:H20C	2.06	0.86
26:A:610:BCR:C21	26:A:610:BCR:H20C	2.05	0.86
26:B:618:BCR:C19	26:B:618:BCR:H20C	2.03	0.86
26:B:619:BCR:C18	26:B:619:BCR:C20	2.51	0.86
26:T:101:BCR:C21	26:T:101:BCR:H20C	2.04	0.86
26:H:101:BCR:H20C	26:H:101:BCR:C21	2.10	0.85
26:A:610:BCR:C20	26:A:610:BCR:C22	2.54	0.85
26:F:101:BCR:C19	26:F:101:BCR:H20C	2.03	0.85
26:H:101:BCR:C22	26:H:101:BCR:C20	2.53	0.84
18:X:24:THR:HA	28:X:101:SQD:H331	2.01	0.84
26:I:101:BCR:C21	26:I:101:BCR:H20C	2.04	0.84
2:B:127:ARG:HH11	2:B:127:ARG:HG3	1.39	0.84
26:B:619:BCR:C20	26:B:619:BCR:C22	2.60	0.83
26:K:101:BCR:H20C	26:K:101:BCR:C21	2.08	0.83
26:C:514:BCR:C21	26:C:514:BCR:C37	2.48	0.83
26:F:101:BCR:C21	26:F:101:BCR:C37	2.44	0.83
26:K:101:BCR:C19	26:K:101:BCR:C36	2.55	0.83
26:B:618:BCR:C20	26:B:618:BCR:C22	2.50	0.83
26:K:102:BCR:C21	26:K:102:BCR:H20C	2.06	0.83
26:H:101:BCR:C20	26:H:101:BCR:C18	2.51	0.82
26:F:101:BCR:C17	26:F:101:BCR:C36	2.58	0.82
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.60	0.82
24:C:511:CLA:HMB1	24:C:511:CLA:HBB1	1.62	0.82
2:B:432:PHE:O	13:O:178:LYS:NZ	2.35	0.82
26:B:620:BCR:H20C	26:B:620:BCR:C21	2.09	0.82
26:K:101:BCR:C22	26:K:101:BCR:C20	2.55	0.82
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:I:101:BCR:C22	26:I:101:BCR:C20	2.49	0.81
24:A:609:CLA:HAC1	26:A:610:BCR:H15C	2.27	0.81
26:C:514:BCR:C18	26:C:514:BCR:C20	2.48	0.81
26:C:514:BCR:C19	26:C:514:BCR:C36	2.57	0.81
26:F:101:BCR:C21	26:F:101:BCR:H20C	2.08	0.81
30:A:615:LHG:H382	30:A:615:LHG:H112	1.63	0.80
7:H:38:PHE:HB2	26:H:101:BCR:H10C	1.62	0.80
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.81	0.79
26:B:618:BCR:H20C	26:B:618:BCR:C21	2.07	0.78
24:C:501:CLA:H193	24:C:507:CLA:HBB1	1.80	0.78
24:C:506:CLA:HMB1	24:C:506:CLA:HBB1	1.65	0.78
24:C:508:CLA:HMB1	24:C:508:CLA:HBB1	1.66	0.77
24:B:603:CLA:HMC2	26:H:101:BCR:H19C	8.86	0.77
26:A:610:BCR:C36	26:A:610:BCR:C19	2.57	0.77
26:T:101:BCR:C19	26:T:101:BCR:C36	2.59	0.76
24:C:513:CLA:HBB1	24:C:513:CLA:HMB1	1.66	0.76
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	1.68	0.76
11:L:14:ARG:HD3	28:L:102:SQD:H241	1.68	0.75
3:C:339:LYS:NZ	15:U:99:ASN:O	2.18	0.75
24:B:613:CLA:HMB1	24:B:613:CLA:HBB1	1.76	0.75
26:B:620:BCR:C36	26:B:620:BCR:C19	2.63	0.75
24:B:603:CLA:H152	26:H:101:BCR:H17C	20.86	0.75
4:D:193:LEU:O	11:L:34:TYR:OH	2.02	0.75
26:K:101:BCR:H16C	17:Y:33:PRO:HD3	1.68	0.75
24:B:602:CLA:HBB1	24:B:602:CLA:HHC	1.68	0.74
10:K:11:LEU:HD11	10:K:22:VAL:HG21	2.05	0.74
5:E:56:TYR:O	16:V:1:ALA:N	2.23	0.74
24:C:510:CLA:H192	24:C:510:CLA:HBC3	1.90	0.74
2:B:479:PHE:O	4:D:139:ARG:NH2	2.21	0.74
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.71	0.73
4:D:87:HIS:ND1	32:H:102:DGD:O2D	2.15	0.73
24:A:607:CLA:H152	27:A:611:PL9:H262	1.83	0.73
2:B:33:TRP:N	26:B:620:BCR:H15C	15.43	0.73
26:I:101:BCR:C37	26:I:101:BCR:C20	2.67	0.72
24:A:607:CLA:HMB1	24:A:607:CLA:HBB1	1.95	0.72
1:A:214:MET:HG2	27:A:611:PL9:H102	1.71	0.72
3:C:213[B]:LEU:HD21	26:I:101:BCR:H20C	1.71	0.72
26:T:101:BCR:C18	26:T:101:BCR:C20	2.57	0.72
26:B:618:BCR:H402	28:B:622:SQD:H82	1.71	0.72
24:C:510:CLA:HBB1	24:C:510:CLA:HMB1	1.71	0.72
24:A:606:CLA:HMB1	24:A:606:CLA:HBB1	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG22	26:A:610:BCR:H271	1.72	0.72
1:A:106:LEU:HD21	26:A:610:BCR:H383	3.27	0.71
3:C:124:VAL:HG11	26:C:514:BCR:C17	2.18	0.71
10:K:34:ALA:HB1	26:K:101:BCR:C20	2.35	0.71
24:C:501:CLA:C1D	24:C:503:CLA:H2	2.21	0.70
4:D:279:LEU:HD22	25:D:401:PHO:HBC3	1.73	0.70
27:D:405:PL9:H411	11:L:29:LEU:HD23	1.74	0.70
10:K:17:ILE:H	10:K:17:ILE:HD13	1.56	0.70
24:B:616:CLA:HMB1	24:B:616:CLA:HBB1	2.75	0.70
2:B:150:CYS:HB2	24:B:605:CLA:HMC3	21.06	0.69
26:F:101:BCR:C20	26:F:101:BCR:C22	2.57	0.69
24:A:609:CLA:HMB1	24:A:609:CLA:HBB1	1.95	0.69
24:D:403:CLA:HMB1	24:D:403:CLA:HBB1	1.74	0.69
24:B:609:CLA:HMC2	26:B:620:BCR:HC8	37.19	0.68
26:B:619:BCR:H381	26:T:101:BCR:H341	49.06	0.68
24:B:611:CLA:HBB1	24:B:611:CLA:HHC	1.74	0.68
26:I:101:BCR:C19	26:I:101:BCR:C36	2.59	0.67
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.76	0.67
24:C:501:CLA:H192	24:C:506:CLA:C1B	2.24	0.67
26:H:101:BCR:C19	26:H:101:BCR:C36	2.61	0.67
5:E:23:HIS:NE2	33:E:103:HEM:ND	2.44	0.66
24:C:501:CLA:C2D	24:C:503:CLA:H2	2.25	0.66
24:B:609:CLA:HMB1	24:B:609:CLA:HBB1	1.77	0.66
18:X:31:ILE:HG23	28:X:101:SQD:H462	1.99	0.66
1:A:310:LYS:NZ	5:E:58:GLN:O	2.29	0.66
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.31	0.66
26:B:619:BCR:C37	26:B:619:BCR:C20	3.77	0.65
26:F:101:BCR:C37	26:F:101:BCR:H20C	2.27	0.65
26:B:618:BCR:C36	26:B:618:BCR:C17	2.70	0.65
16:V:3:LEU:HD23	16:V:23:GLU:HG3	1.78	0.65
4:D:192:THR:HG23	24:D:403:CLA:HBC2	1.78	0.65
24:B:612:CLA:OBD	24:B:612:CLA:H152	13.81	0.65
26:B:618:BCR:C20	26:B:618:BCR:C18	2.59	0.65
28:A:612:SQD:O7	3:C:28:GLN:NE2	2.24	0.65
24:B:616:CLA:H51	26:B:620:BCR:H11C	1.77	0.64
2:B:450:TRP:CD1	24:B:608:CLA:HBA1	2.32	0.64
4:D:186:GLN:HB2	24:D:402:CLA:HBC1	11.53	0.64
26:K:102:BCR:C19	26:K:102:BCR:C36	2.62	0.64
4:D:315:TYR:CZ	4:D:319:LEU:HD11	2.72	0.64
24:C:501:CLA:HBB1	24:C:501:CLA:HMB1	2.06	0.64
2:B:383:PHE:O	13:O:166:SER:HA	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:H:101:BCR:C17	26:H:101:BCR:C36	2.72	0.64
24:A:607:CLA:H122	27:A:611:PL9:H23	1.88	0.64
25:A:608:PHO:HMB1	25:A:608:PHO:HBB1	1.80	0.64
3:C:213[B]:LEU:HD11	26:I:101:BCR:C22	2.27	0.64
3:C:406:SER:HA	3:C:420:VAL:HG23	1.79	0.64
25:D:401:PHO:HMB1	25:D:401:PHO:HBB1	1.80	0.63
26:F:101:BCR:C20	26:F:101:BCR:C18	2.61	0.63
2:B:464:PHE:HD2	24:B:612:CLA:HAC2	1.63	0.63
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.79	0.63
4:D:141:TYR:OH	30:D:406:LHG:O4	2.16	0.63
26:B:619:BCR:H17C	26:T:101:BCR:C17	34.77	0.63
26:F:101:BCR:C36	26:F:101:BCR:C19	2.65	0.63
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.78	0.63
1:A:183:MET:HA	24:A:606:CLA:HMD2	1.80	0.63
28:L:102:SQD:H45	14:T:23:PHE:CD1	2.33	0.63
4:D:261:PHE:HB2	27:D:405:PL9:H522	1.81	0.63
2:B:29:LEU:HD21	26:B:618:BCR:H19C	1.80	0.63
1:A:308:ASP:HB2	5:E:52:PRO:O	2.02	0.62
26:B:618:BCR:C36	26:B:618:BCR:C19	2.60	0.62
24:C:507:CLA:OBD	24:C:509:CLA:H122	1.99	0.62
24:A:609:CLA:HAC2	26:A:610:BCR:H362	1.82	0.62
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.94	0.62
14:T:1[B]:MET:HB3	14:T:4:ILE:HD12	1.81	0.62
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.74	0.62
13:O:57:LYS:O	13:O:58:ASN:HB2	2.03	0.62
26:B:619:BCR:C36	26:B:619:BCR:C17	2.75	0.62
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.23	0.62
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.03	0.62
26:B:619:BCR:C37	26:B:619:BCR:H20C	3.82	0.61
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.82	0.61
24:C:505:CLA:HMB1	24:C:505:CLA:HBB1	2.42	0.61
26:C:514:BCR:H15C	29:C:519:LMG:H401	1.83	0.61
1:A:132:GLU:O	1:A:136:ARG:HG2	2.07	0.61
28:A:614:SQD:H132	26:T:101:BCR:HC41	1.82	0.61
30:A:615:LHG:H371	24:C:508:CLA:H92	1.82	0.61
24:B:614:CLA:H193	26:B:619:BCR:C5	2.31	0.61
26:B:618:BCR:H15C	26:B:619:BCR:H352	1.83	0.61
10:K:36:ALA:HB2	26:K:102:BCR:H391	1.83	0.61
24:C:501:CLA:C1C	24:C:503:CLA:H71	2.30	0.61
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.86	0.61
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:266:TRP:HE3	3:C:271:TYR:HH	2.94	0.60
33:E:103:HEM:HBB2	33:E:103:HEM:HMB2	1.81	0.60
2:B:32:GLY:HA3	26:B:619:BCR:H19C	1.82	0.60
26:B:619:BCR:H333	12:M:13:LEU:HD12	7.64	0.60
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.13	0.60
6:F:20:TRP:CE2	6:F:24:HIS:CE1	2.90	0.60
24:B:610:CLA:HBB1	24:B:610:CLA:HMB1	1.83	0.60
1:A:42:LEU:HD13	26:A:610:BCR:H353	1.83	0.60
11:L:22:LEU:HD23	30:L:101:LHG:H162	1.84	0.60
24:B:614:CLA:H91	24:B:615:CLA:HBB1	12.25	0.59
33:V:201:HEM:HBC2	33:V:201:HEM:HMC1	3.54	0.59
24:B:612:CLA:H162	26:B:619:BCR:H342	1.84	0.59
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.85	0.59
26:C:514:BCR:C17	26:C:514:BCR:C36	2.77	0.59
3:C:324:LEU:HB3	15:U:32:ILE:HD13	1.84	0.59
24:D:404:CLA:H2	18:X:14:LEU:HA	1.83	0.59
1:A:84:PRO:HA	1:A:112:TYR:CG	2.37	0.59
24:B:616:CLA:H171	14:T:8:PHE:CE1	49.21	0.59
24:B:609:CLA:CMC	26:B:620:BCR:HC8	36.29	0.59
26:B:620:BCR:H17C	26:T:101:BCR:C17	49.88	0.59
1:A:126:TYR:CZ	25:A:608:PHO:HBA1	2.38	0.59
29:D:408:LMG:H411	6:F:30:THR:HG21	1.85	0.59
1:A:269:ARG:NH1	4:D:222:LEU:HD13	2.18	0.59
2:B:30:VAL:HG22	24:B:614:CLA:C3C	2.33	0.58
24:B:616:CLA:H101	26:B:619:BCR:H362	22.34	0.58
3:C:210:PHE:HD2	3:C:213[B]:LEU:HD22	1.86	0.58
4:D:123:ILE:HD11	32:H:102:DGD:HAH2	2.13	0.58
26:T:101:BCR:C37	26:T:101:BCR:H20C	2.32	0.58
1:A:323:ARG:HB3	4:D:329:MET:HA	1.95	0.58
24:B:613:CLA:HBB1	24:B:615:CLA:HMB3	1.85	0.58
15:U:27:LEU:HD21	15:U:82:PHE:CG	2.39	0.58
26:F:101:BCR:C23	26:F:101:BCR:C37	2.78	0.58
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.03	0.58
26:T:101:BCR:C37	26:T:101:BCR:C20	2.81	0.58
3:C:206:PRO:HG3	3:C:239:TRP:HZ2	1.69	0.58
26:K:102:BCR:C36	26:K:102:BCR:C16	2.82	0.58
24:C:501:CLA:C3D	24:C:503:CLA:H2	2.34	0.57
2:B:339:ALA:HB2	13:O:58:ASN:HB3	42.39	0.57
3:C:418:ASN:HB2	32:C:517:DGD:O4E	2.03	0.57
1:A:215:HIS:HA	27:A:611:PL9:O1	2.20	0.57
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.47	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:620:BCR:C36	26:B:620:BCR:C17	2.72	0.57
6:F:34:LEU:HD21	26:F:101:BCR:H373	1.87	0.57
1:A:153:SER:HB2	24:A:606:CLA:H43	1.86	0.57
2:B:126:PRO:HB3	7:H:12[B]:ARG:NH1	2.19	0.57
8:I:20:VAL:HG13	26:I:101:BCR:HC41	1.86	0.57
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.86	0.57
3:C:437:PHE:CZ	24:C:510:CLA:HMB3	2.39	0.57
4:D:257:PHE:O	30:D:407:LHG:H351	2.51	0.57
3:C:334:PRO:HA	13:O:153:THR:OG1	2.05	0.57
16:V:41:HIS:CD2	33:V:201:HEM:NB	2.75	0.57
2:B:28:ALA:HB1	28:B:622:SQD:H221	1.87	0.57
32:E:101:DGD:O2D	32:E:101:DGD:O1B	2.21	0.57
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.86	0.56
24:A:607:CLA:HMB3	25:D:401:PHO:H172	1.92	0.56
26:A:610:BCR:C36	26:A:610:BCR:C17	2.74	0.56
3:C:178:LYS:HB2	24:C:502:CLA:H141	1.94	0.56
24:B:605:CLA:H12	24:B:606:CLA:ND	2.21	0.56
10:K:35:LEU:HB2	26:K:101:BCR:H15C	1.85	0.56
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.73	0.56
3:C:429:SER:HA	32:C:517:DGD:HBE1	13.01	0.56
1:A:129:ARG:NH2	4:D:255:GLN:O	2.83	0.56
1:A:328:MET:HE1	4:D:183:LEU:HD13	2.36	0.56
1:A:332:HIS:HA	22:A:603:CL:CL	2.43	0.56
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.13	0.56
27:A:611:PL9:H221	25:D:401:PHO:HMA2	2.05	0.56
24:C:508:CLA:HBC3	24:C:510:CLA:H71	2.32	0.56
26:I:101:BCR:C36	26:I:101:BCR:C17	2.74	0.56
28:L:102:SQD:H181	26:T:101:BCR:H351	1.88	0.56
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.21	0.55
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.36	0.55
24:A:607:CLA:HMD3	4:D:182:LEU:HD11	1.88	0.55
1:A:74:GLY:O	4:D:301:GLN:NE2	2.39	0.55
7:H:65:LEU:HD12	7:H:66:GLY:H	1.78	0.55
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.89	0.55
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.40	0.55
3:C:216:SER:HB3	3:C:221:GLU:HG3	1.89	0.55
16:V:122:GLU:HG3	16:V:126:LEU:HD12	1.88	0.55
7:H:35:MET:CG	26:H:101:BCR:HC42	2.37	0.55
24:C:506:CLA:H162	26:I:101:BCR:H15C	1.89	0.55
10:K:25:LEU:HD21	26:K:101:BCR:HC41	1.89	0.55
1:A:195:HIS:CE1	1:A:197:PHE:HB2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:ALA:HB2	24:B:610:CLA:HMC3	1.88	0.55
14:T:8:PHE:HD1	26:T:101:BCR:H373	1.72	0.55
4:D:149:PRO:HA	24:D:402:CLA:H41	19.50	0.55
16:V:40:CYS:SG	33:V:201:HEM:CAC	2.95	0.55
2:B:25:MET:HG2	26:B:619:BCR:C21	12.96	0.55
26:K:102:BCR:C36	26:K:102:BCR:C17	2.73	0.55
9:J:9:PRO:HD2	9:J:12:ILE:HD12	2.19	0.54
26:T:101:BCR:C17	26:T:101:BCR:C36	2.77	0.54
7:H:36:GLY:O	7:H:40:VAL:HG23	2.31	0.54
1:A:308:ASP:HB3	1:A:314:ILE:HD11	1.88	0.54
2:B:457:VAL:HG11	29:B:621:LMG:H211	1.89	0.54
15:U:76:ARG:HA	15:U:79:LEU:HG	1.89	0.54
4:D:269:PHE:CD2	30:D:406:LHG:HC11	2.43	0.54
26:K:101:BCR:H17C	17:Y:33:PRO:HD3	2.21	0.54
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.08	0.54
14:T:22:PHE:CE2	26:T:101:BCR:H333	2.99	0.54
30:A:615:LHG:H151	30:A:615:LHG:H352	1.90	0.54
2:B:460:LEU:O	2:B:463:PHE:HB3	2.15	0.54
1:A:225:ARG:HA	2:B:480:SER:O	2.08	0.54
24:A:609:CLA:HMA2	29:A:613:LMG:H132	1.90	0.54
2:B:462:PHE:CE1	24:B:614:CLA:HMB3	2.43	0.54
7:H:35:MET:HG2	26:H:101:BCR:HC42	1.90	0.54
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.88	0.54
1:A:276:ALA:HB1	30:A:615:LHG:H262	1.90	0.53
24:B:604:CLA:H3A	24:B:604:CLA:O1A	2.08	0.53
26:K:101:BCR:HC8	19:Z:20:VAL:HG21	1.90	0.53
1:A:105:TRP:HZ3	26:A:610:BCR:H24C	1.72	0.53
2:B:190:PHE:HB3	7:H:45:ILE:HG22	1.90	0.53
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.88	0.53
1:A:210:LEU:HG	25:D:401:PHO:NC	2.57	0.53
1:A:153:SER:HB3	24:A:606:CLA:HED1	2.28	0.53
26:I:101:BCR:C37	26:I:101:BCR:H20C	2.37	0.53
5:E:8:ARG:O	6:F:19:ARG:NH2	2.34	0.53
2:B:145:LEU:HD11	24:B:617:CLA:HMB2	13.24	0.53
1:A:24:THR:O	4:D:255:GLN:NE2	2.41	0.53
20:A:601:OEX:O2	3:C:357:ARG:NH2	2.78	0.53
2:B:274:GLN:HB3	2:B:280:PHE:CE2	2.43	0.53
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.91	0.53
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.91	0.53
4:D:303:ILE:HG21	12:M:2:GLU:HG3	1.89	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:TRP:CD1	25:D:401:PHO:H162	2.43	0.53
5:E:51:ARG:N	5:E:54[B]:SER:OG	2.42	0.53
2:B:12:LEU:HB2	24:B:614:CLA:HMC2	19.19	0.52
1:A:206:PHE:CZ	24:D:403:CLA:HAA1	2.44	0.52
6:F:37:ILE:HA	6:F:40:MET:SD	2.48	0.52
1:A:201:GLY:HA3	1:A:286:ALA:HB2	2.11	0.52
24:C:503:CLA:HMD2	24:C:503:CLA:H193	1.91	0.52
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.44	0.52
2:B:101:ILE:HG23	26:B:620:BCR:C21	17.07	0.52
24:C:506:CLA:C2C	24:C:507:CLA:H122	2.39	0.52
18:X:35:ASP:OD1	28:X:101:SQD:H1	2.46	0.52
24:C:506:CLA:CBB	24:C:507:CLA:HMA3	2.44	0.52
24:B:615:CLA:C12	26:B:618:BCR:H17C	2.40	0.52
3:C:400:PRO:C	3:C:401:LEU:HD12	2.30	0.52
3:C:327:ASN:HB3	13:O:99:ASP:OD2	2.33	0.52
1:A:206:PHE:CZ	24:D:402:CLA:HAA1	14.41	0.52
11:L:21:LEU:HD22	28:L:102:SQD:H361	1.91	0.52
1:A:176:ILE:O	1:A:179:THR:HB	2.09	0.52
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.92	0.52
24:B:617:CLA:H3A	26:B:620:BCR:H17C	1.91	0.52
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.50	0.52
14:T:8:PHE:CD1	26:T:101:BCR:H373	2.46	0.52
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.75	0.52
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.92	0.52
29:D:408:LMG:H172	26:F:101:BCR:H383	1.90	0.52
26:F:101:BCR:C24	26:F:101:BCR:C37	3.06	0.52
3:C:213[B]:LEU:HD11	26:I:101:BCR:C21	2.40	0.52
26:A:610:BCR:H392	26:A:610:BCR:H23C	1.92	0.52
3:C:233:VAL:O	3:C:237:HIS:ND1	2.56	0.52
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.06	0.52
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.45	0.51
24:B:612:CLA:H162	24:B:617:CLA:CAD	29.51	0.51
4:D:49:LEU:HD22	26:F:101:BCR:H362	1.92	0.51
2:B:42:LEU:HD11	2:B:93:PHE:HB3	1.93	0.51
4:D:72:ASN:HA	29:D:408:LMG:HC1	1.92	0.51
29:D:408:LMG:H231	26:F:101:BCR:H381	1.91	0.51
10:K:21:LEU:O	10:K:25:LEU:HG	2.53	0.51
24:A:609:CLA:HMD3	26:A:610:BCR:H361	1.92	0.51
2:B:393:GLU:HB3	15:U:18:GLY:CA	2.40	0.51
28:B:622:SQD:C1	28:B:622:SQD:H462	2.41	0.51
30:A:615:LHG:H223	32:C:517:DGD:HBH2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:ARG:HD3	15:U:102:LEU:HG	2.24	0.51
24:B:602:CLA:HAC1	26:H:101:BCR:H23C	1.93	0.51
2:B:150:CYS:HB2	24:B:604:CLA:HMC3	1.91	0.51
1:A:191:ASN:HB2	3:C:411:ALA:HB1	2.03	0.51
11:L:18:TYR:CE2	14:T:20:ALA:HA	2.45	0.51
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.46	0.51
3:C:170:ILE:HD13	24:C:512:CLA:H111	1.92	0.51
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.45	0.51
4:D:192:THR:HG23	24:D:402:CLA:HBC2	10.67	0.51
7:H:38:PHE:CB	26:H:101:BCR:H10C	2.37	0.51
10:K:21:LEU:HD21	26:K:101:BCR:HC31	2.27	0.51
2:B:208:VAL:HG21	24:B:604:CLA:HMC1	12.34	0.51
3:C:213[B]:LEU:HD21	26:I:101:BCR:C20	2.40	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
26:K:101:BCR:HC21	19:Z:13:VAL:HG13	1.93	0.51
24:B:604:CLA:C1C	24:B:606:CLA:H71	2.40	0.51
4:D:23:LYS:HD3	4:D:135:LEU:HD21	1.92	0.51
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.50
12:M:20:VAL:HG11	12:M:20:VAL:CG2	2.70	0.50
16:V:37:CYS:SG	33:V:201:HEM:CAB	2.99	0.50
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.47	0.50
4:D:53:THR:HA	4:D:67:TYR:HD2	1.75	0.50
27:A:611:PL9:H403	6:F:22:ALA:HB2	1.92	0.50
2:B:138:MET:HE1	24:B:617:CLA:HMD2	12.26	0.50
2:B:29:LEU:HD21	28:B:622:SQD:H191	1.92	0.50
4:D:43:LEU:HD11	24:D:404:CLA:C3C	2.41	0.50
12:M:20:VAL:HG21	12:M:20:VAL:HG11	2.51	0.50
26:T:101:BCR:C23	26:T:101:BCR:C37	2.80	0.50
2:B:71:VAL:HG23	24:B:607[A]:CLA:HMA2	1.92	0.50
24:C:504:CLA:C4B	32:C:516:DGD:HB71	2.42	0.50
4:D:214:HIS:HA	27:D:405:PL9:O2	2.12	0.50
33:E:103:HEM:HBC2	33:E:103:HEM:HMC2	1.92	0.50
3:C:182:PHE:CE2	24:C:502:CLA:H201	2.53	0.50
3:C:323:LYS:NZ	3:C:389:GLU:OE2	2.32	0.50
24:C:512:CLA:HMB1	24:C:512:CLA:HBB1	1.94	0.50
4:D:129:GLN:NE2	25:D:401:PHO:OBD	2.44	0.50
1:A:269:ARG:NH1	4:D:231:THR:HB	2.48	0.50
3:C:116:VAL:HG11	26:C:514:BCR:C5	2.41	0.50
32:C:516:DGD:HB51	29:C:518:LMG:H392	1.93	0.50
2:B:472:ARG:HA	2:B:479:PHE:CE1	2.78	0.50
2:B:71:VAL:HG23	24:B:607[B]:CLA:HMA2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:507:CLA:H142	26:I:101:BCR:H362	1.93	0.50
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.94	0.50
2:B:226:TYR:OH	7:H:19:GLY:HA2	2.22	0.50
26:B:618:BCR:C37	26:B:618:BCR:C23	2.82	0.50
26:H:101:BCR:C20	26:H:101:BCR:C37	2.90	0.50
24:B:609:CLA:HHD	24:B:609:CLA:HBC3	1.94	0.49
3:C:49:LEU:HD23	3:C:149:TYR:OH	2.44	0.49
3:C:60:ILE:HG12	24:C:510:CLA:HMC2	2.06	0.49
4:D:283:ALA:O	4:D:287:VAL:HG23	2.11	0.49
2:B:187:PRO:HD3	24:B:602:CLA:HMD3	1.95	0.49
2:B:442:ILE:HG12	13:O:173:ALA:O	2.67	0.49
2:B:61:PHE:CZ	24:B:608:CLA:HBB1	2.47	0.49
3:C:212:TYR:OH	3:C:232:ASP:OD2	2.24	0.49
1:A:326:LEU:HD22	16:V:134:LYS:HB2	2.38	0.49
1:A:139:MET:HG2	4:D:221:THR:HG22	2.11	0.49
1:A:153:SER:CB	24:A:606:CLA:HED1	2.71	0.49
3:C:206:PRO:HG3	3:C:239:TRP:CZ2	2.46	0.49
26:C:514:BCR:C23	26:C:514:BCR:C37	2.82	0.49
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.02	0.49
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.48	0.49
2:B:347[B]:ARG:NH1	2:B:351:GLY:O	2.43	0.49
2:B:181:VAL:HG11	2:B:195:PRO:HB2	1.94	0.49
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.41	0.49
3:C:437:PHE:CE1	24:C:510:CLA:HMB3	2.48	0.49
10:K:10:LYS:N	10:K:10:LYS:HD2	2.28	0.49
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.54	0.48
2:B:464:PHE:HD2	24:B:613:CLA:HAC2	15.50	0.48
24:B:607[B]:CLA:H93	26:B:620:BCR:H10C	1.95	0.48
30:A:615:LHG:H382	30:A:615:LHG:C11	2.40	0.48
2:B:458:PHE:CD2	24:B:605:CLA:HMC3	2.49	0.48
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.43	0.48
26:F:101:BCR:C20	26:F:101:BCR:C37	2.89	0.48
26:F:101:BCR:H371	26:F:101:BCR:C24	2.60	0.48
5:E:69:ARG:NH2	7:H:50:ASN:O	2.29	0.48
26:K:102:BCR:H371	26:K:102:BCR:H24C	1.95	0.48
24:D:404:CLA:C2	18:X:14:LEU:HA	2.43	0.48
3:C:165:LEU:HD21	24:C:506:CLA:CAB	2.43	0.48
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.96	0.48
4:D:279:LEU:O	4:D:282:SER:OG	2.38	0.48
2:B:450:TRP:NE1	24:B:608:CLA:HBA1	2.27	0.48
24:B:603:CLA:H152	26:H:101:BCR:C17	19.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HA	26:B:619:BCR:H401	1.94	0.48
1:A:217:SER:HB2	4:D:142:ASN:HA	1.95	0.48
26:H:101:BCR:H20C	26:H:101:BCR:C37	2.43	0.48
10:K:28:ILE:O	10:K:31:LEU:HB2	2.15	0.48
16:V:129:LYS:HG2	16:V:136:TYR:O	2.56	0.48
2:B:29:LEU:HD11	26:B:618:BCR:C20	2.44	0.48
4:D:37:LEU:HD22	4:D:128:ARG:HD2	1.96	0.48
26:K:101:BCR:C17	26:K:101:BCR:C36	2.79	0.48
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.17	0.48
24:C:501:CLA:CBB	24:C:501:CLA:H71	2.79	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.49	0.48
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.96	0.48
1:A:306:VAL:HG12	1:A:314:ILE:HB	1.96	0.48
24:B:617:CLA:H3A	24:B:617:CLA:HBA1	1.83	0.48
1:A:64:ARG:NH1	13:O:105:PRO:O	2.47	0.48
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.52	0.48
1:A:106:LEU:CD2	26:A:610:BCR:H383	3.87	0.48
4:D:39:PRO:HG2	24:D:404:CLA:HAB	1.95	0.48
4:D:53:THR:HA	4:D:67:TYR:CD2	2.49	0.48
11:L:20:GLY:HA3	12:M:22:LEU:HD13	2.09	0.48
2:B:479:PHE:HA	4:D:139:ARG:HE	1.79	0.48
3:C:464:GLU:OE2	4:D:245:SER:OG	2.20	0.48
2:B:471:ALA:HB1	4:D:140:PRO:HG2	1.96	0.48
6:F:21:VAL:O	6:F:25:THR:HG23	2.14	0.48
6:F:37:ILE:O	6:F:40:MET:HB2	2.14	0.48
2:B:201:HIS:CE1	24:B:605:CLA:HMB3	22.29	0.47
2:B:208:VAL:HG21	24:B:603:CLA:HMC1	1.95	0.47
2:B:462:PHE:CZ	24:B:615:CLA:HMB3	14.06	0.47
3:C:323:LYS:O	15:U:47:LYS:HD2	2.14	0.47
6:F:20:TRP:NE1	6:F:24:HIS:CE1	2.82	0.47
4:D:123:ILE:HD11	32:H:102:DGD:HAE1	2.06	0.47
24:B:609:CLA:HMD3	26:T:101:BCR:H292	54.66	0.47
27:A:611:PL9:HC2	27:A:611:PL9:H103	2.16	0.47
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.48	0.47
29:C:519:LMG:H171	10:K:27:VAL:HG11	26.46	0.47
7:H:41:PHE:HB2	26:H:101:BCR:C15	2.51	0.47
1:A:267:ASN:HB3	1:A:270[B]:SER:OG	2.14	0.47
24:C:513:CLA:HAB	26:C:514:BCR:H371	2.39	0.47
11:L:10:VAL:O	12:M:28:GLN:NE2	2.36	0.47
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.17	0.47
1:A:215:HIS:ND1	27:A:611:PL9:O1	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:GLY:HA2	2:B:158:LEU:HD12	2.25	0.47
2:B:311:PHE:O	2:B:317:ASN:ND2	2.71	0.47
2:B:33:TRP:CD1	26:T:101:BCR:H381	35.27	0.47
24:B:605:CLA:H3A	24:B:605:CLA:CGA	3.52	0.47
4:D:209:LEU:HD22	27:D:405:PL9:H161	1.96	0.47
10:K:31:LEU:HB3	26:K:101:BCR:C15	2.76	0.47
26:K:101:BCR:C17	17:Y:33:PRO:HD3	2.57	0.47
1:A:296:ASN:HB3	3:C:401:LEU:HG	2.21	0.47
2:B:58:GLN:O	24:B:608:CLA:HED2	2.15	0.47
24:B:605:CLA:HBA1	24:B:605:CLA:H3A	1.69	0.47
26:B:619:BCR:H372	26:B:619:BCR:H20C	4.44	0.47
24:B:615:CLA:H193	26:B:620:BCR:C5	33.28	0.47
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.96	0.47
16:V:76:MET:HG2	33:V:201:HEM:HMB3	1.97	0.47
24:A:606:CLA:HBD	24:D:402:CLA:HAC2	1.97	0.47
3:C:59:LEU:HD13	24:C:510:CLA:HMD2	2.07	0.47
4:D:186:GLN:HB2	24:D:403:CLA:HBC1	1.96	0.47
10:K:17:ILE:N	10:K:17:ILE:HD13	2.28	0.47
2:B:334:ASP:N	2:B:334:ASP:OD2	2.44	0.47
10:K:25:LEU:HB2	10:K:26:PRO:HD3	2.35	0.47
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.97	0.47
2:B:115:TRP:HB2	26:B:619:BCR:H292	17.69	0.47
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.05	0.47
4:D:43:LEU:HD11	24:D:403:CLA:C2C	33.61	0.47
29:B:621:LMG:H411	30:L:101:LHG:H383	1.96	0.47
12:M:16[C]:LEU:HD21	12:M:16[C]:LEU:HD22	1.58	0.47
14:T:22:PHE:CZ	26:T:101:BCR:H333	2.88	0.47
29:A:613:LMG:H382	32:C:516:DGD:HB42	27.23	0.47
2:B:274:GLN:HB3	2:B:280:PHE:HE2	1.79	0.47
26:B:618:BCR:H381	14:T:19:PHE:CZ	34.24	0.47
4:D:43:LEU:HD11	24:D:404:CLA:C2C	2.44	0.47
27:D:405:PL9:H362	11:L:30:LEU:HD13	1.97	0.47
26:K:102:BCR:C37	26:K:102:BCR:C20	2.93	0.47
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.71	0.46
3:C:158:THR:O	3:C:251:HIS:HB3	2.15	0.46
1:A:235:TYR:OH	11:L:11:GLU:OE1	2.17	0.46
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.80	0.46
3:C:330:SER:O	13:O:123:LYS:NZ	2.47	0.46
3:C:55:ALA:HB1	26:K:102:BCR:H373	1.98	0.46
26:T:101:BCR:H373	26:T:101:BCR:H20C	1.96	0.46
24:B:611:CLA:OBD	24:B:611:CLA:H152	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:LEU:HD13	3:C:147:PHE:HB3	1.96	0.46
26:B:619:BCR:HC42	12:M:10:ALA:HA	7.54	0.46
1:A:127:MET:HE3	24:C:505:CLA:HMB1	2.35	0.46
1:A:214:MET:HG2	27:A:611:PL9:C10	2.45	0.46
1:A:271:LEU:HD11	27:A:611:PL9:HC8	1.97	0.46
24:B:604:CLA:C4D	24:B:606:CLA:H43	2.45	0.46
24:B:615:CLA:H101	26:B:618:BCR:C17	2.45	0.46
26:B:619:BCR:C37	26:B:619:BCR:C23	2.81	0.46
26:C:514:BCR:H20C	26:C:514:BCR:C18	2.36	0.46
2:B:193:TYR:OH	32:H:102:DGD:HE1	2.16	0.46
2:B:389:LYS:HE3	2:B:390:TYR:CE1	2.74	0.46
1:A:193:LEU:HD13	4:D:179:PHE:HB3	2.18	0.46
2:B:442:ILE:HD12	4:D:299:ILE:HG12	2.26	0.46
3:C:179:ALA:O	3:C:184:GLY:HA2	2.24	0.46
3:C:321:ASP:OD2	3:C:340:TYR:OH	2.28	0.46
4:D:126:MET:HA	4:D:129:GLN:OE1	2.37	0.46
4:D:342:PRO:O	4:D:345:VAL:HG22	2.15	0.46
1:A:91:LEU:HD21	1:A:163:ILE:HA	1.97	0.46
24:B:607[B]:CLA:H61	24:B:607[B]:CLA:H102	1.62	0.46
26:T:101:BCR:HC8	26:T:101:BCR:H311	1.98	0.46
1:A:58:VAL:HB	1:A:83:VAL:HB	2.05	0.46
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.97	0.46
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.59	0.46
4:D:199:MET:HG2	27:D:405:PL9:H321	1.96	0.46
2:B:383:PHE:CE1	13:O:167:GLY:HA2	2.51	0.46
1:A:296:ASN:HB2	3:C:400:PRO:O	2.33	0.46
2:B:440:ASP:O	13:O:174:LEU:HD22	2.36	0.46
2:B:212:ALA:HB2	24:B:611:CLA:HMC3	12.67	0.46
3:C:393:ALA:HB1	16:V:48:THR:HG21	1.97	0.46
1:A:112:TYR:O	1:A:116:ILE:HG12	2.15	0.46
30:A:615:LHG:H342	24:C:504:CLA:H201	1.97	0.46
4:D:136:VAL:HG12	4:D:138:VAL:HG13	1.98	0.46
4:D:293:LEU:HA	4:D:293:LEU:HD12	1.80	0.46
5:E:20:TRP:HZ2	9:J:13:VAL:HG13	1.81	0.46
26:B:618:BCR:H381	14:T:19:PHE:HZ	34.43	0.46
26:K:101:BCR:H17C	17:Y:33:PRO:HG3	2.09	0.46
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.98	0.45
27:A:611:PL9:H102	27:A:611:PL9:HC72	1.65	0.45
2:B:149:LEU:HD23	24:B:604:CLA:HBC1	1.98	0.45
26:H:101:BCR:H331	26:H:101:BCR:HC8	2.76	0.45
8:I:24:LEU:HG	26:I:101:BCR:HC31	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:102:BCR:H20C	26:K:102:BCR:C22	2.35	0.45
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.13	0.45
1:A:121[B]:LEU:CD2	24:A:609:CLA:HMB3	2.46	0.45
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.45
24:A:606:CLA:HAA1	24:D:403:CLA:HBB2	1.98	0.45
2:B:201:HIS:HB2	24:B:603:CLA:C4A	2.46	0.45
27:D:405:PL9:H471	27:D:405:PL9:H43	1.63	0.45
29:D:408:LMG:H352	26:F:101:BCR:H17C	1.99	0.45
1:A:269:ARG:CZ	4:D:222:LEU:HD13	2.46	0.45
4:D:129:GLN:NE2	4:D:142:ASN:OD1	2.50	0.45
13:O:97:GLU:HB2	13:O:125:LEU:HB3	2.10	0.45
28:L:102:SQD:H321	14:T:16:LEU:HB2	1.98	0.45
2:B:201:HIS:CE1	24:B:604:CLA:HMB3	2.52	0.45
24:B:614:CLA:HBC3	26:B:619:BCR:H11C	1.98	0.45
3:C:38:GLY:HA3	24:C:511:CLA:HMD3	1.99	0.45
4:D:315:TYR:O	4:D:319:LEU:HG	2.33	0.45
1:A:288:LEU:O	1:A:292:THR:HG23	2.38	0.45
2:B:262:THR:C	2:B:264:PRO:HD3	2.50	0.45
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.52	0.45
24:B:606:CLA:H143	24:B:611:CLA:HED2	1.98	0.45
30:D:407:LHG:H141	30:D:407:LHG:H171	1.79	0.45
16:V:12:LEU:O	16:V:70:GLU:HG2	2.16	0.45
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.45
24:B:607[A]:CLA:H72	26:B:620:BCR:C9	2.47	0.45
2:B:26:HIS:HB2	24:B:613:CLA:HMB2	1.98	0.45
26:B:620:BCR:C23	26:B:620:BCR:C37	2.84	0.45
1:A:24:THR:C	4:D:255:GLN:HE22	2.19	0.45
7:H:28:THR:HB	7:H:29:PRO:HD3	1.99	0.45
1:A:153:SER:CB	24:A:606:CLA:H43	2.47	0.45
12:M:20:VAL:HG22	12:M:20:VAL:HG11	3.03	0.45
1:A:77:ILE:HB	11:L:33:SER:OG	2.16	0.45
2:B:102:VAL:HA	26:B:619:BCR:C40	2.47	0.45
2:B:324:LEU:HD21	4:D:196:PHE:HE2	1.81	0.45
26:B:619:BCR:H12C	26:B:620:BCR:C10	21.66	0.45
4:D:155:SER:HA	4:D:159:ILE:HD12	1.99	0.45
30:L:101:LHG:H111	30:L:101:LHG:H241	1.99	0.45
2:B:150:CYS:HB2	24:B:605:CLA:CMC	20.26	0.45
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.61	0.45
24:C:504:CLA:HED3	29:C:519:LMG:O3	22.71	0.45
6:F:29:PRO:HB3	26:F:101:BCR:H12C	1.99	0.45
1:A:127:MET:CE	24:C:505:CLA:HBB1	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:PRO:O	2:B:198:VAL:N	2.60	0.44
24:B:606:CLA:HBB1	24:B:609:CLA:HAB	33.59	0.44
24:B:607[B]:CLA:H161	24:B:607[B]:CLA:H192	1.68	0.44
24:B:616:CLA:H3A	24:B:616:CLA:HBA1	1.62	0.44
26:F:101:BCR:H403	9:J:25:VAL:HG21	2.53	0.44
24:A:609:CLA:H11	8:I:9:TYR:CE1	2.52	0.44
29:A:613:LMG:H201	29:A:613:LMG:H231	1.72	0.44
3:C:297:TYR:HD1	3:C:302:TYR:CZ	2.45	0.44
3:C:307:PRO:HG3	3:C:358:PHE:CE1	2.52	0.44
3:C:424:SER:O	3:C:428:THR:HG23	2.17	0.44
13:O:222:ASP:CG	13:O:224:ASP:H	2.25	0.44
1:A:129:ARG:HH22	4:D:256:ILE:HA	2.26	0.44
1:A:223:LEU:HD22	4:D:265:ARG:HG2	2.19	0.44
24:A:609:CLA:HBA1	24:A:609:CLA:H3A	1.78	0.44
24:B:602:CLA:HMC2	26:H:101:BCR:H19C	2.00	0.44
26:B:620:BCR:H11C	26:B:620:BCR:H341	2.16	0.44
29:Z:101:LMG:O2	29:Z:101:LMG:HC71	2.25	0.44
1:A:131:TRP:CZ3	24:C:505:CLA:HBA1	2.53	0.44
26:A:610:BCR:C37	26:A:610:BCR:H20C	2.47	0.44
2:B:29:LEU:HD11	26:B:618:BCR:C19	2.47	0.44
24:C:506:CLA:H162	24:C:506:CLA:H122	1.72	0.44
6:F:30:THR:HA	26:F:101:BCR:C16	2.52	0.44
7:H:46:LEU:HD11	32:H:102:DGD:HA31	1.99	0.44
27:D:405:PL9:C34	11:L:30:LEU:HD22	2.47	0.44
1:A:202:VAL:HG11	24:A:607:CLA:C3D	2.47	0.44
27:A:611:PL9:H272	27:A:611:PL9:H252	1.74	0.44
2:B:18:ARG:HD3	2:B:115:TRP:CH2	2.78	0.44
2:B:249:ALA:HA	2:B:252:VAL:HG22	1.98	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.00	0.44
24:B:610:CLA:HHD	24:B:610:CLA:HBC3	3.03	0.44
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.48	0.44
24:B:615:CLA:H122	26:B:618:BCR:H16C	1.99	0.44
2:B:63:LEU:HD12	2:B:66:MET:HE3	2.00	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	1.99	0.44
5:E:19:TYR:CE2	5:E:23:HIS:CE1	3.05	0.44
16:V:93:PRO:HG2	33:V:201:HEM:HMC3	1.99	0.44
24:B:602:CLA:HAB	24:B:603:CLA:HMC2	2.00	0.44
3:C:347:GLY:HA3	13:O:17:ASN:HB2	1.99	0.44
4:D:37:LEU:CD2	4:D:128:ARG:HD2	2.48	0.44
7:H:49:TYR:CG	32:H:102:DGD:HB22	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:610:CLA:HAC1	7:H:34:PHE:CE1	2.53	0.44
26:I:101:BCR:H373	26:I:101:BCR:H20C	1.98	0.44
26:K:101:BCR:H17C	17:Y:33:PRO:CG	2.65	0.44
11:L:21:LEU:HD13	28:L:102:SQD:H312	1.99	0.44
27:A:611:PL9:H121	27:A:611:PL9:H103	1.79	0.44
2:B:382:PRO:HG2	2:B:385:ARG:HD2	2.20	0.44
2:B:422:ARG:HH21	13:O:169:ASP:CG	2.23	0.44
24:B:606:CLA:H41	24:B:606:CLA:H62	1.77	0.44
24:C:513:CLA:HMC2	26:C:514:BCR:C21	2.47	0.44
32:H:102:DGD:HB62	32:H:102:DGD:HB91	1.81	0.44
33:V:201:HEM:HHA	33:V:201:HEM:HBA1	2.00	0.44
24:B:614:CLA:HMB3	24:B:615:CLA:HAA1	20.39	0.44
3:C:210:PHE:HA	3:C:213[B]:LEU:HD13	2.20	0.44
30:D:406:LHG:HC91	30:L:101:LHG:HC81	1.99	0.44
27:D:405:PL9:H203	30:D:407:LHG:H122	2.00	0.44
5:E:23:HIS:HA	5:E:26:THR:OG1	2.16	0.44
24:B:607[B]:CLA:H111	24:B:607[B]:CLA:H142	1.76	0.44
2:B:41:GLU:HB3	2:B:60:MET:SD	2.58	0.44
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.53	0.44
24:C:510:CLA:H3A	24:C:510:CLA:HBA1	1.85	0.44
7:H:12[A]:ARG:NH1	7:H:15:ASN:O	2.47	0.44
14:T:18:PHE:HB2	26:T:101:BCR:HC8	1.99	0.44
1:A:116:ILE:HG13	1:A:117:PHE:N	2.36	0.43
2:B:133:LEU:HB3	2:B:138:MET:SD	2.58	0.43
3:C:29:GLU:CD	3:C:29:GLU:H	2.37	0.43
3:C:54:VAL:HG12	3:C:125:LEU:O	2.30	0.43
26:K:102:BCR:C23	26:K:102:BCR:C37	2.82	0.43
1:A:334:ARG:HB2	13:O:157:LEU:HD12	1.99	0.43
24:A:609:CLA:H192	24:C:505:CLA:H142	2.00	0.43
2:B:102:VAL:HA	26:B:620:BCR:C40	17.92	0.43
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.89	0.43
3:C:86:LEU:O	3:C:90:PRO:HG2	2.18	0.43
26:H:101:BCR:H393	18:X:7:LEU:HD21	2.21	0.43
10:K:17:ILE:H	10:K:17:ILE:CD1	2.22	0.43
26:A:610:BCR:C36	26:A:610:BCR:C16	3.49	0.43
24:B:612:CLA:HHC	24:B:612:CLA:HBB1	4.46	0.43
3:C:168:LEU:HD21	24:C:509:CLA:H61	2.11	0.43
26:C:514:BCR:C15	29:C:519:LMG:H401	2.47	0.43
3:C:75:PHE:CZ	3:C:77:PRO:HA	2.59	0.43
4:D:191:TRP:CE2	4:D:197:HIS:HB2	2.53	0.43
24:A:607:CLA:H142	29:D:408:LMG:H232	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:11:VAL:HG13	8:I:15:PHE:HE1	1.83	0.43
1:A:304:HIS:CE1	3:C:414:ILE:HG21	2.59	0.43
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.48	0.43
27:A:611:PL9:H172	27:A:611:PL9:H203	1.80	0.43
4:D:266:TRP:CZ2	11:L:19:LEU:HD13	2.54	0.43
4:D:298:PHE:O	4:D:301:GLN:HB2	2.18	0.43
1:A:121[B]:LEU:HD23	24:A:609:CLA:HMB3	2.00	0.43
2:B:145:LEU:CD1	24:B:617:CLA:HMB2	13.44	0.43
2:B:392:PHE:HA	2:B:397:VAL:HG23	2.18	0.43
24:B:614:CLA:HMB1	24:B:614:CLA:HBB1	2.29	0.43
1:A:288:LEU:HD22	3:C:432:VAL:HA	2.00	0.43
18:X:27:VAL:HG21	28:X:101:SQD:H321	2.00	0.43
24:B:605:CLA:H2	24:B:606:CLA:C4C	2.48	0.43
3:C:185:LEU:HD13	24:C:501:CLA:HED2	2.29	0.43
24:C:501:CLA:ND	24:C:503:CLA:H2	2.33	0.43
27:D:405:PL9:HC72	27:D:405:PL9:H102	1.58	0.43
27:D:405:PL9:H302	27:D:405:PL9:H252	2.01	0.43
7:H:56:ASP:OD2	18:X:2:THR:HB	2.41	0.43
13:O:137:THR:C	13:O:139:SER:H	2.22	0.43
2:B:149:LEU:HD22	24:B:606:CLA:H152	10.75	0.43
3:C:344:SER:OG	3:C:348:GLU:OE2	2.36	0.43
3:C:34:ALA:HB3	3:C:36:TRP:CE2	2.53	0.43
2:B:33:TRP:HD1	26:T:101:BCR:H381	34.48	0.43
1:A:249:VAL:HG12	2:B:491:VAL:HG21	2.04	0.43
1:A:164:GLY:HA3	1:A:294:ALA:O	2.51	0.43
3:C:269:GLU:OE2	3:C:447:ARG:HD3	2.18	0.43
33:E:103:HEM:HBC2	6:F:31:ILE:HG13	1.99	0.43
30:L:101:LHG:H142	30:L:101:LHG:H171	1.87	0.43
1:A:237:TYR:CE1	1:A:241:GLN:HG2	2.64	0.43
1:A:96:ILE:HD12	24:A:609:CLA:HMD1	2.25	0.43
1:A:76:ASN:OD1	1:A:79:THR:HG23	2.26	0.43
2:B:321:LYS:NZ	2:B:363:PHE:O	2.52	0.43
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.43
5:E:34:GLY:HA3	6:F:32:PHE:O	2.19	0.43
24:A:609:CLA:H92	8:I:13:THR:HG23	2.02	0.43
24:C:504:CLA:HBC1	10:K:27:VAL:HA	2.01	0.43
13:O:49[A]:THR:OG1	13:O:236:GLN:HB2	2.23	0.43
18:X:21:LEU:O	18:X:25:PHE:HD1	2.01	0.43
2:B:118:TRP:CE2	11:L:4:ASN:ND2	3.40	0.43
2:B:149:LEU:HD22	24:B:605:CLA:H152	2.00	0.43
2:B:204:ALA:HB3	24:B:604:CLA:HAB	10.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:611:PL9:C22	25:D:401:PHO:HMA2	2.62	0.43
2:B:461:LEU:HD22	30:D:406:LHG:H301	2.02	0.43
30:D:406:LHG:O9	30:L:101:LHG:HC81	2.19	0.43
7:H:49:TYR:CD2	32:H:102:DGD:HB22	2.76	0.43
10:K:15:TYR:CZ	19:Z:5:PHE:HZ	2.66	0.43
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.42
3:C:223:TRP:CG	3:C:224:ILE:N	2.87	0.42
24:C:504:CLA:HED3	29:C:518:LMG:O3	2.19	0.42
4:D:87:HIS:HA	4:D:167:TRP:CD1	2.53	0.42
24:B:602:CLA:H152	26:H:101:BCR:H17C	2.01	0.42
2:B:61:PHE:CE2	24:B:608:CLA:HBB1	2.55	0.42
24:C:502:CLA:H51	24:C:503:CLA:NC	2.33	0.42
27:D:405:PL9:H302	27:D:405:PL9:H271	1.55	0.42
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.54	0.42
16:V:100:ILE:HG13	16:V:101:PHE:CD2	2.91	0.42
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.51	0.42
2:B:58:GLN:C	2:B:329:PRO:HB3	2.58	0.42
32:C:517:DGD:HA41	29:D:408:LMG:H121	2.00	0.42
26:F:101:BCR:H11C	26:F:101:BCR:H341	1.69	0.42
13:O:92:SER:HB3	13:O:131:PRO:HA	2.21	0.42
15:U:59:GLU:CD	15:U:59:GLU:H	2.47	0.42
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.62	0.42
1:A:279:PRO:O	1:A:283:VAL:HG23	2.19	0.42
2:B:204:ALA:CB	24:B:604:CLA:HAB	10.87	0.42
2:B:422:ARG:O	2:B:425:ILE:HG12	2.23	0.42
24:B:616:CLA:HMC2	26:B:619:BCR:H361	30.93	0.42
4:D:17:ILE:O	4:D:20:ASP:HB2	2.42	0.42
4:D:125:PHE:CE1	25:D:401:PHO:HBD	2.54	0.42
24:D:403:CLA:HBB1	18:X:21:LEU:HD21	39.66	0.42
27:D:405:PL9:H421	27:D:405:PL9:H453	1.68	0.42
4:D:65:SER:HB2	4:D:77:ALA:O	2.20	0.42
16:V:37:CYS:HG	33:V:201:HEM:CAB	2.32	0.42
2:B:136:PRO:O	2:B:139:PHE:HB3	2.25	0.42
2:B:243:ALA:HB2	2:B:466:HIS:ND1	2.34	0.42
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	2.01	0.42
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.02	0.42
4:D:154:VAL:HG21	32:H:102:DGD:HAN1	2.02	0.42
25:D:401:PHO:H72	25:D:401:PHO:H112	1.88	0.42
14:T:25[A]:GLU:HA	14:T:26:PRO:HD3	1.89	0.42
24:A:606:CLA:CB	24:D:402:CLA:HAC2	2.49	0.42
24:A:609:CLA:H122	24:A:609:CLA:H162	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:610:CLA:H3A	24:B:610:CLA:HBA1	1.86	0.42
3:C:130:VAL:O	3:C:134:ILE:HG12	2.35	0.42
24:C:508:CLA:HBB2	24:C:509:CLA:HMA3	2.01	0.42
3:C:95:LEU:CD1	24:C:503:CLA:HAA2	2.87	0.42
13:O:81:ILE:HD11	13:O:102:ASP:HA	2.02	0.42
24:B:613:CLA:H91	24:B:614:CLA:HBB1	2.02	0.42
3:C:182:PHE:CG	24:C:502:CLA:H191	2.64	0.42
4:D:72:ASN:O	4:D:76:VAL:HG13	2.20	0.42
1:A:89:ILE:HG23	1:A:92:HIS:HB2	2.02	0.42
2:B:18:ARG:NH2	28:B:622:SQD:O9	2.45	0.42
3:C:76:ILE:HA	3:C:77:PRO:HD3	1.91	0.42
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.54	0.42
27:D:405:PL9:H122	30:D:407:LHG:H111	2.02	0.42
5:E:30:LEU:HD12	33:E:103:HEM:HMC1	2.02	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.97	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.43	0.42
1:A:330:VAL:HG21	4:D:328:TRP:CE2	2.55	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.18	0.42
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.55	0.42
32:C:517:DGD:HD4	32:C:517:DGD:HE5	3.58	0.42
4:D:30:VAL:HA	4:D:38:PHE:HE1	2.15	0.42
11:L:18:TYR:CD2	14:T:20:ALA:HA	2.55	0.42
3:C:390:ARG:HD3	16:V:100:ILE:HD12	2.45	0.42
2:B:18:ARG:HD3	2:B:115:TRP:CZ3	2.67	0.42
3:C:171:GLY:O	3:C:174:LEU:HB2	2.22	0.42
3:C:315:MET:HG2	3:C:392:ALA:HB2	2.13	0.42
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.19	0.42
13:O:184:ARG:HA	15:U:9:LEU:CD1	2.61	0.42
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.95	0.41
4:D:70:GLY:O	9:J:37:GLY:HA3	2.26	0.41
13:O:127:ALA:HA	13:O:144:GLY:HA3	2.02	0.41
13:O:162:ARG:HD2	13:O:186:ASN:HA	2.02	0.41
2:B:399:VAL:HG12	2:B:417:VAL:HG22	2.36	0.41
2:B:65:PHE:HE1	24:B:606:CLA:HED2	10.87	0.41
2:B:69:LEU:HD12	24:B:606:CLA:HAA2	2.02	0.41
2:B:7:ARG:HG2	24:B:613:CLA:O2D	17.20	0.41
3:C:72:LEU:HD11	3:C:108:THR:HB	2.02	0.41
24:C:507:CLA:H61	24:C:507:CLA:H92	1.94	0.41
24:B:605:CLA:H43	24:B:606:CLA:H2	2.01	0.41
24:B:609:CLA:HBA1	24:B:609:CLA:H3A	2.94	0.41
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.84	0.41
1:A:340:PRO:HB3	15:U:103:TYR:CG	2.55	0.41
2:B:385:ARG:HG2	13:O:165:ALA:O	2.22	0.41
3:C:433:LEU:HD22	24:C:510:CLA:H143	2.42	0.41
4:D:317:LYS:O	4:D:321:LEU:HG	2.41	0.41
2:B:383:PHE:CG	4:D:347:PRO:HA	2.55	0.41
4:D:91:LEU:HB3	4:D:93:TRP:CE2	2.56	0.41
24:C:505:CLA:H141	8:I:16:VAL:HG22	2.04	0.41
13:O:42:ARG:HG3	13:O:80:GLN:HA	2.02	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.02	0.41
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.82	0.41
24:B:609:CLA:HBB2	4:D:123:ILE:HG12	2.02	0.41
4:D:80:THR:HB	4:D:168:PHE:HA	2.29	0.41
4:D:101:PHE:HE1	26:F:101:BCR:HC42	2.03	0.41
3:C:27:ASP:HB3	10:K:46:ARG:HD2	2.08	0.41
2:B:325:PHE:CD2	11:L:34:TYR:HB3	2.90	0.41
1:A:297:LEU:HD23	32:C:517:DGD:HBF2	11.51	0.41
28:A:614:SQD:H241	26:B:620:BCR:H383	55.57	0.41
24:B:616:CLA:HAB	26:B:619:BCR:H19C	26.67	0.41
33:V:201:HEM:HMB2	33:V:201:HEM:HBB2	2.03	0.41
24:D:403:CLA:H2	18:X:14:LEU:HA	29.26	0.41
1:A:217:SER:O	1:A:221[A]:SER:HB3	2.21	0.41
1:A:271:LEU:CD1	27:A:611:PL9:HC8	2.49	0.41
2:B:222:PRO:HD2	2:B:225:LEU:HD12	2.05	0.41
2:B:270:PRO:HG2	2:B:317:ASN:O	2.29	0.41
24:B:606:CLA:HBB1	24:B:606:CLA:HHC	2.01	0.41
2:B:25:MET:HE1	26:B:618:BCR:H382	2.01	0.41
24:B:616:CLA:H8	26:B:619:BCR:H362	20.35	0.41
24:B:614:CLA:H151	30:D:406:LHG:H182	2.01	0.41
13:O:43:LEU:HB3	13:O:81:ILE:HB	2.03	0.41
2:B:258:TYR:CZ	32:H:102:DGD:HG12	2.68	0.41
24:B:607[B]:CLA:H72	26:B:620:BCR:C9	2.51	0.41
24:C:501:CLA:H192	24:C:506:CLA:CHB	2.50	0.41
3:C:95:LEU:HD11	24:C:503:CLA:HAA2	2.55	0.41
4:D:48:TRP:NE1	25:D:401:PHO:H162	2.36	0.41
6:F:36:ALA:O	6:F:40:MET:HG3	2.21	0.41
26:H:101:BCR:H20C	26:H:101:BCR:H373	2.02	0.41
24:B:603:CLA:H172	32:H:102:DGD:HAW1	2.03	0.41
30:A:615:LHG:H281	30:A:615:LHG:H251	1.63	0.41
30:A:615:LHG:H302	30:A:615:LHG:H332	1.87	0.41
2:B:24:LEU:HD21	24:B:617:CLA:CAB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLY:O	3:C:403:SER:HB2	2.24	0.41
16:V:41:HIS:NE2	33:V:201:HEM:NB	2.79	0.41
24:D:404:CLA:C2	18:X:14:LEU:HD12	2.51	0.41
28:A:612:SQD:H291	24:C:508:CLA:H71	2.03	0.41
1:A:65:GLU:OE1	1:A:335:ASN:ND2	2.44	0.41
2:B:39:LEU:HA	2:B:39:LEU:HD23	1.76	0.41
3:C:297:TYR:HA	3:C:302:TYR:CE2	2.63	0.41
24:C:505:CLA:HAA1	24:C:505:CLA:CBD	2.50	0.41
24:C:513:CLA:HAB	26:C:514:BCR:H24C	2.82	0.41
2:B:137:LYS:NZ	7:H:17:GLU:OE2	2.65	0.41
2:B:325:PHE:CG	11:L:34:TYR:HB3	2.63	0.41
24:B:613:CLA:HBB1	24:B:615:CLA:CMB	2.51	0.41
2:B:357:ARG:NH2	4:D:337:GLU:HB3	2.53	0.41
24:C:504:CLA:C1D	32:C:517:DGD:HB21	10.31	0.40
13:O:158:ASP:C	13:O:158:ASP:OD1	2.59	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.88	0.40
1:A:57:PRO:HA	1:A:68:SER:HA	2.03	0.40
30:A:615:LHG:H372	30:A:615:LHG:H132	2.03	0.40
2:B:125:ASP:HA	2:B:126:PRO:HD3	2.04	0.40
2:B:246:PHE:CD1	2:B:246:PHE:C	2.94	0.40
2:B:25:MET:HE3	26:B:619:BCR:H382	10.52	0.40
2:B:260:SER:N	2:B:263:THR:OG1	2.67	0.40
24:B:614:CLA:H162	24:B:614:CLA:H121	1.88	0.40
3:C:416[A]:SER:HB2	16:V:42:VAL:HG23	2.02	0.40
25:A:608:PHO:HAB	4:D:205:LEU:HD13	2.08	0.40
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.03	0.40
11:L:24[A]:ILE:HA	11:L:24[A]:ILE:HD13	1.91	0.40
2:B:192:PRO:HB3	7:H:49:TYR:CE2	2.85	0.40
3:C:61:VAL:HG12	3:C:118:HIS:O	2.22	0.40
3:C:221:GLU:O	3:C:226:SER:HB3	2.21	0.40
3:C:51:GLY:HA2	3:C:132:HIS:HB2	2.03	0.40
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.57	0.40
26:K:101:BCR:H17C	17:Y:33:PRO:CD	2.81	0.40
25:A:608:PHO:H2	25:A:608:PHO:H61	1.85	0.40
27:A:611:PL9:H222	27:A:611:PL9:H253	2.05	0.40
2:B:189:GLY:O	2:B:197:GLY:HA3	2.21	0.40
2:B:256:MET:HG3	2:B:448:ARG:HG3	2.03	0.40
26:B:619:BCR:C36	26:B:619:BCR:C20	3.00	0.40
3:C:210:PHE:CD2	3:C:213[B]:LEU:HD22	2.72	0.40
24:C:502:CLA:H61	24:C:512:CLA:H42	2.03	0.40
24:C:508:CLA:CBB	24:C:508:CLA:HMB1	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:D:401:PHO:H62	25:D:401:PHO:H41	1.79	0.40
13:O:126:VAL:O	13:O:144:GLY:HA3	2.37	0.40
14:T:14:ILE:HA	14:T:14:ILE:HD13	1.92	0.40
2:B:105:GLY:O	2:B:108:PHE:HB3	2.20	0.40
2:B:125:ASP:OD1	7:H:18:TYR:HB3	2.22	0.40
2:B:477:ASP:OD1	2:B:478:VAL:N	2.77	0.40
3:C:114:VAL:HG11	24:C:503:CLA:HED2	2.43	0.40
24:C:501:CLA:CHB	26:I:101:BCR:H271	2.51	0.40
24:C:512:CLA:H101	24:C:513:CLA:H141	2.04	0.40
3:C:59:LEU:HD23	3:C:59:LEU:HA	1.77	0.40
5:E:22:ILE:HD13	33:E:103:HEM:HMA1	2.03	0.40
26:F:101:BCR:H281	26:F:101:BCR:H393	1.80	0.40
6:F:34:LEU:HG	26:F:101:BCR:H19C	2.03	0.40
12:M:23:ILE:O	12:M:27:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	46	84
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	46	84
2	B	512/504 (102%)	506 (99%)	6 (1%)	0	100	100
2	b	512/504 (102%)	505 (99%)	7 (1%)	0	100	100
3	C	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	39	81
3	c	454/451 (101%)	444 (98%)	8 (2%)	2 (0%)	39	81
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	81/81 (100%)	80 (99%)	1 (1%)	0	100	100
6	F	32/34 (94%)	32 (100%)	0	0	100	100
6	f	32/34 (94%)	32 (100%)	0	0	100	100
7	H	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
7	h	65/65 (100%)	60 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/38 (95%)	36 (100%)	0	0	100	100
9	j	36/38 (95%)	36 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	6	42
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/34 (97%)	33 (100%)	0	0	100	100
12	m	33/34 (97%)	33 (100%)	0	0	100	100
13	O	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	39	81
13	o	245/243 (101%)	237 (97%)	7 (3%)	1 (0%)	39	81
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/29 (93%)	27 (100%)	0	0	100	100
17	y	27/29 (93%)	27 (100%)	0	0	100	100
18	X	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
18	x	38/39 (97%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5252/5264 (100%)	5139 (98%)	104 (2%)	9 (0%)	56	88

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
10	k	11	LEU
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/269 (102%)	273 (100%)	0	100	100
1	a	273/269 (102%)	273 (100%)	0	100	100
2	B	412/402 (102%)	408 (99%)	4 (1%)	82	93
2	b	412/402 (102%)	410 (100%)	2 (0%)	92	97
3	C	357/352 (101%)	351 (98%)	6 (2%)	68	89
3	c	357/352 (101%)	353 (99%)	4 (1%)	80	92
4	D	277/277 (100%)	274 (99%)	3 (1%)	80	92
4	d	277/277 (100%)	274 (99%)	3 (1%)	80	92
5	E	74/72 (103%)	73 (99%)	1 (1%)	74	91
5	e	74/72 (103%)	73 (99%)	1 (1%)	74	91
6	F	28/28 (100%)	27 (96%)	1 (4%)	42	77
6	f	28/28 (100%)	27 (96%)	1 (4%)	42	77
7	H	56/54 (104%)	52 (93%)	4 (7%)	18	58
7	h	56/54 (104%)	52 (93%)	4 (7%)	18	58
8	I	36/35 (103%)	36 (100%)	0	100	100
8	i	36/35 (103%)	36 (100%)	0	100	100
9	J	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	26/26 (100%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	61
10	k	30/30 (100%)	28 (93%)	2 (7%)	20	61
11	L	36/35 (103%)	35 (97%)	1 (3%)	51	82
11	l	36/35 (103%)	35 (97%)	1 (3%)	51	82
12	M	32/31 (103%)	31 (97%)	1 (3%)	47	81
12	m	32/31 (103%)	31 (97%)	1 (3%)	47	81
13	O	210/206 (102%)	206 (98%)	4 (2%)	65	87
13	o	210/206 (102%)	206 (98%)	4 (2%)	65	87
14	T	29/27 (107%)	29 (100%)	0	100	100
14	t	29/27 (107%)	29 (100%)	0	100	100
15	U	84/84 (100%)	83 (99%)	1 (1%)	78	92
15	u	84/84 (100%)	83 (99%)	1 (1%)	78	92
16	V	118/117 (101%)	117 (99%)	1 (1%)	86	95
16	v	118/117 (101%)	117 (99%)	1 (1%)	86	95
17	Y	22/22 (100%)	21 (96%)	1 (4%)	34	73
17	y	22/22 (100%)	21 (96%)	1 (4%)	34	73
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	51 (98%)	1 (2%)	65	87
19	z	52/52 (100%)	51 (98%)	1 (2%)	65	87
All	All	4370/4302 (102%)	4312 (99%)	58 (1%)	76	91

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	76[A]	SER
2	B	76[B]	SER
2	B	246	PHE
2	B	472	ARG
3	C	24	THR
3	C	289	PHE
3	C	315	MET
3	C	416[A]	SER
3	C	416[B]	SER

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Mol	Chain	Res	Type
3	C	418	ASN
4	D	11	GLU
4	D	90	LEU
4	D	180	ARG
5	E	71	GLU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
12	M	9	ILE
13	O	61	GLN
13	O	118	LEU
13	O	181	GLU
13	O	234	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	27	MET
19	Z	31	GLN
2	b	246	PHE
2	b	472	ARG
3	c	24	THR
3	c	289	PHE
3	c	315	MET
3	c	418	ASN
4	d	11	GLU
4	d	90	LEU
4	d	180	ARG
5	e	71	GLU
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	49	TYR
7	h	65	LEU
10	k	13	GLU
10	k	17	ILE
11	l	1	MET
12	m	9	ILE
13	o	61	GLN

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Mol	Chain	Res	Type
13	o	118	LEU
13	o	181	GLU
13	o	234	LYS
15	u	70	ARG
16	v	30	LYS
17	y	27	MET
19	z	31	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	216	HIS
2	B	409	GLN
4	d	197	HIS
15	u	78	ASN

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 168 ligands modelled in this entry, 16 are monoatomic - leaving 152 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
20	OEX	A	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
23	BCT	A	605	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	606	-	57,73,73	2.60	22 (38%)	61,113,113	1.89	14 (22%)
24	CLA	A	607	-	57,73,73	2.52	21 (36%)	61,113,113	2.11	14 (22%)
25	PHO	A	608	-	67,69,69	1.22	9 (13%)	86,99,99	1.07	5 (5%)
24	CLA	A	609	-	57,73,73	2.59	22 (38%)	61,113,113	1.95	14 (22%)
26	BCR	A	610	-	41,41,41	9.24	30 (73%)	56,56,56	5.60	27 (48%)
27	PL9	A	611	-	54,55,55	3.94	16 (29%)	68,69,69	4.39	34 (50%)
28	SQD	A	612	-	53,54,54	1.49	3 (5%)	62,65,65	1.78	12 (19%)
29	LMG	A	613	-	51,51,55	1.31	5 (9%)	59,59,63	0.96	4 (6%)
28	SQD	A	614	-	53,54,54	1.50	3 (5%)	62,65,65	1.42	6 (9%)
30	LHG	A	615	-	48,48,48	1.09	3 (6%)	49,54,54	1.32	6 (12%)
24	CLA	B	602	-	57,73,73	2.49	22 (38%)	61,113,113	1.84	12 (19%)
24	CLA	B	603	-	57,73,73	2.52	23 (40%)	61,113,113	2.01	11 (18%)
24	CLA	B	604	-	57,73,73	2.48	24 (42%)	61,113,113	2.00	15 (24%)
24	CLA	B	605	-	57,73,73	2.51	21 (36%)	61,113,113	2.19	14 (22%)
24	CLA	B	606	-	57,73,73	2.52	21 (36%)	61,113,113	1.99	11 (18%)
24	CLA	B	607[A]	-	57,73,73	2.52	22 (38%)	61,113,113	2.07	13 (21%)
24	CLA	B	607[B]	-	57,73,73	2.54	22 (38%)	61,113,113	2.07	12 (19%)
24	CLA	B	608	-	57,73,73	2.56	23 (40%)	61,113,113	2.01	14 (22%)
24	CLA	B	609	-	57,73,73	2.48	22 (38%)	61,113,113	2.15	17 (27%)
24	CLA	B	610	-	57,73,73	2.55	23 (40%)	61,113,113	1.95	12 (19%)
24	CLA	B	611	-	57,73,73	2.50	23 (40%)	61,113,113	1.84	13 (21%)
24	CLA	B	612	-	57,73,73	2.51	22 (38%)	61,113,113	2.00	11 (18%)
24	CLA	B	613	-	57,73,73	2.58	24 (42%)	61,113,113	2.08	15 (24%)
24	CLA	B	614	-	57,73,73	2.55	21 (36%)	61,113,113	1.98	10 (16%)
24	CLA	B	615	-	57,73,73	2.52	22 (38%)	61,113,113	1.90	10 (16%)
24	CLA	B	616	-	57,73,73	2.47	19 (33%)	61,113,113	1.94	15 (24%)
24	CLA	B	617	-	57,73,73	2.50	21 (36%)	61,113,113	1.87	13 (21%)
26	BCR	B	618	-	41,41,41	9.01	29 (70%)	56,56,56	6.05	30 (53%)
26	BCR	B	619	-	41,41,41	9.02	29 (70%)	56,56,56	5.63	29 (51%)
26	BCR	B	620	-	41,41,41	9.20	30 (73%)	56,56,56	5.86	32 (57%)
29	LMG	B	621	-	51,51,55	1.27	4 (7%)	59,59,63	1.01	5 (8%)
28	SQD	B	622	-	53,54,54	1.47	4 (7%)	62,65,65	1.73	9 (14%)
24	CLA	C	501	-	57,73,73	2.54	23 (40%)	61,113,113	2.06	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	502	-	57,73,73	2.48	22 (38%)	61,113,113	1.93	13 (21%)
24	CLA	C	503	-	57,73,73	2.56	22 (38%)	61,113,113	1.72	11 (18%)
24	CLA	C	504	-	57,73,73	2.54	22 (38%)	61,113,113	2.04	14 (22%)
24	CLA	C	505	-	57,73,73	2.45	21 (36%)	61,113,113	1.95	11 (18%)
24	CLA	C	506	-	57,73,73	2.49	19 (33%)	61,113,113	1.94	10 (16%)
24	CLA	C	507	-	57,73,73	2.44	21 (36%)	61,113,113	2.22	13 (21%)
24	CLA	C	508	-	57,73,73	2.61	23 (40%)	61,113,113	1.92	10 (16%)
24	CLA	C	509	-	57,73,73	2.49	22 (38%)	61,113,113	1.91	13 (21%)
24	CLA	C	510	-	57,73,73	2.57	23 (40%)	61,113,113	1.79	12 (19%)
24	CLA	C	511	3	57,73,73	2.53	22 (38%)	61,113,113	2.02	16 (26%)
24	CLA	C	512	-	57,73,73	2.50	20 (35%)	61,113,113	1.94	14 (22%)
24	CLA	C	513	-	57,73,73	2.42	20 (35%)	61,113,113	1.96	16 (26%)
26	BCR	C	514	-	41,41,41	9.06	29 (70%)	56,56,56	5.96	33 (58%)
32	DGD	C	515	-	63,63,67	1.66	15 (23%)	77,77,81	1.04	5 (6%)
32	DGD	C	516	-	63,63,67	1.63	14 (22%)	77,77,81	1.21	9 (11%)
32	DGD	C	517	-	63,63,67	1.62	14 (22%)	77,77,81	1.15	6 (7%)
29	LMG	C	518	-	51,51,55	1.39	6 (11%)	59,59,63	1.29	8 (13%)
29	LMG	C	519	-	51,51,55	1.31	5 (9%)	59,59,63	1.03	3 (5%)
25	PHO	D	401	-	67,69,69	1.27	10 (14%)	86,99,99	1.11	6 (6%)
24	CLA	D	402	-	57,73,73	2.61	23 (40%)	61,113,113	1.95	16 (26%)
24	CLA	D	403	-	57,73,73	2.65	21 (36%)	61,113,113	1.91	16 (26%)
24	CLA	D	404	-	57,73,73	2.55	22 (38%)	61,113,113	2.01	14 (22%)
27	PL9	D	405	-	54,55,55	3.98	17 (31%)	68,69,69	4.22	36 (52%)
30	LHG	D	406	-	48,48,48	1.12	3 (6%)	49,54,54	0.98	4 (8%)
30	LHG	D	407	-	48,48,48	1.09	3 (6%)	49,54,54	0.91	3 (6%)
29	LMG	D	408	-	51,51,55	1.31	5 (9%)	59,59,63	1.10	8 (13%)
32	DGD	E	101	-	63,63,67	1.70	15 (23%)	77,77,81	1.24	10 (12%)
30	LHG	E	102	-	41,41,48	1.20	3 (7%)	42,47,54	1.01	2 (4%)
33	HEM	E	103	5,6	24,50,50	2.36	6 (25%)	16,82,82	1.69	1 (6%)
26	BCR	F	101	-	41,41,41	9.10	26 (63%)	56,56,56	6.17	27 (48%)
26	BCR	H	101	-	41,41,41	9.11	30 (73%)	56,56,56	5.80	30 (53%)
32	DGD	H	102	-	63,63,67	1.65	14 (22%)	77,77,81	1.05	6 (7%)
26	BCR	I	101	-	41,41,41	9.12	28 (68%)	56,56,56	6.05	30 (53%)
26	BCR	K	101	-	41,41,41	9.19	31 (75%)	56,56,56	5.50	29 (51%)
26	BCR	K	102	-	41,41,41	9.21	30 (73%)	56,56,56	5.68	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	L	101	-	48,48,48	1.09	2 (4%)	49,54,54	0.89	2 (4%)
28	SQD	L	102	-	53,54,54	1.43	4 (7%)	62,65,65	1.62	7 (11%)
26	BCR	T	101	-	41,41,41	9.12	29 (70%)	56,56,56	6.20	33 (58%)
33	HEM	V	201	16	24,50,50	2.32	6 (25%)	16,82,82	1.64	1 (6%)
28	SQD	X	101	-	42,43,54	1.70	3 (7%)	51,54,65	1.78	8 (15%)
29	LMG	Z	101	-	37,37,55	1.41	4 (10%)	45,45,63	1.42	5 (11%)
20	OEX	a	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
23	BCT	a	605	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	a	606	-	57,73,73	2.59	22 (38%)	61,113,113	1.94	14 (22%)
24	CLA	a	607	-	57,73,73	2.53	21 (36%)	61,113,113	1.88	13 (21%)
25	PHO	a	608	-	67,69,69	1.20	6 (8%)	86,99,99	1.06	6 (6%)
24	CLA	a	609	-	57,73,73	2.52	22 (38%)	61,113,113	1.93	14 (22%)
26	BCR	a	610	-	41,41,41	9.05	30 (73%)	56,56,56	5.69	24 (42%)
27	PL9	a	611	-	54,55,55	3.95	17 (31%)	68,69,69	4.38	37 (54%)
28	SQD	a	612	-	53,54,54	1.49	3 (5%)	62,65,65	1.79	12 (19%)
29	LMG	a	613	-	51,51,55	1.31	5 (9%)	59,59,63	1.02	5 (8%)
28	SQD	a	614	-	53,54,54	1.50	3 (5%)	62,65,65	1.42	6 (9%)
24	CLA	a	615	-	57,73,73	2.60	22 (38%)	61,113,113	2.08	16 (26%)
30	LHG	a	616	-	48,48,48	1.08	2 (4%)	49,54,54	1.20	3 (6%)
28	SQD	b	601	-	53,54,54	1.49	4 (7%)	62,65,65	1.73	9 (14%)
24	CLA	b	603	-	57,73,73	2.52	19 (33%)	61,113,113	1.94	14 (22%)
24	CLA	b	604	-	57,73,73	2.58	21 (36%)	61,113,113	2.08	11 (18%)
24	CLA	b	605	-	57,73,73	2.58	22 (38%)	61,113,113	2.09	15 (24%)
24	CLA	b	606	-	57,73,73	2.55	20 (35%)	61,113,113	2.00	13 (21%)
24	CLA	b	607	-	57,73,73	2.55	22 (38%)	61,113,113	1.95	12 (19%)
24	CLA	b	608[A]	-	57,73,73	2.50	23 (40%)	61,113,113	2.07	13 (21%)
24	CLA	b	608[B]	-	57,73,73	2.52	23 (40%)	61,113,113	2.07	13 (21%)
24	CLA	b	609	-	57,73,73	2.58	22 (38%)	61,113,113	1.94	13 (21%)
24	CLA	b	610	-	57,73,73	2.50	22 (38%)	61,113,113	1.94	12 (19%)
24	CLA	b	611	-	57,73,73	2.50	21 (36%)	61,113,113	1.97	11 (18%)
24	CLA	b	612	-	57,73,73	2.49	23 (40%)	61,113,113	2.00	15 (24%)
24	CLA	b	613	-	57,73,73	2.55	22 (38%)	61,113,113	2.07	11 (18%)
24	CLA	b	614	-	57,73,73	2.58	23 (40%)	61,113,113	2.15	14 (22%)
24	CLA	b	615	-	57,73,73	2.49	22 (38%)	61,113,113	1.89	10 (16%)
24	CLA	b	616	-	57,73,73	2.51	21 (36%)	61,113,113	1.89	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	617	-	57,73,73	2.54	22 (38%)	61,113,113	1.96	12 (19%)
24	CLA	b	618	-	57,73,73	2.53	20 (35%)	61,113,113	2.01	15 (24%)
26	BCR	b	619	-	41,41,41	9.31	29 (70%)	56,56,56	5.89	28 (50%)
26	BCR	b	620	-	41,41,41	8.95	29 (70%)	56,56,56	5.77	29 (51%)
26	BCR	b	621	-	41,41,41	9.20	31 (75%)	56,56,56	6.46	32 (57%)
29	LMG	b	622	-	51,51,55	1.30	4 (7%)	59,59,63	1.05	5 (8%)
24	CLA	c	501	-	57,73,73	2.46	19 (33%)	61,113,113	1.96	15 (24%)
24	CLA	c	502	-	57,73,73	2.52	23 (40%)	61,113,113	1.93	10 (16%)
24	CLA	c	503	-	57,73,73	2.54	22 (38%)	61,113,113	1.77	11 (18%)
24	CLA	c	504	-	57,73,73	2.59	23 (40%)	61,113,113	1.98	14 (22%)
24	CLA	c	505	-	57,73,73	2.48	21 (36%)	61,113,113	1.90	9 (14%)
24	CLA	c	506	-	57,73,73	2.52	20 (35%)	61,113,113	1.95	11 (18%)
24	CLA	c	507	-	57,73,73	2.44	20 (35%)	61,113,113	2.16	13 (21%)
24	CLA	c	508	-	57,73,73	2.51	21 (36%)	61,113,113	2.00	11 (18%)
24	CLA	c	509	-	57,73,73	2.52	23 (40%)	61,113,113	2.02	12 (19%)
24	CLA	c	510	-	57,73,73	2.49	21 (36%)	61,113,113	1.91	12 (19%)
24	CLA	c	511	3	57,73,73	2.54	21 (36%)	61,113,113	1.88	11 (18%)
24	CLA	c	512	-	57,73,73	2.53	24 (42%)	61,113,113	1.90	13 (21%)
24	CLA	c	513	-	57,73,73	2.47	23 (40%)	61,113,113	1.88	11 (18%)
26	BCR	c	514	-	41,41,41	9.06	30 (73%)	56,56,56	5.96	34 (60%)
26	BCR	c	515	-	41,41,41	9.22	31 (75%)	56,56,56	5.69	27 (48%)
32	DGD	c	516	-	63,63,67	1.66	15 (23%)	77,77,81	1.10	6 (7%)
32	DGD	c	517	-	63,63,67	1.58	15 (23%)	77,77,81	1.14	7 (9%)
32	DGD	c	518	-	63,63,67	1.64	14 (22%)	77,77,81	1.29	8 (10%)
29	LMG	c	519	-	51,51,55	1.36	5 (9%)	59,59,63	1.06	5 (8%)
29	LMG	c	520	-	51,51,55	1.35	5 (9%)	59,59,63	1.13	4 (6%)
26	BCR	c	521	-	41,41,41	9.48	29 (70%)	56,56,56	5.66	25 (44%)
25	PHO	d	401	-	67,69,69	1.27	7 (10%)	86,99,99	1.07	6 (6%)
24	CLA	d	402	-	57,73,73	2.57	22 (38%)	61,113,113	1.92	13 (21%)
24	CLA	d	403	-	57,73,73	2.54	21 (36%)	61,113,113	1.91	13 (21%)
27	PL9	d	404	-	54,55,55	3.95	16 (29%)	68,69,69	4.27	35 (51%)
32	DGD	d	405	-	63,63,67	1.67	15 (23%)	77,77,81	1.16	8 (10%)
30	LHG	d	406	-	48,48,48	1.09	3 (6%)	49,54,54	1.04	3 (6%)
30	LHG	d	407	-	48,48,48	1.13	3 (6%)	49,54,54	1.10	3 (6%)
30	LHG	e	101	-	41,41,48	1.21	3 (7%)	42,47,54	1.08	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	HEM	e	102	5,6	24,50,50	2.24	6 (25%)	16,82,82	1.78	2 (12%)
26	BCR	f	101	-	41,41,41	9.06	29 (70%)	56,56,56	5.72	25 (44%)
26	BCR	h	101	-	41,41,41	9.24	30 (73%)	56,56,56	5.73	33 (58%)
32	DGD	h	102	-	63,63,67	1.64	15 (23%)	77,77,81	1.24	8 (10%)
29	LMG	j	101	34	51,51,55	1.29	5 (9%)	59,59,63	0.87	2 (3%)
26	BCR	k	101	-	41,41,41	9.28	31 (75%)	56,56,56	5.71	27 (48%)
28	SQD	l	101	-	53,54,54	1.44	3 (5%)	62,65,65	1.62	7 (11%)
30	LHG	l	102	-	48,48,48	1.16	2 (4%)	49,54,54	0.94	2 (4%)
26	BCR	t	101	-	41,41,41	9.10	29 (70%)	56,56,56	6.04	34 (60%)
33	HEM	v	201	16	24,50,50	2.35	7 (29%)	16,82,82	1.49	3 (18%)
28	SQD	x	101	-	42,43,54	1.69	3 (7%)	51,54,65	1.78	8 (15%)
29	LMG	z	101	-	37,37,55	1.38	4 (10%)	45,45,63	1.25	3 (6%)

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
20	OEX	A	601	1,3	-	0/0/68/68	0/0/6/6
23	BCT	A	605	21	-	0/0/0/0	0/0/0/0
24	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PHO	A	608	-	-	0/53/103/103	0/1/6/6
24	CLA	A	609	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	A	610	-	-	1/29/63/63	0/2/2/2
27	PL9	A	611	-	-	0/53/73/73	0/1/1/1
28	SQD	A	612	-	-	0/49/69/69	0/1/1/1
29	LMG	A	613	-	-	0/46/66/70	0/1/1/1
28	SQD	A	614	-	-	0/49/69/69	0/1/1/1
30	LHG	A	615	-	-	0/53/53/53	0/0/0/0
24	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607[B]	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	617	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	B	618	-	-	1/29/63/63	0/2/2/2
26	BCR	B	619	-	-	4/29/63/63	0/2/2/2
26	BCR	B	620	-	-	2/29/63/63	0/2/2/2
29	LMG	B	621	-	-	0/46/66/70	0/1/1/1
28	SQD	B	622	-	-	0/49/69/69	0/1/1/1
24	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	1/29/63/63	0/2/2/2
32	DGD	C	515	-	-	0/51/91/95	0/2/2/2
32	DGD	C	516	-	-	0/51/91/95	0/2/2/2
32	DGD	C	517	-	-	0/51/91/95	0/2/2/2
29	LMG	C	518	-	-	0/46/66/70	0/1/1/1
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
25	PHO	D	401	-	-	0/53/103/103	0/1/6/6
24	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
27	PL9	D	405	-	-	0/53/73/73	0/1/1/1
30	LHG	D	406	-	-	0/53/53/53	0/0/0/0
30	LHG	D	407	-	-	0/53/53/53	0/0/0/0
29	LMG	D	408	-	-	0/46/66/70	0/1/1/1
32	DGD	E	101	-	-	0/51/91/95	0/2/2/2
30	LHG	E	102	-	-	0/46/46/53	0/0/0/0
33	HEM	E	103	5,6	-	0/6/54/54	0/0/8/8
26	BCR	F	101	-	-	1/29/63/63	0/2/2/2
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
32	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	I	101	-	-	1/29/63/63	0/2/2/2
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
26	BCR	K	102	-	-	0/29/63/63	0/2/2/2
30	LHG	L	101	-	-	0/53/53/53	0/0/0/0
28	SQD	L	102	-	-	0/49/69/69	0/1/1/1
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
33	HEM	V	201	16	-	0/6/54/54	0/0/8/8
28	SQD	X	101	-	-	0/38/58/69	0/1/1/1
29	LMG	Z	101	-	-	1/31/51/70	0/1/1/1
20	OEX	a	601	1,3	-	0/0/68/68	0/0/6/6
23	BCT	a	605	21	-	0/0/0/0	0/0/0/0
24	CLA	a	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PHO	a	608	-	-	0/53/103/103	0/1/6/6
24	CLA	a	609	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	a	610	-	-	1/29/63/63	0/2/2/2
27	PL9	a	611	-	-	0/53/73/73	0/1/1/1
28	SQD	a	612	-	-	0/49/69/69	0/1/1/1
29	LMG	a	613	-	-	0/46/66/70	0/1/1/1
28	SQD	a	614	-	-	0/49/69/69	0/1/1/1
24	CLA	a	615	-	3/3/20/25	0/37/135/135	0/0/9/9
30	LHG	a	616	-	-	0/53/53/53	0/0/0/0
28	SQD	b	601	-	-	0/49/69/69	0/1/1/1
24	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	618	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	b	619	-	-	1/29/63/63	0/2/2/2
26	BCR	b	620	-	-	3/29/63/63	0/2/2/2
26	BCR	b	621	-	-	1/29/63/63	0/2/2/2
29	LMG	b	622	-	-	0/46/66/70	0/1/1/1
24	CLA	c	501	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	c	514	-	-	1/29/63/63	0/2/2/2
26	BCR	c	515	-	-	1/29/63/63	0/2/2/2
32	DGD	c	516	-	-	0/51/91/95	0/2/2/2
32	DGD	c	517	-	-	0/51/91/95	0/2/2/2
32	DGD	c	518	-	-	0/51/91/95	0/2/2/2
29	LMG	c	519	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMG	c	520	-	-	0/46/66/70	0/1/1/1
26	BCR	c	521	-	-	0/29/63/63	0/2/2/2
25	PHO	d	401	-	-	0/53/103/103	0/1/6/6
24	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
27	PL9	d	404	-	-	0/53/73/73	0/1/1/1
32	DGD	d	405	-	-	0/51/91/95	0/2/2/2
30	LHG	d	406	-	-	0/53/53/53	0/0/0/0
30	LHG	d	407	-	-	0/53/53/53	0/0/0/0
30	LHG	e	101	-	-	0/46/46/53	0/0/0/0
33	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
26	BCR	f	101	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	3/29/63/63	0/2/2/2
32	DGD	h	102	-	-	0/51/91/95	0/2/2/2
29	LMG	j	101	34	-	0/46/66/70	0/1/1/1
26	BCR	k	101	-	-	1/29/63/63	0/2/2/2
28	SQD	l	101	-	-	0/49/69/69	0/1/1/1
30	LHG	l	102	-	-	0/53/53/53	0/0/0/0
26	BCR	t	101	-	-	1/29/63/63	0/2/2/2
33	HEM	v	201	16	-	0/6/54/54	0/0/8/8
28	SQD	x	101	-	-	0/38/58/69	0/1/1/1
29	LMG	z	101	-	-	1/31/51/70	0/1/1/1

All (2600) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	620	BCR	C21-C22	-21.97	1.06	1.35
26	T	101	BCR	C21-C22	-21.78	1.06	1.35
26	H	101	BCR	C21-C22	-21.34	1.06	1.35
26	h	101	BCR	C21-C22	-21.33	1.07	1.35
26	b	619	BCR	C21-C22	-20.94	1.07	1.35
26	c	514	BCR	C21-C22	-20.85	1.07	1.35
26	A	610	BCR	C21-C22	-20.71	1.07	1.35
26	B	620	BCR	C21-C22	-20.69	1.07	1.35
26	k	101	BCR	C21-C22	-20.65	1.07	1.35
26	K	101	BCR	C21-C22	-20.59	1.08	1.35
26	t	101	BCR	C21-C22	-20.45	1.08	1.35
26	I	101	BCR	C21-C22	-20.26	1.08	1.35
26	K	102	BCR	C21-C22	-20.05	1.08	1.35
26	a	610	BCR	C21-C22	-19.95	1.08	1.35
26	B	618	BCR	C21-C22	-19.72	1.09	1.35
26	c	515	BCR	C21-C22	-19.70	1.09	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	f	101	BCR	C21-C22	-19.53	1.09	1.35
26	c	521	BCR	C21-C22	-19.46	1.09	1.35
26	C	514	BCR	C21-C22	-19.16	1.09	1.35
26	B	619	BCR	C21-C22	-19.13	1.09	1.35
26	F	101	BCR	C21-C22	-18.77	1.10	1.35
26	b	621	BCR	C21-C22	-16.22	1.13	1.35
26	K	101	BCR	C19-C18	-12.79	1.17	1.45
26	B	618	BCR	C19-C18	-12.55	1.18	1.45
26	k	101	BCR	C19-C18	-12.09	1.19	1.45
26	a	610	BCR	C19-C18	-12.07	1.19	1.45
26	H	101	BCR	C19-C18	-11.91	1.19	1.45
26	c	515	BCR	C19-C18	-11.86	1.19	1.45
26	K	102	BCR	C19-C18	-11.74	1.19	1.45
26	C	514	BCR	C19-C18	-11.63	1.20	1.45
26	A	610	BCR	C19-C18	-11.55	1.20	1.45
26	b	619	BCR	C19-C18	-11.52	1.20	1.45
26	f	101	BCR	C19-C18	-11.44	1.20	1.45
26	I	101	BCR	C19-C18	-11.41	1.20	1.45
26	c	514	BCR	C19-C18	-11.39	1.20	1.45
26	B	620	BCR	C19-C18	-11.33	1.20	1.45
26	b	620	BCR	C19-C18	-11.30	1.20	1.45
26	B	619	BCR	C19-C18	-11.20	1.21	1.45
26	h	101	BCR	C19-C18	-11.19	1.21	1.45
26	t	101	BCR	C19-C18	-11.13	1.21	1.45
26	c	521	BCR	C19-C18	-11.00	1.21	1.45
26	F	101	BCR	C19-C18	-10.96	1.21	1.45
26	T	101	BCR	C19-C18	-10.95	1.21	1.45
26	b	621	BCR	C19-C18	-9.22	1.25	1.45
28	A	612	SQD	C6-S	-8.77	1.67	1.77
28	a	612	SQD	C6-S	-8.73	1.67	1.77
28	A	614	SQD	C6-S	-8.45	1.67	1.77
28	a	614	SQD	C6-S	-8.44	1.67	1.77
28	X	101	SQD	C6-S	-8.28	1.67	1.77
28	x	101	SQD	C6-S	-8.26	1.67	1.77
28	b	601	SQD	C6-S	-8.04	1.68	1.77
28	B	622	SQD	C6-S	-7.92	1.68	1.77
28	l	101	SQD	C6-S	-7.78	1.68	1.77
28	L	102	SQD	C6-S	-7.72	1.68	1.77
26	K	101	BCR	C34-C9	-7.55	1.36	1.50
24	A	606	CLA	C3A-C2A	-7.54	1.32	1.54
26	B	619	BCR	C34-C9	-7.48	1.37	1.50
24	a	606	CLA	C3A-C2A	-7.45	1.32	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C3A-C2A	-7.33	1.33	1.54
24	D	402	CLA	C3A-C2A	-7.29	1.33	1.54
24	b	614	CLA	C3A-C2A	-7.29	1.33	1.54
24	B	608	CLA	C3A-C2A	-7.29	1.33	1.54
26	b	619	BCR	C34-C9	-7.28	1.37	1.50
24	D	403	CLA	C3A-C2A	-7.27	1.33	1.54
24	b	610	CLA	C3A-C2A	-7.27	1.33	1.54
26	B	618	BCR	C34-C9	-7.26	1.37	1.50
26	b	621	BCR	C34-C9	-7.25	1.37	1.50
24	b	605	CLA	C3A-C2A	-7.24	1.33	1.54
26	I	101	BCR	C34-C9	-7.23	1.37	1.50
24	b	618	CLA	C3A-C2A	-7.22	1.33	1.54
26	C	514	BCR	C34-C9	-7.21	1.37	1.50
24	b	604	CLA	C3A-C2A	-7.21	1.33	1.54
24	B	607[A]	CLA	C3A-C2A	-7.20	1.33	1.54
24	B	607[B]	CLA	C3A-C2A	-7.20	1.33	1.54
24	B	609	CLA	C3A-C2A	-7.20	1.33	1.54
24	D	404	CLA	C3A-C2A	-7.19	1.33	1.54
24	C	510	CLA	C3A-C2A	-7.19	1.33	1.54
24	c	506	CLA	C3A-C2A	-7.18	1.33	1.54
24	b	608[A]	CLA	C3A-C2A	-7.18	1.33	1.54
24	b	608[B]	CLA	C3A-C2A	-7.18	1.33	1.54
24	b	609	CLA	C3A-C2A	-7.16	1.33	1.54
26	c	514	BCR	C34-C9	-7.14	1.37	1.50
24	b	612	CLA	C3A-C2A	-7.14	1.33	1.54
26	F	101	BCR	C34-C9	-7.14	1.37	1.50
24	C	504	CLA	C3A-C2A	-7.13	1.33	1.54
26	b	620	BCR	C34-C9	-7.12	1.37	1.50
24	C	501	CLA	C3A-C2A	-7.12	1.33	1.54
24	B	614	CLA	C3A-C2A	-7.11	1.33	1.54
24	B	615	CLA	C3A-C2A	-7.11	1.33	1.54
24	C	509	CLA	C3A-C2A	-7.09	1.33	1.54
24	a	609	CLA	C3A-C2A	-7.09	1.33	1.54
24	A	609	CLA	C3A-C2A	-7.08	1.33	1.54
24	c	512	CLA	C3A-C2A	-7.07	1.33	1.54
26	c	515	BCR	C34-C9	-7.06	1.37	1.50
24	c	511	CLA	C3A-C2A	-7.05	1.33	1.54
24	b	615	CLA	C3A-C2A	-7.04	1.33	1.54
26	t	101	BCR	C34-C9	-7.03	1.37	1.50
24	B	603	CLA	C3A-C2A	-7.02	1.34	1.54
24	a	615	CLA	C3A-C2A	-7.02	1.34	1.54
24	C	511	CLA	C3A-C2A	-7.02	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C3A-C2A	-7.00	1.34	1.54
24	C	512	CLA	C3A-C2A	-6.99	1.34	1.54
24	C	502	CLA	C3A-C2A	-6.99	1.34	1.54
24	c	509	CLA	C3A-C2A	-6.99	1.34	1.54
24	C	508	CLA	C3A-C2A	-6.98	1.34	1.54
24	b	607	CLA	C3A-C2A	-6.98	1.34	1.54
24	c	502	CLA	C3A-C2A	-6.98	1.34	1.54
24	b	613	CLA	C3A-C2A	-6.98	1.34	1.54
24	d	402	CLA	C3A-C2A	-6.96	1.34	1.54
26	c	521	BCR	C34-C9	-6.96	1.37	1.50
26	B	620	BCR	C34-C9	-6.94	1.38	1.50
24	b	606	CLA	C3A-C2A	-6.94	1.34	1.54
24	c	510	CLA	C3A-C2A	-6.94	1.34	1.54
26	f	101	BCR	C34-C9	-6.93	1.38	1.50
24	d	403	CLA	C3A-C2A	-6.92	1.34	1.54
24	b	617	CLA	C3A-C2A	-6.91	1.34	1.54
24	b	616	CLA	C3A-C2A	-6.91	1.34	1.54
24	B	610	CLA	C3A-C2A	-6.91	1.34	1.54
24	b	611	CLA	C3A-C2A	-6.90	1.34	1.54
24	C	503	CLA	C3A-C2A	-6.89	1.34	1.54
24	A	607	CLA	C3A-C2A	-6.86	1.34	1.54
24	c	508	CLA	C3A-C2A	-6.85	1.34	1.54
24	B	612	CLA	C3A-C2A	-6.85	1.34	1.54
24	C	505	CLA	C3A-C2A	-6.84	1.34	1.54
24	c	505	CLA	C3A-C2A	-6.82	1.34	1.54
24	B	605	CLA	C3A-C2A	-6.82	1.34	1.54
26	H	101	BCR	C34-C9	-6.82	1.38	1.50
26	K	102	BCR	C34-C9	-6.81	1.38	1.50
24	B	617	CLA	C3A-C2A	-6.81	1.34	1.54
24	C	506	CLA	C3A-C2A	-6.79	1.34	1.54
24	c	503	CLA	C3A-C2A	-6.79	1.34	1.54
24	a	607	CLA	C3A-C2A	-6.79	1.34	1.54
26	A	610	BCR	C34-C9	-6.78	1.38	1.50
24	C	507	CLA	C3A-C2A	-6.78	1.34	1.54
26	k	101	BCR	C34-C9	-6.78	1.38	1.50
24	c	501	CLA	C3A-C2A	-6.77	1.34	1.54
26	T	101	BCR	C34-C9	-6.75	1.38	1.50
24	B	616	CLA	C3A-C2A	-6.73	1.34	1.54
24	c	513	CLA	C3A-C2A	-6.73	1.34	1.54
24	B	604	CLA	C3A-C2A	-6.72	1.34	1.54
26	h	101	BCR	C34-C9	-6.71	1.38	1.50
24	B	611	CLA	C3A-C2A	-6.70	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	C3A-C2A	-6.67	1.35	1.54
24	b	603	CLA	C3A-C2A	-6.66	1.35	1.54
24	c	507	CLA	C3A-C2A	-6.65	1.35	1.54
24	B	602	CLA	C3A-C2A	-6.60	1.35	1.54
26	a	610	BCR	C34-C9	-6.56	1.38	1.50
24	C	513	CLA	C3A-C2A	-6.56	1.35	1.54
24	b	603	CLA	CHD-C4C	-5.89	1.27	1.41
24	A	606	CLA	CHD-C4C	-5.61	1.27	1.41
24	D	403	CLA	C3D-C2D	-5.61	1.27	1.40
24	a	606	CLA	CHD-C4C	-5.54	1.27	1.41
24	A	607	CLA	CHD-C4C	-5.49	1.28	1.41
24	B	608	CLA	CHD-C4C	-5.48	1.28	1.41
24	B	606	CLA	C3D-C2D	-5.48	1.28	1.40
24	b	616	CLA	CHD-C4C	-5.46	1.28	1.41
24	C	503	CLA	CHD-C4C	-5.43	1.28	1.41
24	b	614	CLA	C3D-C2D	-5.43	1.28	1.40
24	b	617	CLA	CHD-C4C	-5.43	1.28	1.41
24	b	609	CLA	CHD-C4C	-5.41	1.28	1.41
24	B	615	CLA	C3D-C2D	-5.40	1.28	1.40
24	B	614	CLA	C3D-C2D	-5.40	1.28	1.40
24	C	507	CLA	CHD-C4C	-5.38	1.28	1.41
24	A	609	CLA	CHD-C4C	-5.38	1.28	1.41
24	c	511	CLA	CHD-C4C	-5.37	1.28	1.41
24	d	403	CLA	CHD-C4C	-5.37	1.28	1.41
24	b	607	CLA	CHD-C4C	-5.36	1.28	1.41
24	a	609	CLA	CHD-C4C	-5.36	1.28	1.41
24	C	512	CLA	CHD-C4C	-5.34	1.28	1.41
24	C	503	CLA	C3D-C2D	-5.34	1.28	1.40
24	D	404	CLA	CHD-C4C	-5.30	1.28	1.41
27	D	405	PL9	C3-C4	-5.30	1.40	1.49
24	C	511	CLA	C3D-C2D	-5.30	1.28	1.40
24	a	606	CLA	C3D-C2D	-5.30	1.28	1.40
24	B	616	CLA	CHD-C4C	-5.30	1.28	1.41
24	b	615	CLA	CHD-C4C	-5.28	1.28	1.41
24	b	611	CLA	CHD-C4C	-5.27	1.28	1.41
24	b	613	CLA	CHD-C4C	-5.27	1.28	1.41
24	C	509	CLA	CHD-C4C	-5.27	1.28	1.41
24	B	610	CLA	CHD-C4C	-5.27	1.28	1.41
24	b	609	CLA	C3D-C2D	-5.26	1.28	1.40
24	a	607	CLA	CHD-C4C	-5.26	1.28	1.41
24	b	613	CLA	C3D-C2D	-5.25	1.28	1.40
24	b	606	CLA	C3D-C2D	-5.25	1.28	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	615	CLA	C3D-C2D	-5.24	1.28	1.40
24	a	615	CLA	CHD-C4C	-5.23	1.28	1.41
24	D	402	CLA	C3D-C2D	-5.22	1.28	1.40
24	D	403	CLA	CHD-C4C	-5.19	1.28	1.41
24	c	510	CLA	CHD-C4C	-5.19	1.28	1.41
24	D	403	CLA	C4B-CHC	-5.19	1.26	1.40
24	B	612	CLA	CHD-C4C	-5.19	1.28	1.41
24	B	606	CLA	CHD-C4C	-5.17	1.28	1.41
24	B	614	CLA	CHD-C4C	-5.17	1.28	1.41
24	C	508	CLA	C3D-C2D	-5.15	1.28	1.40
24	B	602	CLA	CHD-C4C	-5.15	1.28	1.41
24	B	605	CLA	CHD-C4C	-5.15	1.28	1.41
24	b	606	CLA	CHD-C4C	-5.15	1.28	1.41
24	c	507	CLA	CHD-C4C	-5.15	1.28	1.41
24	B	607[B]	CLA	CHD-C4C	-5.14	1.28	1.41
24	c	504	CLA	C3D-C2D	-5.14	1.28	1.40
24	c	509	CLA	CHD-C4C	-5.13	1.28	1.41
24	b	605	CLA	CHD-C4C	-5.13	1.28	1.41
24	C	508	CLA	C4D-ND	-5.13	1.25	1.37
24	C	511	CLA	CHD-C4C	-5.12	1.28	1.41
24	C	508	CLA	CHD-C4C	-5.10	1.28	1.41
24	B	607[A]	CLA	CHD-C4C	-5.10	1.28	1.41
24	b	618	CLA	CHD-C4C	-5.08	1.29	1.41
24	b	605	CLA	C3D-C2D	-5.08	1.29	1.40
24	b	614	CLA	CHD-C4C	-5.07	1.29	1.41
24	A	609	CLA	C3D-C2D	-5.07	1.29	1.40
24	a	607	CLA	C3D-C2D	-5.06	1.29	1.40
24	B	608	CLA	C3D-C2D	-5.05	1.29	1.40
24	C	510	CLA	CHD-C4C	-5.05	1.29	1.41
24	C	510	CLA	C3D-C2D	-5.05	1.29	1.40
24	B	617	CLA	CHD-C4C	-5.03	1.29	1.41
24	B	615	CLA	CHD-C4C	-5.03	1.29	1.41
24	b	603	CLA	C3D-C2D	-5.02	1.29	1.40
24	c	503	CLA	CHD-C4C	-5.02	1.29	1.41
24	B	614	CLA	C4B-CHC	-5.01	1.26	1.40
24	c	512	CLA	CHD-C4C	-5.00	1.29	1.41
24	c	510	CLA	C3D-C2D	-4.99	1.29	1.40
24	B	617	CLA	C4B-CHC	-4.99	1.26	1.40
24	C	506	CLA	CHD-C4C	-4.98	1.29	1.41
24	d	402	CLA	CHD-C4C	-4.98	1.29	1.41
24	c	503	CLA	C3D-C2D	-4.98	1.29	1.40
24	b	604	CLA	C3D-C2D	-4.98	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	CHD-C4C	-4.97	1.29	1.41
24	b	608[B]	CLA	C3D-C2D	-4.96	1.29	1.40
24	b	604	CLA	CHD-C4C	-4.96	1.29	1.41
24	a	609	CLA	C3D-C2D	-4.95	1.29	1.40
24	B	603	CLA	CHD-C4C	-4.95	1.29	1.41
24	d	402	CLA	C3D-C2D	-4.95	1.29	1.40
24	c	505	CLA	C3D-C2D	-4.95	1.29	1.40
24	B	611	CLA	CHD-C4C	-4.94	1.29	1.41
24	b	608[A]	CLA	C3D-C2D	-4.94	1.29	1.40
24	B	604	CLA	CHD-C4C	-4.93	1.29	1.41
24	B	604	CLA	C4B-CHC	-4.93	1.26	1.40
24	c	511	CLA	C3D-C2D	-4.92	1.29	1.40
24	C	509	CLA	C3D-C2D	-4.92	1.29	1.40
24	a	615	CLA	C4D-ND	-4.92	1.26	1.37
24	a	615	CLA	C4B-CHC	-4.91	1.26	1.40
24	B	604	CLA	C3D-C2D	-4.91	1.29	1.40
24	b	607	CLA	C3D-C2D	-4.90	1.29	1.40
24	C	510	CLA	C4B-CHC	-4.89	1.27	1.40
24	D	402	CLA	C4D-ND	-4.89	1.26	1.37
24	b	618	CLA	C4B-CHC	-4.89	1.27	1.40
24	b	608[B]	CLA	CHD-C4C	-4.88	1.29	1.41
24	C	506	CLA	C3D-C2D	-4.88	1.29	1.40
24	A	607	CLA	C3D-C2D	-4.87	1.29	1.40
24	b	604	CLA	C4D-ND	-4.87	1.26	1.37
24	c	504	CLA	CHD-C4C	-4.87	1.29	1.41
24	C	512	CLA	C4B-CHC	-4.85	1.27	1.40
24	b	605	CLA	C4B-CHC	-4.85	1.27	1.40
24	b	613	CLA	C4D-ND	-4.84	1.26	1.37
24	C	504	CLA	CHD-C4C	-4.84	1.29	1.41
24	C	513	CLA	CHD-C4C	-4.84	1.29	1.41
24	B	610	CLA	C4D-ND	-4.84	1.26	1.37
24	c	501	CLA	CHD-C4C	-4.83	1.29	1.41
24	b	613	CLA	C4B-CHC	-4.82	1.27	1.40
24	C	502	CLA	CHD-C4C	-4.82	1.29	1.41
24	b	617	CLA	C3D-C2D	-4.82	1.29	1.40
24	B	607[B]	CLA	C3D-C2D	-4.81	1.29	1.40
24	B	613	CLA	C4D-ND	-4.80	1.26	1.37
24	c	508	CLA	CHD-C4C	-4.79	1.29	1.41
24	c	506	CLA	CHD-C4C	-4.79	1.29	1.41
24	b	610	CLA	CHD-C4C	-4.78	1.29	1.41
24	B	606	CLA	C4D-ND	-4.78	1.26	1.37
24	c	502	CLA	CHD-C4C	-4.78	1.29	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	404	CLA	C3D-C2D	-4.77	1.29	1.40
24	b	608[A]	CLA	CHD-C4C	-4.77	1.29	1.41
24	B	604	CLA	C4D-ND	-4.76	1.26	1.37
24	c	508	CLA	C4D-ND	-4.76	1.26	1.37
24	C	501	CLA	CHD-C4C	-4.76	1.29	1.41
24	B	607[A]	CLA	C3D-C2D	-4.76	1.29	1.40
24	b	612	CLA	CHD-C4C	-4.75	1.29	1.41
24	A	609	CLA	C4D-ND	-4.75	1.26	1.37
24	b	616	CLA	C3D-C2D	-4.74	1.29	1.40
24	B	613	CLA	C4B-CHC	-4.74	1.27	1.40
24	b	606	CLA	C4D-ND	-4.74	1.26	1.37
24	B	605	CLA	C4B-CHC	-4.74	1.27	1.40
24	C	508	CLA	C4B-CHC	-4.72	1.27	1.40
24	c	502	CLA	C3D-C2D	-4.72	1.29	1.40
24	a	606	CLA	C4D-ND	-4.71	1.26	1.37
24	D	403	CLA	C4D-ND	-4.71	1.26	1.37
24	B	602	CLA	C3D-C2D	-4.70	1.29	1.40
24	c	513	CLA	CHD-C4C	-4.70	1.29	1.41
24	b	617	CLA	C4C-C3C	-4.70	1.36	1.45
24	B	610	CLA	C3D-C2D	-4.70	1.29	1.40
24	B	612	CLA	C3D-C2D	-4.69	1.29	1.40
24	B	603	CLA	C3D-C2D	-4.69	1.29	1.40
24	B	615	CLA	C4D-ND	-4.69	1.26	1.37
24	c	505	CLA	CHD-C4C	-4.68	1.29	1.41
24	A	606	CLA	C3D-C2D	-4.67	1.29	1.40
24	C	507	CLA	C3D-C2D	-4.67	1.29	1.40
24	a	606	CLA	C4B-CHC	-4.67	1.27	1.40
24	D	403	CLA	C4C-C3C	-4.67	1.36	1.45
24	b	605	CLA	C4D-ND	-4.66	1.26	1.37
24	b	616	CLA	C4D-ND	-4.66	1.26	1.37
24	C	509	CLA	C4B-CHC	-4.64	1.27	1.40
24	D	402	CLA	CHD-C4C	-4.64	1.30	1.41
24	b	603	CLA	C4C-C3C	-4.63	1.36	1.45
24	B	609	CLA	C4B-CHC	-4.63	1.27	1.40
24	d	403	CLA	C4C-C3C	-4.62	1.36	1.45
24	c	504	CLA	C4D-ND	-4.62	1.26	1.37
33	E	103	HEM	C3B-C2B	-4.61	1.34	1.40
24	b	618	CLA	C4D-ND	-4.61	1.26	1.37
24	b	609	CLA	C4D-ND	-4.60	1.26	1.37
24	A	606	CLA	C4D-ND	-4.59	1.26	1.37
24	C	506	CLA	C4D-ND	-4.58	1.26	1.37
24	D	404	CLA	C4B-CHC	-4.58	1.27	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	C4B-CHC	-4.58	1.27	1.40
24	B	612	CLA	C4D-ND	-4.58	1.26	1.37
24	b	614	CLA	C4D-ND	-4.58	1.26	1.37
24	C	510	CLA	C1C-NC	-4.57	1.30	1.37
24	c	506	CLA	C3D-C2D	-4.57	1.30	1.40
33	v	201	HEM	C3C-C2C	-4.56	1.34	1.40
24	B	613	CLA	C3D-C2D	-4.56	1.30	1.40
24	C	510	CLA	C4D-ND	-4.55	1.26	1.37
24	b	615	CLA	C3D-C2D	-4.55	1.30	1.40
24	B	608	CLA	C4D-ND	-4.55	1.26	1.37
24	c	504	CLA	C4B-CHC	-4.55	1.27	1.40
24	A	607	CLA	C4B-CHC	-4.54	1.27	1.40
24	b	614	CLA	C4B-CHC	-4.54	1.27	1.40
24	c	508	CLA	C3D-C2D	-4.54	1.30	1.40
24	C	509	CLA	C4D-ND	-4.53	1.26	1.37
24	A	606	CLA	C4B-CHC	-4.52	1.28	1.40
24	b	606	CLA	C4B-CHC	-4.51	1.28	1.40
24	b	607	CLA	C4C-C3C	-4.50	1.36	1.45
24	c	512	CLA	C4B-CHC	-4.50	1.28	1.40
24	B	605	CLA	C3D-C2D	-4.50	1.30	1.40
24	c	505	CLA	C4B-CHC	-4.50	1.28	1.40
24	A	609	CLA	C4C-C3C	-4.49	1.36	1.45
24	c	512	CLA	C3D-C2D	-4.49	1.30	1.40
24	b	618	CLA	C3D-C2D	-4.49	1.30	1.40
24	a	607	CLA	C4D-ND	-4.49	1.27	1.37
24	b	607	CLA	C4D-ND	-4.49	1.27	1.37
24	c	501	CLA	C3D-C2D	-4.49	1.30	1.40
24	B	614	CLA	C4C-C3C	-4.49	1.36	1.45
24	C	504	CLA	C4B-CHC	-4.48	1.28	1.40
24	d	403	CLA	C4B-CHC	-4.48	1.28	1.40
27	a	611	PL9	C3-C4	-4.47	1.41	1.49
24	b	603	CLA	C4B-CHC	-4.46	1.28	1.40
27	d	404	PL9	C3-C4	-4.46	1.41	1.49
24	C	505	CLA	C4B-CHC	-4.46	1.28	1.40
24	B	603	CLA	C4D-ND	-4.45	1.27	1.37
24	A	607	CLA	C1C-NC	-4.44	1.30	1.37
24	C	511	CLA	C4D-ND	-4.44	1.27	1.37
24	b	607	CLA	C4B-CHC	-4.44	1.28	1.40
24	a	615	CLA	C1C-NC	-4.44	1.30	1.37
24	B	611	CLA	C3D-C2D	-4.43	1.30	1.40
24	b	615	CLA	C4B-CHC	-4.43	1.28	1.40
24	b	616	CLA	C4C-C3C	-4.42	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C4B-CHC	-4.42	1.28	1.40
24	b	610	CLA	C4B-CHC	-4.42	1.28	1.40
24	C	502	CLA	C4B-CHC	-4.42	1.28	1.40
24	d	402	CLA	C4B-CHC	-4.41	1.28	1.40
24	b	617	CLA	C4B-CHC	-4.41	1.28	1.40
24	b	610	CLA	C3D-C2D	-4.41	1.30	1.40
24	c	506	CLA	C4B-CHC	-4.41	1.28	1.40
24	b	615	CLA	C4C-C3C	-4.40	1.37	1.45
24	A	609	CLA	C1C-NC	-4.40	1.30	1.37
24	B	609	CLA	C3D-C2D	-4.39	1.30	1.40
24	d	402	CLA	C4D-ND	-4.39	1.27	1.37
24	C	501	CLA	C4D-ND	-4.39	1.27	1.37
24	C	503	CLA	C4D-ND	-4.39	1.27	1.37
24	c	509	CLA	C4B-CHC	-4.39	1.28	1.40
24	B	605	CLA	C4D-ND	-4.39	1.27	1.37
24	b	612	CLA	C4B-CHC	-4.38	1.28	1.40
24	c	510	CLA	C4B-CHC	-4.38	1.28	1.40
24	B	608	CLA	C4B-CHC	-4.38	1.28	1.40
24	B	607[B]	CLA	C4D-ND	-4.38	1.27	1.37
24	d	403	CLA	C3D-C2D	-4.38	1.30	1.40
24	b	611	CLA	C3D-C2D	-4.38	1.30	1.40
24	c	502	CLA	C4D-ND	-4.38	1.27	1.37
24	c	502	CLA	C4B-CHC	-4.37	1.28	1.40
24	b	603	CLA	C1C-NC	-4.37	1.31	1.37
24	c	505	CLA	C4D-ND	-4.37	1.27	1.37
24	B	610	CLA	C4B-CHC	-4.36	1.28	1.40
24	c	503	CLA	C4D-ND	-4.36	1.27	1.37
33	E	103	HEM	C3C-C2C	-4.36	1.34	1.40
24	C	507	CLA	C4B-CHC	-4.36	1.28	1.40
24	C	504	CLA	C4D-ND	-4.36	1.27	1.37
24	B	607[B]	CLA	C4B-CHC	-4.36	1.28	1.40
24	C	511	CLA	C4B-CHC	-4.36	1.28	1.40
24	C	505	CLA	C3D-C2D	-4.36	1.30	1.40
24	B	611	CLA	C4D-ND	-4.35	1.27	1.37
24	b	609	CLA	C4C-C3C	-4.35	1.37	1.45
24	D	402	CLA	C4B-CHC	-4.34	1.28	1.40
24	b	608[B]	CLA	C4D-ND	-4.34	1.27	1.37
24	c	509	CLA	C3D-C2D	-4.34	1.30	1.40
27	A	611	PL9	C3-C4	-4.32	1.42	1.49
24	B	606	CLA	C4B-CHC	-4.32	1.28	1.40
24	c	511	CLA	C1C-NC	-4.32	1.31	1.37
24	C	513	CLA	C3D-C2D	-4.31	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	506	CLA	C4D-ND	-4.31	1.27	1.37
24	C	504	CLA	C4C-C3C	-4.31	1.37	1.45
24	C	502	CLA	C3D-C2D	-4.31	1.30	1.40
24	D	402	CLA	CMA-C3A	-4.30	1.43	1.53
24	C	512	CLA	C4C-C3C	-4.30	1.37	1.45
24	b	611	CLA	C4D-ND	-4.30	1.27	1.37
24	b	603	CLA	C4D-ND	-4.29	1.27	1.37
24	C	513	CLA	C4D-ND	-4.29	1.27	1.37
24	d	403	CLA	C1C-NC	-4.28	1.31	1.37
24	B	607[A]	CLA	C4D-ND	-4.28	1.27	1.37
24	B	612	CLA	C4B-CHC	-4.28	1.28	1.40
24	C	505	CLA	CHD-C4C	-4.28	1.30	1.41
24	b	608[B]	CLA	C4B-CHC	-4.28	1.28	1.40
24	b	612	CLA	C3D-C2D	-4.28	1.30	1.40
24	b	616	CLA	C4B-CHC	-4.28	1.28	1.40
24	a	609	CLA	C4D-ND	-4.27	1.27	1.37
24	c	508	CLA	C4B-CHC	-4.27	1.28	1.40
24	b	609	CLA	C4B-CHC	-4.27	1.28	1.40
24	B	602	CLA	C4B-CHC	-4.26	1.28	1.40
24	B	615	CLA	C4B-CHC	-4.26	1.28	1.40
24	c	513	CLA	C4B-CHC	-4.26	1.28	1.40
24	C	503	CLA	C4C-C3C	-4.26	1.37	1.45
24	b	609	CLA	C1C-NC	-4.25	1.31	1.37
24	b	610	CLA	C4D-ND	-4.25	1.27	1.37
24	b	617	CLA	C4D-ND	-4.25	1.27	1.37
24	b	608[A]	CLA	C4D-ND	-4.25	1.27	1.37
24	C	505	CLA	C4D-ND	-4.25	1.27	1.37
24	B	609	CLA	CHD-C4C	-4.25	1.31	1.41
24	B	607[A]	CLA	C4B-CHC	-4.24	1.28	1.40
33	V	201	HEM	C3B-C2B	-4.23	1.35	1.40
24	c	511	CLA	C4C-C3C	-4.23	1.37	1.45
24	b	616	CLA	C1A-CHA	-4.23	1.25	1.43
24	b	612	CLA	C4D-ND	-4.23	1.27	1.37
24	B	616	CLA	C3D-C2D	-4.22	1.30	1.40
24	B	608	CLA	C4C-C3C	-4.22	1.37	1.45
24	a	607	CLA	C4B-CHC	-4.22	1.28	1.40
24	C	504	CLA	C1C-NC	-4.22	1.31	1.37
24	C	503	CLA	C4B-CHC	-4.21	1.28	1.40
24	C	504	CLA	C3D-C2D	-4.21	1.30	1.40
24	c	507	CLA	C3D-C2D	-4.21	1.30	1.40
24	d	402	CLA	C1C-NC	-4.20	1.31	1.37
24	A	606	CLA	C4C-C3C	-4.19	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C4D-ND	-4.18	1.27	1.37
24	B	613	CLA	C1A-CHA	-4.18	1.25	1.43
24	c	511	CLA	C4B-CHC	-4.18	1.28	1.40
24	B	616	CLA	C4C-C3C	-4.16	1.37	1.45
24	b	604	CLA	C1C-NC	-4.15	1.31	1.37
24	b	608[A]	CLA	C4B-CHC	-4.15	1.29	1.40
24	C	501	CLA	C3D-C2D	-4.14	1.31	1.40
24	c	509	CLA	C4C-C3C	-4.14	1.37	1.45
24	a	607	CLA	C1C-NC	-4.14	1.31	1.37
24	B	606	CLA	C4C-C3C	-4.13	1.37	1.45
24	c	513	CLA	C3D-C2D	-4.13	1.31	1.40
24	D	404	CLA	C4D-ND	-4.11	1.28	1.37
24	b	611	CLA	C4B-CHC	-4.11	1.29	1.40
24	B	617	CLA	C4D-ND	-4.11	1.28	1.37
24	b	618	CLA	C4C-C3C	-4.11	1.37	1.45
24	B	611	CLA	C4B-CHC	-4.11	1.29	1.40
24	b	616	CLA	C1C-NC	-4.10	1.31	1.37
24	c	501	CLA	C4B-CHC	-4.10	1.29	1.40
24	b	604	CLA	C4B-CHC	-4.10	1.29	1.40
24	C	512	CLA	C3D-C2D	-4.10	1.31	1.40
24	B	603	CLA	C4B-CHC	-4.10	1.29	1.40
24	c	513	CLA	C4C-C3C	-4.09	1.37	1.45
24	A	609	CLA	C4B-CHC	-4.09	1.29	1.40
24	c	512	CLA	C4D-ND	-4.09	1.28	1.37
33	e	102	HEM	C3B-C2B	-4.09	1.35	1.40
24	C	513	CLA	C4B-CHC	-4.08	1.29	1.40
24	B	614	CLA	C4D-ND	-4.08	1.28	1.37
24	B	605	CLA	C1C-NC	-4.08	1.31	1.37
24	A	607	CLA	C4D-ND	-4.07	1.28	1.37
24	D	403	CLA	CMA-C3A	-4.07	1.43	1.53
24	B	609	CLA	C4D-ND	-4.07	1.28	1.37
24	B	608	CLA	CAA-C2A	-4.07	1.46	1.54
24	C	504	CLA	CMA-C3A	-4.07	1.43	1.53
24	c	509	CLA	C4D-ND	-4.06	1.28	1.37
24	b	607	CLA	C1C-NC	-4.06	1.31	1.37
24	B	616	CLA	C4B-CHC	-4.05	1.29	1.40
24	d	402	CLA	CHB-C4A	-4.04	1.28	1.33
24	B	612	CLA	C1C-NC	-4.04	1.31	1.37
24	c	503	CLA	C4B-CHC	-4.04	1.29	1.40
24	c	501	CLA	C4D-ND	-4.04	1.28	1.37
24	b	605	CLA	CMA-C3A	-4.04	1.44	1.53
24	C	509	CLA	C1C-NC	-4.03	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	609	CLA	C4B-CHC	-4.03	1.29	1.40
24	C	501	CLA	C1A-CHA	-4.02	1.26	1.43
24	B	607[B]	CLA	CMA-C3A	-4.02	1.44	1.53
24	c	510	CLA	C4D-ND	-4.02	1.28	1.37
24	B	613	CLA	C1C-NC	-4.01	1.31	1.37
24	C	513	CLA	C4C-C3C	-4.01	1.37	1.45
24	B	614	CLA	CMA-C3A	-4.01	1.44	1.53
24	B	607[B]	CLA	C4C-C3C	-4.00	1.37	1.45
33	e	102	HEM	C3C-C2C	-4.00	1.35	1.40
24	C	501	CLA	C4B-CHC	-4.00	1.29	1.40
24	B	608	CLA	CMA-C3A	-3.99	1.44	1.53
24	B	612	CLA	C1A-CHA	-3.99	1.26	1.43
24	B	607[A]	CLA	CMA-C3A	-3.99	1.44	1.53
24	b	614	CLA	CMA-C3A	-3.98	1.44	1.53
24	B	614	CLA	C1C-NC	-3.98	1.31	1.37
24	D	404	CLA	CMA-C3A	-3.98	1.44	1.53
24	C	507	CLA	C4D-ND	-3.98	1.28	1.37
24	B	602	CLA	C4C-C3C	-3.98	1.37	1.45
24	B	613	CLA	CMA-C3A	-3.98	1.44	1.53
24	C	502	CLA	C4C-C3C	-3.97	1.37	1.45
24	B	617	CLA	C1C-NC	-3.97	1.31	1.37
24	C	507	CLA	C1C-NC	-3.97	1.31	1.37
24	b	617	CLA	C1C-NC	-3.97	1.31	1.37
24	c	509	CLA	CMA-C3A	-3.97	1.44	1.53
24	D	403	CLA	C1C-NC	-3.97	1.31	1.37
24	A	606	CLA	CMA-C3A	-3.97	1.44	1.53
24	c	513	CLA	C4D-ND	-3.97	1.28	1.37
24	C	506	CLA	C1C-NC	-3.96	1.31	1.37
24	C	502	CLA	C1C-NC	-3.95	1.31	1.37
24	c	503	CLA	C4C-C3C	-3.95	1.37	1.45
24	b	615	CLA	C4D-ND	-3.95	1.28	1.37
24	B	607[A]	CLA	C4C-C3C	-3.95	1.37	1.45
24	b	611	CLA	C4C-C3C	-3.94	1.37	1.45
24	b	613	CLA	C1C-NC	-3.94	1.31	1.37
24	B	605	CLA	CMA-C3A	-3.93	1.44	1.53
24	C	501	CLA	CMA-C3A	-3.93	1.44	1.53
24	A	606	CLA	C1A-CHA	-3.93	1.26	1.43
24	B	611	CLA	CMA-C3A	-3.93	1.44	1.53
24	b	614	CLA	C1A-CHA	-3.92	1.26	1.43
24	B	617	CLA	C3D-C2D	-3.92	1.31	1.40
24	A	609	CLA	C1A-CHA	-3.92	1.26	1.43
24	a	615	CLA	C4C-C3C	-3.92	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C4D-ND	-3.92	1.28	1.37
24	C	511	CLA	CMA-C3A	-3.92	1.44	1.53
24	c	507	CLA	C1C-NC	-3.92	1.31	1.37
24	B	602	CLA	C4D-ND	-3.91	1.28	1.37
24	c	502	CLA	CMA-C3A	-3.91	1.44	1.53
24	c	512	CLA	C4C-C3C	-3.91	1.37	1.45
24	B	617	CLA	C4C-C3C	-3.91	1.37	1.45
24	c	504	CLA	CMA-C3A	-3.91	1.44	1.53
32	c	517	DGD	O2G-C2G	-3.91	1.36	1.46
24	d	402	CLA	CMA-C3A	-3.90	1.44	1.53
32	c	518	DGD	O2G-C2G	-3.90	1.36	1.46
24	C	510	CLA	CMA-C3A	-3.90	1.44	1.53
27	D	405	PL9	C6-C1	-3.90	1.41	1.48
24	b	608[A]	CLA	CMA-C3A	-3.90	1.44	1.53
24	a	609	CLA	C1C-NC	-3.90	1.31	1.37
24	c	511	CLA	CMA-C3A	-3.89	1.44	1.53
24	b	609	CLA	CMA-C3A	-3.89	1.44	1.53
24	B	605	CLA	C4C-C3C	-3.89	1.38	1.45
24	D	402	CLA	C1A-CHA	-3.89	1.26	1.43
24	B	610	CLA	C1A-CHA	-3.89	1.26	1.43
24	d	402	CLA	C4C-C3C	-3.89	1.38	1.45
24	b	608[B]	CLA	CMA-C3A	-3.89	1.44	1.53
24	A	609	CLA	CMA-C3A	-3.88	1.44	1.53
24	C	508	CLA	C4C-C3C	-3.88	1.38	1.45
24	a	615	CLA	C1A-CHA	-3.88	1.27	1.43
24	a	615	CLA	CMA-C3A	-3.88	1.44	1.53
24	C	502	CLA	CMA-C3A	-3.88	1.44	1.53
24	a	606	CLA	C4C-C3C	-3.88	1.38	1.45
24	c	507	CLA	C4D-ND	-3.88	1.28	1.37
24	B	602	CLA	C1C-NC	-3.88	1.31	1.37
24	c	506	CLA	CMA-C3A	-3.88	1.44	1.53
24	c	511	CLA	C4D-ND	-3.88	1.28	1.37
24	B	612	CLA	C4C-C3C	-3.87	1.38	1.45
24	B	604	CLA	C1C-NC	-3.87	1.31	1.37
24	b	615	CLA	C1C-NC	-3.87	1.31	1.37
24	B	608	CLA	C1C-NC	-3.86	1.31	1.37
24	B	611	CLA	C1C-NC	-3.86	1.31	1.37
24	B	615	CLA	C4C-C3C	-3.85	1.38	1.45
24	C	508	CLA	C1A-CHA	-3.85	1.27	1.43
24	b	607	CLA	CMA-C3A	-3.85	1.44	1.53
24	b	609	CLA	C1A-CHA	-3.84	1.27	1.43
24	C	510	CLA	C4C-C3C	-3.84	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C4C-C3C	-3.84	1.38	1.45
24	B	615	CLA	C1C-NC	-3.84	1.31	1.37
32	c	516	DGD	O2G-C2G	-3.84	1.36	1.46
24	b	604	CLA	C4C-C3C	-3.83	1.38	1.45
24	c	512	CLA	C1C-NC	-3.83	1.31	1.37
24	b	605	CLA	C4C-C3C	-3.83	1.38	1.45
33	V	201	HEM	C3C-C2C	-3.83	1.35	1.40
24	C	511	CLA	C4C-C3C	-3.82	1.38	1.45
24	b	610	CLA	CMA-C3A	-3.82	1.44	1.53
24	b	613	CLA	C4C-C3C	-3.82	1.38	1.45
24	D	403	CLA	CBD-CGD	-3.82	1.39	1.52
24	d	403	CLA	C4D-ND	-3.81	1.28	1.37
24	a	609	CLA	C4C-C3C	-3.81	1.38	1.45
24	a	609	CLA	CMA-C3A	-3.81	1.44	1.53
24	B	609	CLA	CMA-C3A	-3.81	1.44	1.53
24	c	509	CLA	C1C-NC	-3.81	1.31	1.37
32	C	517	DGD	O2G-C2G	-3.81	1.36	1.46
24	B	608	CLA	C1A-CHA	-3.80	1.27	1.43
24	c	508	CLA	C1C-NC	-3.80	1.31	1.37
24	b	604	CLA	CMA-C3A	-3.79	1.44	1.53
32	H	102	DGD	O2G-C2G	-3.79	1.36	1.46
24	C	509	CLA	C4C-C3C	-3.79	1.38	1.45
24	C	504	CLA	C1A-CHA	-3.79	1.27	1.43
24	B	612	CLA	CMA-C3A	-3.79	1.44	1.53
24	D	402	CLA	C1C-NC	-3.79	1.31	1.37
24	B	610	CLA	CMA-C3A	-3.78	1.44	1.53
24	b	611	CLA	C1C-NC	-3.78	1.31	1.37
24	c	502	CLA	C1C-NC	-3.78	1.31	1.37
24	A	606	CLA	C1C-NC	-3.78	1.31	1.37
24	a	606	CLA	CMA-C3A	-3.78	1.44	1.53
24	c	510	CLA	C4C-C3C	-3.77	1.38	1.45
24	C	512	CLA	C1C-NC	-3.77	1.31	1.37
27	d	404	PL9	C6-C1	-3.76	1.41	1.48
24	C	512	CLA	C4D-ND	-3.76	1.28	1.37
24	b	606	CLA	CMA-C3A	-3.75	1.44	1.53
24	b	605	CLA	C1C-NC	-3.75	1.31	1.37
24	c	507	CLA	C4C-C3C	-3.75	1.38	1.45
24	C	508	CLA	C1C-NC	-3.75	1.31	1.37
24	b	606	CLA	C1C-NC	-3.75	1.31	1.37
24	b	613	CLA	CMA-C3A	-3.75	1.44	1.53
24	D	402	CLA	CHB-C4A	-3.75	1.28	1.33
24	B	615	CLA	CMA-C3A	-3.75	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	CMA-C3A	-3.74	1.44	1.53
24	D	404	CLA	C1C-NC	-3.74	1.31	1.37
24	b	611	CLA	CMA-C3A	-3.74	1.44	1.53
24	B	607[B]	CLA	C1C-NC	-3.74	1.32	1.37
24	b	610	CLA	C1C-NC	-3.74	1.32	1.37
24	C	505	CLA	CMA-C3A	-3.73	1.44	1.53
24	C	509	CLA	CMA-C3A	-3.73	1.44	1.53
24	b	615	CLA	CMA-C3A	-3.73	1.44	1.53
24	B	610	CLA	C1C-NC	-3.73	1.32	1.37
24	B	607[A]	CLA	C1C-NC	-3.72	1.32	1.37
24	b	612	CLA	C1C-NC	-3.72	1.32	1.37
24	c	512	CLA	CMA-C3A	-3.72	1.44	1.53
24	A	607	CLA	C1A-CHA	-3.72	1.27	1.43
24	c	510	CLA	CAA-C2A	-3.71	1.46	1.54
24	b	604	CLA	C1A-CHA	-3.71	1.27	1.43
24	c	508	CLA	C4C-C3C	-3.71	1.38	1.45
24	d	403	CLA	CMA-C3A	-3.71	1.44	1.53
24	b	616	CLA	CMA-C3A	-3.71	1.44	1.53
24	b	617	CLA	CMA-C3A	-3.71	1.44	1.53
24	b	604	CLA	CAA-C2A	-3.71	1.46	1.54
24	C	508	CLA	CMA-C3A	-3.69	1.44	1.53
24	c	510	CLA	CMA-C3A	-3.69	1.44	1.53
24	B	606	CLA	CMA-C3A	-3.69	1.44	1.53
24	c	501	CLA	CMA-C3A	-3.68	1.44	1.53
24	a	606	CLA	C1C-NC	-3.68	1.32	1.37
24	C	503	CLA	C1C-NC	-3.68	1.32	1.37
24	c	506	CLA	C1C-NC	-3.68	1.32	1.37
24	c	505	CLA	CMA-C3A	-3.68	1.44	1.53
32	C	516	DGD	O2G-C2G	-3.67	1.36	1.46
24	C	513	CLA	C1C-NC	-3.67	1.32	1.37
24	B	606	CLA	C1C-NC	-3.67	1.32	1.37
24	c	502	CLA	C4C-C3C	-3.67	1.38	1.45
24	c	508	CLA	CMA-C3A	-3.67	1.44	1.53
24	B	614	CLA	C1A-CHA	-3.67	1.27	1.43
24	b	612	CLA	C1A-CHA	-3.67	1.27	1.43
24	b	614	CLA	CAA-C2A	-3.66	1.47	1.54
24	C	513	CLA	C1A-CHA	-3.66	1.27	1.43
24	B	605	CLA	C1A-CHA	-3.66	1.27	1.43
26	B	618	BCR	C1-C6	-3.65	1.48	1.53
24	b	608[B]	CLA	C1A-CHA	-3.65	1.28	1.43
24	d	402	CLA	C1A-CHA	-3.65	1.28	1.43
24	c	503	CLA	CMA-C3A	-3.64	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C4C-C3C	-3.64	1.38	1.45
24	C	506	CLA	C4C-C3C	-3.64	1.38	1.45
24	a	606	CLA	C1A-CHA	-3.64	1.28	1.43
24	A	607	CLA	C4C-C3C	-3.63	1.38	1.45
24	b	618	CLA	CAA-C2A	-3.63	1.47	1.54
32	h	102	DGD	O2G-C2G	-3.63	1.36	1.46
24	B	604	CLA	C1A-CHA	-3.63	1.28	1.43
24	b	606	CLA	C4C-C3C	-3.63	1.38	1.45
24	c	504	CLA	C1C-NC	-3.62	1.32	1.37
24	b	618	CLA	C1C-NC	-3.62	1.32	1.37
24	C	510	CLA	C1A-CHA	-3.62	1.28	1.43
24	b	608[B]	CLA	C4C-C3C	-3.62	1.38	1.45
24	c	505	CLA	C1C-NC	-3.61	1.32	1.37
27	A	611	PL9	C6-C1	-3.61	1.42	1.48
24	C	507	CLA	C4C-C3C	-3.60	1.38	1.45
24	b	608[A]	CLA	C1A-CHA	-3.60	1.28	1.43
24	c	512	CLA	C1A-CHA	-3.59	1.28	1.43
24	B	603	CLA	CMA-C3A	-3.59	1.45	1.53
24	B	603	CLA	C1A-CHA	-3.59	1.28	1.43
24	a	607	CLA	C4C-C3C	-3.59	1.38	1.45
24	B	613	CLA	CAA-C2A	-3.59	1.47	1.54
24	b	614	CLA	C1C-NC	-3.59	1.32	1.37
24	C	505	CLA	CAA-C2A	-3.59	1.47	1.54
24	B	602	CLA	CMA-C3A	-3.59	1.45	1.53
24	D	404	CLA	C1A-CHA	-3.58	1.28	1.43
24	D	404	CLA	C4C-C3C	-3.58	1.38	1.45
24	c	507	CLA	CMA-C3A	-3.58	1.45	1.53
24	d	403	CLA	C1A-CHA	-3.58	1.28	1.43
24	b	615	CLA	CAA-C2A	-3.58	1.47	1.54
24	b	618	CLA	C1A-CHA	-3.58	1.28	1.43
24	B	603	CLA	C1C-NC	-3.57	1.32	1.37
24	a	607	CLA	CMA-C3A	-3.57	1.45	1.53
24	c	513	CLA	CMA-C3A	-3.57	1.45	1.53
24	c	513	CLA	C1C-NC	-3.57	1.32	1.37
24	b	613	CLA	C1A-CHA	-3.57	1.28	1.43
24	B	607[A]	CLA	C1A-CHA	-3.57	1.28	1.43
24	b	610	CLA	C4C-C3C	-3.56	1.38	1.45
24	B	604	CLA	C4C-C3C	-3.56	1.38	1.45
24	B	607[B]	CLA	C1A-CHA	-3.56	1.28	1.43
24	b	618	CLA	CMA-C3A	-3.56	1.45	1.53
24	C	511	CLA	C1A-CHA	-3.54	1.28	1.43
24	c	504	CLA	C1A-CHA	-3.54	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C1C-NC	-3.53	1.32	1.37
24	b	610	CLA	C1A-CHA	-3.53	1.28	1.43
24	D	403	CLA	C1A-CHA	-3.53	1.28	1.43
24	a	607	CLA	C1A-CHA	-3.52	1.28	1.43
27	a	611	PL9	C6-C1	-3.51	1.42	1.48
24	B	610	CLA	C4C-C3C	-3.51	1.38	1.45
32	C	515	DGD	O2G-C2G	-3.51	1.37	1.46
24	B	609	CLA	C1C-NC	-3.51	1.32	1.37
24	b	609	CLA	CAA-C2A	-3.51	1.47	1.54
24	A	606	CLA	CAA-C2A	-3.51	1.47	1.54
24	C	506	CLA	CHB-C4A	-3.50	1.28	1.33
24	B	616	CLA	C1A-CHA	-3.50	1.28	1.43
24	c	501	CLA	C1C-NC	-3.50	1.32	1.37
24	b	614	CLA	C4C-C3C	-3.50	1.38	1.45
24	b	608[A]	CLA	C4C-C3C	-3.50	1.38	1.45
24	b	611	CLA	CAA-C2A	-3.50	1.47	1.54
24	C	507	CLA	CMA-C3A	-3.49	1.45	1.53
24	D	402	CLA	CBD-CGD	-3.49	1.40	1.52
33	v	201	HEM	C3B-C2B	-3.48	1.35	1.40
24	C	511	CLA	C1C-NC	-3.48	1.32	1.37
24	B	614	CLA	CAA-C2A	-3.47	1.47	1.54
24	b	606	CLA	C1A-CHA	-3.47	1.28	1.43
24	C	503	CLA	CMA-C3A	-3.47	1.45	1.53
24	a	615	CLA	CAA-C2A	-3.47	1.47	1.54
24	c	505	CLA	C4C-C3C	-3.47	1.38	1.45
24	c	508	CLA	C1A-CHA	-3.46	1.28	1.43
24	C	513	CLA	CMA-C3A	-3.46	1.45	1.53
24	A	607	CLA	CMA-C3A	-3.46	1.45	1.53
24	b	613	CLA	CBD-CGD	-3.45	1.40	1.52
24	C	502	CLA	C1A-CHA	-3.45	1.28	1.43
24	b	603	CLA	CMA-C3A	-3.44	1.45	1.53
24	b	610	CLA	CAA-C2A	-3.44	1.47	1.54
24	b	608[B]	CLA	C1C-NC	-3.44	1.32	1.37
24	A	609	CLA	CBD-CGD	-3.44	1.40	1.52
24	c	503	CLA	C1C-NC	-3.44	1.32	1.37
24	c	509	CLA	C1A-CHA	-3.43	1.28	1.43
24	C	506	CLA	CMA-C3A	-3.43	1.45	1.53
24	B	609	CLA	C1A-CHA	-3.43	1.28	1.43
24	b	607	CLA	C1A-CHA	-3.42	1.28	1.43
24	c	508	CLA	CAA-C2A	-3.42	1.47	1.54
24	C	512	CLA	CMA-C3A	-3.42	1.45	1.53
24	B	615	CLA	C1A-CHA	-3.41	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	CMA-C3A	-3.41	1.45	1.53
24	b	604	CLA	CHB-C4A	-3.41	1.29	1.33
24	c	507	CLA	C1A-CHA	-3.41	1.29	1.43
24	C	505	CLA	C1C-NC	-3.40	1.32	1.37
24	b	615	CLA	C1A-CHA	-3.39	1.29	1.43
24	a	606	CLA	CAA-C2A	-3.39	1.47	1.54
26	B	620	BCR	C1-C6	-3.39	1.49	1.53
24	B	617	CLA	C1A-CHA	-3.39	1.29	1.43
24	B	607[B]	CLA	CAA-C2A	-3.39	1.47	1.54
24	c	510	CLA	C1C-NC	-3.38	1.32	1.37
24	b	607	CLA	CAA-C2A	-3.38	1.47	1.54
24	D	402	CLA	C4C-C3C	-3.38	1.38	1.45
24	c	503	CLA	C1A-CHA	-3.37	1.29	1.43
24	B	610	CLA	CAA-C2A	-3.37	1.47	1.54
32	d	405	DGD	O2G-C2G	-3.37	1.37	1.46
24	A	607	CLA	CAA-C2A	-3.37	1.47	1.54
24	C	503	CLA	C1A-CHA	-3.37	1.29	1.43
24	c	511	CLA	C1A-CHA	-3.37	1.29	1.43
26	a	610	BCR	C35-C13	-3.36	1.44	1.50
24	C	501	CLA	C1C-NC	-3.36	1.32	1.37
24	c	502	CLA	C1A-CHA	-3.36	1.29	1.43
24	C	510	CLA	CAA-C2A	-3.36	1.47	1.54
24	c	501	CLA	C4C-C3C	-3.36	1.38	1.45
24	c	501	CLA	C1A-CHA	-3.35	1.29	1.43
24	B	611	CLA	CHB-C4A	-3.35	1.29	1.33
24	c	505	CLA	C1A-CHA	-3.35	1.29	1.43
32	c	518	DGD	C3D-C2D	-3.33	1.43	1.52
24	b	608[A]	CLA	C1C-NC	-3.33	1.32	1.37
24	c	506	CLA	C4C-C3C	-3.33	1.39	1.45
24	B	617	CLA	CAA-C2A	-3.33	1.47	1.54
24	c	513	CLA	C1A-CHA	-3.32	1.29	1.43
32	c	516	DGD	C3D-C2D	-3.32	1.43	1.52
24	c	503	CLA	CBD-CGD	-3.32	1.40	1.52
24	C	512	CLA	C1A-CHA	-3.32	1.29	1.43
24	d	402	CLA	CAA-C2A	-3.32	1.47	1.54
24	C	512	CLA	CAA-C2A	-3.31	1.47	1.54
32	C	515	DGD	C3D-C2D	-3.30	1.43	1.52
24	C	510	CLA	CHB-C4A	-3.30	1.29	1.33
24	C	505	CLA	C1A-CHA	-3.30	1.29	1.43
24	C	508	CLA	CAA-C2A	-3.29	1.47	1.54
24	c	508	CLA	CHB-C4A	-3.29	1.29	1.33
24	B	617	CLA	CMA-C3A	-3.29	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	H	102	DGD	C3D-C2D	-3.29	1.43	1.52
32	E	101	DGD	O2G-C2G	-3.29	1.37	1.46
24	a	615	CLA	CBD-CGD	-3.28	1.40	1.52
24	b	611	CLA	C1A-CHA	-3.28	1.29	1.43
24	c	509	CLA	CAA-C2A	-3.28	1.47	1.54
24	b	605	CLA	C1A-CHA	-3.28	1.29	1.43
24	B	614	CLA	CBD-CGD	-3.27	1.40	1.52
24	D	404	CLA	CBD-CGD	-3.27	1.41	1.52
24	B	607[A]	CLA	CAA-C2A	-3.26	1.47	1.54
24	d	403	CLA	CBD-CGD	-3.26	1.41	1.52
24	b	608[A]	CLA	CBD-CGD	-3.26	1.41	1.52
24	C	503	CLA	CBD-CGD	-3.26	1.41	1.52
24	C	509	CLA	CBD-CGD	-3.26	1.41	1.52
24	c	506	CLA	CAA-C2A	-3.25	1.47	1.54
24	C	509	CLA	C1A-CHA	-3.25	1.29	1.43
24	C	504	CLA	CAA-C2A	-3.24	1.47	1.54
24	b	616	CLA	CAA-C2A	-3.24	1.47	1.54
26	T	101	BCR	C35-C13	-3.23	1.44	1.50
24	b	608[B]	CLA	CBD-CGD	-3.23	1.41	1.52
26	c	514	BCR	C35-C13	-3.22	1.44	1.50
24	C	507	CLA	C1A-CHA	-3.22	1.29	1.43
24	B	602	CLA	CBD-CGD	-3.22	1.41	1.52
24	b	603	CLA	C1A-CHA	-3.22	1.29	1.43
24	B	609	CLA	CAA-C2A	-3.22	1.47	1.54
24	A	607	CLA	CBD-CGD	-3.21	1.41	1.52
24	c	505	CLA	CAA-C2A	-3.20	1.47	1.54
24	B	604	CLA	CMA-C3A	-3.19	1.45	1.53
24	a	609	CLA	C1A-CHA	-3.19	1.29	1.43
24	B	613	CLA	CHB-C4A	-3.19	1.29	1.33
24	a	615	CLA	CHB-C4A	-3.19	1.29	1.33
24	b	617	CLA	CAA-C2A	-3.19	1.47	1.54
24	b	610	CLA	CHB-C4A	-3.18	1.29	1.33
26	b	619	BCR	C1-C6	-3.18	1.49	1.53
24	B	615	CLA	CAA-C2A	-3.17	1.47	1.54
24	b	612	CLA	CAA-C2A	-3.17	1.47	1.54
24	B	611	CLA	C1A-CHA	-3.17	1.30	1.43
24	D	402	CLA	CAA-C2A	-3.17	1.47	1.54
32	h	102	DGD	C3D-C2D	-3.16	1.44	1.52
26	b	620	BCR	C1-C6	-3.16	1.49	1.53
24	D	403	CLA	CAA-C2A	-3.15	1.48	1.54
24	c	504	CLA	CAA-C2A	-3.15	1.48	1.54
24	B	613	CLA	C4C-C3C	-3.14	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	607	CLA	CBD-CGD	-3.14	1.41	1.52
24	B	612	CLA	CAA-C2A	-3.13	1.48	1.54
24	c	510	CLA	C1A-CHA	-3.13	1.30	1.43
24	c	506	CLA	CHB-C4A	-3.12	1.29	1.33
24	C	501	CLA	CAA-C2A	-3.10	1.48	1.54
24	b	605	CLA	CBD-CGD	-3.10	1.41	1.52
24	b	617	CLA	C1A-CHA	-3.10	1.30	1.43
24	B	616	CLA	CBD-CGD	-3.10	1.41	1.52
24	C	506	CLA	CAA-C2A	-3.09	1.48	1.54
24	b	609	CLA	CBD-CGD	-3.09	1.41	1.52
24	c	504	CLA	CHB-C4A	-3.09	1.29	1.33
24	C	505	CLA	C4C-C3C	-3.08	1.39	1.45
29	b	622	LMG	O7-C8	-3.08	1.38	1.46
24	B	612	CLA	CHB-C4A	-3.07	1.29	1.33
24	B	611	CLA	CBD-CGD	-3.06	1.41	1.52
24	b	608[B]	CLA	CAA-C2A	-3.06	1.48	1.54
24	B	617	CLA	CBD-CGD	-3.05	1.41	1.52
32	C	517	DGD	C3D-C2D	-3.05	1.44	1.52
24	C	504	CLA	CHB-C4A	-3.04	1.29	1.33
24	B	612	CLA	CBD-CGD	-3.04	1.41	1.52
24	d	402	CLA	CBD-CGD	-3.03	1.41	1.52
24	a	606	CLA	CBD-CGD	-3.03	1.41	1.52
24	B	606	CLA	C1A-CHA	-3.03	1.30	1.43
24	b	605	CLA	CAA-C2A	-3.03	1.48	1.54
26	B	619	BCR	C35-C13	-3.03	1.45	1.50
24	c	501	CLA	CAA-C2A	-3.03	1.48	1.54
24	B	615	CLA	CHB-C4A	-3.03	1.29	1.33
24	D	403	CLA	CHB-C4A	-3.03	1.29	1.33
24	B	602	CLA	C1A-CHA	-3.02	1.30	1.43
24	b	616	CLA	CBD-CGD	-3.01	1.41	1.52
24	c	511	CLA	CAA-C2A	-3.01	1.48	1.54
24	B	611	CLA	C4C-C3C	-3.00	1.39	1.45
29	D	408	LMG	O7-C8	-3.00	1.38	1.46
24	C	508	CLA	CHB-C4A	-2.99	1.29	1.33
32	E	101	DGD	C3D-C2D	-2.99	1.44	1.52
24	B	615	CLA	CBD-CGD	-2.99	1.41	1.52
24	C	504	CLA	CBD-CGD	-2.99	1.41	1.52
24	C	507	CLA	CAA-C2A	-2.99	1.48	1.54
24	B	604	CLA	CBD-CGD	-2.99	1.41	1.52
24	B	605	CLA	CAA-C2A	-2.98	1.48	1.54
24	B	606	CLA	CAA-C2A	-2.98	1.48	1.54
24	C	510	CLA	CBD-CGD	-2.98	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CBD-CGD	-2.97	1.42	1.52
24	c	512	CLA	CBD-CGD	-2.97	1.42	1.52
24	C	508	CLA	CBD-CGD	-2.96	1.42	1.52
24	B	613	CLA	C2A-C1A	-2.96	1.45	1.52
24	C	501	CLA	C4C-C3C	-2.96	1.39	1.45
24	c	513	CLA	CAA-C2A	-2.95	1.48	1.54
24	b	615	CLA	CBD-CGD	-2.95	1.42	1.52
24	c	513	CLA	CHB-C4A	-2.95	1.29	1.33
24	b	612	CLA	C4C-C3C	-2.94	1.39	1.45
24	c	502	CLA	CHB-C4A	-2.93	1.29	1.33
24	c	509	CLA	CBD-CGD	-2.93	1.42	1.52
32	c	517	DGD	C3D-C2D	-2.92	1.44	1.52
24	b	607	CLA	CBD-CGD	-2.92	1.42	1.52
24	b	608[A]	CLA	CAA-C2A	-2.92	1.48	1.54
24	C	506	CLA	C1A-CHA	-2.91	1.31	1.43
24	c	506	CLA	C1A-CHA	-2.91	1.31	1.43
32	H	102	DGD	C6E-C5E	-2.90	1.41	1.51
24	c	502	CLA	CBD-CGD	-2.90	1.42	1.52
26	h	101	BCR	C35-C13	-2.89	1.45	1.50
24	C	512	CLA	CBD-CGD	-2.89	1.42	1.52
24	A	606	CLA	CHB-C4A	-2.89	1.29	1.33
24	b	614	CLA	C2A-C1A	-2.89	1.45	1.52
24	b	612	CLA	CBD-CGD	-2.88	1.42	1.52
24	B	613	CLA	CBD-CGD	-2.88	1.42	1.52
24	A	609	CLA	OBD-CAD	-2.87	1.18	1.22
24	C	510	CLA	C2A-C1A	-2.87	1.45	1.52
24	D	402	CLA	OBD-CAD	-2.85	1.18	1.22
26	H	101	BCR	C1-C6	-2.84	1.49	1.53
32	d	405	DGD	C3D-C2D	-2.84	1.44	1.52
24	B	614	CLA	OBD-CAD	-2.83	1.18	1.22
24	B	608	CLA	CBD-CGD	-2.83	1.42	1.52
32	C	517	DGD	C3E-C2E	-2.82	1.44	1.52
24	B	607[A]	CLA	CBD-CGD	-2.82	1.42	1.52
26	f	101	BCR	C35-C13	-2.82	1.45	1.50
26	t	101	BCR	C35-C13	-2.81	1.45	1.50
24	b	607	CLA	CHB-C4A	-2.81	1.29	1.33
24	A	609	CLA	CAA-C2A	-2.81	1.48	1.54
24	C	509	CLA	CAA-C2A	-2.81	1.48	1.54
24	B	609	CLA	CBD-CGD	-2.80	1.42	1.52
24	B	603	CLA	CAA-C2A	-2.80	1.48	1.54
29	Z	101	LMG	O7-C8	-2.79	1.39	1.46
24	B	604	CLA	CAA-C2A	-2.79	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	621	BCR	C35-C13	-2.78	1.45	1.50
24	d	402	CLA	C2A-C1A	-2.78	1.45	1.52
24	B	607[B]	CLA	CBD-CGD	-2.78	1.42	1.52
29	j	101	LMG	O7-C8	-2.77	1.39	1.46
24	C	503	CLA	OBD-CAD	-2.77	1.18	1.22
24	B	607[A]	CLA	CHB-C4A	-2.77	1.29	1.33
24	D	404	CLA	O2D-CED	-2.76	1.38	1.45
24	b	604	CLA	C2A-C1A	-2.76	1.45	1.52
24	b	609	CLA	C2A-C1A	-2.76	1.45	1.52
24	C	503	CLA	CAA-C2A	-2.76	1.48	1.54
24	a	606	CLA	O2D-CED	-2.75	1.38	1.45
24	b	604	CLA	OBD-CAD	-2.74	1.18	1.22
24	c	507	CLA	CBD-CGD	-2.73	1.42	1.52
26	C	514	BCR	C35-C13	-2.73	1.45	1.50
24	D	403	CLA	OBD-CAD	-2.73	1.18	1.22
24	B	609	CLA	C4C-C3C	-2.73	1.40	1.45
24	c	502	CLA	CAA-C2A	-2.73	1.48	1.54
24	c	503	CLA	O2D-CED	-2.72	1.38	1.45
24	c	503	CLA	CAA-C2A	-2.72	1.48	1.54
24	c	512	CLA	CAA-C2A	-2.72	1.48	1.54
26	k	101	BCR	C35-C13	-2.72	1.45	1.50
26	I	101	BCR	C35-C13	-2.70	1.45	1.50
26	K	101	BCR	C35-C13	-2.70	1.45	1.50
24	C	501	CLA	CBD-CGD	-2.70	1.42	1.52
24	B	602	CLA	CHB-C4A	-2.69	1.30	1.33
24	C	513	CLA	CAA-C2A	-2.69	1.48	1.54
24	a	607	CLA	CHB-C4A	-2.69	1.30	1.33
24	c	510	CLA	CBD-CGD	-2.69	1.43	1.52
24	C	508	CLA	OBD-CAD	-2.68	1.18	1.22
24	B	611	CLA	O2D-CED	-2.68	1.38	1.45
26	C	514	BCR	C31-C1	-2.67	1.48	1.53
24	B	608	CLA	C2A-C1A	-2.67	1.45	1.52
32	c	516	DGD	C6E-C5E	-2.66	1.42	1.51
29	C	518	LMG	O7-C8	-2.66	1.39	1.46
24	C	505	CLA	CHB-C4A	-2.66	1.30	1.33
24	c	504	CLA	CBD-CGD	-2.66	1.43	1.52
24	B	603	CLA	CHB-C4A	-2.65	1.30	1.33
32	c	516	DGD	C3E-C2E	-2.65	1.45	1.52
24	b	603	CLA	CBD-CGD	-2.65	1.43	1.52
24	C	502	CLA	CBD-CGD	-2.65	1.43	1.52
24	b	616	CLA	C2A-C1A	-2.65	1.45	1.52
24	b	612	CLA	OBD-CAD	-2.65	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	515	DGD	C1D-C2D	-2.64	1.44	1.52
26	b	621	BCR	C31-C1	-2.64	1.48	1.53
26	k	101	BCR	C1-C6	-2.64	1.50	1.53
26	c	514	BCR	C31-C1	-2.64	1.48	1.53
24	A	606	CLA	O2D-CED	-2.63	1.38	1.45
25	A	608	PHO	C1C-NC	-2.63	1.32	1.38
24	b	613	CLA	CAA-C2A	-2.63	1.49	1.54
29	c	519	LMG	O7-C8	-2.63	1.39	1.46
26	c	515	BCR	C35-C13	-2.62	1.46	1.50
32	h	102	DGD	C6E-C5E	-2.62	1.42	1.51
24	b	609	CLA	CHB-C4A	-2.62	1.30	1.33
24	D	402	CLA	O2D-CED	-2.62	1.38	1.45
26	B	620	BCR	C31-C1	-2.61	1.48	1.53
24	B	605	CLA	OBD-CAD	-2.61	1.18	1.22
24	C	502	CLA	CAA-C2A	-2.61	1.49	1.54
24	B	610	CLA	C2A-C1A	-2.60	1.46	1.52
26	h	101	BCR	C31-C1	-2.60	1.48	1.53
29	A	613	LMG	O7-C8	-2.60	1.39	1.46
29	B	621	LMG	O7-C8	-2.60	1.39	1.46
24	C	511	CLA	CAA-C2A	-2.59	1.49	1.54
32	h	102	DGD	C3E-C2E	-2.59	1.45	1.52
24	d	403	CLA	O2D-CED	-2.59	1.39	1.45
24	C	511	CLA	CBD-CGD	-2.58	1.43	1.52
24	A	606	CLA	C2A-C1A	-2.58	1.46	1.52
26	b	620	BCR	C35-C13	-2.58	1.46	1.50
32	C	516	DGD	C3D-C2D	-2.58	1.45	1.52
24	D	403	CLA	O2D-CED	-2.58	1.39	1.45
24	B	616	CLA	CAA-C2A	-2.57	1.49	1.54
24	a	609	CLA	CBD-CGD	-2.57	1.43	1.52
24	b	604	CLA	CBD-CGD	-2.57	1.43	1.52
24	b	606	CLA	CBD-CGD	-2.56	1.43	1.52
26	k	101	BCR	C31-C1	-2.56	1.48	1.53
24	c	507	CLA	CAA-C2A	-2.56	1.49	1.54
24	B	607[B]	CLA	CHB-C4A	-2.55	1.30	1.33
25	d	401	PHO	C1C-NC	-2.55	1.32	1.38
24	C	503	CLA	O2D-CED	-2.54	1.39	1.45
24	C	501	CLA	C2A-C1A	-2.54	1.46	1.52
24	C	504	CLA	C2A-C1A	-2.54	1.46	1.52
32	c	517	DGD	C6E-C5E	-2.54	1.42	1.51
24	B	614	CLA	O2D-CED	-2.54	1.39	1.45
32	C	515	DGD	C6E-C5E	-2.54	1.43	1.51
24	a	607	CLA	CAA-C2A	-2.53	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	609	CLA	O2D-CED	-2.53	1.39	1.45
32	c	518	DGD	C6E-C5E	-2.53	1.43	1.51
26	K	102	BCR	C31-C1	-2.52	1.48	1.53
24	d	402	CLA	OBD-CAD	-2.52	1.18	1.22
26	K	101	BCR	C1-C6	-2.52	1.50	1.53
24	b	606	CLA	CHB-C4A	-2.51	1.30	1.33
24	C	502	CLA	O2D-CED	-2.51	1.39	1.45
24	a	609	CLA	CAA-C2A	-2.51	1.49	1.54
32	C	517	DGD	C6E-C5E	-2.51	1.43	1.51
24	B	612	CLA	C2A-C1A	-2.50	1.46	1.52
24	C	509	CLA	OBD-CAD	-2.50	1.18	1.22
32	h	102	DGD	C1D-C2D	-2.50	1.45	1.52
26	c	521	BCR	C35-C13	-2.50	1.46	1.50
24	a	615	CLA	C2A-C1A	-2.49	1.46	1.52
32	d	405	DGD	C6E-C5E	-2.48	1.43	1.51
24	B	611	CLA	OBD-CAD	-2.48	1.18	1.22
24	c	503	CLA	OBD-CAD	-2.48	1.18	1.22
24	b	610	CLA	C2A-C1A	-2.48	1.46	1.52
24	B	610	CLA	CBD-CGD	-2.48	1.43	1.52
26	B	619	BCR	C1-C6	-2.48	1.50	1.53
24	b	603	CLA	CAA-C2A	-2.48	1.49	1.54
24	B	607[B]	CLA	C2A-C1A	-2.47	1.46	1.52
24	c	506	CLA	CBD-CGD	-2.47	1.43	1.52
29	z	101	LMG	O7-C8	-2.47	1.40	1.46
24	C	508	CLA	C2A-C1A	-2.47	1.46	1.52
24	b	608[B]	CLA	O2D-CED	-2.47	1.39	1.45
26	K	101	BCR	C31-C1	-2.46	1.48	1.53
24	C	505	CLA	CBD-CGD	-2.46	1.43	1.52
32	C	516	DGD	C6D-C5D	-2.46	1.43	1.51
32	C	515	DGD	C3E-C2E	-2.45	1.45	1.52
24	B	606	CLA	CBD-CGD	-2.45	1.43	1.52
24	C	505	CLA	C2A-C1A	-2.44	1.46	1.52
26	b	620	BCR	C31-C1	-2.44	1.48	1.53
26	b	621	BCR	C1-C6	-2.44	1.50	1.53
24	c	511	CLA	CBD-CGD	-2.44	1.43	1.52
24	B	611	CLA	CAA-C2A	-2.44	1.49	1.54
24	c	505	CLA	C2A-C1A	-2.43	1.46	1.52
26	H	101	BCR	C35-C13	-2.43	1.46	1.50
24	c	505	CLA	CBD-CGD	-2.43	1.43	1.52
24	A	609	CLA	O2D-CED	-2.42	1.39	1.45
24	D	402	CLA	C2A-C1A	-2.42	1.46	1.52
24	d	403	CLA	CAA-C2A	-2.42	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607[A]	CLA	C2A-C1A	-2.42	1.46	1.52
24	b	608[A]	CLA	CHB-C4A	-2.41	1.30	1.33
24	b	606	CLA	CAA-C2A	-2.41	1.49	1.54
24	b	607	CLA	C2A-C1A	-2.41	1.46	1.52
24	b	613	CLA	CHB-C4A	-2.41	1.30	1.33
24	A	607	CLA	O2D-CED	-2.41	1.39	1.45
24	c	506	CLA	O2D-CED	-2.41	1.39	1.45
24	b	616	CLA	OBD-CAD	-2.41	1.18	1.22
24	D	404	CLA	CHB-C4A	-2.41	1.30	1.33
24	c	511	CLA	O2D-CED	-2.41	1.39	1.45
24	b	615	CLA	OBD-CAD	-2.40	1.18	1.22
24	d	402	CLA	O2D-CED	-2.40	1.39	1.45
24	b	606	CLA	OBD-CAD	-2.40	1.18	1.22
24	b	613	CLA	OBD-CAD	-2.39	1.18	1.22
24	b	608[A]	CLA	O2D-CED	-2.39	1.39	1.45
24	D	404	CLA	CAA-C2A	-2.39	1.49	1.54
25	D	401	PHO	CHC-C4B	-2.38	1.34	1.40
24	B	608	CLA	O2D-CED	-2.38	1.39	1.45
24	B	604	CLA	OBD-CAD	-2.38	1.18	1.22
24	B	603	CLA	CBD-CGD	-2.38	1.44	1.52
24	c	512	CLA	O2D-CED	-2.38	1.39	1.45
26	B	618	BCR	C35-C13	-2.37	1.46	1.50
24	B	616	CLA	O2D-CED	-2.37	1.39	1.45
24	c	504	CLA	OBD-CAD	-2.37	1.18	1.22
24	b	614	CLA	CBD-CGD	-2.37	1.44	1.52
24	B	602	CLA	O2D-CED	-2.37	1.39	1.45
29	C	519	LMG	O7-C8	-2.36	1.40	1.46
24	b	617	CLA	CBD-CGD	-2.36	1.44	1.52
24	B	617	CLA	O2D-CED	-2.36	1.39	1.45
24	C	511	CLA	OBD-CAD	-2.36	1.18	1.22
24	C	509	CLA	O2D-CED	-2.35	1.39	1.45
24	b	615	CLA	O2D-CED	-2.35	1.39	1.45
24	c	508	CLA	C2A-C1A	-2.35	1.46	1.52
24	b	608[A]	CLA	OBD-CAD	-2.34	1.18	1.22
24	B	603	CLA	C2A-C1A	-2.34	1.46	1.52
24	b	614	CLA	CHB-C4A	-2.33	1.30	1.33
24	b	611	CLA	C2A-C1A	-2.33	1.46	1.52
24	C	504	CLA	O2D-CED	-2.33	1.39	1.45
24	B	603	CLA	OBD-CAD	-2.33	1.18	1.22
26	A	610	BCR	C35-C13	-2.33	1.46	1.50
24	B	614	CLA	C2A-C1A	-2.33	1.46	1.52
26	f	101	BCR	C1-C6	-2.33	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	517	DGD	C1E-C2E	-2.32	1.45	1.52
24	a	606	CLA	CHB-C4A	-2.32	1.30	1.33
26	H	101	BCR	C31-C1	-2.32	1.48	1.53
24	b	617	CLA	OBD-CAD	-2.32	1.18	1.22
24	c	504	CLA	O2D-CED	-2.32	1.39	1.45
24	B	606	CLA	CHB-C4A	-2.32	1.30	1.33
24	B	610	CLA	CHB-C4A	-2.31	1.30	1.33
32	c	516	DGD	C6D-C5D	-2.31	1.44	1.51
24	A	607	CLA	C2A-C1A	-2.31	1.46	1.52
24	a	615	CLA	O2D-CED	-2.31	1.39	1.45
24	b	607	CLA	OBD-CAD	-2.31	1.18	1.22
24	C	513	CLA	OBD-CAD	-2.31	1.18	1.22
24	c	507	CLA	O2D-CED	-2.31	1.39	1.45
24	B	605	CLA	C2A-C1A	-2.30	1.46	1.52
24	c	509	CLA	C2A-C1A	-2.30	1.46	1.52
24	A	606	CLA	CBD-CGD	-2.30	1.44	1.52
24	C	510	CLA	O2D-CED	-2.30	1.39	1.45
24	C	513	CLA	C2A-C1A	-2.30	1.46	1.52
24	C	513	CLA	CBD-CGD	-2.30	1.44	1.52
24	D	403	CLA	C2A-C1A	-2.30	1.46	1.52
26	A	610	BCR	C1-C6	-2.30	1.50	1.53
24	c	503	CLA	CHB-C4A	-2.29	1.30	1.33
24	b	610	CLA	O2D-CED	-2.29	1.39	1.45
24	B	615	CLA	OBD-CAD	-2.29	1.18	1.22
24	B	609	CLA	O2D-CED	-2.28	1.39	1.45
26	B	618	BCR	C31-C1	-2.28	1.48	1.53
32	E	101	DGD	C6E-C5E	-2.28	1.43	1.51
24	b	615	CLA	CHB-C4A	-2.28	1.30	1.33
24	C	503	CLA	CHB-C4A	-2.27	1.30	1.33
24	B	610	CLA	O2D-CED	-2.27	1.39	1.45
24	C	508	CLA	C1D-ND	-2.27	1.32	1.37
29	a	613	LMG	O7-C8	-2.27	1.40	1.46
24	b	613	CLA	C1D-ND	-2.27	1.32	1.37
26	I	101	BCR	C1-C6	-2.27	1.50	1.53
24	A	609	CLA	CHB-C4A	-2.27	1.30	1.33
29	c	520	LMG	O7-C8	-2.27	1.40	1.46
24	b	612	CLA	O2D-CED	-2.26	1.39	1.45
24	B	603	CLA	O2D-CED	-2.26	1.39	1.45
24	b	617	CLA	O2D-CED	-2.26	1.39	1.45
26	a	610	BCR	C31-C1	-2.26	1.48	1.53
24	c	513	CLA	C2A-C1A	-2.25	1.46	1.52
24	B	609	CLA	CHB-C4A	-2.25	1.30	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	C6E-C5E	-2.25	1.44	1.51
24	B	607[B]	CLA	O2D-CED	-2.25	1.39	1.45
24	c	501	CLA	CBD-CGD	-2.25	1.44	1.52
24	C	510	CLA	OBD-CAD	-2.25	1.19	1.22
24	B	607[A]	CLA	O2D-CED	-2.24	1.39	1.45
24	C	511	CLA	O2D-CED	-2.24	1.39	1.45
26	c	521	BCR	C31-C1	-2.24	1.49	1.53
24	b	616	CLA	O2D-CED	-2.24	1.39	1.45
24	B	612	CLA	OBD-CAD	-2.23	1.19	1.22
32	C	515	DGD	C1E-C2E	-2.23	1.45	1.52
24	b	608[B]	CLA	CHB-C4A	-2.23	1.30	1.33
24	c	510	CLA	O2D-CED	-2.23	1.39	1.45
24	b	614	CLA	O2D-CED	-2.23	1.39	1.45
26	a	610	BCR	C1-C6	-2.23	1.50	1.53
24	a	607	CLA	O2D-CED	-2.22	1.39	1.45
24	b	617	CLA	CHB-C4A	-2.22	1.30	1.33
24	C	505	CLA	O2D-CED	-2.22	1.39	1.45
24	B	613	CLA	O2D-CED	-2.22	1.39	1.45
24	C	507	CLA	CBD-CGD	-2.22	1.44	1.52
24	B	608	CLA	CHB-C4A	-2.21	1.30	1.33
26	c	515	BCR	C1-C6	-2.21	1.50	1.53
26	K	102	BCR	C1-C6	-2.21	1.50	1.53
24	b	605	CLA	CHB-C4A	-2.21	1.30	1.33
24	b	607	CLA	O2D-CED	-2.21	1.39	1.45
24	B	602	CLA	CAA-C2A	-2.21	1.49	1.54
24	b	618	CLA	CBD-CGD	-2.21	1.44	1.52
24	c	504	CLA	C2A-C1A	-2.21	1.46	1.52
24	b	605	CLA	O2D-CED	-2.20	1.39	1.45
24	b	618	CLA	C2A-C1A	-2.20	1.47	1.52
24	b	603	CLA	O2D-CED	-2.20	1.39	1.45
24	b	612	CLA	CHB-C4A	-2.20	1.30	1.33
32	C	517	DGD	C1D-C2D	-2.20	1.46	1.52
24	b	610	CLA	CBD-CGD	-2.20	1.44	1.52
24	b	613	CLA	O2D-CED	-2.19	1.40	1.45
24	C	501	CLA	CHB-C4A	-2.19	1.30	1.33
24	C	501	CLA	OBD-CAD	-2.19	1.19	1.22
24	B	613	CLA	OBD-CAD	-2.18	1.19	1.22
24	C	502	CLA	CHB-C4A	-2.18	1.30	1.33
24	b	609	CLA	OBD-CAD	-2.18	1.19	1.22
24	B	604	CLA	O2D-CED	-2.18	1.40	1.45
24	B	605	CLA	CHB-C4A	-2.18	1.30	1.33
24	B	606	CLA	O2D-CED	-2.18	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	608	PHO	CHC-C4B	-2.18	1.35	1.40
24	c	505	CLA	OBD-CAD	-2.18	1.19	1.22
25	a	608	PHO	CMD-C2D	-2.18	1.46	1.50
32	d	405	DGD	C6D-C5D	-2.18	1.44	1.51
32	C	516	DGD	C3E-C2E	-2.18	1.46	1.52
24	B	617	CLA	C2A-C1A	-2.18	1.47	1.52
24	B	613	CLA	C1D-ND	-2.17	1.32	1.37
24	C	506	CLA	OBD-CAD	-2.17	1.19	1.22
24	b	617	CLA	C2A-C1A	-2.17	1.47	1.52
24	B	607[A]	CLA	OBD-CAD	-2.17	1.19	1.22
26	t	101	BCR	C31-C1	-2.17	1.49	1.53
24	c	513	CLA	CBD-CGD	-2.16	1.44	1.52
24	b	618	CLA	O2D-CED	-2.16	1.40	1.45
24	b	614	CLA	OBD-CAD	-2.16	1.19	1.22
32	H	102	DGD	C3E-C2E	-2.16	1.46	1.52
24	b	615	CLA	C2A-C1A	-2.16	1.47	1.52
24	b	612	CLA	C3B-C2B	-2.15	1.37	1.40
24	b	608[B]	CLA	C2A-C1A	-2.15	1.47	1.52
24	b	605	CLA	OBD-CAD	-2.15	1.19	1.22
24	b	611	CLA	CHB-C4A	-2.15	1.30	1.33
32	c	518	DGD	C1D-C2D	-2.15	1.46	1.52
26	b	619	BCR	C31-C1	-2.15	1.49	1.53
24	C	512	CLA	O2D-CED	-2.15	1.40	1.45
24	d	403	CLA	C2A-C1A	-2.15	1.47	1.52
24	B	608	CLA	OBD-CAD	-2.14	1.19	1.22
32	H	102	DGD	C6D-C5D	-2.14	1.44	1.51
24	a	615	CLA	OBD-CAD	-2.14	1.19	1.22
24	c	502	CLA	OBD-CAD	-2.14	1.19	1.22
24	c	511	CLA	CHB-C4A	-2.14	1.30	1.33
24	c	508	CLA	O2D-CED	-2.14	1.40	1.45
24	c	509	CLA	O2D-CED	-2.13	1.40	1.45
32	c	517	DGD	C1E-C2E	-2.13	1.46	1.52
26	K	102	BCR	C35-C13	-2.13	1.46	1.50
24	B	615	CLA	O2D-CED	-2.12	1.40	1.45
25	D	401	PHO	CAA-C2A	-2.12	1.50	1.54
24	c	508	CLA	OBD-CAD	-2.12	1.19	1.22
26	A	610	BCR	C31-C1	-2.12	1.49	1.53
24	c	510	CLA	C2A-C1A	-2.12	1.47	1.52
24	C	509	CLA	CHB-C4A	-2.12	1.30	1.33
24	b	612	CLA	C2A-C1A	-2.12	1.47	1.52
24	B	610	CLA	OBD-CAD	-2.11	1.19	1.22
24	B	610	CLA	C1D-ND	-2.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	C1C-NC	-2.11	1.33	1.38
24	c	512	CLA	C2A-C1A	-2.11	1.47	1.52
26	b	619	BCR	C35-C13	-2.11	1.47	1.50
32	c	516	DGD	C1D-C2D	-2.11	1.46	1.52
29	j	101	LMG	O8-C9	-2.11	1.40	1.45
24	C	508	CLA	O2D-CED	-2.11	1.40	1.45
24	c	505	CLA	O2D-CED	-2.11	1.40	1.45
24	c	502	CLA	O2D-CED	-2.11	1.40	1.45
24	c	511	CLA	OBD-CAD	-2.11	1.19	1.22
26	B	620	BCR	C35-C13	-2.10	1.47	1.50
32	c	518	DGD	C3E-C2E	-2.10	1.46	1.52
24	b	611	CLA	OBD-CAD	-2.10	1.19	1.22
24	a	606	CLA	C2A-C1A	-2.10	1.47	1.52
24	c	507	CLA	OBD-CAD	-2.10	1.19	1.22
24	B	617	CLA	OBD-CAD	-2.10	1.19	1.22
24	C	507	CLA	O2D-CED	-2.10	1.40	1.45
24	B	609	CLA	OBD-CAD	-2.10	1.19	1.22
24	c	502	CLA	C2A-C1A	-2.09	1.47	1.52
24	B	604	CLA	CHB-C4A	-2.09	1.30	1.33
24	B	612	CLA	O2D-CED	-2.09	1.40	1.45
24	b	609	CLA	O2D-CED	-2.09	1.40	1.45
26	c	515	BCR	C31-C1	-2.09	1.49	1.53
24	b	618	CLA	OBD-CAD	-2.09	1.19	1.22
24	c	509	CLA	OBD-CAD	-2.08	1.19	1.22
24	c	513	CLA	O2D-CED	-2.08	1.40	1.45
24	c	512	CLA	CHB-C4A	-2.08	1.30	1.33
24	c	512	CLA	OBD-CAD	-2.08	1.19	1.22
26	h	101	BCR	C1-C6	-2.07	1.51	1.53
24	A	609	CLA	C2A-C1A	-2.07	1.47	1.52
24	c	513	CLA	OBD-CAD	-2.07	1.19	1.22
24	b	608[B]	CLA	OBD-CAD	-2.06	1.19	1.22
24	b	616	CLA	CHB-C4A	-2.06	1.30	1.33
24	C	513	CLA	O2D-CED	-2.05	1.40	1.45
32	E	101	DGD	C6D-C5D	-2.05	1.45	1.51
32	c	517	DGD	C6D-C5D	-2.05	1.45	1.51
24	c	509	CLA	CHB-C4A	-2.05	1.30	1.33
24	B	604	CLA	C2A-C1A	-2.04	1.47	1.52
32	c	517	DGD	C1D-C2D	-2.04	1.46	1.52
32	c	517	DGD	C3E-C2E	-2.03	1.47	1.52
24	b	608[A]	CLA	C2A-C1A	-2.03	1.47	1.52
32	h	102	DGD	C6D-C5D	-2.03	1.45	1.51
25	A	608	PHO	CHD-C4C	-2.03	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	101	BCR	C35-C13	-2.03	1.47	1.50
24	B	604	CLA	C1D-ND	-2.03	1.33	1.37
24	B	607[B]	CLA	OBD-CAD	-2.02	1.19	1.22
24	C	501	CLA	O2D-CED	-2.01	1.40	1.45
24	C	511	CLA	C2A-C1A	-2.01	1.47	1.52
24	C	502	CLA	C2A-C1A	-2.01	1.47	1.52
25	a	608	PHO	C1C-NC	-2.01	1.34	1.38
24	a	609	CLA	OBD-CAD	-2.00	1.19	1.22
24	b	611	CLA	C1D-ND	-2.00	1.33	1.37
24	C	507	CLA	C3B-CAB	2.00	1.52	1.47
32	c	517	DGD	O6D-C1D	2.00	1.47	1.41
25	d	401	PHO	C1C-C2C	2.01	1.50	1.45
24	B	609	CLA	CMC-C2C	2.01	1.55	1.50
28	b	601	SQD	O6-C1	2.01	1.43	1.40
30	D	406	LHG	C8-C7	2.01	1.56	1.50
26	T	101	BCR	C32-C1	2.02	1.58	1.53
24	A	606	CLA	CMC-C2C	2.02	1.55	1.50
24	D	402	CLA	CMC-C2C	2.02	1.55	1.50
24	C	507	CLA	CBA-CGA	2.02	1.56	1.50
30	d	406	LHG	C8-C7	2.02	1.56	1.50
25	D	401	PHO	C1C-C2C	2.02	1.50	1.45
24	c	509	CLA	CMC-C2C	2.02	1.55	1.50
24	C	502	CLA	CBA-CGA	2.03	1.56	1.50
24	C	504	CLA	CMC-C2C	2.03	1.55	1.50
24	B	613	CLA	CMC-C2C	2.03	1.55	1.50
24	B	607[A]	CLA	C3B-CAB	2.03	1.52	1.47
24	B	603	CLA	CMC-C2C	2.03	1.55	1.50
28	L	102	SQD	O6-C1	2.03	1.43	1.40
25	A	608	PHO	C1B-C2B	2.04	1.50	1.45
26	k	101	BCR	C33-C5	2.04	1.54	1.51
24	B	614	CLA	O2D-CGD	2.04	1.38	1.33
28	B	622	SQD	O6-C1	2.04	1.43	1.40
24	b	610	CLA	CMC-C2C	2.05	1.55	1.50
24	b	608[A]	CLA	CMC-C2C	2.05	1.55	1.50
29	D	408	LMG	O6-C5	2.05	1.49	1.44
24	a	609	CLA	CMC-C2C	2.06	1.55	1.50
27	a	611	PL9	C41-C39	2.06	1.56	1.51
24	B	611	CLA	CMC-C2C	2.06	1.55	1.50
26	B	618	BCR	C17-C18	2.06	1.38	1.35
24	a	606	CLA	CMC-C2C	2.06	1.55	1.50
24	B	611	CLA	CBA-CGA	2.06	1.56	1.50
30	d	407	LHG	C8-C7	2.06	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	101	BCR	C7-C6	2.07	1.53	1.45
24	a	606	CLA	C3B-CAB	2.07	1.52	1.47
24	b	614	CLA	CMC-C2C	2.07	1.55	1.50
24	b	612	CLA	CMC-C2C	2.07	1.55	1.50
26	b	621	BCR	C7-C6	2.07	1.53	1.45
30	D	407	LHG	C8-C7	2.08	1.56	1.50
32	h	102	DGD	O6D-C1D	2.09	1.47	1.41
32	C	515	DGD	O3D-C3D	2.09	1.47	1.43
27	A	611	PL9	C2-C3	2.10	1.40	1.34
26	c	514	BCR	C7-C6	2.10	1.53	1.45
29	A	613	LMG	C7-C8	2.10	1.56	1.50
25	A	608	PHO	C1A-NA	2.10	1.41	1.37
32	h	102	DGD	O3D-C3D	2.11	1.47	1.43
32	C	517	DGD	O6D-C1D	2.11	1.47	1.41
32	c	518	DGD	O6D-C1D	2.11	1.47	1.41
25	d	401	PHO	CHD-C1D	2.11	1.42	1.38
30	A	615	LHG	C8-C7	2.11	1.56	1.50
26	c	515	BCR	C33-C5	2.12	1.54	1.51
24	B	607[B]	CLA	C3B-CAB	2.12	1.52	1.47
26	T	101	BCR	C7-C6	2.12	1.53	1.45
24	c	502	CLA	CBA-CGA	2.12	1.56	1.50
26	c	515	BCR	C7-C6	2.13	1.53	1.45
32	H	102	DGD	O6D-C1D	2.13	1.47	1.41
26	f	101	BCR	C7-C6	2.13	1.53	1.45
32	C	516	DGD	O6D-C1D	2.13	1.47	1.41
26	H	101	BCR	C7-C6	2.13	1.53	1.45
25	D	401	PHO	CHD-C1D	2.14	1.43	1.38
24	b	608[A]	CLA	C3B-CAB	2.14	1.52	1.47
33	v	201	HEM	CAD-C3D	2.14	1.55	1.52
24	B	602	CLA	CBA-CGA	2.14	1.56	1.50
24	B	606	CLA	CMC-C2C	2.15	1.55	1.50
24	b	608[B]	CLA	C3B-CAB	2.15	1.52	1.47
24	c	513	CLA	CMC-C2C	2.15	1.55	1.50
26	t	101	BCR	C7-C6	2.15	1.53	1.45
24	b	608[B]	CLA	CMC-C2C	2.16	1.55	1.50
24	d	403	CLA	CBA-CGA	2.16	1.56	1.50
24	C	509	CLA	CMC-C2C	2.16	1.55	1.50
24	B	604	CLA	CMC-C2C	2.16	1.55	1.50
32	C	515	DGD	O5D-C1E	2.16	1.44	1.40
26	K	102	BCR	C7-C6	2.16	1.53	1.45
32	c	517	DGD	O5D-C1E	2.16	1.44	1.40
24	b	605	CLA	CMC-C2C	2.16	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3B-CAB	2.16	1.52	1.47
27	a	611	PL9	C2-C3	2.17	1.40	1.34
26	a	610	BCR	C27-C26	2.17	1.55	1.51
26	a	610	BCR	C7-C6	2.17	1.53	1.45
25	D	401	PHO	C1B-C2B	2.17	1.50	1.45
29	a	613	LMG	C7-C8	2.18	1.57	1.50
33	V	201	HEM	CMC-C2C	2.18	1.56	1.51
24	c	512	CLA	CBA-CGA	2.19	1.57	1.50
24	C	510	CLA	CMC-C2C	2.19	1.55	1.50
26	A	610	BCR	C7-C6	2.20	1.53	1.45
26	b	621	BCR	C33-C5	2.20	1.54	1.51
24	B	609	CLA	C3B-CAB	2.20	1.52	1.47
24	c	510	CLA	CMC-C2C	2.21	1.55	1.50
26	I	101	BCR	C4-C5	2.21	1.55	1.51
24	A	607	CLA	CMC-C2C	2.21	1.55	1.50
26	K	101	BCR	C7-C6	2.22	1.53	1.45
26	B	618	BCR	C4-C5	2.22	1.55	1.51
24	D	404	CLA	CBA-CGA	2.23	1.57	1.50
24	c	512	CLA	CMC-C2C	2.23	1.55	1.50
29	Z	101	LMG	O8-C28	2.23	1.44	1.33
24	b	610	CLA	C3B-CAB	2.24	1.52	1.47
32	d	405	DGD	C3G-C2G	2.24	1.57	1.50
29	z	101	LMG	O8-C28	2.24	1.45	1.33
25	a	608	PHO	C1A-NA	2.24	1.42	1.37
29	c	519	LMG	C11-C10	2.25	1.57	1.50
26	c	514	BCR	C33-C5	2.26	1.54	1.51
30	E	102	LHG	C8-C7	2.26	1.57	1.50
24	D	404	CLA	CMC-C2C	2.26	1.55	1.50
32	c	516	DGD	O3D-C3D	2.26	1.48	1.43
24	B	615	CLA	CMC-C2C	2.26	1.55	1.50
32	C	516	DGD	O3D-C3D	2.27	1.48	1.43
26	K	101	BCR	C33-C5	2.27	1.54	1.51
32	h	102	DGD	O5D-C1E	2.27	1.44	1.40
32	C	517	DGD	O6E-C1E	2.28	1.47	1.41
24	a	607	CLA	CMC-C2C	2.28	1.55	1.50
24	B	602	CLA	CMC-C2C	2.29	1.55	1.50
26	B	620	BCR	C33-C5	2.29	1.54	1.51
24	C	503	CLA	O2D-CGD	2.29	1.39	1.33
24	a	609	CLA	CBA-CGA	2.29	1.57	1.50
24	C	507	CLA	CMC-C2C	2.30	1.55	1.50
27	D	405	PL9	C26-C24	2.30	1.56	1.51
29	C	518	LMG	O6-C5	2.30	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	518	LMG	C11-C10	2.30	1.57	1.50
24	C	511	CLA	CBA-CGA	2.31	1.57	1.50
32	E	101	DGD	C3G-C2G	2.31	1.57	1.50
26	T	101	BCR	C12-C13	2.32	1.51	1.45
29	C	519	LMG	C7-C8	2.32	1.57	1.50
32	E	101	DGD	O2D-C2D	2.32	1.48	1.43
24	C	512	CLA	CMC-C2C	2.33	1.55	1.50
24	B	608	CLA	CMC-C2C	2.33	1.55	1.50
24	B	608	CLA	C3B-CAB	2.34	1.52	1.47
24	B	614	CLA	C3D-CAD	2.34	1.52	1.45
32	c	516	DGD	O5D-C1E	2.34	1.44	1.40
32	d	405	DGD	O3D-C3D	2.34	1.48	1.43
26	B	618	BCR	C27-C26	2.35	1.56	1.51
25	A	608	PHO	CHC-C1C	2.35	1.43	1.38
26	B	619	BCR	C30-C25	2.35	1.57	1.53
24	A	606	CLA	C3B-CAB	2.35	1.52	1.47
24	D	403	CLA	O2D-CGD	2.35	1.39	1.33
30	e	101	LHG	C8-C7	2.36	1.57	1.50
32	C	515	DGD	O6D-C1D	2.36	1.47	1.41
32	c	516	DGD	O6D-C1D	2.36	1.47	1.41
32	H	102	DGD	O3D-C3D	2.36	1.48	1.43
24	C	511	CLA	C3D-CAD	2.36	1.52	1.45
32	c	517	DGD	O2D-C2D	2.37	1.48	1.43
32	C	516	DGD	O6D-C5D	2.37	1.50	1.44
32	C	515	DGD	O2D-C2D	2.38	1.48	1.43
32	d	405	DGD	O5D-C1E	2.38	1.44	1.40
24	b	609	CLA	C3D-CAD	2.38	1.52	1.45
29	c	520	LMG	C7-C8	2.38	1.57	1.50
32	E	101	DGD	O3G-C1D	2.39	1.44	1.40
32	c	518	DGD	O3D-C3D	2.39	1.48	1.43
25	a	608	PHO	C4C-NC	2.40	1.42	1.36
32	E	101	DGD	O6D-C1D	2.40	1.48	1.41
24	c	503	CLA	O2D-CGD	2.40	1.39	1.33
24	C	505	CLA	C3B-CAB	2.40	1.52	1.47
24	b	607	CLA	C3B-CAB	2.41	1.52	1.47
24	c	501	CLA	CMC-C2C	2.41	1.56	1.50
32	h	102	DGD	O2D-C2D	2.42	1.48	1.43
26	T	101	BCR	C27-C26	2.42	1.56	1.51
26	c	521	BCR	C27-C26	2.42	1.56	1.51
32	C	517	DGD	O3D-C3D	2.42	1.48	1.43
26	c	521	BCR	C7-C6	2.42	1.54	1.45
26	c	515	BCR	C27-C26	2.42	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	C3B-CAB	2.43	1.52	1.47
24	c	503	CLA	CMC-C2C	2.43	1.56	1.50
24	B	617	CLA	C3B-CAB	2.43	1.52	1.47
24	c	509	CLA	C3B-CAB	2.43	1.52	1.47
24	c	502	CLA	C3B-CAB	2.43	1.53	1.47
24	c	507	CLA	C3B-CAB	2.43	1.53	1.47
32	c	518	DGD	O6E-C1E	2.44	1.48	1.41
24	d	402	CLA	O2D-CGD	2.44	1.39	1.33
26	a	610	BCR	C12-C13	2.44	1.51	1.45
24	D	402	CLA	C3D-CAD	2.44	1.52	1.45
24	b	606	CLA	C3D-CAD	2.45	1.52	1.45
24	b	616	CLA	O2D-CGD	2.45	1.39	1.33
26	b	621	BCR	C27-C26	2.45	1.56	1.51
32	C	515	DGD	O6E-C1E	2.45	1.48	1.41
24	b	604	CLA	C3D-CAD	2.46	1.52	1.45
24	D	402	CLA	O2D-CGD	2.46	1.39	1.33
32	E	101	DGD	O3D-C3D	2.46	1.48	1.43
24	c	504	CLA	CMC-C2C	2.47	1.56	1.50
25	A	608	PHO	C4C-C3C	2.47	1.49	1.45
32	c	517	DGD	O6E-C1E	2.47	1.48	1.41
24	B	604	CLA	C3D-CAD	2.47	1.52	1.45
26	C	514	BCR	C33-C5	2.47	1.55	1.51
26	b	619	BCR	C4-C5	2.48	1.56	1.51
24	A	609	CLA	C3D-CAD	2.48	1.52	1.45
24	B	605	CLA	C3B-CAB	2.48	1.53	1.47
32	d	405	DGD	O2D-C2D	2.48	1.48	1.43
26	k	101	BCR	C7-C6	2.49	1.54	1.45
26	t	101	BCR	C27-C26	2.49	1.56	1.51
27	D	405	PL9	C41-C39	2.49	1.57	1.51
24	a	615	CLA	C3D-CAD	2.49	1.52	1.45
25	A	608	PHO	C4C-NC	2.49	1.42	1.36
24	B	606	CLA	C3D-CAD	2.50	1.52	1.45
24	c	512	CLA	O2D-CGD	2.50	1.39	1.33
24	B	612	CLA	C3B-CAB	2.50	1.53	1.47
24	C	503	CLA	CMC-C2C	2.50	1.56	1.50
24	C	509	CLA	C3B-CAB	2.50	1.53	1.47
25	d	401	PHO	C4C-C3C	2.50	1.49	1.45
24	d	403	CLA	O2D-CGD	2.51	1.39	1.33
24	C	506	CLA	C3B-CAB	2.51	1.53	1.47
24	A	609	CLA	O2D-CGD	2.51	1.39	1.33
24	b	615	CLA	C3B-CAB	2.51	1.53	1.47
24	B	608	CLA	C3D-CAD	2.51	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	H	102	DGD	O2D-C2D	2.51	1.48	1.43
24	A	607	CLA	O2D-CGD	2.51	1.39	1.33
24	b	609	CLA	C3B-CAB	2.51	1.53	1.47
32	d	405	DGD	O6D-C1D	2.51	1.48	1.41
32	h	102	DGD	O6E-C1E	2.52	1.48	1.41
26	b	619	BCR	C27-C26	2.52	1.56	1.51
24	C	503	CLA	C3D-CAD	2.53	1.53	1.45
24	B	615	CLA	C3D-CAD	2.53	1.53	1.45
26	I	101	BCR	C27-C26	2.54	1.56	1.51
26	b	620	BCR	C12-C13	2.54	1.51	1.45
24	C	508	CLA	C3B-CAB	2.54	1.53	1.47
24	C	502	CLA	C3B-CAB	2.54	1.53	1.47
24	B	603	CLA	C3B-CAB	2.54	1.53	1.47
25	D	401	PHO	C4C-C3C	2.55	1.50	1.45
26	A	610	BCR	C4-C5	2.55	1.56	1.51
26	B	619	BCR	C4-C5	2.55	1.56	1.51
24	C	501	CLA	CMC-C2C	2.56	1.56	1.50
24	b	617	CLA	C3D-CAD	2.56	1.53	1.45
24	a	615	CLA	C3B-CAB	2.56	1.53	1.47
24	b	613	CLA	C3D-CAD	2.56	1.53	1.45
24	b	608[B]	CLA	O2D-CGD	2.56	1.39	1.33
32	c	516	DGD	O2D-C2D	2.56	1.49	1.43
26	b	620	BCR	C4-C5	2.56	1.56	1.51
33	e	102	HEM	CAA-C2A	2.57	1.56	1.52
24	B	611	CLA	C3B-CAB	2.57	1.53	1.47
26	F	101	BCR	C4-C5	2.57	1.56	1.51
24	B	615	CLA	C3B-CAB	2.57	1.53	1.47
24	b	616	CLA	O2A-CGA	2.57	1.41	1.33
32	C	516	DGD	O5D-C1E	2.57	1.44	1.40
26	a	610	BCR	C4-C5	2.57	1.56	1.51
27	d	404	PL9	C21-C19	2.57	1.57	1.51
24	B	604	CLA	C3B-CAB	2.58	1.53	1.47
24	b	604	CLA	C3B-CAB	2.58	1.53	1.47
24	a	609	CLA	C3B-CAB	2.59	1.53	1.47
24	D	404	CLA	O2D-CGD	2.59	1.39	1.33
24	C	502	CLA	O2D-CGD	2.59	1.39	1.33
32	c	517	DGD	O6D-C5D	2.60	1.50	1.44
26	b	620	BCR	C40-C30	2.61	1.59	1.53
24	c	505	CLA	C3D-CAD	2.61	1.53	1.45
32	d	405	DGD	O3G-C1D	2.61	1.44	1.40
24	b	613	CLA	O2D-CGD	2.61	1.39	1.33
24	c	506	CLA	C3B-CAB	2.62	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C3B-CAB	2.62	1.53	1.47
24	a	606	CLA	C3D-CAD	2.62	1.53	1.45
24	b	605	CLA	C3D-CAD	2.62	1.53	1.45
24	b	608[A]	CLA	O2D-CGD	2.63	1.40	1.33
32	c	518	DGD	O5D-C1E	2.63	1.44	1.40
26	B	620	BCR	C12-C13	2.63	1.51	1.45
32	H	102	DGD	O5D-C1E	2.63	1.44	1.40
24	d	403	CLA	C3B-CAB	2.64	1.53	1.47
26	K	102	BCR	C4-C5	2.64	1.56	1.51
32	c	518	DGD	O2D-C2D	2.64	1.49	1.43
24	b	607	CLA	C3D-CAD	2.64	1.53	1.45
24	b	608[B]	CLA	C3D-CAD	2.64	1.53	1.45
24	B	613	CLA	C3B-CAB	2.65	1.53	1.47
24	c	508	CLA	C3B-CAB	2.65	1.53	1.47
32	C	517	DGD	O2D-C2D	2.65	1.49	1.43
24	b	614	CLA	C3D-CAD	2.65	1.53	1.45
26	K	102	BCR	C27-C26	2.66	1.56	1.51
24	c	503	CLA	C3D-CAD	2.66	1.53	1.45
24	c	505	CLA	C3B-CAB	2.66	1.53	1.47
24	C	504	CLA	O2D-CGD	2.66	1.40	1.33
24	b	608[A]	CLA	C3D-CAD	2.66	1.53	1.45
24	b	616	CLA	C3D-CAD	2.67	1.53	1.45
26	C	514	BCR	C12-C13	2.67	1.51	1.45
26	B	619	BCR	C40-C30	2.68	1.59	1.53
26	B	620	BCR	C27-C26	2.68	1.56	1.51
27	d	404	PL9	C41-C39	2.68	1.57	1.51
24	B	611	CLA	O2D-CGD	2.68	1.40	1.33
24	B	608	CLA	O2D-CGD	2.69	1.40	1.33
26	c	514	BCR	C27-C26	2.69	1.56	1.51
24	D	402	CLA	C3B-CAB	2.69	1.53	1.47
24	B	602	CLA	O2D-CGD	2.70	1.40	1.33
24	c	511	CLA	C3B-CAB	2.70	1.53	1.47
24	c	507	CLA	O2D-CGD	2.70	1.40	1.33
26	K	101	BCR	C27-C26	2.70	1.56	1.51
26	H	101	BCR	C4-C5	2.70	1.56	1.51
25	d	401	PHO	C4C-NC	2.71	1.43	1.36
24	B	606	CLA	C3B-CAB	2.71	1.53	1.47
24	B	605	CLA	C3D-CAD	2.71	1.53	1.45
32	c	516	DGD	O6D-C5D	2.71	1.51	1.44
24	b	606	CLA	C3B-CAB	2.72	1.53	1.47
24	c	504	CLA	O2D-CGD	2.72	1.40	1.33
32	H	102	DGD	O6E-C1E	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	402	CLA	C1B-CHB	2.72	1.47	1.40
24	C	510	CLA	O2D-CGD	2.72	1.40	1.33
24	A	607	CLA	C3B-CAB	2.72	1.53	1.47
24	C	512	CLA	O2D-CGD	2.72	1.40	1.33
24	c	510	CLA	C3B-CAB	2.73	1.53	1.47
24	b	615	CLA	O2D-CGD	2.73	1.40	1.33
26	f	101	BCR	C17-C18	2.73	1.39	1.35
26	t	101	BCR	C12-C13	2.73	1.51	1.45
24	C	510	CLA	C3D-CAD	2.73	1.53	1.45
24	C	510	CLA	C3B-CAB	2.74	1.53	1.47
24	C	508	CLA	C3D-CAD	2.74	1.53	1.45
26	c	514	BCR	C12-C13	2.74	1.52	1.45
24	c	506	CLA	O2D-CGD	2.74	1.40	1.33
32	d	405	DGD	O6E-C1E	2.74	1.48	1.41
24	B	616	CLA	C3B-CAB	2.75	1.53	1.47
24	a	615	CLA	O2D-CGD	2.75	1.40	1.33
24	b	611	CLA	C3B-CAB	2.76	1.53	1.47
24	B	613	CLA	O2D-CGD	2.76	1.40	1.33
24	c	504	CLA	C3D-CAD	2.76	1.53	1.45
24	a	609	CLA	C3D-CAD	2.76	1.53	1.45
24	D	404	CLA	C3B-CAB	2.76	1.53	1.47
33	v	201	HEM	C4D-ND	2.76	1.40	1.36
32	c	516	DGD	O6E-C1E	2.77	1.48	1.41
24	a	606	CLA	O2D-CGD	2.77	1.40	1.33
24	c	511	CLA	C3D-CAD	2.77	1.53	1.45
26	t	101	BCR	C4-C5	2.77	1.56	1.51
24	c	513	CLA	C3B-CAB	2.77	1.53	1.47
24	b	603	CLA	C3D-CAD	2.77	1.53	1.45
24	b	614	CLA	O2D-CGD	2.78	1.40	1.33
24	C	512	CLA	C3B-CAB	2.79	1.53	1.47
26	c	521	BCR	C4-C5	2.79	1.56	1.51
26	f	101	BCR	C12-C13	2.79	1.52	1.45
24	C	501	CLA	C3B-CAB	2.80	1.53	1.47
24	b	614	CLA	C3B-CAB	2.81	1.53	1.47
24	C	509	CLA	O2D-CGD	2.81	1.40	1.33
24	D	404	CLA	C3D-CAD	2.81	1.53	1.45
24	c	510	CLA	C3D-CAD	2.81	1.53	1.45
26	C	514	BCR	C27-C26	2.82	1.57	1.51
24	b	607	CLA	O2D-CGD	2.82	1.40	1.33
27	D	405	PL9	C36-C34	2.83	1.57	1.51
24	d	402	CLA	C3D-CAD	2.83	1.53	1.45
24	B	610	CLA	C3B-CAB	2.84	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	O2D-CGD	2.84	1.40	1.33
24	b	604	CLA	C1B-CHB	2.85	1.47	1.40
24	a	609	CLA	O2D-CGD	2.85	1.40	1.33
24	C	503	CLA	C3B-CAB	2.86	1.53	1.47
24	C	506	CLA	C3D-CAD	2.86	1.53	1.45
24	B	607[B]	CLA	C3D-CAD	2.86	1.53	1.45
24	B	604	CLA	O2D-CGD	2.87	1.40	1.33
26	K	101	BCR	C12-C13	2.87	1.52	1.45
32	C	516	DGD	O2D-C2D	2.88	1.49	1.43
24	c	512	CLA	C3D-CAD	2.88	1.54	1.45
24	b	609	CLA	O2A-CGA	2.88	1.41	1.33
27	a	611	PL9	C21-C19	2.88	1.57	1.51
24	a	607	CLA	C3D-CAD	2.88	1.54	1.45
26	h	101	BCR	C4-C5	2.88	1.57	1.51
24	B	602	CLA	C3B-CAB	2.88	1.53	1.47
24	C	510	CLA	C1B-CHB	2.88	1.47	1.40
24	b	610	CLA	O2A-CGA	2.88	1.41	1.33
26	k	101	BCR	C27-C26	2.89	1.57	1.51
32	H	102	DGD	O6D-C5D	2.89	1.51	1.44
32	E	101	DGD	O5D-C1E	2.89	1.45	1.40
24	b	617	CLA	C3B-CAB	2.89	1.53	1.47
24	c	508	CLA	O2A-CGA	2.91	1.42	1.33
24	B	617	CLA	O2D-CGD	2.91	1.40	1.33
26	T	101	BCR	C4-C5	2.91	1.57	1.51
26	B	618	BCR	C12-C13	2.91	1.52	1.45
26	B	620	BCR	C4-C5	2.91	1.57	1.51
32	C	516	DGD	O6E-C1E	2.91	1.49	1.41
24	c	506	CLA	C3D-CAD	2.91	1.54	1.45
24	B	615	CLA	O2D-CGD	2.91	1.40	1.33
24	B	607[A]	CLA	C3D-CAD	2.91	1.54	1.45
26	b	619	BCR	C12-C13	2.92	1.52	1.45
24	A	606	CLA	O2D-CGD	2.93	1.40	1.33
33	E	103	HEM	CAA-C2A	2.93	1.57	1.52
24	b	609	CLA	O2D-CGD	2.94	1.40	1.33
24	c	503	CLA	C3B-CAB	2.94	1.54	1.47
26	c	514	BCR	C4-C5	2.95	1.57	1.51
24	C	509	CLA	C3D-CAD	2.95	1.54	1.45
24	B	603	CLA	O2D-CGD	2.95	1.40	1.33
24	b	612	CLA	C3D-CAD	2.96	1.54	1.45
24	B	611	CLA	C1B-CHB	2.96	1.48	1.40
26	h	101	BCR	C27-C26	2.97	1.57	1.51
24	a	607	CLA	O2D-CGD	2.97	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	C3B-CAB	2.97	1.54	1.47
26	c	515	BCR	C4-C5	2.97	1.57	1.51
24	b	612	CLA	O2D-CGD	2.97	1.40	1.33
24	c	504	CLA	C3B-CAB	2.98	1.54	1.47
24	b	605	CLA	C3B-CAB	2.98	1.54	1.47
24	B	611	CLA	C3D-CAD	2.99	1.54	1.45
27	D	405	PL9	C21-C19	2.99	1.58	1.51
24	D	403	CLA	C3B-CAB	2.99	1.54	1.47
24	C	507	CLA	O2D-CGD	2.99	1.40	1.33
24	b	617	CLA	O2D-CGD	2.99	1.40	1.33
24	B	612	CLA	C3D-CAD	3.00	1.54	1.45
26	A	610	BCR	C40-C30	3.00	1.60	1.53
27	d	404	PL9	C36-C34	3.00	1.58	1.51
24	C	505	CLA	O2D-CGD	3.00	1.40	1.33
24	b	605	CLA	O2D-CGD	3.01	1.40	1.33
24	B	603	CLA	C3D-CAD	3.01	1.54	1.45
24	c	502	CLA	C3D-CAD	3.01	1.54	1.45
24	B	616	CLA	C3D-CAD	3.01	1.54	1.45
26	k	101	BCR	C2-C3	3.01	1.60	1.52
24	c	510	CLA	O2D-CGD	3.01	1.41	1.33
32	E	101	DGD	O6E-C1E	3.02	1.49	1.41
24	B	612	CLA	O2D-CGD	3.03	1.41	1.33
24	B	612	CLA	C1B-CHB	3.03	1.48	1.40
24	B	610	CLA	C3D-CAD	3.03	1.54	1.45
24	C	504	CLA	C3B-CAB	3.04	1.54	1.47
24	C	501	CLA	O2D-CGD	3.04	1.41	1.33
24	C	507	CLA	C3D-CAD	3.04	1.54	1.45
24	B	609	CLA	C3D-CAD	3.04	1.54	1.45
26	K	101	BCR	C4-C5	3.04	1.57	1.51
24	B	605	CLA	O2D-CGD	3.04	1.41	1.33
24	B	602	CLA	C3D-CAD	3.04	1.54	1.45
32	h	102	DGD	O6D-C5D	3.04	1.52	1.44
24	b	615	CLA	O2A-CGA	3.05	1.42	1.33
25	a	608	PHO	CHC-C1C	3.05	1.44	1.38
24	B	610	CLA	O2D-CGD	3.05	1.41	1.33
24	c	502	CLA	O2D-CGD	3.05	1.41	1.33
24	A	607	CLA	C3D-CAD	3.05	1.54	1.45
24	B	607[B]	CLA	O2D-CGD	3.05	1.41	1.33
24	c	511	CLA	O2D-CGD	3.06	1.41	1.33
24	D	402	CLA	C1B-CHB	3.06	1.48	1.40
26	k	101	BCR	C12-C13	3.06	1.52	1.45
27	A	611	PL9	C21-C19	3.07	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	O2A-CGA	3.07	1.42	1.33
29	a	613	LMG	O6-C1	3.07	1.49	1.41
24	C	506	CLA	O2A-CGA	3.07	1.42	1.33
24	d	403	CLA	C3D-CAD	3.07	1.54	1.45
25	D	401	PHO	CHC-C1C	3.07	1.44	1.38
24	c	501	CLA	C3B-CAB	3.08	1.54	1.47
26	B	619	BCR	C12-C13	3.08	1.52	1.45
24	B	607[A]	CLA	O2D-CGD	3.09	1.41	1.33
26	b	621	BCR	C4-C5	3.09	1.57	1.51
24	C	505	CLA	O2A-CGA	3.09	1.42	1.33
25	d	401	PHO	CHC-C1C	3.09	1.44	1.38
26	h	101	BCR	C12-C13	3.10	1.52	1.45
25	a	608	PHO	C3B-C4B	3.10	1.49	1.43
32	c	518	DGD	O6D-C5D	3.10	1.52	1.44
24	C	512	CLA	C3D-CAD	3.11	1.54	1.45
24	c	505	CLA	O2D-CGD	3.11	1.41	1.33
24	B	613	CLA	C3D-CAD	3.11	1.54	1.45
24	B	609	CLA	O2D-CGD	3.11	1.41	1.33
24	c	505	CLA	O2A-CGA	3.11	1.42	1.33
24	b	613	CLA	C3B-CAB	3.12	1.54	1.47
24	C	513	CLA	C3D-CAD	3.12	1.54	1.45
24	B	603	CLA	C1B-CHB	3.12	1.48	1.40
24	C	508	CLA	O2D-CGD	3.12	1.41	1.33
24	b	618	CLA	C3D-CAD	3.12	1.54	1.45
26	H	101	BCR	C27-C26	3.13	1.57	1.51
24	b	603	CLA	O2D-CGD	3.13	1.41	1.33
24	c	509	CLA	C3D-CAD	3.13	1.54	1.45
26	t	101	BCR	C40-C30	3.13	1.60	1.53
24	B	612	CLA	O2A-CGA	3.14	1.42	1.33
24	C	505	CLA	C3D-CAD	3.14	1.54	1.45
24	a	607	CLA	C3B-CAB	3.15	1.54	1.47
24	b	615	CLA	C3D-CAD	3.15	1.54	1.45
24	c	513	CLA	O2D-CGD	3.15	1.41	1.33
24	b	607	CLA	C1B-CHB	3.15	1.48	1.40
24	c	507	CLA	C3D-CAD	3.15	1.54	1.45
24	b	609	CLA	C1B-CHB	3.16	1.48	1.40
24	b	610	CLA	O2D-CGD	3.16	1.41	1.33
25	D	401	PHO	C4C-NC	3.16	1.44	1.36
26	b	620	BCR	C17-C18	3.16	1.40	1.35
24	c	510	CLA	O2A-CGA	3.16	1.42	1.33
32	E	101	DGD	O6D-C5D	3.16	1.52	1.44
26	K	101	BCR	C2-C3	3.16	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	101	BCR	C4-C5	3.16	1.57	1.51
24	c	508	CLA	O2D-CGD	3.17	1.41	1.33
26	H	101	BCR	C12-C13	3.17	1.52	1.45
26	f	101	BCR	C4-C5	3.17	1.57	1.51
24	C	504	CLA	C1B-CHB	3.17	1.48	1.40
24	B	614	CLA	O2A-CGA	3.17	1.42	1.33
24	c	501	CLA	C3D-CAD	3.18	1.54	1.45
24	C	510	CLA	O2A-CGA	3.18	1.42	1.33
24	B	615	CLA	O2A-CGA	3.19	1.42	1.33
24	c	509	CLA	O2D-CGD	3.19	1.41	1.33
26	b	621	BCR	C12-C13	3.20	1.53	1.45
26	h	101	BCR	C40-C30	3.20	1.60	1.53
24	C	504	CLA	C3D-CAD	3.20	1.54	1.45
24	c	508	CLA	C1B-CHB	3.21	1.48	1.40
26	I	101	BCR	C2-C3	3.21	1.61	1.52
32	d	405	DGD	O6D-C5D	3.21	1.52	1.44
24	B	613	CLA	C1B-CHB	3.21	1.48	1.40
26	f	101	BCR	C40-C30	3.21	1.60	1.53
24	b	611	CLA	C3D-CAD	3.22	1.54	1.45
24	d	402	CLA	C3B-CAB	3.22	1.54	1.47
24	b	618	CLA	O2D-CGD	3.22	1.41	1.33
26	b	620	BCR	C27-C26	3.22	1.57	1.51
24	a	615	CLA	C1B-CHB	3.23	1.48	1.40
24	c	513	CLA	C1B-CHB	3.23	1.48	1.40
27	A	611	PL9	C36-C34	3.23	1.58	1.51
24	c	508	CLA	C3D-CAD	3.24	1.55	1.45
24	c	513	CLA	O2A-CGA	3.24	1.42	1.33
24	c	504	CLA	C1B-CHB	3.24	1.48	1.40
26	T	101	BCR	C40-C30	3.24	1.60	1.53
24	b	606	CLA	O2D-CGD	3.25	1.41	1.33
26	A	610	BCR	C27-C26	3.25	1.57	1.51
26	b	621	BCR	C23-C22	3.25	1.53	1.45
24	B	613	CLA	O2A-CGA	3.25	1.43	1.33
24	C	509	CLA	C1B-CHB	3.25	1.48	1.40
24	B	615	CLA	C1B-CHB	3.26	1.48	1.40
24	C	509	CLA	O2A-CGA	3.26	1.43	1.33
24	C	504	CLA	O2A-CGA	3.26	1.43	1.33
24	a	615	CLA	O2A-CGA	3.26	1.43	1.33
26	a	610	BCR	C40-C30	3.26	1.60	1.53
24	D	403	CLA	C1B-CHB	3.27	1.48	1.40
32	C	517	DGD	O6D-C5D	3.27	1.52	1.44
26	K	101	BCR	C40-C30	3.27	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	514	BCR	C2-C3	3.27	1.61	1.52
24	C	513	CLA	O2D-CGD	3.27	1.41	1.33
24	b	604	CLA	O2A-CGA	3.27	1.43	1.33
29	j	101	LMG	O8-C28	3.28	1.43	1.33
24	b	610	CLA	C3D-CAD	3.28	1.55	1.45
24	C	506	CLA	C1B-CHB	3.28	1.49	1.40
26	H	101	BCR	C2-C3	3.28	1.61	1.52
24	C	507	CLA	C1B-CHB	3.29	1.49	1.40
26	F	101	BCR	C27-C26	3.29	1.58	1.51
24	B	608	CLA	O2A-CGA	3.29	1.43	1.33
27	a	611	PL9	C36-C34	3.30	1.58	1.51
24	c	501	CLA	O2D-CGD	3.31	1.41	1.33
26	C	514	BCR	C4-C5	3.31	1.58	1.51
24	B	605	CLA	C1B-CHB	3.31	1.49	1.40
26	t	101	BCR	C2-C3	3.31	1.61	1.52
24	D	403	CLA	O2A-CGA	3.31	1.43	1.33
24	a	607	CLA	C1B-CHB	3.33	1.49	1.40
24	C	502	CLA	C3D-CAD	3.33	1.55	1.45
24	B	617	CLA	C3D-CAD	3.33	1.55	1.45
24	C	503	CLA	O2A-CGA	3.33	1.43	1.33
32	c	516	DGD	O6E-C5E	3.33	1.52	1.44
24	A	606	CLA	C3D-CAD	3.33	1.55	1.45
26	A	610	BCR	C2-C3	3.33	1.61	1.52
24	B	605	CLA	O2A-CGA	3.33	1.43	1.33
26	b	619	BCR	C2-C3	3.34	1.61	1.52
24	b	614	CLA	O2A-CGA	3.34	1.43	1.33
24	C	501	CLA	C3D-CAD	3.34	1.55	1.45
24	d	402	CLA	O2A-CGA	3.34	1.43	1.33
24	B	616	CLA	C1B-CHB	3.34	1.49	1.40
24	b	611	CLA	O2A-CGA	3.35	1.43	1.33
24	B	606	CLA	O2D-CGD	3.35	1.41	1.33
24	C	508	CLA	C1B-CHB	3.35	1.49	1.40
24	b	617	CLA	C1B-CHB	3.35	1.49	1.40
26	c	514	BCR	C2-C3	3.35	1.61	1.52
24	b	606	CLA	C1B-CHB	3.35	1.49	1.40
26	I	101	BCR	C40-C30	3.36	1.61	1.53
29	A	613	LMG	O6-C1	3.36	1.50	1.41
26	h	101	BCR	C2-C3	3.36	1.61	1.52
24	B	607[A]	CLA	C1B-CHB	3.37	1.49	1.40
26	b	621	BCR	C2-C3	3.37	1.61	1.52
24	B	602	CLA	C1B-CHB	3.37	1.49	1.40
26	b	620	BCR	C2-C3	3.37	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	404	CLA	C1B-CHB	3.37	1.49	1.40
26	a	610	BCR	C2-C3	3.38	1.61	1.52
26	B	618	BCR	C40-C30	3.38	1.61	1.53
26	F	101	BCR	C12-C13	3.38	1.53	1.45
24	c	506	CLA	C1B-CHB	3.38	1.49	1.40
24	c	513	CLA	C3D-CAD	3.39	1.55	1.45
24	C	512	CLA	O2A-CGA	3.39	1.43	1.33
24	C	501	CLA	C1B-CHB	3.39	1.49	1.40
26	B	619	BCR	C27-C26	3.39	1.58	1.51
24	B	604	CLA	C1B-CHB	3.40	1.49	1.40
24	c	502	CLA	C1B-CHB	3.40	1.49	1.40
24	b	604	CLA	O2D-CGD	3.40	1.42	1.33
24	A	607	CLA	C1B-CHB	3.40	1.49	1.40
24	B	616	CLA	O2A-CGA	3.41	1.43	1.33
24	C	511	CLA	O2D-CGD	3.41	1.42	1.33
24	C	503	CLA	C1B-CHB	3.41	1.49	1.40
24	b	617	CLA	O2A-CGA	3.42	1.43	1.33
24	b	608[A]	CLA	C1B-CHB	3.42	1.49	1.40
24	A	609	CLA	O2A-CGA	3.42	1.43	1.33
24	b	610	CLA	C1B-CHB	3.42	1.49	1.40
29	B	621	LMG	O6-C1	3.42	1.50	1.41
24	b	616	CLA	C1B-CHB	3.43	1.49	1.40
24	B	603	CLA	O2A-CGA	3.43	1.43	1.33
24	b	608[B]	CLA	C1B-CHB	3.43	1.49	1.40
24	a	606	CLA	O2A-CGA	3.43	1.43	1.33
24	B	611	CLA	O2A-CGA	3.44	1.43	1.33
24	B	607[B]	CLA	C1B-CHB	3.44	1.49	1.40
26	c	515	BCR	C2-C3	3.44	1.61	1.52
26	F	101	BCR	C40-C30	3.44	1.61	1.53
25	D	401	PHO	C3B-C4B	3.45	1.50	1.43
26	C	514	BCR	C40-C30	3.45	1.61	1.53
26	c	515	BCR	C40-C30	3.45	1.61	1.53
26	K	102	BCR	C2-C3	3.46	1.61	1.52
32	C	515	DGD	O6D-C5D	3.46	1.53	1.44
24	a	607	CLA	O2A-CGA	3.46	1.43	1.33
24	B	607[B]	CLA	O2A-CGA	3.47	1.43	1.33
24	b	607	CLA	O2A-CGA	3.48	1.43	1.33
24	A	606	CLA	C1B-CHB	3.48	1.49	1.40
26	c	514	BCR	C40-C30	3.48	1.61	1.53
24	A	606	CLA	O2A-CGA	3.49	1.43	1.33
32	c	517	DGD	O6E-C5E	3.49	1.53	1.44
26	B	620	BCR	C2-C3	3.49	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	609	CLA	C1B-CHB	3.49	1.49	1.40
24	A	609	CLA	C3B-CAB	3.50	1.55	1.47
24	b	614	CLA	C1B-CHB	3.50	1.49	1.40
24	D	402	CLA	O2A-CGA	3.50	1.43	1.33
24	a	606	CLA	C1B-CHB	3.50	1.49	1.40
24	B	606	CLA	C1B-CHB	3.51	1.49	1.40
24	c	509	CLA	C1B-CHB	3.51	1.49	1.40
24	B	617	CLA	CHC-C1C	3.51	1.45	1.35
24	B	606	CLA	O2A-CGA	3.51	1.43	1.33
24	B	608	CLA	C1B-CHB	3.51	1.49	1.40
24	C	508	CLA	O2A-CGA	3.52	1.43	1.33
26	b	619	BCR	C40-C30	3.53	1.61	1.53
24	c	501	CLA	O2A-CGA	3.54	1.43	1.33
24	b	603	CLA	O2A-CGA	3.54	1.43	1.33
26	T	101	BCR	C24-C25	3.54	1.58	1.45
24	B	607[A]	CLA	O2A-CGA	3.55	1.43	1.33
24	b	613	CLA	O2A-CGA	3.55	1.43	1.33
26	A	610	BCR	C12-C13	3.55	1.53	1.45
32	C	517	DGD	O6E-C5E	3.56	1.53	1.44
29	c	520	LMG	O6-C1	3.56	1.51	1.41
26	c	521	BCR	C2-C3	3.56	1.62	1.52
24	D	403	CLA	CHC-C1C	3.56	1.45	1.35
25	A	608	PHO	C3B-C4B	3.56	1.50	1.43
24	C	513	CLA	C1B-CHB	3.57	1.49	1.40
26	B	619	BCR	C2-C3	3.57	1.62	1.52
26	K	102	BCR	C12-C13	3.57	1.53	1.45
24	b	611	CLA	C1B-CHB	3.57	1.49	1.40
24	C	510	CLA	CHC-C1C	3.58	1.45	1.35
32	H	102	DGD	O6E-C5E	3.58	1.53	1.44
24	C	506	CLA	O2D-CGD	3.58	1.42	1.33
24	b	608[B]	CLA	O2A-CGA	3.58	1.44	1.33
26	f	101	BCR	C2-C3	3.59	1.62	1.52
24	b	605	CLA	CHC-C1C	3.59	1.45	1.35
29	z	101	LMG	O6-C1	3.59	1.51	1.41
24	c	507	CLA	C1B-CHB	3.59	1.49	1.40
24	b	612	CLA	O2A-CGA	3.59	1.44	1.33
24	a	615	CLA	CHC-C1C	3.59	1.45	1.35
24	b	615	CLA	C1B-CHB	3.59	1.49	1.40
29	C	519	LMG	O6-C1	3.59	1.51	1.41
24	C	504	CLA	CHC-C1C	3.59	1.45	1.35
24	b	618	CLA	O2A-CGA	3.59	1.44	1.33
24	C	512	CLA	C1B-CHB	3.60	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	t	101	BCR	C24-C25	3.61	1.58	1.45
24	b	611	CLA	O2D-CGD	3.61	1.42	1.33
32	c	517	DGD	O2G-C1B	3.61	1.44	1.34
26	b	621	BCR	C24-C23	3.61	1.43	1.32
32	d	405	DGD	O6E-C5E	3.61	1.53	1.44
24	b	613	CLA	CHC-C1C	3.63	1.46	1.35
29	Z	101	LMG	O6-C1	3.63	1.51	1.41
24	c	503	CLA	O2A-CGA	3.63	1.44	1.33
24	b	608[A]	CLA	O2A-CGA	3.64	1.44	1.33
29	C	519	LMG	O8-C28	3.64	1.44	1.33
24	c	502	CLA	O2A-CGA	3.64	1.44	1.33
26	c	514	BCR	C24-C25	3.65	1.59	1.45
29	D	408	LMG	O8-C28	3.66	1.44	1.33
24	C	511	CLA	O2A-CGA	3.66	1.44	1.33
24	c	501	CLA	C1B-CHB	3.66	1.50	1.40
24	c	511	CLA	O2A-CGA	3.66	1.44	1.33
24	B	610	CLA	O2A-CGA	3.66	1.44	1.33
32	C	515	DGD	O6E-C5E	3.66	1.53	1.44
24	c	503	CLA	C1B-CHB	3.67	1.50	1.40
24	b	618	CLA	CHC-C1C	3.67	1.46	1.35
24	B	604	CLA	CHC-C1C	3.67	1.46	1.35
24	C	509	CLA	CHC-C1C	3.67	1.46	1.35
32	H	102	DGD	O2G-C1B	3.68	1.45	1.34
26	t	101	BCR	C17-C18	3.68	1.40	1.35
24	c	509	CLA	O2A-CGA	3.68	1.44	1.33
26	T	101	BCR	C2-C3	3.69	1.62	1.52
29	b	622	LMG	O8-C28	3.69	1.44	1.33
24	b	612	CLA	C1B-CHB	3.69	1.50	1.40
24	c	506	CLA	O2A-CGA	3.69	1.44	1.33
24	c	512	CLA	O2A-CGA	3.69	1.44	1.33
26	B	618	BCR	C2-C3	3.69	1.62	1.52
24	B	609	CLA	CHC-C1C	3.69	1.46	1.35
29	B	621	LMG	O8-C28	3.70	1.44	1.33
26	H	101	BCR	C40-C30	3.70	1.61	1.53
24	C	513	CLA	O2A-CGA	3.70	1.44	1.33
24	B	610	CLA	C1B-CHB	3.70	1.50	1.40
24	b	613	CLA	C1B-CHB	3.70	1.50	1.40
32	C	516	DGD	O6E-C5E	3.70	1.53	1.44
24	B	614	CLA	CHC-C1C	3.71	1.46	1.35
32	h	102	DGD	O6E-C5E	3.72	1.53	1.44
24	B	604	CLA	O2A-CGA	3.73	1.44	1.33
24	C	502	CLA	C1B-CHB	3.74	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	I	101	BCR	C12-C13	3.74	1.54	1.45
30	D	406	LHG	O7-C7	3.74	1.45	1.34
24	C	501	CLA	O2A-CGA	3.74	1.44	1.33
26	f	101	BCR	C27-C26	3.75	1.59	1.51
26	K	102	BCR	C24-C25	3.75	1.59	1.45
29	c	519	LMG	O6-C1	3.76	1.51	1.41
26	c	515	BCR	C12-C13	3.76	1.54	1.45
24	b	605	CLA	C1B-CHB	3.76	1.50	1.40
24	b	612	CLA	CHC-C1C	3.76	1.46	1.35
24	c	507	CLA	CHC-C1C	3.77	1.46	1.35
32	E	101	DGD	O6E-C5E	3.78	1.53	1.44
26	b	621	BCR	C24-C25	3.78	1.59	1.45
24	C	505	CLA	C1B-CHB	3.78	1.50	1.40
26	k	101	BCR	C40-C30	3.78	1.61	1.53
29	a	613	LMG	O8-C28	3.79	1.44	1.33
24	c	512	CLA	C1B-CHB	3.80	1.50	1.40
26	b	621	BCR	C40-C30	3.81	1.61	1.53
29	A	613	LMG	O8-C28	3.81	1.44	1.33
24	C	505	CLA	CHC-C1C	3.81	1.46	1.35
32	c	518	DGD	O6E-C5E	3.82	1.53	1.44
26	C	514	BCR	C24-C25	3.82	1.59	1.45
24	c	510	CLA	C1B-CHB	3.82	1.50	1.40
33	e	102	HEM	C3B-CAB	3.83	1.55	1.47
29	b	622	LMG	O6-C1	3.83	1.51	1.41
24	B	617	CLA	O2A-CGA	3.83	1.44	1.33
24	A	607	CLA	O2A-CGA	3.83	1.44	1.33
24	c	511	CLA	C1B-CHB	3.84	1.50	1.40
32	C	515	DGD	O1G-C1A	3.84	1.44	1.33
24	B	612	CLA	CHC-C1C	3.84	1.46	1.35
32	C	517	DGD	O2G-C1B	3.84	1.45	1.34
26	c	521	BCR	C24-C25	3.84	1.59	1.45
24	B	613	CLA	CHC-C1C	3.84	1.46	1.35
29	D	408	LMG	O7-C10	3.84	1.45	1.34
30	a	616	LHG	O7-C7	3.84	1.45	1.34
29	j	101	LMG	O6-C1	3.85	1.51	1.41
24	b	610	CLA	CHC-C1C	3.85	1.46	1.35
24	B	602	CLA	O2A-CGA	3.85	1.44	1.33
24	b	603	CLA	CHC-C1C	3.85	1.46	1.35
30	L	101	LHG	O7-C7	3.85	1.45	1.34
26	F	101	BCR	C2-C3	3.86	1.62	1.52
32	h	102	DGD	O1G-C1A	3.86	1.44	1.33
32	c	518	DGD	O1G-C1A	3.86	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	O2A-CGA	3.87	1.44	1.33
24	a	609	CLA	C1B-CHB	3.89	1.50	1.40
33	E	103	HEM	C3B-CAB	3.89	1.56	1.47
33	e	102	HEM	C3C-CAC	3.89	1.55	1.47
24	c	507	CLA	O2A-CGA	3.90	1.44	1.33
24	D	402	CLA	CHC-C1C	3.90	1.46	1.35
26	a	610	BCR	C24-C25	3.90	1.60	1.45
26	c	521	BCR	C12-C13	3.91	1.54	1.45
29	D	408	LMG	O6-C1	3.91	1.51	1.41
24	C	507	CLA	O2A-CGA	3.91	1.44	1.33
28	A	612	SQD	O48-C23	3.91	1.44	1.33
24	B	605	CLA	CHC-C1C	3.91	1.46	1.35
26	B	620	BCR	C24-C25	3.91	1.60	1.45
26	B	618	BCR	C24-C25	3.92	1.60	1.45
24	C	502	CLA	CHC-C1C	3.92	1.46	1.35
24	A	609	CLA	CHC-C1C	3.93	1.46	1.35
24	B	609	CLA	C1B-CHB	3.93	1.50	1.40
24	c	505	CLA	CHC-C1C	3.93	1.46	1.35
26	h	101	BCR	C24-C25	3.93	1.60	1.45
32	C	516	DGD	O2G-C1B	3.93	1.45	1.34
32	c	516	DGD	O2G-C1B	3.93	1.45	1.34
24	d	403	CLA	C1B-CHB	3.93	1.50	1.40
26	a	610	BCR	C17-C18	3.93	1.41	1.35
24	B	615	CLA	CHC-C1C	3.94	1.46	1.35
24	C	506	CLA	CHC-C1C	3.94	1.46	1.35
24	B	614	CLA	C1B-CHB	3.94	1.50	1.40
24	C	512	CLA	CHC-C1C	3.94	1.46	1.35
29	j	101	LMG	O7-C10	3.94	1.45	1.34
24	B	602	CLA	CHC-C1C	3.95	1.47	1.35
26	c	521	BCR	C40-C30	3.95	1.62	1.53
32	C	517	DGD	O1G-C1A	3.95	1.45	1.33
29	c	520	LMG	O8-C28	3.95	1.45	1.33
24	B	607[A]	CLA	CHC-C1C	3.95	1.47	1.35
26	c	515	BCR	C24-C25	3.95	1.60	1.45
24	c	504	CLA	O2A-CGA	3.95	1.45	1.33
24	b	617	CLA	CHC-C1C	3.96	1.47	1.35
30	A	615	LHG	O7-C7	3.96	1.45	1.34
28	a	612	SQD	O47-C7	3.96	1.45	1.34
28	A	612	SQD	O47-C7	3.97	1.46	1.34
30	d	406	LHG	O7-C7	3.97	1.46	1.34
24	A	606	CLA	CHC-C1C	3.97	1.47	1.35
24	B	610	CLA	CHC-C1C	3.97	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	d	405	DGD	O1G-C1A	3.97	1.45	1.33
24	b	618	CLA	C1B-CHB	3.97	1.50	1.40
24	b	615	CLA	CHC-C1C	3.97	1.47	1.35
32	c	516	DGD	O1G-C1A	3.97	1.45	1.33
32	c	518	DGD	O2G-C1B	3.98	1.46	1.34
28	a	612	SQD	O48-C23	3.98	1.45	1.33
24	C	508	CLA	CHC-C1C	3.98	1.47	1.35
30	l	102	LHG	O7-C7	3.99	1.46	1.34
26	b	619	BCR	C24-C25	3.99	1.60	1.45
24	d	402	CLA	CHC-C1C	3.99	1.47	1.35
24	D	404	CLA	O2A-CGA	3.99	1.45	1.33
24	C	507	CLA	CHC-C1C	3.99	1.47	1.35
33	V	201	HEM	C3B-CAB	3.99	1.56	1.47
24	a	609	CLA	O2A-CGA	4.00	1.45	1.33
29	C	518	LMG	O8-C28	4.00	1.45	1.33
32	E	101	DGD	O1G-C1A	4.00	1.45	1.33
24	B	608	CLA	CHC-C1C	4.00	1.47	1.35
24	c	505	CLA	C1B-CHB	4.01	1.50	1.40
30	D	407	LHG	O8-C23	4.01	1.45	1.33
32	c	517	DGD	O1G-C1A	4.01	1.45	1.33
30	A	615	LHG	O8-C23	4.01	1.45	1.33
24	b	603	CLA	C1B-CHB	4.01	1.50	1.40
26	I	101	BCR	C24-C25	4.01	1.60	1.45
24	c	502	CLA	CHC-C1C	4.03	1.47	1.35
24	B	611	CLA	CHC-C1C	4.03	1.47	1.35
24	B	607[B]	CLA	CHC-C1C	4.03	1.47	1.35
26	K	102	BCR	C40-C30	4.04	1.62	1.53
24	d	403	CLA	CHC-C1C	4.04	1.47	1.35
26	B	620	BCR	C40-C30	4.04	1.62	1.53
24	C	511	CLA	CHC-C1C	4.04	1.47	1.35
30	d	407	LHG	O7-C7	4.04	1.46	1.34
28	L	102	SQD	O48-C23	4.05	1.45	1.33
24	b	608[A]	CLA	CHC-C1C	4.06	1.47	1.35
32	C	516	DGD	O1G-C1A	4.06	1.45	1.33
24	c	513	CLA	CHC-C1C	4.06	1.47	1.35
28	l	101	SQD	O48-C23	4.06	1.45	1.33
32	h	102	DGD	O2G-C1B	4.06	1.46	1.34
24	B	606	CLA	CHC-C1C	4.06	1.47	1.35
24	b	614	CLA	CHC-C1C	4.06	1.47	1.35
29	c	519	LMG	O8-C28	4.07	1.45	1.33
24	c	506	CLA	CHC-C1C	4.07	1.47	1.35
24	b	605	CLA	O2A-CGA	4.07	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	609	CLA	CHC-C1C	4.08	1.47	1.35
33	E	103	HEM	C3C-CAC	4.08	1.56	1.47
24	c	509	CLA	CHC-C1C	4.08	1.47	1.35
24	b	607	CLA	CHC-C1C	4.08	1.47	1.35
24	B	617	CLA	C1B-CHB	4.09	1.51	1.40
24	C	511	CLA	C1B-CHB	4.09	1.51	1.40
24	A	607	CLA	CHC-C1C	4.09	1.47	1.35
26	A	610	BCR	C17-C18	4.09	1.41	1.35
24	b	608[B]	CLA	CHC-C1C	4.09	1.47	1.35
24	c	512	CLA	CHC-C1C	4.09	1.47	1.35
24	b	606	CLA	O2A-CGA	4.10	1.45	1.33
24	a	606	CLA	CHC-C1C	4.10	1.47	1.35
29	C	518	LMG	O6-C1	4.10	1.52	1.41
28	a	614	SQD	O47-C7	4.10	1.46	1.34
28	A	614	SQD	O47-C7	4.11	1.46	1.34
30	d	406	LHG	O8-C23	4.11	1.45	1.33
32	H	102	DGD	O1G-C1A	4.12	1.45	1.33
29	B	621	LMG	O7-C10	4.13	1.46	1.34
24	b	611	CLA	CHC-C1C	4.14	1.47	1.35
29	b	622	LMG	O7-C10	4.15	1.46	1.34
24	d	403	CLA	O2A-CGA	4.15	1.45	1.33
24	c	510	CLA	CHC-C1C	4.16	1.47	1.35
24	c	508	CLA	CHC-C1C	4.16	1.47	1.35
25	d	401	PHO	C3B-C4B	4.16	1.51	1.43
24	D	404	CLA	CHC-C1C	4.16	1.47	1.35
32	C	515	DGD	O2G-C1B	4.17	1.46	1.34
26	k	101	BCR	C24-C25	4.17	1.61	1.45
33	v	201	HEM	C3C-CAC	4.17	1.56	1.47
24	c	511	CLA	CHC-C1C	4.18	1.47	1.35
26	H	101	BCR	C24-C25	4.19	1.61	1.45
24	c	504	CLA	CHC-C1C	4.20	1.47	1.35
28	L	102	SQD	O47-C7	4.20	1.46	1.34
24	B	616	CLA	CHC-C1C	4.21	1.47	1.35
24	c	501	CLA	CHC-C1C	4.21	1.47	1.35
24	b	609	CLA	CHC-C1C	4.22	1.47	1.35
28	B	622	SQD	O47-C7	4.22	1.46	1.34
24	b	616	CLA	CHC-C1C	4.22	1.47	1.35
24	C	513	CLA	CHC-C1C	4.22	1.47	1.35
24	c	503	CLA	CHC-C1C	4.22	1.47	1.35
28	l	101	SQD	O47-C7	4.22	1.46	1.34
30	e	101	LHG	O7-C7	4.24	1.46	1.34
28	b	601	SQD	O47-C7	4.24	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Z	101	LMG	O7-C10	4.25	1.46	1.34
30	a	616	LHG	O8-C23	4.26	1.46	1.33
28	x	101	SQD	O47-C7	4.26	1.46	1.34
26	K	101	BCR	C24-C25	4.27	1.61	1.45
30	E	102	LHG	O8-C23	4.28	1.46	1.33
30	D	407	LHG	O7-C7	4.28	1.46	1.34
24	a	607	CLA	CHC-C1C	4.28	1.48	1.35
28	X	101	SQD	O47-C7	4.29	1.46	1.34
33	V	201	HEM	C3C-CAC	4.30	1.56	1.47
30	E	102	LHG	O7-C7	4.31	1.47	1.34
30	e	101	LHG	O8-C23	4.32	1.46	1.33
24	b	604	CLA	CHC-C1C	4.33	1.48	1.35
28	B	622	SQD	O48-C23	4.33	1.46	1.33
28	b	601	SQD	O48-C23	4.34	1.46	1.33
24	C	503	CLA	CHC-C1C	4.35	1.48	1.35
33	v	201	HEM	C3B-CAB	4.36	1.57	1.47
26	k	101	BCR	C23-C22	4.36	1.55	1.45
29	A	613	LMG	O7-C10	4.36	1.47	1.34
26	T	101	BCR	C17-C18	4.38	1.41	1.35
32	d	405	DGD	O2G-C1B	4.38	1.47	1.34
24	C	501	CLA	CHC-C1C	4.39	1.48	1.35
24	b	606	CLA	CHC-C1C	4.39	1.48	1.35
26	K	102	BCR	C17-C18	4.39	1.41	1.35
28	A	614	SQD	O48-C23	4.40	1.46	1.33
28	a	614	SQD	O48-C23	4.40	1.46	1.33
29	z	101	LMG	O7-C10	4.40	1.47	1.34
32	E	101	DGD	O2G-C1B	4.43	1.47	1.34
28	x	101	SQD	O48-C23	4.44	1.46	1.33
30	L	101	LHG	O8-C23	4.45	1.46	1.33
26	c	514	BCR	C23-C22	4.49	1.55	1.45
28	X	101	SQD	O48-C23	4.49	1.46	1.33
29	C	519	LMG	O7-C10	4.50	1.47	1.34
26	f	101	BCR	C24-C25	4.53	1.62	1.45
26	c	521	BCR	C24-C23	4.55	1.46	1.32
26	b	620	BCR	C24-C25	4.55	1.62	1.45
29	c	519	LMG	O7-C10	4.57	1.47	1.34
26	B	619	BCR	C17-C18	4.58	1.42	1.35
26	I	101	BCR	C23-C22	4.60	1.56	1.45
24	B	603	CLA	CHC-C1C	4.60	1.48	1.35
26	F	101	BCR	C24-C25	4.61	1.62	1.45
26	A	610	BCR	C24-C25	4.62	1.62	1.45
26	K	102	BCR	C23-C22	4.62	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	101	BCR	C23-C22	4.62	1.56	1.45
26	b	620	BCR	C23-C22	4.63	1.56	1.45
26	c	514	BCR	C17-C18	4.64	1.42	1.35
26	b	619	BCR	C17-C18	4.65	1.42	1.35
26	c	515	BCR	C17-C18	4.65	1.42	1.35
26	K	102	BCR	C24-C23	4.66	1.47	1.32
30	D	406	LHG	O8-C23	4.68	1.47	1.33
26	I	101	BCR	C24-C23	4.71	1.47	1.32
26	k	101	BCR	C17-C18	4.71	1.42	1.35
29	a	613	LMG	O7-C10	4.72	1.48	1.34
30	d	407	LHG	O8-C23	4.73	1.47	1.33
29	C	518	LMG	O7-C10	4.76	1.48	1.34
26	B	620	BCR	C24-C23	4.78	1.47	1.32
29	c	520	LMG	O7-C10	4.79	1.48	1.34
26	K	101	BCR	C23-C22	4.80	1.56	1.45
26	c	515	BCR	C23-C22	4.80	1.56	1.45
26	B	620	BCR	C23-C22	4.87	1.56	1.45
26	T	101	BCR	C24-C23	4.87	1.47	1.32
26	t	101	BCR	C24-C23	4.88	1.47	1.32
26	k	101	BCR	C24-C23	4.93	1.47	1.32
26	c	514	BCR	C24-C23	4.94	1.48	1.32
33	E	103	HEM	C3D-C2D	4.96	1.52	1.37
30	l	102	LHG	O8-C23	4.97	1.48	1.33
26	b	619	BCR	C24-C23	5.03	1.48	1.32
26	C	514	BCR	C24-C23	5.04	1.48	1.32
26	B	620	BCR	C17-C18	5.06	1.42	1.35
26	b	619	BCR	C23-C22	5.09	1.57	1.45
26	B	619	BCR	C24-C25	5.09	1.64	1.45
33	e	102	HEM	C3D-C2D	5.14	1.52	1.37
26	c	515	BCR	C24-C23	5.15	1.48	1.32
26	h	101	BCR	C17-C18	5.15	1.42	1.35
26	H	101	BCR	C23-C22	5.16	1.57	1.45
33	V	201	HEM	C3D-C2D	5.17	1.53	1.37
26	f	101	BCR	C23-C22	5.17	1.57	1.45
26	K	101	BCR	C24-C23	5.18	1.48	1.32
26	a	610	BCR	C24-C23	5.27	1.49	1.32
26	B	618	BCR	C24-C23	5.28	1.49	1.32
26	A	610	BCR	C23-C22	5.32	1.57	1.45
26	T	101	BCR	C23-C22	5.33	1.57	1.45
26	T	101	BCR	C38-C26	5.34	1.59	1.51
26	h	101	BCR	C24-C23	5.38	1.49	1.32
26	K	101	BCR	C17-C18	5.39	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	610	BCR	C23-C22	5.41	1.57	1.45
26	C	514	BCR	C23-C22	5.45	1.58	1.45
26	f	101	BCR	C24-C23	5.46	1.49	1.32
26	K	101	BCR	C11-C12	5.46	1.47	1.34
26	c	521	BCR	C23-C22	5.46	1.58	1.45
26	t	101	BCR	C23-C22	5.47	1.58	1.45
26	H	101	BCR	C17-C18	5.48	1.43	1.35
26	b	620	BCR	C24-C23	5.51	1.49	1.32
33	v	201	HEM	C3D-C2D	5.56	1.54	1.37
26	b	621	BCR	C17-C18	5.57	1.43	1.35
26	A	610	BCR	C24-C23	5.58	1.49	1.32
26	B	618	BCR	C23-C22	5.58	1.58	1.45
26	a	610	BCR	C38-C26	5.58	1.60	1.51
26	f	101	BCR	C11-C12	5.61	1.47	1.34
26	b	619	BCR	C11-C12	5.61	1.47	1.34
26	b	620	BCR	C11-C12	5.65	1.47	1.34
26	B	619	BCR	C23-C22	5.66	1.58	1.45
26	H	101	BCR	C24-C23	5.75	1.50	1.32
26	t	101	BCR	C38-C26	5.81	1.60	1.51
24	A	609	CLA	C4C-NC	5.81	1.46	1.37
26	F	101	BCR	C11-C12	5.83	1.48	1.34
26	K	101	BCR	C38-C26	5.83	1.60	1.51
26	I	101	BCR	C17-C18	5.84	1.43	1.35
24	A	607	CLA	C4C-NC	5.86	1.46	1.37
26	C	514	BCR	C38-C26	5.86	1.60	1.51
26	B	618	BCR	C11-C12	5.89	1.48	1.34
26	F	101	BCR	C23-C22	5.91	1.59	1.45
26	B	620	BCR	C11-C12	5.92	1.48	1.34
24	b	615	CLA	C4C-NC	5.94	1.46	1.37
24	B	614	CLA	C4C-NC	5.94	1.46	1.37
26	c	515	BCR	C38-C26	5.94	1.60	1.51
26	B	618	BCR	C38-C26	5.94	1.60	1.51
26	b	619	BCR	C38-C26	5.95	1.60	1.51
24	C	509	CLA	C4C-NC	6.02	1.46	1.37
24	b	616	CLA	C4C-NC	6.03	1.46	1.37
24	b	613	CLA	C4C-NC	6.03	1.46	1.37
24	C	510	CLA	C4C-NC	6.04	1.46	1.37
26	F	101	BCR	C24-C23	6.04	1.51	1.32
26	b	621	BCR	C38-C26	6.06	1.60	1.51
26	k	101	BCR	C11-C12	6.09	1.48	1.34
26	B	620	BCR	C38-C26	6.10	1.60	1.51
24	a	615	CLA	C4C-NC	6.12	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	101	BCR	C38-C26	6.12	1.60	1.51
24	B	608	CLA	C4C-NC	6.15	1.46	1.37
26	c	514	BCR	C38-C26	6.15	1.61	1.51
24	b	603	CLA	C4C-NC	6.16	1.46	1.37
26	c	514	BCR	C11-C12	6.16	1.49	1.34
26	a	610	BCR	C11-C12	6.16	1.49	1.34
24	B	612	CLA	C4C-NC	6.17	1.46	1.37
27	D	405	PL9	O2-C1	6.18	1.41	1.24
27	d	404	PL9	O2-C1	6.18	1.41	1.24
26	K	102	BCR	C38-C26	6.19	1.61	1.51
26	c	521	BCR	C38-C26	6.19	1.61	1.51
26	B	619	BCR	C24-C23	6.22	1.51	1.32
26	B	619	BCR	C38-C26	6.24	1.61	1.51
26	T	101	BCR	C11-C12	6.24	1.49	1.34
24	B	615	CLA	C4C-NC	6.25	1.46	1.37
24	C	507	CLA	C4C-NC	6.25	1.46	1.37
26	t	101	BCR	C11-C12	6.26	1.49	1.34
26	C	514	BCR	C11-C12	6.27	1.49	1.34
26	A	610	BCR	C38-C26	6.27	1.61	1.51
24	d	402	CLA	C4C-NC	6.27	1.46	1.37
24	C	513	CLA	C4C-NC	6.28	1.46	1.37
24	B	610	CLA	C4C-NC	6.29	1.46	1.37
26	C	514	BCR	C17-C18	6.30	1.44	1.35
26	H	101	BCR	C11-C12	6.31	1.49	1.34
24	B	604	CLA	C4C-NC	6.31	1.46	1.37
26	B	619	BCR	C11-C12	6.31	1.49	1.34
26	c	515	BCR	C11-C12	6.32	1.49	1.34
26	I	101	BCR	C38-C26	6.34	1.61	1.51
26	K	102	BCR	C11-C12	6.35	1.49	1.34
24	A	606	CLA	C4C-NC	6.35	1.46	1.37
26	h	101	BCR	C11-C12	6.36	1.49	1.34
24	b	607	CLA	C4C-NC	6.38	1.46	1.37
26	b	621	BCR	C11-C12	6.43	1.49	1.34
24	C	504	CLA	C4C-NC	6.43	1.46	1.37
24	B	613	CLA	C4C-NC	6.44	1.46	1.37
24	c	507	CLA	C4C-NC	6.48	1.46	1.37
26	A	610	BCR	C11-C12	6.48	1.49	1.34
27	A	611	PL9	O2-C1	6.49	1.42	1.24
26	T	101	BCR	C26-C25	6.49	1.46	1.34
24	c	510	CLA	C4C-NC	6.50	1.47	1.37
26	B	620	BCR	C8-C9	6.50	1.60	1.45
24	b	609	CLA	C4C-NC	6.50	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C4C-NC	6.55	1.47	1.37
24	c	511	CLA	C4C-NC	6.55	1.47	1.37
24	C	511	CLA	C4C-NC	6.56	1.47	1.37
24	D	403	CLA	C4C-NC	6.56	1.47	1.37
24	a	607	CLA	C4C-NC	6.57	1.47	1.37
24	a	606	CLA	C4C-NC	6.60	1.47	1.37
24	a	609	CLA	C4C-NC	6.60	1.47	1.37
24	b	611	CLA	C4C-NC	6.60	1.47	1.37
24	B	607[A]	CLA	C4C-NC	6.60	1.47	1.37
24	b	605	CLA	C4C-NC	6.62	1.47	1.37
27	a	611	PL9	O2-C1	6.62	1.42	1.24
24	B	605	CLA	C4C-NC	6.63	1.47	1.37
24	d	403	CLA	C4C-NC	6.63	1.47	1.37
26	t	101	BCR	C26-C25	6.63	1.46	1.34
24	b	604	CLA	C4C-NC	6.64	1.47	1.37
26	I	101	BCR	C11-C12	6.64	1.50	1.34
24	C	512	CLA	C4C-NC	6.65	1.47	1.37
24	b	612	CLA	C4C-NC	6.65	1.47	1.37
26	F	101	BCR	C8-C9	6.66	1.60	1.45
26	H	101	BCR	C38-C26	6.66	1.61	1.51
26	b	620	BCR	C38-C26	6.68	1.61	1.51
24	b	614	CLA	C4C-NC	6.69	1.47	1.37
26	F	101	BCR	C38-C26	6.73	1.61	1.51
26	h	101	BCR	C38-C26	6.73	1.61	1.51
24	B	607[B]	CLA	C4C-NC	6.73	1.47	1.37
26	c	521	BCR	C11-C12	6.75	1.50	1.34
24	C	503	CLA	C4C-NC	6.79	1.47	1.37
24	C	508	CLA	C4C-NC	6.79	1.47	1.37
24	D	404	CLA	C4C-NC	6.80	1.47	1.37
24	C	502	CLA	C4C-NC	6.81	1.47	1.37
26	B	618	BCR	C8-C9	6.81	1.61	1.45
24	b	610	CLA	C4C-NC	6.81	1.47	1.37
24	c	505	CLA	C4C-NC	6.81	1.47	1.37
24	c	502	CLA	C4C-NC	6.84	1.47	1.37
24	C	506	CLA	C4C-NC	6.84	1.47	1.37
24	c	501	CLA	C4C-NC	6.85	1.47	1.37
24	B	617	CLA	C4C-NC	6.85	1.47	1.37
24	c	512	CLA	C4C-NC	6.85	1.47	1.37
24	B	602	CLA	C4C-NC	6.86	1.47	1.37
26	B	619	BCR	C8-C9	6.86	1.61	1.45
24	D	402	CLA	C4C-NC	6.87	1.47	1.37
24	B	606	CLA	C4C-NC	6.88	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	C4C-NC	6.89	1.47	1.37
24	B	616	CLA	C4C-NC	6.89	1.47	1.37
24	c	508	CLA	C4C-NC	6.90	1.47	1.37
24	c	509	CLA	C4C-NC	6.91	1.47	1.37
24	b	608[A]	CLA	C4C-NC	6.96	1.47	1.37
26	K	102	BCR	C8-C9	6.96	1.61	1.45
26	a	610	BCR	C26-C25	6.97	1.46	1.34
24	B	603	CLA	C4C-NC	6.99	1.47	1.37
27	a	611	PL9	O1-C4	7.00	1.39	1.23
26	b	620	BCR	C8-C9	7.01	1.61	1.45
27	D	405	PL9	O1-C4	7.01	1.39	1.23
26	c	514	BCR	C26-C25	7.03	1.47	1.34
24	B	611	CLA	C4C-NC	7.05	1.47	1.37
24	b	608[B]	CLA	C4C-NC	7.05	1.47	1.37
26	b	619	BCR	C8-C9	7.06	1.61	1.45
26	h	101	BCR	C8-C9	7.07	1.61	1.45
24	c	503	CLA	C4C-NC	7.12	1.47	1.37
26	b	621	BCR	C26-C25	7.13	1.47	1.34
24	b	617	CLA	C4C-NC	7.14	1.47	1.37
26	T	101	BCR	C8-C9	7.16	1.61	1.45
26	B	620	BCR	C26-C25	7.16	1.47	1.34
24	C	505	CLA	C4C-NC	7.17	1.47	1.37
26	f	101	BCR	C8-C9	7.17	1.61	1.45
26	H	101	BCR	C8-C9	7.18	1.61	1.45
24	c	504	CLA	C4C-NC	7.18	1.48	1.37
24	c	513	CLA	C4C-NC	7.19	1.48	1.37
27	d	404	PL9	C33-C34	7.21	1.51	1.32
24	C	501	CLA	C4C-NC	7.23	1.48	1.37
26	t	101	BCR	C8-C9	7.23	1.61	1.45
27	D	405	PL9	C33-C34	7.25	1.51	1.32
26	f	101	BCR	C38-C26	7.26	1.62	1.51
26	B	618	BCR	C26-C25	7.26	1.47	1.34
26	b	621	BCR	C8-C9	7.28	1.62	1.45
24	B	609	CLA	C4C-NC	7.35	1.48	1.37
26	c	515	BCR	C8-C9	7.35	1.62	1.45
26	I	101	BCR	C8-C9	7.42	1.62	1.45
27	A	611	PL9	O1-C4	7.42	1.40	1.23
24	c	506	CLA	C4C-NC	7.43	1.48	1.37
27	A	611	PL9	C33-C34	7.46	1.52	1.32
26	c	521	BCR	C26-C25	7.48	1.47	1.34
26	a	610	BCR	C8-C9	7.49	1.62	1.45
26	C	514	BCR	C8-C9	7.50	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	BCR	C8-C9	7.54	1.62	1.45
26	c	521	BCR	C17-C18	7.56	1.46	1.35
26	c	521	BCR	C8-C9	7.58	1.62	1.45
27	a	611	PL9	C33-C34	7.58	1.52	1.32
26	C	514	BCR	C26-C25	7.58	1.48	1.34
26	K	101	BCR	C26-C25	7.60	1.48	1.34
27	d	404	PL9	C8-C9	7.60	1.52	1.32
26	c	515	BCR	C26-C25	7.63	1.48	1.34
26	K	102	BCR	C26-C25	7.63	1.48	1.34
26	K	101	BCR	C8-C9	7.67	1.62	1.45
27	a	611	PL9	C43-C44	7.72	1.52	1.32
27	d	404	PL9	O1-C4	7.72	1.41	1.23
27	A	611	PL9	C43-C44	7.74	1.52	1.32
27	a	611	PL9	C13-C14	7.80	1.52	1.32
27	A	611	PL9	C8-C9	7.80	1.52	1.32
27	D	405	PL9	C8-C9	7.81	1.52	1.32
27	d	404	PL9	C43-C44	7.84	1.53	1.32
26	k	101	BCR	C8-C9	7.86	1.63	1.45
27	a	611	PL9	C8-C9	7.91	1.53	1.32
26	A	610	BCR	C8-C9	7.92	1.63	1.45
27	A	611	PL9	C28-C29	7.94	1.53	1.32
26	k	101	BCR	C26-C25	7.98	1.48	1.34
27	D	405	PL9	C43-C44	7.99	1.53	1.32
27	A	611	PL9	C13-C14	7.99	1.53	1.32
27	a	611	PL9	C28-C29	8.01	1.53	1.32
26	b	619	BCR	C26-C25	8.11	1.49	1.34
26	I	101	BCR	C26-C25	8.14	1.49	1.34
27	d	404	PL9	C48-C49	8.21	1.56	1.32
27	D	405	PL9	C13-C14	8.22	1.54	1.32
27	d	404	PL9	C13-C14	8.23	1.54	1.32
27	D	405	PL9	C48-C49	8.24	1.56	1.32
27	D	405	PL9	C28-C29	8.28	1.54	1.32
26	H	101	BCR	C26-C25	8.30	1.49	1.34
26	h	101	BCR	C26-C25	8.35	1.49	1.34
26	A	610	BCR	C26-C25	8.36	1.49	1.34
27	d	404	PL9	C28-C29	8.43	1.54	1.32
27	A	611	PL9	C48-C49	8.50	1.57	1.32
27	a	611	PL9	C48-C49	8.55	1.57	1.32
27	d	404	PL9	C23-C24	8.88	1.55	1.32
27	A	611	PL9	C38-C39	8.91	1.55	1.32
27	a	611	PL9	C23-C24	8.95	1.55	1.32
27	A	611	PL9	C23-C24	9.10	1.56	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	101	BCR	C26-C25	9.17	1.50	1.34
26	b	620	BCR	C26-C25	9.18	1.50	1.34
27	D	405	PL9	C23-C24	9.19	1.56	1.32
26	B	618	BCR	C16-C17	9.20	1.70	1.43
27	a	611	PL9	C38-C39	9.23	1.56	1.32
27	d	404	PL9	C38-C39	9.24	1.56	1.32
26	f	101	BCR	C26-C25	9.26	1.51	1.34
26	B	619	BCR	C16-C17	9.29	1.70	1.43
27	D	405	PL9	C38-C39	9.34	1.56	1.32
26	c	515	BCR	C16-C17	9.36	1.70	1.43
26	B	619	BCR	C26-C25	9.36	1.51	1.34
26	f	101	BCR	C16-C17	9.44	1.71	1.43
26	c	521	BCR	C16-C17	9.49	1.71	1.43
26	b	620	BCR	C16-C17	9.56	1.71	1.43
26	a	610	BCR	C16-C17	9.62	1.71	1.43
26	F	101	BCR	C16-C17	9.65	1.71	1.43
26	I	101	BCR	C16-C17	9.72	1.71	1.43
27	d	404	PL9	C18-C19	9.75	1.57	1.32
26	b	621	BCR	C16-C17	9.76	1.72	1.43
26	A	610	BCR	C16-C17	9.84	1.72	1.43
27	D	405	PL9	C18-C19	9.87	1.58	1.32
27	A	611	PL9	C18-C19	9.91	1.58	1.32
27	a	611	PL9	C18-C19	9.92	1.58	1.32
26	b	619	BCR	C16-C17	9.98	1.72	1.43
26	B	620	BCR	C16-C17	10.00	1.72	1.43
26	c	514	BCR	C16-C17	10.00	1.72	1.43
26	K	102	BCR	C16-C17	10.01	1.72	1.43
26	k	101	BCR	C16-C17	10.06	1.72	1.43
26	h	101	BCR	C16-C17	10.08	1.73	1.43
26	t	101	BCR	C16-C17	10.19	1.73	1.43
26	K	101	BCR	C16-C17	10.24	1.73	1.43
26	H	101	BCR	C16-C17	10.24	1.73	1.43
26	T	101	BCR	C16-C17	10.26	1.73	1.43
26	B	620	BCR	C8-C7	10.37	1.64	1.32
26	H	101	BCR	C37-C22	10.46	1.70	1.50
26	C	514	BCR	C16-C17	10.47	1.74	1.43
26	b	620	BCR	C8-C7	10.66	1.65	1.32
26	B	619	BCR	C8-C7	10.70	1.65	1.32
26	B	618	BCR	C8-C7	10.74	1.65	1.32
26	h	101	BCR	C8-C7	10.77	1.65	1.32
26	F	101	BCR	C8-C7	10.81	1.65	1.32
26	t	101	BCR	C8-C7	10.81	1.65	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	619	BCR	C8-C7	10.84	1.65	1.32
26	K	102	BCR	C8-C7	10.84	1.65	1.32
26	I	101	BCR	C8-C7	10.84	1.65	1.32
26	c	515	BCR	C8-C7	10.85	1.66	1.32
26	T	101	BCR	C8-C7	10.86	1.66	1.32
26	f	101	BCR	C8-C7	10.87	1.66	1.32
26	a	610	BCR	C8-C7	10.89	1.66	1.32
26	H	101	BCR	C8-C7	10.97	1.66	1.32
26	A	610	BCR	C8-C7	11.00	1.66	1.32
26	b	621	BCR	C8-C7	11.01	1.66	1.32
26	C	514	BCR	C8-C7	11.03	1.66	1.32
26	c	514	BCR	C8-C7	11.19	1.67	1.32
26	H	101	BCR	C20-C21	11.20	1.76	1.43
26	c	521	BCR	C8-C7	11.31	1.67	1.32
26	c	514	BCR	C20-C21	11.33	1.76	1.43
26	K	101	BCR	C8-C7	11.39	1.67	1.32
26	a	610	BCR	C20-C21	11.45	1.77	1.43
26	k	101	BCR	C8-C7	11.51	1.67	1.32
26	b	620	BCR	C20-C21	11.59	1.77	1.43
26	A	610	BCR	C20-C21	11.74	1.77	1.43
26	I	101	BCR	C20-C21	11.82	1.78	1.43
26	c	521	BCR	C16-C15	11.93	1.67	1.35
26	b	620	BCR	C5-C6	11.93	1.55	1.34
26	C	514	BCR	C20-C21	11.94	1.78	1.43
26	T	101	BCR	C20-C21	11.94	1.78	1.43
26	h	101	BCR	C20-C21	12.03	1.78	1.43
26	f	101	BCR	C20-C21	12.06	1.78	1.43
26	B	620	BCR	C20-C21	12.06	1.78	1.43
26	k	101	BCR	C20-C21	12.07	1.78	1.43
26	K	101	BCR	C20-C21	12.09	1.78	1.43
26	H	101	BCR	C5-C6	12.10	1.56	1.34
26	c	515	BCR	C20-C21	12.11	1.78	1.43
26	t	101	BCR	C20-C21	12.16	1.79	1.43
26	B	618	BCR	C16-C15	12.17	1.68	1.35
26	h	101	BCR	C37-C22	12.25	1.73	1.50
26	I	101	BCR	C37-C22	12.31	1.73	1.50
26	b	620	BCR	C37-C22	12.33	1.73	1.50
26	B	618	BCR	C5-C6	12.35	1.56	1.34
26	b	619	BCR	C5-C6	12.40	1.56	1.34
26	F	101	BCR	C37-C22	12.42	1.74	1.50
26	b	619	BCR	C20-C21	12.42	1.79	1.43
26	B	619	BCR	C5-C6	12.43	1.56	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	102	BCR	C20-C21	12.46	1.79	1.43
26	B	618	BCR	C20-C21	12.53	1.80	1.43
26	c	515	BCR	C37-C22	12.56	1.74	1.50
26	c	514	BCR	C37-C22	12.58	1.74	1.50
26	B	619	BCR	C37-C22	12.61	1.74	1.50
26	F	101	BCR	C20-C21	12.66	1.80	1.43
26	T	101	BCR	C37-C22	12.68	1.74	1.50
26	B	619	BCR	C20-C21	12.72	1.80	1.43
26	h	101	BCR	C5-C6	12.74	1.57	1.34
26	B	619	BCR	C16-C15	12.79	1.69	1.35
26	f	101	BCR	C16-C15	12.85	1.70	1.35
26	c	515	BCR	C16-C15	12.86	1.70	1.35
26	b	619	BCR	C37-C22	12.91	1.75	1.50
26	I	101	BCR	C16-C15	12.91	1.70	1.35
26	b	621	BCR	C16-C15	12.92	1.70	1.35
26	k	101	BCR	C37-C22	12.97	1.75	1.50
26	f	101	BCR	C5-C6	12.97	1.57	1.34
26	a	610	BCR	C5-C6	12.98	1.57	1.34
26	B	618	BCR	C37-C22	13.01	1.75	1.50
26	F	101	BCR	C5-C6	13.02	1.57	1.34
26	f	101	BCR	C37-C22	13.06	1.75	1.50
26	K	101	BCR	C37-C22	13.13	1.75	1.50
26	A	610	BCR	C5-C6	13.15	1.58	1.34
26	t	101	BCR	C37-C22	13.16	1.75	1.50
26	b	620	BCR	C16-C15	13.26	1.71	1.35
26	h	101	BCR	C16-C15	13.27	1.71	1.35
26	I	101	BCR	C5-C6	13.28	1.58	1.34
26	c	514	BCR	C16-C15	13.32	1.71	1.35
26	H	101	BCR	C16-C15	13.36	1.71	1.35
26	t	101	BCR	C5-C6	13.37	1.58	1.34
26	a	610	BCR	C37-C22	13.37	1.75	1.50
26	A	610	BCR	C37-C22	13.40	1.75	1.50
26	B	620	BCR	C5-C6	13.44	1.58	1.34
26	K	102	BCR	C16-C15	13.44	1.71	1.35
26	A	610	BCR	C16-C15	13.47	1.71	1.35
26	b	619	BCR	C16-C15	13.48	1.71	1.35
26	K	102	BCR	C5-C6	13.48	1.58	1.34
26	a	610	BCR	C16-C15	13.52	1.71	1.35
26	K	102	BCR	C37-C22	13.54	1.76	1.50
26	F	101	BCR	C16-C15	13.57	1.71	1.35
26	K	101	BCR	C5-C6	13.58	1.58	1.34
26	C	514	BCR	C16-C15	13.66	1.72	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C36-C18	13.68	1.76	1.50
26	C	514	BCR	C37-C22	13.70	1.76	1.50
26	k	101	BCR	C16-C15	13.76	1.72	1.35
26	B	620	BCR	C37-C22	13.78	1.76	1.50
26	B	620	BCR	C16-C15	13.78	1.72	1.35
26	k	101	BCR	C5-C6	13.78	1.59	1.34
26	c	521	BCR	C20-C21	13.83	1.83	1.43
26	c	521	BCR	C5-C6	13.84	1.59	1.34
26	t	101	BCR	C16-C15	13.85	1.72	1.35
26	K	101	BCR	C16-C15	13.89	1.72	1.35
26	T	101	BCR	C16-C15	13.91	1.72	1.35
26	b	621	BCR	C5-C6	13.92	1.59	1.34
26	C	514	BCR	C5-C6	13.97	1.59	1.34
26	c	515	BCR	C5-C6	13.97	1.59	1.34
26	T	101	BCR	C5-C6	14.03	1.59	1.34
26	F	101	BCR	C36-C18	14.17	1.77	1.50
26	c	514	BCR	C5-C6	14.28	1.60	1.34
26	B	618	BCR	C36-C18	14.42	1.77	1.50
26	b	621	BCR	C37-C22	14.45	1.77	1.50
26	b	621	BCR	C36-C18	14.64	1.78	1.50
26	f	101	BCR	C36-C18	14.68	1.78	1.50
26	t	101	BCR	C36-C18	14.75	1.78	1.50
26	K	101	BCR	C36-C18	14.91	1.78	1.50
26	a	610	BCR	C36-C18	14.95	1.78	1.50
26	T	101	BCR	C36-C18	15.19	1.79	1.50
26	b	619	BCR	C36-C18	15.19	1.79	1.50
26	A	610	BCR	C36-C18	15.20	1.79	1.50
26	b	620	BCR	C36-C18	15.27	1.79	1.50
26	I	101	BCR	C36-C18	15.49	1.79	1.50
26	H	101	BCR	C36-C18	15.57	1.79	1.50
26	k	101	BCR	C36-C18	15.59	1.80	1.50
26	H	101	BCR	C20-C19	15.69	1.71	1.34
26	C	514	BCR	C36-C18	15.76	1.80	1.50
26	c	515	BCR	C36-C18	15.83	1.80	1.50
26	K	102	BCR	C36-C18	15.83	1.80	1.50
26	B	620	BCR	C36-C18	15.88	1.80	1.50
26	b	621	BCR	C20-C21	16.01	1.90	1.43
26	c	514	BCR	C36-C18	16.02	1.80	1.50
26	h	101	BCR	C36-C18	16.18	1.81	1.50
26	I	101	BCR	C20-C19	16.34	1.72	1.34
26	K	101	BCR	C20-C19	16.40	1.73	1.34
26	C	514	BCR	C20-C19	16.45	1.73	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	f	101	BCR	C20-C19	16.53	1.73	1.34
26	a	610	BCR	C20-C19	16.61	1.73	1.34
26	k	101	BCR	C20-C19	16.65	1.73	1.34
26	b	620	BCR	C20-C19	16.78	1.74	1.34
26	K	102	BCR	C20-C19	16.85	1.74	1.34
26	B	620	BCR	C20-C19	16.86	1.74	1.34
26	c	521	BCR	C36-C18	16.93	1.82	1.50
26	A	610	BCR	C20-C19	16.93	1.74	1.34
26	c	514	BCR	C20-C19	17.00	1.74	1.34
26	c	515	BCR	C20-C19	17.12	1.74	1.34
26	F	101	BCR	C20-C19	17.21	1.74	1.34
26	c	521	BCR	C37-C22	17.25	1.83	1.50
26	h	101	BCR	C20-C19	17.38	1.75	1.34
26	B	618	BCR	C20-C19	17.40	1.75	1.34
26	b	619	BCR	C20-C19	17.49	1.75	1.34
26	T	101	BCR	C20-C19	17.56	1.75	1.34
26	B	619	BCR	C20-C19	17.68	1.76	1.34
26	t	101	BCR	C20-C19	17.77	1.76	1.34
26	b	620	BCR	C10-C9	19.12	1.61	1.35
26	b	619	BCR	C10-C9	19.33	1.62	1.35
26	c	521	BCR	C20-C19	19.47	1.80	1.34
26	K	101	BCR	C10-C9	19.68	1.62	1.35
26	B	619	BCR	C10-C9	19.77	1.62	1.35
26	c	514	BCR	C10-C9	19.85	1.62	1.35
26	B	620	BCR	C10-C9	19.90	1.62	1.35
26	C	514	BCR	C10-C9	19.90	1.62	1.35
26	B	618	BCR	C10-C9	20.11	1.63	1.35
26	f	101	BCR	C10-C9	20.12	1.63	1.35
26	c	521	BCR	C10-C9	20.17	1.63	1.35
26	K	102	BCR	C10-C9	20.21	1.63	1.35
26	F	101	BCR	C10-C9	20.25	1.63	1.35
26	t	101	BCR	C10-C9	20.26	1.63	1.35
26	A	610	BCR	C10-C9	20.43	1.63	1.35
26	T	101	BCR	C10-C9	20.55	1.63	1.35
26	b	621	BCR	C10-C9	20.58	1.63	1.35
26	I	101	BCR	C10-C9	20.59	1.63	1.35
26	b	621	BCR	C20-C19	20.60	1.82	1.34
26	H	101	BCR	C10-C9	20.72	1.63	1.35
26	k	101	BCR	C10-C9	20.74	1.63	1.35
26	c	515	BCR	C10-C9	20.76	1.63	1.35
26	a	610	BCR	C10-C9	20.86	1.64	1.35
26	h	101	BCR	C10-C9	21.03	1.64	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	620	BCR	C14-C13	23.70	1.67	1.35
26	T	101	BCR	C14-C13	23.80	1.68	1.35
26	c	514	BCR	C14-C13	23.93	1.68	1.35
26	C	514	BCR	C14-C13	23.94	1.68	1.35
26	c	521	BCR	C14-C13	24.78	1.69	1.35
26	t	101	BCR	C14-C13	24.85	1.69	1.35
26	b	621	BCR	C14-C13	24.92	1.69	1.35
26	a	610	BCR	C14-C13	25.11	1.69	1.35
26	h	101	BCR	C14-C13	25.13	1.69	1.35
26	B	619	BCR	C14-C13	25.28	1.70	1.35
26	K	101	BCR	C14-C13	25.49	1.70	1.35
26	H	101	BCR	C14-C13	25.55	1.70	1.35
26	B	618	BCR	C14-C13	25.59	1.70	1.35
26	f	101	BCR	C14-C13	25.73	1.70	1.35
26	I	101	BCR	C14-C13	25.78	1.70	1.35
26	k	101	BCR	C14-C13	25.79	1.70	1.35
26	A	610	BCR	C14-C13	25.93	1.70	1.35
26	B	620	BCR	C14-C13	26.11	1.71	1.35
26	K	102	BCR	C14-C13	26.14	1.71	1.35
26	c	515	BCR	C14-C13	26.57	1.71	1.35
26	F	101	BCR	C14-C13	26.59	1.71	1.35
26	b	619	BCR	C14-C13	28.20	1.74	1.35

All (1981) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	101	BCR	C33-C5-C6	-16.30	107.26	124.62
26	B	618	BCR	C33-C5-C6	-15.99	107.59	124.62
26	T	101	BCR	C38-C26-C25	-15.84	107.75	124.62
26	B	618	BCR	C38-C26-C25	-15.46	108.15	124.62
26	b	619	BCR	C33-C5-C6	-15.27	108.36	124.62
26	f	101	BCR	C33-C5-C6	-15.07	108.56	124.62
26	b	621	BCR	C38-C26-C25	-14.94	108.71	124.62
26	H	101	BCR	C33-C5-C6	-14.71	108.95	124.62
26	b	620	BCR	C33-C5-C6	-14.68	108.98	124.62
26	B	620	BCR	C38-C26-C25	-14.53	109.14	124.62
26	C	514	BCR	C38-C26-C25	-14.49	109.18	124.62
26	K	101	BCR	C38-C26-C25	-14.37	109.31	124.62
26	k	101	BCR	C33-C5-C6	-14.26	109.42	124.62
26	B	619	BCR	C33-C5-C6	-14.13	109.57	124.62
26	t	101	BCR	C38-C26-C25	-14.11	109.59	124.62
26	c	515	BCR	C38-C26-C25	-14.03	109.68	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C33-C5-C6	-13.89	109.83	124.62
26	a	610	BCR	C33-C5-C6	-13.85	109.86	124.62
26	A	610	BCR	C33-C5-C6	-13.82	109.90	124.62
26	I	101	BCR	C38-C26-C25	-13.81	109.91	124.62
26	c	514	BCR	C38-C26-C25	-13.73	110.00	124.62
26	k	101	BCR	C38-C26-C25	-13.60	110.13	124.62
26	a	610	BCR	C38-C26-C25	-13.43	110.31	124.62
26	I	101	BCR	C4-C5-C6	-13.42	107.98	122.73
26	b	619	BCR	C38-C26-C25	-13.41	110.33	124.62
26	K	102	BCR	C33-C5-C6	-13.30	110.45	124.62
26	A	610	BCR	C38-C26-C25	-13.13	110.63	124.62
26	T	101	BCR	C33-C5-C6	-13.11	110.66	124.62
26	t	101	BCR	C33-C5-C6	-13.00	110.78	124.62
26	b	621	BCR	C15-C14-C13	-12.92	108.44	127.22
26	h	101	BCR	C33-C5-C6	-12.67	111.12	124.62
26	H	101	BCR	C38-C26-C25	-12.21	111.62	124.62
26	c	521	BCR	C33-C5-C6	-12.14	111.69	124.62
26	C	514	BCR	C33-C5-C6	-12.14	111.69	124.62
26	h	101	BCR	C38-C26-C25	-12.06	111.78	124.62
26	b	621	BCR	C33-C5-C6	-11.96	111.88	124.62
26	c	521	BCR	C38-C26-C25	-11.89	111.95	124.62
26	B	620	BCR	C33-C5-C6	-11.75	112.10	124.62
26	f	101	BCR	C4-C5-C6	-11.67	109.90	122.73
26	b	620	BCR	C24-C23-C22	-11.63	108.64	126.21
26	c	514	BCR	C33-C5-C6	-11.48	112.39	124.62
26	F	101	BCR	C16-C17-C18	-11.35	110.72	127.22
26	b	619	BCR	C4-C5-C6	-11.33	110.28	122.73
26	b	621	BCR	C16-C17-C18	-11.32	110.77	127.22
27	D	405	PL9	C7-C8-C9	-11.15	107.74	126.70
26	F	101	BCR	C4-C5-C6	-11.13	110.50	122.73
26	K	102	BCR	C16-C17-C18	-11.09	111.09	127.22
26	b	619	BCR	C16-C17-C18	-11.07	111.13	127.22
27	d	404	PL9	C7-C8-C9	-10.99	108.00	126.70
26	b	621	BCR	C24-C23-C22	-10.98	109.62	126.21
26	c	514	BCR	C16-C17-C18	-10.98	111.27	127.22
26	c	521	BCR	C20-C21-C22	-10.83	111.48	127.22
26	f	101	BCR	C16-C17-C18	-10.82	111.49	127.22
26	t	101	BCR	C27-C26-C25	-10.78	110.88	122.73
26	a	610	BCR	C27-C26-C25	-10.75	110.91	122.73
26	T	101	BCR	C27-C26-C25	-10.71	110.96	122.73
26	c	515	BCR	C33-C5-C6	-10.63	113.30	124.62
26	c	521	BCR	C24-C23-C22	-10.56	110.26	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	515	BCR	C4-C5-C6	-10.52	111.17	122.73
26	b	621	BCR	C20-C21-C22	-10.51	111.94	127.22
26	a	610	BCR	C4-C5-C6	-10.50	111.19	122.73
26	K	102	BCR	C38-C26-C25	-10.33	113.61	124.62
26	B	620	BCR	C16-C17-C18	-10.29	112.26	127.22
26	c	514	BCR	C24-C23-C22	-10.22	110.77	126.21
26	F	101	BCR	C7-C8-C9	-10.17	110.85	126.21
26	B	620	BCR	C27-C26-C25	-10.16	111.56	122.73
26	t	101	BCR	C24-C23-C22	-10.14	110.89	126.21
26	I	101	BCR	C27-C26-C25	-10.12	111.61	122.73
26	I	101	BCR	C33-C5-C6	-10.06	113.91	124.62
26	h	101	BCR	C15-C14-C13	-10.00	112.69	127.22
26	F	101	BCR	C11-C10-C9	-9.91	112.81	127.22
26	c	521	BCR	C16-C17-C18	-9.89	112.85	127.22
26	B	618	BCR	C4-C5-C6	-9.83	111.92	122.73
26	A	610	BCR	C4-C5-C6	-9.79	111.97	122.73
26	f	101	BCR	C30-C25-C26	-9.75	109.45	122.50
26	b	620	BCR	C4-C5-C6	-9.74	112.03	122.73
26	a	610	BCR	C16-C17-C18	-9.70	113.11	127.22
26	T	101	BCR	C24-C23-C22	-9.70	111.55	126.21
26	H	101	BCR	C4-C5-C6	-9.63	112.15	122.73
26	B	619	BCR	C11-C10-C9	-9.58	113.30	127.22
26	h	101	BCR	C16-C17-C18	-9.57	113.31	127.22
26	B	619	BCR	C16-C17-C18	-9.51	113.40	127.22
26	b	620	BCR	C38-C26-C25	-9.45	114.55	124.62
26	I	101	BCR	C24-C23-C22	-9.44	111.95	126.21
26	c	515	BCR	C27-C26-C25	-9.37	112.44	122.73
26	t	101	BCR	C30-C25-C26	-9.36	109.97	122.50
26	F	101	BCR	C36-C18-C17	-9.17	109.56	122.89
26	C	514	BCR	C11-C10-C9	-9.06	114.05	127.22
26	B	619	BCR	C38-C26-C25	-9.06	114.97	124.62
26	F	101	BCR	C38-C26-C25	-9.06	114.97	124.62
26	c	514	BCR	C27-C26-C25	-9.05	112.79	122.73
26	K	102	BCR	C24-C23-C22	-9.03	112.57	126.21
26	T	101	BCR	C30-C25-C26	-9.01	110.44	122.50
26	I	101	BCR	C11-C10-C9	-8.99	114.15	127.22
26	B	620	BCR	C8-C7-C6	-8.91	101.36	127.24
26	B	618	BCR	C16-C17-C18	-8.89	114.30	127.22
26	K	102	BCR	C27-C26-C25	-8.88	112.97	122.73
26	H	101	BCR	C15-C14-C13	-8.87	114.33	127.22
26	H	101	BCR	C37-C22-C21	-8.82	110.06	122.89
27	A	611	PL9	C37-C38-C39	-8.81	108.31	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	F	101	BCR	C24-C23-C22	-8.78	112.94	126.21
26	A	610	BCR	C16-C17-C18	-8.75	114.50	127.22
26	B	620	BCR	C4-C5-C6	-8.68	113.19	122.73
26	K	101	BCR	C30-C25-C26	-8.67	110.90	122.50
27	A	611	PL9	C42-C43-C44	-8.67	108.62	127.75
26	F	101	BCR	C30-C25-C26	-8.63	110.96	122.50
26	c	515	BCR	C11-C10-C9	-8.60	114.71	127.22
26	I	101	BCR	C16-C17-C18	-8.58	114.74	127.22
26	f	101	BCR	C27-C26-C25	-8.58	113.30	122.73
26	I	101	BCR	C7-C8-C9	-8.57	113.27	126.21
26	T	101	BCR	C16-C17-C18	-8.52	114.84	127.22
26	K	101	BCR	C27-C26-C25	-8.45	113.44	122.73
27	a	611	PL9	C37-C38-C39	-8.45	109.11	127.75
26	b	621	BCR	C27-C26-C25	-8.40	113.50	122.73
26	b	619	BCR	C11-C10-C9	-8.40	115.01	127.22
26	k	101	BCR	C27-C26-C25	-8.40	113.50	122.73
26	F	101	BCR	C27-C26-C25	-8.32	113.59	122.73
26	b	620	BCR	C8-C7-C6	-8.31	103.13	127.24
26	f	101	BCR	C38-C26-C25	-8.30	115.78	124.62
27	d	404	PL9	C12-C13-C14	-8.30	109.44	127.75
26	k	101	BCR	C16-C17-C18	-8.29	115.18	127.22
27	D	405	PL9	C32-C33-C34	-8.27	109.51	127.75
26	B	619	BCR	C7-C8-C9	-8.26	113.73	126.21
26	b	620	BCR	C11-C10-C9	-8.22	115.27	127.22
26	b	619	BCR	C7-C8-C9	-8.20	113.82	126.21
27	D	405	PL9	C22-C23-C24	-8.20	109.67	127.75
27	a	611	PL9	C40-C39-C38	-8.19	107.73	123.58
26	C	514	BCR	C7-C8-C9	-8.15	113.90	126.21
27	a	611	PL9	C16-C14-C13	-8.13	105.84	120.98
27	A	611	PL9	C40-C39-C38	-8.07	107.95	123.58
26	B	618	BCR	C7-C8-C9	-8.04	114.06	126.21
27	a	611	PL9	C45-C44-C43	-7.99	108.11	123.58
26	c	515	BCR	C24-C23-C22	-7.96	114.18	126.21
26	K	102	BCR	C20-C21-C22	-7.96	115.66	127.22
27	a	611	PL9	C27-C28-C29	-7.95	110.22	127.75
27	A	611	PL9	C16-C14-C13	-7.94	106.19	120.98
26	b	620	BCR	C15-C14-C13	-7.94	115.68	127.22
27	a	611	PL9	C42-C43-C44	-7.93	110.26	127.75
27	a	611	PL9	C22-C23-C24	-7.92	110.29	127.75
27	A	611	PL9	C10-C9-C8	-7.88	108.33	123.58
27	D	405	PL9	C27-C28-C29	-7.87	110.39	127.75
27	A	611	PL9	C27-C28-C29	-7.87	110.39	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	611	PL9	C45-C44-C43	-7.84	108.40	123.58
26	T	101	BCR	C15-C14-C13	-7.84	115.83	127.22
26	H	101	BCR	C16-C17-C18	-7.84	115.83	127.22
27	d	404	PL9	C32-C33-C34	-7.83	110.47	127.75
26	H	101	BCR	C24-C23-C22	-7.83	114.38	126.21
26	t	101	BCR	C7-C6-C5	-7.83	103.20	121.36
26	C	514	BCR	C16-C17-C18	-7.80	115.88	127.22
26	C	514	BCR	C24-C23-C22	-7.75	114.50	126.21
26	c	514	BCR	C11-C10-C9	-7.74	115.97	127.22
26	b	621	BCR	C4-C5-C6	-7.73	114.23	122.73
27	d	404	PL9	C22-C23-C24	-7.71	110.75	127.75
26	I	101	BCR	C1-C6-C5	-7.66	112.26	122.50
26	c	521	BCR	C27-C26-C25	-7.64	114.33	122.73
26	C	514	BCR	C20-C21-C22	-7.61	116.17	127.22
26	a	610	BCR	C30-C25-C26	-7.59	112.35	122.50
26	c	514	BCR	C30-C25-C26	-7.59	112.35	122.50
26	B	618	BCR	C27-C26-C25	-7.58	114.40	122.73
27	a	611	PL9	C10-C9-C8	-7.58	108.91	123.58
27	d	404	PL9	C35-C34-C33	-7.57	108.93	123.58
26	B	619	BCR	C8-C7-C6	-7.52	105.41	127.24
26	T	101	BCR	C7-C8-C9	-7.51	114.86	126.21
27	a	611	PL9	C7-C8-C9	-7.51	113.93	126.70
26	K	101	BCR	C11-C10-C9	-7.49	116.33	127.22
27	A	611	PL9	C7-C8-C9	-7.48	113.98	126.70
26	f	101	BCR	C24-C23-C22	-7.47	114.93	126.21
26	f	101	BCR	C1-C6-C5	-7.47	112.51	122.50
26	K	102	BCR	C30-C25-C26	-7.46	112.52	122.50
27	A	611	PL9	C41-C39-C38	-7.45	107.10	120.98
26	C	514	BCR	C15-C14-C13	-7.43	116.41	127.22
27	D	405	PL9	C16-C14-C13	-7.42	107.15	120.98
26	c	514	BCR	C15-C14-C13	-7.42	116.44	127.22
26	c	521	BCR	C4-C5-C6	-7.40	114.60	122.73
26	B	618	BCR	C11-C10-C9	-7.38	116.49	127.22
26	B	619	BCR	C4-C5-C6	-7.38	114.62	122.73
26	f	101	BCR	C11-C10-C9	-7.37	116.51	127.22
27	A	611	PL9	C17-C18-C19	-7.36	111.51	127.75
27	a	611	PL9	C35-C34-C33	-7.34	109.36	123.58
27	a	611	PL9	C15-C14-C13	-7.33	109.39	123.58
26	B	620	BCR	C30-C25-C26	-7.31	112.72	122.50
26	k	101	BCR	C24-C23-C22	-7.28	115.21	126.21
27	a	611	PL9	C17-C18-C19	-7.28	111.70	127.75
26	k	101	BCR	C30-C25-C26	-7.27	112.77	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	H	101	BCR	C8-C7-C6	-7.27	106.14	127.24
27	d	404	PL9	C46-C44-C43	-7.26	107.47	120.98
26	b	619	BCR	C1-C6-C5	-7.24	112.82	122.50
26	b	621	BCR	C36-C18-C19	-7.22	106.28	118.08
26	B	618	BCR	C1-C6-C5	-7.18	112.89	122.50
26	f	101	BCR	C7-C8-C9	-7.17	115.37	126.21
27	a	611	PL9	C32-C33-C34	-7.17	111.94	127.75
26	T	101	BCR	C7-C6-C5	-7.17	104.73	121.36
26	c	515	BCR	C7-C8-C9	-7.14	115.42	126.21
26	h	101	BCR	C4-C5-C6	-7.12	114.90	122.73
26	c	515	BCR	C1-C6-C5	-7.11	112.99	122.50
26	b	621	BCR	C8-C7-C6	-7.07	106.71	127.24
27	D	405	PL9	C30-C29-C28	-7.06	109.90	123.58
26	a	610	BCR	C1-C6-C5	-7.06	113.05	122.50
27	A	611	PL9	C15-C14-C13	-7.03	109.97	123.58
26	t	101	BCR	C11-C10-C9	-7.02	117.02	127.22
27	d	404	PL9	C16-C14-C13	-7.01	107.93	120.98
27	A	611	PL9	C22-C23-C24	-7.00	112.31	127.75
26	B	619	BCR	C7-C6-C5	-6.97	105.20	121.36
26	C	514	BCR	C27-C26-C25	-6.91	115.13	122.73
27	D	405	PL9	C25-C24-C23	-6.90	110.22	123.58
27	D	405	PL9	C10-C9-C8	-6.89	110.23	123.58
27	d	404	PL9	C21-C19-C18	-6.89	108.14	120.98
26	c	521	BCR	C30-C25-C26	-6.88	113.29	122.50
27	d	404	PL9	C25-C24-C23	-6.88	110.26	123.58
26	h	101	BCR	C27-C26-C25	-6.86	115.19	122.73
26	H	101	BCR	C27-C26-C25	-6.86	115.19	122.73
27	D	405	PL9	C45-C44-C43	-6.86	110.30	123.58
27	A	611	PL9	C26-C24-C23	-6.85	108.22	120.98
27	d	404	PL9	C17-C18-C19	-6.82	112.70	127.75
27	D	405	PL9	C15-C14-C13	-6.80	110.41	123.58
27	a	611	PL9	C12-C13-C14	-6.79	112.76	127.75
26	b	620	BCR	C16-C17-C18	-6.77	117.37	127.22
27	A	611	PL9	C12-C13-C14	-6.77	112.83	127.75
27	a	611	PL9	C25-C24-C23	-6.76	110.49	123.58
27	d	404	PL9	C11-C9-C8	-6.76	108.39	120.98
27	d	404	PL9	C15-C14-C13	-6.75	110.50	123.58
27	d	404	PL9	C27-C28-C29	-6.75	112.87	127.75
26	b	621	BCR	C11-C10-C9	-6.74	117.42	127.22
24	B	605	CLA	O1D-CGD-CBD	-6.73	114.17	124.64
27	A	611	PL9	C32-C33-C34	-6.73	112.90	127.75
26	c	514	BCR	C20-C21-C22	-6.67	117.52	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	611	PL9	C35-C34-C33	-6.67	110.67	123.58
27	D	405	PL9	C20-C19-C18	-6.67	110.67	123.58
27	d	404	PL9	C10-C9-C8	-6.62	110.75	123.58
27	D	405	PL9	C40-C39-C38	-6.61	110.78	123.58
27	d	404	PL9	C37-C38-C39	-6.60	113.19	127.75
26	t	101	BCR	C4-C5-C6	-6.59	115.49	122.73
26	c	514	BCR	C4-C5-C6	-6.58	115.50	122.73
27	d	404	PL9	C42-C43-C44	-6.57	113.26	127.75
27	d	404	PL9	C45-C44-C43	-6.56	110.88	123.58
26	c	515	BCR	C15-C14-C13	-6.54	117.72	127.22
27	a	611	PL9	C30-C29-C28	-6.53	110.93	123.58
26	c	514	BCR	C34-C9-C10	-6.49	113.46	122.89
26	t	101	BCR	C15-C14-C13	-6.43	117.88	127.22
26	c	515	BCR	C16-C17-C18	-6.42	117.89	127.22
26	h	101	BCR	C36-C18-C17	-6.41	113.56	122.89
26	H	101	BCR	C1-C6-C5	-6.41	113.92	122.50
26	a	610	BCR	C24-C23-C22	-6.40	116.53	126.21
27	a	611	PL9	C11-C9-C8	-6.39	109.08	120.98
27	a	611	PL9	C40-C39-C41	-6.38	105.65	115.37
26	C	514	BCR	C4-C5-C6	-6.37	115.73	122.73
27	D	405	PL9	C35-C34-C33	-6.37	111.25	123.58
26	h	101	BCR	C24-C23-C22	-6.34	116.63	126.21
27	D	405	PL9	C17-C18-C19	-6.34	113.77	127.75
26	A	610	BCR	C1-C6-C5	-6.32	114.04	122.50
27	A	611	PL9	C11-C9-C8	-6.32	109.21	120.98
27	d	404	PL9	C30-C29-C28	-6.31	111.35	123.58
26	H	101	BCR	C31-C1-C6	-6.29	100.72	110.33
26	A	610	BCR	C15-C14-C13	-6.27	118.11	127.22
26	h	101	BCR	C1-C6-C5	-6.25	114.14	122.50
26	B	618	BCR	C20-C21-C22	-6.24	118.15	127.22
26	f	101	BCR	C36-C18-C17	-6.23	113.83	122.89
26	b	620	BCR	C1-C6-C5	-6.23	114.16	122.50
27	A	611	PL9	C30-C29-C28	-6.23	111.53	123.58
26	C	514	BCR	C30-C25-C26	-6.22	114.17	122.50
26	K	101	BCR	C8-C7-C6	-6.21	109.21	127.24
27	A	611	PL9	C46-C44-C43	-6.20	109.43	120.98
27	d	404	PL9	C40-C39-C38	-6.20	111.58	123.58
27	D	405	PL9	C11-C9-C8	-6.16	109.50	120.98
26	f	101	BCR	C15-C14-C13	-6.16	118.27	127.22
26	c	514	BCR	C8-C7-C6	-6.15	109.38	127.24
27	D	405	PL9	C21-C19-C18	-6.14	109.54	120.98
27	A	611	PL9	C20-C19-C18	-6.12	111.72	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	611	PL9	C26-C24-C23	-6.11	109.59	120.98
26	B	620	BCR	C24-C23-C22	-6.11	116.98	126.21
26	b	619	BCR	C36-C18-C17	-6.10	114.01	122.89
26	k	101	BCR	C8-C7-C6	-6.10	109.55	127.24
26	b	620	BCR	C7-C6-C5	-6.09	107.23	121.36
26	t	101	BCR	C16-C17-C18	-6.09	118.37	127.22
26	k	101	BCR	C1-C6-C5	-6.07	114.38	122.50
26	c	514	BCR	C24-C25-C26	-6.07	107.28	121.36
26	K	101	BCR	C4-C5-C6	-6.06	116.07	122.73
26	A	610	BCR	C11-C10-C9	-6.06	118.41	127.22
26	A	610	BCR	C30-C25-C26	-6.04	114.42	122.50
26	B	619	BCR	C24-C23-C22	-6.03	117.09	126.21
27	D	405	PL9	C42-C43-C44	-6.03	114.45	127.75
26	c	515	BCR	C30-C25-C26	-6.03	114.44	122.50
26	B	619	BCR	C15-C14-C13	-6.02	118.46	127.22
26	K	102	BCR	C4-C5-C6	-5.97	116.17	122.73
26	b	620	BCR	C12-C13-C14	-5.95	109.37	118.95
26	C	514	BCR	C23-C24-C25	-5.94	110.00	127.24
33	e	102	HEM	CBD-CAD-C3D	-5.92	102.08	112.47
26	C	514	BCR	C8-C7-C6	-5.91	110.08	127.24
26	F	101	BCR	C7-C6-C5	-5.91	107.66	121.36
26	I	101	BCR	C37-C22-C21	-5.90	114.32	122.89
27	A	611	PL9	C25-C24-C23	-5.89	112.17	123.58
27	D	405	PL9	C37-C38-C39	-5.89	114.76	127.75
26	B	620	BCR	C15-C14-C13	-5.88	118.67	127.22
26	h	101	BCR	C7-C6-C5	-5.88	107.72	121.36
27	D	405	PL9	C46-C44-C43	-5.83	110.11	120.98
26	T	101	BCR	C4-C5-C6	-5.83	116.33	122.73
26	B	620	BCR	C36-C18-C17	-5.80	114.46	122.89
27	a	611	PL9	C20-C19-C18	-5.79	112.37	123.58
26	K	102	BCR	C7-C6-C5	-5.78	107.95	121.36
26	B	620	BCR	C11-C10-C9	-5.78	118.81	127.22
26	K	101	BCR	C7-C8-C9	-5.77	117.49	126.21
26	k	101	BCR	C34-C9-C10	-5.73	114.55	122.89
26	c	521	BCR	C11-C10-C9	-5.73	118.89	127.22
26	c	514	BCR	C7-C6-C5	-5.72	108.09	121.36
33	E	103	HEM	CBD-CAD-C3D	-5.71	102.45	112.47
26	h	101	BCR	C20-C21-C22	-5.71	118.92	127.22
26	C	514	BCR	C7-C6-C5	-5.70	108.14	121.36
26	H	101	BCR	C36-C18-C17	-5.69	114.62	122.89
26	a	610	BCR	C7-C8-C9	-5.68	117.62	126.21
26	K	101	BCR	C34-C9-C10	-5.62	114.71	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	619	BCR	C38-C26-C27	-5.61	102.62	113.47
27	A	611	PL9	C21-C19-C18	-5.61	110.53	120.98
26	t	101	BCR	C7-C8-C9	-5.61	117.74	126.21
26	a	610	BCR	C20-C21-C22	-5.60	119.09	127.22
27	a	611	PL9	C46-C44-C43	-5.58	110.59	120.98
26	b	620	BCR	C20-C21-C22	-5.56	119.13	127.22
26	K	101	BCR	C7-C6-C5	-5.56	108.47	121.36
26	F	101	BCR	C1-C6-C5	-5.55	115.08	122.50
26	k	101	BCR	C15-C14-C13	-5.54	119.16	127.22
26	K	102	BCR	C15-C14-C13	-5.52	119.19	127.22
24	D	402	CLA	O1D-CGD-CBD	-5.52	116.05	124.64
26	c	521	BCR	C7-C6-C5	-5.52	108.57	121.36
26	a	610	BCR	C15-C14-C13	-5.51	119.22	127.22
27	d	404	PL9	C20-C19-C18	-5.50	112.92	123.58
26	B	618	BCR	C24-C23-C22	-5.50	117.90	126.21
26	b	619	BCR	C20-C21-C22	-5.48	119.26	127.22
26	b	619	BCR	C24-C23-C22	-5.48	117.93	126.21
26	B	618	BCR	C8-C7-C6	-5.47	111.35	127.24
26	B	620	BCR	C7-C6-C5	-5.46	108.69	121.36
26	b	621	BCR	C30-C25-C26	-5.45	115.21	122.50
26	a	610	BCR	C11-C10-C9	-5.45	119.30	127.22
26	I	101	BCR	C20-C21-C22	-5.44	119.31	127.22
27	d	404	PL9	C26-C24-C23	-5.42	110.88	120.98
26	C	514	BCR	C24-C25-C26	-5.41	108.80	121.36
26	K	102	BCR	C11-C10-C9	-5.41	119.36	127.22
26	B	618	BCR	C15-C14-C13	-5.41	119.36	127.22
27	a	611	PL9	C41-C39-C38	-5.37	110.98	120.98
24	a	607	CLA	O1D-CGD-CBD	-5.34	116.33	124.64
26	k	101	BCR	C4-C5-C6	-5.34	116.87	122.73
26	B	618	BCR	C37-C22-C21	-5.32	115.15	122.89
26	B	618	BCR	C30-C25-C26	-5.32	115.38	122.50
27	D	405	PL9	C12-C13-C14	-5.30	116.06	127.75
26	T	101	BCR	C11-C10-C9	-5.26	119.57	127.22
26	B	619	BCR	C1-C6-C5	-5.23	115.50	122.50
26	K	102	BCR	C8-C7-C6	-5.22	112.10	127.24
26	c	521	BCR	C8-C7-C6	-5.20	112.16	127.24
33	V	201	HEM	CBA-CAA-C2A	-5.18	103.38	112.49
27	A	611	PL9	C40-C39-C41	-5.16	107.51	115.37
26	B	619	BCR	C38-C26-C27	-5.13	103.55	113.47
26	B	620	BCR	C7-C8-C9	-5.12	118.48	126.21
27	D	405	PL9	C45-C44-C46	-5.12	107.58	115.37
26	B	619	BCR	C34-C9-C10	-5.10	115.47	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C7-C8-C9	-5.08	118.54	126.21
26	C	514	BCR	C31-C1-C6	-5.07	102.59	110.33
26	K	101	BCR	C16-C17-C18	-5.06	119.87	127.22
24	b	604	CLA	O1D-CGD-CBD	-5.05	116.78	124.64
26	H	101	BCR	C24-C25-C26	-5.05	109.65	121.36
24	b	605	CLA	O1D-CGD-CBD	-5.04	116.80	124.64
26	K	101	BCR	C1-C6-C5	-5.04	115.76	122.50
26	b	621	BCR	C31-C1-C6	-5.04	102.64	110.33
26	K	102	BCR	C36-C18-C17	-5.03	115.58	122.89
26	b	621	BCR	C24-C25-C26	-5.02	109.72	121.36
26	C	514	BCR	C16-C15-C14	-5.02	112.42	123.23
26	b	621	BCR	C35-C13-C14	-5.01	115.60	122.89
26	B	618	BCR	C7-C6-C5	-5.01	109.74	121.36
26	c	514	BCR	C7-C8-C9	-5.01	118.64	126.21
26	B	618	BCR	C24-C25-C26	-4.99	109.78	121.36
26	T	101	BCR	C23-C24-C25	-4.97	112.80	127.24
26	I	101	BCR	C34-C9-C10	-4.95	115.69	122.89
26	t	101	BCR	C35-C13-C12	-4.93	110.02	118.08
26	K	101	BCR	C38-C26-C27	-4.91	103.97	113.47
26	k	101	BCR	C7-C6-C5	-4.91	109.98	121.36
26	A	610	BCR	C24-C23-C22	-4.88	118.84	126.21
26	B	620	BCR	C31-C1-C6	-4.87	102.89	110.33
26	I	101	BCR	C16-C15-C14	-4.86	112.75	123.23
26	K	102	BCR	C1-C6-C5	-4.85	116.01	122.50
26	b	621	BCR	C7-C6-C5	-4.85	110.12	121.36
26	T	101	BCR	C8-C7-C6	-4.83	113.23	127.24
26	c	514	BCR	C23-C24-C25	-4.82	113.24	127.24
26	B	620	BCR	C20-C19-C18	-4.82	112.22	126.34
27	a	611	PL9	C21-C19-C18	-4.82	112.01	120.98
26	H	101	BCR	C7-C6-C5	-4.81	110.20	121.36
26	t	101	BCR	C24-C25-C26	-4.81	110.21	121.36
26	b	619	BCR	C23-C24-C25	-4.79	113.33	127.24
26	t	101	BCR	C8-C7-C6	-4.77	113.40	127.24
26	b	620	BCR	C7-C8-C9	-4.75	119.03	126.21
26	h	101	BCR	C8-C7-C6	-4.75	113.46	127.24
26	a	610	BCR	C7-C6-C5	-4.74	110.37	121.36
26	K	102	BCR	C7-C8-C9	-4.72	119.08	126.21
27	A	611	PL9	C36-C34-C33	-4.71	112.20	120.98
24	b	613	CLA	O1D-CGD-CBD	-4.70	117.32	124.64
26	T	101	BCR	C35-C13-C12	-4.70	110.41	118.08
26	b	619	BCR	C34-C9-C10	-4.69	116.07	122.89
26	I	101	BCR	C36-C18-C17	-4.67	116.09	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C11-C10-C9	-4.66	120.45	127.22
24	B	604	CLA	O1D-CGD-CBD	-4.66	117.39	124.64
26	h	101	BCR	C35-C13-C14	-4.66	116.12	122.89
26	B	619	BCR	C30-C25-C26	-4.64	116.30	122.50
26	B	620	BCR	C20-C21-C22	-4.62	120.50	127.22
26	K	101	BCR	C15-C14-C13	-4.61	120.51	127.22
26	K	101	BCR	C24-C23-C22	-4.61	119.25	126.21
26	c	515	BCR	C38-C26-C27	-4.61	104.56	113.47
26	b	619	BCR	C7-C6-C5	-4.60	110.70	121.36
26	c	521	BCR	C1-C6-C5	-4.59	116.36	122.50
26	I	101	BCR	C33-C5-C4	-4.58	104.62	113.47
26	h	101	BCR	C23-C24-C25	-4.54	114.06	127.24
26	H	101	BCR	C38-C26-C27	-4.54	104.70	113.47
26	b	620	BCR	C27-C26-C25	-4.53	117.75	122.73
26	H	101	BCR	C30-C25-C26	-4.51	116.46	122.50
26	c	521	BCR	C38-C26-C27	-4.51	104.75	113.47
26	A	610	BCR	C7-C8-C9	-4.50	119.42	126.21
26	h	101	BCR	C24-C25-C26	-4.47	110.98	121.36
26	T	101	BCR	C24-C25-C26	-4.47	111.00	121.36
26	I	101	BCR	C30-C25-C26	-4.47	116.52	122.50
27	d	404	PL9	C31-C29-C28	-4.46	112.67	120.98
26	h	101	BCR	C38-C26-C27	-4.46	104.84	113.47
24	A	607	CLA	O1D-CGD-CBD	-4.46	117.70	124.64
26	F	101	BCR	C8-C7-C6	-4.44	114.36	127.24
26	F	101	BCR	C15-C14-C13	-4.43	120.78	127.22
26	c	514	BCR	C36-C18-C17	-4.43	116.45	122.89
27	d	404	PL9	C36-C34-C33	-4.41	112.76	120.98
26	T	101	BCR	C11-C12-C13	-4.41	113.42	126.34
26	t	101	BCR	C11-C12-C13	-4.40	113.44	126.34
26	c	515	BCR	C8-C7-C6	-4.38	114.51	127.24
26	B	618	BCR	C34-C9-C10	-4.38	116.52	122.89
27	D	405	PL9	C47-C48-C49	-4.38	110.76	127.72
26	A	610	BCR	C7-C6-C5	-4.37	111.21	121.36
24	c	509	CLA	O1D-CGD-CBD	-4.37	117.83	124.64
26	a	610	BCR	C38-C26-C27	-4.36	105.05	113.47
26	f	101	BCR	C7-C6-C5	-4.35	111.28	121.36
24	b	618	CLA	C4B-CHC-C1C	-4.34	120.72	129.34
24	b	606	CLA	O1D-CGD-CBD	-4.33	117.91	124.64
26	K	102	BCR	C38-C26-C27	-4.33	105.10	113.47
27	a	611	PL9	C31-C29-C28	-4.31	112.95	120.98
27	A	611	PL9	C31-C29-C28	-4.31	112.96	120.98
24	B	605	CLA	O2D-CGD-O1D	-4.28	114.76	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C38-C26-C27	-4.26	105.22	113.47
26	a	610	BCR	C24-C25-C26	-4.25	111.51	121.36
26	c	521	BCR	C15-C14-C13	-4.23	121.07	127.22
27	D	405	PL9	C10-C9-C11	-4.23	108.93	115.37
26	b	619	BCR	C27-C26-C25	-4.22	118.09	122.73
26	T	101	BCR	C35-C13-C14	-4.22	116.75	122.89
24	D	404	CLA	O1D-CGD-CBD	-4.22	118.07	124.64
26	b	620	BCR	C38-C26-C27	-4.20	105.35	113.47
24	B	609	CLA	O1D-CGD-CBD	-4.18	118.14	124.64
24	B	617	CLA	C4B-CHC-C1C	-4.17	121.06	129.34
27	d	404	PL9	C47-C48-C49	-4.15	111.63	127.72
26	f	101	BCR	C8-C7-C6	-4.15	115.20	127.24
26	T	101	BCR	C20-C21-C22	-4.14	121.20	127.22
26	B	619	BCR	C36-C18-C19	-4.14	111.32	118.08
26	B	619	BCR	C27-C26-C25	-4.14	118.19	122.73
27	D	405	PL9	C41-C39-C38	-4.13	113.29	120.98
26	H	101	BCR	C23-C24-C25	-4.13	115.26	127.24
24	B	614	CLA	C4B-CHC-C1C	-4.13	121.14	129.34
24	a	615	CLA	O1D-CGD-CBD	-4.13	118.22	124.64
26	h	101	BCR	C31-C1-C6	-4.12	104.04	110.33
26	b	619	BCR	C37-C22-C21	-4.12	116.90	122.89
27	a	611	PL9	C45-C44-C46	-4.11	109.11	115.37
24	c	507	CLA	C4B-CHC-C1C	-4.10	121.20	129.34
24	B	612	CLA	O1D-CGD-CBD	-4.10	118.26	124.64
26	t	101	BCR	C23-C24-C25	-4.09	115.36	127.24
26	b	621	BCR	C37-C22-C21	-4.08	116.95	122.89
27	d	404	PL9	C41-C39-C38	-4.08	113.39	120.98
26	h	101	BCR	C40-C30-C25	-4.08	104.11	110.33
24	a	615	CLA	C4B-CHC-C1C	-4.06	121.28	129.34
26	b	621	BCR	C38-C26-C27	-4.05	105.64	113.47
26	B	620	BCR	C23-C22-C21	-4.05	112.43	118.95
26	C	514	BCR	C20-C19-C18	-4.04	114.50	126.34
24	c	502	CLA	O1D-CGD-CBD	-4.02	118.39	124.64
26	A	610	BCR	C27-C26-C25	-4.01	118.32	122.73
26	C	514	BCR	C38-C26-C27	-4.01	105.72	113.47
26	C	514	BCR	C36-C18-C17	-4.00	117.07	122.89
26	b	619	BCR	C30-C25-C26	-4.00	117.15	122.50
26	b	620	BCR	C30-C25-C26	-3.99	117.17	122.50
26	c	521	BCR	C35-C13-C14	-3.98	117.10	122.89
26	k	101	BCR	C23-C24-C25	-3.97	115.71	127.24
26	B	619	BCR	C20-C19-C18	-3.97	114.70	126.34
26	B	618	BCR	C23-C24-C25	-3.96	115.73	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C4B-CHC-C1C	-3.95	121.49	129.34
24	A	609	CLA	O1D-CGD-CBD	-3.94	118.51	124.64
27	A	611	PL9	C15-C14-C16	-3.93	109.38	115.37
26	B	618	BCR	C36-C18-C17	-3.93	117.17	122.89
24	C	505	CLA	O1D-CGD-CBD	-3.93	118.53	124.64
26	K	102	BCR	C23-C24-C25	-3.92	115.85	127.24
27	A	611	PL9	C45-C44-C46	-3.92	109.40	115.37
26	a	610	BCR	C36-C18-C17	-3.92	117.19	122.89
26	a	610	BCR	C8-C7-C6	-3.91	115.89	127.24
26	c	521	BCR	C24-C25-C26	-3.90	112.31	121.36
24	b	608[A]	CLA	O1D-CGD-CBD	-3.89	118.58	124.64
26	K	101	BCR	C23-C22-C21	-3.89	112.68	118.95
26	I	101	BCR	C38-C26-C27	-3.89	105.96	113.47
26	F	101	BCR	C37-C22-C21	-3.88	117.24	122.89
24	D	402	CLA	CHA-C1A-NA	-3.88	116.50	126.21
26	A	610	BCR	C34-C9-C10	-3.87	117.25	122.89
26	B	619	BCR	C11-C12-C13	-3.87	114.99	126.34
24	b	605	CLA	C4B-CHC-C1C	-3.86	121.66	129.34
26	B	618	BCR	C33-C5-C4	-3.86	106.00	113.47
32	c	518	DGD	O3G-C3G-C2G	-3.86	101.80	110.99
26	c	515	BCR	C20-C21-C22	-3.84	121.64	127.22
26	B	620	BCR	C24-C25-C26	-3.83	112.47	121.36
24	b	612	CLA	O1D-CGD-CBD	-3.82	118.69	124.64
26	B	619	BCR	C35-C13-C14	-3.82	117.33	122.89
27	a	611	PL9	C15-C14-C16	-3.81	109.56	115.37
32	C	517	DGD	O3G-C3G-C2G	-3.79	101.96	110.99
26	b	620	BCR	C37-C22-C21	-3.79	117.38	122.89
26	c	514	BCR	C16-C15-C14	-3.77	115.10	123.23
24	B	605	CLA	C4B-CHC-C1C	-3.75	121.88	129.34
24	C	511	CLA	C4B-CHC-C1C	-3.74	121.91	129.34
26	f	101	BCR	C37-C22-C23	-3.72	112.00	118.08
24	b	615	CLA	C4B-CHC-C1C	-3.72	121.94	129.34
24	B	607[A]	CLA	C4B-CHC-C1C	-3.72	121.96	129.34
24	b	613	CLA	C4B-CHC-C1C	-3.72	121.96	129.34
26	h	101	BCR	C30-C25-C26	-3.71	117.53	122.50
27	D	405	PL9	C15-C14-C16	-3.71	109.72	115.37
24	B	613	CLA	CBA-CAA-C2A	-3.71	104.40	113.96
27	a	611	PL9	C36-C34-C33	-3.71	114.08	120.98
24	a	606	CLA	C4B-CHC-C1C	-3.71	121.97	129.34
24	C	507	CLA	C4B-CHC-C1C	-3.70	121.98	129.34
26	I	101	BCR	C7-C6-C5	-3.70	112.78	121.36
26	c	515	BCR	C7-C6-C5	-3.70	112.79	121.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	610	BCR	C8-C7-C6	-3.69	116.52	127.24
25	D	401	PHO	CBA-CAA-C2A	-3.69	104.44	113.96
26	B	618	BCR	C38-C26-C27	-3.68	106.36	113.47
26	K	101	BCR	C35-C13-C14	-3.68	117.54	122.89
24	C	511	CLA	O1D-CGD-CBD	-3.67	118.93	124.64
26	b	619	BCR	C8-C7-C6	-3.67	116.60	127.24
26	A	610	BCR	C23-C22-C21	-3.66	113.05	118.95
24	c	508	CLA	O2D-CGD-O1D	-3.65	116.08	123.77
26	k	101	BCR	C24-C25-C26	-3.65	112.89	121.36
24	B	607[B]	CLA	C4B-CHC-C1C	-3.64	122.10	129.34
24	C	513	CLA	CMB-C2B-C1B	-3.64	122.12	128.31
26	B	620	BCR	C38-C26-C27	-3.63	106.45	113.47
24	b	603	CLA	O1D-CGD-CBD	-3.62	119.00	124.64
27	A	611	PL9	C47-C48-C49	-3.62	113.70	127.72
24	b	610	CLA	C4B-CHC-C1C	-3.62	122.15	129.34
26	h	101	BCR	C33-C5-C4	-3.61	106.49	113.47
24	B	607[A]	CLA	O1D-CGD-CBD	-3.61	119.03	124.64
26	A	610	BCR	C36-C18-C17	-3.60	117.64	122.89
26	K	102	BCR	C24-C25-C26	-3.60	113.00	121.36
26	C	514	BCR	C34-C9-C10	-3.59	117.66	122.89
27	D	405	PL9	C3-C2-C1	-3.59	118.70	122.59
24	b	608[B]	CLA	O1D-CGD-CBD	-3.59	119.06	124.64
24	C	505	CLA	C4B-CHC-C1C	-3.58	122.22	129.34
25	D	401	PHO	O2D-CGD-O1D	-3.58	116.23	123.77
24	A	606	CLA	C4B-CHC-C1C	-3.58	122.23	129.34
24	C	509	CLA	O1D-CGD-CBD	-3.58	119.08	124.64
27	a	611	PL9	C47-C48-C49	-3.57	113.88	127.72
24	b	608[A]	CLA	C4B-CHC-C1C	-3.57	122.25	129.34
24	a	609	CLA	CHA-C1A-NA	-3.57	117.29	126.21
24	B	604	CLA	C4B-CHC-C1C	-3.57	122.25	129.34
24	B	608	CLA	C3B-CAB-CBB	-3.56	119.24	126.40
24	c	510	CLA	C4B-CHC-C1C	-3.55	122.28	129.34
26	b	619	BCR	C24-C25-C26	-3.55	113.13	121.36
27	D	405	PL9	C51-C49-C48	-3.55	111.17	122.63
24	D	402	CLA	C4B-CHC-C1C	-3.54	122.30	129.34
26	I	101	BCR	C8-C7-C6	-3.54	116.96	127.24
24	b	614	CLA	O2D-CGD-O1D	-3.54	116.32	123.77
26	B	619	BCR	C37-C22-C21	-3.53	117.75	122.89
24	b	609	CLA	O1D-CGD-CBD	-3.53	119.15	124.64
24	b	608[B]	CLA	C4B-CHC-C1C	-3.53	122.33	129.34
26	c	514	BCR	C20-C19-C18	-3.53	116.00	126.34
24	c	505	CLA	C4B-CHC-C1C	-3.52	122.34	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	515	BCR	C23-C24-C25	-3.51	117.06	127.24
24	c	505	CLA	O1D-CGD-CBD	-3.50	119.20	124.64
26	t	101	BCR	C1-C6-C5	-3.50	117.82	122.50
28	a	612	SQD	C1-C2-C3	-3.49	103.06	109.98
27	d	404	PL9	C3-C2-C1	-3.49	118.81	122.59
26	I	101	BCR	C30-C25-C24	-3.48	106.00	115.96
28	A	612	SQD	C1-C2-C3	-3.47	103.10	109.98
24	B	602	CLA	O1D-CGD-CBD	-3.46	119.25	124.64
26	K	102	BCR	C33-C5-C4	-3.46	106.78	113.47
24	C	509	CLA	C4B-CHC-C1C	-3.46	122.47	129.34
26	c	515	BCR	C34-C9-C10	-3.45	117.86	122.89
24	C	502	CLA	C4B-CHC-C1C	-3.45	122.49	129.34
26	b	621	BCR	C1-C6-C5	-3.45	117.89	122.50
24	C	512	CLA	C4B-CHC-C1C	-3.45	122.49	129.34
27	d	404	PL9	C50-C49-C48	-3.44	111.52	122.63
24	b	615	CLA	O1D-CGD-CBD	-3.44	119.29	124.64
24	c	505	CLA	CMB-C2B-C1B	-3.44	122.47	128.31
26	c	515	BCR	C33-C5-C4	-3.43	106.83	113.47
26	I	101	BCR	C20-C19-C18	-3.43	116.28	126.34
24	D	404	CLA	CMB-C2B-C1B	-3.43	122.48	128.31
27	A	611	PL9	C50-C49-C48	-3.43	111.55	122.63
26	A	610	BCR	C33-C5-C4	-3.42	106.85	113.47
24	C	508	CLA	C4B-CHC-C1C	-3.42	122.54	129.34
27	D	405	PL9	C31-C29-C28	-3.41	114.62	120.98
26	t	101	BCR	C34-C9-C10	-3.41	117.93	122.89
24	c	509	CLA	C4B-CHC-C1C	-3.39	122.61	129.34
24	b	613	CLA	CMB-C2B-C1B	-3.39	122.55	128.31
24	B	607[B]	CLA	O1D-CGD-CBD	-3.38	119.38	124.64
26	k	101	BCR	C20-C21-C22	-3.38	122.31	127.22
26	B	620	BCR	C16-C15-C14	-3.38	115.95	123.23
24	C	504	CLA	O1D-CGD-CBD	-3.38	119.38	124.64
24	C	504	CLA	C4B-CHC-C1C	-3.38	122.63	129.34
24	C	510	CLA	C4B-CHC-C1C	-3.37	122.64	129.34
26	a	610	BCR	C34-C9-C10	-3.37	117.98	122.89
24	b	612	CLA	C4B-CHC-C1C	-3.36	122.66	129.34
24	B	612	CLA	C4B-CHC-C1C	-3.34	122.70	129.34
24	b	610	CLA	CMB-C2B-C1B	-3.34	122.64	128.31
24	D	403	CLA	O1D-CGD-CBD	-3.33	119.45	124.64
24	C	512	CLA	O1D-CGD-CBD	-3.33	119.46	124.64
24	b	603	CLA	C4B-CHC-C1C	-3.33	122.73	129.34
24	D	403	CLA	C4B-CHC-C1C	-3.32	122.73	129.34
24	b	614	CLA	C4B-CHC-C1C	-3.32	122.74	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	615	CLA	O1D-CGD-CBD	-3.32	119.47	124.64
27	D	405	PL9	C26-C24-C23	-3.32	114.80	120.98
24	C	508	CLA	O1D-CGD-CBD	-3.32	119.48	124.64
24	D	404	CLA	C4B-CHC-C1C	-3.32	122.75	129.34
24	C	507	CLA	O1D-CGD-CBD	-3.31	119.48	124.64
24	B	613	CLA	C4B-CHC-C1C	-3.31	122.77	129.34
27	a	611	PL9	C25-C24-C26	-3.29	110.36	115.37
24	B	608	CLA	C4B-CHC-C1C	-3.29	122.81	129.34
27	d	404	PL9	C45-C44-C46	-3.27	110.38	115.37
24	C	510	CLA	O1D-CGD-CBD	-3.27	119.55	124.64
24	c	507	CLA	C3B-CAB-CBB	-3.25	119.86	126.40
24	B	612	CLA	CMB-C2B-C1B	-3.25	122.79	128.31
24	B	610	CLA	C4B-CHC-C1C	-3.24	122.89	129.34
27	D	405	PL9	C36-C34-C33	-3.24	114.94	120.98
27	d	404	PL9	C51-C49-C48	-3.24	112.17	122.63
24	C	507	CLA	C3B-CAB-CBB	-3.23	119.90	126.40
24	b	611	CLA	O1D-CGD-CBD	-3.23	119.62	124.64
24	A	607	CLA	C4B-CHC-C1C	-3.22	122.93	129.34
24	c	507	CLA	O1D-CGD-CBD	-3.22	119.62	124.64
24	b	607	CLA	O1D-CGD-CBD	-3.22	119.63	124.64
24	B	616	CLA	O1D-CGD-CBD	-3.22	119.63	124.64
24	C	501	CLA	O1D-CGD-CBD	-3.22	119.63	124.64
24	d	403	CLA	C4B-CHC-C1C	-3.21	122.95	129.34
26	b	619	BCR	C30-C25-C24	-3.21	106.78	115.96
27	D	405	PL9	C50-C49-C48	-3.21	112.26	122.63
24	C	508	CLA	CMB-C2B-C1B	-3.21	122.85	128.31
27	a	611	PL9	C50-C49-C48	-3.21	112.26	122.63
24	b	611	CLA	O2D-CGD-O1D	-3.21	117.02	123.77
24	C	506	CLA	CMB-C2B-C1B	-3.20	122.86	128.31
24	c	502	CLA	C4B-CHC-C1C	-3.20	122.98	129.34
26	A	610	BCR	C16-C15-C14	-3.19	116.35	123.23
24	a	607	CLA	CHA-C1A-NA	-3.19	118.24	126.21
24	a	615	CLA	CHA-C1A-NA	-3.18	118.25	126.21
24	B	603	CLA	O1D-CGD-CBD	-3.18	119.69	124.64
24	b	617	CLA	C4B-CHC-C1C	-3.18	123.02	129.34
26	c	514	BCR	C31-C1-C6	-3.18	105.48	110.33
26	b	621	BCR	C7-C8-C9	-3.17	121.41	126.21
24	b	616	CLA	CMB-C2B-C1B	-3.17	122.92	128.31
24	C	513	CLA	C4B-CHC-C1C	-3.17	123.05	129.34
24	b	616	CLA	O2D-CGD-O1D	-3.16	117.11	123.77
24	C	507	CLA	O2D-CGD-O1D	-3.16	117.11	123.77
30	d	406	LHG	C5-O7-C7	-3.16	110.10	117.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C4B-CHC-C1C	-3.16	123.06	129.34
26	t	101	BCR	C35-C13-C14	-3.16	118.30	122.89
24	b	609	CLA	CMB-C2B-C1B	-3.15	122.95	128.31
26	b	620	BCR	C16-C15-C14	-3.15	116.44	123.23
26	K	101	BCR	C23-C24-C25	-3.15	118.10	127.24
26	F	101	BCR	C20-C21-C22	-3.15	122.64	127.22
24	c	508	CLA	CMB-C2B-C1B	-3.15	122.96	128.31
26	B	620	BCR	C37-C22-C21	-3.14	118.31	122.89
24	B	615	CLA	C4B-CHC-C1C	-3.14	123.10	129.34
26	c	521	BCR	C34-C9-C10	-3.14	118.32	122.89
24	B	603	CLA	O2D-CGD-O1D	-3.14	117.17	123.77
27	d	404	PL9	C30-C29-C31	-3.13	110.60	115.37
24	b	616	CLA	O1D-CGD-CBD	-3.13	119.76	124.64
24	b	618	CLA	O1D-CGD-CBD	-3.13	119.76	124.64
26	t	101	BCR	C38-C26-C27	-3.13	107.42	113.47
26	T	101	BCR	C37-C22-C21	-3.13	118.34	122.89
26	T	101	BCR	C33-C5-C4	-3.12	107.43	113.47
26	B	620	BCR	C12-C13-C14	-3.12	113.92	118.95
26	c	514	BCR	C3-C4-C5	-3.12	108.69	113.87
24	b	610	CLA	O2D-CGD-O1D	-3.12	117.20	123.77
24	a	615	CLA	CMB-C2B-C1B	-3.12	123.00	128.31
26	K	101	BCR	C33-C5-C4	-3.12	107.44	113.47
26	k	101	BCR	C23-C22-C21	-3.11	113.94	118.95
26	h	101	BCR	C37-C22-C21	-3.10	118.38	122.89
24	B	606	CLA	O1D-CGD-CBD	-3.10	119.82	124.64
26	k	101	BCR	C33-C5-C4	-3.10	107.48	113.47
24	D	404	CLA	CHA-C1A-NA	-3.09	118.47	126.21
26	K	101	BCR	C11-C12-C13	-3.09	117.27	126.34
26	h	101	BCR	C20-C19-C18	-3.08	117.30	126.34
24	d	402	CLA	O1D-CGD-CBD	-3.08	119.84	124.64
27	D	405	PL9	C40-C39-C41	-3.08	110.68	115.37
26	K	101	BCR	C37-C22-C21	-3.08	118.41	122.89
26	c	515	BCR	C24-C25-C26	-3.07	114.23	121.36
24	d	403	CLA	O1D-CGD-CBD	-3.07	119.86	124.64
29	Z	101	LMG	O2-C2-C3	-3.07	103.44	110.36
24	b	617	CLA	O2D-CGD-O1D	-3.07	117.31	123.77
26	T	101	BCR	C38-C26-C27	-3.07	107.54	113.47
24	c	504	CLA	O1D-CGD-CBD	-3.06	119.88	124.64
24	C	506	CLA	C4B-CHC-C1C	-3.06	123.27	129.34
26	H	101	BCR	C10-C11-C12	-3.05	113.67	123.11
24	c	501	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
26	A	610	BCR	C38-C26-C27	-3.04	107.58	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	O1D-CGD-CBD	-3.04	119.90	124.64
26	k	101	BCR	C37-C22-C21	-3.04	118.46	122.89
26	b	621	BCR	C20-C19-C18	-3.04	117.44	126.34
24	a	606	CLA	CMB-C2B-C1B	-3.03	123.15	128.31
24	B	610	CLA	O1D-CGD-CBD	-3.03	119.93	124.64
24	b	616	CLA	C4B-CHC-C1C	-3.03	123.33	129.34
24	c	505	CLA	O2D-CGD-O1D	-3.02	117.41	123.77
30	A	615	LHG	C5-O7-C7	-3.02	110.45	117.91
24	c	512	CLA	C4B-CHC-C1C	-3.01	123.35	129.34
24	c	506	CLA	CMB-C2B-C1B	-3.01	123.19	128.31
24	C	505	CLA	O2D-CGD-O1D	-3.01	117.43	123.77
24	A	609	CLA	CHA-C1A-NA	-3.00	118.70	126.21
26	a	610	BCR	C11-C12-C13	-2.99	117.57	126.34
32	C	516	DGD	O6D-C5D-C4D	-2.99	103.96	109.67
24	B	609	CLA	CAC-C3C-C2C	-2.99	122.37	127.51
26	b	620	BCR	C20-C19-C18	-2.99	117.58	126.34
32	C	517	DGD	C3G-C2G-C1G	-2.99	105.12	112.08
27	d	404	PL9	C15-C14-C16	-2.98	110.83	115.37
27	A	611	PL9	C51-C49-C48	-2.98	113.00	122.63
24	B	614	CLA	O2D-CGD-O1D	-2.98	117.50	123.77
26	B	620	BCR	C1-C6-C7	-2.98	107.44	115.96
24	b	604	CLA	O2D-CGD-O1D	-2.98	117.50	123.77
24	c	501	CLA	C4B-CHC-C1C	-2.97	123.44	129.34
26	K	101	BCR	C24-C25-C26	-2.97	114.48	121.36
33	v	201	HEM	CBA-CAA-C2A	-2.96	107.28	112.49
26	t	101	BCR	C16-C15-C14	-2.96	116.85	123.23
26	B	620	BCR	C23-C24-C25	-2.96	118.65	127.24
26	T	101	BCR	C16-C15-C14	-2.96	116.85	123.23
26	H	101	BCR	C8-C9-C10	-2.96	114.19	118.95
32	C	516	DGD	C1D-O6D-C5D	-2.95	107.95	113.74
26	I	101	BCR	C15-C14-C13	-2.95	122.93	127.22
24	B	603	CLA	C4B-CHC-C1C	-2.94	123.49	129.34
24	c	504	CLA	C4B-CHC-C1C	-2.94	123.50	129.34
26	H	101	BCR	C35-C13-C14	-2.94	118.61	122.89
24	C	512	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
24	B	617	CLA	C3B-CAB-CBB	-2.94	120.49	126.40
26	f	101	BCR	C34-C9-C10	-2.94	118.61	122.89
26	c	521	BCR	C33-C5-C4	-2.92	107.81	113.47
24	c	511	CLA	O1D-CGD-CBD	-2.92	120.09	124.64
24	d	402	CLA	C3C-C4C-NC	-2.92	107.25	110.21
24	c	503	CLA	C4B-CHC-C1C	-2.92	123.53	129.34
24	C	510	CLA	O2D-CGD-O1D	-2.92	117.63	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	O1D-CGD-CBD	-2.91	120.11	124.64
26	b	620	BCR	C34-C9-C10	-2.91	118.65	122.89
24	d	402	CLA	CMB-C2B-C1B	-2.91	123.36	128.31
24	b	609	CLA	C3B-CAB-CBB	-2.91	120.55	126.40
24	B	617	CLA	O1D-CGD-CBD	-2.90	120.12	124.64
26	B	620	BCR	C1-C6-C5	-2.90	118.62	122.50
29	B	621	LMG	C6-C5-C4	-2.90	105.72	112.99
28	A	612	SQD	C45-O47-C7	-2.90	110.75	117.91
26	F	101	BCR	C12-C13-C14	-2.90	114.29	118.95
24	B	608	CLA	O1D-CGD-CBD	-2.89	120.14	124.64
24	a	609	CLA	C4B-CHC-C1C	-2.89	123.59	129.34
28	a	612	SQD	C45-O47-C7	-2.89	110.76	117.91
26	c	515	BCR	C36-C18-C17	-2.88	118.69	122.89
24	c	508	CLA	C4B-CHC-C1C	-2.88	123.61	129.34
26	a	610	BCR	C33-C5-C4	-2.88	107.90	113.47
24	a	607	CLA	CMB-C2B-C1B	-2.88	123.41	128.31
24	c	512	CLA	CMB-C2B-C1B	-2.87	123.42	128.31
26	t	101	BCR	C20-C21-C22	-2.87	123.05	127.22
32	c	517	DGD	O6D-C5D-C4D	-2.87	104.19	109.67
24	b	612	CLA	O2D-CGD-O1D	-2.86	117.75	123.77
30	A	615	LHG	O8-C23-O10	-2.86	116.01	123.51
24	b	618	CLA	CBA-CAA-C2A	-2.86	106.59	113.96
24	C	505	CLA	C3B-CAB-CBB	-2.86	120.65	126.40
29	b	622	LMG	C6-C5-C4	-2.86	105.83	112.99
24	b	614	CLA	O1D-CGD-CBD	-2.85	120.20	124.64
24	c	513	CLA	C4B-CHC-C1C	-2.84	123.69	129.34
26	H	101	BCR	C33-C5-C4	-2.84	107.98	113.47
24	B	617	CLA	CHC-C1C-C2C	-2.84	118.45	126.31
26	a	610	BCR	C23-C24-C25	-2.84	119.01	127.24
26	c	514	BCR	C10-C11-C12	-2.84	114.35	123.11
24	B	604	CLA	CMB-C2B-C1B	-2.83	123.49	128.31
26	B	618	BCR	C30-C25-C24	-2.83	107.88	115.96
25	d	401	PHO	CMB-C2B-C1B	-2.82	120.55	125.06
26	b	620	BCR	C35-C13-C14	-2.82	118.78	122.89
28	l	101	SQD	C1-O5-C5	-2.82	108.21	113.74
26	t	101	BCR	C36-C18-C17	-2.82	118.79	122.89
24	B	604	CLA	O2D-CGD-O1D	-2.81	117.84	123.77
28	L	102	SQD	C1-O5-C5	-2.81	108.22	113.74
26	F	101	BCR	C37-C22-C23	-2.81	113.49	118.08
26	I	101	BCR	C1-C6-C7	-2.81	107.93	115.96
24	b	606	CLA	C4B-CHC-C1C	-2.80	123.77	129.34
24	c	507	CLA	O2D-CGD-O1D	-2.80	117.88	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	606	CLA	O1D-CGD-CBD	-2.80	120.28	124.64
24	a	615	CLA	CHC-C1C-C2C	-2.80	118.55	126.31
24	B	613	CLA	CMB-C2B-C1B	-2.79	123.57	128.31
24	b	611	CLA	CBA-CAA-C2A	-2.78	106.79	113.96
24	c	506	CLA	C4B-CHC-C1C	-2.78	123.81	129.34
26	A	610	BCR	C24-C25-C26	-2.78	114.91	121.36
26	I	101	BCR	C24-C25-C26	-2.77	114.94	121.36
26	T	101	BCR	C1-C6-C5	-2.77	118.80	122.50
24	b	607	CLA	C4B-CHC-C1C	-2.76	123.85	129.34
26	A	610	BCR	C20-C19-C18	-2.76	118.25	126.34
24	b	612	CLA	C3B-CAB-CBB	-2.75	120.86	126.40
32	c	516	DGD	O6D-C5D-C4D	-2.75	104.41	109.67
24	C	510	CLA	CMB-C2B-C1B	-2.75	123.63	128.31
24	d	403	CLA	CHA-C1A-NA	-2.75	119.33	126.21
30	D	406	LHG	C5-O7-C7	-2.75	111.11	117.91
24	b	614	CLA	CBA-CAA-C2A	-2.75	106.88	113.96
24	c	513	CLA	CMB-C2B-C1B	-2.75	123.64	128.31
24	a	607	CLA	C4B-CHC-C1C	-2.74	123.89	129.34
24	b	614	CLA	CHA-C1A-NA	-2.73	119.37	126.21
24	B	612	CLA	CHA-C1A-NA	-2.73	119.39	126.21
24	c	512	CLA	O1D-CGD-CBD	-2.73	120.40	124.64
26	b	620	BCR	C10-C11-C12	-2.72	114.71	123.11
24	b	618	CLA	C3B-CAB-CBB	-2.72	120.93	126.40
26	b	621	BCR	C23-C24-C25	-2.71	119.39	127.24
24	C	504	CLA	CMB-C2B-C1B	-2.70	123.72	128.31
27	a	611	PL9	C51-C49-C48	-2.70	113.90	122.63
26	c	515	BCR	C1-C6-C7	-2.70	108.24	115.96
32	c	518	DGD	C2G-O2G-C1B	-2.70	111.24	117.91
24	b	603	CLA	CHA-C1A-NA	-2.70	119.47	126.21
24	A	606	CLA	C4A-NA-C1A	-2.69	102.96	106.38
24	b	604	CLA	C4B-CHC-C1C	-2.69	124.00	129.34
24	b	608[B]	CLA	C3B-CAB-CBB	-2.69	120.99	126.40
26	H	101	BCR	C20-C19-C18	-2.69	118.46	126.34
32	C	517	DGD	O2E-C2E-C3E	-2.68	104.31	110.36
24	b	618	CLA	CHC-C1C-C2C	-2.68	118.90	126.31
30	d	407	LHG	C5-O7-C7	-2.67	111.30	117.91
26	k	101	BCR	C35-C13-C14	-2.67	119.00	122.89
26	C	514	BCR	C37-C22-C21	-2.67	119.00	122.89
24	A	606	CLA	CMB-C2B-C1B	-2.67	123.77	128.31
24	B	614	CLA	CHC-C1C-C2C	-2.67	118.91	126.31
24	C	510	CLA	C4A-NA-C1A	-2.67	102.99	106.38
24	b	608[A]	CLA	C3B-CAB-CBB	-2.67	121.04	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	CMB-C2B-C1B	-2.67	123.78	128.31
24	C	510	CLA	CHA-C1A-NA	-2.66	119.56	126.21
26	A	610	BCR	C40-C30-C25	-2.66	106.27	110.33
26	t	101	BCR	C30-C25-C24	-2.66	108.36	115.96
28	a	612	SQD	C44-O6-C1	-2.65	108.27	113.81
26	h	101	BCR	C30-C25-C24	-2.65	108.37	115.96
24	b	613	CLA	CHC-C1C-C2C	-2.65	118.96	126.31
24	B	609	CLA	CMB-C2B-C1B	-2.65	123.81	128.31
24	c	511	CLA	C4B-CHC-C1C	-2.64	124.09	129.34
28	A	612	SQD	C44-O6-C1	-2.63	108.31	113.81
24	b	613	CLA	CHA-C1A-NA	-2.63	119.63	126.21
24	c	512	CLA	O2D-CGD-O1D	-2.63	118.24	123.77
24	A	607	CLA	CHA-C1A-NA	-2.62	119.64	126.21
24	a	606	CLA	CHA-C1A-NA	-2.62	119.65	126.21
24	b	605	CLA	CHA-C1A-NA	-2.62	119.65	126.21
26	c	521	BCR	C7-C8-C9	-2.62	122.25	126.21
32	c	518	DGD	C3G-C2G-C1G	-2.61	106.00	112.08
24	c	507	CLA	CHC-C1C-C2C	-2.61	119.09	126.31
32	c	516	DGD	O3G-C3G-C2G	-2.60	104.81	110.99
24	c	501	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
24	B	605	CLA	C3B-CAB-CBB	-2.60	121.17	126.40
24	b	609	CLA	C4B-CHC-C1C	-2.60	124.18	129.34
29	z	101	LMG	O2-C2-C3	-2.60	104.51	110.36
24	b	615	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
24	c	513	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
26	t	101	BCR	C3-C4-C5	-2.59	109.57	113.87
24	B	606	CLA	C4B-CHC-C1C	-2.59	124.19	129.34
26	C	514	BCR	C1-C6-C5	-2.59	119.03	122.50
24	B	607[B]	CLA	C3B-CAB-CBB	-2.59	121.19	126.40
24	d	402	CLA	C4B-CHC-C1C	-2.59	124.20	129.34
24	B	602	CLA	C4B-CHC-C1C	-2.59	124.20	129.34
26	c	515	BCR	C30-C25-C24	-2.58	108.57	115.96
26	c	514	BCR	C30-C25-C24	-2.58	108.57	115.96
24	B	607[A]	CLA	C3B-CAB-CBB	-2.58	121.21	126.40
28	A	612	SQD	C1-O5-C5	-2.58	108.69	113.74
26	b	621	BCR	C34-C9-C10	-2.57	119.14	122.89
24	c	502	CLA	C3B-CAB-CBB	-2.57	121.23	126.40
24	A	609	CLA	CMB-C2B-C1B	-2.57	123.94	128.31
32	c	516	DGD	C2G-O2G-C1B	-2.57	111.56	117.91
26	B	618	BCR	C2-C1-C6	-2.57	106.66	110.48
26	h	101	BCR	C11-C12-C13	-2.56	118.82	126.34
24	b	615	CLA	C3B-CAB-CBB	-2.56	121.24	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	O1D-CGD-CBD	-2.56	120.66	124.64
26	b	619	BCR	C33-C5-C4	-2.55	108.53	113.47
24	d	402	CLA	O2D-CGD-O1D	-2.55	118.41	123.77
24	b	606	CLA	CHA-C1A-NA	-2.55	119.84	126.21
24	A	606	CLA	CHA-C1A-NA	-2.55	119.84	126.21
24	C	503	CLA	C4B-CHC-C1C	-2.54	124.30	129.34
32	c	518	DGD	C3G-O3G-C1D	-2.54	108.51	113.81
24	a	609	CLA	CMB-C2B-C1B	-2.54	124.00	128.31
28	a	612	SQD	C1-O5-C5	-2.53	108.78	113.74
26	C	514	BCR	C12-C13-C14	-2.53	114.88	118.95
24	B	614	CLA	O1D-CGD-CBD	-2.53	120.71	124.64
30	a	616	LHG	C5-O7-C7	-2.52	111.67	117.91
24	A	606	CLA	CHC-C1C-C2C	-2.52	119.33	126.31
25	D	401	PHO	CMB-C2B-C1B	-2.51	121.05	125.06
24	B	608	CLA	O2D-CGD-O1D	-2.51	118.48	123.77
24	B	611	CLA	O2A-CGA-O1A	-2.51	116.93	123.51
24	b	611	CLA	C4B-CHC-C1C	-2.51	124.36	129.34
24	C	502	CLA	O2D-CGD-O1D	-2.51	118.50	123.77
26	C	514	BCR	C30-C25-C24	-2.50	108.81	115.96
24	A	607	CLA	CMB-C2B-C1B	-2.50	124.06	128.31
24	c	501	CLA	O1D-CGD-CBD	-2.50	120.75	124.64
26	B	619	BCR	C24-C25-C26	-2.50	115.57	121.36
26	c	514	BCR	C38-C26-C27	-2.49	108.67	113.47
26	T	101	BCR	C20-C19-C18	-2.48	119.06	126.34
26	B	620	BCR	C33-C5-C4	-2.48	108.67	113.47
32	C	515	DGD	O3G-C3G-C2G	-2.48	105.10	110.99
24	B	613	CLA	O1D-CGD-CBD	-2.47	120.79	124.64
26	t	101	BCR	C8-C9-C10	-2.47	114.97	118.95
24	A	607	CLA	CHC-C1C-C2C	-2.47	119.48	126.31
24	D	402	CLA	O2D-CGD-O1D	-2.47	118.58	123.77
27	D	405	PL9	C7-C3-C2	-2.46	119.08	122.66
25	d	401	PHO	O2D-CGD-O1D	-2.46	118.58	123.77
24	C	509	CLA	CHC-C1C-C2C	-2.46	119.48	126.31
26	k	101	BCR	C36-C18-C17	-2.46	119.31	122.89
24	C	502	CLA	CMB-C2B-C1B	-2.46	124.13	128.31
24	b	615	CLA	CHC-C1C-C2C	-2.46	119.50	126.31
24	b	605	CLA	CHC-C1C-C2C	-2.46	119.50	126.31
24	c	511	CLA	O2D-CGD-O1D	-2.46	118.60	123.77
24	B	602	CLA	C4-C3-C2	-2.45	118.83	123.58
24	D	402	CLA	C3B-CAB-CBB	-2.45	121.47	126.40
24	C	502	CLA	O1D-CGD-CBD	-2.45	120.82	124.64
24	B	611	CLA	C4B-CHC-C1C	-2.45	124.47	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	607	CLA	O2D-CGD-O1D	-2.45	118.62	123.77
24	b	618	CLA	O2D-CGD-O1D	-2.44	118.62	123.77
26	F	101	BCR	C34-C9-C10	-2.44	119.33	122.89
24	C	513	CLA	C3C-C4C-NC	-2.44	107.73	110.21
26	B	619	BCR	C36-C18-C17	-2.44	119.33	122.89
26	K	102	BCR	C39-C30-C25	-2.44	106.61	110.33
24	D	402	CLA	CMB-C2B-C1B	-2.44	124.17	128.31
24	a	615	CLA	O2A-CGA-O1A	-2.44	117.12	123.51
26	K	102	BCR	C16-C15-C14	-2.44	117.98	123.23
24	A	606	CLA	O2D-CGD-O1D	-2.43	118.65	123.77
26	f	101	BCR	C30-C25-C24	-2.43	109.00	115.96
26	K	101	BCR	C1-C6-C7	-2.43	109.01	115.96
25	A	608	PHO	O2D-CGD-O1D	-2.43	118.66	123.77
24	b	611	CLA	C3B-CAB-CBB	-2.43	121.52	126.40
24	a	606	CLA	CBA-CAA-C2A	-2.43	107.71	113.96
33	v	201	HEM	CAA-CBA-CGA	-2.42	108.07	112.78
24	C	512	CLA	CHC-C1C-C2C	-2.42	119.59	126.31
24	b	603	CLA	C4-C3-C2	-2.42	118.89	123.58
26	B	618	BCR	C1-C6-C7	-2.41	109.06	115.96
27	d	404	PL9	C7-C3-C2	-2.41	119.16	122.66
24	B	614	CLA	C3B-CAB-CBB	-2.41	121.56	126.40
26	T	101	BCR	C36-C18-C17	-2.41	119.39	122.89
26	a	610	BCR	C20-C19-C18	-2.40	119.29	126.34
24	C	511	CLA	CMB-C2B-C1B	-2.40	124.23	128.31
24	B	606	CLA	CBA-CAA-C2A	-2.40	107.77	113.96
32	C	515	DGD	C3G-C2G-C1G	-2.40	106.49	112.08
24	b	618	CLA	CHA-C1A-NA	-2.40	120.21	126.21
24	D	403	CLA	CHA-C1A-NA	-2.40	120.21	126.21
26	I	101	BCR	C23-C22-C21	-2.40	115.09	118.95
24	c	506	CLA	O2D-CGD-O1D	-2.40	118.73	123.77
26	h	101	BCR	C1-C6-C7	-2.39	109.13	115.96
32	H	102	DGD	O5E-C6E-C5E	-2.39	103.34	111.30
24	c	512	CLA	CHA-C1A-NA	-2.39	120.24	126.21
24	c	509	CLA	CMB-C2B-C1B	-2.38	124.26	128.31
24	D	404	CLA	C3B-CAB-CBB	-2.38	121.61	126.40
26	h	101	BCR	C10-C11-C12	-2.38	115.76	123.11
24	A	609	CLA	C4B-CHC-C1C	-2.38	124.62	129.34
24	a	615	CLA	CAA-CBA-CGA	-2.38	106.41	113.28
24	b	617	CLA	O1D-CGD-CBD	-2.37	120.94	124.64
26	T	101	BCR	C1-C6-C7	-2.37	109.18	115.96
26	K	101	BCR	C16-C15-C14	-2.37	118.13	123.23
24	c	510	CLA	CHC-C1C-C2C	-2.36	119.76	126.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	610	CLA	O1D-CGD-CBD	-2.36	120.96	124.64
32	C	517	DGD	C2G-O2G-C1B	-2.36	112.06	117.91
24	C	513	CLA	O1D-CGD-CBD	-2.36	120.96	124.64
24	B	607[B]	CLA	CHC-C1C-C2C	-2.36	119.77	126.31
24	D	403	CLA	CMB-C2B-C1B	-2.36	124.31	128.31
24	C	513	CLA	CHA-C1A-NA	-2.35	120.32	126.21
24	c	504	CLA	CMB-C2B-C1B	-2.35	124.31	128.31
25	a	608	PHO	O2A-CGA-O1A	-2.35	117.35	123.51
24	a	606	CLA	CHC-C1C-C2C	-2.35	119.80	126.31
27	D	405	PL9	C20-C19-C21	-2.35	111.79	115.37
27	d	404	PL9	C10-C9-C11	-2.35	111.79	115.37
24	D	402	CLA	CHC-C1C-C2C	-2.34	119.82	126.31
26	c	514	BCR	C33-C5-C4	-2.34	108.94	113.47
24	C	511	CLA	CHC-C1C-C2C	-2.34	119.82	126.31
24	b	612	CLA	CHC-C1C-C2C	-2.34	119.83	126.31
26	t	101	BCR	C39-C30-C25	-2.34	106.76	110.33
24	b	608[A]	CLA	CHA-C1A-NA	-2.33	120.37	126.21
26	b	621	BCR	C11-C12-C13	-2.33	119.50	126.34
25	d	401	PHO	C6-C5-C3	-2.33	108.59	112.76
27	A	611	PL9	C3-C2-C1	-2.33	120.07	122.59
24	b	607	CLA	CBA-CAA-C2A	-2.32	107.97	113.96
29	C	518	LMG	O1-C7-C8	-2.32	105.46	110.99
26	b	621	BCR	C33-C5-C4	-2.32	108.98	113.47
32	c	518	DGD	O4D-C4D-C3D	-2.32	105.13	110.36
24	B	608	CLA	CMB-C2B-C1B	-2.32	124.37	128.31
24	C	512	CLA	O2D-CGD-O1D	-2.31	118.90	123.77
27	A	611	PL9	C25-C24-C26	-2.31	111.85	115.37
24	B	609	CLA	CHC-C1C-C2C	-2.31	119.91	126.31
24	c	510	CLA	CMB-C2B-C1B	-2.31	124.38	128.31
24	B	607[A]	CLA	CHC-C1C-C2C	-2.30	119.92	126.31
24	c	506	CLA	O1D-CGD-CBD	-2.30	121.06	124.64
24	C	501	CLA	O2D-CGD-O1D	-2.30	118.92	123.77
24	b	607	CLA	C3B-CAB-CBB	-2.30	121.77	126.40
29	D	408	LMG	O8-C28-O10	-2.30	117.48	123.51
26	F	101	BCR	C30-C25-C24	-2.30	109.39	115.96
30	D	406	LHG	O7-C7-O9	-2.29	117.43	123.67
24	b	603	CLA	CHC-C1C-C2C	-2.29	119.96	126.31
24	C	503	CLA	O1D-CGD-CBD	-2.29	121.08	124.64
24	C	507	CLA	CHC-C1C-C2C	-2.28	119.98	126.31
26	h	101	BCR	C11-C10-C9	-2.28	123.91	127.22
24	a	615	CLA	C3B-CAB-CBB	-2.27	121.83	126.40
24	C	507	CLA	OBD-CAD-C3D	-2.27	124.08	128.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	BCR	C28-C27-C26	-2.26	110.11	113.87
24	C	502	CLA	CHA-C1A-NA	-2.26	120.55	126.21
24	c	513	CLA	C3C-C4C-NC	-2.26	107.92	110.21
24	C	509	CLA	CMB-C2B-C1B	-2.26	124.47	128.31
26	k	101	BCR	C12-C13-C14	-2.26	115.31	118.95
27	D	405	PL9	C30-C29-C31	-2.26	111.93	115.37
32	E	101	DGD	C6D-C5D-C4D	-2.26	106.85	112.00
24	b	605	CLA	CAA-C2A-C3A	-2.25	106.67	112.79
24	c	501	CLA	CHA-C1A-NA	-2.25	120.57	126.21
24	B	608	CLA	CHC-C1C-C2C	-2.25	120.07	126.31
26	A	610	BCR	C1-C6-C7	-2.25	109.52	115.96
26	c	514	BCR	C12-C13-C14	-2.25	115.33	118.95
24	b	608[B]	CLA	CHA-C1A-NA	-2.25	120.58	126.21
24	B	609	CLA	O2D-CGD-O1D	-2.24	119.04	123.77
26	T	101	BCR	C30-C25-C24	-2.24	109.56	115.96
24	b	606	CLA	O2D-CGD-O1D	-2.24	119.06	123.77
26	B	620	BCR	C3-C4-C5	-2.24	110.16	113.87
24	B	615	CLA	CHA-C1A-NA	-2.24	120.62	126.21
24	b	610	CLA	C11-C12-C13	-2.23	108.55	115.46
24	C	503	CLA	C3B-CAB-CBB	-2.23	121.92	126.40
26	B	618	BCR	C39-C30-C25	-2.23	106.93	110.33
32	c	516	DGD	O1G-C1A-O1A	-2.23	117.67	123.51
24	b	614	CLA	CHC-C1C-C2C	-2.22	120.15	126.31
26	c	515	BCR	C16-C15-C14	-2.22	118.44	123.23
24	c	507	CLA	CHA-C1A-NA	-2.22	120.66	126.21
26	b	620	BCR	C32-C1-C6	-2.22	106.94	110.33
24	a	609	CLA	O1D-CGD-CBD	-2.22	121.19	124.64
24	b	617	CLA	OBD-CAD-C3D	-2.22	124.17	128.09
27	d	404	PL9	C35-C34-C36	-2.21	112.00	115.37
24	b	618	CLA	O2A-CGA-O1A	-2.21	117.71	123.51
24	B	616	CLA	CHA-C1A-NA	-2.21	120.68	126.21
32	d	405	DGD	O2G-C1B-O1B	-2.21	117.66	123.67
26	T	101	BCR	C3-C4-C5	-2.21	110.21	113.87
24	B	604	CLA	CHC-C1C-C2C	-2.21	120.19	126.31
24	B	606	CLA	C3D-CAD-CBD	-2.20	104.48	107.60
26	t	101	BCR	C33-C5-C4	-2.20	109.21	113.47
26	t	101	BCR	C1-C6-C7	-2.20	109.66	115.96
24	B	605	CLA	CHC-C1C-C2C	-2.20	120.21	126.31
24	D	404	CLA	C4A-NA-C1A	-2.20	103.58	106.38
24	B	610	CLA	CHC-C1C-C2C	-2.20	120.22	126.31
24	B	609	CLA	C11-C12-C13	-2.20	108.65	115.46
24	C	504	CLA	C3C-C4C-NC	-2.20	107.98	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	CHC-C1C-C2C	-2.20	120.22	126.31
24	C	511	CLA	O2A-CGA-O1A	-2.20	117.75	123.51
24	B	616	CLA	O2A-CGA-O1A	-2.19	117.77	123.51
24	c	503	CLA	C3B-CAB-CBB	-2.19	121.99	126.40
24	C	501	CLA	C4B-CHC-C1C	-2.19	124.99	129.34
24	C	502	CLA	C3B-CAB-CBB	-2.19	122.00	126.40
26	c	515	BCR	C35-C13-C14	-2.19	119.71	122.89
24	B	608	CLA	CBA-CAA-C2A	-2.19	108.32	113.96
25	a	608	PHO	CMB-C2B-C1B	-2.18	121.57	125.06
27	a	611	PL9	C20-C19-C21	-2.18	112.05	115.37
26	B	620	BCR	C11-C12-C13	-2.18	119.95	126.34
24	c	501	CLA	CHC-C1C-C2C	-2.18	120.27	126.31
26	C	514	BCR	C1-C6-C7	-2.18	109.73	115.96
26	C	514	BCR	C11-C12-C13	-2.18	119.95	126.34
32	h	102	DGD	O2G-C1B-O1B	-2.18	117.75	123.67
24	B	612	CLA	CHC-C1C-C2C	-2.18	120.28	126.31
24	B	613	CLA	O2D-CGD-O1D	-2.18	119.19	123.77
24	C	504	CLA	C3B-CAB-CBB	-2.18	122.02	126.40
24	b	612	CLA	CHA-C1A-NA	-2.17	120.78	126.21
24	A	606	CLA	C3C-C4C-NC	-2.17	108.01	110.21
26	b	619	BCR	C39-C30-C25	-2.17	107.02	110.33
24	B	617	CLA	C4-C3-C2	-2.17	119.39	123.58
32	C	516	DGD	O1G-C1A-O1A	-2.17	117.83	123.51
24	c	504	CLA	CHA-C1A-NA	-2.16	120.80	126.21
24	C	513	CLA	C3B-CAB-CBB	-2.16	122.05	126.40
24	B	604	CLA	CHA-C1A-NA	-2.16	120.81	126.21
24	b	604	CLA	CHA-C1A-NA	-2.16	120.81	126.21
29	D	408	LMG	O7-C10-O9	-2.16	117.80	123.67
24	C	513	CLA	O2D-CGD-O1D	-2.15	119.24	123.77
24	c	504	CLA	O2D-CGD-O1D	-2.15	119.24	123.77
26	k	101	BCR	C11-C12-C13	-2.15	120.04	126.34
26	F	101	BCR	C38-C26-C27	-2.15	109.32	113.47
24	b	608[B]	CLA	CHC-C1C-C2C	-2.15	120.36	126.31
24	b	605	CLA	CMB-C2B-C1B	-2.15	124.66	128.31
24	b	618	CLA	C4-C3-C2	-2.15	119.43	123.58
24	C	511	CLA	CHA-C1A-NA	-2.14	120.85	126.21
26	I	101	BCR	C23-C24-C25	-2.14	121.03	127.24
24	b	605	CLA	O2D-CGD-O1D	-2.14	119.26	123.77
24	B	607[B]	CLA	C3C-C4C-NC	-2.14	108.05	110.21
32	h	102	DGD	O3G-C3G-C2G	-2.14	105.90	110.99
26	T	101	BCR	C31-C1-C6	-2.14	107.07	110.33
30	A	615	LHG	C6-C5-C4	-2.14	107.11	112.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	C3C-C4C-NC	-2.13	108.05	110.21
29	b	622	LMG	O1-C7-C8	-2.13	105.92	110.99
29	A	613	LMG	O8-C28-O10	-2.13	117.92	123.51
29	j	101	LMG	O8-C28-O10	-2.13	117.93	123.51
26	C	514	BCR	C3-C4-C5	-2.13	110.34	113.87
24	D	402	CLA	C3C-C4C-NC	-2.13	108.06	110.21
24	a	607	CLA	O2D-CGD-O1D	-2.13	119.30	123.77
24	d	403	CLA	CMB-C2B-C1B	-2.12	124.70	128.31
24	c	511	CLA	CHA-C1A-NA	-2.12	120.90	126.21
26	k	101	BCR	C20-C19-C18	-2.12	120.11	126.34
24	C	503	CLA	CHA-C1A-NA	-2.12	120.90	126.21
24	b	614	CLA	CAC-C3C-C2C	-2.12	123.87	127.51
24	C	512	CLA	CHA-C1A-NA	-2.12	120.90	126.21
24	B	616	CLA	C3B-CAB-CBB	-2.12	122.13	126.40
24	b	608[A]	CLA	C6-C5-C3	-2.12	108.97	112.76
28	b	601	SQD	O5-C1-C2	-2.12	105.88	110.28
26	t	101	BCR	C31-C1-C6	-2.12	107.10	110.33
24	C	504	CLA	CHC-C1C-C2C	-2.11	120.45	126.31
26	c	521	BCR	C16-C15-C14	-2.11	118.68	123.23
24	B	607[A]	CLA	C6-C5-C3	-2.11	108.97	112.76
24	a	607	CLA	CHC-C1C-C2C	-2.11	120.47	126.31
24	B	613	CLA	CHA-C1A-NA	-2.11	120.93	126.21
24	d	403	CLA	C3B-CAB-CBB	-2.11	122.16	126.40
29	a	613	LMG	O8-C28-O10	-2.10	118.00	123.51
27	a	611	PL9	C10-C9-C11	-2.10	112.17	115.37
24	B	616	CLA	CHC-C1C-C2C	-2.10	120.48	126.31
28	B	622	SQD	O5-C1-C2	-2.10	105.91	110.28
24	B	610	CLA	O2D-CGD-O1D	-2.10	119.35	123.77
26	c	514	BCR	C37-C22-C21	-2.10	119.83	122.89
29	B	621	LMG	O1-C1-C2	-2.10	105.42	108.00
24	B	603	CLA	C2C-C1C-NC	-2.10	108.78	110.22
28	x	101	SQD	O48-C23-O10	-2.10	118.01	123.51
27	a	611	PL9	C35-C34-C36	-2.10	112.17	115.37
26	F	101	BCR	C28-C27-C26	-2.10	110.39	113.87
26	f	101	BCR	C16-C15-C14	-2.10	118.71	123.23
26	b	621	BCR	C1-C6-C7	-2.09	109.97	115.96
28	X	101	SQD	O48-C23-O10	-2.09	118.03	123.51
27	A	611	PL9	C10-C9-C11	-2.09	112.19	115.37
24	C	509	CLA	CHA-C1A-NA	-2.09	120.98	126.21
24	B	611	CLA	CHC-C1C-C2C	-2.09	120.52	126.31
26	c	521	BCR	C23-C24-C25	-2.09	121.19	127.24
24	D	403	CLA	CBC-CAC-C3C	-2.08	106.05	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	519	LMG	O1-C7-C8	-2.08	106.03	110.99
24	a	609	CLA	O2D-CGD-O1D	-2.08	119.39	123.77
24	B	603	CLA	CMB-C2B-C1B	-2.08	124.78	128.31
30	A	615	LHG	O7-C7-O9	-2.08	118.02	123.67
24	C	501	CLA	CHA-C1A-NA	-2.08	121.02	126.21
24	B	607[A]	CLA	C3C-C4C-NC	-2.07	108.11	110.21
29	C	518	LMG	O8-C28-O10	-2.07	118.07	123.51
26	H	101	BCR	C11-C12-C13	-2.07	120.26	126.34
29	b	622	LMG	C8-O7-C10	-2.07	112.78	117.91
24	C	502	CLA	CHC-C1C-C2C	-2.07	120.57	126.31
32	E	101	DGD	O1B-C1B-C2B	-2.07	115.83	123.76
24	A	607	CLA	O2D-CGD-O1D	-2.07	119.41	123.77
28	a	612	SQD	O48-C23-O10	-2.07	118.09	123.51
32	c	517	DGD	C1E-O6E-C5E	-2.07	109.69	113.74
24	B	602	CLA	CHA-C1A-NA	-2.07	121.04	126.21
28	A	612	SQD	O9-S-O7	-2.06	108.13	113.96
28	a	612	SQD	O9-S-O7	-2.06	108.13	113.96
32	H	102	DGD	O3D-C3D-C2D	-2.06	105.71	110.36
24	c	501	CLA	C6-C5-C3	-2.06	109.06	112.76
24	b	609	CLA	O2A-CGA-O1A	-2.06	118.11	123.51
24	D	404	CLA	CHC-C1C-C2C	-2.06	120.60	126.31
25	a	608	PHO	O2D-CGD-O1D	-2.06	119.43	123.77
26	K	102	BCR	C1-C6-C7	-2.06	110.07	115.96
28	A	612	SQD	O48-C23-O10	-2.06	118.12	123.51
28	A	612	SQD	O5-C1-C2	-2.06	106.00	110.28
29	c	519	LMG	O7-C10-O9	-2.05	118.08	123.67
24	c	512	CLA	O2A-CGA-O1A	-2.05	118.12	123.51
32	H	102	DGD	O3G-C3G-C2G	-2.05	106.10	110.99
24	a	606	CLA	C4A-NA-C1A	-2.05	103.77	106.38
24	b	603	CLA	C3B-CAB-CBB	-2.05	122.27	126.40
24	C	511	CLA	C3C-C4C-NC	-2.05	108.13	110.21
24	c	509	CLA	CHC-C1C-C2C	-2.05	120.62	126.31
25	d	401	PHO	CBA-CAA-C2A	-2.05	108.67	113.96
24	b	608[A]	CLA	CHC-C1C-C2C	-2.05	120.63	126.31
26	f	101	BCR	C20-C19-C18	-2.05	120.33	126.34
32	h	102	DGD	C2G-O2G-C1B	-2.05	112.84	117.91
24	c	506	CLA	CHA-C1A-NA	-2.05	121.09	126.21
30	D	407	LHG	O8-C23-O10	-2.04	118.15	123.51
24	d	403	CLA	CHC-C1C-C2C	-2.04	120.65	126.31
24	c	508	CLA	C3C-C4C-NC	-2.04	108.14	110.21
24	C	501	CLA	C6-C5-C3	-2.04	109.10	112.76
28	x	101	SQD	O9-S-O7	-2.04	108.20	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	CHA-C1A-NA	-2.04	121.11	126.21
32	d	405	DGD	O1G-C1A-O1A	-2.04	118.17	123.51
26	b	621	BCR	C30-C25-C24	-2.03	110.14	115.96
26	c	514	BCR	C37-C22-C23	-2.03	114.76	118.08
29	D	408	LMG	O1-C7-C8	-2.03	106.15	110.99
28	a	612	SQD	O5-C1-C2	-2.03	106.05	110.28
24	B	609	CLA	C11-C10-C8	-2.03	109.17	115.46
24	B	610	CLA	CHA-C1A-NA	-2.03	121.13	126.21
24	b	610	CLA	C11-C10-C8	-2.03	109.17	115.46
26	C	514	BCR	C35-C13-C14	-2.03	119.93	122.89
26	f	101	BCR	C28-C29-C30	-2.03	107.38	114.77
24	B	608	CLA	CHA-C1A-NA	-2.03	121.13	126.21
24	A	609	CLA	CBC-CAC-C3C	-2.03	106.22	112.38
24	a	609	CLA	CHC-C1C-C2C	-2.03	120.69	126.31
24	b	617	CLA	C11-C10-C8	-2.03	109.18	115.46
28	B	622	SQD	O9-S-O7	-2.03	108.23	113.96
24	C	511	CLA	OBD-CAD-C3D	-2.03	124.51	128.09
24	b	617	CLA	CHC-C1C-C2C	-2.03	120.69	126.31
24	c	503	CLA	CMB-C2B-C1B	-2.02	124.87	128.31
24	B	607[A]	CLA	CHA-C1A-NA	-2.02	121.15	126.21
29	a	613	LMG	C1-O6-C5	-2.02	109.78	113.74
28	b	601	SQD	O9-S-O7	-2.02	108.25	113.96
24	d	402	CLA	C5-C3-C2	-2.02	117.22	120.98
24	C	507	CLA	CHA-C1A-NA	-2.02	121.16	126.21
32	E	101	DGD	O2G-C1B-O1B	-2.02	118.18	123.67
26	K	101	BCR	C20-C21-C22	-2.02	124.29	127.22
26	H	101	BCR	C30-C25-C24	-2.01	110.20	115.96
24	B	616	CLA	C11-C10-C8	-2.01	109.23	115.46
24	A	609	CLA	C5-C3-C2	-2.01	117.23	120.98
24	B	615	CLA	CBA-CAA-C2A	-2.01	108.77	113.96
24	D	403	CLA	C5-C3-C2	-2.01	117.23	120.98
24	C	509	CLA	CAA-CBA-CGA	-2.01	107.47	113.28
24	B	607[B]	CLA	CMB-C2B-C1B	-2.01	124.90	128.31
26	B	620	BCR	C10-C11-C12	-2.01	116.91	123.11
24	B	611	CLA	O1D-CGD-CBD	-2.01	121.52	124.64
28	X	101	SQD	O9-S-O7	-2.00	108.30	113.96
24	c	507	CLA	C4A-NA-C1A	-2.00	103.83	106.38
32	C	515	DGD	O1G-C1A-O1A	-2.00	118.25	123.51
32	c	517	DGD	C4E-C3E-C2E	2.00	114.47	110.79
27	a	611	PL9	C36-C37-C38	2.00	116.86	111.61
24	B	602	CLA	C4-C3-C5	2.00	118.42	115.37
24	B	612	CLA	CHD-C4C-C3C	2.01	128.01	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	O2A-CGA-CBA	2.01	118.03	111.85
24	c	504	CLA	CAD-CBD-CHA	2.01	109.41	103.29
24	b	608[B]	CLA	CHD-C4C-C3C	2.02	128.02	124.91
27	a	611	PL9	C3-C4-C5	2.02	121.55	118.64
24	C	503	CLA	CAD-CBD-CHA	2.02	109.43	103.29
29	B	621	LMG	O8-C28-C29	2.02	118.07	111.85
26	T	101	BCR	C23-C22-C21	2.02	122.22	118.95
24	a	607	CLA	CED-O2D-CGD	2.03	120.78	115.97
26	b	619	BCR	C35-C13-C14	2.03	125.83	122.89
26	b	620	BCR	C40-C30-C25	2.03	113.43	110.33
24	d	402	CLA	CAD-CBD-CHA	2.03	109.46	103.29
24	B	604	CLA	CMD-C2D-C3D	2.03	129.06	125.09
24	A	606	CLA	CAD-CBD-CHA	2.03	109.47	103.29
24	C	512	CLA	CMD-C2D-C3D	2.04	129.08	125.09
24	c	501	CLA	CHD-C4C-C3C	2.04	128.06	124.91
24	C	505	CLA	CMD-C2D-C3D	2.04	129.09	125.09
24	b	603	CLA	C4-C3-C5	2.05	118.49	115.37
24	C	506	CLA	CMB-C2B-C3B	2.05	129.10	125.09
24	A	607	CLA	CHD-C4C-C3C	2.05	128.08	124.91
29	Z	101	LMG	C1-C2-C3	2.05	114.06	109.98
28	x	101	SQD	C3-C4-C5	2.05	113.89	110.23
26	I	101	BCR	C19-C18-C17	2.06	122.27	118.95
24	c	511	CLA	CAD-CBD-CHA	2.06	109.55	103.29
32	c	518	DGD	C3D-C4D-C5D	2.07	113.91	110.23
24	c	501	CLA	CED-O2D-CGD	2.07	120.88	115.97
24	b	613	CLA	O2A-CGA-CBA	2.07	118.21	111.85
26	B	618	BCR	C2-C3-C4	2.07	116.66	111.42
24	b	609	CLA	CMB-C2B-C3B	2.07	129.14	125.09
24	c	510	CLA	CED-O2D-CGD	2.07	120.89	115.97
32	c	518	DGD	O3G-C1D-C2D	2.08	110.56	108.00
24	D	403	CLA	CED-O2D-CGD	2.08	120.91	115.97
24	B	610	CLA	CHD-C4C-C3C	2.08	128.13	124.91
26	c	514	BCR	C35-C13-C12	2.08	121.49	118.08
24	B	611	CLA	CAD-CBD-CHA	2.09	109.62	103.29
28	X	101	SQD	C3-C4-C5	2.09	113.95	110.23
24	A	609	CLA	CHD-C4C-C3C	2.09	128.13	124.91
24	b	612	CLA	C2C-C1C-NC	2.09	111.66	110.22
24	B	613	CLA	CHD-C4C-C3C	2.09	128.14	124.91
32	H	102	DGD	O6D-C1D-C2D	2.09	114.63	110.28
32	H	102	DGD	O5D-C1E-C2E	2.09	110.58	108.00
26	C	514	BCR	C8-C9-C10	2.10	122.33	118.95
24	B	604	CLA	CHD-C4C-C3C	2.10	128.15	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CED-O2D-CGD	2.10	120.96	115.97
24	B	605	CLA	CMD-C2D-C3D	2.10	129.20	125.09
24	C	501	CLA	CHC-C1C-NC	2.11	127.82	123.92
24	C	501	CLA	CAC-C3C-C4C	2.11	127.93	124.82
24	C	502	CLA	O2A-CGA-CBA	2.11	118.34	111.85
24	C	513	CLA	CMC-C2C-C1C	2.11	128.12	125.00
24	b	607	CLA	CED-O2D-CGD	2.12	121.00	115.97
24	b	612	CLA	CAD-CBD-CHA	2.13	109.75	103.29
24	C	503	CLA	O2A-CGA-CBA	2.13	118.39	111.85
29	C	518	LMG	O4-C4-C5	2.13	114.83	109.23
24	b	608[B]	CLA	O2A-CGA-CBA	2.13	118.40	111.85
24	C	505	CLA	CHD-C4C-C3C	2.13	128.20	124.91
24	b	605	CLA	O2A-CGA-CBA	2.13	118.41	111.85
32	E	101	DGD	O6E-C5E-C6E	2.14	111.91	106.38
24	a	609	CLA	CED-O2D-CGD	2.14	121.05	115.97
24	b	614	CLA	CAC-C3C-C4C	2.14	127.98	124.82
29	C	519	LMG	C3-C4-C5	2.14	114.05	110.23
26	h	101	BCR	C3-C4-C5	2.15	117.43	113.87
24	B	617	CLA	CAD-CBD-CHA	2.15	109.82	103.29
24	b	608[A]	CLA	CAD-CBD-CHA	2.16	109.85	103.29
29	D	408	LMG	C3-C4-C5	2.16	114.08	110.23
24	c	505	CLA	CAD-CBD-CHA	2.16	109.86	103.29
29	a	613	LMG	O1-C1-C2	2.17	110.66	108.00
24	B	613	CLA	CAC-C3C-C4C	2.17	128.02	124.82
24	c	510	CLA	C4-C3-C5	2.17	118.68	115.37
25	D	401	PHO	C3D-C4D-CHA	2.17	112.43	107.14
30	L	101	LHG	O8-C23-C24	2.18	118.54	111.85
24	B	615	CLA	CHC-C1C-NC	2.18	127.94	123.92
24	C	509	CLA	O2A-CGA-CBA	2.18	118.55	111.85
24	c	508	CLA	CMD-C2D-C3D	2.18	129.35	125.09
24	B	610	CLA	CED-O2D-CGD	2.19	121.16	115.97
29	c	519	LMG	O6-C5-C4	2.19	113.84	109.67
24	c	502	CLA	CAD-CBD-CHA	2.19	109.94	103.29
24	B	609	CLA	CAD-CBD-CHA	2.19	109.95	103.29
24	c	513	CLA	CMD-C2D-C3D	2.19	129.38	125.09
24	b	608[B]	CLA	CAD-CBD-CHA	2.20	109.97	103.29
24	b	608[A]	CLA	O2A-CGA-CBA	2.20	118.62	111.85
24	b	606	CLA	CAD-CBD-CHA	2.20	109.98	103.29
26	F	101	BCR	C8-C9-C10	2.20	122.50	118.95
29	Z	101	LMG	O6-C5-C4	2.20	113.87	109.67
24	C	512	CLA	CAD-CBD-CHA	2.21	109.99	103.29
24	C	510	CLA	C4-C3-C5	2.21	118.73	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	e	102	HEM	CMB-C2B-C3B	2.21	129.41	125.09
24	b	609	CLA	CED-O2D-CGD	2.21	121.22	115.97
24	c	508	CLA	O2A-CGA-CBA	2.21	118.65	111.85
24	C	505	CLA	CAD-CBD-CHA	2.21	110.00	103.29
24	D	402	CLA	CHD-C4C-C3C	2.21	128.33	124.91
29	C	519	LMG	O8-C28-C29	2.21	118.66	111.85
29	D	408	LMG	C1-O6-C5	2.22	118.09	113.74
24	c	504	CLA	CED-O2D-CGD	2.22	121.23	115.97
24	B	606	CLA	CAD-CBD-CHA	2.22	110.03	103.29
25	d	401	PHO	C3D-C4D-CHA	2.22	112.54	107.14
25	D	401	PHO	O2D-CGD-CBD	2.23	114.43	111.22
24	B	602	CLA	CHC-C1C-NC	2.23	128.04	123.92
24	C	510	CLA	CAD-CBD-CHA	2.23	110.06	103.29
24	b	612	CLA	CED-O2D-CGD	2.23	121.27	115.97
24	C	509	CLA	C4-C3-C5	2.23	118.77	115.37
24	A	607	CLA	CAD-CBD-CHA	2.24	110.08	103.29
24	c	506	CLA	O2A-CGA-CBA	2.24	118.75	111.85
26	c	521	BCR	C29-C28-C27	2.24	117.10	111.42
24	A	609	CLA	CAD-CBD-CHA	2.25	110.11	103.29
29	j	101	LMG	O7-C10-C11	2.25	116.26	111.53
24	c	503	CLA	O2A-CGA-CBA	2.25	118.78	111.85
25	A	608	PHO	CBD-CHA-C1A	2.25	130.67	126.70
29	A	613	LMG	O8-C28-C29	2.25	118.78	111.85
24	B	617	CLA	CED-O2D-CGD	2.25	121.32	115.97
24	B	617	CLA	C4-C3-C5	2.26	118.81	115.37
29	B	621	LMG	O7-C10-C11	2.26	116.28	111.53
24	c	509	CLA	C4-C3-C5	2.26	118.81	115.37
24	b	618	CLA	C4-C3-C5	2.26	118.81	115.37
26	b	620	BCR	C29-C30-C25	2.26	113.84	110.48
24	c	503	CLA	CAD-CBD-CHA	2.26	110.16	103.29
28	a	612	SQD	O48-C23-C24	2.26	118.81	111.85
24	C	504	CLA	CAD-CBD-CHA	2.26	110.16	103.29
24	B	603	CLA	O2A-CGA-CBA	2.26	118.81	111.85
32	c	516	DGD	O6D-C5D-C6D	2.26	111.29	106.61
24	B	607[B]	CLA	O2A-CGA-CBA	2.27	118.83	111.85
24	b	609	CLA	CAD-CBD-CHA	2.27	110.18	103.29
24	c	510	CLA	CAD-CBD-CHA	2.27	110.18	103.29
32	d	405	DGD	C3E-C4E-C5E	2.27	114.28	110.23
28	A	614	SQD	C3-C4-C5	2.27	114.28	110.23
28	A	612	SQD	O48-C23-C24	2.28	118.86	111.85
24	b	607	CLA	CAD-CBD-CHA	2.29	110.23	103.29
24	A	609	CLA	O2A-CGA-CBA	2.29	118.91	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	CAD-CBD-CHA	2.29	110.26	103.29
32	h	102	DGD	O6D-C5D-C6D	2.30	111.35	106.61
24	B	608	CLA	O2A-CGA-CBA	2.30	118.92	111.85
26	B	619	BCR	C12-C13-C14	2.30	122.66	118.95
24	B	605	CLA	CED-O2D-CGD	2.30	121.44	115.97
24	C	513	CLA	CHC-C1C-NC	2.30	128.18	123.92
28	A	614	SQD	O8-S-C6	2.30	109.78	104.99
26	b	619	BCR	C19-C18-C17	2.31	122.67	118.95
24	C	511	CLA	O2A-CGA-CBA	2.31	118.95	111.85
25	A	608	PHO	C4D-C3D-CAD	2.31	109.88	105.61
24	b	603	CLA	CAD-CBD-CHA	2.31	110.30	103.29
33	v	201	HEM	CMB-C2B-C3B	2.31	129.61	125.09
24	b	605	CLA	CAD-CBD-CHA	2.31	110.31	103.29
24	a	615	CLA	CMB-C2B-C3B	2.31	129.62	125.09
28	a	614	SQD	O8-S-C6	2.31	109.80	104.99
28	a	614	SQD	C3-C4-C5	2.31	114.36	110.23
24	B	605	CLA	CAD-CBD-CHA	2.32	110.33	103.29
26	b	620	BCR	C34-C9-C8	2.32	121.87	118.08
26	K	101	BCR	C34-C9-C8	2.32	121.88	118.08
24	a	609	CLA	CAD-CBD-CHA	2.33	110.36	103.29
24	a	606	CLA	CAD-CBD-CHA	2.33	110.36	103.29
30	A	615	LHG	O8-C23-C24	2.33	119.01	111.85
24	C	511	CLA	CAD-CBD-CHA	2.33	110.38	103.29
24	B	612	CLA	CED-O2D-CGD	2.33	121.52	115.97
24	c	512	CLA	CAD-CBD-CHA	2.33	110.38	103.29
24	a	615	CLA	CAD-CBD-CHA	2.34	110.39	103.29
24	D	402	CLA	CAD-CBD-CHA	2.34	110.40	103.29
24	c	501	CLA	C4-C3-C5	2.34	118.94	115.37
26	A	610	BCR	C34-C9-C8	2.34	121.91	118.08
32	C	517	DGD	O6E-C5E-C6E	2.34	112.45	106.38
24	d	403	CLA	CAD-CBD-CHA	2.35	110.42	103.29
30	d	407	LHG	O8-C23-C24	2.35	119.07	111.85
24	C	501	CLA	C4-C3-C5	2.35	118.95	115.37
26	c	515	BCR	C8-C9-C10	2.35	122.74	118.95
32	C	516	DGD	C1E-C2E-C3E	2.35	114.65	109.98
24	D	404	CLA	O2A-CGA-CBA	2.35	119.09	111.85
24	c	503	CLA	CHC-C1C-NC	2.36	128.28	123.92
29	D	408	LMG	O8-C28-C29	2.36	119.11	111.85
24	b	616	CLA	CMB-C2B-C3B	2.36	129.70	125.09
29	B	621	LMG	C3-C4-C5	2.36	114.44	110.23
24	b	604	CLA	CED-O2D-CGD	2.36	121.58	115.97
24	B	604	CLA	CAD-CBD-CHA	2.38	110.51	103.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	OBD-CAD-CBD	2.38	129.53	125.94
24	b	617	CLA	O2A-CGA-CBA	2.38	119.19	111.85
24	B	607[A]	CLA	O2A-CGA-CBA	2.39	119.19	111.85
24	b	613	CLA	CAD-CBD-CHA	2.39	110.54	103.29
24	b	610	CLA	CMB-C2B-C3B	2.39	129.76	125.09
24	c	513	CLA	CHC-C1C-NC	2.40	128.36	123.92
28	l	101	SQD	O8-S-C6	2.40	109.98	104.99
24	b	604	CLA	O2A-CGA-CBA	2.40	119.25	111.85
24	A	609	CLA	CED-O2D-CGD	2.41	121.69	115.97
24	a	606	CLA	C4-C3-C5	2.41	119.04	115.37
32	d	405	DGD	C1E-C2E-C3E	2.41	114.77	109.98
24	b	603	CLA	CED-O2D-CGD	2.42	121.71	115.97
32	d	405	DGD	O6D-C5D-C6D	2.42	111.60	106.61
24	B	610	CLA	O2A-CGA-CBA	2.42	119.29	111.85
28	L	102	SQD	O8-S-C6	2.43	110.03	104.99
32	E	101	DGD	O6D-C5D-C6D	2.43	111.64	106.61
26	c	521	BCR	C19-C18-C17	2.43	122.88	118.95
29	c	520	LMG	O6-C5-C4	2.44	114.32	109.67
27	d	404	PL9	C53-C6-C1	2.44	119.85	114.66
24	C	501	CLA	CHD-C4C-C3C	2.44	128.68	124.91
24	a	607	CLA	CAD-CBD-CHA	2.44	110.71	103.29
24	D	404	CLA	CAD-CBD-CHA	2.44	110.71	103.29
32	c	517	DGD	O6E-C5E-C6E	2.45	112.72	106.38
24	A	606	CLA	C4-C3-C5	2.45	119.11	115.37
24	B	602	CLA	CMC-C2C-C1C	2.45	128.63	125.00
24	C	504	CLA	O2A-CGA-CBA	2.45	119.40	111.85
24	b	611	CLA	CHC-C1C-NC	2.45	128.46	123.92
24	c	505	CLA	CHC-C1C-NC	2.46	128.46	123.92
24	B	609	CLA	C4-C3-C5	2.46	119.11	115.37
24	C	512	CLA	C2A-C1A-CHA	2.46	127.76	123.80
24	b	618	CLA	O2A-CGA-CBA	2.46	119.42	111.85
26	b	620	BCR	C28-C27-C26	2.46	117.95	113.87
24	b	610	CLA	C4-C3-C5	2.46	119.12	115.37
26	B	619	BCR	C28-C27-C26	2.47	117.95	113.87
24	a	609	CLA	CHC-C1C-NC	2.47	128.49	123.92
24	b	614	CLA	C2A-C1A-CHA	2.47	127.78	123.80
25	a	608	PHO	C4D-C3D-CAD	2.47	110.19	105.61
24	B	616	CLA	CAD-CBD-CHA	2.48	110.81	103.29
29	a	613	LMG	O8-C28-C29	2.48	119.47	111.85
24	b	612	CLA	CHC-C1C-NC	2.48	128.51	123.92
26	b	619	BCR	C2-C3-C4	2.48	117.70	111.42
24	C	511	CLA	CED-O2D-CGD	2.48	121.87	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CED-O2D-CGD	2.49	121.88	115.97
24	C	513	CLA	CED-O2D-CGD	2.49	121.89	115.97
24	c	513	CLA	O2A-CGA-CBA	2.50	119.53	111.85
24	B	605	CLA	O2A-CGA-CBA	2.50	119.53	111.85
24	C	509	CLA	CAD-CBD-CHA	2.51	110.90	103.29
26	T	101	BCR	C2-C1-C6	2.51	114.21	110.48
29	C	518	LMG	C1-C2-C3	2.51	114.96	109.98
24	c	506	CLA	CHC-C1C-NC	2.51	128.57	123.92
26	B	619	BCR	C40-C30-C25	2.51	114.17	110.33
32	C	515	DGD	O6D-C5D-C6D	2.52	111.81	106.61
24	B	609	CLA	O2A-CGA-CBA	2.52	119.60	111.85
32	H	102	DGD	C1D-C2D-C3D	2.52	114.98	109.98
26	I	101	BCR	C8-C9-C10	2.53	123.03	118.95
24	C	508	CLA	CED-O2D-CGD	2.53	121.97	115.97
24	b	616	CLA	CHC-C1C-NC	2.54	128.61	123.92
24	b	609	CLA	CHC-C1C-NC	2.54	128.62	123.92
24	B	613	CLA	CHC-C1C-NC	2.55	128.64	123.92
24	D	402	CLA	O2D-CGD-CBD	2.55	114.90	111.22
25	A	608	PHO	O1D-CGD-CBD	2.55	128.61	124.64
28	B	622	SQD	C4-C3-C2	2.55	115.49	110.79
26	b	619	BCR	C36-C18-C19	2.56	122.26	118.08
24	b	610	CLA	CHC-C1C-NC	2.56	128.66	123.92
28	b	601	SQD	C4-C3-C2	2.56	115.50	110.79
25	a	608	PHO	CBD-CHA-C1A	2.56	131.22	126.70
24	C	504	CLA	CED-O2D-CGD	2.56	122.06	115.97
24	c	509	CLA	CED-O2D-CGD	2.56	122.06	115.97
24	B	611	CLA	CMD-C2D-C3D	2.57	130.10	125.09
26	H	101	BCR	C19-C18-C17	2.57	123.10	118.95
24	C	504	CLA	CHC-C1C-NC	2.58	128.70	123.92
24	C	506	CLA	CHC-C1C-NC	2.58	128.70	123.92
24	B	602	CLA	CAD-CBD-CHA	2.58	111.14	103.29
26	K	101	BCR	C35-C13-C12	2.59	122.31	118.08
24	b	606	CLA	O2A-CGA-CBA	2.59	119.82	111.85
24	B	612	CLA	CHC-C1C-NC	2.59	128.72	123.92
26	B	618	BCR	C36-C18-C19	2.59	122.32	118.08
24	B	613	CLA	CMD-C2D-C3D	2.60	130.17	125.09
24	b	611	CLA	CED-O2D-CGD	2.60	122.15	115.97
24	C	505	CLA	CHC-C1C-NC	2.60	128.73	123.92
24	D	402	CLA	O2A-CGA-CBA	2.61	119.88	111.85
24	C	503	CLA	CHC-C1C-NC	2.61	128.76	123.92
26	B	620	BCR	C2-C1-C6	2.62	114.38	110.48
24	b	605	CLA	CED-O2D-CGD	2.62	122.20	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	616	LHG	O8-C23-C24	2.63	119.93	111.85
24	c	513	CLA	C4-C3-C5	2.63	119.37	115.37
24	C	513	CLA	C4-C3-C5	2.63	119.37	115.37
24	b	606	CLA	CED-O2D-CGD	2.64	122.24	115.97
26	f	101	BCR	C19-C18-C17	2.64	123.21	118.95
32	h	102	DGD	O1G-C1A-C2A	2.64	119.99	111.85
24	B	611	CLA	CHC-C1C-NC	2.65	128.82	123.92
24	B	604	CLA	CHC-C1C-NC	2.65	128.83	123.92
24	B	604	CLA	O2A-CGA-CBA	2.65	120.02	111.85
27	D	405	PL9	C53-C6-C1	2.66	120.32	114.66
24	B	613	CLA	O2A-CGA-CBA	2.66	120.03	111.85
24	a	609	CLA	O2A-CGA-CBA	2.68	120.08	111.85
26	B	619	BCR	C29-C30-C25	2.68	114.47	110.48
24	b	607	CLA	CHC-C1C-NC	2.68	128.88	123.92
29	c	520	LMG	C3-C4-C5	2.68	115.01	110.23
32	d	405	DGD	O1G-C1A-C2A	2.69	120.13	111.85
32	h	102	DGD	C4D-C3D-C2D	2.70	115.75	110.79
24	b	608[A]	CLA	CHC-C1C-NC	2.70	128.91	123.92
24	b	612	CLA	C4-C3-C5	2.70	119.48	115.37
24	c	509	CLA	O2A-CGA-CBA	2.70	120.16	111.85
26	t	101	BCR	C29-C30-C25	2.71	114.51	110.48
24	D	404	CLA	CHC-C1C-NC	2.71	128.94	123.92
24	C	513	CLA	CMB-C2B-C3B	2.71	130.39	125.09
24	B	608	CLA	CHC-C1C-NC	2.71	128.94	123.92
24	B	615	CLA	CAD-CBD-CHA	2.71	111.53	103.29
24	C	510	CLA	C2A-C1A-CHA	2.71	128.17	123.80
30	D	407	LHG	O8-C23-C24	2.71	120.20	111.85
24	d	402	CLA	O2A-CGA-CBA	2.72	120.21	111.85
24	B	606	CLA	CHC-C1C-NC	2.72	128.95	123.92
26	c	514	BCR	C29-C30-C25	2.72	114.53	110.48
24	D	404	CLA	C4-C3-C5	2.72	119.52	115.37
24	d	403	CLA	C4-C3-C5	2.72	119.52	115.37
32	E	101	DGD	O1G-C1A-C2A	2.72	120.23	111.85
24	B	611	CLA	CED-O2D-CGD	2.73	122.45	115.97
24	b	603	CLA	O2A-CGA-CBA	2.74	120.27	111.85
24	c	511	CLA	O2A-CGA-CBA	2.74	120.28	111.85
26	c	514	BCR	C19-C18-C17	2.74	123.38	118.95
24	C	510	CLA	CHC-C1C-NC	2.75	129.00	123.92
24	D	403	CLA	CHC-C1C-NC	2.75	129.01	123.92
24	d	402	CLA	CHC-C1C-NC	2.75	129.01	123.92
24	b	606	CLA	CHC-C1C-NC	2.75	129.01	123.92
30	d	406	LHG	O8-C23-C24	2.75	120.32	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	502	CLA	CED-O2D-CGD	2.76	122.52	115.97
24	a	606	CLA	O2A-CGA-CBA	2.76	120.34	111.85
30	e	101	LHG	O8-C23-C24	2.76	120.35	111.85
29	C	518	LMG	O6-C5-C4	2.76	114.93	109.67
24	B	614	CLA	C4-C3-C5	2.76	119.58	115.37
24	D	403	CLA	CAD-CBD-CHA	2.76	111.69	103.29
24	C	512	CLA	O2A-CGA-CBA	2.77	120.37	111.85
24	b	615	CLA	C4-C3-C5	2.77	119.60	115.37
24	B	611	CLA	C4-C3-C5	2.78	119.60	115.37
29	b	622	LMG	O8-C28-C29	2.78	120.40	111.85
24	B	616	CLA	C4-C3-C5	2.78	119.61	115.37
28	l	101	SQD	O48-C23-C24	2.78	120.41	111.85
24	C	502	CLA	C4-C3-C5	2.78	119.61	115.37
28	L	102	SQD	O48-C23-C24	2.79	120.42	111.85
24	c	511	CLA	C4-C3-C5	2.79	119.61	115.37
27	A	611	PL9	C53-C6-C1	2.79	120.59	114.66
32	C	516	DGD	C4E-C3E-C2E	2.79	115.92	110.79
32	h	102	DGD	O5D-C1E-C2E	2.79	111.43	108.00
30	l	102	LHG	O8-C23-C24	2.79	120.44	111.85
30	E	102	LHG	O8-C23-C24	2.79	120.44	111.85
28	b	601	SQD	O48-C23-C24	2.79	120.44	111.85
24	c	502	CLA	CHC-C1C-NC	2.79	129.09	123.92
29	C	518	LMG	C4-C3-C2	2.80	115.94	110.79
26	H	101	BCR	C34-C9-C8	2.80	122.66	118.08
24	D	403	CLA	C2A-C1A-CHA	2.81	128.32	123.80
28	B	622	SQD	O48-C23-C24	2.81	120.50	111.85
24	b	617	CLA	C4-C3-C5	2.81	119.65	115.37
32	C	516	DGD	O6E-C5E-C6E	2.81	113.67	106.38
24	b	614	CLA	CHC-C1C-NC	2.81	129.13	123.92
24	c	512	CLA	C2A-C1A-CHA	2.81	128.33	123.80
24	b	604	CLA	CHC-C1C-NC	2.82	129.13	123.92
24	C	511	CLA	C4-C3-C5	2.82	119.66	115.37
24	C	502	CLA	CHC-C1C-NC	2.82	129.14	123.92
24	C	513	CLA	O2A-CGA-CBA	2.82	120.53	111.85
24	c	502	CLA	C4-C3-C5	2.83	119.68	115.37
24	c	511	CLA	CHC-C1C-NC	2.83	129.16	123.92
24	c	501	CLA	CHC-C1C-NC	2.83	129.16	123.92
30	D	406	LHG	O8-C23-C24	2.84	120.58	111.85
24	D	402	CLA	CHC-C1C-NC	2.84	129.18	123.92
24	C	509	CLA	CHC-C1C-NC	2.84	129.18	123.92
24	b	608[B]	CLA	CHC-C1C-NC	2.84	129.18	123.92
24	C	507	CLA	CHC-C1C-NC	2.85	129.19	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	504	CLA	CHC-C1C-NC	2.85	129.20	123.92
24	c	512	CLA	CHC-C1C-NC	2.85	129.20	123.92
25	A	608	PHO	CMD-C2D-C1D	2.86	129.64	125.06
24	c	501	CLA	O2A-CGA-CBA	2.88	120.70	111.85
24	C	503	CLA	C4-C3-C5	2.88	119.75	115.37
24	b	611	CLA	O2A-CGA-CBA	2.88	120.70	111.85
24	d	403	CLA	O2A-CGA-CBA	2.88	120.72	111.85
24	d	402	CLA	C4-C3-C5	2.88	119.76	115.37
24	a	607	CLA	CHC-C1C-NC	2.89	129.26	123.92
24	c	512	CLA	O2A-CGA-CBA	2.90	120.77	111.85
28	a	612	SQD	O8-S-C6	2.90	111.02	104.99
29	z	101	LMG	O1-C1-C2	2.91	111.58	108.00
24	c	503	CLA	C4-C3-C5	2.91	119.80	115.37
24	D	403	CLA	C4-C3-C5	2.91	119.80	115.37
29	c	520	LMG	O8-C28-C29	2.92	120.83	111.85
29	c	519	LMG	O8-C28-C29	2.93	120.86	111.85
28	A	612	SQD	O8-S-C6	2.93	111.08	104.99
24	b	614	CLA	O2A-CGA-CBA	2.94	120.90	111.85
26	B	618	BCR	C29-C30-C25	2.95	114.86	110.48
32	E	101	DGD	C1E-C2E-C3E	2.96	115.84	109.98
24	B	609	CLA	CHD-C4C-C3C	2.96	129.48	124.91
24	B	605	CLA	C4-C3-C5	2.96	119.89	115.37
26	f	101	BCR	C36-C18-C19	2.97	122.93	118.08
24	B	609	CLA	CHC-C1C-NC	2.97	129.41	123.92
24	B	616	CLA	O2A-CGA-CBA	2.98	121.02	111.85
24	c	507	CLA	O2A-CGA-CBA	2.98	121.02	111.85
24	c	508	CLA	C4-C3-C5	2.98	119.91	115.37
24	C	508	CLA	C4-C3-C5	2.98	119.92	115.37
24	b	606	CLA	C4-C3-C5	2.99	119.92	115.37
24	c	508	CLA	CHC-C1C-NC	2.99	129.45	123.92
28	A	614	SQD	O48-C23-C24	3.00	121.08	111.85
30	D	406	LHG	O7-C7-C8	3.00	117.86	111.53
28	x	101	SQD	O48-C23-C24	3.01	121.11	111.85
32	d	405	DGD	C4E-C3E-C2E	3.01	116.33	110.79
28	X	101	SQD	O48-C23-C24	3.01	121.12	111.85
24	B	616	CLA	CHC-C1C-NC	3.01	129.50	123.92
25	D	401	PHO	O1D-CGD-CBD	3.02	129.33	124.64
28	a	614	SQD	O48-C23-C24	3.02	121.13	111.85
25	d	401	PHO	O1D-CGD-CBD	3.02	129.33	124.64
24	B	610	CLA	CHC-C1C-NC	3.02	129.51	123.92
24	B	605	CLA	CHC-C1C-NC	3.02	129.51	123.92
24	b	605	CLA	CHC-C1C-NC	3.03	129.53	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	509	CLA	CHC-C1C-NC	3.03	129.53	123.92
24	D	403	CLA	O2A-CGA-CBA	3.04	121.19	111.85
24	b	617	CLA	CHC-C1C-NC	3.04	129.55	123.92
24	b	609	CLA	C4-C3-C5	3.05	120.02	115.37
26	t	101	BCR	C2-C1-C6	3.06	115.04	110.48
32	E	101	DGD	C3E-C4E-C5E	3.07	115.69	110.23
24	D	402	CLA	C4-C3-C5	3.07	120.05	115.37
24	B	608	CLA	C4-C3-C5	3.08	120.06	115.37
32	c	517	DGD	O1G-C1A-C2A	3.09	121.34	111.85
24	b	612	CLA	O2A-CGA-CBA	3.09	121.36	111.85
24	B	611	CLA	O2A-CGA-CBA	3.10	121.38	111.85
24	a	615	CLA	C4-C3-C5	3.11	120.11	115.37
27	a	611	PL9	C53-C6-C1	3.11	121.28	114.66
24	b	608[A]	CLA	C4-C3-C5	3.11	120.11	115.37
24	b	615	CLA	CHC-C1C-NC	3.11	129.68	123.92
24	B	617	CLA	O2A-CGA-CBA	3.13	121.48	111.85
24	a	606	CLA	CHC-C1C-NC	3.15	129.74	123.92
29	b	622	LMG	O7-C10-C11	3.15	118.17	111.53
24	B	617	CLA	C2A-C1A-CHA	3.16	128.88	123.80
24	C	507	CLA	O2A-CGA-CBA	3.16	121.56	111.85
32	C	516	DGD	C3E-C4E-C5E	3.16	115.86	110.23
24	A	606	CLA	O2A-CGA-CBA	3.16	121.56	111.85
32	E	101	DGD	C4E-C3E-C2E	3.16	116.60	110.79
24	B	607[A]	CLA	C4-C3-C5	3.16	120.18	115.37
24	c	507	CLA	CHC-C1C-NC	3.17	129.78	123.92
24	b	608[B]	CLA	C4-C3-C5	3.17	120.20	115.37
24	B	607[B]	CLA	C4-C3-C5	3.18	120.21	115.37
32	C	516	DGD	O2G-C1B-C2B	3.18	118.22	111.53
29	A	613	LMG	O7-C10-C11	3.18	118.23	111.53
24	d	403	CLA	CHC-C1C-NC	3.21	129.86	123.92
29	A	613	LMG	O1-C1-C2	3.21	111.95	108.00
24	C	511	CLA	CHC-C1C-NC	3.22	129.87	123.92
24	D	403	CLA	CMC-C2C-C1C	3.23	129.79	125.00
24	B	607[A]	CLA	CHC-C1C-NC	3.24	129.91	123.92
24	B	602	CLA	O2A-CGA-CBA	3.25	121.86	111.85
24	c	504	CLA	C4-C3-C5	3.25	120.33	115.37
24	b	603	CLA	CHC-C1C-NC	3.26	129.95	123.92
24	b	605	CLA	C4-C3-C5	3.27	120.36	115.37
24	B	604	CLA	C4-C3-C5	3.28	120.36	115.37
25	a	608	PHO	O1D-CGD-CBD	3.29	129.75	124.64
24	C	504	CLA	C4-C3-C5	3.29	120.38	115.37
24	C	507	CLA	C4-C3-C5	3.30	120.39	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607[B]	CLA	CHC-C1C-NC	3.30	130.02	123.92
24	b	613	CLA	CHC-C1C-NC	3.30	130.03	123.92
24	b	618	CLA	C2A-C1A-CHA	3.31	129.13	123.80
24	A	606	CLA	CHC-C1C-NC	3.31	130.05	123.92
24	C	501	CLA	O2A-CGA-CBA	3.32	122.06	111.85
24	A	607	CLA	CHC-C1C-NC	3.32	130.06	123.92
24	a	607	CLA	O2D-CGD-CBD	3.34	116.04	111.22
24	c	506	CLA	C4-C3-C5	3.35	120.47	115.37
24	a	615	CLA	CHC-C1C-NC	3.36	130.13	123.92
29	D	408	LMG	O6-C5-C4	3.36	116.08	109.67
32	C	516	DGD	O1G-C1A-C2A	3.36	122.20	111.85
24	C	508	CLA	CHC-C1C-NC	3.37	130.15	123.92
24	b	617	CLA	C2A-C1A-CHA	3.37	129.22	123.80
24	C	506	CLA	C4-C3-C5	3.38	120.52	115.37
24	B	612	CLA	C2A-C1A-CHA	3.38	129.24	123.80
24	c	510	CLA	CHC-C1C-NC	3.38	130.18	123.92
24	c	507	CLA	C4-C3-C5	3.38	120.52	115.37
24	b	618	CLA	CHC-C1C-NC	3.39	130.19	123.92
32	c	517	DGD	O2G-C1B-C2B	3.39	118.67	111.53
24	A	607	CLA	C4-C3-C5	3.39	120.54	115.37
24	B	613	CLA	C2A-C1A-CHA	3.40	129.27	123.80
24	a	607	CLA	C4-C3-C5	3.41	120.57	115.37
29	D	408	LMG	O7-C10-C11	3.42	118.73	111.53
24	b	604	CLA	C4-C3-C5	3.42	120.58	115.37
28	l	101	SQD	O9-S-C6	3.43	109.34	106.92
24	C	513	CLA	C2A-C1A-CHA	3.43	129.33	123.80
28	L	102	SQD	O9-S-C6	3.44	109.34	106.92
28	a	614	SQD	O47-C7-C8	3.44	118.77	111.53
28	A	614	SQD	O47-C7-C8	3.44	118.77	111.53
29	C	518	LMG	O8-C28-C29	3.44	122.44	111.85
32	c	517	DGD	O3G-C1D-C2D	3.46	112.26	108.00
24	B	603	CLA	C4-C3-C5	3.46	120.64	115.37
24	B	603	CLA	CHC-C1C-NC	3.47	130.34	123.92
24	C	512	CLA	CHC-C1C-NC	3.48	130.36	123.92
24	B	613	CLA	C4-C3-C5	3.48	120.68	115.37
30	L	101	LHG	O7-C7-C8	3.48	118.87	111.53
24	B	614	CLA	CHC-C1C-NC	3.51	130.41	123.92
24	B	609	CLA	CAC-C3C-C4C	3.51	130.00	124.82
24	b	614	CLA	C4-C3-C5	3.52	120.74	115.37
24	c	512	CLA	C4-C3-C5	3.56	120.80	115.37
24	D	403	CLA	O2D-CGD-CBD	3.57	116.37	111.22
24	A	607	CLA	O2A-CGA-CBA	3.58	122.86	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	C4-C3-C5	3.58	120.82	115.37
29	c	519	LMG	O7-C10-C11	3.60	119.11	111.53
30	D	407	LHG	O7-C7-C8	3.60	119.12	111.53
24	C	506	CLA	CED-O2D-CGD	3.61	124.56	115.97
24	b	609	CLA	C2A-C1A-CHA	3.63	129.64	123.80
26	K	102	BCR	C40-C30-C25	3.64	115.89	110.33
29	Z	101	LMG	O7-C10-C11	3.64	119.20	111.53
29	z	101	LMG	O7-C10-C11	3.67	119.25	111.53
26	b	621	BCR	C19-C18-C17	3.68	124.88	118.95
24	b	604	CLA	C2A-C1A-CHA	3.68	129.73	123.80
24	B	611	CLA	O2D-CGD-CBD	3.72	116.58	111.22
24	B	615	CLA	C4-C3-C5	3.73	121.06	115.37
28	l	101	SQD	O47-C7-C8	3.74	119.42	111.53
24	b	616	CLA	C4-C3-C5	3.75	121.08	115.37
24	C	509	CLA	C2A-C1A-CHA	3.77	129.87	123.80
24	B	610	CLA	C2A-C1A-CHA	3.79	129.91	123.80
28	L	102	SQD	O47-C7-C8	3.79	119.52	111.53
24	B	608	CLA	O2D-CGD-CBD	3.82	116.73	111.22
24	B	617	CLA	CHC-C1C-NC	3.82	131.00	123.92
29	a	613	LMG	O7-C10-C11	3.82	119.59	111.53
28	b	601	SQD	C3-C4-C5	3.83	117.05	110.23
28	B	622	SQD	C3-C4-C5	3.84	117.07	110.23
28	x	101	SQD	O47-C7-C8	3.84	119.62	111.53
28	X	101	SQD	O47-C7-C8	3.85	119.63	111.53
24	a	615	CLA	O2A-CGA-CBA	3.86	123.72	111.85
26	F	101	BCR	C36-C18-C19	3.87	124.41	118.08
24	A	609	CLA	C4-C3-C5	3.89	121.29	115.37
24	a	609	CLA	C4-C3-C5	3.89	121.30	115.37
24	d	402	CLA	C2A-C1A-CHA	3.90	130.09	123.80
26	b	621	BCR	C2-C1-C6	3.91	116.30	110.48
29	C	519	LMG	O7-C10-C11	3.93	119.82	111.53
30	l	102	LHG	O7-C7-C8	3.95	119.86	111.53
24	C	509	CLA	O2D-CGD-CBD	3.98	116.96	111.22
24	a	615	CLA	C2A-C1A-CHA	4.00	130.24	123.80
32	C	517	DGD	O2G-C1B-C2B	4.03	120.02	111.53
24	a	606	CLA	O2D-CGD-CBD	4.04	117.04	111.22
32	E	101	DGD	O2G-C1B-C2B	4.05	120.05	111.53
28	B	622	SQD	O47-C7-C8	4.05	120.05	111.53
28	b	601	SQD	O47-C7-C8	4.05	120.06	111.53
24	B	604	CLA	C2A-C1A-CHA	4.06	130.34	123.80
24	C	501	CLA	C2A-C1A-CHA	4.08	130.37	123.80
32	C	515	DGD	O2G-C1B-C2B	4.11	120.18	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	614	SQD	O6-C1-C2	4.14	113.09	108.00
24	b	605	CLA	O2D-CGD-CBD	4.15	117.20	111.22
29	C	518	LMG	O7-C10-C11	4.16	120.30	111.53
24	C	503	CLA	C2A-C1A-CHA	4.20	130.56	123.80
32	d	405	DGD	O2G-C1B-C2B	4.20	120.39	111.53
28	a	614	SQD	O6-C1-C2	4.21	113.18	108.00
24	B	602	CLA	O2D-CGD-CBD	4.24	117.34	111.22
24	b	607	CLA	C4-C3-C5	4.24	121.83	115.37
30	E	102	LHG	O7-C7-C8	4.26	120.50	111.53
24	B	606	CLA	C4-C3-C5	4.27	121.88	115.37
24	b	611	CLA	C2A-C1A-CHA	4.30	130.73	123.80
32	c	516	DGD	O2G-C1B-C2B	4.30	120.60	111.53
24	d	403	CLA	O2D-CGD-CBD	4.31	117.44	111.22
26	A	610	BCR	C39-C30-C25	4.37	117.01	110.33
24	A	609	CLA	C2A-C1A-CHA	4.38	130.85	123.80
30	d	406	LHG	O7-C7-C8	4.39	120.77	111.53
24	D	402	CLA	C2A-C1A-CHA	4.39	130.87	123.80
24	C	503	CLA	O2D-CGD-CBD	4.40	117.56	111.22
28	A	612	SQD	O47-C7-C8	4.40	120.80	111.53
28	a	612	SQD	O47-C7-C8	4.41	120.82	111.53
24	B	616	CLA	O2D-CGD-CBD	4.48	117.69	111.22
29	c	520	LMG	O7-C10-C11	4.53	121.07	111.53
28	B	622	SQD	O9-S-C6	4.54	110.12	106.92
24	c	501	CLA	C2A-C1A-CHA	4.55	131.13	123.80
24	B	607[B]	CLA	C2A-C1A-CHA	4.56	131.14	123.80
24	b	616	CLA	C2A-C1A-CHA	4.56	131.15	123.80
28	b	601	SQD	O9-S-C6	4.56	110.14	106.92
24	c	503	CLA	C2A-C1A-CHA	4.57	131.15	123.80
24	D	404	CLA	O2D-CGD-CBD	4.59	117.84	111.22
24	c	513	CLA	C2A-C1A-CHA	4.60	131.21	123.80
24	C	504	CLA	C2A-C1A-CHA	4.61	131.22	123.80
26	c	514	BCR	C2-C1-C6	4.61	117.34	110.48
24	B	616	CLA	C2A-C1A-CHA	4.62	131.24	123.80
24	C	505	CLA	C2A-C1A-CHA	4.67	131.32	123.80
32	h	102	DGD	O2G-C1B-C2B	4.68	121.38	111.53
24	C	502	CLA	C2A-C1A-CHA	4.71	131.38	123.80
24	c	507	CLA	C2A-C1A-CHA	4.71	131.39	123.80
24	c	508	CLA	C2A-C1A-CHA	4.74	131.44	123.80
24	B	607[A]	CLA	C2A-C1A-CHA	4.77	131.48	123.80
24	b	607	CLA	C2A-C1A-CHA	4.78	131.51	123.80
24	b	610	CLA	C2A-C1A-CHA	4.79	131.51	123.80
32	c	518	DGD	O2G-C1B-C2B	4.79	121.62	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	614	CLA	C2A-C1A-CHA	4.80	131.53	123.80
24	b	603	CLA	O2D-CGD-CBD	4.81	118.16	111.22
30	e	101	LHG	O7-C7-C8	4.83	121.71	111.53
24	B	617	CLA	O2D-CGD-CBD	4.84	118.21	111.22
24	A	606	CLA	C2A-C1A-CHA	4.86	131.63	123.80
24	c	502	CLA	C2A-C1A-CHA	4.86	131.63	123.80
24	c	505	CLA	C2A-C1A-CHA	4.86	131.63	123.80
24	b	612	CLA	C2A-C1A-CHA	4.87	131.65	123.80
24	c	509	CLA	C2A-C1A-CHA	4.91	131.71	123.80
24	c	503	CLA	O2D-CGD-CBD	4.91	118.30	111.22
24	b	613	CLA	C2A-C1A-CHA	4.91	131.71	123.80
26	b	621	BCR	C37-C22-C23	4.92	126.13	118.08
30	d	407	LHG	O7-C7-C8	4.98	122.03	111.53
24	c	504	CLA	C2A-C1A-CHA	4.99	131.83	123.80
30	a	616	LHG	O7-C7-C8	4.99	122.04	111.53
24	C	508	CLA	C2A-C1A-CHA	5.00	131.86	123.80
29	Z	101	LMG	O1-C1-C2	5.03	114.19	108.00
26	H	101	BCR	C2-C1-C6	5.07	118.02	110.48
26	h	101	BCR	C29-C30-C25	5.09	118.05	110.48
24	C	510	CLA	O2D-CGD-CBD	5.09	118.57	111.22
24	b	609	CLA	O2D-CGD-CBD	5.10	118.58	111.22
24	B	602	CLA	C2A-C1A-CHA	5.12	132.05	123.80
24	A	607	CLA	C2A-C1A-CHA	5.14	132.07	123.80
24	b	615	CLA	C2A-C1A-CHA	5.15	132.10	123.80
24	C	507	CLA	C2A-C1A-CHA	5.16	132.10	123.80
24	B	605	CLA	C2A-C1A-CHA	5.17	132.12	123.80
24	B	608	CLA	C2A-C1A-CHA	5.18	132.14	123.80
24	b	608[B]	CLA	C2A-C1A-CHA	5.18	132.15	123.80
24	B	615	CLA	O2D-CGD-CBD	5.18	118.70	111.22
24	B	603	CLA	C2A-C1A-CHA	5.19	132.16	123.80
24	b	608[B]	CLA	O2D-CGD-CBD	5.22	118.75	111.22
28	x	101	SQD	O9-S-C6	5.22	110.60	106.92
24	C	508	CLA	O2D-CGD-CBD	5.24	118.78	111.22
24	a	606	CLA	C2A-C1A-CHA	5.26	132.27	123.80
28	X	101	SQD	O9-S-C6	5.26	110.63	106.92
24	B	604	CLA	O2D-CGD-CBD	5.27	118.82	111.22
24	a	609	CLA	C2A-C1A-CHA	5.27	132.29	123.80
24	d	403	CLA	C2A-C1A-CHA	5.27	132.29	123.80
24	b	608[A]	CLA	O2D-CGD-CBD	5.27	118.83	111.22
24	c	509	CLA	O2D-CGD-CBD	5.28	118.83	111.22
24	B	611	CLA	C2A-C1A-CHA	5.28	132.30	123.80
24	b	616	CLA	O2D-CGD-CBD	5.29	118.86	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C2A-C1A-CHA	5.34	132.40	123.80
24	b	615	CLA	O2D-CGD-CBD	5.37	118.96	111.22
28	X	101	SQD	O7-S-C6	5.38	110.71	106.92
24	b	608[A]	CLA	C2A-C1A-CHA	5.40	132.50	123.80
24	c	511	CLA	C2A-C1A-CHA	5.40	132.50	123.80
24	A	606	CLA	O2D-CGD-CBD	5.41	119.02	111.22
24	c	510	CLA	C2A-C1A-CHA	5.42	132.52	123.80
24	A	606	CLA	C2A-C3A-C4A	5.42	107.40	101.84
24	B	605	CLA	O2D-CGD-CBD	5.42	119.04	111.22
28	x	101	SQD	O7-S-C6	5.45	110.76	106.92
28	x	101	SQD	O6-C1-C2	5.45	114.71	108.00
28	X	101	SQD	O6-C1-C2	5.47	114.73	108.00
24	B	609	CLA	C2A-C1A-CHA	5.49	132.65	123.80
24	C	504	CLA	O2D-CGD-CBD	5.52	119.18	111.22
24	A	609	CLA	O2D-CGD-CBD	5.52	119.19	111.22
24	B	615	CLA	C2A-C1A-CHA	5.54	132.72	123.80
24	D	404	CLA	C2A-C1A-CHA	5.56	132.76	123.80
26	C	514	BCR	C2-C1-C6	5.58	118.79	110.48
24	b	611	CLA	O2D-CGD-CBD	5.59	119.29	111.22
28	b	601	SQD	O6-C1-C2	5.60	114.89	108.00
28	B	622	SQD	O6-C1-C2	5.60	114.90	108.00
24	C	506	CLA	O2D-CGD-CBD	5.63	119.35	111.22
24	a	607	CLA	C2A-C1A-CHA	5.65	132.90	123.80
24	c	504	CLA	O2D-CGD-CBD	5.65	119.37	111.22
24	b	603	CLA	C2A-C1A-CHA	5.65	132.90	123.80
24	c	502	CLA	O2D-CGD-CBD	5.65	119.37	111.22
26	H	101	BCR	C29-C30-C25	5.66	118.90	110.48
24	a	609	CLA	O2D-CGD-CBD	5.68	119.42	111.22
24	C	511	CLA	C2A-C1A-CHA	5.68	132.95	123.80
30	A	615	LHG	O7-C7-C8	5.68	123.50	111.53
24	B	606	CLA	O2D-CGD-CBD	5.71	119.46	111.22
26	h	101	BCR	C2-C1-C6	5.73	119.00	110.48
24	B	606	CLA	C2A-C1A-CHA	5.74	133.04	123.80
28	a	614	SQD	O9-S-C6	5.78	110.99	106.92
24	c	506	CLA	C2A-C1A-CHA	5.79	133.13	123.80
24	C	513	CLA	O2D-CGD-CBD	5.80	119.58	111.22
24	b	607	CLA	O2D-CGD-CBD	5.82	119.62	111.22
24	b	606	CLA	O2D-CGD-CBD	5.85	119.67	111.22
28	A	614	SQD	O9-S-C6	5.86	111.05	106.92
24	C	506	CLA	C2A-C1A-CHA	5.86	133.24	123.80
26	F	101	BCR	C23-C22-C21	5.89	128.45	118.95
24	C	502	CLA	O2D-CGD-CBD	5.94	119.79	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C2A-C1A-CHA	5.94	133.37	123.80
24	c	513	CLA	O2D-CGD-CBD	5.97	119.83	111.22
24	c	511	CLA	O2D-CGD-CBD	6.03	119.92	111.22
24	c	506	CLA	O2D-CGD-CBD	6.06	119.96	111.22
24	B	607[B]	CLA	O2D-CGD-CBD	6.07	119.98	111.22
24	b	610	CLA	O2D-CGD-CBD	6.08	119.99	111.22
28	L	102	SQD	O6-C1-C2	6.09	115.49	108.00
28	l	101	SQD	O6-C1-C2	6.09	115.49	108.00
24	B	613	CLA	O2D-CGD-CBD	6.09	120.01	111.22
24	c	510	CLA	O2D-CGD-CBD	6.13	120.07	111.22
24	B	607[A]	CLA	O2D-CGD-CBD	6.13	120.07	111.22
28	a	612	SQD	O6-C1-C2	6.17	115.59	108.00
28	A	612	SQD	O6-C1-C2	6.19	115.62	108.00
28	l	101	SQD	O7-S-C6	6.22	111.31	106.92
24	d	402	CLA	O2D-CGD-CBD	6.23	120.20	111.22
28	L	102	SQD	O7-S-C6	6.23	111.31	106.92
24	B	609	CLA	O2D-CGD-CBD	6.25	120.23	111.22
26	B	619	BCR	C19-C18-C17	6.27	129.06	118.95
24	b	617	CLA	O2D-CGD-CBD	6.32	120.34	111.22
24	a	615	CLA	C2A-C3A-C4A	6.38	108.38	101.84
24	B	614	CLA	O2D-CGD-CBD	6.38	120.43	111.22
24	a	615	CLA	O2D-CGD-CBD	6.48	120.56	111.22
24	B	610	CLA	O2D-CGD-CBD	6.51	120.61	111.22
24	B	603	CLA	C2A-C3A-C4A	6.52	108.52	101.84
24	C	511	CLA	O2D-CGD-CBD	6.56	120.69	111.22
28	B	622	SQD	O7-S-C6	6.59	111.56	106.92
24	b	612	CLA	O2D-CGD-CBD	6.59	120.73	111.22
24	C	505	CLA	C2A-C3A-C4A	6.60	108.61	101.84
24	c	501	CLA	O2D-CGD-CBD	6.62	120.78	111.22
28	b	601	SQD	O7-S-C6	6.64	111.60	106.92
24	c	508	CLA	O2D-CGD-CBD	6.64	120.80	111.22
24	C	506	CLA	C2A-C3A-C4A	6.75	108.75	101.84
24	B	617	CLA	C2A-C3A-C4A	6.80	108.81	101.84
24	c	505	CLA	O2D-CGD-CBD	6.83	121.07	111.22
24	B	612	CLA	O2D-CGD-CBD	6.84	121.09	111.22
24	a	607	CLA	C2A-C3A-C4A	6.85	108.86	101.84
24	c	505	CLA	C2A-C3A-C4A	6.87	108.88	101.84
24	C	512	CLA	O2D-CGD-CBD	6.89	121.17	111.22
24	a	606	CLA	C2A-C3A-C4A	6.91	108.92	101.84
24	b	618	CLA	C2A-C3A-C4A	6.91	108.92	101.84
24	A	607	CLA	O2D-CGD-CBD	6.91	121.19	111.22
24	c	510	CLA	C2A-C3A-C4A	6.92	108.93	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	O2D-CGD-CBD	6.98	121.30	111.22
24	c	511	CLA	C2A-C3A-C4A	6.98	109.00	101.84
24	D	402	CLA	C2A-C3A-C4A	7.02	109.04	101.84
24	C	501	CLA	O2D-CGD-CBD	7.03	121.36	111.22
24	B	615	CLA	C2A-C3A-C4A	7.05	109.07	101.84
24	C	512	CLA	C2A-C3A-C4A	7.06	109.08	101.84
24	b	618	CLA	O2D-CGD-CBD	7.16	121.55	111.22
24	C	511	CLA	C2A-C3A-C4A	7.17	109.19	101.84
24	b	616	CLA	C2A-C3A-C4A	7.18	109.20	101.84
24	d	402	CLA	C2A-C3A-C4A	7.19	109.21	101.84
24	b	610	CLA	C2A-C3A-C4A	7.22	109.24	101.84
24	b	613	CLA	O2D-CGD-CBD	7.25	121.68	111.22
24	c	512	CLA	C2A-C3A-C4A	7.26	109.28	101.84
24	c	508	CLA	C2A-C3A-C4A	7.28	109.30	101.84
24	C	510	CLA	C2A-C3A-C4A	7.29	109.32	101.84
24	a	609	CLA	C2A-C3A-C4A	7.29	109.32	101.84
28	A	612	SQD	O9-S-C6	7.30	112.06	106.92
24	B	609	CLA	C2A-C3A-C4A	7.33	109.36	101.84
24	b	612	CLA	C2A-C3A-C4A	7.33	109.36	101.84
24	b	604	CLA	C2A-C3A-C4A	7.35	109.38	101.84
28	a	612	SQD	O9-S-C6	7.36	112.11	106.92
24	C	508	CLA	C2A-C3A-C4A	7.46	109.49	101.84
24	c	507	CLA	O2D-CGD-CBD	7.47	122.00	111.22
24	c	513	CLA	C2A-C3A-C4A	7.57	109.60	101.84
24	b	613	CLA	C2A-C3A-C4A	7.68	109.71	101.84
24	b	606	CLA	C2A-C3A-C4A	7.70	109.73	101.84
24	b	615	CLA	C2A-C3A-C4A	7.71	109.75	101.84
24	c	501	CLA	C2A-C3A-C4A	7.72	109.76	101.84
24	A	607	CLA	C2A-C3A-C4A	7.73	109.77	101.84
24	C	513	CLA	C2A-C3A-C4A	7.73	109.77	101.84
24	B	604	CLA	C2A-C3A-C4A	7.79	109.82	101.84
24	D	404	CLA	C2A-C3A-C4A	7.79	109.82	101.84
24	A	609	CLA	C2A-C3A-C4A	7.81	109.85	101.84
24	C	503	CLA	C2A-C3A-C4A	7.82	109.86	101.84
24	c	506	CLA	C2A-C3A-C4A	7.86	109.89	101.84
24	B	603	CLA	O2D-CGD-CBD	7.90	122.62	111.22
24	B	611	CLA	C2A-C3A-C4A	7.90	109.94	101.84
24	C	505	CLA	O2D-CGD-CBD	7.93	122.66	111.22
24	b	603	CLA	C2A-C3A-C4A	7.94	109.98	101.84
24	D	403	CLA	C2A-C3A-C4A	7.96	110.00	101.84
24	c	503	CLA	C2A-C3A-C4A	8.01	110.05	101.84
24	c	502	CLA	C2A-C3A-C4A	8.08	110.12	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	O2D-CGD-CBD	8.11	122.92	111.22
24	b	604	CLA	O2D-CGD-CBD	8.14	122.97	111.22
24	c	504	CLA	C2A-C3A-C4A	8.15	110.20	101.84
24	d	403	CLA	C2A-C3A-C4A	8.22	110.27	101.84
24	B	602	CLA	C2A-C3A-C4A	8.24	110.29	101.84
24	B	612	CLA	C2A-C3A-C4A	8.31	110.36	101.84
24	B	605	CLA	C2A-C3A-C4A	8.31	110.36	101.84
24	C	502	CLA	C2A-C3A-C4A	8.35	110.40	101.84
24	b	607	CLA	C2A-C3A-C4A	8.36	110.41	101.84
24	B	606	CLA	C2A-C3A-C4A	8.38	110.43	101.84
24	B	614	CLA	C2A-C3A-C4A	8.42	110.47	101.84
24	C	507	CLA	O2D-CGD-CBD	8.44	123.40	111.22
24	b	609	CLA	C2A-C3A-C4A	8.48	110.53	101.84
24	C	507	CLA	C2A-C3A-C4A	8.54	110.59	101.84
24	B	610	CLA	C2A-C3A-C4A	8.54	110.60	101.84
24	c	507	CLA	C2A-C3A-C4A	8.55	110.61	101.84
24	C	509	CLA	C2A-C3A-C4A	8.55	110.61	101.84
24	C	504	CLA	C2A-C3A-C4A	8.59	110.65	101.84
24	B	607[A]	CLA	C2A-C3A-C4A	8.61	110.67	101.84
24	b	614	CLA	C2A-C3A-C4A	8.65	110.71	101.84
24	B	608	CLA	C2A-C3A-C4A	8.80	110.86	101.84
24	B	607[B]	CLA	C2A-C3A-C4A	8.83	110.89	101.84
24	b	605	CLA	C2A-C3A-C4A	8.86	110.93	101.84
24	b	611	CLA	C2A-C3A-C4A	8.88	110.94	101.84
24	c	509	CLA	C2A-C3A-C4A	8.90	110.96	101.84
24	b	617	CLA	C2A-C3A-C4A	8.92	110.99	101.84
24	B	616	CLA	C2A-C3A-C4A	8.94	111.00	101.84
24	b	608[A]	CLA	C2A-C3A-C4A	8.99	111.06	101.84
24	C	501	CLA	C2A-C3A-C4A	9.00	111.07	101.84
24	B	613	CLA	C2A-C3A-C4A	9.12	111.19	101.84
24	b	608[B]	CLA	C2A-C3A-C4A	9.18	111.25	101.84
26	H	101	BCR	C21-C20-C19	14.35	167.40	123.11
26	B	620	BCR	C21-C20-C19	15.70	171.57	123.11
26	K	101	BCR	C21-C20-C19	16.02	172.58	123.11
26	f	101	BCR	C21-C20-C19	16.11	172.85	123.11
26	k	101	BCR	C21-C20-C19	16.27	173.33	123.11
26	B	619	BCR	C21-C20-C19	16.53	174.13	123.11
26	c	521	BCR	C21-C20-C19	16.74	174.78	123.11
26	C	514	BCR	C21-C20-C19	16.91	175.30	123.11
26	B	618	BCR	C21-C20-C19	17.00	175.59	123.11
26	F	101	BCR	C21-C20-C19	17.01	175.63	123.11
26	b	620	BCR	C21-C20-C19	17.04	175.72	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	621	BCR	C21-C20-C19	17.13	175.99	123.11
26	A	610	BCR	C21-C20-C19	17.30	176.52	123.11
26	t	101	BCR	C21-C20-C19	17.33	176.60	123.11
26	h	101	BCR	C21-C20-C19	17.36	176.72	123.11
26	K	102	BCR	C21-C20-C19	17.40	176.83	123.11
26	c	515	BCR	C21-C20-C19	17.47	177.04	123.11
26	I	101	BCR	C21-C20-C19	17.56	177.31	123.11
26	c	514	BCR	C21-C20-C19	17.64	177.57	123.11
26	a	610	BCR	C21-C20-C19	17.65	177.61	123.11
26	T	101	BCR	C21-C20-C19	17.96	178.57	123.11
26	b	619	BCR	C21-C20-C19	18.24	179.43	123.11
26	a	610	BCR	C15-C16-C17	19.39	165.06	123.23
26	K	101	BCR	C15-C16-C17	20.25	166.92	123.23
26	b	619	BCR	C15-C16-C17	20.31	167.04	123.23
26	c	514	BCR	C15-C16-C17	20.62	167.72	123.23
26	h	101	BCR	C15-C16-C17	20.63	167.74	123.23
26	f	101	BCR	C15-C16-C17	20.75	167.99	123.23
26	B	619	BCR	C15-C16-C17	21.08	168.72	123.23
26	b	620	BCR	C15-C16-C17	21.31	169.19	123.23
26	K	102	BCR	C15-C16-C17	21.43	169.46	123.23
26	c	515	BCR	C15-C16-C17	21.55	169.72	123.23
26	H	101	BCR	C15-C16-C17	21.66	169.95	123.23
26	c	521	BCR	C15-C16-C17	21.75	170.15	123.23
26	B	618	BCR	C15-C16-C17	21.75	170.16	123.23
26	C	514	BCR	C15-C16-C17	21.94	170.57	123.23
26	F	101	BCR	C15-C16-C17	22.01	170.72	123.23
26	I	101	BCR	C15-C16-C17	22.03	170.75	123.23
26	B	620	BCR	C15-C16-C17	22.03	170.76	123.23
26	A	610	BCR	C15-C16-C17	22.73	172.26	123.23
26	t	101	BCR	C15-C16-C17	23.62	174.19	123.23
26	T	101	BCR	C15-C16-C17	23.77	174.50	123.23
26	k	101	BCR	C15-C16-C17	23.82	174.62	123.23
26	b	621	BCR	C15-C16-C17	23.85	174.68	123.23

All (205) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	508	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	ND
24	b	607	CLA	NA
24	b	607	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	607	CLA	ND
24	c	511	CLA	NA
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	504	CLA	NC
24	c	504	CLA	ND
24	c	504	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	a	609	CLA	NC
24	a	609	CLA	ND
24	a	609	CLA	NA
24	d	402	CLA	NC
24	d	402	CLA	ND
24	d	402	CLA	NA
24	a	606	CLA	NA
24	a	606	CLA	NC
24	a	606	CLA	ND
24	B	607[A]	CLA	NA
24	B	607[A]	CLA	NC
24	B	607[A]	CLA	ND
24	B	607[B]	CLA	NA
24	B	607[B]	CLA	NC
24	B	607[B]	CLA	ND
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	c	513	CLA	NA
24	c	513	CLA	NC
24	c	513	CLA	ND
24	C	501	CLA	NA
24	C	501	CLA	NC
24	C	501	CLA	ND
24	c	507	CLA	NC
24	c	507	CLA	ND
24	c	507	CLA	NA
24	b	605	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	605	CLA	ND
24	b	605	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	c	503	CLA	NC
24	c	503	CLA	ND
24	c	503	CLA	NA
24	b	603	CLA	NC
24	b	603	CLA	ND
24	b	603	CLA	NA
24	C	505	CLA	NC
24	C	505	CLA	ND
24	C	505	CLA	NA
24	b	616	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	606	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	A	606	CLA	NA
24	A	606	CLA	NC
24	A	606	CLA	ND
24	C	511	CLA	NC
24	C	511	CLA	ND
24	c	501	CLA	NC
24	c	501	CLA	ND
24	C	510	CLA	NC
24	C	510	CLA	ND
24	D	403	CLA	NA
24	D	403	CLA	NC
24	D	403	CLA	ND
24	B	610	CLA	NC
24	B	610	CLA	ND
24	B	610	CLA	NA
24	c	502	CLA	NA
24	c	502	CLA	NC
24	c	502	CLA	ND
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	c	508	CLA	NA
24	c	508	CLA	NC

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Mol	Chain	Res	Type	Atom
24	c	508	CLA	ND
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	a	607	CLA	NC
24	a	607	CLA	ND
24	a	607	CLA	NA
24	D	404	CLA	NA
24	D	404	CLA	NC
24	D	404	CLA	ND
24	d	403	CLA	NA
24	d	403	CLA	NC
24	d	403	CLA	ND
24	b	615	CLA	NC
24	b	615	CLA	ND
24	b	615	CLA	NA
24	B	609	CLA	NC
24	B	609	CLA	ND
24	B	609	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	b	612	CLA	NA
24	D	402	CLA	NC
24	D	402	CLA	ND
24	D	402	CLA	NA
24	B	603	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	b	608[A]	CLA	NA
24	b	608[A]	CLA	NC
24	b	608[A]	CLA	ND

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Mol	Chain	Res	Type	Atom
24	c	505	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	ND
24	A	607	CLA	NC
24	A	607	CLA	ND
24	A	607	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	616	CLA	NC
24	B	616	CLA	ND
24	B	616	CLA	NA
24	C	509	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	b	608[B]	CLA	NA
24	b	608[B]	CLA	NC
24	b	608[B]	CLA	ND
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	A	609	CLA	NC
24	A	609	CLA	ND
24	A	609	CLA	NA
24	b	604	CLA	NC
24	b	604	CLA	ND
24	b	604	CLA	NA
24	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	b	613	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	614	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	ND
24	B	612	CLA	NA
24	B	612	CLA	NC

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Mol	Chain	Res	Type	Atom
24	B	612	CLA	ND
24	b	618	CLA	NC
24	b	618	CLA	ND
24	a	615	CLA	NC
24	a	615	CLA	ND
24	a	615	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	ND
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA
24	B	611	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	b	611	CLA	NA
24	C	502	CLA	NA
24	C	502	CLA	NC
24	C	502	CLA	ND

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	t	101	BCR	C21-C20-C19-C18
26	b	620	BCR	C17-C16-C15-C14
26	a	610	BCR	C21-C20-C19-C18
26	C	514	BCR	C16-C17-C18-C19
26	c	514	BCR	C20-C21-C22-C23
26	h	101	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
26	h	101	BCR	C16-C17-C18-C19
26	B	619	BCR	C16-C17-C18-C19
26	A	610	BCR	C17-C16-C15-C14
26	B	620	BCR	C17-C16-C15-C14
26	B	620	BCR	C16-C17-C18-C19
26	b	620	BCR	C20-C21-C22-C37
26	F	101	BCR	C17-C16-C15-C14
26	b	620	BCR	C16-C17-C18-C19
26	h	101	BCR	C17-C16-C15-C14
26	K	101	BCR	C16-C17-C18-C19
26	c	515	BCR	C17-C16-C15-C14
26	B	619	BCR	C20-C21-C22-C37
26	K	101	BCR	C16-C17-C18-C36
26	k	101	BCR	C16-C17-C18-C36
26	B	619	BCR	C16-C17-C18-C36
26	B	618	BCR	C20-C21-C22-C23
26	H	101	BCR	C17-C16-C15-C14
26	b	619	BCR	C17-C16-C15-C14
26	b	621	BCR	C21-C20-C19-C18
26	H	101	BCR	C10-C11-C12-C13
26	B	619	BCR	C21-C20-C19-C18
26	I	101	BCR	C21-C20-C19-C18
29	Z	101	LMG	C8-O7-C10-C11
29	z	101	LMG	C8-O7-C10-C11

There are no ring outliers.

73 monomers are involved in 571 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	601	OEX	1	0
24	A	606	CLA	9	0
24	A	607	CLA	7	0
25	A	608	PHO	4	0
24	A	609	CLA	13	0
26	A	610	BCR	19	0
27	A	611	PL9	17	0
28	A	612	SQD	2	0
29	A	613	LMG	3	0
28	A	614	SQD	2	0
30	A	615	LHG	10	0
24	B	602	CLA	6	0
24	B	603	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	604	CLA	10	0
24	B	605	CLA	11	0
24	B	606	CLA	14	0
24	B	607[A]	CLA	2	0
24	B	607[B]	CLA	6	0
24	B	608	CLA	5	0
24	B	609	CLA	8	0
24	B	610	CLA	5	0
24	B	611	CLA	5	0
24	B	612	CLA	5	0
24	B	613	CLA	8	0
24	B	614	CLA	11	0
24	B	615	CLA	10	0
24	B	616	CLA	9	0
24	B	617	CLA	9	0
26	B	618	BCR	24	0
26	B	619	BCR	36	0
26	B	620	BCR	25	0
29	B	621	LMG	2	0
28	B	622	SQD	6	0
24	C	501	CLA	13	0
24	C	502	CLA	5	0
24	C	503	CLA	11	0
24	C	504	CLA	6	0
24	C	505	CLA	9	0
24	C	506	CLA	10	0
24	C	507	CLA	7	0
24	C	508	CLA	6	0
24	C	509	CLA	4	0
24	C	510	CLA	9	0
24	C	511	CLA	3	0
24	C	512	CLA	4	0
24	C	513	CLA	5	0
26	C	514	BCR	21	0
32	C	516	DGD	3	0
32	C	517	DGD	7	0
29	C	518	LMG	2	0
29	C	519	LMG	4	0
25	D	401	PHO	12	0
24	D	402	CLA	6	0
24	D	403	CLA	8	0
24	D	404	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	405	PL9	14	0
30	D	406	LHG	6	0
30	D	407	LHG	4	0
29	D	408	LMG	7	0
32	E	101	DGD	1	0
33	E	103	HEM	6	0
26	F	101	BCR	28	0
26	H	101	BCR	25	0
32	H	102	DGD	11	0
26	I	101	BCR	18	0
26	K	101	BCR	21	0
26	K	102	BCR	15	0
30	L	101	LHG	6	0
28	L	102	SQD	6	0
26	T	101	BCR	29	0
33	V	201	HEM	10	0
28	X	101	SQD	4	0
29	Z	101	LMG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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(Å²)	Q<0.9	
1	A	334/334 (100%)	0.96	20 (5%)	25	19	57, 63, 84, 93	0
1	a	334/334 (100%)	0.88	24 (7%)	18	15	78, 84, 104, 114	0
2	B	504/504 (100%)	0.76	16 (3%)	51	42	59, 68, 89, 111	0
2	b	504/504 (100%)	0.94	46 (9%)	11	10	80, 88, 110, 131	0
3	C	451/451 (100%)	0.88	27 (5%)	25	19	61, 72, 85, 97	0
3	c	451/451 (100%)	0.85	39 (8%)	13	12	82, 93, 105, 118	0
4	D	342/342 (100%)	0.92	16 (4%)	35	28	57, 64, 80, 102	0
4	d	342/342 (100%)	0.93	25 (7%)	18	14	78, 85, 101, 123	0
5	E	81/81 (100%)	0.75	5 (6%)	24	19	68, 81, 98, 104	0
5	e	81/81 (100%)	0.84	8 (9%)	9	9	89, 102, 119, 125	0
6	F	34/34 (100%)	0.85	1 (2%)	55	45	68, 74, 99, 102	0
6	f	34/34 (100%)	0.93	4 (11%)	6	6	89, 95, 120, 122	0
7	H	65/65 (100%)	0.74	4 (6%)	24	19	64, 74, 81, 99	0
7	h	65/65 (100%)	0.85	8 (12%)	5	6	85, 95, 102, 120	0
8	I	38/38 (100%)	0.56	1 (2%)	59	49	70, 74, 105, 109	0
8	i	38/38 (100%)	0.73	2 (5%)	30	23	90, 95, 126, 130	0
9	J	38/38 (100%)	0.72	2 (5%)	30	23	66, 78, 109, 112	0
9	j	38/38 (100%)	0.69	2 (5%)	30	23	87, 99, 129, 133	0
10	K	37/37 (100%)	0.75	1 (2%)	58	47	74, 79, 86, 88	0
10	k	37/37 (100%)	1.02	4 (10%)	8	7	94, 100, 107, 108	0
11	L	37/37 (100%)	0.69	2 (5%)	29	23	58, 62, 90, 99	0
11	l	37/37 (100%)	0.78	2 (5%)	29	23	79, 83, 111, 120	0
12	M	34/34 (100%)	0.79	2 (5%)	26	20	62, 64, 77, 93	0
12	m	34/34 (100%)	0.87	2 (5%)	26	20	83, 84, 98, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/243 (100%)	0.77	15 (6%) 24 19	59, 73, 95, 111	0
13	o	243/243 (100%)	0.96	27 (11%) 7 7	79, 94, 116, 132	0
14	T	30/30 (100%)	0.50	0 100 100	60, 64, 85, 93	0
14	t	30/30 (100%)	0.58	0 100 100	80, 85, 105, 114	0
15	U	97/97 (100%)	0.77	3 (3%) 52 43	64, 71, 89, 90	0
15	u	97/97 (100%)	0.85	6 (6%) 24 19	84, 92, 110, 111	0
16	V	137/137 (100%)	0.84	9 (6%) 22 16	64, 69, 80, 88	0
16	v	137/137 (100%)	0.79	10 (7%) 18 14	84, 89, 101, 109	0
17	Y	29/29 (100%)	0.75	1 (3%) 49 40	82, 89, 115, 118	0
17	y	29/29 (100%)	0.70	5 (17%) 2 2	103, 110, 136, 138	0
18	X	39/39 (100%)	0.55	1 (2%) 59 49	74, 80, 107, 108	0
18	x	39/39 (100%)	0.52	0 100 100	95, 101, 127, 129	0
19	Z	62/62 (100%)	0.56	2 (3%) 51 42	80, 89, 109, 112	0
19	z	62/62 (100%)	0.50	3 (4%) 34 27	101, 110, 129, 133	0
All	All	5264/5264 (100%)	0.84	345 (6%) 22 16	57, 83, 107, 138	0

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	d	11	GLU	5.3
9	j	3	SER	5.0
16	v	77	LYS	4.7
1	a	137	LEU	4.6
3	c	293	ASN	4.5
4	d	217	THR	4.4
3	c	129	GLY	4.3
13	O	29	ALA	4.2
13	o	86	LYS	4.2
5	e	6	GLY	4.1
2	b	267	LEU	4.0
4	d	221	THR	4.0
10	k	10	LYS	4.0
8	i	38	GLU	4.0
3	C	266	TRP	3.9
3	c	183	GLY	3.9
13	O	207	ARG	3.9
4	d	64	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	b	268	PHE	3.8
13	o	164	LEU	3.7
2	b	12	LEU	3.7
2	b	218	LEU	3.6
7	H	64	ALA	3.6
3	c	392	ALA	3.5
3	c	292	PHE	3.5
6	f	12	SER	3.5
5	e	84	LYS	3.5
3	c	302	TYR	3.4
16	V	34	GLN	3.4
2	b	124	ARG	3.4
15	u	27	LEU	3.4
4	d	218	VAL	3.3
3	c	457	LYS	3.3
10	k	11	LEU	3.3
13	o	161	GLY	3.3
11	l	1	MET	3.3
3	c	296	VAL	3.3
7	h	2	ALA	3.2
2	b	137	LYS	3.2
2	b	494	GLY	3.2
1	a	314	ILE	3.2
1	a	139	MET	3.2
19	z	1	MET	3.2
2	b	310	ALA	3.2
15	u	17	LEU	3.1
3	C	135	ARG	3.1
4	D	135	LEU	3.1
1	a	302	PHE	3.1
3	c	44	ASN	3.1
1	a	220	THR	3.1
1	A	86	SER	3.1
1	a	294	ALA	3.1
3	c	227	VAL	3.1
2	b	65	PHE	3.1
1	A	178	GLY	3.0
9	j	40	LEU	3.0
1	A	170	ASP	3.0
13	o	163	GLY	3.0
13	o	40	ILE	3.0
13	o	87	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
13	o	93	LEU	2.9
13	o	71	VAL	2.9
1	A	292	THR	2.9
2	b	321	LYS	2.9
13	o	204	VAL	2.9
4	d	229	ALA	2.8
1	a	224	ILE	2.8
4	D	80	THR	2.8
2	b	443	PHE	2.8
4	D	172	SER	2.8
13	o	46	GLN	2.8
3	c	226	SER	2.8
3	C	145[A]	SER	2.8
7	H	66	GLY	2.8
13	O	213	GLY	2.8
2	b	425	ILE	2.7
3	c	294	ASN	2.7
1	a	140	ARG	2.7
2	b	492	GLU	2.7
2	b	225	LEU	2.7
1	a	337	HIS	2.7
2	b	485	GLU	2.7
7	h	12[A]	ARG	2.7
3	C	311	GLN	2.7
12	m	31	SER	2.7
19	z	24	PRO	2.7
3	c	95	LEU	2.7
1	a	138	GLY	2.7
1	A	246	TYR	2.7
5	E	60	GLN	2.7
17	y	41	VAL	2.7
2	b	70	GLY	2.7
2	b	161	LEU	2.6
5	e	7	GLU	2.6
5	e	26	THR	2.6
2	b	69	LEU	2.6
3	C	95	LEU	2.6
17	y	38	LEU	2.6
1	a	188	ALA	2.6
3	c	161	LEU	2.6
16	v	100	ILE	2.6
1	a	130	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
7	h	30	LEU	2.6
1	A	139	MET	2.6
2	b	226	TYR	2.6
2	B	203	ILE	2.6
3	c	163	PHE	2.6
4	D	52	THR	2.6
3	c	201	ASN	2.6
4	d	17	ILE	2.6
9	J	4	GLU	2.6
13	o	97	GLU	2.6
3	c	338	GLY	2.6
3	C	417	VAL	2.6
3	c	375	LEU	2.6
7	H	2	ALA	2.6
3	C	411	ALA	2.5
13	o	4	THR	2.5
15	U	91	LEU	2.5
5	e	42	LEU	2.5
16	v	47	LYS	2.5
4	D	352	LEU	2.5
2	b	11	VAL	2.5
19	z	3	ILE	2.5
8	I	24	LEU	2.5
4	d	183	LEU	2.5
13	O	243	ILE	2.5
3	c	342	MET	2.5
2	b	264	PRO	2.5
3	c	184	GLY	2.5
4	D	208	ALA	2.5
16	v	59	LEU	2.5
3	C	293	ASN	2.5
13	O	16	ALA	2.5
1	a	340	PRO	2.5
15	u	28	ASN	2.5
5	e	79	PHE	2.5
2	b	120	LEU	2.4
3	C	69	LEU	2.4
4	d	264	LYS	2.4
13	O	86	LYS	2.4
4	d	60	THR	2.4
13	o	57	LYS	2.4
2	B	322	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	490	GLN	2.4
6	f	44	GLN	2.4
13	o	201	VAL	2.4
16	v	48	THR	2.4
4	d	71	CYS	2.4
4	d	219	GLU	2.4
16	V	52	LEU	2.4
2	b	183	PRO	2.4
3	c	416[A]	SER	2.4
16	v	94	SER	2.4
2	b	493	TRP	2.4
2	B	315	ILE	2.4
1	A	307	ILE	2.4
3	C	70	PHE	2.4
16	v	34	GLN	2.4
1	a	223	LEU	2.4
1	A	314	ILE	2.4
3	C	309	ALA	2.4
1	a	222	SER	2.4
13	O	238	VAL	2.4
1	A	19	ASN	2.4
3	c	93	ALA	2.4
2	b	241	SER	2.4
4	d	245	SER	2.4
12	M	34	LYS	2.4
13	O	241	ALA	2.4
16	V	121	VAL	2.4
3	C	457	LYS	2.4
8	i	37	LEU	2.4
1	A	108	ASN	2.4
4	D	219	GLU	2.4
13	O	204	VAL	2.4
3	C	347	GLY	2.3
1	A	294	ALA	2.3
3	c	411	ALA	2.3
7	h	53	LEU	2.3
4	D	212	ALA	2.3
4	D	292	ASN	2.3
2	B	490	GLN	2.3
2	b	168	VAL	2.3
6	f	42	PHE	2.3
16	v	66	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	52	LEU	2.3
3	C	129	GLY	2.3
1	a	275	LEU	2.3
2	B	323	GLY	2.3
16	v	30	LYS	2.3
4	D	54	PHE	2.3
16	V	100	ILE	2.3
1	a	335	ASN	2.3
17	y	36	ILE	2.3
4	D	218	VAL	2.3
4	d	54	PHE	2.3
2	B	321	LYS	2.3
13	o	126	VAL	2.3
1	A	60	ILE	2.3
2	B	8	VAL	2.3
15	U	17	LEU	2.3
13	O	74[A]	GLU	2.3
2	B	207	ILE	2.3
3	c	48	LYS	2.3
4	d	141	TYR	2.3
7	H	49	TYR	2.3
12	m	5	GLN	2.3
16	V	75	TYR	2.3
3	C	66	ALA	2.3
13	o	166	SER	2.3
13	o	76	THR	2.3
2	b	50	PRO	2.2
4	D	254	SER	2.2
3	C	401	LEU	2.2
13	O	42	ARG	2.2
1	A	232	SER	2.2
4	D	295	SER	2.2
16	V	65	PRO	2.2
3	c	45	LEU	2.2
3	c	172	ALA	2.2
2	B	178	VAL	2.2
1	A	213	ALA	2.2
1	a	257	ARG	2.2
4	D	107	LEU	2.2
16	V	54	LEU	2.2
3	C	336	GLY	2.2
13	o	88	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
5	E	49	THR	2.2
9	J	3	SER	2.2
3	c	415	ASN	2.2
11	L	1	MET	2.2
2	b	193	TYR	2.2
2	b	302	TRP	2.2
3	c	135	ARG	2.2
4	d	98	GLN	2.2
13	o	103	PHE	2.2
19	Z	35	ARG	2.2
2	B	382	PRO	2.2
3	c	49	LEU	2.2
5	E	79	PHE	2.2
10	k	46	ARG	2.2
13	O	212	ALA	2.2
1	A	220	THR	2.2
3	C	272	LEU	2.2
4	d	22	LEU	2.2
2	b	361	ALA	2.2
3	c	273	SER	2.2
2	B	57	ARG	2.2
2	b	123	PHE	2.2
18	X	2	THR	2.2
17	y	25	ILE	2.2
15	u	101	GLY	2.2
2	b	448	ARG	2.2
3	C	151	TRP	2.2
2	B	341	LYS	2.1
2	b	167	TRP	2.1
3	c	69	LEU	2.1
13	o	125	LEU	2.1
5	e	22	ILE	2.1
17	Y	21	GLN	2.1
3	C	396	MET	2.1
3	c	196	VAL	2.1
13	o	118	LEU	2.1
1	a	108	ASN	2.1
1	a	303	ASN	2.1
1	a	306	VAL	2.1
2	b	491	VAL	2.1
13	o	151	TYR	2.1
5	e	41	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	320	ALA	2.1
3	c	133	ALA	2.1
6	F	41	GLN	2.1
11	l	17	LEU	2.1
13	o	110[A]	MET	2.1
2	b	206	GLY	2.1
3	c	373	ASN	2.1
3	C	134	ILE	2.1
3	C	265	ILE	2.1
5	E	84	LYS	2.1
13	O	123	LYS	2.1
13	O	163	GLY	2.1
1	A	312	ASN	2.1
4	D	132	ILE	2.1
7	h	26	GLY	2.1
1	A	222	SER	2.1
4	d	314	PHE	2.1
19	Z	24	PRO	2.1
2	b	330	MET	2.1
1	A	296	ASN	2.1
2	b	52	LEU	2.1
3	C	294	ASN	2.1
16	v	121	VAL	2.1
13	o	202	ALA	2.1
1	A	224	ILE	2.1
3	c	297	TYR	2.1
6	f	37	ILE	2.1
3	C	225	VAL	2.1
11	L	6	ASN	2.1
13	o	58	ASN	2.1
1	a	293	MET	2.1
4	d	82	ALA	2.1
2	b	203	ILE	2.1
3	C	222	GLY	2.1
3	C	361	PHE	2.1
4	d	223	PHE	2.1
4	d	258	GLY	2.1
2	b	53	ASN	2.1
13	o	238	VAL	2.1
13	o	55	GLU	2.1
2	b	320	ALA	2.0
10	k	20	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	a	296	ASN	2.0
3	c	328	VAL	2.0
3	c	341	LEU	2.0
7	h	15	ASN	2.0
2	b	322	GLY	2.0
2	B	67	ALA	2.0
2	b	482	ILE	2.0
2	b	370	LEU	2.0
1	A	90	GLY	2.0
7	h	66	GLY	2.0
2	B	425	ILE	2.0
2	b	169	SER	2.0
7	h	51	SER	2.0
15	U	90	ALA	2.0
17	y	40	ALA	2.0
4	d	222	LEU	2.0
5	E	73	LYS	2.0
2	b	301	ALA	2.0
4	d	309	PRO	2.0
15	u	70	ARG	2.0
16	V	38	ALA	2.0
10	K	42	ALA	2.0
13	O	186	ASN	2.0
4	d	84	SER	2.0
4	d	230	SER	2.0
15	u	81	HIS	2.0
1	a	89	ILE	2.0
4	D	290	ALA	2.0
12	M	11	THR	2.0
3	c	131	TYR	2.0
3	c	168	LEU	2.0
16	V	12	LEU	2.0
3	C	421	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
26	BCR	H	101	40/40	0.73	0.78	6.73	67,74,83,83	0
29	LMG	C	519	51/55	0.67	0.77	6.56	83,117,122,123	0
28	SQD	a	614	54/54	0.69	0.70	5.98	111,124,129,130	0
30	LHG	E	102	42/49	0.50	0.79	5.80	110,124,127,127	0
32	DGD	d	405	62/66	0.55	0.81	5.40	138,151,164,165	0
27	PL9	A	611	55/55	0.51	0.93	5.36	93,109,118,119	0
29	LMG	b	622	51/55	0.69	0.60	5.11	91,100,112,116	0
29	LMG	c	520	51/55	0.60	0.87	5.07	104,137,142,143	0
29	LMG	z	101	37/55	0.74	0.96	4.54	117,145,149,150	0
26	BCR	K	102	40/40	0.84	0.83	4.10	70,74,78,78	0
29	LMG	B	621	51/55	0.77	0.56	3.90	70,80,92,95	0
26	BCR	C	514	40/40	0.76	0.71	3.88	78,84,87,88	0
28	SQD	x	101	43/54	0.59	0.83	3.81	128,136,140,140	0
29	LMG	A	613	51/55	0.77	0.73	3.70	94,100,105,105	0
26	BCR	k	101	40/40	0.76	0.69	3.62	95,99,100,100	0
26	BCR	t	101	40/40	0.79	0.54	3.60	86,99,106,106	0
28	SQD	L	102	54/54	0.78	0.58	3.54	119,131,146,147	0
22	CL	A	604	1/1	0.82	0.64	3.54	62,62,62,62	0
26	BCR	c	521	40/40	0.76	0.78	3.50	91,95,98,99	0
28	SQD	X	101	43/54	0.76	0.68	3.47	108,115,119,119	0
29	LMG	c	519	51/55	0.62	0.71	3.40	92,118,134,135	0
32	DGD	E	101	62/66	0.56	0.78	3.34	118,130,143,144	0
24	CLA	B	606	65/65	0.87	0.68	3.33	59,64,75,76	0
24	CLA	c	509	65/65	0.89	0.80	3.21	91,93,108,108	0
26	BCR	b	619	40/40	0.83	0.54	3.16	84,88,90,90	0
26	BCR	T	101	40/40	0.78	0.49	3.06	65,78,85,86	0
30	LHG	d	407	49/49	0.84	0.63	3.02	85,89,98,102	0
28	SQD	b	601	54/54	0.72	0.55	2.98	99,107,121,121	0
29	LMG	a	613	51/55	0.82	0.71	2.93	114,121,126,126	0
30	LHG	e	101	42/49	0.56	0.82	2.86	131,145,147,148	0
28	SQD	A	614	54/54	0.72	0.56	2.86	91,103,109,109	0
24	CLA	B	608	65/65	0.85	0.54	2.80	58,61,73,74	0
24	CLA	b	603	65/65	0.77	0.67	2.70	94,102,127,128	0
27	PL9	a	611	55/55	0.52	0.71	2.69	113,130,139,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	BCR	B	618	40/40	0.80	0.55	2.66	63,68,69,70	0
30	LHG	a	616	49/49	0.73	0.74	2.49	87,94,124,125	0
26	BCR	K	101	40/40	0.83	0.63	2.48	75,78,79,80	0
24	CLA	c	508	65/65	0.83	0.52	2.47	87,90,115,119	0
30	LHG	D	406	49/49	0.80	0.61	2.46	70,75,81,82	0
26	BCR	h	101	40/40	0.72	0.60	2.40	87,94,103,104	0
24	CLA	B	602	65/65	0.80	0.55	2.36	73,82,107,107	0
24	CLA	B	611	65/65	0.89	0.60	2.33	62,65,73,77	0
30	LHG	d	406	49/49	0.80	0.63	2.30	91,96,102,102	0
27	PL9	d	404	55/55	0.74	0.67	2.30	80,84,91,93	0
24	CLA	b	615	65/65	0.87	0.48	2.29	80,84,106,108	0
26	BCR	f	101	40/40	0.73	0.56	2.27	87,91,109,110	0
24	CLA	b	609	65/65	0.82	0.51	2.27	79,82,94,95	0
26	BCR	c	514	40/40	0.74	0.63	2.18	99,105,108,108	0
32	DGD	h	102	62/66	0.84	0.62	2.15	87,93,99,101	0
30	LHG	D	407	49/49	0.82	0.55	2.12	64,69,78,81	0
24	CLA	b	612	65/65	0.88	0.61	2.05	82,86,94,98	0
29	LMG	Z	101	37/55	0.55	0.67	2.01	96,124,129,129	0
24	CLA	C	510	65/65	0.90	0.55	1.97	65,69,76,78	0
32	DGD	H	102	62/66	0.85	0.57	1.90	66,72,79,81	0
24	CLA	C	509	65/65	0.88	0.65	1.86	70,72,87,88	0
24	CLA	B	613	65/65	0.87	0.58	1.84	61,64,71,72	0
24	CLA	C	511	65/65	0.89	0.61	1.82	70,75,78,79	0
24	CLA	C	513	65/65	0.79	0.57	1.81	80,85,105,105	0
26	BCR	I	101	40/40	0.74	0.63	1.79	71,78,81,82	0
24	CLA	B	607[B]	65/65	0.81	0.54	1.78	63,67,72,75	65
24	CLA	D	403	65/65	0.88	0.56	1.77	54,59,75,76	0
24	CLA	C	512	65/65	0.90	0.54	1.76	78,82,103,104	0
26	BCR	b	621	40/40	0.78	0.47	1.74	89,94,100,101	0
26	BCR	B	620	40/40	0.79	0.47	1.73	68,74,80,80	0
27	PL9	D	405	55/55	0.80	0.56	1.70	60,64,70,72	0
26	BCR	c	515	40/40	0.76	0.61	1.69	92,98,102,102	0
24	CLA	B	607[A]	65/65	0.81	0.54	1.68	65,69,81,82	65
28	SQD	A	612	54/54	0.83	0.47	1.68	90,98,107,108	0
26	BCR	b	620	40/40	0.81	0.44	1.65	83,89,101,101	0
24	CLA	c	510	65/65	0.86	0.52	1.62	86,90,96,99	0
24	CLA	b	604	65/65	0.89	0.55	1.58	85,88,93,94	0
24	CLA	b	608[A]	65/65	0.78	0.57	1.54	85,90,102,103	65
24	CLA	B	605	65/65	0.88	0.54	1.54	60,63,91,91	0
24	CLA	B	617	65/65	0.84	0.50	1.52	63,69,118,119	0
24	CLA	b	608[B]	65/65	0.78	0.57	1.51	83,87,93,95	65
24	CLA	b	605	65/65	0.89	0.56	1.50	79,84,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	LHG	A	615	49/49	0.82	0.56	1.44	67,74,103,104	0
24	CLA	b	607	65/65	0.91	0.59	1.35	80,84,95,97	0
24	CLA	B	614	65/65	0.88	0.46	1.34	60,63,85,87	0
26	BCR	a	610	40/40	0.85	0.49	1.33	83,89,93,94	0
24	CLA	B	610	65/65	0.91	0.50	1.28	64,69,72,73	0
24	CLA	c	513	65/65	0.72	0.56	1.27	101,106,125,126	0
24	CLA	b	614	65/65	0.86	0.62	1.26	81,85,91,92	0
24	CLA	C	505	65/65	0.86	0.54	1.24	69,71,85,85	0
24	CLA	c	507	65/65	0.89	0.56	1.23	91,94,113,115	0
26	BCR	F	101	40/40	0.81	0.49	1.22	66,71,88,90	0
24	CLA	C	504	65/65	0.86	0.53	1.19	66,68,95,95	0
28	SQD	a	612	54/54	0.68	0.44	1.15	110,119,128,128	0
24	CLA	B	604	65/65	0.90	0.54	1.14	58,63,72,76	0
24	CLA	b	606	65/65	0.89	0.53	1.11	81,84,111,112	0
24	CLA	c	506	65/65	0.85	0.48	1.07	93,100,136,136	0
24	CLA	B	603	65/65	0.88	0.53	1.05	64,67,72,73	0
24	CLA	c	505	65/65	0.87	0.52	1.05	89,92,106,106	0
29	LMG	D	408	51/55	0.76	0.50	1.03	66,76,106,108	0
24	CLA	b	617	65/65	0.82	0.55	1.03	86,89,107,108	0
25	PHO	a	608	64/64	0.88	0.51	1.02	78,83,86,87	0
32	DGD	c	517	62/66	0.83	0.46	1.01	84,96,124,124	0
24	CLA	b	613	65/65	0.89	0.49	1.00	80,83,94,96	0
26	BCR	A	610	40/40	0.84	0.48	0.99	63,68,73,73	0
24	CLA	a	615	65/65	0.93	0.47	0.97	75,79,91,96	0
24	CLA	C	503	65/65	0.89	0.52	0.96	68,72,76,77	0
24	CLA	c	504	65/65	0.86	0.46	0.94	86,89,115,116	0
24	CLA	B	616	65/65	0.86	0.51	0.91	65,68,86,87	0
24	CLA	C	501	65/65	0.85	0.53	0.91	69,73,85,87	0
33	HEM	V	201	43/43	0.92	0.54	0.90	63,65,68,69	0
29	LMG	C	518	51/55	0.64	0.54	0.90	72,98,113,114	0
24	CLA	c	511	65/65	0.88	0.55	0.90	90,95,99,99	0
24	CLA	a	609	65/65	0.88	0.47	0.89	83,85,133,133	0
24	CLA	c	503	65/65	0.87	0.53	0.89	89,93,96,97	0
24	CLA	A	606	65/65	0.91	0.52	0.89	56,59,66,75	0
24	CLA	B	612	65/65	0.89	0.49	0.88	60,62,73,75	0
32	DGD	c	516	62/66	0.70	0.55	0.86	84,94,122,124	0
24	CLA	a	606	65/65	0.88	0.52	0.85	77,80,87,95	0
33	HEM	E	103	43/43	0.92	0.46	0.79	80,82,86,87	0
24	CLA	A	609	65/65	0.90	0.46	0.79	62,65,112,113	0
24	CLA	b	618	65/65	0.88	0.54	0.78	83,90,139,139	0
24	CLA	c	502	65/65	0.90	0.50	0.77	85,87,101,103	0
24	CLA	b	616	65/65	0.84	0.56	0.76	82,86,121,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	b	611	65/65	0.88	0.52	0.73	85,90,92,93	0
24	CLA	D	402	65/65	0.91	0.47	0.72	54,59,70,76	0
33	HEM	v	201	43/43	0.91	0.52	0.72	84,86,88,90	0
33	HEM	e	102	43/43	0.92	0.48	0.70	101,103,107,108	0
24	CLA	C	502	65/65	0.88	0.46	0.69	65,67,80,83	0
32	DGD	C	515	62/66	0.80	0.48	0.69	64,73,102,103	0
25	PHO	A	608	64/64	0.89	0.49	0.68	57,62,65,67	0
24	CLA	b	610	65/65	0.85	0.47	0.66	82,86,92,93	0
24	CLA	d	402	65/65	0.87	0.52	0.66	75,80,95,96	0
24	CLA	B	609	65/65	0.89	0.45	0.64	61,65,71,72	0
24	CLA	B	615	65/65	0.87	0.49	0.63	61,65,101,102	0
26	BCR	B	619	40/40	0.80	0.42	0.59	62,69,81,81	0
28	SQD	l	101	54/54	0.83	0.42	0.55	98,110,125,126	0
25	PHO	d	401	64/64	0.87	0.46	0.54	80,84,90,94	0
25	PHO	D	401	64/64	0.88	0.45	0.53	59,63,69,73	0
24	CLA	c	512	65/65	0.81	0.50	0.50	99,102,124,124	0
30	LHG	l	102	49/49	0.77	0.45	0.49	84,92,104,106	0
28	SQD	B	622	54/54	0.81	0.42	0.47	119,127,141,142	0
23	BCT	A	605	4/4	0.85	0.52	0.46	79,80,81,82	0
24	CLA	C	508	65/65	0.88	0.46	0.46	66,70,95,99	0
24	CLA	A	607	65/65	0.92	0.46	0.45	60,62,104,106	0
24	CLA	C	507	65/65	0.85	0.49	0.44	70,74,92,94	0
34	MG	j	102	1/1	0.97	0.43	0.41	89,89,89,89	0
24	CLA	a	607	65/65	0.87	0.47	0.41	80,83,124,126	0
32	DGD	c	518	62/66	0.79	0.47	0.33	83,93,113,117	0
29	LMG	j	101	51/55	0.71	0.44	0.32	87,96,126,129	0
24	CLA	c	501	65/65	0.85	0.51	0.31	90,93,106,108	0
24	CLA	D	404	65/65	0.91	0.42	0.30	65,68,106,107	0
22	CL	A	603	1/1	0.75	0.45	0.29	65,65,65,65	0
32	DGD	C	517	62/66	0.82	0.46	0.18	62,72,93,97	0
32	DGD	C	516	62/66	0.84	0.42	0.03	63,75,103,104	0
30	LHG	L	101	49/49	0.83	0.41	0.01	63,72,83,85	0
24	CLA	C	506	65/65	0.88	0.40	-0.00	72,79,115,115	0
24	CLA	d	403	65/65	0.89	0.40	0.00	86,89,126,128	0
23	BCT	a	605	4/4	0.95	0.48	-0.03	100,101,101,103	0
34	MG	J	101	1/1	0.95	0.38	-0.20	68,68,68,68	0
20	OEX	a	601	10/10	0.96	0.40	-0.26	83,84,87,88	0
22	CL	a	603	1/1	0.90	0.39	-0.31	86,86,86,86	0
22	CL	a	604	1/1	0.60	0.32	-0.80	83,83,83,83	0
31	CA	o	301	1/1	0.84	0.41	-1.00	110,110,110,110	0
21	FE2	a	602	1/1	0.95	0.30	-1.13	88,88,88,88	0
20	OEX	A	601	10/10	0.97	0.39	-1.28	63,64,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
21	FE2	A	602	1/1	0.94	0.32	-1.39	67,67,67,67	0
31	CA	f	102	1/1	0.86	0.15	-	118,118,118,118	0
31	CA	B	601	1/1	0.20	0.46	-	117,117,117,117	0
31	CA	O	301	1/1	0.47	0.21	-	90,90,90,90	0
31	CA	b	602	1/1	0.47	0.39	-	137,137,137,137	0
22	CL	U	201	1/1	0.67	0.53	-	91,91,91,91	0
31	CA	F	102	1/1	0.33	0.18	-	97,97,97,97	0
22	CL	u	201	1/1	0.34	0.61	-	112,112,112,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.