



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2018 – 04:42 PM EST

PDB ID : 5E7C
Title : Macromolecular diffractive imaging using imperfect crystals - Bragg data
Authors : Ayer, K.; Yefanov, O.; Oberthuer, D.; Roy-Chowdhury, S.; Galli, L.; Mariani, V.; Basu, S.; Coe, J.; Conrad, C.E.; Fromme, R.; Schaffner, A.; Doerner, 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.; Robinson, J.S.; Koglin, J.E.; Boutet, S.; Fromme, P.; Barty, A.; Chapman, H.N.
Deposited on : 2015-10-12
Resolution : 4.50 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

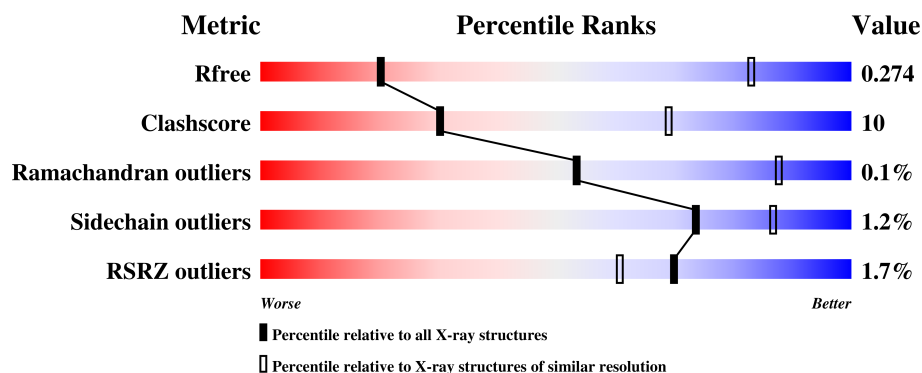
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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.



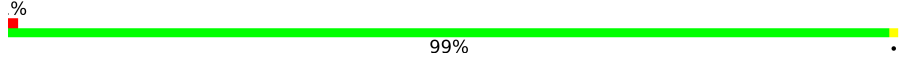

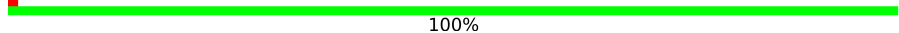

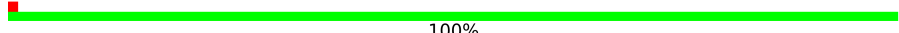

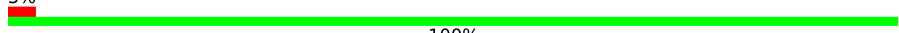




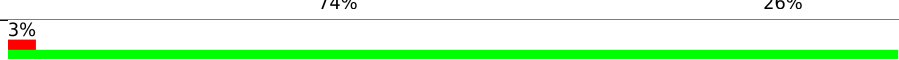


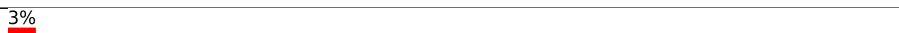
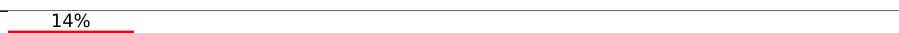

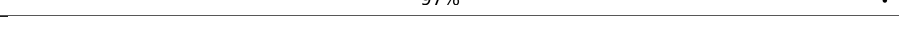

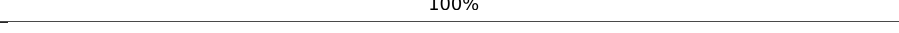

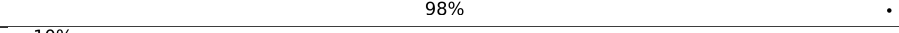

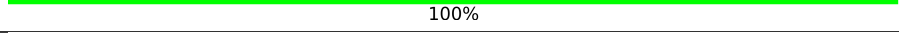

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1068 (5.30-3.70)
Clashscore	122126	1013 (5.28-3.72)
Ramachandran outliers	120053	1085 (5.30-3.70)
Sidechain outliers	120020	1067 (5.30-3.70)
RSRZ outliers	108989	1006 (5.30-3.62)

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>%</div> <div> <div></div> <div>73%</div> <div>27%</div> </div> </div>
1	a	334	<div> <div>%</div> <div> <div></div> <div>99%</div> <div>.</div> </div> </div>
2	B	504	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>23%</div> </div> </div>
2	b	504	<div> <div>%</div> <div> <div></div> <div>99%</div> <div>.</div> </div> </div>
3	C	451	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	c	451	 99%
4	D	342	 77% 23%
4	d	342	 100%
5	E	81	 62% 38%
5	e	81	 100%
6	F	34	 47% 53%
6	f	34	 100%
7	H	65	 9% 80% 17%
7	h	65	 6% 97%
8	I	38	 74% 26%
8	i	38	 3% 100%
9	J	38	 3% 74% 26%
9	j	38	 3% 100%
10	K	37	 51% 46%
10	k	37	 3% 95% 5%
11	L	37	 14% 81% 19%
11	l	37	 5% 97%
12	M	34	 82% 18%
12	m	34	 100%
13	O	243	 82% 17%
13	o	243	 2% 98%
14	T	30	 10% 77% 23%
14	t	30	 100%
15	U	97	 81% 19%
15	u	97	 99%

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Mol	Chain	Length	Quality of chain
16	V	137	
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
23	CLA	A	605	X	-	-	-
23	CLA	A	606	X	-	-	-
23	CLA	A	608	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607[A]	X	-	-	-
23	CLA	B	607[B]	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	X
23	CLA	C	501	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	X
23	CLA	C	513	X	-	-	X
23	CLA	D	402	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	604	X	-	-	-
23	CLA	a	605	X	-	-	-
23	CLA	a	607	X	-	-	-
23	CLA	a	613	X	-	-	-
23	CLA	b	604	X	-	-	X
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609[A]	X	-	-	X
23	CLA	b	609[B]	X	-	-	X
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	X
23	CLA	c	514	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
25	BCR	A	609	-	-	-	X
25	BCR	B	618	-	-	X	-
25	BCR	B	619	-	-	X	-
25	BCR	B	620	-	-	X	-
25	BCR	C	515	-	-	X	-
25	BCR	F	101	-	-	X	-
25	BCR	H	101	-	X	X	X
25	BCR	K	101	-	-	X	-
25	BCR	T	101	-	-	X	X
25	BCR	a	608	-	-	-	X
25	BCR	b	620	-	-	-	X
25	BCR	b	622	-	-	-	X
25	BCR	c	515	-	-	-	X
25	BCR	h	101	-	X	-	X
26	PL9	a	609	-	-	-	X
27	SQD	A	611	-	-	-	X
27	SQD	a	610	-	-	-	X
27	SQD	b	602	-	-	-	X
27	SQD	x	101	-	-	-	X
28	LMG	C	519	-	-	-	X
28	LMG	C	520	-	-	-	X
28	LMG	c	521	-	-	-	X
28	LMG	z	101	-	-	-	X
30	CA	B	601	-	-	-	X
30	CA	F	102	-	-	-	X
30	CA	b	603	-	-	-	X
32	DGD	D	406	-	-	-	X
32	DGD	d	405	-	-	-	X

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 49966 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	0	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	6	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	0	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			

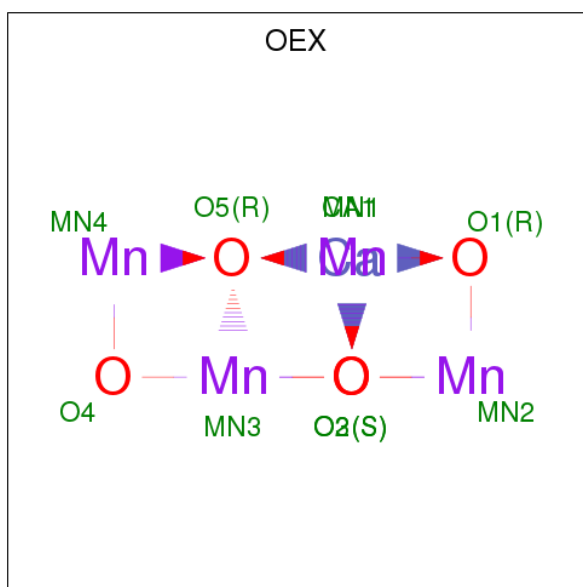
- Molecule 18 is a protein called Photosystem II reaction center X protein.

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).

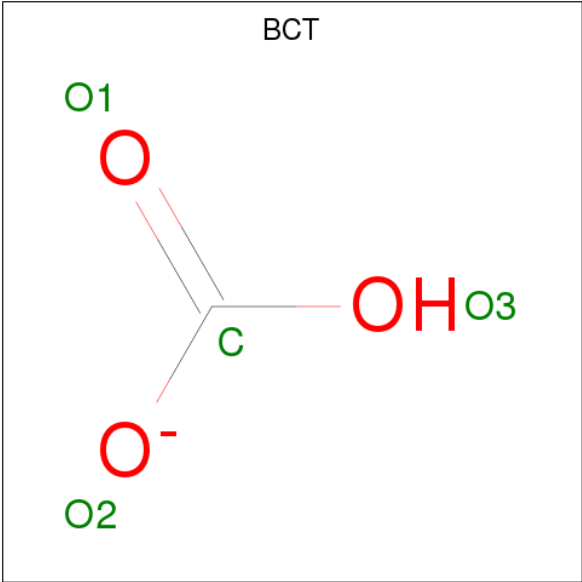


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

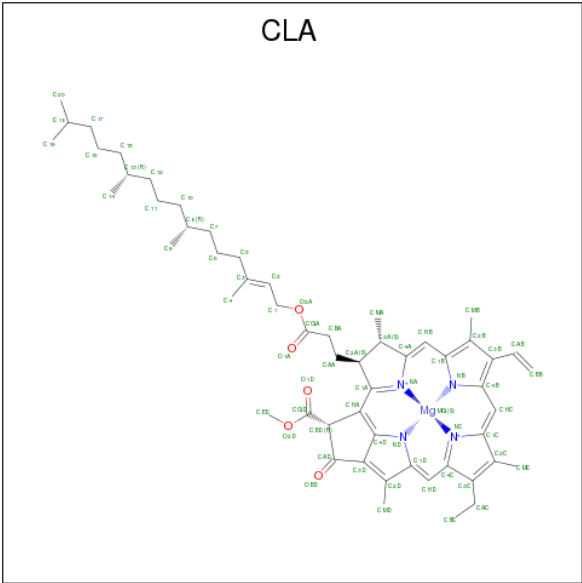
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Cl	0	0
			1	1		
21	A	2	Total	Cl	0	0
			2	2		
21	c	1	Total	Cl	0	0
			1	1		
21	V	1	Total	Cl	0	0
			1	1		
21	u	1	Total	Cl	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



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

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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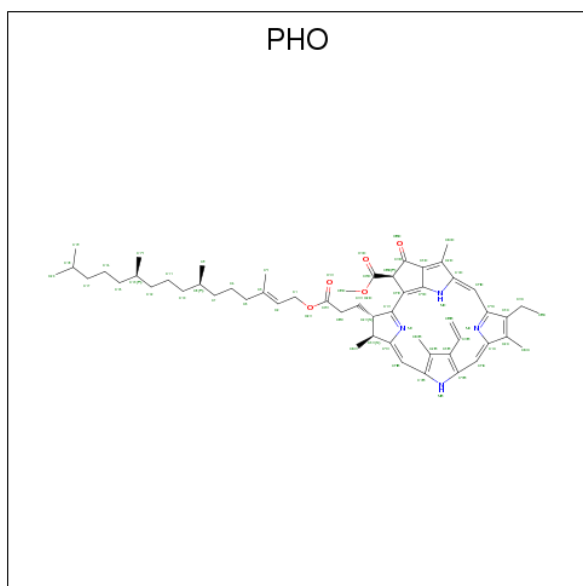
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1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

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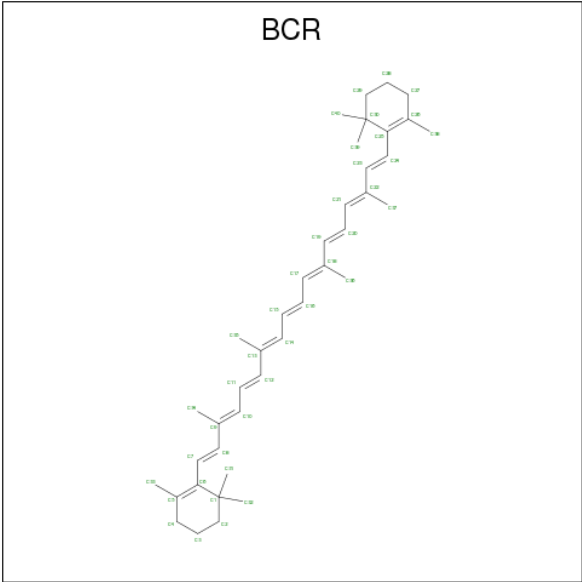
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



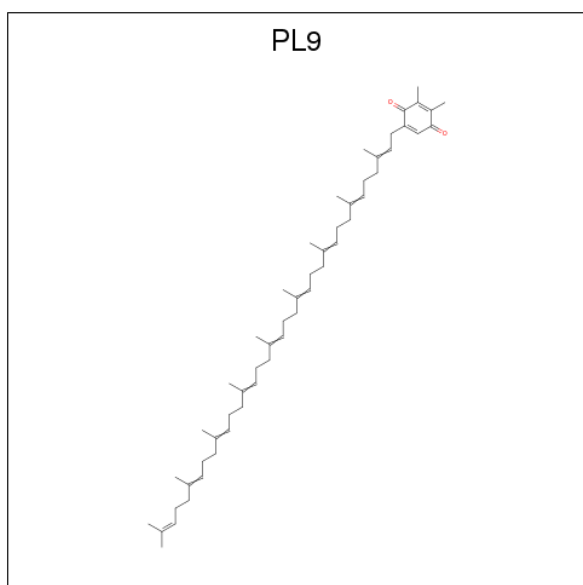
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total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

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

- Molecule 26 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: $C_{53}H_{80}O_2$).



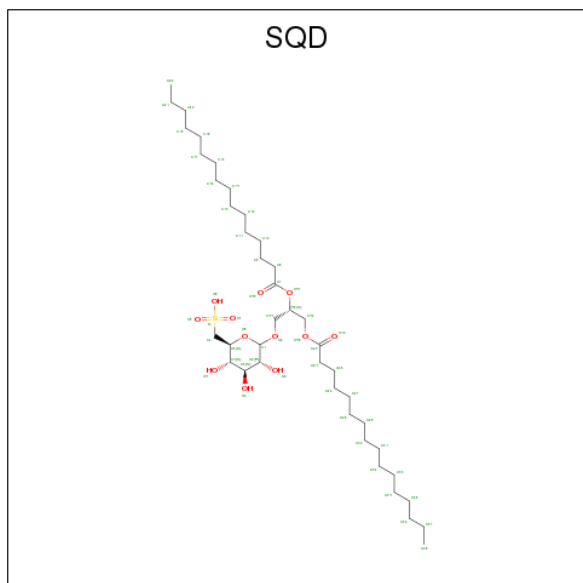
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 55 53 2	0	0
26	D	1	Total C O 55 53 2	0	0

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

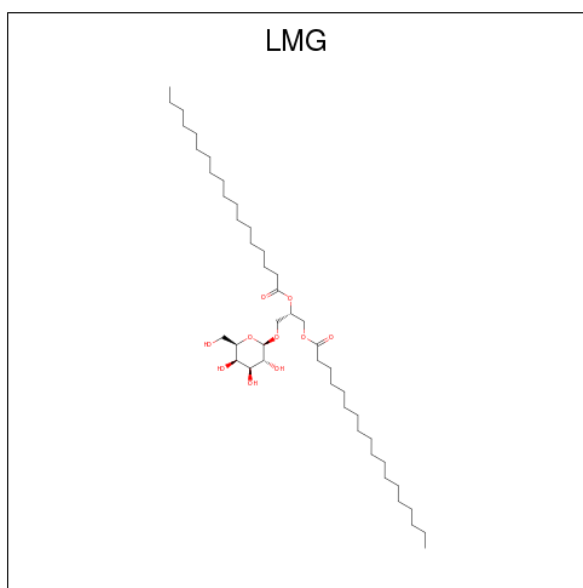
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



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

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			51	41	10		
28	B	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	C	1	Total	C	O	0	0
			51	41	10		
28	J	1	Total	C	O	0	0
			51	41	10		
28	Z	1	Total	C	O	0	0
			37	27	10		
28	a	1	Total	C	O	0	0
			51	41	10		
28	b	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	c	1	Total	C	O	0	0
			51	41	10		
28	j	1	Total	C	O	0	0
			51	41	10		
28	z	1	Total	C	O	0	0
			37	27	10		

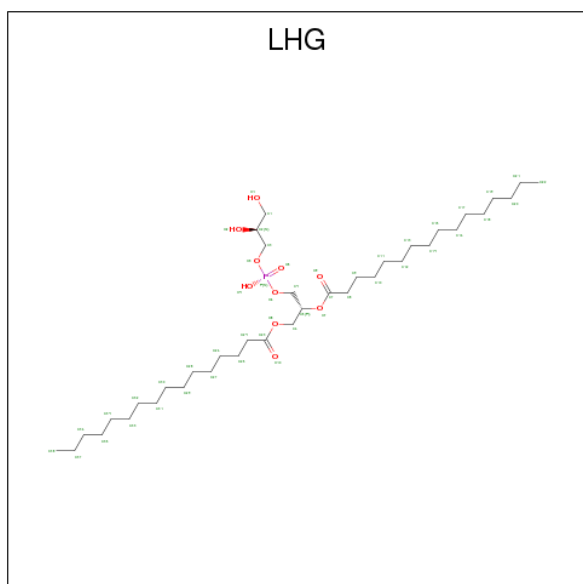
- Molecule 29 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



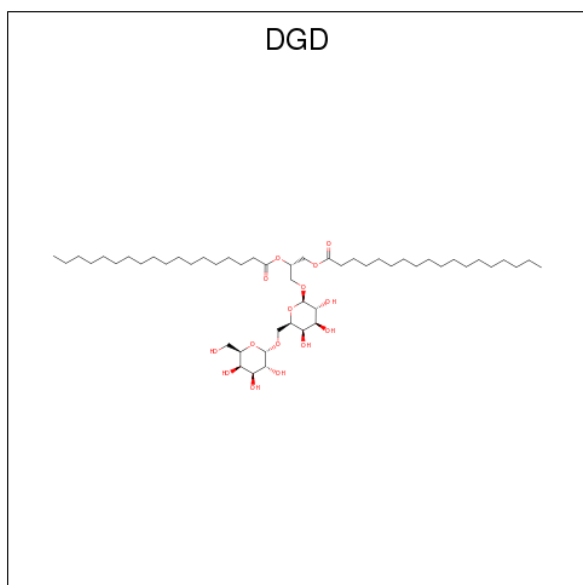
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O P 49 38 10 1	0	0

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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



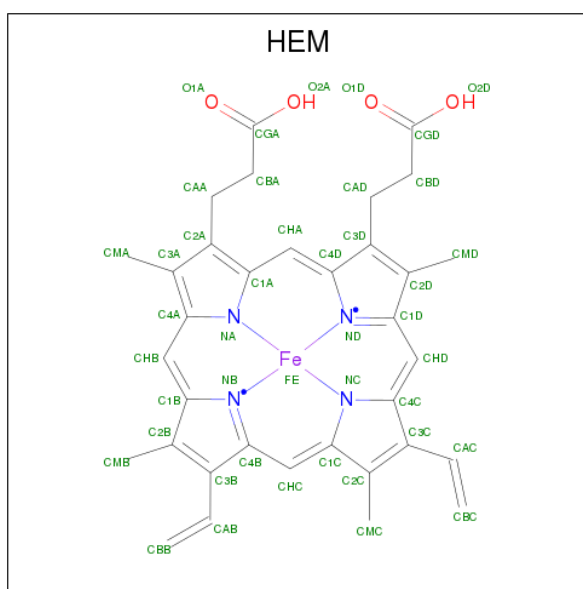
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	C	1	Total	C	O	0	0
			62	47	15		
32	C	1	Total	C	O	0	0
			62	47	15		

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

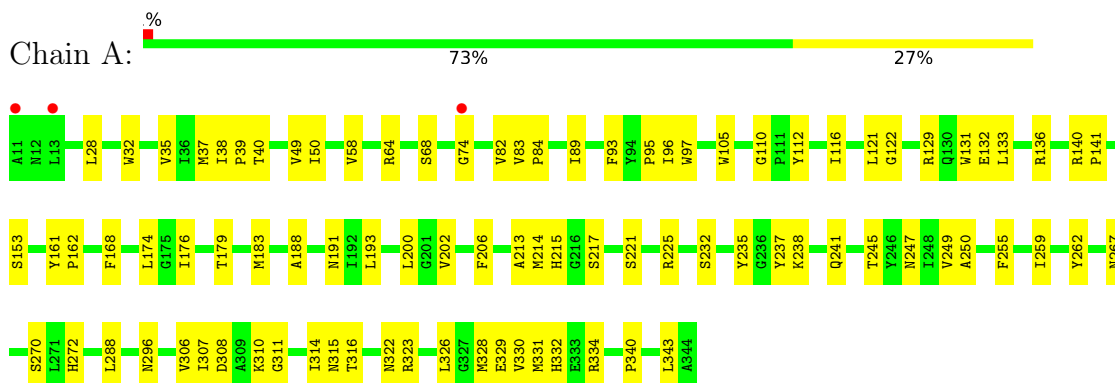
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

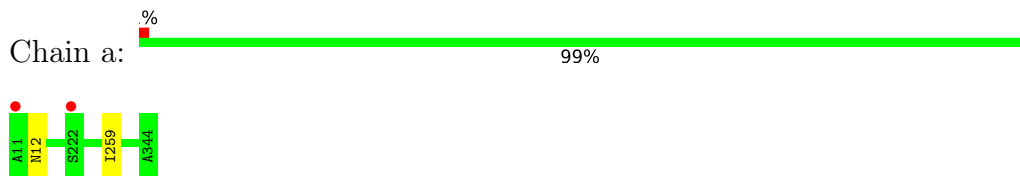
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

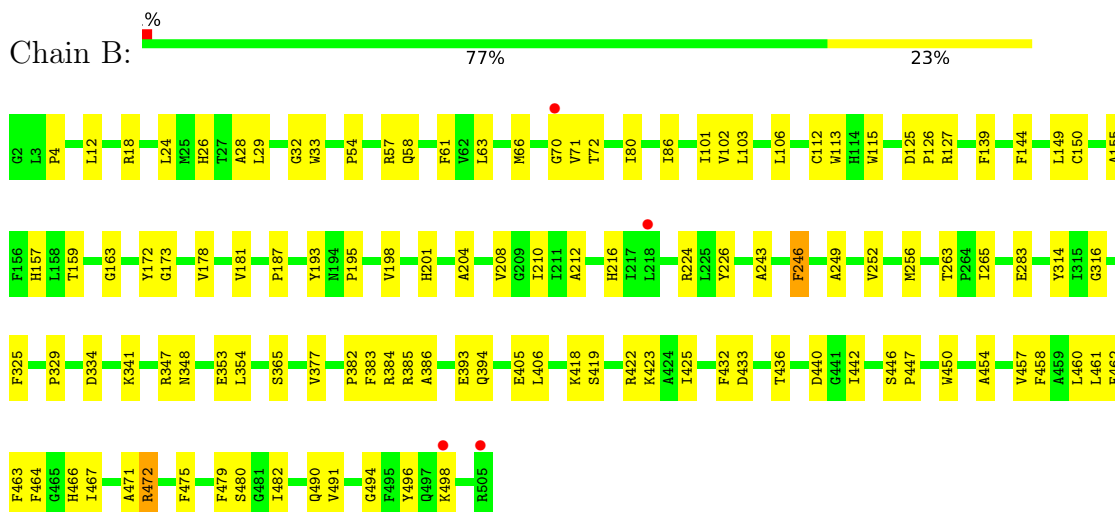
- Molecule 1: Photosystem II protein D1 1



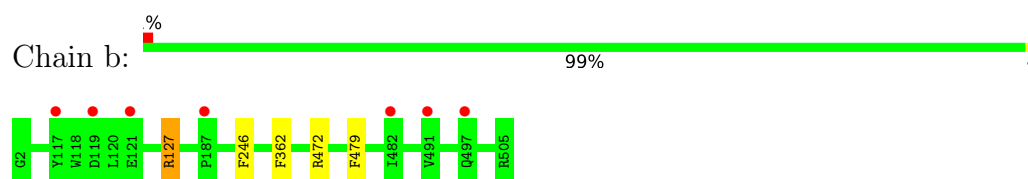
- Molecule 1: Photosystem II protein D1 1



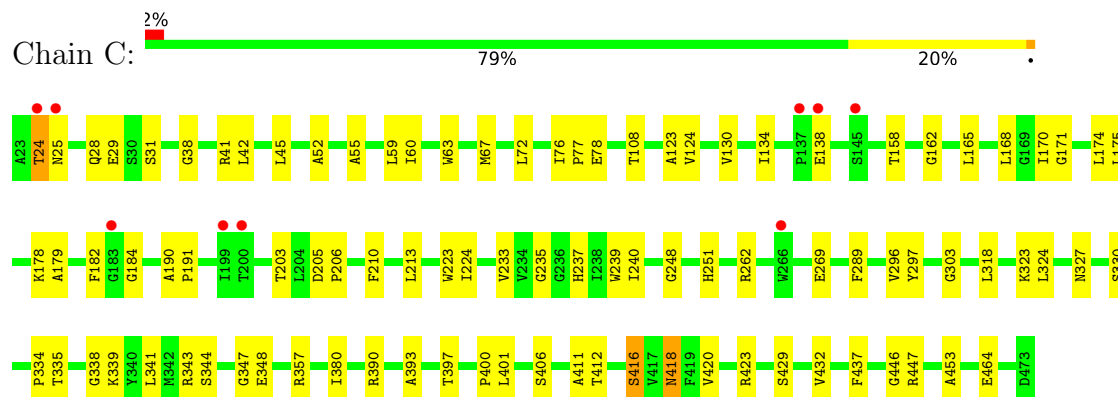
- Molecule 2: Photosystem II CP47 reaction center protein



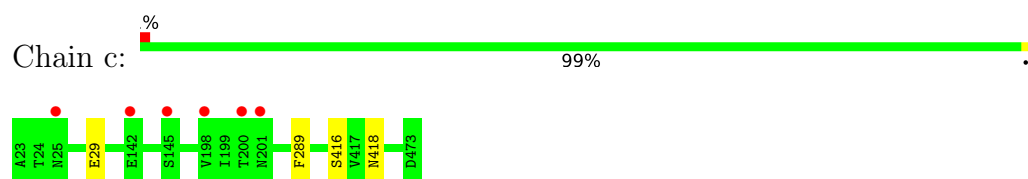
- Molecule 2: Photosystem II CP47 reaction center protein



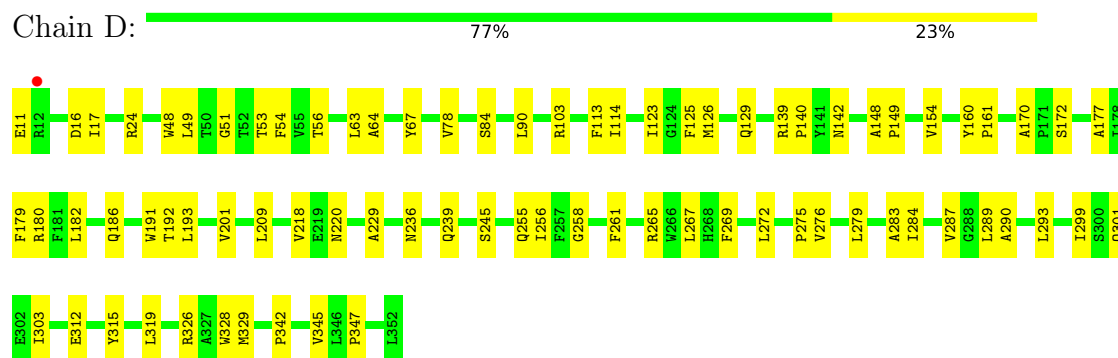
- Molecule 3: Photosystem II CP43 reaction center protein



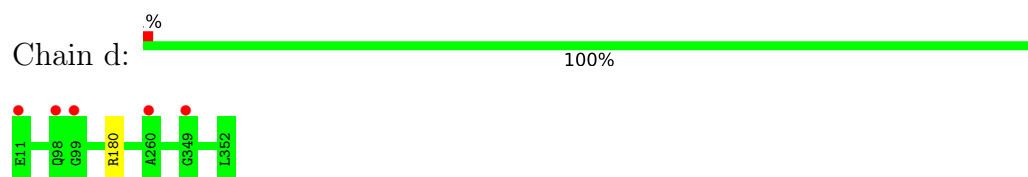
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein



- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha

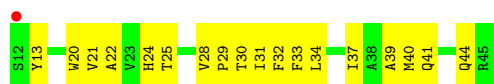




- Molecule 5: Cytochrome b559 subunit alpha



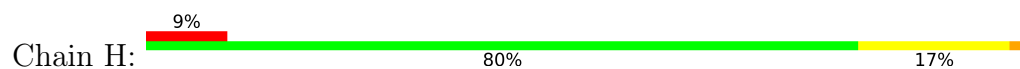
- Molecule 6: Cytochrome b559 subunit beta



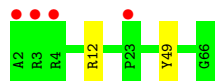
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

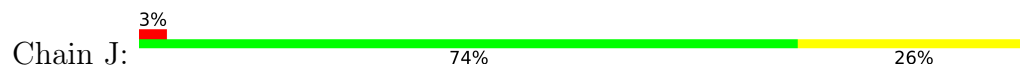


- Molecule 8: Photosystem II reaction center protein I





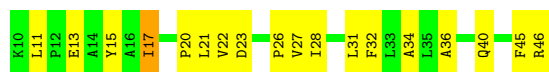
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



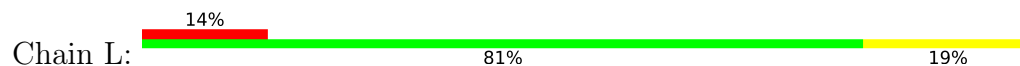
- Molecule 10: Photosystem II reaction center protein K



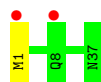
- Molecule 10: Photosystem II reaction center protein K



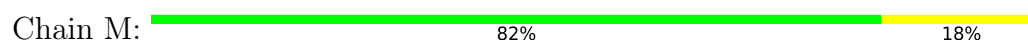
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M





- Molecule 12: Photosystem II reaction center protein M

Chain m: 100%

There are no outlier residues recorded for this chain.

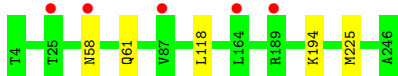
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 82% 17%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 2% 98% .



- Molecule 14: Photosystem II reaction center protein T

Chain T: 10% 77% 23%



- Molecule 14: Photosystem II reaction center protein T

Chain t: 100%

There are no outlier residues recorded for this chain.

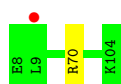
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: % 81% 19%

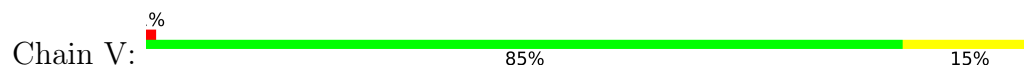


- Molecule 15: Photosystem II 12 kDa extrinsic protein

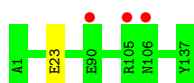
Chain u: % 99% .



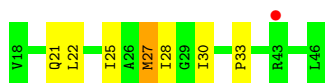
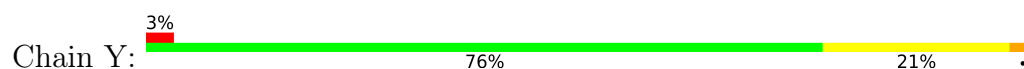
- Molecule 16: Cytochrome c-550



- Molecule 16: Cytochrome c-550



- Molecule 17: Photosystem II reaction center protein Ycf12

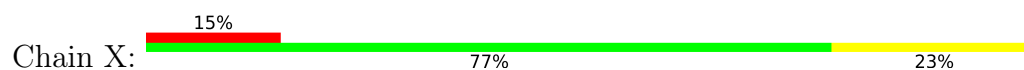


- Molecule 17: Photosystem II reaction center protein Ycf12



There are no outlier residues recorded for this chain.

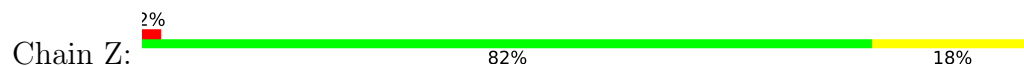
- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein

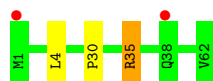


- Molecule 19: Photosystem II reaction center protein Z





- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 4.50 36.50 – 4.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-4.50) 99.9 (36.50-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 4.44Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.246 , 0.275 0.250 , 0.274	Depositor DCC
R_{free} test set	2721 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	211.4	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 13.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	49966	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.33	0/2734	0.53	0/3727
1	a	0.33	0/2734	0.53	0/3727
2	B	0.30	0/4194	0.51	0/5713
2	b	0.31	0/4194	0.52	1/5713 (0.0%)
3	C	0.31	0/3634	0.49	0/4947
3	c	0.32	0/3634	0.52	0/4947
4	D	0.31	0/2821	0.50	0/3844
4	d	0.30	0/2821	0.50	0/3844
5	E	0.30	0/693	0.49	0/944
5	e	0.31	0/693	0.55	0/944
6	F	0.34	0/284	0.49	0/387
6	f	0.40	0/284	0.74	0/387
7	H	0.29	0/544	0.52	0/739
7	h	0.28	0/544	0.52	0/739
8	I	0.31	0/327	0.54	0/439
8	i	0.31	0/327	0.60	0/439
9	J	0.27	0/278	0.44	0/376
9	j	0.31	0/278	0.50	0/376
10	K	0.31	0/303	0.57	0/416
10	k	0.34	0/303	0.55	0/416
11	L	0.28	0/319	0.44	0/433
11	l	0.28	0/319	0.45	0/433
12	M	0.33	0/278	0.56	0/378
12	m	0.34	0/278	0.57	0/378
13	O	0.29	0/1926	0.53	0/2611
13	o	0.32	0/1926	0.58	0/2611
14	T	0.34	0/282	0.52	0/382
14	t	0.34	0/282	0.51	0/382
15	U	0.28	0/785	0.51	0/1064
15	u	0.31	0/785	0.56	0/1064
16	V	0.29	0/1096	0.50	0/1487
16	v	0.29	0/1096	0.56	0/1487

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	Y	0.33	0/216	0.49	0/289
17	y	0.36	0/216	0.59	0/289
18	X	0.29	0/298	0.42	0/403
18	x	0.32	0/298	0.54	0/403
19	Z	0.32	0/490	0.46	0/669
19	z	0.41	0/490	0.68	1/669 (0.1%)
All	All	0.31	0/43004	0.52	2/58496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	z	35	ARG	CB-CG-CD	6.51	128.53	111.60
2	b	127	ARG	CG-CD-NE	5.53	123.42	111.80

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	93	0
1	a	2637	0	2551	0	0
2	B	4024	0	3901	139	0
2	b	4024	0	3901	0	0
3	C	3506	0	3439	104	0
3	c	3506	0	3439	0	0
4	D	2726	0	2627	81	0
4	d	2726	0	2627	0	0
5	E	668	0	658	30	0
5	e	668	0	658	0	0
6	F	275	0	282	23	0
6	f	275	0	282	0	0
7	H	525	0	558	12	0
7	h	525	0	558	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	320	0	339	13	0
8	i	320	0	339	0	0
9	J	272	0	279	10	0
9	j	272	0	279	0	0
10	K	293	0	305	18	0
10	k	293	0	305	0	0
11	L	309	0	327	8	0
11	l	309	0	327	0	0
12	M	272	0	300	7	0
12	m	272	0	300	0	0
13	O	1883	0	1865	33	0
13	o	1883	0	1865	0	0
14	T	270	0	278	14	0
14	t	270	0	278	0	0
15	U	774	0	773	17	0
15	u	774	0	773	0	0
16	V	1072	0	1088	19	0
16	v	1072	0	1088	0	0
17	Y	215	0	246	12	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	6	0
19	z	479	0	516	0	0
20	A	10	0	0	1	0
20	a	10	0	0	0	0
21	A	2	0	0	0	0
21	V	1	0	0	0	0
21	a	1	0	0	0	0
21	c	1	0	0	0	0
21	u	1	0	0	0	0
22	A	4	0	1	0	0
22	a	4	0	1	0	0
23	A	195	0	216	21	0
23	B	1105	0	1224	105	0
23	C	845	0	936	87	0
23	D	195	0	216	17	0
23	a	260	0	288	0	0
23	b	1105	0	1224	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	64	0	74	11	0
24	a	64	0	74	0	0
24	d	64	0	74	0	0
25	A	40	0	55	16	0
25	B	120	0	165	86	0
25	C	120	0	164	48	0
25	F	40	0	54	29	0
25	H	40	0	55	21	0
25	K	40	0	55	30	0
25	T	40	0	55	38	0
25	a	40	0	55	0	0
25	b	120	0	165	0	0
25	c	120	0	165	0	0
25	f	40	0	55	0	0
25	h	40	0	55	0	0
25	k	40	0	55	0	0
25	t	40	0	55	0	0
26	A	55	0	80	15	0
26	D	55	0	80	7	0
26	a	55	0	80	0	0
26	d	55	0	80	0	0
27	A	54	0	78	4	0
27	B	54	0	78	9	0
27	X	43	0	53	4	0
27	a	108	0	156	0	0
27	b	108	0	156	0	0
27	x	43	0	53	0	0
28	A	51	0	72	2	0
28	B	51	0	72	4	0
28	C	102	0	144	2	0
28	J	51	0	72	5	0
28	Z	37	0	44	2	0
28	a	51	0	72	0	0
28	b	51	0	72	0	0
28	c	102	0	144	0	0
28	j	51	0	72	0	0
28	z	37	0	44	0	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	B	49	0	74	3	0
31	D	98	0	148	11	0
31	E	42	0	57	4	0
31	L	49	0	74	4	0
31	a	49	0	74	0	0
31	b	49	0	74	0	0
31	d	49	0	74	0	0
31	e	42	0	57	0	0
31	l	49	0	74	0	0
32	C	186	0	246	11	0
32	D	62	0	82	1	0
32	H	62	0	82	5	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	5	0
33	V	43	0	30	3	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	49966	0	51358	844	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 (844) 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)
25:B:620:BCR:C20	25:B:620:BCR:C19	1.74	1.66
25:T:101:BCR:C16	25:T:101:BCR:C17	1.75	1.64
25:K:101:BCR:C19	25:K:101:BCR:C20	1.75	1.64
25:K:101:BCR:C37	25:K:101:BCR:C22	1.75	1.63
25:A:609:BCR:C19	25:A:609:BCR:C20	1.74	1.63
25:T:101:BCR:C19	25:T:101:BCR:C20	1.75	1.63
25:B:618:BCR:C19	25:B:618:BCR:C20	1.76	1.62
25:T:101:BCR:C37	25:T:101:BCR:C22	1.76	1.62
25:C:514:BCR:C19	25:C:514:BCR:C20	1.75	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:F:101:BCR:C20	25:F:101:BCR:C19	1.73	1.62
25:F:101:BCR:C20	25:F:101:BCR:C21	1.77	1.61
25:F:101:BCR:C22	25:F:101:BCR:C37	1.73	1.61
25:H:101:BCR:C18	25:H:101:BCR:C36	1.80	1.61
25:A:609:BCR:C22	25:A:609:BCR:C37	1.75	1.61
25:B:619:BCR:C37	25:B:619:BCR:C22	1.76	1.61
25:C:514:BCR:C21	25:C:514:BCR:C20	1.78	1.61
25:B:620:BCR:C20	25:B:620:BCR:C21	1.79	1.60
25:C:521:BCR:C21	25:C:521:BCR:C20	1.77	1.60
25:C:515:BCR:C21	25:C:515:BCR:C20	1.77	1.59
25:K:101:BCR:C20	25:K:101:BCR:C21	1.80	1.59
25:A:609:BCR:C21	25:A:609:BCR:C20	1.79	1.59
25:T:101:BCR:C21	25:T:101:BCR:C20	1.80	1.59
25:B:620:BCR:C22	25:B:620:BCR:C37	1.75	1.59
25:K:101:BCR:C36	25:K:101:BCR:C18	1.77	1.59
25:C:515:BCR:C37	25:C:515:BCR:C22	1.74	1.59
25:A:609:BCR:C36	25:A:609:BCR:C18	1.79	1.58
25:T:101:BCR:C18	25:T:101:BCR:C36	1.77	1.58
25:C:521:BCR:C36	25:C:521:BCR:C18	1.79	1.58
25:B:618:BCR:C36	25:B:618:BCR:C18	1.78	1.58
25:H:101:BCR:C20	25:H:101:BCR:C21	1.77	1.58
25:H:101:BCR:C22	25:H:101:BCR:C37	1.73	1.57
25:C:514:BCR:C36	25:C:514:BCR:C18	1.80	1.57
25:B:618:BCR:C22	25:B:618:BCR:C37	1.77	1.57
25:B:618:BCR:C20	25:B:618:BCR:C21	1.79	1.56
25:B:620:BCR:C18	25:B:620:BCR:C36	1.78	1.56
25:F:101:BCR:C36	25:F:101:BCR:C18	1.77	1.56
25:B:619:BCR:C21	25:B:619:BCR:C20	1.77	1.56
25:C:515:BCR:C18	25:C:515:BCR:C36	1.79	1.55
25:B:619:BCR:C18	25:B:619:BCR:C36	1.81	1.53
25:F:101:BCR:C20	25:F:101:BCR:C22	2.42	0.95
25:C:521:BCR:C20	25:C:521:BCR:C22	2.44	0.95
25:C:515:BCR:C21	25:C:515:BCR:C37	2.41	0.94
25:T:101:BCR:C21	25:T:101:BCR:C37	2.43	0.94
3:C:165:LEU:HD21	23:C:507:CLA:HAB	11.38	0.94
25:B:620:BCR:C21	25:B:620:BCR:C37	2.42	0.94
25:F:101:BCR:C21	25:F:101:BCR:C37	2.42	0.93
25:B:618:BCR:C37	25:B:618:BCR:C21	2.42	0.92
25:B:619:BCR:C21	25:B:619:BCR:C37	2.44	0.92
25:B:620:BCR:H20C	25:B:620:BCR:C19	2.01	0.91
25:A:609:BCR:C19	25:A:609:BCR:H20C	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:H:101:BCR:C37	25:H:101:BCR:C21	2.42	0.89
25:K:101:BCR:C37	25:K:101:BCR:C21	2.48	0.89
25:B:618:BCR:C22	25:B:618:BCR:C20	2.45	0.89
23:B:615:CLA:H43	27:B:623:SQD:H121	1.54	0.89
25:A:609:BCR:C21	25:A:609:BCR:C37	2.45	0.88
3:C:165:LEU:HD21	23:C:506:CLA:HAB	1.55	0.88
25:H:101:BCR:C22	25:H:101:BCR:C20	2.46	0.88
25:C:514:BCR:C19	25:C:514:BCR:H20C	2.01	0.88
25:C:515:BCR:C20	25:C:515:BCR:C22	2.47	0.88
25:B:619:BCR:C20	25:B:619:BCR:C22	2.47	0.87
23:B:604:CLA:HMC2	25:H:101:BCR:H19C	20.13	0.87
25:T:101:BCR:H16C	25:T:101:BCR:C17	2.03	0.87
25:T:101:BCR:C18	25:T:101:BCR:C20	2.51	0.87
25:T:101:BCR:C19	25:T:101:BCR:H20C	2.05	0.86
25:F:101:BCR:C19	25:F:101:BCR:H20C	2.03	0.85
25:A:609:BCR:C21	25:A:609:BCR:H20C	2.06	0.85
25:C:515:BCR:C21	25:C:515:BCR:H20C	2.04	0.85
25:K:101:BCR:H20C	25:K:101:BCR:C19	2.04	0.85
25:B:620:BCR:H20C	25:B:620:BCR:C21	2.04	0.84
23:B:617:CLA:H3A	25:B:620:BCR:H17C	1.60	0.84
25:H:101:BCR:H20C	25:H:101:BCR:C21	2.04	0.84
25:F:101:BCR:C21	25:F:101:BCR:H20C	2.06	0.84
25:T:101:BCR:C21	25:T:101:BCR:H20C	2.10	0.83
25:C:514:BCR:C20	25:C:514:BCR:C22	2.48	0.83
25:K:101:BCR:C19	25:K:101:BCR:C36	2.53	0.83
25:C:521:BCR:H15C	25:K:101:BCR:H342	1.60	0.83
25:B:618:BCR:C19	25:B:618:BCR:H20C	2.05	0.83
25:B:620:BCR:C36	25:B:620:BCR:C19	2.55	0.83
25:C:521:BCR:H20C	25:C:521:BCR:C21	2.03	0.83
25:F:101:BCR:C20	25:F:101:BCR:C18	2.62	0.82
25:C:514:BCR:C21	25:C:514:BCR:H20C	2.04	0.82
25:K:101:BCR:H20C	25:K:101:BCR:C21	2.08	0.82
7:H:38:PHE:HB2	25:H:101:BCR:H10C	1.61	0.81
25:T:101:BCR:C22	25:T:101:BCR:C20	2.51	0.81
25:B:618:BCR:H12C	25:B:619:BCR:H10C	1.60	0.81
25:B:620:BCR:C20	25:B:620:BCR:C22	2.51	0.81
31:D:408:LHG:H382	31:D:408:LHG:H112	1.62	0.81
2:B:432:PHE:O	13:O:178:LYS:NZ	2.24	0.80
1:A:50:ILE:HG22	25:A:609:BCR:H271	1.63	0.79
25:B:619:BCR:C36	25:B:619:BCR:C19	2.56	0.79
2:B:127:ARG:HH11	2:B:127:ARG:HG3	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:101:BCR:C19	25:T:101:BCR:C36	2.55	0.79
10:K:17:ILE:H	10:K:17:ILE:HD13	1.48	0.79
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.65	0.78
25:B:620:BCR:C20	25:B:620:BCR:C18	2.53	0.78
23:C:505:CLA:HMB1	23:C:505:CLA:HBB1	1.66	0.77
3:C:124:VAL:HG11	25:C:515:BCR:H17C	30.64	0.77
3:C:24:THR:OG1	3:C:138:GLU:OE1	3.06	0.76
25:B:618:BCR:H20C	25:B:618:BCR:C21	2.09	0.76
25:A:609:BCR:C20	25:A:609:BCR:C18	2.55	0.76
5:E:56:TYR:O	16:V:1:ALA:N	2.21	0.76
3:C:210:PHE:HA	3:C:213[B]:LEU:HD13	2.15	0.76
25:C:514:BCR:C18	25:C:514:BCR:C20	2.56	0.76
25:H:101:BCR:C19	25:H:101:BCR:C36	2.63	0.76
23:C:507:CLA:H142	25:C:515:BCR:H362	1.68	0.76
31:D:408:LHG:H151	31:D:408:LHG:H352	1.67	0.75
25:C:515:BCR:C36	25:C:515:BCR:C19	2.55	0.75
23:A:605:CLA:HMB1	23:A:605:CLA:HBB1	1.68	0.75
23:B:617:CLA:HAB	25:B:620:BCR:H19C	10.64	0.75
27:A:611:SQD:O7	3:C:28:GLN:NE2	2.16	0.75
23:C:513:CLA:HBB1	23:C:513:CLA:HMB1	1.68	0.75
25:F:101:BCR:C36	25:F:101:BCR:C19	2.58	0.74
2:B:103:LEU:HD21	23:B:608:CLA:HMC3	16.10	0.74
25:B:618:BCR:C18	25:B:618:BCR:C20	2.59	0.74
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.68	0.74
25:B:619:BCR:C21	25:B:619:BCR:H20C	2.13	0.73
25:B:619:BCR:H17C	25:T:101:BCR:C17	34.95	0.73
25:K:101:BCR:H10C	17:Y:28:ILE:HG23	2.23	0.73
23:A:606:CLA:HMB1	23:A:606:CLA:HBB1	1.71	0.73
32:D:406:DGD:HA72	25:F:101:BCR:HC22	1.70	0.72
25:A:609:BCR:C19	25:A:609:BCR:C36	2.57	0.72
20:A:601:OEX:O2	3:C:357:ARG:NH2	2.46	0.72
23:C:512:CLA:HMB1	23:C:512:CLA:HBB1	1.71	0.72
14:T:15:ALA:HA	25:T:101:BCR:H12C	1.70	0.72
25:A:609:BCR:C22	25:A:609:BCR:C20	2.54	0.72
25:C:521:BCR:C19	25:C:521:BCR:C36	2.57	0.72
23:C:508:CLA:HMB1	23:C:508:CLA:HBB1	1.71	0.72
25:K:101:BCR:C22	25:K:101:BCR:C20	2.61	0.72
23:C:506:CLA:HMB1	23:C:506:CLA:HBB1	1.71	0.71
18:X:35:ASP:OD1	27:X:101:SQD:H5	2.36	0.71
18:X:24:THR:HA	27:X:101:SQD:H331	1.95	0.71
2:B:103:LEU:HD21	23:B:606:CLA:HMC3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.74	0.71
23:C:507:CLA:HMB1	23:C:507:CLA:HBB1	2.82	0.71
25:K:101:BCR:H17C	17:Y:33:PRO:HD3	1.72	0.71
23:C:510:CLA:HBB1	23:C:510:CLA:HMB1	1.71	0.70
3:C:124:VAL:HG11	25:C:514:BCR:H17C	1.72	0.70
1:A:310:LYS:NZ	5:E:58:GLN:O	2.26	0.70
23:C:506:CLA:HMC2	23:C:507:CLA:H102	1.74	0.70
23:B:609:CLA:HMB1	23:B:609:CLA:HBB1	1.74	0.70
25:F:101:BCR:C17	25:F:101:BCR:C36	2.63	0.69
23:B:602:CLA:HMC2	25:H:101:BCR:H19C	1.74	0.69
25:K:101:BCR:C17	17:Y:33:PRO:HD3	2.21	0.69
25:K:101:BCR:HC8	19:Z:20:VAL:HG21	1.73	0.69
1:A:40:THR:HG23	23:A:608:CLA:HBB1	1.74	0.69
25:K:101:BCR:C20	25:K:101:BCR:C18	2.59	0.69
3:C:213[B]:LEU:HD21	25:C:515:BCR:H20C	1.74	0.69
25:T:101:BCR:H17C	25:T:101:BCR:H20C	1.75	0.69
23:A:606:CLA:H152	26:A:610:PL9:H262	1.74	0.69
23:B:615:CLA:H18	28:B:621:LMG:H421	1.75	0.67
4:D:279:LEU:HD22	24:D:401:PHO:HBC3	1.79	0.67
23:B:617:CLA:H101	25:B:620:BCR:H362	6.41	0.67
4:D:49:LEU:HD13	25:F:101:BCR:H16C	1.92	0.67
25:T:101:BCR:C37	25:T:101:BCR:C20	2.72	0.67
3:C:464:GLU:OE2	4:D:245:SER:OG	2.11	0.67
25:B:618:BCR:C37	25:B:618:BCR:C20	2.73	0.66
25:K:101:BCR:H17C	17:Y:33:PRO:HG3	1.75	0.66
10:K:34:ALA:HB1	25:K:101:BCR:C20	2.26	0.66
23:B:610:CLA:HMD3	25:T:101:BCR:H292	69.62	0.66
2:B:106:LEU:HB3	25:B:620:BCR:H15C	1.78	0.65
3:C:25:ASN:HD21	3:C:45:LEU:HD11	4.27	0.65
23:C:501:CLA:C1D	23:C:503:CLA:H2	2.27	0.65
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.17	0.65
3:C:78:GLU:OE2	16:V:106:ASN:ND2	2.50	0.65
1:A:214:MET:HG2	26:A:610:PL9:H102	1.79	0.65
23:A:606:CLA:H122	26:A:610:PL9:H23	1.79	0.65
25:C:514:BCR:C19	25:C:514:BCR:C36	2.60	0.65
5:E:69:ARG:NH2	7:H:50:ASN:O	2.48	0.64
25:C:515:BCR:C37	25:C:515:BCR:C20	2.75	0.64
23:C:501:CLA:C1C	23:C:503:CLA:H71	2.26	0.64
3:C:123:ALA:HB2	25:C:521:BCR:H12C	1.78	0.64
25:C:521:BCR:C17	25:C:521:BCR:C36	2.70	0.64
2:B:150:CYS:HB2	23:B:606:CLA:HMC3	15.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:623:SQD:H462	27:B:623:SQD:H1	1.79	0.63
6:F:29:PRO:HB3	25:F:101:BCR:H12C	2.23	0.63
24:D:401:PHO:HMB1	24:D:401:PHO:HBB1	1.80	0.63
25:B:618:BCR:H15C	25:B:619:BCR:C13	2.28	0.63
25:K:101:BCR:H17C	17:Y:33:PRO:CG	2.28	0.63
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.87	0.63
23:C:501:CLA:C2D	23:C:503:CLA:H2	2.29	0.63
23:D:402:CLA:HBB1	23:D:402:CLA:HMB1	1.81	0.63
25:B:618:BCR:C37	25:B:618:BCR:H20C	2.29	0.63
23:B:614:CLA:HMB1	23:B:614:CLA:HBB1	2.41	0.62
3:C:123:ALA:HB2	25:C:521:BCR:C12	2.29	0.62
23:C:511:CLA:H192	23:C:511:CLA:HBC3	20.78	0.62
25:K:101:BCR:HC21	19:Z:13:VAL:HG13	1.81	0.62
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.31	0.62
3:C:429:SER:HB3	32:C:517:DGD:HBT2	1.82	0.62
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.81	0.61
3:C:72:LEU:HD23	10:K:11:LEU:HD23	2.55	0.61
25:B:619:BCR:H17C	25:T:101:BCR:H17C	35.28	0.61
1:A:326:LEU:HD22	16:V:134:LYS:HB2	2.07	0.61
16:V:93:PRO:HG2	33:V:202:HEM:HMC3	1.82	0.61
18:X:31:ILE:HG23	27:X:101:SQD:H462	1.97	0.61
23:C:508:CLA:H92	31:D:408:LHG:H371	1.81	0.61
2:B:150:CYS:HB2	23:B:604:CLA:HMC3	1.83	0.61
6:F:30:THR:HG23	25:F:101:BCR:C19	2.89	0.61
3:C:124:VAL:HG11	25:C:514:BCR:C17	2.30	0.61
23:C:502:CLA:C1C	23:C:504:CLA:H71	14.56	0.61
25:F:101:BCR:H17C	28:J:101:LMG:H352	2.01	0.61
2:B:383:PHE:O	13:O:166:SER:HA	2.05	0.61
5:E:8:ARG:NH2	9:J:3:SER:O	3.61	0.60
24:A:607:PHO:HMB1	24:A:607:PHO:HBB1	1.83	0.60
2:B:471:ALA:HB1	4:D:140:PRO:HG2	1.83	0.60
2:B:393:GLU:HB3	15:U:18:GLY:CA	2.41	0.60
25:K:101:BCR:H17C	17:Y:33:PRO:CD	2.31	0.60
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.60
4:D:315:TYR:CZ	4:D:319:LEU:HD11	2.61	0.60
1:A:74:GLY:O	4:D:301:GLN:NE2	2.41	0.60
23:B:611:CLA:HBB1	23:B:611:CLA:HMB1	4.49	0.60
33:E:102:HEM:HMC2	33:E:102:HEM:HBC2	1.82	0.60
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.89	0.60
23:B:606:CLA:HBB2	25:B:620:BCR:H342	1.84	0.60
3:C:339:LYS:NZ	15:U:99:ASN:O	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TYR:OH	11:L:11:GLU:OE1	2.13	0.60
18:X:3:ILE:HG23	18:X:7:LEU:HD23	2.43	0.59
25:B:619:BCR:C17	25:T:101:BCR:H17C	35.72	0.59
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.59
1:A:323:ARG:HB3	4:D:329:MET:HA	1.92	0.59
3:C:52:ALA:HA	23:C:511:CLA:HMB3	1.85	0.59
1:A:84:PRO:HA	1:A:112:TYR:CG	2.37	0.59
25:F:101:BCR:H383	28:J:101:LMG:H172	2.22	0.59
25:B:618:BCR:H402	27:B:623:SQD:H82	1.83	0.59
3:C:38:GLY:HA3	23:C:511:CLA:HMD3	1.84	0.58
23:C:505:CLA:H141	8:I:16:VAL:HG13	1.84	0.58
3:C:347:GLY:HA3	13:O:17:ASN:HB2	1.87	0.58
2:B:33:TRP:N	25:B:619:BCR:H15C	2.18	0.58
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.85	0.58
23:C:501:CLA:C3D	23:C:503:CLA:H2	2.34	0.58
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.34	0.58
4:D:186:GLN:HB2	23:D:402:CLA:HBC1	11.56	0.58
2:B:450:TRP:CD1	23:B:608:CLA:HBA1	2.39	0.58
2:B:12:LEU:HB2	23:B:615:CLA:HMC2	14.17	0.58
3:C:429:SER:HB3	32:C:518:DGD:HBT2	11.56	0.58
23:C:501:CLA:H192	23:C:506:CLA:C1B	2.34	0.58
25:T:101:BCR:C17	25:T:101:BCR:H20C	2.34	0.58
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.02	0.58
25:B:618:BCR:C36	25:B:618:BCR:C19	2.62	0.57
13:O:57:LYS:O	13:O:58:ASN:HB2	2.03	0.57
2:B:127:ARG:HG3	2:B:127:ARG:NH1	2.19	0.57
23:C:502:CLA:C2D	23:C:504:CLA:H2	18.36	0.57
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.39	0.57
23:B:605:CLA:HBB1	23:B:605:CLA:HMB1	1.85	0.57
25:B:618:BCR:H353	25:T:101:BCR:H372	25.15	0.57
4:D:123:ILE:HD11	32:H:102:DGD:HAE1	1.90	0.57
33:E:102:HEM:HMB2	33:E:102:HEM:HBB2	1.87	0.57
6:F:25:THR:O	6:F:29:PRO:HG2	2.48	0.57
3:C:213[B]:LEU:HD11	25:C:515:BCR:C21	2.34	0.57
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.99	0.57
6:F:34:LEU:HD21	25:F:101:BCR:H373	1.87	0.57
23:C:502:CLA:C1D	23:C:504:CLA:H2	17.51	0.57
23:D:404:CLA:H2	18:X:14:LEU:HA	1.85	0.57
3:C:170:ILE:HD13	23:C:512:CLA:H111	1.87	0.57
3:C:72:LEU:HD11	3:C:108:THR:HB	2.10	0.56
33:V:202:HEM:HMB1	33:V:202:HEM:HBB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LEU:HD21	23:C:506:CLA:CAB	2.32	0.56
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.46	0.56
2:B:32:GLY:HA3	25:B:619:BCR:H19C	1.85	0.56
4:D:261:PHE:HB2	26:D:405:PL9:H522	1.87	0.56
5:E:23:HIS:NE2	33:E:102:HEM:ND	2.33	0.56
7:H:65:LEU:HD12	7:H:66:GLY:H	1.70	0.56
25:A:609:BCR:C36	25:A:609:BCR:C17	2.73	0.56
3:C:262:ARG:HG2	8:I:38:GLU:HG2	2.04	0.56
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.35	0.56
31:L:101:LHG:H272	12:M:22:LEU:HD21	2.00	0.56
23:A:608:CLA:C1B	8:I:12:VAL:HG22	2.35	0.56
25:B:619:BCR:H381	25:T:101:BCR:H341	48.88	0.56
2:B:115:TRP:HB2	25:B:620:BCR:H292	8.58	0.56
2:B:29:LEU:CD2	25:B:618:BCR:H17C	2.35	0.56
3:C:124:VAL:HG11	25:C:515:BCR:C17	31.31	0.56
25:B:620:BCR:C23	25:B:620:BCR:C37	2.87	0.55
23:C:507:CLA:H91	25:C:515:BCR:C17	2.36	0.55
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.88	0.55
5:E:35:TRP:HA	6:F:39:ALA:HB2	2.23	0.55
1:A:64:ARG:NH1	13:O:105:PRO:O	2.41	0.55
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.39	0.55
23:B:614:CLA:H193	25:B:619:BCR:C5	2.37	0.55
2:B:461:LEU:HD22	31:B:622:LHG:H301	1.89	0.55
2:B:26:HIS:HB2	23:B:613:CLA:HMB2	1.87	0.55
23:B:613:CLA:H152	23:B:613:CLA:OBD	13.46	0.55
23:C:504:CLA:H193	23:C:504:CLA:HMD2	20.38	0.55
26:A:610:PL9:H403	6:F:22:ALA:HB2	1.89	0.55
18:X:27:VAL:HG21	27:X:101:SQD:H321	1.88	0.55
23:A:605:CLA:HBD	23:D:402:CLA:HAC2	1.88	0.55
1:A:330:VAL:HG21	4:D:328:TRP:CE2	2.41	0.55
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.40	0.55
2:B:12:LEU:HB2	23:B:613:CLA:HMC2	1.88	0.55
23:C:509:CLA:HBC3	23:C:511:CLA:H71	20.60	0.55
25:C:521:BCR:H391	10:K:36:ALA:HB2	1.87	0.55
23:B:606:CLA:C4D	23:B:608:CLA:H43	22.73	0.54
4:D:201:VAL:HG13	23:D:402:CLA:HBB1	12.00	0.54
11:L:26:VAL:HG21	31:L:101:LHG:H192	2.05	0.54
26:A:610:PL9:H221	24:D:401:PHO:HMA2	1.88	0.54
31:E:101:LHG:H152	6:F:22:ALA:HB1	2.06	0.54
3:C:178:LYS:HB2	23:C:503:CLA:H141	19.51	0.54
31:L:101:LHG:H271	12:M:22:LEU:HD11	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:8:PHE:CD1	25:T:101:BCR:H373	2.64	0.54
2:B:112:CYS:HG	14:T:18:PHE:HZ	44.91	0.54
3:C:170:ILE:HD13	23:C:513:CLA:H111	10.41	0.54
2:B:384:ARG:HD3	15:U:102:LEU:HG	2.13	0.54
23:B:611:CLA:OBD	23:B:611:CLA:H152	2.07	0.54
2:B:29:LEU:HD21	25:B:618:BCR:H17C	1.90	0.54
2:B:61:PHE:CZ	23:B:608:CLA:HBB1	2.42	0.54
25:F:101:BCR:C23	25:F:101:BCR:C37	2.80	0.54
23:C:502:CLA:C3D	23:C:504:CLA:H2	18.16	0.54
25:K:101:BCR:C37	25:K:101:BCR:C23	2.79	0.54
3:C:397:THR:HG21	16:V:40:CYS:SG	2.55	0.54
1:A:129:ARG:NH2	4:D:255:GLN:O	2.75	0.54
25:B:618:BCR:H341	25:T:101:BCR:H24C	25.24	0.54
4:D:192:THR:HG23	23:D:402:CLA:HBC2	10.79	0.54
1:A:308:ASP:HB2	5:E:52:PRO:O	2.07	0.54
23:B:617:CLA:H171	14:T:8:PHE:CE1	51.10	0.54
2:B:325:PHE:CG	11:L:34:TYR:HB3	2.43	0.53
3:C:178:LYS:HB2	23:C:502:CLA:H141	1.90	0.53
1:A:245:THR:OG1	4:D:265:ARG:NE	2.60	0.53
2:B:28:ALA:HB1	27:B:623:SQD:H221	1.90	0.53
25:C:515:BCR:C23	25:C:515:BCR:C37	2.81	0.53
5:E:20:TRP:HZ2	9:J:13:VAL:HG13	1.72	0.53
2:B:29:LEU:HD21	25:B:620:BCR:H17C	16.90	0.53
23:B:604:CLA:H152	25:H:101:BCR:H17C	15.46	0.53
25:C:521:BCR:C15	25:K:101:BCR:H342	2.35	0.53
4:D:24:ARG:NH2	18:X:35:ASP:OD2	2.72	0.53
23:B:605:CLA:H12	23:B:606:CLA:ND	2.24	0.53
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	2.42	0.53
4:D:303:ILE:HG21	12:M:2:GLU:HG3	1.90	0.53
25:F:101:BCR:C24	25:F:101:BCR:C37	3.09	0.53
1:A:191:ASN:HB2	3:C:411:ALA:HB1	1.94	0.53
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.44	0.53
2:B:393:GLU:HB3	15:U:18:GLY:N	2.35	0.53
25:C:515:BCR:C37	25:C:515:BCR:H20C	2.39	0.53
23:B:602:CLA:HAC1	25:H:101:BCR:H23C	1.91	0.53
23:B:604:CLA:H202	25:H:101:BCR:H12C	7.99	0.53
25:K:101:BCR:H16C	17:Y:33:PRO:HD3	1.91	0.53
25:T:101:BCR:C17	25:T:101:BCR:C36	2.76	0.53
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.99	0.53
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.90	0.53
10:K:31:LEU:HB3	25:K:101:BCR:C15	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.44	0.52
23:C:502:CLA:HMB1	23:C:502:CLA:HBB1	2.63	0.52
2:B:365:SER:OG	4:D:326:ARG:NH2	2.38	0.52
2:B:71:VAL:HG23	23:B:607[B]:CLA:HMA2	1.91	0.52
2:B:63:LEU:HD12	2:B:66:MET:HE3	1.91	0.52
3:C:324:LEU:HB3	15:U:32:ILE:HD13	1.89	0.52
9:J:9:PRO:HD2	9:J:12:ILE:HD12	1.91	0.52
25:K:101:BCR:HC8	25:K:101:BCR:H311	2.22	0.52
2:B:106:LEU:HB3	25:B:620:BCR:C15	2.38	0.52
1:A:221[B]:SER:HA	4:D:139:ARG:HB2	2.18	0.52
23:D:404:CLA:C2	18:X:14:LEU:HA	2.39	0.52
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.91	0.52
2:B:433:ASP:OD1	2:B:436:THR:OG1	2.33	0.52
25:C:521:BCR:C36	25:C:521:BCR:C16	2.88	0.52
1:A:121[A]:LEU:HG	28:A:612:LMG:H182	1.90	0.52
23:C:510:CLA:H192	23:C:510:CLA:HBC3	1.92	0.52
23:C:502:CLA:C4D	23:C:504:CLA:H2	17.17	0.52
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.47	0.52
25:C:521:BCR:C37	25:C:521:BCR:C20	2.87	0.52
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.92	0.52
2:B:472:ARG:HA	2:B:479:PHE:CE1	2.44	0.52
3:C:213[B]:LEU:HD21	25:C:515:BCR:C20	2.40	0.52
3:C:296:VAL:HG11	23:C:502:CLA:HMA2	13.42	0.52
3:C:393:ALA:HB1	16:V:48:THR:HG21	1.92	0.52
2:B:385:ARG:HG2	13:O:165:ALA:O	2.20	0.52
23:A:608:CLA:HAC2	25:A:609:BCR:H362	1.90	0.52
2:B:71:VAL:HG23	23:B:607[A]:CLA:HMA2	1.92	0.52
3:C:38:GLY:HA3	23:C:512:CLA:HMD3	17.92	0.52
4:D:129:GLN:NE2	24:D:401:PHO:OBD	2.43	0.52
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.07	0.51
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.39	0.51
23:B:613:CLA:H91	23:B:614:CLA:HBB1	1.92	0.51
5:E:8:ARG:HB3	5:E:13:ILE:HD11	2.13	0.51
3:C:206:PRO:HG3	3:C:239:TRP:HZ2	1.74	0.51
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.45	0.51
23:D:403:CLA:C2	18:X:14:LEU:HA	29.77	0.51
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.28	0.51
23:A:606:CLA:HMB3	24:D:401:PHO:H172	1.91	0.51
1:A:247:ASN:HB3	2:B:482:ILE:HD11	2.08	0.51
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.04	0.51
2:B:382:PRO:HG2	2:B:385:ARG:HD2	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:THR:HB	5:E:49:THR:HG23	2.10	0.51
25:B:620:BCR:H383	25:B:620:BCR:H23C	2.99	0.51
1:A:217:SER:HB2	4:D:142:ASN:HA	1.93	0.51
1:A:232:SER:HB2	2:B:4:PRO:HG3	1.92	0.51
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.46	0.51
4:D:186:GLN:HB2	23:D:403:CLA:HBC1	1.93	0.51
4:D:53:THR:HA	4:D:67:TYR:CD2	2.46	0.51
10:K:21:LEU:HD21	25:K:101:BCR:HC31	2.14	0.51
5:E:53:ASP:HB2	16:V:2:GLU:HG2	2.21	0.51
1:A:183:MET:HA	23:A:605:CLA:HMD2	1.93	0.51
23:B:604:CLA:C1C	23:B:606:CLA:H71	2.40	0.51
33:E:102:HEM:HMC1	6:F:31:ILE:HG13	3.35	0.51
23:D:403:CLA:H2	18:X:14:LEU:HA	29.17	0.51
25:B:618:BCR:C37	25:B:618:BCR:C23	2.82	0.50
2:B:18:ARG:NH2	27:B:623:SQD:O9	2.41	0.50
6:F:29:PRO:HB3	25:F:101:BCR:C12	2.78	0.50
25:F:101:BCR:C20	25:F:101:BCR:C37	2.89	0.50
23:B:613:CLA:HBB1	23:B:615:CLA:HMB3	1.93	0.50
23:B:617:CLA:H11	25:B:620:BCR:H362	1.93	0.50
23:C:503:CLA:HMD2	23:C:503:CLA:H193	1.93	0.50
2:B:442:ILE:HG12	13:O:173:ALA:O	2.37	0.50
19:Z:15:LEU:HD22	19:Z:46:LEU:HD23	2.56	0.50
2:B:208:VAL:HG21	23:B:603:CLA:HMC1	1.94	0.50
23:B:612:CLA:HMC2	25:H:101:BCR:H343	24.24	0.50
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.49	0.50
1:A:215:HIS:ND1	26:A:610:PL9:O1	2.39	0.50
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.94	0.50
23:B:617:CLA:H3A	25:B:620:BCR:C17	2.39	0.50
1:A:68:SER:N	4:D:312:GLU:O	2.64	0.50
25:H:101:BCR:C17	25:H:101:BCR:C36	2.77	0.50
23:B:605:CLA:H2	23:B:606:CLA:C4C	2.41	0.50
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.94	0.50
3:C:168:LEU:HD21	23:C:510:CLA:H61	20.22	0.50
3:C:213[B]:LEU:HD11	25:C:515:BCR:C22	2.41	0.50
2:B:113:TRP:HB2	25:B:620:BCR:C21	2.42	0.49
3:C:158:THR:O	3:C:251:HIS:HB3	2.13	0.49
2:B:181:VAL:HG11	2:B:195:PRO:HB2	1.94	0.49
27:B:623:SQD:H462	27:B:623:SQD:C1	2.41	0.49
19:Z:26:ALA:HB1	19:Z:36:SER:HB3	2.11	0.49
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.95	0.49
23:B:606:CLA:C1C	23:B:608:CLA:H71	26.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:617:CLA:C3A	25:B:620:BCR:H17C	2.39	0.49
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.05	0.49
1:A:132:GLU:O	1:A:136:ARG:HG2	2.12	0.49
3:C:25:ASN:O	3:C:31:SER:HB3	2.62	0.49
3:C:55:ALA:HB1	25:C:521:BCR:H373	1.93	0.49
23:C:501:CLA:HBB1	23:C:501:CLA:HMB1	1.93	0.49
31:B:622:LHG:HC11	4:D:269:PHE:CD2	2.48	0.49
13:O:49[A]:THR:OG1	13:O:236:GLN:HB2	2.21	0.49
3:C:59:LEU:HD13	23:C:510:CLA:HMD2	1.95	0.49
4:D:193:LEU:O	11:L:34:TYR:OH	2.29	0.49
13:O:127:ALA:HA	13:O:144:GLY:HA3	1.95	0.49
2:B:422:ARG:HH21	13:O:169:ASP:CG	2.17	0.49
26:D:405:PL9:H421	26:D:405:PL9:H453	1.68	0.48
1:A:136:ARG:HH12	8:I:27:ASP:CG	2.28	0.48
1:A:202:VAL:HG11	23:A:605:CLA:C3D	10.99	0.48
25:B:619:BCR:C23	25:B:619:BCR:C37	2.81	0.48
25:B:620:BCR:C36	25:B:620:BCR:C17	2.79	0.48
2:B:394:GLN:HG2	15:U:22:GLY:HA3	2.29	0.48
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.48
25:C:521:BCR:H15C	25:K:101:BCR:C34	2.39	0.48
4:D:209:LEU:HD22	26:D:405:PL9:H161	1.94	0.48
25:C:515:BCR:HC31	10:K:15:TYR:OH	53.97	0.48
1:A:37:MET:HG3	1:A:122:GLY:O	2.21	0.48
23:C:509:CLA:HMB3	23:C:510:CLA:HAA1	1.95	0.48
2:B:422:ARG:O	2:B:425:ILE:HG12	2.14	0.48
1:A:58:VAL:HB	1:A:83:VAL:HB	2.01	0.48
2:B:204:ALA:CB	23:B:605:CLA:HAB	29.67	0.48
2:B:440:ASP:OD1	4:D:299:ILE:HD13	2.14	0.48
23:B:606:CLA:H162	23:B:610:CLA:HBB2	1.96	0.48
25:B:618:BCR:C36	25:B:618:BCR:C17	2.75	0.48
23:C:506:CLA:H141	8:I:16:VAL:HG13	9.05	0.48
2:B:29:LEU:CD2	25:B:620:BCR:H17C	17.01	0.48
23:C:506:CLA:CBB	23:C:507:CLA:HMA3	2.43	0.48
1:A:296:ASN:HB2	3:C:400:PRO:O	2.28	0.48
1:A:334:ARG:HG3	13:O:157:LEU:HB2	1.96	0.48
2:B:149:LEU:HD22	23:B:605:CLA:H152	1.96	0.48
25:B:618:BCR:C20	25:B:618:BCR:H372	2.43	0.48
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.86	0.48
2:B:33:TRP:CD1	25:T:101:BCR:H381	35.32	0.48
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.48
1:A:306:VAL:HG12	1:A:314:ILE:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TRP:CD1	23:B:610:CLA:HBA1	36.69	0.48
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.48	0.48
5:E:9:PRO:HA	31:E:101:LHG:O3	2.37	0.48
14:T:22:PHE:CE2	25:T:101:BCR:H333	2.95	0.48
23:B:616:CLA:H51	25:B:620:BCR:H11C	1.96	0.47
2:B:101:ILE:HG23	25:B:619:BCR:C21	2.44	0.47
25:B:618:BCR:H15C	25:B:619:BCR:C35	2.43	0.47
1:A:215:HIS:HA	26:A:610:PL9:O1	2.14	0.47
2:B:29:LEU:HD21	27:B:623:SQD:H191	1.97	0.47
1:A:217:SER:HA	4:D:272:LEU:HD12	1.96	0.47
23:B:613:CLA:CMB	23:B:615:CLA:HBB1	2.44	0.47
32:C:517:DGD:HB22	28:C:519:LMG:H302	1.96	0.47
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.78	0.47
25:T:101:BCR:HC8	25:T:101:BCR:H311	1.97	0.47
2:B:193:TYR:OH	32:H:102:DGD:HE1	2.17	0.47
16:V:95:LEU:HD11	16:V:112:LEU:HD11	2.18	0.47
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.97	0.47
1:A:131:TRP:CH2	23:C:505:CLA:HAA2	2.49	0.47
3:C:42:LEU:HD21	23:C:512:CLA:H2A	18.79	0.47
5:E:34:GLY:HA3	6:F:32:PHE:O	2.14	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.54	0.47
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.97	0.47
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.50	0.47
2:B:112:CYS:HA	25:B:620:BCR:H281	5.92	0.47
4:D:283:ALA:O	4:D:287:VAL:HG23	2.14	0.47
3:C:323:LYS:O	15:U:47:LYS:HD2	2.15	0.47
2:B:126:PRO:HB3	7:H:12[B]:ARG:NH1	2.30	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.50	0.47
23:D:402:CLA:H41	26:D:405:PL9:H202	1.96	0.47
25:B:620:BCR:H333	12:M:13:LEU:HD12	38.17	0.47
2:B:57:ARG:HH22	2:B:334:ASP:CG	2.50	0.47
3:C:233:VAL:O	3:C:237:HIS:ND1	2.41	0.47
1:A:49:VAL:HG13	26:D:405:PL9:H503	1.97	0.47
4:D:84:SER:O	5:E:69:ARG:HB2	2.25	0.47
1:A:32:TRP:CD2	8:I:22:GLY:HA3	2.50	0.47
3:C:416[A]:SER:HB2	16:V:42:VAL:HG23	1.96	0.47
2:B:139:PHE:HE2	2:B:216:HIS:CE1	2.33	0.47
23:B:616:CLA:H2	23:B:617:CLA:HBB2	1.96	0.47
1:A:331:MET:SD	4:D:347:PRO:HB2	2.62	0.47
10:K:11:LEU:HD11	10:K:22:VAL:HG21	2.21	0.47
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.05	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Y:27:MET:O	17:Y:30:ILE:HG22	2.26	0.47
23:A:606:CLA:HMD3	4:D:182:LEU:HD11	1.97	0.47
23:B:602:CLA:HBB1	23:B:602:CLA:HHC	1.97	0.47
25:B:619:BCR:HC31	28:B:621:LMG:H131	1.96	0.47
2:B:72:THR:HG22	2:B:80:ILE:HD11	1.97	0.47
2:B:464:PHE:HD2	23:B:612:CLA:HAC2	1.80	0.46
25:B:620:BCR:C20	25:B:620:BCR:C37	3.43	0.46
3:C:344:SER:O	13:O:75:THR:HG22	2.15	0.46
19:Z:5:PHE:HB2	19:Z:57:LEU:HB3	2.47	0.46
1:A:340:PRO:HB3	15:U:103:TYR:CG	2.49	0.46
26:A:610:PL9:H252	26:A:610:PL9:H272	1.65	0.46
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.97	0.46
26:A:610:PL9:H203	26:A:610:PL9:H172	1.74	0.46
3:C:25:ASN:ND2	3:C:45:LEU:HD11	3.62	0.46
6:F:37:ILE:O	6:F:40:MET:HB2	2.25	0.46
13:O:154:ALA:HB1	13:O:165:ALA:HB2	2.01	0.46
23:B:607[B]:CLA:H61	23:B:607[B]:CLA:H102	1.62	0.46
3:C:168:LEU:HD21	23:C:509:CLA:H61	1.98	0.46
3:C:418:ASN:HB2	32:C:518:DGD:O4E	2.15	0.46
4:D:149:PRO:HA	23:D:402:CLA:H41	19.51	0.46
1:A:105:TRP:NE1	1:A:110:GLY:HA3	2.31	0.46
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.46
4:D:113:PHE:CE1	25:F:101:BCR:H332	2.51	0.46
28:C:520:LMG:H171	10:K:27:VAL:HG11	26.62	0.46
25:T:101:BCR:C17	25:T:101:BCR:C20	2.92	0.46
1:A:105:TRP:HZ3	25:A:609:BCR:H24C	1.80	0.46
2:B:57:ARG:NH2	2:B:334:ASP:OD2	2.66	0.46
2:B:150:CYS:HB2	23:B:604:CLA:CMC	2.46	0.46
23:B:617:CLA:HBB1	23:B:617:CLA:HMB1	2.70	0.46
1:A:288:LEU:HD22	3:C:432:VAL:HA	1.98	0.46
4:D:342:PRO:O	4:D:345:VAL:HG22	2.17	0.46
2:B:454:ALA:HB2	28:B:621:LMG:H172	1.98	0.46
23:C:506:CLA:H3A	23:C:506:CLA:HBA2	3.73	0.46
3:C:429:SER:HA	32:C:518:DGD:HBE1	12.65	0.46
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.98	0.46
25:B:619:BCR:C37	25:B:619:BCR:H24C	2.46	0.45
3:C:344:SER:OG	3:C:348:GLU:OE2	2.32	0.45
23:C:502:CLA:H193	23:C:508:CLA:HBB1	29.57	0.45
4:D:154:VAL:HG21	32:H:102:DGD:HAN1	1.97	0.45
6:F:28:VAL:N	6:F:29:PRO:CD	3.06	0.45
1:A:131:TRP:CH2	23:C:506:CLA:HAA2	16.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:TRP:NE1	23:B:608:CLA:HBA1	2.31	0.45
3:C:24:THR:O	3:C:25:ASN:OD1	5.33	0.45
3:C:60:ILE:HG12	23:C:511:CLA:HMC2	13.52	0.45
23:C:506:CLA:H162	25:C:515:BCR:H15C	1.99	0.45
32:C:518:DGD:HBH2	31:D:408:LHG:H223	1.97	0.45
1:A:202:VAL:HG11	23:A:606:CLA:C3D	2.47	0.45
2:B:419:SER:HA	2:B:422:ARG:NH1	2.37	0.45
25:B:619:BCR:C36	25:B:619:BCR:C17	2.77	0.45
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.56	0.45
2:B:460:LEU:O	2:B:463:PHE:HB3	2.16	0.45
3:C:171:GLY:O	3:C:174:LEU:HB2	2.16	0.45
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.06	0.45
6:F:37:ILE:HG22	6:F:41:GLN:HE21	1.90	0.45
5:E:17:VAL:HG23	9:J:7:ARG:HB2	1.97	0.45
2:B:155:ALA:O	2:B:159:THR:OG1	2.29	0.45
2:B:226:TYR:OH	7:H:19:GLY:HA2	2.25	0.45
4:D:53:THR:HA	4:D:67:TYR:HD2	1.81	0.45
3:C:223:TRP:HE3	32:C:516:DGD:HB21	1.82	0.45
23:C:509:CLA:H52	23:C:511:CLA:HED3	25.37	0.45
23:A:605:CLA:HMD3	4:D:182:LEU:HD11	10.99	0.45
32:C:518:DGD:HE4	9:J:40:LEU:HD21	1.99	0.45
3:C:41:ARG:NH2	10:K:46:ARG:O	2.42	0.45
25:T:101:BCR:C23	25:T:101:BCR:C37	2.84	0.45
3:C:343:ARG:NH1	3:C:347:GLY:O	2.50	0.45
5:E:30:LEU:HD12	33:E:102:HEM:HMC1	1.99	0.45
25:B:618:BCR:H342	25:T:101:BCR:H402	24.46	0.45
28:Z:101:LMG:O2	28:Z:101:LMG:HC71	2.19	0.45
23:B:607[B]:CLA:H161	23:B:607[B]:CLA:H192	1.68	0.45
14:T:15:ALA:HB2	25:T:101:BCR:H14C	1.99	0.45
1:A:267:ASN:HB3	1:A:270[B]:SER:OG	2.26	0.44
26:A:610:PL9:H122	26:A:610:PL9:H152	1.79	0.44
31:D:408:LHG:H382	31:D:408:LHG:C11	2.41	0.44
23:B:604:CLA:H202	25:H:101:BCR:C12	7.95	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.44
2:B:386:ALA:HB1	15:U:100:ASN:ND2	2.33	0.44
2:B:24:LEU:HD21	23:B:617:CLA:CAB	2.46	0.44
3:C:182:PHE:CG	23:C:503:CLA:H191	21.99	0.44
4:D:125:PHE:CE2	24:D:401:PHO:HBA1	2.52	0.44
31:D:408:LHG:H132	31:D:408:LHG:H372	1.99	0.44
3:C:390:ARG:HD3	16:V:100:ILE:HD12	2.16	0.44
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:TRP:CE3	25:B:620:BCR:H401	10.10	0.44
25:B:620:BCR:H24C	25:B:620:BCR:H371	1.99	0.44
25:C:515:BCR:C36	25:C:515:BCR:C17	2.80	0.44
23:D:404:CLA:HMD3	25:F:101:BCR:HC21	1.99	0.44
5:E:70:PHE:HZ	7:H:51:SER:HB3	2.18	0.44
13:O:85:LEU:HD22	13:O:243:ILE:HD12	2.14	0.44
26:A:610:PL9:H503	18:X:24:THR:OG1	2.17	0.44
25:B:619:BCR:C37	25:B:619:BCR:C24	2.95	0.44
7:H:65:LEU:CD1	7:H:66:GLY:H	2.31	0.44
16:V:12:LEU:O	16:V:70:GLU:HG2	2.17	0.44
1:A:176:ILE:O	1:A:179:THR:HB	2.18	0.44
2:B:208:VAL:HG21	23:B:605:CLA:HMC1	26.53	0.44
23:C:506:CLA:H162	23:C:506:CLA:H122	1.72	0.44
1:A:316:THR:HG22	4:D:64:ALA:HB3	1.99	0.44
7:H:35:MET:CG	25:H:101:BCR:HC42	2.48	0.44
23:A:608:CLA:HAB	8:I:15:PHE:CD1	2.52	0.44
23:B:606:CLA:H41	23:B:606:CLA:H62	1.77	0.44
25:B:618:BCR:H12C	25:B:619:BCR:C10	2.41	0.44
25:F:101:BCR:H381	28:J:101:LMG:H231	2.00	0.44
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.12	0.44
23:B:615:CLA:HBB1	23:B:617:CLA:HMB3	16.16	0.44
3:C:338:GLY:HA3	3:C:341:LEU:O	2.18	0.44
4:D:201:VAL:HG13	23:D:403:CLA:HBB1	2.00	0.44
1:A:136:ARG:NH1	8:I:27:ASP:OD2	2.34	0.44
1:A:214:MET:HG2	26:A:610:PL9:C10	2.47	0.44
1:A:326:LEU:HD11	16:V:137:TYR:HB2	1.98	0.44
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.53	0.44
3:C:179:ALA:O	3:C:184:GLY:HA2	2.22	0.44
3:C:269:GLU:OE2	3:C:447:ARG:HD3	2.17	0.44
23:C:505:CLA:C1D	32:C:518:DGD:HB21	37.28	0.44
23:C:511:CLA:HMB1	23:C:511:CLA:HBB1	2.24	0.44
26:D:405:PL9:HC72	26:D:405:PL9:H102	1.63	0.44
2:B:212:ALA:HB2	23:B:612:CLA:HMC3	25.50	0.44
2:B:348:ASN:HB3	2:B:354:LEU:HD11	2.11	0.44
2:B:201:HIS:CE1	23:B:604:CLA:HMB3	2.53	0.44
6:F:33:PHE:HB3	25:F:101:BCR:H363	2.39	0.44
2:B:458:PHE:HB3	23:B:605:CLA:HBC2	2.00	0.43
23:A:608:CLA:H192	23:C:505:CLA:H142	2.00	0.43
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.53	0.43
23:B:607[B]:CLA:H111	23:B:607[B]:CLA:H142	1.76	0.43
3:C:330:SER:O	13:O:123:LYS:NZ	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D:401:PHO:H61	23:D:402:CLA:H111	34.56	0.43
9:J:19:MET:HG3	25:K:101:BCR:H372	2.00	0.43
23:C:511:CLA:H111	19:Z:24:PRO:HB3	2.00	0.43
23:C:513:CLA:H172	25:C:514:BCR:H19C	2.00	0.43
4:D:293:LEU:HA	4:D:293:LEU:HD12	1.90	0.43
6:F:21:VAL:O	6:F:25:THR:HG23	2.18	0.43
23:B:604:CLA:CMC	25:H:101:BCR:H19C	20.11	0.43
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.43
4:D:125:PHE:CE1	24:D:401:PHO:HBD	2.54	0.43
26:D:405:PL9:H471	26:D:405:PL9:H43	1.80	0.43
31:B:622:LHG:O9	31:L:101:LHG:HC81	2.18	0.43
2:B:383:PHE:CE1	13:O:167:GLY:HA2	2.54	0.43
1:A:329:GLU:O	1:A:332:HIS:ND1	2.52	0.43
3:C:205:ASP:HA	3:C:206:PRO:HD3	1.85	0.43
2:B:467:ILE:HG13	4:D:126:MET:HE2	2.01	0.43
23:B:610:CLA:HMC2	25:H:101:BCR:H343	1.99	0.43
23:B:612:CLA:HMB1	23:B:612:CLA:HBB1	2.00	0.43
3:C:130:VAL:O	3:C:134:ILE:HG12	2.18	0.43
3:C:206:PRO:HG3	3:C:239:TRP:CZ2	2.52	0.43
3:C:60:ILE:HG12	23:C:510:CLA:HMC2	1.99	0.43
2:B:33:TRP:HD1	25:T:101:BCR:H381	34.54	0.43
27:A:611:SQD:H132	31:D:408:LHG:H142	2.00	0.43
2:B:347[B]:ARG:HG2	2:B:353:GLU:HA	2.16	0.43
23:B:604:CLA:H3A	23:B:604:CLA:CGA	2.49	0.43
5:E:51:ARG:N	5:E:54[B]:SER:OG	2.53	0.43
3:C:416[B]:SER:HB3	16:V:42:VAL:HG23	2.01	0.43
3:C:327:ASN:HB3	13:O:99:ASP:OD2	2.20	0.43
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	2.01	0.43
15:U:76:ARG:HA	15:U:79:LEU:HG	2.01	0.43
28:Z:101:LMG:HC8	28:Z:101:LMG:H111	2.09	0.43
1:A:136:ARG:NH2	8:I:30:ARG:HB2	2.34	0.43
2:B:462:PHE:CE1	23:B:614:CLA:HMB3	2.54	0.43
23:C:505:CLA:CMD	23:C:507:CLA:HAB	2.49	0.43
2:B:440:ASP:O	13:O:174:LEU:HD22	2.26	0.43
2:B:201:HIS:HB2	23:B:605:CLA:C4A	19.74	0.43
3:C:175:LEU:HD23	3:C:237:HIS:CD2	2.82	0.43
23:C:502:CLA:H192	23:C:507:CLA:C1B	29.30	0.43
2:B:33:TRP:HD1	25:B:619:BCR:H12C	1.84	0.42
1:A:225:ARG:HA	2:B:480:SER:O	2.19	0.42
23:B:613:CLA:HHC	23:B:613:CLA:HBB1	4.42	0.42
2:B:498:LYS:HA	4:D:24:ARG:HA	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:408:LHG:H302	31:D:408:LHG:H332	1.96	0.42
5:E:23:HIS:HA	5:E:26:THR:OG1	2.23	0.42
23:A:608:CLA:HMA2	28:A:612:LMG:H132	2.01	0.42
2:B:341:LYS:HD3	2:B:406:LEU:HD11	2.02	0.42
2:B:33:TRP:CD1	23:B:614:CLA:HBC1	2.54	0.42
23:C:507:CLA:HMC2	23:C:508:CLA:H102	28.45	0.42
1:A:28:LEU:HD21	4:D:258:GLY:HA2	2.00	0.42
27:B:623:SQD:O8	11:L:7:ARG:HD2	2.19	0.42
2:B:386:ALA:HB1	15:U:100:ASN:HD22	2.15	0.42
16:V:41:HIS:HA	16:V:45:ILE:O	2.24	0.42
1:A:183:MET:HB3	23:A:605:CLA:HBC2	2.00	0.42
27:A:611:SQD:O10	31:D:408:LHG:H122	2.19	0.42
2:B:187:PRO:HD3	23:B:602:CLA:HMD3	2.00	0.42
10:K:40:GLN:HB3	10:K:45:PHE:CD1	2.54	0.42
1:A:237:TYR:CE1	1:A:241:GLN:HG2	2.54	0.42
2:B:418:LYS:HZ1	15:U:14:ASP:HB3	2.12	0.42
2:B:32:GLY:CA	25:B:619:BCR:H19C	2.50	0.42
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.54	0.42
3:C:29:GLU:CD	3:C:29:GLU:H	2.23	0.42
3:C:335:THR:O	13:O:152:ARG:NH2	2.50	0.42
3:C:437:PHE:CE1	23:C:510:CLA:HMB3	2.55	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.12	0.42
2:B:256:MET:HA	2:B:263:THR:HG21	2.00	0.42
2:B:462:PHE:CZ	23:B:616:CLA:HMB3	24.19	0.42
2:B:458:PHE:CD2	23:B:605:CLA:HMC3	2.55	0.42
2:B:201:HIS:CE1	23:B:606:CLA:HMB3	19.12	0.42
3:C:303:GLY:O	3:C:423:ARG:NE	2.38	0.42
4:D:17:ILE:HD12	18:X:36:LYS:HE3	2.01	0.42
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.11	0.42
5:E:67:THR:OG1	5:E:75:GLN:NE2	2.74	0.42
6:F:30:THR:HA	25:F:101:BCR:C16	2.49	0.42
1:A:97:TRP:CZ2	8:I:9:TYR:HE2	2.37	0.42
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.02	0.42
1:A:153:SER:HB3	23:A:605:CLA:HED1	2.02	0.42
25:A:609:BCR:C37	25:A:609:BCR:C23	2.83	0.42
3:C:318:LEU:HD21	3:C:380:ILE:CG2	2.61	0.42
3:C:453:ALA:O	8:I:33:LYS:HB3	2.19	0.42
1:A:262:TYR:CE2	31:E:101:LHG:HC31	2.70	0.42
10:K:34:ALA:HB3	25:K:101:BCR:H19C	2.01	0.42
2:B:102:VAL:HA	25:B:619:BCR:C40	2.50	0.42
2:B:377:VAL:HG11	4:D:342:PRO:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338:GLY:HA2	13:O:103:PHE:HZ	1.85	0.42
23:C:502:CLA:H51	23:C:503:CLA:NC	2.35	0.42
23:C:505:CLA:H3A	23:C:505:CLA:HBA2	1.63	0.42
3:C:76:ILE:HA	3:C:77:PRO:HD3	1.89	0.42
10:K:32:PHE:CE2	25:K:101:BCR:H352	2.62	0.42
1:A:310:LYS:HE3	16:V:7:VAL:HG21	2.02	0.42
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.01	0.42
23:B:611:CLA:HBB1	23:B:611:CLA:HHC	2.00	0.42
2:B:112:CYS:HA	25:B:618:BCR:H281	2.02	0.42
23:C:508:CLA:OBD	23:C:510:CLA:H122	13.29	0.42
4:D:48:TRP:CD1	24:D:401:PHO:H162	2.54	0.42
5:E:8:ARG:HG3	6:F:13:TYR:CD1	2.61	0.42
23:B:602:CLA:CMC	25:H:101:BCR:H19C	2.47	0.42
7:H:61:SER:HA	32:H:102:DGD:HE2	2.01	0.42
10:K:17:ILE:N	10:K:17:ILE:HD13	2.26	0.42
14:T:22:PHE:HE2	25:T:101:BCR:H312	2.33	0.42
4:D:328:TRP:CZ3	16:V:135:VAL:HA	2.57	0.42
2:B:149:LEU:HD23	23:B:604:CLA:HBC1	2.02	0.42
23:B:608:CLA:H122	23:B:613:CLA:HMA2	19.77	0.42
3:C:210:PHE:HD2	3:C:213[B]:LEU:HD22	1.94	0.42
14:T:8:PHE:HD1	25:T:101:BCR:H373	1.90	0.42
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.52	0.41
2:B:198:VAL:HG13	23:B:606:CLA:HMA3	16.08	0.41
23:B:612:CLA:H41	23:B:615:CLA:HAC2	2.02	0.41
23:C:503:CLA:H51	23:C:504:CLA:NC	18.74	0.41
23:C:504:CLA:H202	31:D:408:LHG:H172	2.02	0.41
23:C:507:CLA:H61	23:C:507:CLA:H92	1.94	0.41
26:A:610:PL9:C22	24:D:401:PHO:HMA2	2.49	0.41
23:D:402:CLA:HMD2	23:D:403:CLA:CBB	2.50	0.41
5:E:20:TRP:CZ2	9:J:13:VAL:HG13	2.53	0.41
2:B:204:ALA:CB	23:B:603:CLA:HAB	2.51	0.41
2:B:325:PHE:CD2	11:L:34:TYR:HB3	2.55	0.41
2:B:382:PRO:HG2	2:B:385:ARG:CD	2.72	0.41
23:B:604:CLA:H152	25:H:101:BCR:C17	14.59	0.41
3:C:447:ARG:NH2	4:D:229:ALA:HB1	2.44	0.41
23:C:501:CLA:CGA	23:C:501:CLA:H3A	2.50	0.41
23:C:507:CLA:OBD	23:C:509:CLA:H122	2.20	0.41
4:D:67:TYR:O	28:J:101:LMG:O5	2.25	0.41
7:H:48:ILE:HG13	7:H:53:LEU:HD23	2.02	0.41
13:O:42:ARG:O	13:O:241:ALA:HA	2.19	0.41
1:A:35:VAL:HG22	25:A:609:BCR:HC21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.58	0.41
23:B:612:CLA:HBA1	23:B:612:CLA:H3A	2.22	0.41
23:B:615:CLA:H91	23:B:616:CLA:HBB1	34.00	0.41
4:D:103:ARG:HE	5:E:77:GLU:HG3	2.21	0.41
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.03	0.41
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.03	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	2.00	0.41
2:B:139:PHE:CZ	23:B:612:CLA:HMB3	16.82	0.41
23:B:605:CLA:H43	23:B:606:CLA:H2	2.01	0.41
3:C:437:PHE:CZ	23:C:511:CLA:HMB3	13.84	0.41
6:F:34:LEU:HD22	9:J:24:ILE:HG12	2.71	0.41
1:A:112:TYR:O	1:A:116:ILE:HG12	2.22	0.41
1:A:200:LEU:HG	32:C:518:DGD:HAT2	2.03	0.41
1:A:217:SER:O	1:A:221[A]:SER:HB3	2.20	0.41
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.64	0.41
23:B:606:CLA:HAB	23:B:608:CLA:H171	35.58	0.41
3:C:223:TRP:CG	3:C:224:ILE:N	2.88	0.41
4:D:123:ILE:HD11	32:H:102:DGD:HAH2	2.35	0.41
13:O:137:THR:C	13:O:139:SER:H	2.24	0.41
1:A:326:LEU:CD2	16:V:134:LYS:HB2	2.57	0.41
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.51	0.41
26:A:610:PL9:H103	26:A:610:PL9:H121	1.79	0.41
2:B:150:CYS:HB2	23:B:606:CLA:CMC	14.82	0.41
31:E:101:LHG:H241	31:E:101:LHG:HC61	1.92	0.41
14:T:15:ALA:CA	25:T:101:BCR:H12C	2.45	0.41
1:A:141:PRO:HG3	3:C:446:GLY:C	2.41	0.41
1:A:193:LEU:HD13	4:D:179:PHE:HB3	2.10	0.41
27:B:623:SQD:H302	14:T:19:PHE:CD2	30.38	0.41
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.02	0.41
4:D:236:ASN:O	4:D:239:GLN:HG2	2.33	0.41
8:I:33:LYS:HB3	8:I:34:ARG:H	1.45	0.41
1:A:235:TYR:O	1:A:238[B]:LYS:HE3	2.81	0.41
2:B:187:PRO:HD3	23:B:604:CLA:HMD3	24.60	0.41
2:B:86:ILE:HG13	2:B:86:ILE:H	1.72	0.41
3:C:52:ALA:HA	23:C:512:CLA:HMB3	18.95	0.41
6:F:37:ILE:HA	6:F:40:MET:SD	2.60	0.41
1:A:343:LEU:O	3:C:401:LEU:HD11	2.21	0.41
23:C:503:CLA:H51	23:C:504:CLA:C4C	19.74	0.41
25:C:515:BCR:H11C	25:C:515:BCR:H341	1.83	0.41
13:O:19:CYS:SG	13:O:46:GLN:HB2	2.85	0.41
1:A:89:ILE:HG12	13:O:73:ARG:HH22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:22:PHE:CE2	25:T:101:BCR:H312	3.04	0.41
1:A:188:ALA:HB2	1:A:328:MET:CB	2.51	0.41
1:A:330:VAL:HG21	4:D:328:TRP:NE1	2.36	0.41
1:A:206:PHE:CZ	23:D:403:CLA:HAA1	2.55	0.41
5:E:82:GLN:C	5:E:84:LYS:H	2.25	0.41
12:M:16[C]:LEU:CD2	12:M:16[C]:LEU:HD22	0.97	0.41
23:A:608:CLA:H122	23:A:608:CLA:H162	1.76	0.41
27:A:611:SQD:H291	23:C:508:CLA:H71	2.03	0.41
23:B:608:CLA:C4A	23:B:608:CLA:HBA2	2.50	0.41
23:B:608:CLA:H162	23:B:612:CLA:HBB2	18.81	0.41
3:C:223:TRP:CE3	32:C:516:DGD:HB21	2.56	0.41
23:A:605:CLA:HMB3	24:D:401:PHO:H172	13.84	0.40
23:B:614:CLA:H162	23:B:614:CLA:H121	1.89	0.40
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.98	0.40
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.05	0.40
23:C:504:CLA:HAC2	10:K:26:PRO:O	2.21	0.40
12:M:16[C]:LEU:HD21	12:M:16[C]:LEU:HD22	1.58	0.40
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.03	0.40
25:B:620:BCR:H351	25:B:620:BCR:H15C	1.95	0.40
23:C:507:CLA:CBB	23:C:508:CLA:HMA3	18.81	0.40
25:F:101:BCR:H20C	28:J:101:LMG:H301	2.03	0.40
25:F:101:BCR:H403	9:J:25:VAL:HG21	2.15	0.40
15:U:64:ILE:HA	15:U:65:PRO:HD3	1.99	0.40
16:V:40:CYS:SG	33:V:202:HEM:CAC	3.09	0.40
10:K:28:ILE:HG12	17:Y:28:ILE:HG21	2.22	0.40
1:A:334:ARG:HB2	13:O:157:LEU:HD12	2.02	0.40
26:A:610:PL9:HC72	26:A:610:PL9:H102	1.79	0.40
2:B:249:ALA:HA	2:B:252:VAL:HG22	2.02	0.40
23:B:616:CLA:H3A	23:B:616:CLA:HBA1	1.65	0.40
23:B:617:CLA:H203	25:B:620:BCR:C10	7.14	0.40
2:B:457:VAL:HG11	28:B:621:LMG:H211	2.03	0.40
23:C:502:CLA:H61	23:C:512:CLA:H42	2.03	0.40
31:D:407:LHG:H141	11:L:22:LEU:HD21	2.03	0.40
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.85	0.40
2:B:494:GLY:HA3	5:E:4:THR:O	2.38	0.40
23:B:608:CLA:C14	23:B:613:CLA:HED2	21.29	0.40
23:B:608:CLA:H41	23:B:608:CLA:H62	2.44	0.40
23:B:610:CLA:H3A	23:B:610:CLA:HBA1	1.80	0.40
23:B:617:CLA:HBA1	23:B:617:CLA:H3A	1.90	0.40
23:B:617:CLA:C10	25:B:620:BCR:H362	6.24	0.40
3:C:63:TRP:CZ2	3:C:67:MET:HG2	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.56	0.40
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.57	0.40
25:B:620:BCR:H353	25:T:101:BCR:H372	46.03	0.40
1:A:322:ASN:OD1	3:C:412:THR:HA	2.22	0.40
2:B:383:PHE:CG	4:D:347:PRO:HA	2.56	0.40
23:B:604:CLA:HMB1	23:B:604:CLA:HBB1	2.03	0.40
25:B:618:BCR:H15C	25:B:619:BCR:H352	2.03	0.40
23:C:503:CLA:H61	23:C:513:CLA:H42	26.72	0.40
1:A:315:ASN:O	4:D:63:LEU:HA	2.23	0.40
5:E:8:ARG:HB2	6:F:13:TYR:HB3	2.02	0.40
23:C:505:CLA:H202	8:I:12:VAL:HG11	2.04	0.40
15:U:38:TYR:HB2	15:U:41:LEU:HD12	2.03	0.40
13:O:184:ARG:HA	15:U:9:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/334 (101%)	332 (99%)	3 (1%)	1 (0%)	43	80
1	a	336/334 (101%)	330 (98%)	5 (2%)	1 (0%)	43	80
2	B	512/504 (102%)	507 (99%)	5 (1%)	0	100	100
2	b	512/504 (102%)	503 (98%)	9 (2%)	0	100	100
3	C	454/451 (101%)	443 (98%)	9 (2%)	2 (0%)	36	76
3	c	454/451 (101%)	441 (97%)	11 (2%)	2 (0%)	36	76
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	340/342 (99%)	333 (98%)	7 (2%)	0	100	100
5	E	81/81 (100%)	80 (99%)	1 (1%)	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	
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%)	57 (88%)	8 (12%)	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%)	35 (100%)	0	0	100	100
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%)	36	76
13	o	245/243 (101%)	235 (96%)	9 (4%)	1 (0%)	36	76
14	T	29/30 (97%)	28 (97%)	1 (3%)	0	100	100
14	t	29/30 (97%)	29 (100%)	0	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%)	131 (96%)	5 (4%)	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%)	5134 (98%)	110 (2%)	8 (0%)	53	84

All (8) 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
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%)	272 (100%)	1 (0%)	92	95
2	B	412/402 (102%)	410 (100%)	2 (0%)	90	94
2	b	412/402 (102%)	407 (99%)	5 (1%)	74	87
3	C	357/352 (101%)	354 (99%)	3 (1%)	83	91
3	c	357/352 (101%)	354 (99%)	3 (1%)	83	91
4	D	277/277 (100%)	274 (99%)	3 (1%)	76	87
4	d	277/277 (100%)	276 (100%)	1 (0%)	92	95
5	E	74/72 (103%)	73 (99%)	1 (1%)	69	85
5	e	74/72 (103%)	74 (100%)	0	100	100
6	F	28/28 (100%)	27 (96%)	1 (4%)	38	66
6	f	28/28 (100%)	28 (100%)	0	100	100
7	H	56/54 (104%)	52 (93%)	4 (7%)	16	47
7	h	56/54 (104%)	53 (95%)	3 (5%)	24	56
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
9	j	26/26 (100%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	30/30 (100%)	28 (93%)	2 (7%)	18	49
10	k	30/30 (100%)	28 (93%)	2 (7%)	18	49
11	L	36/35 (103%)	35 (97%)	1 (3%)	47	71
11	l	36/35 (103%)	35 (97%)	1 (3%)	47	71
12	M	32/31 (103%)	31 (97%)	1 (3%)	43	69
12	m	32/31 (103%)	32 (100%)	0	100	100
13	O	210/206 (102%)	206 (98%)	4 (2%)	60	80
13	o	210/206 (102%)	206 (98%)	4 (2%)	60	80
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%)	74	87
15	u	84/84 (100%)	83 (99%)	1 (1%)	74	87
16	V	118/117 (101%)	117 (99%)	1 (1%)	83	91
16	v	118/117 (101%)	117 (99%)	1 (1%)	83	91
17	Y	22/22 (100%)	21 (96%)	1 (4%)	30	61
17	y	22/22 (100%)	22 (100%)	0	100	100
18	X	33/32 (103%)	33 (100%)	0	100	100
18	x	33/32 (103%)	32 (97%)	1 (3%)	44	69
19	Z	52/52 (100%)	50 (96%)	2 (4%)	36	64
19	z	52/52 (100%)	49 (94%)	3 (6%)	22	54
All	All	4370/4302 (102%)	4317 (99%)	53 (1%)	74	87

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	246	PHE
2	B	472	ARG
3	C	24	THR
3	C	289	PHE
3	C	418	ASN
4	D	11	GLU
4	D	90	LEU
4	D	180	ARG
5	E	71	GLU
6	F	44	GLN

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Mol	Chain	Res	Type
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	6	GLN
19	Z	31	GLN
1	a	12	ASN
2	b	127	ARG
2	b	246	PHE
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
3	c	29	GLU
3	c	289	PHE
3	c	418	ASN
4	d	180	ARG
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	49	TYR
10	k	13	GLU
10	k	17	ILE
11	l	1	MET
13	o	61	GLN
13	o	118	LEU
13	o	194	LYS
13	o	225	MET
15	u	70	ARG
16	v	23	GLU
18	x	2	THR
19	z	4	LEU
19	z	30	PRO

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Mol	Chain	Res	Type
19	z	35	ARG

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

Mol	Chain	Res	Type
12	M	33	GLN
1	a	198	HIS
3	c	25	ASN
12	m	33	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 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	-
22	BCT	A	604	29	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	605	-	58,73,73	2.64	23 (39%)	66,113,113	1.67	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	606	-	58,73,73	2.61	23 (39%)	66,113,113	1.84	13 (19%)
24	PHO	A	607	-	67,69,69	1.26	8 (11%)	85,99,99	1.03	4 (4%)
23	CLA	A	608	-	58,73,73	2.59	24 (41%)	66,113,113	1.81	14 (21%)
25	BCR	A	609	-	41,41,41	9.33	30 (73%)	56,56,56	5.61	28 (50%)
26	PL9	A	610	-	55,55,55	4.15	19 (34%)	69,69,69	3.64	38 (55%)
27	SQD	A	611	-	53,54,54	0.97	3 (5%)	63,65,65	1.54	12 (19%)
28	LMG	A	612	-	51,51,55	1.29	5 (9%)	59,59,63	0.98	2 (3%)
23	CLA	B	602	-	58,73,73	2.63	23 (39%)	66,113,113	1.75	11 (16%)
23	CLA	B	603	-	58,73,73	2.61	23 (39%)	66,113,113	1.83	16 (24%)
23	CLA	B	604	-	58,73,73	2.62	23 (39%)	66,113,113	1.81	15 (22%)
23	CLA	B	605	-	58,73,73	2.59	22 (37%)	66,113,113	1.86	15 (22%)
23	CLA	B	606	-	58,73,73	2.63	23 (39%)	66,113,113	1.77	11 (16%)
23	CLA	B	607[A]	-	58,73,73	2.61	23 (39%)	66,113,113	1.87	16 (24%)
23	CLA	B	607[B]	-	58,73,73	2.61	23 (39%)	66,113,113	1.89	16 (24%)
23	CLA	B	608	-	58,73,73	2.62	23 (39%)	66,113,113	1.80	17 (25%)
23	CLA	B	609	-	58,73,73	2.63	23 (39%)	66,113,113	1.87	17 (25%)
23	CLA	B	610	-	58,73,73	2.59	23 (39%)	66,113,113	1.79	12 (18%)
23	CLA	B	611	-	58,73,73	2.62	22 (37%)	66,113,113	1.72	13 (19%)
23	CLA	B	612	-	58,73,73	2.59	23 (39%)	66,113,113	1.86	14 (21%)
23	CLA	B	613	-	58,73,73	2.61	23 (39%)	66,113,113	1.80	15 (22%)
23	CLA	B	614	-	58,73,73	2.63	23 (39%)	66,113,113	1.73	13 (19%)
23	CLA	B	615	-	58,73,73	2.62	23 (39%)	66,113,113	1.79	14 (21%)
23	CLA	B	616	-	58,73,73	2.61	23 (39%)	66,113,113	1.77	13 (19%)
23	CLA	B	617	-	58,73,73	2.61	23 (39%)	66,113,113	1.78	12 (18%)
25	BCR	B	618	-	41,41,41	9.12	29 (70%)	56,56,56	6.03	30 (53%)
25	BCR	B	619	-	41,41,41	9.57	30 (73%)	56,56,56	5.30	29 (51%)
25	BCR	B	620	-	41,41,41	9.14	30 (73%)	56,56,56	6.04	32 (57%)
28	LMG	B	621	-	51,51,55	1.26	4 (7%)	59,59,63	0.92	2 (3%)
31	LHG	B	622	-	48,48,48	1.13	3 (6%)	51,54,54	0.99	5 (9%)
27	SQD	B	623	-	53,54,54	1.06	4 (7%)	63,65,65	1.43	9 (14%)
23	CLA	C	501	-	58,73,73	2.60	23 (39%)	66,113,113	1.85	15 (22%)
23	CLA	C	502	-	58,73,73	2.60	23 (39%)	66,113,113	1.72	14 (21%)
23	CLA	C	503	-	58,73,73	2.62	22 (37%)	66,113,113	1.71	13 (19%)
23	CLA	C	504	-	58,73,73	2.59	23 (39%)	66,113,113	1.79	14 (21%)
23	CLA	C	505	-	58,73,73	2.64	23 (39%)	66,113,113	1.84	14 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	506	-	58,73,73	2.61	23 (39%)	66,113,113	1.83	13 (19%)
23	CLA	C	507	-	58,73,73	2.57	23 (39%)	66,113,113	1.91	15 (22%)
23	CLA	C	508	-	58,73,73	2.63	23 (39%)	66,113,113	1.81	15 (22%)
23	CLA	C	509	-	58,73,73	2.59	22 (37%)	66,113,113	1.84	15 (22%)
23	CLA	C	510	-	58,73,73	2.63	23 (39%)	66,113,113	1.70	14 (21%)
23	CLA	C	511	3	58,73,73	2.61	23 (39%)	66,113,113	1.75	13 (19%)
23	CLA	C	512	-	58,73,73	2.63	23 (39%)	66,113,113	1.81	17 (25%)
23	CLA	C	513	-	58,73,73	2.58	23 (39%)	66,113,113	1.82	15 (22%)
25	BCR	C	514	-	41,41,41	9.09	31 (75%)	56,56,56	6.12	31 (55%)
25	BCR	C	515	-	41,41,41	9.24	29 (70%)	56,56,56	5.92	30 (53%)
32	DGD	C	516	-	63,63,67	1.69	16 (25%)	77,77,81	0.94	4 (5%)
32	DGD	C	517	-	63,63,67	1.63	18 (28%)	77,77,81	1.03	5 (6%)
32	DGD	C	518	-	63,63,67	1.66	16 (25%)	77,77,81	1.05	5 (6%)
28	LMG	C	519	-	51,51,55	1.31	4 (7%)	59,59,63	1.08	2 (3%)
28	LMG	C	520	-	51,51,55	1.30	5 (9%)	59,59,63	1.02	4 (6%)
25	BCR	C	521	-	41,41,41	9.24	29 (70%)	56,56,56	5.85	26 (46%)
24	PHO	D	401	-	67,69,69	1.26	7 (10%)	85,99,99	1.05	4 (4%)
23	CLA	D	402	-	58,73,73	2.61	23 (39%)	66,113,113	1.82	16 (24%)
23	CLA	D	403	-	58,73,73	2.63	23 (39%)	66,113,113	1.71	13 (19%)
23	CLA	D	404	-	58,73,73	2.60	23 (39%)	66,113,113	1.84	14 (21%)
26	PL9	D	405	-	55,55,55	4.15	18 (32%)	69,69,69	3.63	35 (50%)
32	DGD	D	406	-	63,63,67	1.71	15 (23%)	77,77,81	1.13	7 (9%)
31	LHG	D	407	-	48,48,48	1.11	3 (6%)	51,54,54	0.92	3 (5%)
31	LHG	D	408	-	48,48,48	1.10	3 (6%)	51,54,54	0.99	4 (7%)
31	LHG	E	101	-	41,41,48	1.19	3 (7%)	44,47,54	0.93	3 (6%)
33	HEM	E	102	5,6	27,50,50	2.10	5 (18%)	17,82,82	1.75	3 (17%)
25	BCR	F	101	-	41,41,41	9.20	29 (70%)	56,56,56	6.03	29 (51%)
25	BCR	H	101	-	41,41,41	9.18	29 (70%)	56,56,56	5.80	36 (64%)
32	DGD	H	102	-	63,63,67	1.68	15 (23%)	77,77,81	0.93	3 (3%)
28	LMG	J	101	34	51,51,55	1.30	4 (7%)	59,59,63	1.01	5 (8%)
25	BCR	K	101	-	41,41,41	9.14	30 (73%)	56,56,56	5.84	26 (46%)
31	LHG	L	101	-	48,48,48	1.10	3 (6%)	51,54,54	0.89	3 (5%)
25	BCR	T	101	-	41,41,41	9.19	29 (70%)	56,56,56	5.95	29 (51%)
33	HEM	V	202	16	27,50,50	2.06	5 (18%)	17,82,82	1.82	6 (35%)
27	SQD	X	101	-	42,43,54	1.20	3 (7%)	52,54,65	1.48	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	Z	101	-	37,37,55	1.41	5 (13%)	45,45,63	1.24	3 (6%)
20	OEX	a	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
22	BCT	a	603	29	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	a	604	-	58,73,73	2.63	23 (39%)	66,113,113	1.68	14 (21%)
23	CLA	a	605	-	58,73,73	2.61	23 (39%)	66,113,113	1.82	16 (24%)
24	PHO	a	606	-	67,69,69	1.25	8 (11%)	85,99,99	1.03	4 (4%)
23	CLA	a	607	-	58,73,73	2.62	23 (39%)	66,113,113	1.79	14 (21%)
25	BCR	a	608	-	41,41,41	9.24	30 (73%)	56,56,56	5.62	26 (46%)
26	PL9	a	609	-	55,55,55	4.13	18 (32%)	69,69,69	3.69	35 (50%)
27	SQD	a	610	-	53,54,54	0.97	3 (5%)	63,65,65	1.54	11 (17%)
28	LMG	a	611	-	51,51,55	1.29	5 (9%)	59,59,63	1.01	2 (3%)
27	SQD	a	612	-	53,54,54	1.03	3 (5%)	63,65,65	1.25	7 (11%)
23	CLA	a	613	-	58,73,73	2.61	23 (39%)	66,113,113	1.86	15 (22%)
31	LHG	a	614	-	48,48,48	1.09	3 (6%)	51,54,54	1.05	3 (5%)
27	SQD	b	601	-	53,54,54	1.03	3 (5%)	63,65,65	1.25	7 (11%)
27	SQD	b	602	-	53,54,54	1.07	4 (7%)	63,65,65	1.43	9 (14%)
23	CLA	b	604	-	58,73,73	2.61	23 (39%)	66,113,113	1.75	12 (18%)
23	CLA	b	605	-	58,73,73	2.62	23 (39%)	66,113,113	1.84	15 (22%)
23	CLA	b	606	-	58,73,73	2.64	23 (39%)	66,113,113	1.84	16 (24%)
23	CLA	b	607	-	58,73,73	2.60	23 (39%)	66,113,113	1.84	15 (22%)
23	CLA	b	608	-	58,73,73	2.63	23 (39%)	66,113,113	1.76	12 (18%)
23	CLA	b	609[A]	-	58,73,73	2.60	23 (39%)	66,113,113	1.87	16 (24%)
23	CLA	b	609[B]	-	58,73,73	2.62	23 (39%)	66,113,113	1.88	16 (24%)
23	CLA	b	610	-	58,73,73	2.64	23 (39%)	66,113,113	1.81	16 (24%)
23	CLA	b	611	-	58,73,73	2.62	23 (39%)	66,113,113	1.84	16 (24%)
23	CLA	b	612	-	58,73,73	2.61	23 (39%)	66,113,113	1.77	12 (18%)
23	CLA	b	613	-	58,73,73	2.63	23 (39%)	66,113,113	1.73	12 (18%)
23	CLA	b	614	-	58,73,73	2.61	23 (39%)	66,113,113	1.86	15 (22%)
23	CLA	b	615	-	58,73,73	2.60	23 (39%)	66,113,113	1.83	14 (21%)
23	CLA	b	616	-	58,73,73	2.59	23 (39%)	66,113,113	1.77	16 (24%)
23	CLA	b	617	-	58,73,73	2.61	23 (39%)	66,113,113	1.79	13 (19%)
23	CLA	b	618	-	58,73,73	2.63	23 (39%)	66,113,113	1.77	13 (19%)
23	CLA	b	619	-	58,73,73	2.60	23 (39%)	66,113,113	1.81	13 (19%)
25	BCR	b	620	-	41,41,41	9.04	30 (73%)	56,56,56	5.84	29 (51%)
25	BCR	b	621	-	41,41,41	9.12	29 (70%)	56,56,56	5.62	31 (55%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	b	622	-	41,41,41	9.26	30 (73%)	56,56,56	5.79	32 (57%)
28	LMG	b	623	-	51,51,55	1.28	4 (7%)	59,59,63	0.96	2 (3%)
31	LHG	b	624	-	48,48,48	1.10	3 (6%)	51,54,54	0.98	3 (5%)
23	CLA	c	502	-	58,73,73	2.59	23 (39%)	66,113,113	1.79	10 (15%)
23	CLA	c	503	-	58,73,73	2.61	23 (39%)	66,113,113	1.78	14 (21%)
23	CLA	c	504	-	58,73,73	2.62	23 (39%)	66,113,113	1.72	13 (19%)
23	CLA	c	505	-	58,73,73	2.61	23 (39%)	66,113,113	1.78	14 (21%)
23	CLA	c	506	-	58,73,73	2.63	23 (39%)	66,113,113	1.81	11 (16%)
23	CLA	c	507	-	58,73,73	2.63	23 (39%)	66,113,113	1.85	14 (21%)
23	CLA	c	508	-	58,73,73	2.57	22 (37%)	66,113,113	1.93	15 (22%)
23	CLA	c	509	-	58,73,73	2.60	23 (39%)	66,113,113	1.85	15 (22%)
23	CLA	c	510	-	58,73,73	2.60	23 (39%)	66,113,113	1.83	14 (21%)
23	CLA	c	511	-	58,73,73	2.63	23 (39%)	66,113,113	1.69	13 (19%)
23	CLA	c	512	3	58,73,73	2.62	23 (39%)	66,113,113	1.73	14 (21%)
23	CLA	c	513	-	58,73,73	2.61	22 (37%)	66,113,113	1.80	17 (25%)
23	CLA	c	514	-	58,73,73	2.60	23 (39%)	66,113,113	1.71	11 (16%)
25	BCR	c	515	-	41,41,41	9.09	29 (70%)	56,56,56	6.21	32 (57%)
25	BCR	c	516	-	41,41,41	9.29	30 (73%)	56,56,56	5.77	27 (48%)
32	DGD	c	517	-	63,63,67	1.69	16 (25%)	77,77,81	0.94	4 (5%)
32	DGD	c	518	-	63,63,67	1.64	16 (25%)	77,77,81	1.00	5 (6%)
32	DGD	c	519	-	63,63,67	1.65	16 (25%)	77,77,81	1.09	4 (5%)
28	LMG	c	520	-	51,51,55	1.31	4 (7%)	59,59,63	1.04	2 (3%)
28	LMG	c	521	-	51,51,55	1.31	5 (9%)	59,59,63	1.02	3 (5%)
25	BCR	c	522	-	41,41,41	9.17	30 (73%)	56,56,56	5.81	28 (50%)
24	PHO	d	401	-	67,69,69	1.26	7 (10%)	85,99,99	1.03	4 (4%)
23	CLA	d	402	-	58,73,73	2.62	23 (39%)	66,113,113	1.70	11 (16%)
23	CLA	d	403	-	58,73,73	2.59	22 (37%)	66,113,113	1.76	14 (21%)
26	PL9	d	404	-	55,55,55	4.16	19 (34%)	69,69,69	3.61	35 (50%)
32	DGD	d	405	-	63,63,67	1.69	16 (25%)	77,77,81	1.04	7 (9%)
31	LHG	d	406	-	48,48,48	1.11	3 (6%)	51,54,54	0.92	3 (5%)
31	LHG	e	101	-	41,41,48	1.20	3 (7%)	44,47,54	0.98	2 (4%)
33	HEM	e	102	5,6	27,50,50	2.06	5 (18%)	17,82,82	1.78	4 (23%)
25	BCR	f	101	-	41,41,41	9.18	30 (73%)	56,56,56	5.75	28 (50%)
25	BCR	h	101	-	41,41,41	9.17	30 (73%)	56,56,56	5.81	37 (66%)
32	DGD	h	102	-	63,63,67	1.67	15 (23%)	77,77,81	0.99	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LMG	j	101	34	51,51,55	1.30	4 (7%)	59,59,63	0.94	4 (6%)
25	BCR	k	101	-	41,41,41	9.24	30 (73%)	56,56,56	5.65	26 (46%)
31	LHG	l	101	-	48,48,48	1.11	3 (6%)	51,54,54	0.90	3 (5%)
25	BCR	t	101	-	41,41,41	9.25	29 (70%)	56,56,56	5.72	26 (46%)
33	HEM	v	201	16	27,50,50	2.12	5 (18%)	17,82,82	1.81	4 (23%)
27	SQD	x	101	-	42,43,54	1.19	3 (7%)	52,54,65	1.48	7 (13%)
28	LMG	z	101	-	37,37,55	1.42	5 (13%)	45,45,63	1.20	4 (8%)

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
22	BCT	A	604	29	-	0/0/0/0	0/0/0/0
23	CLA	A	605	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	607	-	-	0/53/103/103	0/5/6/6
23	CLA	A	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	A	609	-	-	1/29/63/63	0/2/2/2
26	PL9	A	610	-	-	0/53/73/73	0/1/1/1
27	SQD	A	611	-	-	0/49/69/69	0/1/1/1
28	LMG	A	612	-	-	0/46/66/70	0/1/1/1
23	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	1/29/63/63	0/2/2/2
25	BCR	B	619	-	-	1/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	LMG	B	621	-	-	0/46/66/70	0/1/1/1
31	LHG	B	622	-	-	0/53/53/53	0/0/0/0
27	SQD	B	623	-	-	0/49/69/69	0/1/1/1
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
25	BCR	C	515	-	-	2/29/63/63	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
28	LMG	C	519	-	-	0/46/66/70	0/1/1/1
28	LMG	C	520	-	-	0/46/66/70	0/1/1/1
25	BCR	C	521	-	-	0/29/63/63	0/2/2/2
24	PHO	D	401	-	-	0/53/103/103	0/5/6/6
23	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	D	405	-	-	0/53/73/73	0/1/1/1
32	DGD	D	406	-	-	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LHG	D	407	-	-	0/53/53/53	0/0/0/0
31	LHG	D	408	-	-	0/53/53/53	0/0/0/0
31	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
25	BCR	F	101	-	-	0/29/63/63	0/2/2/2
25	BCR	H	101	-	-	0/29/63/63	0/2/2/2
32	DGD	H	102	-	-	0/51/91/95	0/2/2/2
28	LMG	J	101	34	-	0/46/66/70	0/1/1/1
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
31	LHG	L	101	-	-	0/53/53/53	0/0/0/0
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	HEM	V	202	16	-	0/6/54/54	0/0/8/8
27	SQD	X	101	-	-	0/38/58/69	0/1/1/1
28	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
22	BCT	a	603	29	-	0/0/0/0	0/0/0/0
23	CLA	a	604	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	a	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	606	-	-	0/53/103/103	0/5/6/6
23	CLA	a	607	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	a	608	-	-	1/29/63/63	0/2/2/2
26	PL9	a	609	-	-	0/53/73/73	0/1/1/1
27	SQD	a	610	-	-	0/49/69/69	0/1/1/1
28	LMG	a	611	-	-	0/46/66/70	0/1/1/1
27	SQD	a	612	-	-	0/49/69/69	0/1/1/1
23	CLA	a	613	-	3/3/20/25	0/37/135/135	0/0/9/9
31	LHG	a	614	-	-	0/53/53/53	0/0/0/0
27	SQD	b	601	-	-	0/49/69/69	0/1/1/1
27	SQD	b	602	-	-	0/49/69/69	0/1/1/1
23	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609[A]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609[B]	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	618	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
25	BCR	b	621	-	-	4/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
28	LMG	b	623	-	-	0/46/66/70	0/1/1/1
31	LHG	b	624	-	-	0/53/53/53	0/0/0/0
23	CLA	c	502	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	512	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	514	-	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
25	BCR	c	516	-	-	0/29/63/63	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
32	DGD	c	519	-	-	0/51/91/95	0/2/2/2
28	LMG	c	520	-	-	0/46/66/70	0/1/1/1
28	LMG	c	521	-	-	0/46/66/70	0/1/1/1
25	BCR	c	522	-	-	1/29/63/63	0/2/2/2
24	PHO	d	401	-	-	0/53/103/103	0/5/6/6
23	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
26	PL9	d	404	-	-	0/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	DGD	d	405	-	-	0/51/91/95	0/2/2/2
31	LHG	d	406	-	-	0/53/53/53	0/0/0/0
31	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
25	BCR	f	101	-	-	0/29/63/63	0/2/2/2
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
32	DGD	h	102	-	-	0/51/91/95	0/2/2/2
28	LMG	j	101	34	-	0/46/66/70	0/1/1/1
25	BCR	k	101	-	-	2/29/63/63	0/2/2/2
31	LHG	l	101	-	-	0/53/53/53	0/0/0/0
25	BCR	t	101	-	-	1/29/63/63	0/2/2/2
33	HEM	v	201	16	-	0/6/54/54	0/0/8/8
27	SQD	x	101	-	-	0/38/58/69	0/1/1/1
28	LMG	z	101	-	-	1/31/51/70	0/1/1/1

All (2695) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	619	BCR	C21-C22	-26.31	1.00	1.35
25	H	101	BCR	C21-C22	-23.87	1.04	1.35
25	F	101	BCR	C21-C22	-23.08	1.05	1.35
25	C	514	BCR	C21-C22	-23.08	1.05	1.35
25	c	516	BCR	C21-C22	-23.01	1.05	1.35
25	c	515	BCR	C21-C22	-22.95	1.05	1.35
25	C	515	BCR	C21-C22	-22.94	1.05	1.35
25	C	521	BCR	C21-C22	-22.88	1.05	1.35
25	B	620	BCR	C21-C22	-22.45	1.06	1.35
25	k	101	BCR	C21-C22	-22.32	1.06	1.35
25	B	618	BCR	C21-C22	-22.29	1.06	1.35
25	h	101	BCR	C21-C22	-22.12	1.06	1.35
25	b	622	BCR	C21-C22	-22.09	1.06	1.35
25	A	609	BCR	C21-C22	-22.05	1.06	1.35
25	b	620	BCR	C21-C22	-21.93	1.06	1.35
25	f	101	BCR	C21-C22	-21.73	1.07	1.35
25	t	101	BCR	C21-C22	-21.67	1.07	1.35
25	c	522	BCR	C21-C22	-21.29	1.07	1.35
25	b	621	BCR	C21-C22	-21.10	1.07	1.35
25	K	101	BCR	C21-C22	-21.03	1.07	1.35
25	a	608	BCR	C21-C22	-20.66	1.08	1.35
25	T	101	BCR	C21-C22	-20.63	1.08	1.35
25	B	619	BCR	C19-C18	-15.23	1.12	1.45
25	F	101	BCR	C19-C18	-13.69	1.16	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	101	BCR	C19-C18	-13.63	1.16	1.45
25	h	101	BCR	C19-C18	-13.41	1.16	1.45
25	C	521	BCR	C19-C18	-13.34	1.16	1.45
25	b	621	BCR	C19-C18	-13.34	1.16	1.45
25	T	101	BCR	C19-C18	-13.25	1.17	1.45
25	c	515	BCR	C19-C18	-13.22	1.17	1.45
25	k	101	BCR	C19-C18	-13.22	1.17	1.45
25	c	522	BCR	C19-C18	-13.07	1.17	1.45
25	f	101	BCR	C19-C18	-12.95	1.17	1.45
25	b	620	BCR	C19-C18	-12.61	1.18	1.45
25	t	101	BCR	C19-C18	-12.60	1.18	1.45
25	B	620	BCR	C19-C18	-12.58	1.18	1.45
25	C	514	BCR	C19-C18	-12.56	1.18	1.45
25	A	609	BCR	C19-C18	-12.56	1.18	1.45
25	a	608	BCR	C19-C18	-12.48	1.18	1.45
25	b	622	BCR	C19-C18	-12.38	1.19	1.45
25	c	516	BCR	C19-C18	-12.34	1.19	1.45
25	C	515	BCR	C19-C18	-12.31	1.19	1.45
25	H	101	BCR	C19-C18	-12.31	1.19	1.45
25	B	618	BCR	C19-C18	-12.24	1.19	1.45
23	A	605	CLA	C3A-C2A	-7.60	1.33	1.54
23	a	604	CLA	C3A-C2A	-7.55	1.33	1.54
23	a	607	CLA	C3A-C2A	-7.53	1.33	1.54
23	b	611	CLA	C3A-C2A	-7.53	1.33	1.54
23	B	609	CLA	C3A-C2A	-7.48	1.33	1.54
23	b	610	CLA	C3A-C2A	-7.46	1.33	1.54
23	B	607[A]	CLA	C3A-C2A	-7.45	1.33	1.54
23	C	510	CLA	C3A-C2A	-7.45	1.33	1.54
23	B	607[B]	CLA	C3A-C2A	-7.45	1.33	1.54
23	b	613	CLA	C3A-C2A	-7.44	1.33	1.54
23	b	615	CLA	C3A-C2A	-7.43	1.33	1.54
23	D	404	CLA	C3A-C2A	-7.43	1.33	1.54
23	C	505	CLA	C3A-C2A	-7.43	1.33	1.54
23	b	607	CLA	C3A-C2A	-7.42	1.33	1.54
23	b	605	CLA	C3A-C2A	-7.42	1.33	1.54
23	c	511	CLA	C3A-C2A	-7.42	1.33	1.54
23	d	403	CLA	C3A-C2A	-7.41	1.33	1.54
23	c	507	CLA	C3A-C2A	-7.41	1.33	1.54
23	B	613	CLA	C3A-C2A	-7.40	1.33	1.54
23	B	611	CLA	C3A-C2A	-7.39	1.33	1.54
23	A	608	CLA	C3A-C2A	-7.39	1.33	1.54
23	b	609[B]	CLA	C3A-C2A	-7.39	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C3A-C2A	-7.38	1.33	1.54
23	B	615	CLA	C3A-C2A	-7.38	1.33	1.54
23	b	617	CLA	C3A-C2A	-7.38	1.33	1.54
23	D	402	CLA	C3A-C2A	-7.37	1.33	1.54
23	B	614	CLA	C3A-C2A	-7.37	1.33	1.54
23	C	508	CLA	C3A-C2A	-7.36	1.33	1.54
23	b	606	CLA	C3A-C2A	-7.35	1.33	1.54
23	b	612	CLA	C3A-C2A	-7.34	1.33	1.54
23	C	512	CLA	C3A-C2A	-7.34	1.33	1.54
23	b	604	CLA	C3A-C2A	-7.34	1.33	1.54
23	C	501	CLA	C3A-C2A	-7.33	1.33	1.54
23	c	513	CLA	C3A-C2A	-7.33	1.33	1.54
23	B	605	CLA	C3A-C2A	-7.33	1.33	1.54
23	b	616	CLA	C3A-C2A	-7.33	1.33	1.54
23	d	402	CLA	C3A-C2A	-7.32	1.33	1.54
23	b	619	CLA	C3A-C2A	-7.32	1.33	1.54
23	C	502	CLA	C3A-C2A	-7.32	1.33	1.54
23	B	603	CLA	C3A-C2A	-7.32	1.33	1.54
23	c	512	CLA	C3A-C2A	-7.32	1.33	1.54
23	c	506	CLA	C3A-C2A	-7.32	1.33	1.54
23	a	613	CLA	C3A-C2A	-7.32	1.33	1.54
23	b	609[A]	CLA	C3A-C2A	-7.32	1.33	1.54
23	b	614	CLA	C3A-C2A	-7.31	1.33	1.54
23	c	503	CLA	C3A-C2A	-7.29	1.33	1.54
23	B	606	CLA	C3A-C2A	-7.29	1.33	1.54
23	b	608	CLA	C3A-C2A	-7.29	1.33	1.54
23	a	605	CLA	C3A-C2A	-7.29	1.33	1.54
23	C	503	CLA	C3A-C2A	-7.29	1.33	1.54
23	C	511	CLA	C3A-C2A	-7.29	1.33	1.54
23	B	612	CLA	C3A-C2A	-7.28	1.34	1.54
23	c	514	CLA	C3A-C2A	-7.27	1.34	1.54
23	B	608	CLA	C3A-C2A	-7.27	1.34	1.54
23	B	604	CLA	C3A-C2A	-7.27	1.34	1.54
23	c	502	CLA	C3A-C2A	-7.27	1.34	1.54
23	b	618	CLA	C3A-C2A	-7.26	1.34	1.54
23	c	509	CLA	C3A-C2A	-7.26	1.34	1.54
23	c	510	CLA	C3A-C2A	-7.25	1.34	1.54
23	C	504	CLA	C3A-C2A	-7.24	1.34	1.54
23	C	506	CLA	C3A-C2A	-7.24	1.34	1.54
23	A	606	CLA	C3A-C2A	-7.23	1.34	1.54
23	B	617	CLA	C3A-C2A	-7.23	1.34	1.54
23	c	505	CLA	C3A-C2A	-7.23	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C3A-C2A	-7.23	1.34	1.54
23	B	602	CLA	C3A-C2A	-7.22	1.34	1.54
23	C	509	CLA	C3A-C2A	-7.21	1.34	1.54
23	c	504	CLA	C3A-C2A	-7.20	1.34	1.54
23	C	513	CLA	C3A-C2A	-7.14	1.34	1.54
23	B	616	CLA	C3A-C2A	-7.11	1.34	1.54
23	c	508	CLA	C3A-C2A	-7.11	1.34	1.54
23	C	507	CLA	C3A-C2A	-7.04	1.34	1.54
25	c	515	BCR	C34-C9	-6.89	1.35	1.50
25	B	618	BCR	C34-C9	-6.83	1.36	1.50
25	B	619	BCR	C34-C9	-6.81	1.36	1.50
25	K	101	BCR	C34-C9	-6.80	1.36	1.50
25	b	621	BCR	C34-C9	-6.80	1.36	1.50
25	k	101	BCR	C34-C9	-6.72	1.36	1.50
25	c	516	BCR	C34-C9	-6.66	1.36	1.50
25	B	620	BCR	C34-C9	-6.59	1.36	1.50
25	H	101	BCR	C34-C9	-6.56	1.36	1.50
25	b	620	BCR	C34-C9	-6.56	1.36	1.50
25	C	515	BCR	C34-C9	-6.55	1.36	1.50
25	f	101	BCR	C34-C9	-6.53	1.36	1.50
25	T	101	BCR	C34-C9	-6.52	1.36	1.50
25	t	101	BCR	C34-C9	-6.52	1.36	1.50
25	C	514	BCR	C34-C9	-6.51	1.36	1.50
25	a	608	BCR	C34-C9	-6.51	1.36	1.50
25	F	101	BCR	C34-C9	-6.49	1.36	1.50
25	A	609	BCR	C34-C9	-6.47	1.36	1.50
25	h	101	BCR	C34-C9	-6.46	1.36	1.50
25	C	521	BCR	C34-C9	-6.45	1.36	1.50
25	b	622	BCR	C34-C9	-6.43	1.36	1.50
25	c	522	BCR	C34-C9	-6.40	1.36	1.50
23	b	606	CLA	C3D-C2D	-5.60	1.28	1.39
23	b	610	CLA	C3D-C2D	-5.57	1.28	1.39
23	B	606	CLA	C3D-C2D	-5.56	1.28	1.39
23	b	608	CLA	C3D-C2D	-5.56	1.28	1.39
23	C	503	CLA	C3D-C2D	-5.51	1.28	1.39
23	a	605	CLA	C3D-C2D	-5.44	1.28	1.39
23	A	606	CLA	C3D-C2D	-5.43	1.28	1.39
23	C	509	CLA	C3D-C2D	-5.41	1.28	1.39
23	b	617	CLA	C3D-C2D	-5.40	1.28	1.39
23	b	615	CLA	C3D-C2D	-5.39	1.28	1.39
23	b	609[B]	CLA	C3D-C2D	-5.38	1.28	1.39
23	c	506	CLA	C3D-C2D	-5.38	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3D-C2D	-5.38	1.28	1.39
23	B	614	CLA	C3D-C2D	-5.37	1.28	1.39
23	b	618	CLA	C3D-C2D	-5.36	1.28	1.39
23	C	510	CLA	C3D-C2D	-5.36	1.28	1.39
23	c	504	CLA	C3D-C2D	-5.33	1.28	1.39
23	c	505	CLA	C3D-C2D	-5.33	1.29	1.39
23	c	511	CLA	C3D-C2D	-5.33	1.29	1.39
23	d	402	CLA	C3D-C2D	-5.33	1.29	1.39
23	B	604	CLA	C3D-C2D	-5.32	1.29	1.39
23	c	510	CLA	C3D-C2D	-5.31	1.29	1.39
23	A	605	CLA	C3D-C2D	-5.31	1.29	1.39
23	b	607	CLA	C3D-C2D	-5.31	1.29	1.39
23	D	403	CLA	C3D-C2D	-5.30	1.29	1.39
23	a	607	CLA	C3D-C2D	-5.29	1.29	1.39
23	C	506	CLA	C3D-C2D	-5.29	1.29	1.39
23	a	613	CLA	C3D-C2D	-5.29	1.29	1.39
26	d	404	PL9	C3-C4	-5.29	1.40	1.49
23	B	615	CLA	C3D-C2D	-5.27	1.29	1.39
23	b	616	CLA	C3D-C2D	-5.26	1.29	1.39
23	C	511	CLA	C3D-C2D	-5.26	1.29	1.39
23	B	607[B]	CLA	C3D-C2D	-5.25	1.29	1.39
23	D	402	CLA	C3D-C2D	-5.25	1.29	1.39
23	C	505	CLA	C3D-C2D	-5.25	1.29	1.39
23	B	613	CLA	C3D-C2D	-5.25	1.29	1.39
23	a	604	CLA	C3D-C2D	-5.24	1.29	1.39
23	B	609	CLA	C3D-C2D	-5.23	1.29	1.39
23	B	605	CLA	C3D-C2D	-5.23	1.29	1.39
23	b	605	CLA	C3D-C2D	-5.21	1.29	1.39
23	c	507	CLA	C3D-C2D	-5.21	1.29	1.39
23	C	508	CLA	C3D-C2D	-5.21	1.29	1.39
23	c	513	CLA	C3D-C2D	-5.20	1.29	1.39
23	c	512	CLA	C3D-C2D	-5.20	1.29	1.39
23	B	602	CLA	C3D-C2D	-5.19	1.29	1.39
23	B	603	CLA	C3D-C2D	-5.19	1.29	1.39
23	b	614	CLA	C3D-C2D	-5.18	1.29	1.39
23	B	617	CLA	C3D-C2D	-5.18	1.29	1.39
23	B	608	CLA	C3D-C2D	-5.18	1.29	1.39
23	D	404	CLA	C3D-C2D	-5.17	1.29	1.39
23	b	604	CLA	C3D-C2D	-5.17	1.29	1.39
23	C	513	CLA	C3D-C2D	-5.16	1.29	1.39
23	b	619	CLA	C3D-C2D	-5.15	1.29	1.39
23	B	607[A]	CLA	C3D-C2D	-5.15	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	C3D-C2D	-5.14	1.29	1.39
23	C	504	CLA	C3D-C2D	-5.14	1.29	1.39
23	b	611	CLA	C3D-C2D	-5.12	1.29	1.39
23	C	507	CLA	C3D-C2D	-5.12	1.29	1.39
23	b	613	CLA	C3D-C2D	-5.09	1.29	1.39
23	b	609[A]	CLA	C3D-C2D	-5.08	1.29	1.39
23	c	514	CLA	C3D-C2D	-5.07	1.29	1.39
23	c	503	CLA	C3D-C2D	-5.07	1.29	1.39
23	A	608	CLA	C3D-C2D	-5.07	1.29	1.39
23	B	612	CLA	C3D-C2D	-5.06	1.29	1.39
23	c	508	CLA	C3D-C2D	-5.06	1.29	1.39
23	c	502	CLA	C3D-C2D	-5.05	1.29	1.39
23	C	512	CLA	C3D-C2D	-5.02	1.29	1.39
23	B	610	CLA	C3D-C2D	-5.00	1.29	1.39
26	A	610	PL9	C3-C4	-4.99	1.41	1.49
26	D	405	PL9	C3-C4	-4.98	1.41	1.49
23	C	501	CLA	C3D-C2D	-4.97	1.29	1.39
23	B	611	CLA	C3D-C2D	-4.96	1.29	1.39
23	C	502	CLA	C3D-C2D	-4.96	1.29	1.39
23	d	403	CLA	C3D-C2D	-4.94	1.29	1.39
23	b	612	CLA	C3D-C2D	-4.93	1.29	1.39
26	a	609	PL9	C3-C4	-4.91	1.41	1.49
23	a	613	CLA	C4B-CHC	-4.78	1.27	1.40
23	B	605	CLA	C4B-CHC	-4.77	1.27	1.40
23	b	610	CLA	C4B-CHC	-4.74	1.27	1.40
23	b	614	CLA	C4B-CHC	-4.72	1.27	1.40
23	B	617	CLA	C4B-CHC	-4.68	1.27	1.40
26	d	404	PL9	C6-C1	-4.68	1.40	1.48
26	D	405	PL9	C6-C1	-4.67	1.40	1.48
23	b	618	CLA	C4C-C3C	-4.63	1.37	1.45
23	b	607	CLA	C4B-CHC	-4.63	1.27	1.40
23	c	510	CLA	C4B-CHC	-4.63	1.27	1.40
23	B	608	CLA	C4B-CHC	-4.62	1.27	1.40
23	b	606	CLA	C4B-CHC	-4.61	1.27	1.40
23	c	513	CLA	C4B-CHC	-4.61	1.27	1.40
23	B	614	CLA	C4B-CHC	-4.61	1.27	1.40
23	B	612	CLA	C4B-CHC	-4.60	1.28	1.40
23	C	512	CLA	C4B-CHC	-4.59	1.28	1.40
23	C	510	CLA	C4B-CHC	-4.59	1.28	1.40
23	b	619	CLA	C4B-CHC	-4.58	1.28	1.40
23	B	604	CLA	C4B-CHC	-4.57	1.28	1.40
23	C	504	CLA	C4B-CHC	-4.57	1.28	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C4B-CHC	-4.57	1.28	1.40
23	C	508	CLA	C4B-CHC	-4.56	1.28	1.40
23	B	613	CLA	C4B-CHC	-4.56	1.28	1.40
23	C	503	CLA	C4C-C3C	-4.55	1.37	1.45
23	C	509	CLA	C4B-CHC	-4.54	1.28	1.40
23	c	511	CLA	C4B-CHC	-4.54	1.28	1.40
23	D	402	CLA	C4B-CHC	-4.53	1.28	1.40
23	C	506	CLA	C4B-CHC	-4.53	1.28	1.40
23	C	507	CLA	C4B-CHC	-4.53	1.28	1.40
23	d	402	CLA	C4B-CHC	-4.52	1.28	1.40
23	b	616	CLA	C4B-CHC	-4.52	1.28	1.40
23	B	606	CLA	C4B-CHC	-4.52	1.28	1.40
23	c	506	CLA	C4B-CHC	-4.52	1.28	1.40
23	a	605	CLA	C4B-CHC	-4.52	1.28	1.40
23	c	503	CLA	C4B-CHC	-4.51	1.28	1.40
23	B	602	CLA	C4B-CHC	-4.51	1.28	1.40
23	c	508	CLA	C4B-CHC	-4.51	1.28	1.40
23	b	604	CLA	C4B-CHC	-4.51	1.28	1.40
23	b	608	CLA	C4C-C3C	-4.51	1.37	1.45
23	B	610	CLA	C4B-CHC	-4.50	1.28	1.40
23	c	512	CLA	C4B-CHC	-4.50	1.28	1.40
23	b	617	CLA	C4B-CHC	-4.49	1.28	1.40
23	A	606	CLA	C4B-CHC	-4.49	1.28	1.40
23	a	604	CLA	C4B-CHC	-4.48	1.28	1.40
23	D	403	CLA	C4B-CHC	-4.48	1.28	1.40
23	c	505	CLA	C4B-CHC	-4.48	1.28	1.40
23	C	501	CLA	C4B-CHC	-4.48	1.28	1.40
23	B	616	CLA	C4B-CHC	-4.47	1.28	1.40
23	c	507	CLA	C4B-CHC	-4.46	1.28	1.40
23	C	503	CLA	C4B-CHC	-4.46	1.28	1.40
23	d	403	CLA	C4B-CHC	-4.45	1.28	1.40
23	c	504	CLA	C4B-CHC	-4.45	1.28	1.40
23	B	607[A]	CLA	C4B-CHC	-4.45	1.28	1.40
23	C	502	CLA	C4B-CHC	-4.45	1.28	1.40
23	B	614	CLA	C4C-C3C	-4.44	1.37	1.45
23	D	404	CLA	C4B-CHC	-4.44	1.28	1.40
23	B	609	CLA	C4B-CHC	-4.44	1.28	1.40
23	b	608	CLA	C4B-CHC	-4.43	1.28	1.40
23	b	618	CLA	C4B-CHC	-4.43	1.28	1.40
23	C	511	CLA	C4B-CHC	-4.43	1.28	1.40
23	B	606	CLA	C4C-C3C	-4.43	1.37	1.45
23	c	502	CLA	C4B-CHC	-4.42	1.28	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C4C-C3C	-4.41	1.37	1.45
23	c	509	CLA	C4B-CHC	-4.41	1.28	1.40
23	B	615	CLA	C4B-CHC	-4.41	1.28	1.40
23	b	609[B]	CLA	C4B-CHC	-4.40	1.28	1.40
23	b	612	CLA	C4B-CHC	-4.40	1.28	1.40
23	B	603	CLA	C4B-CHC	-4.39	1.28	1.40
26	A	610	PL9	C6-C1	-4.39	1.40	1.48
23	B	607[B]	CLA	C4C-C3C	-4.39	1.37	1.45
23	b	605	CLA	C4B-CHC	-4.39	1.28	1.40
23	b	613	CLA	C4B-CHC	-4.37	1.28	1.40
23	c	514	CLA	C4B-CHC	-4.37	1.28	1.40
23	b	609[A]	CLA	C4B-CHC	-4.36	1.28	1.40
23	A	605	CLA	C4B-CHC	-4.36	1.28	1.40
23	a	607	CLA	CHD-C4C	-4.36	1.28	1.41
23	b	616	CLA	C4C-C3C	-4.36	1.37	1.45
23	b	605	CLA	C4C-C3C	-4.36	1.37	1.45
23	C	505	CLA	C4B-CHC	-4.35	1.28	1.40
23	A	608	CLA	C4B-CHC	-4.35	1.28	1.40
23	B	607[B]	CLA	C4B-CHC	-4.35	1.28	1.40
23	C	504	CLA	C4C-C3C	-4.33	1.37	1.45
26	a	609	PL9	C6-C1	-4.33	1.41	1.48
23	B	611	CLA	C4B-CHC	-4.33	1.28	1.40
23	c	512	CLA	C4C-C3C	-4.32	1.37	1.45
23	C	513	CLA	C4B-CHC	-4.32	1.28	1.40
23	c	504	CLA	C4C-C3C	-4.32	1.37	1.45
23	b	611	CLA	C4B-CHC	-4.31	1.28	1.40
23	b	614	CLA	C4C-C3C	-4.31	1.37	1.45
23	A	608	CLA	C4C-C3C	-4.29	1.37	1.45
23	B	616	CLA	C4C-C3C	-4.28	1.37	1.45
23	B	607[A]	CLA	C4C-C3C	-4.28	1.37	1.45
23	a	607	CLA	C4B-CHC	-4.28	1.28	1.40
23	B	604	CLA	C4C-C3C	-4.28	1.37	1.45
23	b	617	CLA	C4C-C3C	-4.28	1.37	1.45
23	c	502	CLA	C4C-C3C	-4.27	1.37	1.45
23	b	610	CLA	C4C-C3C	-4.25	1.37	1.45
23	C	507	CLA	CHD-C4C	-4.25	1.28	1.41
23	B	615	CLA	C4C-C3C	-4.25	1.37	1.45
23	c	508	CLA	CHD-C4C	-4.23	1.28	1.41
23	b	609[B]	CLA	C4C-C3C	-4.23	1.37	1.45
23	c	513	CLA	C4C-C3C	-4.23	1.37	1.45
23	c	503	CLA	C4C-C3C	-4.22	1.37	1.45
23	C	510	CLA	C4C-C3C	-4.21	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CHD-C4C	-4.21	1.28	1.41
23	B	616	CLA	CHD-C4C	-4.21	1.28	1.41
23	A	608	CLA	CHD-C4C	-4.21	1.28	1.41
23	C	505	CLA	C4C-C3C	-4.21	1.37	1.45
23	c	506	CLA	CHD-C4C	-4.21	1.28	1.41
23	b	616	CLA	CHD-C4C	-4.20	1.28	1.41
23	b	614	CLA	CHD-C4C	-4.20	1.28	1.41
23	b	608	CLA	CHD-C4C	-4.20	1.28	1.41
23	c	509	CLA	C4C-C3C	-4.20	1.37	1.45
23	b	609[A]	CLA	C4C-C3C	-4.19	1.37	1.45
23	b	618	CLA	CHD-C4C	-4.19	1.28	1.41
23	c	507	CLA	C4C-C3C	-4.19	1.37	1.45
23	C	502	CLA	C4C-C3C	-4.19	1.37	1.45
23	b	606	CLA	CHD-C4C	-4.19	1.28	1.41
23	d	402	CLA	C4C-C3C	-4.18	1.37	1.45
23	C	509	CLA	CHD-C4C	-4.18	1.28	1.41
23	b	619	CLA	C4C-C3C	-4.18	1.37	1.45
23	b	612	CLA	C4C-C3C	-4.17	1.37	1.45
33	v	201	HEM	C3C-C2C	-4.17	1.34	1.40
23	c	508	CLA	C4C-C3C	-4.17	1.37	1.45
23	c	510	CLA	CHD-C4C	-4.17	1.28	1.41
23	B	612	CLA	C4C-C3C	-4.17	1.37	1.45
23	B	613	CLA	CHD-C4C	-4.16	1.28	1.41
23	b	612	CLA	CHD-C4C	-4.16	1.28	1.41
23	D	404	CLA	CHD-C4C	-4.16	1.28	1.41
23	b	615	CLA	CHD-C4C	-4.15	1.28	1.41
23	C	508	CLA	CHD-C4C	-4.15	1.28	1.41
23	c	511	CLA	C4C-C3C	-4.15	1.37	1.45
23	C	505	CLA	CHD-C4C	-4.15	1.28	1.41
23	b	604	CLA	CHD-C4C	-4.15	1.28	1.41
23	B	606	CLA	CHD-C4C	-4.15	1.28	1.41
23	b	610	CLA	CHD-C4C	-4.15	1.28	1.41
23	b	613	CLA	CHD-C4C	-4.15	1.28	1.41
23	C	503	CLA	CHD-C4C	-4.15	1.28	1.41
23	b	619	CLA	CHD-C4C	-4.15	1.28	1.41
23	B	607[B]	CLA	CHD-C4C	-4.15	1.28	1.41
23	c	514	CLA	C4C-C3C	-4.14	1.37	1.45
23	B	607[A]	CLA	CHD-C4C	-4.14	1.28	1.41
23	d	403	CLA	C4C-C3C	-4.14	1.37	1.45
23	C	512	CLA	CHD-C4C	-4.14	1.28	1.41
23	c	511	CLA	CHD-C4C	-4.13	1.28	1.41
23	C	502	CLA	CHD-C4C	-4.13	1.28	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C4C-C3C	-4.13	1.37	1.45
23	C	506	CLA	CHD-C4C	-4.13	1.28	1.41
23	C	507	CLA	C4C-C3C	-4.13	1.37	1.45
23	b	609[B]	CLA	CHD-C4C	-4.13	1.28	1.41
23	b	617	CLA	CHD-C4C	-4.13	1.28	1.41
23	A	605	CLA	C4C-C3C	-4.13	1.37	1.45
23	B	617	CLA	C4C-C3C	-4.12	1.37	1.45
23	B	611	CLA	CHD-C4C	-4.12	1.28	1.41
23	d	403	CLA	CHD-C4C	-4.12	1.28	1.41
23	c	503	CLA	CHD-C4C	-4.12	1.28	1.41
23	A	606	CLA	CHD-C4C	-4.12	1.28	1.41
23	c	505	CLA	C4C-C3C	-4.12	1.37	1.45
23	B	605	CLA	CHD-C4C	-4.11	1.28	1.41
23	c	506	CLA	C1D-C2D	-4.11	1.33	1.42
23	c	510	CLA	C4C-C3C	-4.11	1.37	1.45
23	B	610	CLA	CHD-C4C	-4.11	1.28	1.41
23	c	512	CLA	CHD-C4C	-4.10	1.28	1.41
23	C	513	CLA	C4C-C3C	-4.10	1.37	1.45
23	c	504	CLA	CHD-C4C	-4.10	1.28	1.41
23	C	501	CLA	CHD-C4C	-4.09	1.28	1.41
23	C	511	CLA	C4C-C3C	-4.09	1.38	1.45
23	D	403	CLA	CHD-C4C	-4.08	1.29	1.41
23	a	607	CLA	C4C-C3C	-4.08	1.38	1.45
23	C	501	CLA	C4C-C3C	-4.08	1.38	1.45
23	C	511	CLA	CHD-C4C	-4.08	1.29	1.41
23	c	513	CLA	CHD-C4C	-4.07	1.29	1.41
23	B	608	CLA	C4C-C3C	-4.07	1.38	1.45
23	C	506	CLA	C4C-C3C	-4.07	1.38	1.45
23	B	615	CLA	CHD-C4C	-4.06	1.29	1.41
23	B	610	CLA	C4C-C3C	-4.06	1.38	1.45
32	C	518	DGD	O2G-C2G	-4.06	1.36	1.46
23	D	404	CLA	C4C-C3C	-4.06	1.38	1.45
23	B	608	CLA	CHD-C4C	-4.06	1.29	1.41
23	B	602	CLA	CHD-C4C	-4.06	1.29	1.41
23	b	609[A]	CLA	CHD-C4C	-4.05	1.29	1.41
23	b	605	CLA	CHD-C4C	-4.05	1.29	1.41
23	B	612	CLA	CHD-C4C	-4.05	1.29	1.41
23	B	617	CLA	CHD-C4C	-4.05	1.29	1.41
23	b	607	CLA	CHD-C4C	-4.05	1.29	1.41
23	c	509	CLA	CHD-C4C	-4.05	1.29	1.41
23	b	604	CLA	C4C-C3C	-4.05	1.38	1.45
23	b	606	CLA	C1D-C2D	-4.05	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	CHD-C4C	-4.05	1.29	1.41
23	C	513	CLA	CHD-C4C	-4.04	1.29	1.41
23	B	613	CLA	C4C-C3C	-4.04	1.38	1.45
23	d	402	CLA	CHD-C4C	-4.04	1.29	1.41
23	D	403	CLA	C4C-C3C	-4.04	1.38	1.45
23	a	613	CLA	CMA-C3A	-4.04	1.44	1.53
23	a	604	CLA	C4C-C3C	-4.03	1.38	1.45
23	c	505	CLA	CHD-C4C	-4.03	1.29	1.41
23	c	507	CLA	CHD-C4C	-4.03	1.29	1.41
23	B	605	CLA	CMA-C3A	-4.02	1.44	1.53
23	c	506	CLA	C4C-C3C	-4.02	1.38	1.45
23	C	504	CLA	CHD-C4C	-4.02	1.29	1.41
23	a	605	CLA	CHD-C4C	-4.02	1.29	1.41
32	c	519	DGD	O2G-C2G	-4.01	1.36	1.46
23	c	502	CLA	CHD-C4C	-4.01	1.29	1.41
23	a	604	CLA	CHD-C4C	-4.01	1.29	1.41
23	C	508	CLA	C4C-C3C	-4.01	1.38	1.45
23	B	604	CLA	CHD-C4C	-4.01	1.29	1.41
23	B	607[B]	CLA	CMA-C3A	-4.00	1.44	1.53
23	B	603	CLA	CHD-C4C	-4.00	1.29	1.41
23	B	613	CLA	CMA-C3A	-4.00	1.44	1.53
23	b	615	CLA	C4C-C3C	-4.00	1.38	1.45
23	A	605	CLA	CHD-C4C	-4.00	1.29	1.41
23	A	608	CLA	CMA-C3A	-3.99	1.44	1.53
23	c	512	CLA	CMA-C3A	-3.99	1.44	1.53
23	C	511	CLA	CMA-C3A	-3.99	1.44	1.53
23	B	603	CLA	C4C-C3C	-3.98	1.38	1.45
23	a	605	CLA	C4C-C3C	-3.97	1.38	1.45
23	D	402	CLA	CMA-C3A	-3.97	1.44	1.53
23	c	510	CLA	CMA-C3A	-3.97	1.44	1.53
23	B	609	CLA	CHD-C4C	-3.97	1.29	1.41
23	B	607[A]	CLA	CMA-C3A	-3.95	1.44	1.53
23	c	514	CLA	CHD-C4C	-3.95	1.29	1.41
32	c	518	DGD	O2G-C2G	-3.95	1.36	1.46
23	b	608	CLA	CMA-C3A	-3.95	1.44	1.53
32	c	517	DGD	O2G-C2G	-3.94	1.36	1.46
23	D	402	CLA	CHD-C4C	-3.94	1.29	1.41
23	b	611	CLA	CHD-C4C	-3.94	1.29	1.41
23	B	605	CLA	C4C-C3C	-3.94	1.38	1.45
23	C	504	CLA	CMA-C3A	-3.94	1.44	1.53
23	C	510	CLA	CMA-C3A	-3.93	1.44	1.53
23	b	612	CLA	CMA-C3A	-3.93	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CMA-C3A	-3.93	1.44	1.53
23	A	606	CLA	C4C-C3C	-3.93	1.38	1.45
23	b	609[B]	CLA	CMA-C3A	-3.93	1.44	1.53
23	C	505	CLA	C1D-C2D	-3.93	1.33	1.42
23	b	615	CLA	CMA-C3A	-3.92	1.44	1.53
23	B	608	CLA	CMA-C3A	-3.92	1.44	1.53
23	a	613	CLA	CHD-C4C	-3.92	1.29	1.41
23	B	612	CLA	CMA-C3A	-3.91	1.44	1.53
23	c	505	CLA	CMA-C3A	-3.91	1.44	1.53
23	C	509	CLA	C4C-C3C	-3.91	1.38	1.45
23	C	505	CLA	CMA-C3A	-3.91	1.44	1.53
23	a	605	CLA	CMA-C3A	-3.91	1.44	1.53
32	C	516	DGD	O2G-C2G	-3.90	1.36	1.46
23	b	610	CLA	CMA-C3A	-3.90	1.44	1.53
23	B	611	CLA	C4C-C3C	-3.90	1.38	1.45
23	b	611	CLA	CMA-C3A	-3.90	1.44	1.53
23	c	506	CLA	CMA-C3A	-3.90	1.44	1.53
23	B	609	CLA	CMA-C3A	-3.90	1.44	1.53
23	c	507	CLA	CMA-C3A	-3.89	1.44	1.53
23	a	607	CLA	CMA-C3A	-3.89	1.44	1.53
23	b	604	CLA	CMA-C3A	-3.89	1.44	1.53
23	b	611	CLA	C4C-C3C	-3.88	1.38	1.45
32	H	102	DGD	O2G-C2G	-3.88	1.36	1.46
23	D	403	CLA	CMA-C3A	-3.88	1.44	1.53
23	B	606	CLA	CMA-C3A	-3.88	1.44	1.53
23	c	509	CLA	CMA-C3A	-3.87	1.44	1.53
23	B	602	CLA	C4C-C3C	-3.87	1.38	1.45
23	a	604	CLA	CMA-C3A	-3.87	1.44	1.53
23	b	617	CLA	CMA-C3A	-3.87	1.44	1.53
23	b	609[A]	CLA	CMA-C3A	-3.87	1.44	1.53
33	V	202	HEM	C3C-C2C	-3.87	1.35	1.40
23	A	606	CLA	CMA-C3A	-3.87	1.44	1.53
23	B	615	CLA	CMA-C3A	-3.87	1.44	1.53
23	B	604	CLA	C1D-C2D	-3.86	1.33	1.42
23	d	403	CLA	CMA-C3A	-3.86	1.44	1.53
23	B	610	CLA	CMA-C3A	-3.86	1.44	1.53
23	d	402	CLA	CMA-C3A	-3.85	1.44	1.53
23	C	501	CLA	CMA-C3A	-3.85	1.44	1.53
23	C	509	CLA	CMA-C3A	-3.85	1.44	1.53
23	c	514	CLA	CMA-C3A	-3.85	1.44	1.53
23	A	605	CLA	CMA-C3A	-3.84	1.44	1.53
23	c	503	CLA	CMA-C3A	-3.84	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	CMA-C3A	-3.83	1.44	1.53
33	E	102	HEM	C3B-C2B	-3.83	1.35	1.40
23	C	506	CLA	CMA-C3A	-3.83	1.44	1.53
23	B	614	CLA	CMA-C3A	-3.83	1.44	1.53
23	C	508	CLA	CMA-C3A	-3.83	1.44	1.53
23	c	511	CLA	CMA-C3A	-3.83	1.44	1.53
23	b	618	CLA	CMA-C3A	-3.82	1.44	1.53
23	B	611	CLA	CMA-C3A	-3.82	1.44	1.53
23	c	513	CLA	CMA-C3A	-3.82	1.44	1.53
23	D	404	CLA	CMA-C3A	-3.82	1.44	1.53
32	C	517	DGD	O2G-C2G	-3.82	1.36	1.46
23	c	504	CLA	CMA-C3A	-3.82	1.44	1.53
23	a	604	CLA	C1A-CHA	-3.81	1.27	1.43
23	b	614	CLA	CMA-C3A	-3.81	1.44	1.53
23	C	512	CLA	CMA-C3A	-3.81	1.44	1.53
23	a	613	CLA	C4C-C3C	-3.81	1.38	1.45
23	D	402	CLA	C4C-C3C	-3.80	1.38	1.45
23	b	607	CLA	CMA-C3A	-3.80	1.44	1.53
23	C	502	CLA	CMA-C3A	-3.79	1.44	1.53
23	b	613	CLA	C4C-C3C	-3.79	1.38	1.45
23	B	613	CLA	C1A-CHA	-3.78	1.27	1.43
23	b	617	CLA	C1A-CHA	-3.78	1.27	1.43
32	D	406	DGD	O2G-C2G	-3.78	1.37	1.46
23	b	613	CLA	CMA-C3A	-3.77	1.44	1.53
23	C	513	CLA	CMA-C3A	-3.77	1.44	1.53
23	c	502	CLA	CMA-C3A	-3.77	1.44	1.53
23	B	602	CLA	CMA-C3A	-3.77	1.44	1.53
23	B	603	CLA	CMA-C3A	-3.77	1.44	1.53
23	B	612	CLA	C1A-CHA	-3.77	1.27	1.43
32	h	102	DGD	O2G-C2G	-3.75	1.37	1.46
23	C	501	CLA	C1A-CHA	-3.75	1.27	1.43
23	A	605	CLA	C1A-CHA	-3.74	1.27	1.43
23	C	508	CLA	C1D-C2D	-3.74	1.34	1.42
33	e	102	HEM	C3B-C2B	-3.74	1.35	1.40
23	c	508	CLA	CMA-C3A	-3.74	1.44	1.53
23	b	607	CLA	C4C-C3C	-3.74	1.38	1.45
23	C	504	CLA	C1A-CHA	-3.74	1.27	1.43
23	B	609	CLA	C1A-CHA	-3.73	1.27	1.43
23	D	403	CLA	C1A-CHA	-3.73	1.27	1.43
23	c	503	CLA	C1A-CHA	-3.73	1.27	1.43
23	b	611	CLA	C1A-CHA	-3.73	1.27	1.43
32	d	405	DGD	O2G-C2G	-3.73	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	619	CLA	CMA-C3A	-3.72	1.44	1.53
23	C	510	CLA	C1A-CHA	-3.72	1.27	1.43
23	b	616	CLA	CMA-C3A	-3.72	1.44	1.53
23	C	507	CLA	CMA-C3A	-3.71	1.44	1.53
23	B	604	CLA	CMA-C3A	-3.71	1.44	1.53
23	A	608	CLA	C1A-CHA	-3.71	1.27	1.43
23	B	604	CLA	C1A-CHA	-3.71	1.27	1.43
23	B	615	CLA	C1A-CHA	-3.71	1.27	1.43
23	B	617	CLA	CMA-C3A	-3.71	1.44	1.53
23	B	608	CLA	C1A-CHA	-3.70	1.27	1.43
23	a	607	CLA	C1D-C2D	-3.70	1.34	1.42
23	C	503	CLA	CMA-C3A	-3.70	1.45	1.53
23	c	511	CLA	CAA-C2A	-3.69	1.47	1.54
23	d	402	CLA	C1D-C2D	-3.69	1.34	1.42
33	e	102	HEM	C3C-C2C	-3.69	1.35	1.40
23	b	605	CLA	C1A-CHA	-3.69	1.27	1.43
23	d	402	CLA	C1A-CHA	-3.68	1.27	1.43
23	B	605	CLA	C1D-C2D	-3.68	1.34	1.42
23	b	619	CLA	C1D-C2D	-3.68	1.34	1.42
23	c	505	CLA	C1A-CHA	-3.67	1.27	1.43
23	D	402	CLA	C1A-CHA	-3.67	1.27	1.43
23	b	615	CLA	C1A-CHA	-3.67	1.27	1.43
23	B	613	CLA	C1D-C2D	-3.67	1.34	1.42
23	C	508	CLA	C1A-CHA	-3.67	1.27	1.43
23	A	606	CLA	C1A-CHA	-3.67	1.27	1.43
23	b	614	CLA	C1D-C2D	-3.67	1.34	1.42
23	C	505	CLA	CAA-C2A	-3.67	1.47	1.54
23	b	609[B]	CLA	C1D-C2D	-3.67	1.34	1.42
23	C	513	CLA	C1A-CHA	-3.66	1.28	1.43
23	B	606	CLA	C1D-C2D	-3.66	1.34	1.42
23	b	609[B]	CLA	C1A-CHA	-3.66	1.28	1.43
23	b	608	CLA	C1A-CHA	-3.65	1.28	1.43
23	a	607	CLA	C1A-CHA	-3.65	1.28	1.43
23	b	608	CLA	C1D-C2D	-3.65	1.34	1.42
33	E	102	HEM	C3C-C2C	-3.65	1.35	1.40
23	b	619	CLA	C1A-CHA	-3.64	1.28	1.43
23	B	614	CLA	CBD-CGD	-3.64	1.41	1.52
23	B	609	CLA	C4C-C3C	-3.64	1.38	1.45
23	B	616	CLA	CMA-C3A	-3.64	1.45	1.53
23	b	615	CLA	C1D-C2D	-3.64	1.34	1.42
23	a	613	CLA	C1A-CHA	-3.63	1.28	1.43
23	B	614	CLA	C1A-CHA	-3.63	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C1A-CHA	-3.63	1.28	1.43
23	C	511	CLA	C1D-C2D	-3.63	1.34	1.42
23	B	603	CLA	C1A-CHA	-3.63	1.28	1.43
23	b	612	CLA	C1D-C2D	-3.62	1.34	1.42
23	B	608	CLA	CAA-C2A	-3.62	1.47	1.54
23	a	604	CLA	CAA-C2A	-3.62	1.47	1.54
23	c	511	CLA	C1A-CHA	-3.62	1.28	1.43
23	C	506	CLA	C1D-C2D	-3.62	1.34	1.42
23	A	605	CLA	CAA-C2A	-3.62	1.47	1.54
23	b	613	CLA	C1A-CHA	-3.61	1.28	1.43
23	D	403	CLA	C1D-C2D	-3.61	1.34	1.42
23	b	607	CLA	C1A-CHA	-3.61	1.28	1.43
23	b	614	CLA	C1A-CHA	-3.61	1.28	1.43
23	c	507	CLA	C1D-C2D	-3.61	1.34	1.42
23	B	607[A]	CLA	C1A-CHA	-3.60	1.28	1.43
23	b	610	CLA	C1A-CHA	-3.60	1.28	1.43
23	C	509	CLA	C1D-C2D	-3.60	1.34	1.42
23	C	512	CLA	C1D-C2D	-3.60	1.34	1.42
23	C	511	CLA	C1A-CHA	-3.60	1.28	1.43
23	c	511	CLA	C1D-C2D	-3.60	1.34	1.42
23	B	607[B]	CLA	C1D-C2D	-3.60	1.34	1.42
23	B	616	CLA	C1A-CHA	-3.60	1.28	1.43
23	c	506	CLA	C1A-CHA	-3.60	1.28	1.43
23	b	609[A]	CLA	C1A-CHA	-3.59	1.28	1.43
23	c	502	CLA	C1A-CHA	-3.59	1.28	1.43
23	b	612	CLA	CAA-C2A	-3.59	1.47	1.54
23	c	505	CLA	C1D-C2D	-3.59	1.34	1.42
23	B	617	CLA	C1A-CHA	-3.58	1.28	1.43
33	V	202	HEM	C3B-C2B	-3.58	1.35	1.40
23	C	502	CLA	C1A-CHA	-3.58	1.28	1.43
23	b	614	CLA	CBD-CGD	-3.58	1.41	1.52
23	B	610	CLA	C1A-CHA	-3.58	1.28	1.43
23	c	504	CLA	CBD-CGD	-3.58	1.41	1.52
23	c	506	CLA	CAA-C2A	-3.58	1.47	1.54
23	B	607[B]	CLA	C1A-CHA	-3.58	1.28	1.43
23	D	404	CLA	C1A-CHA	-3.58	1.28	1.43
23	b	607	CLA	C1D-C2D	-3.57	1.34	1.42
23	B	616	CLA	C1D-C2D	-3.57	1.34	1.42
23	C	505	CLA	C1A-CHA	-3.57	1.28	1.43
23	C	510	CLA	CAA-C2A	-3.57	1.47	1.54
23	c	509	CLA	C1A-CHA	-3.56	1.28	1.43
23	a	605	CLA	C1A-CHA	-3.56	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C1A-CHA	-3.56	1.28	1.43
23	b	612	CLA	C1A-CHA	-3.56	1.28	1.43
23	C	512	CLA	C1A-CHA	-3.56	1.28	1.43
23	b	605	CLA	C1D-C2D	-3.56	1.34	1.42
23	D	403	CLA	CBD-CGD	-3.56	1.41	1.52
23	d	403	CLA	C1A-CHA	-3.55	1.28	1.43
23	B	603	CLA	C1D-C2D	-3.55	1.34	1.42
23	b	613	CLA	CAA-C2A	-3.55	1.47	1.54
23	b	617	CLA	C1D-C2D	-3.55	1.34	1.42
23	a	613	CLA	CBD-CGD	-3.55	1.41	1.52
23	c	507	CLA	C1A-CHA	-3.55	1.28	1.43
23	c	507	CLA	CAA-C2A	-3.55	1.47	1.54
23	b	616	CLA	C1D-C2D	-3.55	1.34	1.42
23	B	606	CLA	C1A-CHA	-3.55	1.28	1.43
23	b	610	CLA	C1D-C2D	-3.55	1.34	1.42
23	B	608	CLA	CBD-CGD	-3.55	1.41	1.52
23	c	509	CLA	C1D-C2D	-3.54	1.34	1.42
23	b	605	CLA	CHB-C4A	-3.54	1.29	1.33
23	b	618	CLA	C1D-C2D	-3.54	1.34	1.42
23	b	613	CLA	C1D-C2D	-3.54	1.34	1.42
23	b	605	CLA	CAA-C2A	-3.54	1.47	1.54
23	b	609[A]	CLA	C1D-C2D	-3.53	1.34	1.42
23	C	507	CLA	C1D-C2D	-3.53	1.34	1.42
33	v	201	HEM	C3B-C2B	-3.53	1.35	1.40
23	b	604	CLA	C1A-CHA	-3.53	1.28	1.43
23	c	504	CLA	C1A-CHA	-3.53	1.28	1.43
23	B	607[A]	CLA	C1D-C2D	-3.53	1.34	1.42
23	B	612	CLA	C1D-C2D	-3.52	1.34	1.42
23	B	613	CLA	CAA-C2A	-3.52	1.47	1.54
23	c	508	CLA	C1A-CHA	-3.52	1.28	1.43
23	B	611	CLA	C1D-C2D	-3.52	1.34	1.42
23	c	513	CLA	C1D-C2D	-3.52	1.34	1.42
23	c	511	CLA	CBD-CGD	-3.52	1.41	1.52
23	A	606	CLA	C1D-C2D	-3.52	1.34	1.42
23	b	613	CLA	CBD-CGD	-3.51	1.41	1.52
23	C	506	CLA	C1A-CHA	-3.51	1.28	1.43
23	C	503	CLA	C1D-C2D	-3.51	1.34	1.42
23	B	611	CLA	CBD-CGD	-3.51	1.41	1.52
23	c	510	CLA	C1A-CHA	-3.51	1.28	1.43
23	c	512	CLA	C1A-CHA	-3.51	1.28	1.43
23	c	510	CLA	C1D-C2D	-3.51	1.34	1.42
23	D	402	CLA	CBD-CGD	-3.50	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	C1D-C2D	-3.50	1.34	1.42
23	c	508	CLA	C1D-C2D	-3.50	1.34	1.42
23	b	615	CLA	CAA-C2A	-3.50	1.47	1.54
23	C	501	CLA	CBD-CGD	-3.50	1.41	1.52
23	d	402	CLA	CBD-CGD	-3.50	1.41	1.52
23	B	605	CLA	C1A-CHA	-3.50	1.28	1.43
23	C	513	CLA	C1D-C2D	-3.50	1.34	1.42
23	C	504	CLA	CBD-CGD	-3.50	1.41	1.52
23	C	509	CLA	C1A-CHA	-3.50	1.28	1.43
23	a	605	CLA	C1D-C2D	-3.49	1.34	1.42
23	b	616	CLA	CAA-C2A	-3.49	1.47	1.54
23	c	514	CLA	C1A-CHA	-3.49	1.28	1.43
23	b	618	CLA	C1A-CHA	-3.49	1.28	1.43
23	b	606	CLA	C1A-CHA	-3.49	1.28	1.43
23	B	602	CLA	CBD-CGD	-3.48	1.41	1.52
23	B	611	CLA	C1A-CHA	-3.48	1.28	1.43
23	B	610	CLA	CAA-C2A	-3.48	1.47	1.54
32	C	518	DGD	C3D-C2D	-3.48	1.43	1.52
23	B	617	CLA	C1D-C2D	-3.48	1.34	1.42
23	c	507	CLA	CHB-C4A	-3.48	1.29	1.33
23	c	503	CLA	C1D-C2D	-3.47	1.34	1.42
23	B	614	CLA	CAA-C2A	-3.47	1.47	1.54
23	C	512	CLA	CBD-CGD	-3.47	1.41	1.52
23	B	608	CLA	C1D-C2D	-3.47	1.34	1.42
23	C	512	CLA	CAA-C2A	-3.46	1.47	1.54
23	B	614	CLA	C1D-C2D	-3.46	1.34	1.42
23	b	616	CLA	C1A-CHA	-3.46	1.28	1.43
23	A	606	CLA	CBD-CGD	-3.46	1.41	1.52
32	c	519	DGD	C3D-C2D	-3.46	1.43	1.52
23	A	605	CLA	C1D-C2D	-3.46	1.34	1.42
23	C	510	CLA	CBD-CGD	-3.46	1.41	1.52
23	b	610	CLA	CBD-CGD	-3.46	1.41	1.52
23	D	402	CLA	C1D-C2D	-3.46	1.34	1.42
23	b	604	CLA	C1D-C2D	-3.45	1.34	1.42
23	D	403	CLA	CAA-C2A	-3.45	1.47	1.54
23	A	608	CLA	CBD-CGD	-3.45	1.41	1.52
23	c	502	CLA	C1D-C2D	-3.45	1.34	1.42
23	C	501	CLA	C1D-C2D	-3.45	1.34	1.42
23	c	504	CLA	C1D-C2D	-3.45	1.34	1.42
23	a	604	CLA	C1D-C2D	-3.45	1.34	1.42
23	a	604	CLA	CBD-CGD	-3.45	1.41	1.52
23	c	509	CLA	CAA-C2A	-3.45	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	608	CLA	C1D-C2D	-3.44	1.34	1.42
23	C	503	CLA	C1A-CHA	-3.44	1.28	1.43
23	B	610	CLA	C1D-C2D	-3.43	1.34	1.42
23	c	512	CLA	CBD-CGD	-3.43	1.41	1.52
23	B	616	CLA	CBD-CGD	-3.43	1.41	1.52
23	c	505	CLA	CBD-CGD	-3.43	1.41	1.52
23	C	504	CLA	C1D-C2D	-3.43	1.34	1.42
23	d	403	CLA	C1D-C2D	-3.42	1.34	1.42
23	B	607[B]	CLA	CAA-C2A	-3.42	1.47	1.54
23	C	507	CLA	C1A-CHA	-3.42	1.29	1.43
23	c	513	CLA	CBD-CGD	-3.41	1.41	1.52
23	C	508	CLA	CAA-C2A	-3.41	1.47	1.54
23	a	605	CLA	CBD-CGD	-3.41	1.41	1.52
23	D	404	CLA	C1D-C2D	-3.40	1.34	1.42
23	C	503	CLA	CBD-CGD	-3.40	1.41	1.52
23	B	609	CLA	C1D-C2D	-3.40	1.34	1.42
23	b	609[A]	CLA	CBD-CGD	-3.40	1.41	1.52
23	B	615	CLA	CBD-CGD	-3.40	1.41	1.52
23	B	615	CLA	C1D-C2D	-3.40	1.34	1.42
23	B	603	CLA	CHB-C4A	-3.39	1.29	1.33
23	B	617	CLA	CAA-C2A	-3.39	1.47	1.54
23	D	404	CLA	CBD-CGD	-3.39	1.41	1.52
23	c	512	CLA	C1D-C2D	-3.39	1.34	1.42
23	b	609[B]	CLA	CAA-C2A	-3.39	1.47	1.54
23	B	604	CLA	CBD-CGD	-3.39	1.41	1.52
23	B	612	CLA	CBD-CGD	-3.38	1.42	1.52
23	C	503	CLA	CAA-C2A	-3.38	1.47	1.54
23	b	618	CLA	CBD-CGD	-3.38	1.42	1.52
23	C	502	CLA	C1D-C2D	-3.38	1.34	1.42
23	C	510	CLA	C1D-C2D	-3.37	1.34	1.42
23	C	506	CLA	CHB-C4A	-3.37	1.29	1.33
23	B	607[A]	CLA	CBD-CGD	-3.36	1.42	1.52
23	c	502	CLA	CAA-C2A	-3.36	1.47	1.54
23	b	609[B]	CLA	CBD-CGD	-3.36	1.42	1.52
23	C	511	CLA	CBD-CGD	-3.35	1.42	1.52
23	B	602	CLA	C1D-C2D	-3.35	1.34	1.42
23	b	619	CLA	CAA-C2A	-3.35	1.47	1.54
25	K	101	BCR	C1-C6	-3.35	1.49	1.53
23	C	506	CLA	CAA-C2A	-3.35	1.47	1.54
23	a	613	CLA	C1D-C2D	-3.34	1.35	1.42
23	B	617	CLA	CBD-CGD	-3.34	1.42	1.52
23	c	503	CLA	CBD-CGD	-3.34	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	605	CLA	CBD-CGD	-3.34	1.42	1.52
23	C	502	CLA	CAA-C2A	-3.34	1.47	1.54
23	C	508	CLA	CBD-CGD	-3.33	1.42	1.52
23	b	606	CLA	CBD-CGD	-3.33	1.42	1.52
23	C	511	CLA	CAA-C2A	-3.33	1.47	1.54
23	B	611	CLA	CAA-C2A	-3.33	1.47	1.54
23	d	402	CLA	CAA-C2A	-3.33	1.47	1.54
23	b	608	CLA	CBD-CGD	-3.33	1.42	1.52
23	b	605	CLA	CBD-CGD	-3.32	1.42	1.52
23	B	613	CLA	CBD-CGD	-3.32	1.42	1.52
23	C	502	CLA	CBD-CGD	-3.32	1.42	1.52
23	d	402	CLA	CHB-C4A	-3.32	1.29	1.33
23	b	608	CLA	CAA-C2A	-3.31	1.47	1.54
23	B	603	CLA	CAA-C2A	-3.31	1.47	1.54
23	b	606	CLA	CAA-C2A	-3.30	1.47	1.54
23	b	616	CLA	CBD-CGD	-3.30	1.42	1.52
23	c	512	CLA	CAA-C2A	-3.30	1.47	1.54
23	B	606	CLA	CBD-CGD	-3.30	1.42	1.52
23	B	606	CLA	CAA-C2A	-3.29	1.47	1.54
23	d	403	CLA	CBD-CGD	-3.29	1.42	1.52
23	B	605	CLA	CBD-CGD	-3.29	1.42	1.52
25	b	620	BCR	C1-C6	-3.29	1.49	1.53
23	B	607[A]	CLA	CAA-C2A	-3.29	1.47	1.54
23	c	509	CLA	CHB-C4A	-3.29	1.29	1.33
23	b	614	CLA	CAA-C2A	-3.29	1.47	1.54
23	C	501	CLA	CAA-C2A	-3.28	1.47	1.54
23	c	505	CLA	CAA-C2A	-3.28	1.47	1.54
23	B	607[A]	CLA	CHB-C4A	-3.28	1.29	1.33
32	c	517	DGD	C3D-C2D	-3.27	1.43	1.52
23	B	607[B]	CLA	CBD-CGD	-3.27	1.42	1.52
23	b	604	CLA	CBD-CGD	-3.27	1.42	1.52
23	b	609[A]	CLA	CAA-C2A	-3.27	1.47	1.54
23	c	508	CLA	CBD-CGD	-3.27	1.42	1.52
23	B	615	CLA	CAA-C2A	-3.26	1.47	1.54
23	C	509	CLA	CBD-CGD	-3.26	1.42	1.52
23	c	502	CLA	CBD-CGD	-3.26	1.42	1.52
23	b	617	CLA	CBD-CGD	-3.26	1.42	1.52
23	B	609	CLA	CBD-CGD	-3.26	1.42	1.52
32	H	102	DGD	C3D-C2D	-3.25	1.44	1.52
23	c	504	CLA	CAA-C2A	-3.25	1.47	1.54
23	c	514	CLA	CAA-C2A	-3.24	1.47	1.54
23	b	611	CLA	C1D-C2D	-3.24	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	605	CLA	CAA-C2A	-3.24	1.47	1.54
23	b	607	CLA	CBD-CGD	-3.24	1.42	1.52
23	a	604	CLA	CHB-C4A	-3.23	1.29	1.33
23	D	402	CLA	CAA-C2A	-3.23	1.48	1.54
23	A	606	CLA	CAA-C2A	-3.22	1.48	1.54
23	D	402	CLA	CHB-C4A	-3.22	1.30	1.33
23	a	605	CLA	CHB-C4A	-3.22	1.30	1.33
23	a	613	CLA	CAA-C2A	-3.21	1.48	1.54
23	c	507	CLA	CBD-CGD	-3.21	1.42	1.52
23	B	612	CLA	CHB-C4A	-3.21	1.30	1.33
23	C	505	CLA	CBD-CGD	-3.20	1.42	1.52
23	B	609	CLA	CAA-C2A	-3.19	1.48	1.54
23	a	607	CLA	CBD-CGD	-3.19	1.42	1.52
23	B	604	CLA	CAA-C2A	-3.19	1.48	1.54
23	c	510	CLA	CAA-C2A	-3.19	1.48	1.54
32	D	406	DGD	C3D-C2D	-3.19	1.44	1.52
23	c	514	CLA	CBD-CGD	-3.18	1.42	1.52
23	b	617	CLA	CAA-C2A	-3.18	1.48	1.54
25	K	101	BCR	C31-C1	-3.17	1.47	1.53
23	b	611	CLA	CBD-CGD	-3.16	1.42	1.52
23	b	619	CLA	CBD-CGD	-3.16	1.42	1.52
25	B	618	BCR	C1-C6	-3.16	1.49	1.53
23	b	618	CLA	CAA-C2A	-3.16	1.48	1.54
23	b	611	CLA	CAA-C2A	-3.16	1.48	1.54
23	C	507	CLA	CBD-CGD	-3.15	1.42	1.52
23	A	605	CLA	CHB-C4A	-3.15	1.30	1.33
23	b	611	CLA	CHB-C4A	-3.15	1.30	1.33
23	B	607[B]	CLA	CHB-C4A	-3.15	1.30	1.33
23	c	510	CLA	CBD-CGD	-3.15	1.42	1.52
25	k	101	BCR	C1-C6	-3.15	1.49	1.53
32	h	102	DGD	C3D-C2D	-3.14	1.44	1.52
32	C	516	DGD	C3D-C2D	-3.14	1.44	1.52
23	C	513	CLA	CAA-C2A	-3.14	1.48	1.54
25	C	515	BCR	C1-C6	-3.14	1.49	1.53
23	B	603	CLA	CBD-CGD	-3.13	1.42	1.52
23	B	604	CLA	OBD-CAD	-3.13	1.17	1.22
23	b	610	CLA	CAA-C2A	-3.13	1.48	1.54
23	B	602	CLA	CAA-C2A	-3.13	1.48	1.54
23	b	612	CLA	CBD-CGD	-3.13	1.42	1.52
23	c	503	CLA	CAA-C2A	-3.12	1.48	1.54
23	B	605	CLA	CAA-C2A	-3.12	1.48	1.54
23	C	504	CLA	CAA-C2A	-3.12	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	J	101	LMG	O7-C8	-3.12	1.38	1.46
23	D	403	CLA	CHB-C4A	-3.11	1.30	1.33
23	C	506	CLA	CBD-CGD	-3.11	1.42	1.52
23	B	610	CLA	CBD-CGD	-3.11	1.42	1.52
32	d	405	DGD	C3D-C2D	-3.11	1.44	1.52
23	C	513	CLA	CBD-CGD	-3.11	1.42	1.52
23	B	612	CLA	CAA-C2A	-3.10	1.48	1.54
23	b	615	CLA	CBD-CGD	-3.09	1.42	1.52
23	C	508	CLA	CHB-C4A	-3.09	1.30	1.33
23	C	509	CLA	CAA-C2A	-3.09	1.48	1.54
28	b	623	LMG	O7-C8	-3.08	1.38	1.46
23	c	514	CLA	CHB-C4A	-3.08	1.30	1.33
23	b	614	CLA	CHB-C4A	-3.08	1.30	1.33
23	c	509	CLA	CBD-CGD	-3.08	1.42	1.52
23	b	607	CLA	CAA-C2A	-3.07	1.48	1.54
23	C	501	CLA	CHB-C4A	-3.06	1.30	1.33
23	a	613	CLA	CHB-C4A	-3.06	1.30	1.33
23	c	506	CLA	CBD-CGD	-3.05	1.43	1.52
23	b	604	CLA	CAA-C2A	-3.05	1.48	1.54
23	b	609[A]	CLA	CHB-C4A	-3.04	1.30	1.33
23	c	513	CLA	CAA-C2A	-3.04	1.48	1.54
25	f	101	BCR	C1-C6	-3.04	1.49	1.53
32	c	518	DGD	C3D-C2D	-3.03	1.44	1.52
23	B	609	CLA	CHB-C4A	-3.03	1.30	1.33
23	B	611	CLA	CHB-C4A	-3.02	1.30	1.33
25	B	620	BCR	C1-C6	-3.01	1.49	1.53
23	B	614	CLA	OBD-CAD	-3.01	1.18	1.22
25	k	101	BCR	C31-C1	-3.01	1.47	1.53
23	b	613	CLA	CHB-C4A	-3.01	1.30	1.33
23	C	507	CLA	CAA-C2A	-3.01	1.48	1.54
23	c	508	CLA	CAA-C2A	-3.00	1.48	1.54
23	b	609[B]	CLA	CHB-C4A	-2.98	1.30	1.33
23	b	608	CLA	CHB-C4A	-2.98	1.30	1.33
23	c	505	CLA	CHB-C4A	-2.98	1.30	1.33
23	B	616	CLA	CAA-C2A	-2.98	1.48	1.54
23	a	607	CLA	CAA-C2A	-2.97	1.48	1.54
23	D	403	CLA	OBD-CAD	-2.97	1.18	1.22
23	b	606	CLA	OBD-CAD	-2.96	1.18	1.22
23	B	613	CLA	CHB-C4A	-2.96	1.30	1.33
28	j	101	LMG	O7-C8	-2.95	1.39	1.46
28	B	621	LMG	O7-C8	-2.93	1.39	1.46
25	h	101	BCR	C35-C13	-2.93	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	k	101	BCR	C35-C13	-2.93	1.44	1.50
23	b	615	CLA	CHB-C4A	-2.92	1.30	1.33
23	C	510	CLA	OBD-CAD	-2.92	1.18	1.22
23	c	502	CLA	CHB-C4A	-2.91	1.30	1.33
23	C	504	CLA	CHB-C4A	-2.91	1.30	1.33
23	b	612	CLA	CHB-C4A	-2.91	1.30	1.33
23	c	503	CLA	CHB-C4A	-2.91	1.30	1.33
23	C	512	CLA	CHB-C4A	-2.90	1.30	1.33
28	C	519	LMG	O7-C8	-2.89	1.39	1.46
32	C	517	DGD	C3D-C2D	-2.89	1.44	1.52
23	C	510	CLA	CHB-C4A	-2.89	1.30	1.33
23	C	505	CLA	CHB-C4A	-2.89	1.30	1.33
25	B	618	BCR	C35-C13	-2.88	1.44	1.50
28	c	520	LMG	O7-C8	-2.88	1.39	1.46
23	b	619	CLA	OBD-CAD	-2.88	1.18	1.22
25	B	619	BCR	C31-C1	-2.87	1.47	1.53
23	d	403	CLA	CHB-C4A	-2.86	1.30	1.33
28	Z	101	LMG	O7-C8	-2.86	1.39	1.46
28	z	101	LMG	O7-C8	-2.86	1.39	1.46
25	b	621	BCR	C31-C1	-2.84	1.47	1.53
23	d	402	CLA	OBD-CAD	-2.84	1.18	1.22
23	b	613	CLA	OBD-CAD	-2.84	1.18	1.22
28	A	612	LMG	O7-C8	-2.84	1.39	1.46
32	C	517	DGD	C6E-C5E	-2.82	1.42	1.51
23	A	605	CLA	O2D-CED	-2.82	1.38	1.45
23	c	507	CLA	OBD-CAD	-2.82	1.18	1.22
23	a	604	CLA	O2D-CED	-2.82	1.38	1.45
23	B	610	CLA	CHB-C4A	-2.82	1.30	1.33
23	B	602	CLA	CHB-C4A	-2.81	1.30	1.33
23	B	604	CLA	CHB-C4A	-2.81	1.30	1.33
23	c	511	CLA	CHB-C4A	-2.81	1.30	1.33
23	C	503	CLA	CHB-C4A	-2.81	1.30	1.33
23	B	614	CLA	CHB-C4A	-2.81	1.30	1.33
25	b	622	BCR	C35-C13	-2.81	1.44	1.50
23	b	606	CLA	CHB-C4A	-2.81	1.30	1.33
23	A	608	CLA	CAA-C2A	-2.81	1.48	1.54
25	C	515	BCR	C35-C13	-2.81	1.44	1.50
25	f	101	BCR	C35-C13	-2.81	1.44	1.50
28	c	521	LMG	O7-C8	-2.80	1.39	1.46
25	B	619	BCR	C35-C13	-2.80	1.44	1.50
23	C	502	CLA	CHB-C4A	-2.80	1.30	1.33
32	C	518	DGD	C6E-C5E	-2.80	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	619	BCR	C1-C6	-2.80	1.50	1.53
23	B	615	CLA	CHB-C4A	-2.80	1.30	1.33
28	a	611	LMG	O7-C8	-2.79	1.39	1.46
23	B	617	CLA	OBD-CAD	-2.79	1.18	1.22
32	c	519	DGD	C6E-C5E	-2.79	1.42	1.51
32	c	517	DGD	C6E-C5E	-2.79	1.42	1.51
25	t	101	BCR	C31-C1	-2.79	1.48	1.53
32	H	102	DGD	C6E-C5E	-2.79	1.42	1.51
23	C	509	CLA	CHB-C4A	-2.79	1.30	1.33
23	C	506	CLA	C1C-NC	-2.78	1.31	1.37
23	B	606	CLA	OBD-CAD	-2.78	1.18	1.22
32	c	518	DGD	C6E-C5E	-2.78	1.42	1.51
23	a	605	CLA	C1C-NC	-2.78	1.31	1.37
25	a	608	BCR	C35-C13	-2.78	1.44	1.50
23	a	613	CLA	C1C-NC	-2.78	1.31	1.37
23	B	611	CLA	O2D-CED	-2.78	1.38	1.45
25	F	101	BCR	C1-C6	-2.78	1.50	1.53
23	b	605	CLA	C1C-NC	-2.78	1.31	1.37
23	b	606	CLA	C1C-NC	-2.78	1.31	1.37
23	b	607	CLA	CHB-C4A	-2.77	1.30	1.33
23	a	613	CLA	OBD-CAD	-2.77	1.18	1.22
23	A	605	CLA	OBD-CAD	-2.77	1.18	1.22
32	h	102	DGD	C6E-C5E	-2.77	1.42	1.51
32	C	516	DGD	C6E-C5E	-2.77	1.42	1.51
23	c	504	CLA	O2D-CED	-2.76	1.38	1.45
23	A	606	CLA	C1C-NC	-2.76	1.31	1.37
25	c	516	BCR	C1-C6	-2.76	1.50	1.53
23	b	617	CLA	CHB-C4A	-2.76	1.30	1.33
23	B	608	CLA	C1C-NC	-2.75	1.31	1.37
23	d	403	CLA	CAA-C2A	-2.75	1.48	1.54
28	C	520	LMG	O7-C8	-2.75	1.39	1.46
23	c	513	CLA	CHB-C4A	-2.75	1.30	1.33
32	d	405	DGD	C6E-C5E	-2.74	1.42	1.51
23	B	604	CLA	C1C-NC	-2.74	1.31	1.37
23	A	606	CLA	CHB-C4A	-2.74	1.30	1.33
23	B	611	CLA	OBD-CAD	-2.74	1.18	1.22
23	D	402	CLA	OBD-CAD	-2.74	1.18	1.22
23	b	604	CLA	CHB-C4A	-2.73	1.30	1.33
23	b	608	CLA	C1C-NC	-2.73	1.31	1.37
23	C	504	CLA	OBD-CAD	-2.73	1.18	1.22
23	b	616	CLA	OBD-CAD	-2.73	1.18	1.22
25	T	101	BCR	C35-C13	-2.73	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	C1C-NC	-2.73	1.31	1.37
23	b	613	CLA	O2D-CED	-2.73	1.38	1.45
25	b	621	BCR	C35-C13	-2.72	1.44	1.50
23	a	605	CLA	OBD-CAD	-2.72	1.18	1.22
23	b	610	CLA	OBD-CAD	-2.72	1.18	1.22
23	B	617	CLA	C1C-NC	-2.72	1.31	1.37
23	b	614	CLA	OBD-CAD	-2.72	1.18	1.22
23	c	512	CLA	O2D-CED	-2.72	1.38	1.45
23	c	512	CLA	C1C-NC	-2.71	1.31	1.37
23	D	402	CLA	C1C-NC	-2.71	1.32	1.37
23	D	404	CLA	CAA-C2A	-2.71	1.48	1.54
23	c	504	CLA	CHB-C4A	-2.71	1.30	1.33
23	B	608	CLA	CHB-C4A	-2.71	1.30	1.33
25	B	620	BCR	C35-C13	-2.70	1.45	1.50
32	D	406	DGD	C6E-C5E	-2.70	1.42	1.51
23	b	618	CLA	CHB-C4A	-2.70	1.30	1.33
23	d	402	CLA	C1C-NC	-2.69	1.32	1.37
23	b	615	CLA	C1C-NC	-2.69	1.32	1.37
25	h	101	BCR	C1-C6	-2.69	1.50	1.53
23	c	504	CLA	OBD-CAD	-2.69	1.18	1.22
23	b	618	CLA	OBD-CAD	-2.69	1.18	1.22
23	c	511	CLA	OBD-CAD	-2.69	1.18	1.22
23	C	501	CLA	C1C-NC	-2.69	1.32	1.37
23	B	610	CLA	C1C-NC	-2.69	1.32	1.37
23	c	508	CLA	OBD-CAD	-2.68	1.18	1.22
23	C	513	CLA	CHB-C4A	-2.68	1.30	1.33
23	A	608	CLA	CHB-C4A	-2.68	1.30	1.33
23	c	511	CLA	O2D-CED	-2.68	1.38	1.45
23	A	608	CLA	C1C-NC	-2.68	1.32	1.37
23	C	507	CLA	CHB-C4A	-2.68	1.30	1.33
25	c	516	BCR	C35-C13	-2.68	1.45	1.50
23	C	502	CLA	C1C-NC	-2.67	1.32	1.37
23	C	501	CLA	OBD-CAD	-2.67	1.18	1.22
23	A	606	CLA	OBD-CAD	-2.67	1.18	1.22
25	C	514	BCR	C35-C13	-2.67	1.45	1.50
23	B	614	CLA	C1C-NC	-2.67	1.32	1.37
23	D	403	CLA	C1C-NC	-2.67	1.32	1.37
23	C	504	CLA	C1C-NC	-2.66	1.32	1.37
23	C	510	CLA	C1C-NC	-2.66	1.32	1.37
23	b	605	CLA	OBD-CAD	-2.66	1.18	1.22
23	B	608	CLA	O2D-CED	-2.66	1.39	1.45
23	B	615	CLA	OBD-CAD	-2.66	1.18	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C1C-NC	-2.66	1.32	1.37
23	D	403	CLA	O2D-CED	-2.65	1.39	1.45
25	c	515	BCR	C31-C1	-2.65	1.48	1.53
25	A	609	BCR	C35-C13	-2.65	1.45	1.50
25	A	609	BCR	C1-C6	-2.65	1.50	1.53
23	C	503	CLA	O2D-CED	-2.65	1.39	1.45
23	d	402	CLA	O2D-CED	-2.65	1.39	1.45
23	C	503	CLA	OBD-CAD	-2.65	1.18	1.22
23	b	611	CLA	C1C-NC	-2.65	1.32	1.37
23	c	513	CLA	C1C-NC	-2.64	1.32	1.37
25	c	522	BCR	C35-C13	-2.64	1.45	1.50
23	b	607	CLA	OBD-CAD	-2.64	1.18	1.22
23	B	606	CLA	CHB-C4A	-2.64	1.30	1.33
23	b	617	CLA	OBD-CAD	-2.64	1.18	1.22
23	C	505	CLA	OBD-CAD	-2.64	1.18	1.22
27	A	611	SQD	C6-S	-2.63	1.67	1.77
25	B	620	BCR	C31-C1	-2.63	1.48	1.53
23	C	508	CLA	OBD-CAD	-2.63	1.18	1.22
32	C	516	DGD	C3E-C2E	-2.63	1.45	1.52
27	a	610	SQD	C6-S	-2.62	1.67	1.77
23	c	506	CLA	C1C-NC	-2.62	1.32	1.37
23	B	606	CLA	C1C-NC	-2.62	1.32	1.37
23	a	613	CLA	O2D-CED	-2.62	1.39	1.45
23	c	502	CLA	OBD-CAD	-2.62	1.18	1.22
23	c	512	CLA	OBD-CAD	-2.62	1.18	1.22
25	c	515	BCR	C35-C13	-2.62	1.45	1.50
23	B	607[B]	CLA	C1C-NC	-2.62	1.32	1.37
23	c	508	CLA	CHB-C4A	-2.61	1.30	1.33
23	b	612	CLA	C1C-NC	-2.61	1.32	1.37
32	c	517	DGD	C3E-C2E	-2.61	1.45	1.52
23	c	514	CLA	OBD-CAD	-2.61	1.18	1.22
23	B	615	CLA	C1C-NC	-2.61	1.32	1.37
23	C	511	CLA	OBD-CAD	-2.61	1.18	1.22
23	d	403	CLA	C1C-NC	-2.61	1.32	1.37
23	B	607[A]	CLA	C1C-NC	-2.60	1.32	1.37
23	b	610	CLA	C1C-NC	-2.60	1.32	1.37
23	b	614	CLA	C1C-NC	-2.60	1.32	1.37
23	B	613	CLA	C1C-NC	-2.60	1.32	1.37
23	b	613	CLA	C1C-NC	-2.60	1.32	1.37
23	B	603	CLA	OBD-CAD	-2.60	1.18	1.22
23	C	504	CLA	O2D-CED	-2.60	1.39	1.45
25	b	620	BCR	C35-C13	-2.60	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHB-C4A	-2.60	1.30	1.33
23	B	611	CLA	C1C-NC	-2.59	1.32	1.37
23	C	509	CLA	C1C-NC	-2.59	1.32	1.37
23	c	506	CLA	OBD-CAD	-2.59	1.18	1.22
25	b	620	BCR	C31-C1	-2.59	1.48	1.53
23	C	511	CLA	C1C-NC	-2.59	1.32	1.37
23	b	611	CLA	OBD-CAD	-2.59	1.18	1.22
23	B	616	CLA	OBD-CAD	-2.59	1.18	1.22
23	B	614	CLA	O2D-CED	-2.59	1.39	1.45
23	b	617	CLA	C1C-NC	-2.59	1.32	1.37
23	C	513	CLA	OBD-CAD	-2.59	1.18	1.22
25	t	101	BCR	C35-C13	-2.59	1.45	1.50
25	b	622	BCR	C31-C1	-2.59	1.48	1.53
23	c	513	CLA	OBD-CAD	-2.58	1.18	1.22
25	b	622	BCR	C1-C6	-2.58	1.50	1.53
23	C	505	CLA	C1C-NC	-2.58	1.32	1.37
23	C	503	CLA	C1C-NC	-2.57	1.32	1.37
23	c	509	CLA	C1C-NC	-2.57	1.32	1.37
23	b	604	CLA	C1C-NC	-2.57	1.32	1.37
23	c	514	CLA	C1C-NC	-2.57	1.32	1.37
23	b	619	CLA	C1C-NC	-2.57	1.32	1.37
23	c	509	CLA	OBD-CAD	-2.57	1.18	1.22
23	C	512	CLA	C1C-NC	-2.56	1.32	1.37
23	B	609	CLA	C1C-NC	-2.56	1.32	1.37
25	F	101	BCR	C35-C13	-2.56	1.45	1.50
23	c	505	CLA	O2D-CED	-2.56	1.39	1.45
23	B	612	CLA	OBD-CAD	-2.56	1.18	1.22
23	c	505	CLA	OBD-CAD	-2.56	1.18	1.22
23	c	508	CLA	C1C-NC	-2.56	1.32	1.37
23	B	616	CLA	C1C-NC	-2.56	1.32	1.37
23	C	510	CLA	O2D-CED	-2.56	1.39	1.45
27	b	601	SQD	C6-S	-2.56	1.67	1.77
23	C	507	CLA	C1C-NC	-2.56	1.32	1.37
23	c	507	CLA	C1C-NC	-2.55	1.32	1.37
23	B	603	CLA	C1C-NC	-2.55	1.32	1.37
23	D	404	CLA	O2D-CED	-2.55	1.39	1.45
23	B	610	CLA	OBD-CAD	-2.55	1.18	1.22
23	B	602	CLA	C1C-NC	-2.55	1.32	1.37
23	a	604	CLA	C1C-NC	-2.55	1.32	1.37
23	B	605	CLA	OBD-CAD	-2.55	1.18	1.22
23	A	608	CLA	OBD-CAD	-2.55	1.18	1.22
25	C	521	BCR	C1-C6	-2.55	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	O2D-CED	-2.54	1.39	1.45
23	B	617	CLA	CHB-C4A	-2.54	1.30	1.33
23	D	402	CLA	O2D-CED	-2.54	1.39	1.45
25	C	514	BCR	C31-C1	-2.54	1.48	1.53
23	b	608	CLA	OBD-CAD	-2.54	1.18	1.22
23	B	610	CLA	O2D-CED	-2.54	1.39	1.45
23	B	605	CLA	C1C-NC	-2.54	1.32	1.37
23	a	604	CLA	C2A-C1A	-2.54	1.46	1.52
27	a	612	SQD	C6-S	-2.54	1.67	1.77
23	B	613	CLA	OBD-CAD	-2.53	1.18	1.22
23	b	615	CLA	OBD-CAD	-2.53	1.18	1.22
23	a	607	CLA	OBD-CAD	-2.53	1.18	1.22
23	b	610	CLA	O2D-CED	-2.53	1.39	1.45
23	b	604	CLA	O2D-CED	-2.52	1.39	1.45
23	b	607	CLA	C1C-NC	-2.52	1.32	1.37
23	B	612	CLA	C1C-NC	-2.52	1.32	1.37
23	C	502	CLA	O2D-CED	-2.52	1.39	1.45
23	A	605	CLA	C1C-NC	-2.52	1.32	1.37
23	C	502	CLA	OBD-CAD	-2.52	1.18	1.22
23	A	606	CLA	O2D-CED	-2.52	1.39	1.45
23	b	609[A]	CLA	OBD-CAD	-2.51	1.18	1.22
25	C	521	BCR	C31-C1	-2.51	1.48	1.53
23	b	617	CLA	O2D-CED	-2.51	1.39	1.45
23	b	616	CLA	O2D-CED	-2.51	1.39	1.45
23	c	503	CLA	OBD-CAD	-2.51	1.18	1.22
23	b	618	CLA	O2D-CED	-2.51	1.39	1.45
23	d	403	CLA	O2D-CED	-2.51	1.39	1.45
23	c	502	CLA	C1C-NC	-2.51	1.32	1.37
23	b	615	CLA	O2D-CED	-2.51	1.39	1.45
23	b	609[B]	CLA	C1C-NC	-2.51	1.32	1.37
23	C	501	CLA	O2D-CED	-2.50	1.39	1.45
23	B	606	CLA	O2D-CED	-2.50	1.39	1.45
23	C	506	CLA	OBD-CAD	-2.50	1.18	1.22
23	C	512	CLA	OBD-CAD	-2.50	1.18	1.22
23	C	513	CLA	C1C-NC	-2.50	1.32	1.37
25	b	621	BCR	C1-C6	-2.50	1.50	1.53
23	C	508	CLA	C1C-NC	-2.50	1.32	1.37
27	X	101	SQD	C6-S	-2.49	1.67	1.77
23	c	513	CLA	O2D-CED	-2.49	1.39	1.45
23	B	607[A]	CLA	OBD-CAD	-2.49	1.18	1.22
23	B	604	CLA	O2D-CED	-2.49	1.39	1.45
23	B	613	CLA	O2D-CED	-2.49	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	OBD-CAD	-2.49	1.18	1.22
23	A	605	CLA	C2A-C1A	-2.49	1.46	1.52
23	c	505	CLA	C1C-NC	-2.48	1.32	1.37
23	B	607[A]	CLA	O2D-CED	-2.48	1.39	1.45
27	x	101	SQD	C6-S	-2.48	1.67	1.77
23	B	608	CLA	C2A-C1A	-2.48	1.46	1.52
23	C	512	CLA	O2D-CED	-2.48	1.39	1.45
23	B	607[B]	CLA	O2D-CED	-2.48	1.39	1.45
23	C	511	CLA	O2D-CED	-2.48	1.39	1.45
23	D	404	CLA	CHB-C4A	-2.47	1.30	1.33
23	c	503	CLA	O2D-CED	-2.47	1.39	1.45
23	D	404	CLA	C1C-NC	-2.47	1.32	1.37
23	B	609	CLA	OBD-CAD	-2.47	1.18	1.22
23	b	612	CLA	O2D-CED	-2.47	1.39	1.45
23	c	504	CLA	C1C-NC	-2.47	1.32	1.37
23	b	609[B]	CLA	O2D-CED	-2.47	1.39	1.45
23	c	502	CLA	O2D-CED	-2.47	1.39	1.45
23	a	607	CLA	CHB-C4A	-2.47	1.30	1.33
23	B	608	CLA	OBD-CAD	-2.47	1.18	1.22
25	H	101	BCR	C35-C13	-2.47	1.45	1.50
23	B	615	CLA	O2D-CED	-2.46	1.39	1.45
23	a	607	CLA	C1C-NC	-2.46	1.32	1.37
23	b	606	CLA	O2D-CED	-2.46	1.39	1.45
23	C	507	CLA	OBD-CAD	-2.46	1.18	1.22
23	a	604	CLA	OBD-CAD	-2.46	1.18	1.22
23	C	509	CLA	OBD-CAD	-2.46	1.18	1.22
23	C	505	CLA	O2D-CED	-2.46	1.39	1.45
23	c	510	CLA	C1C-NC	-2.46	1.32	1.37
25	C	521	BCR	C35-C13	-2.46	1.45	1.50
32	h	102	DGD	C3E-C2E	-2.46	1.46	1.52
32	C	518	DGD	C3E-C2E	-2.46	1.46	1.52
23	b	619	CLA	CHB-C4A	-2.45	1.30	1.33
23	B	602	CLA	O2D-CED	-2.45	1.39	1.45
25	B	618	BCR	C31-C1	-2.45	1.48	1.53
23	B	617	CLA	O2D-CED	-2.45	1.39	1.45
23	c	506	CLA	CHB-C4A	-2.45	1.30	1.33
23	c	507	CLA	O2D-CED	-2.44	1.39	1.45
23	b	616	CLA	C1C-NC	-2.44	1.32	1.37
23	b	604	CLA	OBD-CAD	-2.44	1.18	1.22
23	b	609[A]	CLA	O2D-CED	-2.44	1.39	1.45
23	c	511	CLA	C1C-NC	-2.44	1.32	1.37
25	c	516	BCR	C31-C1	-2.44	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	CHB-C4A	-2.44	1.30	1.33
23	a	607	CLA	O2D-CED	-2.43	1.39	1.45
25	c	522	BCR	C31-C1	-2.43	1.48	1.53
23	c	509	CLA	O2D-CED	-2.43	1.39	1.45
23	b	611	CLA	O2D-CED	-2.43	1.39	1.45
23	B	602	CLA	OBD-CAD	-2.42	1.18	1.22
23	b	609[A]	CLA	C1C-NC	-2.42	1.32	1.37
27	b	602	SQD	C6-S	-2.42	1.68	1.77
23	b	614	CLA	O2D-CED	-2.42	1.39	1.45
23	B	609	CLA	O2D-CED	-2.42	1.39	1.45
23	b	608	CLA	O2D-CED	-2.41	1.39	1.45
23	b	610	CLA	CHB-C4A	-2.41	1.30	1.33
25	f	101	BCR	C31-C1	-2.41	1.48	1.53
25	H	101	BCR	C1-C6	-2.41	1.50	1.53
23	c	510	CLA	OBD-CAD	-2.41	1.18	1.22
23	b	608	CLA	C2A-C1A	-2.41	1.46	1.52
25	h	101	BCR	C31-C1	-2.41	1.48	1.53
23	b	617	CLA	C2A-C1A	-2.40	1.46	1.52
23	C	505	CLA	C2A-C1A	-2.40	1.46	1.52
23	a	605	CLA	O2D-CED	-2.40	1.39	1.45
23	c	506	CLA	O2D-CED	-2.40	1.39	1.45
32	H	102	DGD	C3E-C2E	-2.40	1.46	1.52
23	C	506	CLA	O2D-CED	-2.40	1.39	1.45
23	A	608	CLA	O2D-CED	-2.40	1.39	1.45
23	D	403	CLA	C2A-C1A	-2.39	1.46	1.52
25	A	609	BCR	C31-C1	-2.39	1.48	1.53
23	b	609[B]	CLA	OBD-CAD	-2.39	1.18	1.22
23	B	603	CLA	O2D-CED	-2.38	1.39	1.45
27	B	623	SQD	C6-S	-2.38	1.68	1.77
23	c	510	CLA	CHB-C4A	-2.38	1.30	1.33
23	c	506	CLA	C2A-C1A	-2.38	1.46	1.52
23	C	508	CLA	O2D-CED	-2.38	1.39	1.45
23	B	616	CLA	CHB-C4A	-2.38	1.30	1.33
23	B	612	CLA	O2D-CED	-2.38	1.39	1.45
23	b	619	CLA	O2D-CED	-2.37	1.39	1.45
25	C	515	BCR	C31-C1	-2.37	1.48	1.53
23	c	510	CLA	O2D-CED	-2.36	1.39	1.45
23	b	607	CLA	O2D-CED	-2.36	1.39	1.45
23	b	605	CLA	C2A-C1A	-2.36	1.46	1.52
25	K	101	BCR	C35-C13	-2.36	1.45	1.50
32	c	519	DGD	C3E-C2E	-2.36	1.46	1.52
32	c	518	DGD	C3E-C2E	-2.36	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C2A-C1A	-2.36	1.46	1.52
23	B	605	CLA	O2D-CED	-2.35	1.39	1.45
23	c	514	CLA	O2D-CED	-2.35	1.39	1.45
23	B	607[B]	CLA	OBD-CAD	-2.34	1.18	1.22
25	a	608	BCR	C1-C6	-2.34	1.50	1.53
23	B	606	CLA	C2A-C1A	-2.34	1.46	1.52
25	a	608	BCR	C31-C1	-2.34	1.48	1.53
23	d	402	CLA	C2A-C1A	-2.34	1.46	1.52
23	C	513	CLA	O2D-CED	-2.34	1.39	1.45
23	c	512	CLA	CHB-C4A	-2.34	1.31	1.33
23	C	507	CLA	O2D-CED	-2.34	1.39	1.45
23	B	609	CLA	C2A-C1A	-2.33	1.46	1.52
23	c	508	CLA	O2D-CED	-2.33	1.39	1.45
23	C	504	CLA	C2A-C1A	-2.33	1.46	1.52
23	b	611	CLA	C2A-C1A	-2.32	1.46	1.52
32	C	517	DGD	C3E-C2E	-2.32	1.46	1.52
23	C	509	CLA	O2D-CED	-2.32	1.39	1.45
23	C	511	CLA	CHB-C4A	-2.32	1.31	1.33
23	c	514	CLA	C2A-C1A	-2.31	1.46	1.52
24	d	401	PHO	C1C-NC	-2.30	1.33	1.38
23	C	510	CLA	C2A-C1A	-2.29	1.46	1.52
23	B	615	CLA	C2A-C1A	-2.29	1.46	1.52
25	H	101	BCR	C31-C1	-2.29	1.49	1.53
32	C	518	DGD	C1D-C2D	-2.29	1.45	1.52
23	b	605	CLA	O2D-CED	-2.28	1.39	1.45
23	C	513	CLA	C2A-C1A	-2.27	1.47	1.52
23	B	617	CLA	C2A-C1A	-2.27	1.47	1.52
23	B	604	CLA	C2A-C1A	-2.26	1.47	1.52
23	B	610	CLA	C2A-C1A	-2.26	1.47	1.52
23	B	603	CLA	C2A-C1A	-2.26	1.47	1.52
23	B	613	CLA	C2A-C1A	-2.26	1.47	1.52
32	c	519	DGD	C1D-C2D	-2.26	1.45	1.52
23	d	403	CLA	OBD-CAD	-2.25	1.19	1.22
32	C	516	DGD	C1D-C2D	-2.25	1.45	1.52
23	b	615	CLA	C2A-C1A	-2.25	1.47	1.52
23	b	612	CLA	C2A-C1A	-2.25	1.47	1.52
25	F	101	BCR	C31-C1	-2.25	1.49	1.53
23	b	610	CLA	C2A-C1A	-2.25	1.47	1.52
23	D	404	CLA	OBD-CAD	-2.24	1.19	1.22
23	c	511	CLA	C2A-C1A	-2.24	1.47	1.52
32	c	517	DGD	C6D-C5D	-2.24	1.44	1.51
32	c	519	DGD	C6D-C5D	-2.23	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C2A-C1A	-2.23	1.47	1.52
23	c	507	CLA	C2A-C1A	-2.23	1.47	1.52
23	D	402	CLA	C2A-C1A	-2.22	1.47	1.52
32	C	518	DGD	C6D-C5D	-2.21	1.44	1.51
32	c	518	DGD	C6D-C5D	-2.21	1.44	1.51
23	B	614	CLA	C2A-C1A	-2.20	1.47	1.52
32	c	518	DGD	C1E-C2E	-2.20	1.46	1.52
23	b	609[B]	CLA	C2A-C1A	-2.19	1.47	1.52
24	D	401	PHO	C1C-NC	-2.19	1.33	1.38
23	c	509	CLA	C2A-C1A	-2.18	1.47	1.52
23	C	511	CLA	C2A-C1A	-2.18	1.47	1.52
23	A	608	CLA	C2A-C1A	-2.17	1.47	1.52
32	h	102	DGD	C1D-C2D	-2.17	1.46	1.52
32	C	516	DGD	C6D-C5D	-2.16	1.44	1.51
23	B	602	CLA	C2A-C1A	-2.16	1.47	1.52
23	b	619	CLA	C2A-C1A	-2.16	1.47	1.52
25	T	101	BCR	C31-C1	-2.16	1.49	1.53
23	A	606	CLA	C2A-C1A	-2.16	1.47	1.52
32	C	516	DGD	C1E-C2E	-2.16	1.46	1.52
24	A	607	PHO	C1C-NC	-2.15	1.33	1.38
23	c	502	CLA	C2A-C1A	-2.15	1.47	1.52
23	C	502	CLA	C2A-C1A	-2.14	1.47	1.52
23	a	613	CLA	C2A-C1A	-2.14	1.47	1.52
32	H	102	DGD	C6D-C5D	-2.14	1.44	1.51
32	c	517	DGD	C1E-C2E	-2.14	1.46	1.52
23	b	618	CLA	C2A-C1A	-2.14	1.47	1.52
23	b	613	CLA	C2A-C1A	-2.13	1.47	1.52
32	d	405	DGD	C6D-C5D	-2.13	1.44	1.51
32	d	405	DGD	C3E-C2E	-2.13	1.46	1.52
24	a	606	PHO	C1C-NC	-2.13	1.33	1.38
23	b	606	CLA	C2A-C1A	-2.13	1.47	1.52
23	a	605	CLA	C2A-C1A	-2.13	1.47	1.52
32	H	102	DGD	C1D-C2D	-2.13	1.46	1.52
23	B	612	CLA	C2A-C1A	-2.12	1.47	1.52
23	c	503	CLA	C2A-C1A	-2.12	1.47	1.52
32	C	518	DGD	C1E-C2E	-2.12	1.46	1.52
25	c	522	BCR	C1-C6	-2.12	1.50	1.53
23	c	504	CLA	C2A-C1A	-2.12	1.47	1.52
32	C	517	DGD	C1E-C2E	-2.11	1.46	1.52
23	b	609[A]	CLA	C2A-C1A	-2.10	1.47	1.52
23	B	607[B]	CLA	C2A-C1A	-2.10	1.47	1.52
32	c	517	DGD	C1D-C2D	-2.09	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	406	DGD	C6D-C5D	-2.09	1.44	1.51
25	C	514	BCR	C1-C6	-2.08	1.50	1.53
32	c	519	DGD	C1E-C2E	-2.08	1.46	1.52
23	C	512	CLA	C2A-C1A	-2.07	1.47	1.52
23	c	512	CLA	C2A-C1A	-2.07	1.47	1.52
23	b	614	CLA	C2A-C1A	-2.07	1.47	1.52
23	B	616	CLA	C2A-C1A	-2.06	1.47	1.52
23	c	510	CLA	C2A-C1A	-2.06	1.47	1.52
32	C	517	DGD	C6D-C5D	-2.06	1.45	1.51
23	C	501	CLA	C2A-C1A	-2.06	1.47	1.52
23	B	607[A]	CLA	C2A-C1A	-2.05	1.47	1.52
32	h	102	DGD	C6D-C5D	-2.05	1.45	1.51
32	C	517	DGD	C1D-C2D	-2.04	1.46	1.52
23	C	506	CLA	C2A-C1A	-2.03	1.47	1.52
23	b	604	CLA	C2A-C1A	-2.02	1.47	1.52
23	a	607	CLA	C2A-C1A	-2.02	1.47	1.52
23	b	607	CLA	C2A-C1A	-2.01	1.47	1.52
23	b	616	CLA	C2A-C1A	-2.00	1.47	1.52
25	b	620	BCR	C7-C6	2.00	1.52	1.45
26	a	609	PL9	C17-C18	2.02	1.57	1.50
31	l	101	LHG	C8-C7	2.02	1.56	1.50
32	C	518	DGD	O5D-C1E	2.02	1.43	1.40
28	Z	101	LMG	C7-C8	2.02	1.56	1.50
26	A	610	PL9	C22-C23	2.02	1.57	1.50
23	C	507	CLA	CMC-C2C	2.02	1.55	1.50
25	T	101	BCR	C7-C6	2.02	1.52	1.45
31	a	614	LHG	C8-C7	2.03	1.56	1.50
23	A	608	CLA	CBA-CGA	2.03	1.56	1.50
26	D	405	PL9	C37-C38	2.04	1.57	1.50
25	C	514	BCR	C33-C5	2.04	1.54	1.51
25	c	522	BCR	C7-C6	2.04	1.52	1.45
32	c	518	DGD	O3G-C1D	2.05	1.43	1.40
26	a	609	PL9	C41-C39	2.05	1.55	1.51
28	z	101	LMG	C7-C8	2.05	1.56	1.50
25	F	101	BCR	C7-C6	2.05	1.52	1.45
25	K	101	BCR	C7-C6	2.05	1.52	1.45
32	C	517	DGD	C3G-C2G	2.06	1.56	1.50
26	d	404	PL9	C37-C38	2.06	1.57	1.50
31	L	101	LHG	C8-C7	2.06	1.56	1.50
28	A	612	LMG	C7-C8	2.06	1.56	1.50
26	d	404	PL9	C22-C23	2.06	1.57	1.50
24	a	606	PHO	CHD-C1D	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	101	BCR	C7-C6	2.07	1.53	1.45
26	A	610	PL9	C37-C38	2.07	1.57	1.50
25	c	515	BCR	C7-C6	2.08	1.53	1.45
24	a	606	PHO	C1B-C2B	2.08	1.50	1.45
27	B	623	SQD	O6-C1	2.08	1.43	1.40
32	C	517	DGD	O3G-C1D	2.08	1.43	1.40
31	b	624	LHG	C8-C7	2.08	1.56	1.50
31	d	406	LHG	C8-C7	2.08	1.56	1.50
31	D	407	LHG	C8-C7	2.09	1.56	1.50
32	d	405	DGD	C3G-C2G	2.09	1.56	1.50
23	C	507	CLA	C3B-CAB	2.09	1.52	1.47
28	c	521	LMG	C7-C8	2.09	1.56	1.50
23	D	404	CLA	CBA-CGA	2.10	1.56	1.50
26	A	610	PL9	C41-C39	2.10	1.55	1.51
28	a	611	LMG	C7-C8	2.10	1.56	1.50
32	D	406	DGD	C3G-C2G	2.11	1.56	1.50
27	b	602	SQD	O6-C1	2.11	1.43	1.40
25	f	101	BCR	C7-C6	2.12	1.53	1.45
24	A	607	PHO	C1B-C2B	2.12	1.50	1.45
25	C	514	BCR	C12-C13	2.12	1.50	1.45
25	B	619	BCR	C12-C13	2.13	1.50	1.45
24	D	401	PHO	C1A-NA	2.13	1.41	1.37
32	c	518	DGD	O6D-C1D	2.14	1.47	1.41
32	c	518	DGD	O5D-C1E	2.14	1.43	1.40
32	C	518	DGD	O6D-C1D	2.14	1.47	1.41
28	C	520	LMG	C7-C8	2.15	1.56	1.50
32	h	102	DGD	O3D-C3D	2.15	1.48	1.43
24	A	607	PHO	CHD-C1D	2.15	1.42	1.38
32	C	517	DGD	O6D-C1D	2.16	1.47	1.41
32	c	519	DGD	O6D-C1D	2.16	1.47	1.41
32	c	517	DGD	O5D-C1E	2.17	1.43	1.40
25	a	608	BCR	C7-C6	2.18	1.53	1.45
32	c	518	DGD	O6E-C1E	2.18	1.47	1.41
31	B	622	LHG	C8-C7	2.18	1.56	1.50
25	B	620	BCR	C7-C6	2.18	1.53	1.45
25	c	516	BCR	C7-C6	2.19	1.53	1.45
32	C	517	DGD	O5D-C1E	2.20	1.44	1.40
31	E	101	LHG	C8-C7	2.20	1.57	1.50
31	D	408	LHG	C8-C7	2.21	1.57	1.50
31	e	101	LHG	C8-C7	2.22	1.57	1.50
24	D	401	PHO	CHD-C1D	2.23	1.43	1.38
23	c	508	CLA	C3B-CAB	2.24	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	O5D-C1E	2.24	1.44	1.40
25	A	609	BCR	C7-C6	2.24	1.53	1.45
32	c	519	DGD	O3D-C3D	2.25	1.48	1.43
32	C	517	DGD	O6E-C1E	2.25	1.47	1.41
32	c	519	DGD	O5D-C1E	2.25	1.44	1.40
25	b	622	BCR	C7-C6	2.25	1.53	1.45
32	C	518	DGD	O3D-C3D	2.26	1.48	1.43
24	d	401	PHO	C1A-NA	2.26	1.42	1.37
28	Z	101	LMG	O8-C28	2.26	1.44	1.33
25	C	514	BCR	C7-C6	2.26	1.53	1.45
32	H	102	DGD	O6D-C1D	2.27	1.47	1.41
28	z	101	LMG	O8-C28	2.27	1.44	1.33
25	k	101	BCR	C7-C6	2.27	1.53	1.45
25	B	619	BCR	C7-C6	2.27	1.53	1.45
24	d	401	PHO	CHD-C1D	2.28	1.43	1.38
25	t	101	BCR	C7-C6	2.29	1.53	1.45
32	c	517	DGD	O3D-C3D	2.29	1.48	1.43
32	H	102	DGD	O3D-C3D	2.30	1.48	1.43
32	c	519	DGD	O6E-C1E	2.30	1.47	1.41
32	c	518	DGD	O3D-C3D	2.30	1.48	1.43
25	b	620	BCR	C12-C13	2.30	1.50	1.45
32	d	405	DGD	O3D-C3D	2.31	1.48	1.43
23	B	607[B]	CLA	C3B-CAB	2.31	1.52	1.47
23	B	607[A]	CLA	C3B-CAB	2.32	1.52	1.47
32	C	516	DGD	O3D-C3D	2.33	1.48	1.43
32	c	517	DGD	O6E-C1E	2.33	1.47	1.41
32	D	406	DGD	O3D-C3D	2.33	1.48	1.43
32	h	102	DGD	O6D-C1D	2.34	1.47	1.41
32	C	517	DGD	O3D-C3D	2.35	1.48	1.43
32	D	406	DGD	O3G-C1D	2.35	1.44	1.40
23	b	619	CLA	C3B-CAB	2.36	1.52	1.47
32	C	516	DGD	O6D-C1D	2.37	1.48	1.41
32	d	405	DGD	O3G-C1D	2.37	1.44	1.40
23	b	609[B]	CLA	C3B-CAB	2.37	1.52	1.47
32	D	406	DGD	O6D-C1D	2.39	1.48	1.41
25	b	621	BCR	C7-C6	2.39	1.54	1.45
32	C	518	DGD	O6E-C1E	2.39	1.48	1.41
32	c	517	DGD	O6D-C1D	2.40	1.48	1.41
23	b	606	CLA	C3D-CAD	2.40	1.52	1.46
23	b	609[A]	CLA	C3B-CAB	2.40	1.52	1.47
32	d	405	DGD	O6D-C1D	2.43	1.48	1.41
23	b	610	CLA	C3D-CAD	2.43	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	516	DGD	O6E-C1E	2.44	1.48	1.41
26	D	405	PL9	C41-C39	2.44	1.56	1.51
26	d	404	PL9	C41-C39	2.45	1.56	1.51
23	B	606	CLA	C3D-CAD	2.46	1.53	1.46
23	C	503	CLA	C3D-CAD	2.46	1.53	1.46
25	B	620	BCR	C12-C13	2.47	1.51	1.45
32	D	406	DGD	O2D-C2D	2.48	1.49	1.43
24	a	606	PHO	C4C-C3C	2.49	1.49	1.45
25	c	515	BCR	C12-C13	2.49	1.51	1.45
23	B	614	CLA	C3D-CAD	2.50	1.53	1.46
25	B	618	BCR	C12-C13	2.50	1.51	1.45
23	c	504	CLA	O2D-CGD	2.50	1.39	1.33
23	c	511	CLA	O2D-CGD	2.51	1.39	1.33
23	a	604	CLA	O2D-CGD	2.51	1.39	1.33
32	h	102	DGD	O2D-C2D	2.51	1.49	1.43
32	H	102	DGD	O2D-C2D	2.51	1.49	1.43
23	B	617	CLA	C3B-CAB	2.51	1.52	1.47
23	B	616	CLA	C3B-CAB	2.51	1.52	1.47
23	b	608	CLA	C3B-CAB	2.52	1.52	1.47
23	B	604	CLA	C3D-CAD	2.52	1.53	1.46
23	b	608	CLA	C3D-CAD	2.52	1.53	1.46
23	B	603	CLA	C3B-CAB	2.52	1.52	1.47
23	a	613	CLA	O2D-CGD	2.52	1.39	1.33
24	a	606	PHO	C1A-NA	2.52	1.42	1.37
23	d	402	CLA	O2D-CGD	2.53	1.39	1.33
23	C	510	CLA	O2D-CGD	2.53	1.39	1.33
23	B	606	CLA	C3B-CAB	2.53	1.52	1.47
32	c	517	DGD	O2D-C2D	2.53	1.49	1.43
32	d	405	DGD	O2D-C2D	2.53	1.49	1.43
32	h	102	DGD	O5D-C1E	2.53	1.44	1.40
23	b	612	CLA	C3B-CAB	2.54	1.52	1.47
32	d	405	DGD	O5D-C1E	2.54	1.44	1.40
32	c	519	DGD	O2D-C2D	2.54	1.49	1.43
23	c	503	CLA	C3B-CAB	2.54	1.52	1.47
23	b	605	CLA	C3B-CAB	2.54	1.52	1.47
32	h	102	DGD	O6E-C1E	2.54	1.48	1.41
25	F	101	BCR	C12-C13	2.54	1.51	1.45
23	B	614	CLA	O2D-CGD	2.54	1.39	1.33
32	C	518	DGD	O2D-C2D	2.55	1.49	1.43
23	D	403	CLA	O2D-CGD	2.55	1.39	1.33
25	b	620	BCR	C27-C26	2.55	1.56	1.51
23	B	605	CLA	C3D-CAD	2.55	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C3B-CAB	2.55	1.52	1.47
23	b	618	CLA	C3D-CAD	2.55	1.53	1.46
23	C	506	CLA	C3B-CAB	2.56	1.53	1.47
23	b	618	CLA	C3B-CAB	2.56	1.53	1.47
23	B	616	CLA	C3D-CAD	2.57	1.53	1.46
23	c	507	CLA	C3B-CAB	2.57	1.53	1.47
23	c	512	CLA	C3D-CAD	2.57	1.53	1.46
32	d	405	DGD	O6E-C1E	2.57	1.48	1.41
23	D	402	CLA	O2D-CGD	2.57	1.39	1.33
32	C	516	DGD	O2D-C2D	2.58	1.49	1.43
23	C	510	CLA	C3D-CAD	2.58	1.53	1.46
23	c	510	CLA	C3D-CAD	2.58	1.53	1.46
32	H	102	DGD	O5D-C1E	2.58	1.44	1.40
23	a	613	CLA	C3D-CAD	2.58	1.53	1.46
24	A	607	PHO	C1A-NA	2.59	1.42	1.37
23	b	616	CLA	C3D-CAD	2.59	1.53	1.46
32	c	518	DGD	O2D-C2D	2.59	1.49	1.43
23	b	617	CLA	C3D-CAD	2.59	1.53	1.46
23	A	606	CLA	C3D-CAD	2.60	1.53	1.46
23	A	608	CLA	C3B-CAB	2.61	1.53	1.47
23	b	607	CLA	C3D-CAD	2.61	1.53	1.46
23	B	616	CLA	O2D-CGD	2.62	1.39	1.33
24	A	607	PHO	C4C-C3C	2.62	1.49	1.45
23	c	504	CLA	C3D-CAD	2.62	1.53	1.46
23	c	513	CLA	C3D-CAD	2.62	1.53	1.46
23	D	403	CLA	C3D-CAD	2.62	1.53	1.46
23	c	505	CLA	C3B-CAB	2.62	1.53	1.47
23	b	614	CLA	C3D-CAD	2.62	1.53	1.46
24	a	606	PHO	C4C-NC	2.63	1.42	1.36
23	B	611	CLA	C3B-CAB	2.63	1.53	1.47
23	C	504	CLA	O2D-CGD	2.63	1.39	1.33
24	d	401	PHO	C4C-C3C	2.64	1.49	1.45
23	B	617	CLA	C3D-CAD	2.64	1.53	1.46
23	d	402	CLA	C3D-CAD	2.64	1.53	1.46
23	b	605	CLA	C3D-CAD	2.64	1.53	1.46
23	C	501	CLA	O2D-CGD	2.64	1.39	1.33
23	b	617	CLA	C3B-CAB	2.65	1.53	1.47
23	b	619	CLA	C3D-CAD	2.65	1.53	1.46
23	C	511	CLA	C3D-CAD	2.65	1.53	1.46
25	K	101	BCR	C12-C13	2.65	1.51	1.45
23	B	615	CLA	C3D-CAD	2.65	1.53	1.46
23	c	510	CLA	C3B-CAB	2.65	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C3D-CAD	2.65	1.53	1.46
32	C	517	DGD	O2D-C2D	2.66	1.49	1.43
23	b	609[B]	CLA	C3D-CAD	2.66	1.53	1.46
25	b	622	BCR	C12-C13	2.66	1.51	1.45
23	a	607	CLA	C3D-CAD	2.66	1.53	1.46
23	C	503	CLA	O2D-CGD	2.66	1.39	1.33
23	A	605	CLA	O2D-CGD	2.67	1.39	1.33
23	c	511	CLA	C3D-CAD	2.67	1.53	1.46
23	b	609[A]	CLA	C3D-CAD	2.67	1.53	1.46
23	c	513	CLA	O2D-CGD	2.67	1.39	1.33
23	c	512	CLA	O2D-CGD	2.67	1.39	1.33
23	b	610	CLA	C3B-CAB	2.68	1.53	1.47
23	B	615	CLA	C3B-CAB	2.68	1.53	1.47
23	a	605	CLA	C3D-CAD	2.68	1.53	1.46
23	A	606	CLA	O2D-CGD	2.68	1.39	1.33
23	B	607[A]	CLA	C3D-CAD	2.68	1.53	1.46
23	c	506	CLA	C3D-CAD	2.69	1.53	1.46
25	H	101	BCR	C4-C5	2.69	1.56	1.51
23	B	605	CLA	C3B-CAB	2.69	1.53	1.47
23	C	502	CLA	O2D-CGD	2.69	1.39	1.33
23	c	507	CLA	C3D-CAD	2.69	1.53	1.46
23	C	513	CLA	C3B-CAB	2.69	1.53	1.47
23	c	514	CLA	C3D-CAD	2.69	1.53	1.46
23	C	509	CLA	C3D-CAD	2.69	1.53	1.46
23	C	513	CLA	C3D-CAD	2.69	1.53	1.46
23	b	613	CLA	C3B-CAB	2.69	1.53	1.47
23	c	502	CLA	C3D-CAD	2.69	1.53	1.46
23	C	505	CLA	C3D-CAD	2.70	1.53	1.46
23	B	608	CLA	C3B-CAB	2.70	1.53	1.47
23	b	615	CLA	C3D-CAD	2.70	1.53	1.46
32	D	406	DGD	O6E-C1E	2.70	1.48	1.41
23	b	615	CLA	C3B-CAB	2.70	1.53	1.47
23	B	608	CLA	C3D-CAD	2.70	1.53	1.46
23	B	608	CLA	O2D-CGD	2.70	1.40	1.33
23	c	511	CLA	C3B-CAB	2.70	1.53	1.47
23	C	508	CLA	O2D-CGD	2.71	1.40	1.33
23	b	613	CLA	O2D-CGD	2.71	1.40	1.33
23	b	613	CLA	C3D-CAD	2.71	1.53	1.46
23	D	402	CLA	C3D-CAD	2.71	1.53	1.46
23	C	511	CLA	C3B-CAB	2.71	1.53	1.47
23	c	505	CLA	O2D-CGD	2.71	1.40	1.33
32	D	406	DGD	O5D-C1E	2.71	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	522	BCR	C27-C26	2.71	1.56	1.51
32	H	102	DGD	O6E-C1E	2.71	1.48	1.41
23	C	504	CLA	C3B-CAB	2.71	1.53	1.47
23	A	605	CLA	C3D-CAD	2.72	1.53	1.46
23	b	614	CLA	O2D-CGD	2.72	1.40	1.33
25	B	618	BCR	C4-C5	2.72	1.56	1.51
23	b	618	CLA	O2D-CGD	2.72	1.40	1.33
23	B	607[B]	CLA	C3D-CAD	2.72	1.53	1.46
23	C	504	CLA	C3D-CAD	2.72	1.53	1.46
23	B	611	CLA	O2D-CGD	2.73	1.40	1.33
25	t	101	BCR	C2-C3	2.73	1.59	1.52
23	B	604	CLA	O2D-CGD	2.74	1.40	1.33
23	b	604	CLA	C3B-CAB	2.74	1.53	1.47
24	A	607	PHO	C4C-NC	2.74	1.43	1.36
23	B	613	CLA	C3D-CAD	2.74	1.53	1.46
25	T	101	BCR	C4-C5	2.74	1.56	1.51
23	D	404	CLA	C3B-CAB	2.74	1.53	1.47
25	f	101	BCR	C12-C13	2.75	1.51	1.45
23	c	514	CLA	C3B-CAB	2.75	1.53	1.47
24	D	401	PHO	C4C-C3C	2.75	1.50	1.45
25	t	101	BCR	C4-C5	2.75	1.56	1.51
25	H	101	BCR	C12-C13	2.75	1.51	1.45
23	C	507	CLA	C3D-CAD	2.75	1.53	1.46
23	c	505	CLA	C3D-CAD	2.75	1.53	1.46
23	c	503	CLA	O2D-CGD	2.76	1.40	1.33
25	B	618	BCR	C27-C26	2.76	1.56	1.51
23	a	604	CLA	C3B-CAB	2.76	1.53	1.47
23	b	604	CLA	C3D-CAD	2.76	1.54	1.46
23	C	506	CLA	C3D-CAD	2.77	1.54	1.46
23	a	613	CLA	C3B-CAB	2.77	1.53	1.47
23	C	512	CLA	O2D-CGD	2.77	1.40	1.33
23	b	609[B]	CLA	O2D-CGD	2.77	1.40	1.33
23	b	609[A]	CLA	O2D-CGD	2.77	1.40	1.33
23	B	602	CLA	C3D-CAD	2.77	1.54	1.46
23	b	616	CLA	C3B-CAB	2.77	1.53	1.47
23	b	610	CLA	O2D-CGD	2.77	1.40	1.33
23	B	614	CLA	C3B-CAB	2.77	1.53	1.47
23	b	616	CLA	O2D-CGD	2.77	1.40	1.33
23	c	506	CLA	C3B-CAB	2.77	1.53	1.47
23	d	403	CLA	C3B-CAB	2.78	1.53	1.47
23	d	403	CLA	O2D-CGD	2.78	1.40	1.33
23	B	612	CLA	C3D-CAD	2.78	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	h	101	BCR	C4-C5	2.78	1.56	1.51
23	C	507	CLA	O2D-CGD	2.79	1.40	1.33
23	c	509	CLA	O2D-CGD	2.79	1.40	1.33
23	B	610	CLA	C3B-CAB	2.79	1.53	1.47
23	B	607[A]	CLA	O2D-CGD	2.79	1.40	1.33
25	k	101	BCR	C12-C13	2.79	1.52	1.45
23	c	502	CLA	C3B-CAB	2.79	1.53	1.47
23	D	404	CLA	C3D-CAD	2.79	1.54	1.46
25	C	515	BCR	C27-C26	2.79	1.56	1.51
25	c	516	BCR	C27-C26	2.80	1.56	1.51
25	b	620	BCR	C4-C5	2.80	1.56	1.51
23	B	611	CLA	C3D-CAD	2.80	1.54	1.46
23	B	613	CLA	C3B-CAB	2.80	1.53	1.47
25	c	515	BCR	C4-C5	2.80	1.56	1.51
23	B	617	CLA	O2D-CGD	2.80	1.40	1.33
23	B	615	CLA	O2D-CGD	2.80	1.40	1.33
25	C	521	BCR	C12-C13	2.81	1.52	1.45
23	d	402	CLA	C3B-CAB	2.81	1.53	1.47
23	B	602	CLA	O2D-CGD	2.81	1.40	1.33
23	C	512	CLA	C3D-CAD	2.81	1.54	1.46
23	b	617	CLA	O2D-CGD	2.81	1.40	1.33
23	B	603	CLA	C3D-CAD	2.81	1.54	1.46
24	d	401	PHO	C4C-NC	2.81	1.43	1.36
23	A	608	CLA	C3D-CAD	2.81	1.54	1.46
23	C	508	CLA	C3D-CAD	2.81	1.54	1.46
32	c	518	DGD	O6D-C5D	2.81	1.51	1.44
23	B	610	CLA	C3D-CAD	2.81	1.54	1.46
23	B	609	CLA	C3D-CAD	2.81	1.54	1.46
23	C	501	CLA	C3D-CAD	2.81	1.54	1.46
23	b	604	CLA	O2D-CGD	2.82	1.40	1.33
25	C	515	BCR	C4-C5	2.82	1.56	1.51
23	b	611	CLA	O2D-CGD	2.82	1.40	1.33
23	c	512	CLA	C3B-CAB	2.82	1.53	1.47
23	D	404	CLA	O2D-CGD	2.82	1.40	1.33
23	C	508	CLA	C3B-CAB	2.82	1.53	1.47
25	c	522	BCR	C4-C5	2.83	1.56	1.51
23	C	505	CLA	O2D-CGD	2.83	1.40	1.33
23	c	508	CLA	O2D-CGD	2.83	1.40	1.33
23	B	607[B]	CLA	O2D-CGD	2.83	1.40	1.33
23	b	611	CLA	C3D-CAD	2.84	1.54	1.46
23	D	403	CLA	C3B-CAB	2.84	1.53	1.47
25	C	521	BCR	C27-C26	2.84	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	O2D-CGD	2.84	1.40	1.33
23	B	603	CLA	O2D-CGD	2.84	1.40	1.33
23	a	604	CLA	C3D-CAD	2.84	1.54	1.46
23	c	509	CLA	C3D-CAD	2.84	1.54	1.46
23	C	501	CLA	C3B-CAB	2.84	1.53	1.47
23	c	503	CLA	C3D-CAD	2.85	1.54	1.46
23	B	609	CLA	C3B-CAB	2.85	1.53	1.47
23	b	608	CLA	O2D-CGD	2.85	1.40	1.33
23	c	502	CLA	O2D-CGD	2.85	1.40	1.33
23	b	607	CLA	C3B-CAB	2.85	1.53	1.47
23	a	605	CLA	O2D-CGD	2.85	1.40	1.33
23	b	615	CLA	O2D-CGD	2.86	1.40	1.33
23	C	512	CLA	C3B-CAB	2.86	1.53	1.47
23	c	509	CLA	C3B-CAB	2.86	1.53	1.47
25	a	608	BCR	C12-C13	2.86	1.52	1.45
23	b	607	CLA	O2D-CGD	2.86	1.40	1.33
23	C	502	CLA	C3D-CAD	2.86	1.54	1.46
23	c	513	CLA	C3B-CAB	2.86	1.53	1.47
23	B	602	CLA	C3B-CAB	2.86	1.53	1.47
23	c	504	CLA	C3B-CAB	2.86	1.53	1.47
23	c	507	CLA	O2D-CGD	2.87	1.40	1.33
25	B	619	BCR	C40-C30	2.88	1.59	1.53
23	C	509	CLA	C3B-CAB	2.88	1.53	1.47
23	b	606	CLA	O2D-CGD	2.89	1.40	1.33
23	A	605	CLA	C3B-CAB	2.89	1.53	1.47
23	B	609	CLA	O2D-CGD	2.89	1.40	1.33
24	D	401	PHO	C4C-NC	2.90	1.43	1.36
23	C	505	CLA	C3B-CAB	2.90	1.53	1.47
23	C	503	CLA	C3B-CAB	2.90	1.53	1.47
26	D	405	PL9	C21-C19	2.91	1.57	1.51
23	B	612	CLA	O2D-CGD	2.91	1.40	1.33
23	C	511	CLA	O2D-CGD	2.91	1.40	1.33
25	C	521	BCR	C4-C5	2.91	1.56	1.51
25	B	620	BCR	C4-C5	2.91	1.56	1.51
26	d	404	PL9	C21-C19	2.91	1.57	1.51
23	B	606	CLA	O2D-CGD	2.92	1.40	1.33
32	C	517	DGD	O6D-C5D	2.92	1.51	1.44
25	H	101	BCR	C27-C26	2.92	1.56	1.51
23	d	403	CLA	C3D-CAD	2.92	1.54	1.46
23	B	605	CLA	O2D-CGD	2.92	1.40	1.33
23	A	608	CLA	O2D-CGD	2.93	1.40	1.33
23	a	607	CLA	C3B-CAB	2.93	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3B-CAB	2.93	1.53	1.47
25	K	101	BCR	C27-C26	2.93	1.57	1.51
25	b	622	BCR	C4-C5	2.93	1.57	1.51
23	b	612	CLA	C3D-CAD	2.93	1.54	1.46
25	h	101	BCR	C27-C26	2.93	1.57	1.51
23	c	506	CLA	O2D-CGD	2.94	1.40	1.33
25	C	514	BCR	C4-C5	2.94	1.57	1.51
23	b	605	CLA	O2D-CGD	2.94	1.40	1.33
23	a	605	CLA	C3B-CAB	2.94	1.53	1.47
23	a	607	CLA	O2D-CGD	2.95	1.40	1.33
23	b	619	CLA	O2D-CGD	2.96	1.40	1.33
23	D	402	CLA	C3B-CAB	2.96	1.53	1.47
24	d	401	PHO	CHC-C1C	2.96	1.44	1.38
25	K	101	BCR	C17-C18	2.97	1.39	1.35
25	c	515	BCR	C27-C26	2.97	1.57	1.51
23	B	610	CLA	O2D-CGD	2.97	1.40	1.33
25	b	621	BCR	C40-C30	2.97	1.59	1.53
25	B	620	BCR	C27-C26	2.98	1.57	1.51
25	c	516	BCR	C4-C5	2.98	1.57	1.51
25	k	101	BCR	C2-C3	2.98	1.60	1.52
25	C	514	BCR	C27-C26	2.98	1.57	1.51
23	b	611	CLA	C3B-CAB	2.98	1.53	1.47
25	a	608	BCR	C4-C5	2.99	1.57	1.51
26	a	609	PL9	C21-C19	2.99	1.57	1.51
25	C	515	BCR	C12-C13	3.00	1.52	1.45
26	A	610	PL9	C21-C19	3.01	1.57	1.51
25	A	609	BCR	C12-C13	3.01	1.52	1.45
23	c	514	CLA	O2D-CGD	3.01	1.40	1.33
23	B	604	CLA	C3B-CAB	3.01	1.53	1.47
24	A	607	PHO	CHC-C1C	3.02	1.44	1.38
26	d	404	PL9	C7-C3	3.02	1.54	1.51
25	t	101	BCR	C12-C13	3.03	1.52	1.45
23	A	606	CLA	C3B-CAB	3.03	1.53	1.47
25	c	515	BCR	C2-C3	3.04	1.60	1.52
25	b	622	BCR	C27-C26	3.04	1.57	1.51
25	A	609	BCR	C4-C5	3.04	1.57	1.51
23	c	510	CLA	O2D-CGD	3.04	1.40	1.33
23	C	510	CLA	C3B-CAB	3.04	1.53	1.47
25	F	101	BCR	C4-C5	3.04	1.57	1.51
25	T	101	BCR	C27-C26	3.05	1.57	1.51
25	t	101	BCR	C27-C26	3.05	1.57	1.51
23	b	606	CLA	C3B-CAB	3.05	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	401	PHO	CHC-C1C	3.06	1.44	1.38
25	K	101	BCR	C4-C5	3.06	1.57	1.51
25	k	101	BCR	C27-C26	3.07	1.57	1.51
25	K	101	BCR	C2-C3	3.07	1.60	1.52
23	C	506	CLA	O2D-CGD	3.09	1.40	1.33
26	D	405	PL9	C7-C3	3.09	1.54	1.51
23	C	509	CLA	O2D-CGD	3.10	1.41	1.33
23	c	506	CLA	O2A-CGA	3.10	1.42	1.33
25	h	101	BCR	C12-C13	3.12	1.52	1.45
25	T	101	BCR	C12-C13	3.12	1.52	1.45
25	t	101	BCR	C40-C30	3.12	1.60	1.53
23	C	513	CLA	O2D-CGD	3.12	1.41	1.33
25	a	608	BCR	C27-C26	3.12	1.57	1.51
32	c	519	DGD	O6D-C5D	3.13	1.52	1.44
23	b	614	CLA	C3B-CAB	3.13	1.54	1.47
24	a	606	PHO	CHC-C1C	3.13	1.44	1.38
25	C	514	BCR	C2-C3	3.13	1.60	1.52
32	H	102	DGD	O6D-C5D	3.14	1.52	1.44
23	b	612	CLA	O2D-CGD	3.15	1.41	1.33
23	b	605	CLA	C1B-CHB	3.16	1.48	1.40
32	c	517	DGD	O6D-C5D	3.17	1.52	1.44
25	b	621	BCR	C17-C18	3.17	1.40	1.35
25	C	521	BCR	C17-C18	3.19	1.40	1.35
25	T	101	BCR	C40-C30	3.19	1.60	1.53
25	B	618	BCR	C17-C18	3.20	1.40	1.35
23	b	616	CLA	O2A-CGA	3.20	1.42	1.33
25	k	101	BCR	C4-C5	3.20	1.57	1.51
25	B	619	BCR	C4-C5	3.21	1.57	1.51
25	a	608	BCR	C40-C30	3.22	1.60	1.53
25	b	621	BCR	C2-C3	3.23	1.60	1.52
25	b	621	BCR	C4-C5	3.23	1.57	1.51
25	b	622	BCR	C2-C3	3.23	1.60	1.52
32	h	102	DGD	O6D-C5D	3.23	1.52	1.44
23	C	510	CLA	O2A-CGA	3.24	1.42	1.33
23	c	509	CLA	O2A-CGA	3.24	1.42	1.33
26	a	609	PL9	C36-C34	3.25	1.58	1.51
25	f	101	BCR	C4-C5	3.25	1.57	1.51
23	B	609	CLA	O2A-CGA	3.26	1.42	1.33
23	b	617	CLA	O2A-CGA	3.26	1.42	1.33
25	f	101	BCR	C40-C30	3.27	1.60	1.53
23	B	603	CLA	C1B-CHB	3.27	1.48	1.40
25	F	101	BCR	C27-C26	3.27	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	405	PL9	C36-C34	3.27	1.58	1.51
24	a	606	PHO	C3B-C4B	3.27	1.50	1.43
25	B	620	BCR	C2-C3	3.28	1.61	1.52
23	B	608	CLA	O2A-CGA	3.28	1.42	1.33
23	c	511	CLA	O2A-CGA	3.29	1.42	1.33
23	b	610	CLA	O2A-CGA	3.30	1.42	1.33
32	d	405	DGD	O6D-C5D	3.30	1.52	1.44
23	B	610	CLA	O2A-CGA	3.30	1.42	1.33
25	c	522	BCR	C12-C13	3.30	1.53	1.45
23	c	507	CLA	C1B-CHB	3.30	1.48	1.40
25	B	618	BCR	C40-C30	3.31	1.60	1.53
23	C	505	CLA	O2A-CGA	3.31	1.42	1.33
32	C	516	DGD	O6D-C5D	3.31	1.52	1.44
25	C	514	BCR	C40-C30	3.31	1.60	1.53
25	C	515	BCR	C2-C3	3.32	1.61	1.52
25	H	101	BCR	C2-C3	3.32	1.61	1.52
25	B	619	BCR	C2-C3	3.33	1.61	1.52
23	a	604	CLA	O2A-CGA	3.33	1.43	1.33
23	C	503	CLA	O2A-CGA	3.33	1.43	1.33
25	b	620	BCR	C40-C30	3.33	1.60	1.53
23	D	402	CLA	O2A-CGA	3.35	1.43	1.33
25	F	101	BCR	C40-C30	3.35	1.60	1.53
32	C	518	DGD	O6D-C5D	3.35	1.52	1.44
23	B	614	CLA	O2A-CGA	3.35	1.43	1.33
25	c	516	BCR	C2-C3	3.35	1.61	1.52
25	A	609	BCR	C40-C30	3.35	1.60	1.53
23	b	612	CLA	O2A-CGA	3.35	1.43	1.33
25	T	101	BCR	C2-C3	3.35	1.61	1.52
23	b	611	CLA	O2A-CGA	3.36	1.43	1.33
23	B	607[A]	CLA	C1B-CHB	3.37	1.49	1.40
23	c	509	CLA	C1B-CHB	3.37	1.49	1.40
25	f	101	BCR	C27-C26	3.37	1.57	1.51
32	D	406	DGD	O6D-C5D	3.37	1.52	1.44
24	A	607	PHO	C3B-C4B	3.37	1.50	1.43
23	B	603	CLA	O2A-CGA	3.38	1.43	1.33
23	D	403	CLA	O2A-CGA	3.38	1.43	1.33
25	A	609	BCR	C27-C26	3.38	1.57	1.51
23	c	514	CLA	O2A-CGA	3.39	1.43	1.33
25	c	516	BCR	C12-C13	3.39	1.53	1.45
23	B	613	CLA	O2A-CGA	3.39	1.43	1.33
25	B	619	BCR	C27-C26	3.39	1.57	1.51
25	c	515	BCR	C40-C30	3.39	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	O2A-CGA	3.39	1.43	1.33
23	d	402	CLA	C1B-CHB	3.39	1.49	1.40
23	c	507	CLA	O2A-CGA	3.40	1.43	1.33
23	B	607[B]	CLA	C1B-CHB	3.40	1.49	1.40
23	C	501	CLA	C1B-CHB	3.40	1.49	1.40
23	b	605	CLA	O2A-CGA	3.41	1.43	1.33
23	A	605	CLA	O2A-CGA	3.42	1.43	1.33
23	B	607[B]	CLA	O2A-CGA	3.42	1.43	1.33
23	a	613	CLA	O2A-CGA	3.43	1.43	1.33
23	D	403	CLA	C1B-CHB	3.43	1.49	1.40
23	D	402	CLA	C1B-CHB	3.43	1.49	1.40
25	b	621	BCR	C27-C26	3.43	1.58	1.51
25	h	101	BCR	C40-C30	3.43	1.60	1.53
23	b	615	CLA	O2A-CGA	3.43	1.43	1.33
23	B	606	CLA	O2A-CGA	3.43	1.43	1.33
28	a	611	LMG	O6-C1	3.44	1.50	1.41
23	a	613	CLA	C1B-CHB	3.44	1.49	1.40
32	C	517	DGD	O6E-C5E	3.44	1.52	1.44
23	a	605	CLA	C1B-CHB	3.44	1.49	1.40
23	a	605	CLA	O2A-CGA	3.44	1.43	1.33
23	c	504	CLA	O2A-CGA	3.44	1.43	1.33
23	c	505	CLA	O2A-CGA	3.44	1.43	1.33
23	b	609[B]	CLA	C1B-CHB	3.45	1.49	1.40
23	C	506	CLA	C1B-CHB	3.45	1.49	1.40
23	C	508	CLA	O2A-CGA	3.45	1.43	1.33
28	A	612	LMG	O6-C1	3.46	1.50	1.41
25	A	609	BCR	C2-C3	3.46	1.61	1.52
23	C	512	CLA	O2A-CGA	3.46	1.43	1.33
23	B	607[A]	CLA	O2A-CGA	3.46	1.43	1.33
23	b	608	CLA	O2A-CGA	3.47	1.43	1.33
25	h	101	BCR	C2-C3	3.47	1.61	1.52
23	C	501	CLA	O2A-CGA	3.47	1.43	1.33
23	c	505	CLA	C1B-CHB	3.47	1.49	1.40
26	d	404	PL9	C36-C34	3.48	1.58	1.51
23	b	618	CLA	C1B-CHB	3.48	1.49	1.40
23	B	611	CLA	O2A-CGA	3.48	1.43	1.33
23	B	615	CLA	O2A-CGA	3.48	1.43	1.33
23	b	609[A]	CLA	C1B-CHB	3.48	1.49	1.40
23	c	502	CLA	C1B-CHB	3.48	1.49	1.40
23	C	504	CLA	O2A-CGA	3.48	1.43	1.33
23	d	402	CLA	O2A-CGA	3.49	1.43	1.33
23	b	615	CLA	C1B-CHB	3.49	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C1B-CHB	3.49	1.49	1.40
23	b	610	CLA	C1B-CHB	3.49	1.49	1.40
28	C	520	LMG	O6-C1	3.49	1.50	1.41
23	c	502	CLA	O2A-CGA	3.49	1.43	1.33
23	B	604	CLA	C1B-CHB	3.50	1.49	1.40
25	C	521	BCR	C2-C3	3.50	1.61	1.52
23	C	504	CLA	C1B-CHB	3.50	1.49	1.40
23	B	604	CLA	O2A-CGA	3.51	1.43	1.33
23	B	611	CLA	C1B-CHB	3.51	1.49	1.40
25	K	101	BCR	C40-C30	3.51	1.61	1.53
23	B	612	CLA	C1B-CHB	3.51	1.49	1.40
23	b	609[A]	CLA	O2A-CGA	3.51	1.43	1.33
25	c	522	BCR	C2-C3	3.51	1.61	1.52
23	a	604	CLA	C1B-CHB	3.51	1.49	1.40
23	b	607	CLA	C1B-CHB	3.51	1.49	1.40
23	C	512	CLA	C1B-CHB	3.52	1.49	1.40
23	C	507	CLA	C1B-CHB	3.52	1.49	1.40
23	b	609[B]	CLA	O2A-CGA	3.52	1.43	1.33
23	A	605	CLA	C1B-CHB	3.52	1.49	1.40
23	B	612	CLA	O2A-CGA	3.52	1.43	1.33
23	C	508	CLA	C1B-CHB	3.52	1.49	1.40
23	B	605	CLA	O2A-CGA	3.52	1.43	1.33
28	B	621	LMG	O6-C1	3.53	1.51	1.41
25	b	622	BCR	C40-C30	3.53	1.61	1.53
23	b	612	CLA	C1B-CHB	3.54	1.49	1.40
23	b	617	CLA	C1B-CHB	3.54	1.49	1.40
23	b	614	CLA	O2A-CGA	3.54	1.43	1.33
23	b	613	CLA	O2A-CGA	3.54	1.43	1.33
23	b	619	CLA	O2A-CGA	3.54	1.43	1.33
32	c	518	DGD	O6E-C5E	3.54	1.53	1.44
23	b	608	CLA	C1B-CHB	3.54	1.49	1.40
23	C	511	CLA	O2A-CGA	3.55	1.43	1.33
23	c	503	CLA	C1B-CHB	3.55	1.49	1.40
23	B	615	CLA	C1B-CHB	3.55	1.49	1.40
25	a	608	BCR	C2-C3	3.55	1.61	1.52
28	J	101	LMG	O8-C28	3.56	1.43	1.33
28	c	521	LMG	O6-C1	3.56	1.51	1.41
23	B	606	CLA	C1B-CHB	3.57	1.49	1.40
24	D	401	PHO	C3B-C4B	3.57	1.50	1.43
28	j	101	LMG	O8-C28	3.57	1.43	1.33
23	C	509	CLA	C1B-CHB	3.57	1.49	1.40
25	T	101	BCR	C24-C25	3.57	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	O2A-CGA	3.58	1.43	1.33
25	H	101	BCR	C40-C30	3.58	1.61	1.53
23	C	510	CLA	C1B-CHB	3.58	1.49	1.40
32	C	518	DGD	O6E-C5E	3.58	1.53	1.44
23	c	512	CLA	O2A-CGA	3.58	1.43	1.33
23	B	610	CLA	C1B-CHB	3.58	1.49	1.40
23	b	618	CLA	O2A-CGA	3.59	1.43	1.33
25	b	620	BCR	C2-C3	3.59	1.61	1.52
32	c	517	DGD	O6E-C5E	3.59	1.53	1.44
23	b	604	CLA	O2A-CGA	3.60	1.43	1.33
23	c	513	CLA	C1B-CHB	3.60	1.49	1.40
23	B	616	CLA	C1B-CHB	3.60	1.49	1.40
23	C	509	CLA	O2A-CGA	3.61	1.43	1.33
23	B	614	CLA	C1B-CHB	3.61	1.49	1.40
23	c	513	CLA	O2A-CGA	3.61	1.43	1.33
23	B	616	CLA	O2A-CGA	3.61	1.43	1.33
23	c	511	CLA	C1B-CHB	3.62	1.49	1.40
23	A	608	CLA	O2A-CGA	3.62	1.43	1.33
24	d	401	PHO	C3B-C4B	3.62	1.50	1.43
23	A	606	CLA	O2A-CGA	3.62	1.43	1.33
23	A	606	CLA	C1B-CHB	3.62	1.49	1.40
28	b	623	LMG	O6-C1	3.62	1.51	1.41
23	c	508	CLA	C1B-CHB	3.62	1.49	1.40
23	C	503	CLA	C1B-CHB	3.62	1.49	1.40
23	c	504	CLA	C1B-CHB	3.62	1.49	1.40
23	b	616	CLA	C1B-CHB	3.62	1.49	1.40
23	C	502	CLA	C1B-CHB	3.63	1.49	1.40
23	b	613	CLA	C1B-CHB	3.63	1.49	1.40
23	B	617	CLA	O2A-CGA	3.64	1.43	1.33
25	f	101	BCR	C2-C3	3.64	1.61	1.52
23	b	611	CLA	C1B-CHB	3.64	1.49	1.40
23	C	513	CLA	O2A-CGA	3.64	1.43	1.33
23	c	508	CLA	O2A-CGA	3.64	1.43	1.33
23	c	503	CLA	O2A-CGA	3.64	1.43	1.33
28	c	520	LMG	O6-C1	3.65	1.51	1.41
23	b	606	CLA	O2A-CGA	3.65	1.43	1.33
32	c	519	DGD	O6E-C5E	3.65	1.53	1.44
23	B	602	CLA	O2A-CGA	3.65	1.43	1.33
28	C	520	LMG	O8-C28	3.65	1.43	1.33
25	c	515	BCR	C24-C25	3.65	1.58	1.45
23	c	514	CLA	C1B-CHB	3.65	1.49	1.40
23	B	602	CLA	C1B-CHB	3.65	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C1B-CHB	3.65	1.49	1.40
25	C	515	BCR	C40-C30	3.65	1.61	1.53
23	b	606	CLA	C1B-CHB	3.65	1.49	1.40
23	b	619	CLA	C1B-CHB	3.65	1.49	1.40
28	B	621	LMG	O8-C28	3.66	1.43	1.33
23	B	605	CLA	C1B-CHB	3.66	1.49	1.40
32	C	516	DGD	O6E-C5E	3.66	1.53	1.44
23	C	505	CLA	C1B-CHB	3.66	1.49	1.40
23	A	608	CLA	C1B-CHB	3.66	1.49	1.40
23	B	609	CLA	C1B-CHB	3.67	1.49	1.40
25	k	101	BCR	C40-C30	3.67	1.61	1.53
23	b	614	CLA	C1B-CHB	3.67	1.49	1.40
23	c	510	CLA	O2A-CGA	3.68	1.44	1.33
23	C	513	CLA	C1B-CHB	3.69	1.49	1.40
25	B	620	BCR	C40-C30	3.69	1.61	1.53
28	b	623	LMG	O8-C28	3.69	1.44	1.33
25	C	521	BCR	C40-C30	3.69	1.61	1.53
28	J	101	LMG	O6-C1	3.70	1.51	1.41
23	b	607	CLA	O2A-CGA	3.70	1.44	1.33
32	d	405	DGD	O6E-C5E	3.70	1.53	1.44
25	B	618	BCR	C2-C3	3.71	1.62	1.52
32	D	406	DGD	O6E-C5E	3.71	1.53	1.44
23	a	607	CLA	O2A-CGA	3.71	1.44	1.33
26	A	610	PL9	C36-C34	3.71	1.59	1.51
25	F	101	BCR	C2-C3	3.71	1.62	1.52
23	d	403	CLA	C1B-CHB	3.71	1.50	1.40
25	b	620	BCR	C24-C25	3.72	1.59	1.45
23	a	607	CLA	C1B-CHB	3.72	1.50	1.40
23	b	604	CLA	C1B-CHB	3.72	1.50	1.40
28	C	519	LMG	O6-C1	3.72	1.51	1.41
23	D	404	CLA	C1B-CHB	3.72	1.50	1.40
28	Z	101	LMG	O6-C1	3.73	1.51	1.41
25	c	516	BCR	C40-C30	3.73	1.61	1.53
25	c	522	BCR	C40-C30	3.73	1.61	1.53
28	a	611	LMG	O8-C28	3.73	1.44	1.33
25	t	101	BCR	C17-C18	3.74	1.40	1.35
23	C	507	CLA	O2A-CGA	3.74	1.44	1.33
28	j	101	LMG	O6-C1	3.74	1.51	1.41
25	C	514	BCR	C24-C25	3.74	1.59	1.45
28	c	520	LMG	O8-C28	3.75	1.44	1.33
28	z	101	LMG	O6-C1	3.75	1.51	1.41
28	c	521	LMG	O8-C28	3.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C1B-CHB	3.76	1.50	1.40
23	d	403	CLA	O2A-CGA	3.78	1.44	1.33
23	B	617	CLA	C1B-CHB	3.78	1.50	1.40
25	t	101	BCR	C24-C25	3.78	1.59	1.45
23	c	506	CLA	C1B-CHB	3.80	1.50	1.40
32	h	102	DGD	O6E-C5E	3.80	1.53	1.44
28	A	612	LMG	O8-C28	3.80	1.44	1.33
23	c	512	CLA	C1B-CHB	3.81	1.50	1.40
23	C	511	CLA	C1B-CHB	3.83	1.50	1.40
23	D	404	CLA	O2A-CGA	3.85	1.44	1.33
32	c	519	DGD	O1G-C1A	3.86	1.44	1.33
25	B	618	BCR	C24-C25	3.87	1.59	1.45
32	H	102	DGD	O6E-C5E	3.87	1.53	1.44
28	C	519	LMG	O8-C28	3.87	1.44	1.33
33	V	202	HEM	C3C-CAC	3.88	1.55	1.47
33	e	102	HEM	C3C-CAC	3.88	1.55	1.47
23	B	617	CLA	CHC-C1C	3.89	1.46	1.35
31	b	624	LHG	O7-C7	3.90	1.45	1.34
32	H	102	DGD	O2G-C1B	3.90	1.45	1.34
23	b	606	CLA	CHC-C1C	3.91	1.46	1.35
23	b	614	CLA	CHC-C1C	3.92	1.46	1.35
33	e	102	HEM	C3B-CAB	3.92	1.55	1.47
32	C	518	DGD	O1G-C1A	3.92	1.44	1.33
23	B	604	CLA	CHC-C1C	3.92	1.46	1.35
31	a	614	LHG	O7-C7	3.93	1.45	1.34
33	v	201	HEM	C3C-CAC	3.93	1.55	1.47
32	C	518	DGD	O2G-C1B	3.94	1.45	1.34
23	a	613	CLA	CHC-C1C	3.94	1.46	1.35
33	V	202	HEM	C3B-CAB	3.95	1.55	1.47
23	c	508	CLA	CHC-C1C	3.95	1.46	1.35
25	C	515	BCR	C24-C25	3.95	1.59	1.45
33	E	102	HEM	C3B-CAB	3.96	1.55	1.47
31	D	407	LHG	O7-C7	3.96	1.45	1.34
23	B	602	CLA	CHC-C1C	3.96	1.46	1.35
23	C	504	CLA	CHC-C1C	3.96	1.46	1.35
32	C	517	DGD	O1G-C1A	3.97	1.44	1.33
23	B	612	CLA	CHC-C1C	3.97	1.46	1.35
23	B	614	CLA	CHC-C1C	3.97	1.46	1.35
23	B	605	CLA	CHC-C1C	3.97	1.46	1.35
32	c	519	DGD	O2G-C1B	3.98	1.45	1.34
25	k	101	BCR	C17-C18	3.98	1.41	1.35
23	b	604	CLA	CHC-C1C	3.98	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	518	DGD	O2G-C1B	3.98	1.45	1.34
31	B	622	LHG	O7-C7	3.98	1.45	1.34
23	B	610	CLA	CHC-C1C	3.99	1.46	1.35
32	h	102	DGD	O1G-C1A	4.00	1.44	1.33
25	T	101	BCR	C17-C18	4.00	1.41	1.35
25	c	516	BCR	C24-C25	4.00	1.60	1.45
31	L	101	LHG	O7-C7	4.00	1.45	1.34
23	C	510	CLA	CHC-C1C	4.00	1.46	1.35
23	B	606	CLA	CHC-C1C	4.00	1.46	1.35
25	C	521	BCR	C24-C25	4.00	1.60	1.45
23	b	610	CLA	CHC-C1C	4.01	1.46	1.35
27	a	610	SQD	O47-C7	4.02	1.45	1.34
23	B	608	CLA	CHC-C1C	4.02	1.46	1.35
31	d	406	LHG	O7-C7	4.02	1.45	1.34
25	h	101	BCR	C24-C25	4.02	1.60	1.45
27	A	611	SQD	O48-C23	4.02	1.45	1.33
27	A	611	SQD	O47-C7	4.02	1.45	1.34
23	C	509	CLA	CHC-C1C	4.03	1.46	1.35
23	C	506	CLA	CHC-C1C	4.03	1.46	1.35
25	B	620	BCR	C17-C18	4.05	1.41	1.35
23	C	507	CLA	CHC-C1C	4.05	1.46	1.35
26	A	610	PL9	C7-C3	4.05	1.55	1.51
25	b	622	BCR	C24-C25	4.05	1.60	1.45
25	h	101	BCR	C17-C18	4.05	1.41	1.35
23	b	613	CLA	CHC-C1C	4.05	1.46	1.35
31	D	408	LHG	O7-C7	4.06	1.46	1.34
23	b	619	CLA	CHC-C1C	4.06	1.46	1.35
27	a	610	SQD	O48-C23	4.06	1.45	1.33
23	c	513	CLA	CHC-C1C	4.06	1.46	1.35
32	C	517	DGD	O2G-C1B	4.06	1.46	1.34
23	B	609	CLA	CHC-C1C	4.07	1.46	1.35
23	b	608	CLA	CHC-C1C	4.07	1.46	1.35
32	c	517	DGD	O2G-C1B	4.07	1.46	1.34
23	c	506	CLA	CHC-C1C	4.07	1.47	1.35
32	h	102	DGD	O2G-C1B	4.07	1.46	1.34
23	c	510	CLA	CHC-C1C	4.07	1.47	1.35
23	b	607	CLA	CHC-C1C	4.08	1.47	1.35
26	a	609	PL9	C7-C3	4.08	1.55	1.51
23	C	511	CLA	CHC-C1C	4.09	1.47	1.35
33	v	201	HEM	C3B-CAB	4.09	1.56	1.47
23	b	615	CLA	CHC-C1C	4.09	1.47	1.35
23	C	512	CLA	CHC-C1C	4.09	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHC-C1C	4.09	1.47	1.35
23	D	402	CLA	CHC-C1C	4.09	1.47	1.35
25	B	620	BCR	C24-C25	4.09	1.60	1.45
25	K	101	BCR	C24-C25	4.10	1.60	1.45
23	d	402	CLA	CHC-C1C	4.10	1.47	1.35
23	C	503	CLA	CHC-C1C	4.10	1.47	1.35
23	C	501	CLA	CHC-C1C	4.10	1.47	1.35
23	c	512	CLA	CHC-C1C	4.10	1.47	1.35
23	b	618	CLA	CHC-C1C	4.10	1.47	1.35
23	B	613	CLA	CHC-C1C	4.10	1.47	1.35
31	e	101	LHG	O7-C7	4.10	1.46	1.34
31	E	101	LHG	O7-C7	4.10	1.46	1.34
32	C	516	DGD	O2G-C1B	4.10	1.46	1.34
23	C	502	CLA	CHC-C1C	4.11	1.47	1.35
32	c	518	DGD	O1G-C1A	4.11	1.45	1.33
23	a	605	CLA	CHC-C1C	4.11	1.47	1.35
28	J	101	LMG	O7-C10	4.11	1.46	1.34
23	A	608	CLA	CHC-C1C	4.12	1.47	1.35
25	A	609	BCR	C17-C18	4.12	1.41	1.35
33	E	102	HEM	C3C-CAC	4.12	1.55	1.47
32	C	516	DGD	O1G-C1A	4.12	1.45	1.33
23	C	508	CLA	CHC-C1C	4.12	1.47	1.35
23	B	616	CLA	CHC-C1C	4.12	1.47	1.35
23	c	509	CLA	CHC-C1C	4.13	1.47	1.35
28	j	101	LMG	O7-C10	4.13	1.46	1.34
23	c	507	CLA	CHC-C1C	4.13	1.47	1.35
23	A	606	CLA	CHC-C1C	4.13	1.47	1.35
31	l	101	LHG	O7-C7	4.13	1.46	1.34
23	c	503	CLA	CHC-C1C	4.13	1.47	1.35
25	k	101	BCR	C24-C25	4.14	1.60	1.45
23	B	607[A]	CLA	CHC-C1C	4.14	1.47	1.35
28	B	621	LMG	O7-C10	4.14	1.46	1.34
23	b	612	CLA	CHC-C1C	4.14	1.47	1.35
23	b	617	CLA	CHC-C1C	4.14	1.47	1.35
23	B	611	CLA	CHC-C1C	4.14	1.47	1.35
32	d	405	DGD	O1G-C1A	4.14	1.45	1.33
32	H	102	DGD	O1G-C1A	4.15	1.45	1.33
23	c	502	CLA	CHC-C1C	4.15	1.47	1.35
23	c	511	CLA	CHC-C1C	4.15	1.47	1.35
25	b	622	BCR	C17-C18	4.16	1.41	1.35
23	c	514	CLA	CHC-C1C	4.16	1.47	1.35
32	c	517	DGD	O1G-C1A	4.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHC-C1C	4.16	1.47	1.35
23	B	615	CLA	CHC-C1C	4.16	1.47	1.35
23	b	609[A]	CLA	CHC-C1C	4.16	1.47	1.35
23	B	607[B]	CLA	CHC-C1C	4.16	1.47	1.35
23	b	611	CLA	CHC-C1C	4.16	1.47	1.35
25	H	101	BCR	C24-C25	4.16	1.60	1.45
23	d	403	CLA	CHC-C1C	4.16	1.47	1.35
23	c	504	CLA	CHC-C1C	4.16	1.47	1.35
23	A	605	CLA	CHC-C1C	4.17	1.47	1.35
23	b	609[B]	CLA	CHC-C1C	4.17	1.47	1.35
27	a	612	SQD	O47-C7	4.18	1.46	1.34
23	C	513	CLA	CHC-C1C	4.18	1.47	1.35
27	b	601	SQD	O47-C7	4.19	1.46	1.34
23	a	604	CLA	CHC-C1C	4.19	1.47	1.35
25	c	522	BCR	C24-C25	4.19	1.60	1.45
23	D	403	CLA	CHC-C1C	4.19	1.47	1.35
23	D	404	CLA	CHC-C1C	4.20	1.47	1.35
28	b	623	LMG	O7-C10	4.21	1.46	1.34
32	d	405	DGD	O2G-C1B	4.22	1.46	1.34
23	c	505	CLA	CHC-C1C	4.22	1.47	1.35
23	b	605	CLA	CHC-C1C	4.25	1.47	1.35
25	c	515	BCR	C17-C18	4.25	1.41	1.35
32	D	406	DGD	O1G-C1A	4.27	1.45	1.33
28	Z	101	LMG	O7-C10	4.28	1.46	1.34
23	B	603	CLA	CHC-C1C	4.29	1.47	1.35
27	B	623	SQD	O47-C7	4.29	1.46	1.34
27	b	602	SQD	O47-C7	4.30	1.46	1.34
32	D	406	DGD	O2G-C1B	4.30	1.46	1.34
28	A	612	LMG	O7-C10	4.32	1.46	1.34
28	C	519	LMG	O7-C10	4.35	1.46	1.34
28	z	101	LMG	O7-C10	4.35	1.46	1.34
31	D	408	LHG	O8-C23	4.35	1.45	1.33
27	x	101	SQD	O47-C7	4.36	1.46	1.34
27	X	101	SQD	O47-C7	4.37	1.46	1.34
28	a	611	LMG	O7-C10	4.39	1.47	1.34
23	a	607	CLA	CHC-C1C	4.40	1.47	1.35
31	a	614	LHG	O8-C23	4.40	1.46	1.33
31	b	624	LHG	O8-C23	4.40	1.46	1.33
25	f	101	BCR	C17-C18	4.41	1.41	1.35
31	L	101	LHG	O8-C23	4.41	1.46	1.33
28	c	520	LMG	O7-C10	4.41	1.47	1.34
25	c	522	BCR	C17-C18	4.42	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	E	101	LHG	O8-C23	4.42	1.46	1.33
25	A	609	BCR	C24-C25	4.43	1.61	1.45
25	c	516	BCR	C17-C18	4.44	1.41	1.35
27	b	602	SQD	O48-C23	4.45	1.46	1.33
27	B	623	SQD	O48-C23	4.45	1.46	1.33
28	C	520	LMG	O7-C10	4.46	1.47	1.34
25	f	101	BCR	C24-C25	4.46	1.61	1.45
25	C	514	BCR	C17-C18	4.47	1.41	1.35
28	c	521	LMG	O7-C10	4.47	1.47	1.34
31	D	407	LHG	O8-C23	4.49	1.46	1.33
31	e	101	LHG	O8-C23	4.49	1.46	1.33
27	a	612	SQD	O48-C23	4.52	1.46	1.33
27	b	601	SQD	O48-C23	4.52	1.46	1.33
31	d	406	LHG	O8-C23	4.53	1.46	1.33
25	a	608	BCR	C24-C25	4.54	1.62	1.45
31	l	101	LHG	O8-C23	4.57	1.46	1.33
27	x	101	SQD	O48-C23	4.57	1.46	1.33
27	X	101	SQD	O48-C23	4.59	1.46	1.33
25	b	621	BCR	C24-C25	4.60	1.62	1.45
25	B	619	BCR	C23-C22	4.61	1.55	1.45
25	F	101	BCR	C24-C25	4.63	1.62	1.45
25	h	101	BCR	C24-C23	4.64	1.47	1.33
31	B	622	LHG	O8-C23	4.66	1.46	1.33
25	H	101	BCR	C17-C18	4.70	1.42	1.35
25	b	621	BCR	C11-C12	4.71	1.46	1.34
25	H	101	BCR	C23-C22	4.72	1.56	1.45
25	B	619	BCR	C24-C25	4.72	1.62	1.45
25	a	608	BCR	C17-C18	4.74	1.42	1.35
25	b	620	BCR	C17-C18	4.76	1.42	1.35
25	b	620	BCR	C24-C23	4.77	1.47	1.33
25	T	101	BCR	C24-C23	4.78	1.47	1.33
25	H	101	BCR	C24-C23	4.79	1.47	1.33
25	c	515	BCR	C24-C23	4.81	1.47	1.33
25	b	620	BCR	C23-C22	4.82	1.56	1.45
25	B	619	BCR	C11-C12	4.82	1.46	1.34
25	b	620	BCR	C11-C12	4.86	1.46	1.34
25	C	514	BCR	C11-C12	4.91	1.47	1.34
25	F	101	BCR	C23-C22	4.95	1.56	1.45
25	F	101	BCR	C11-C12	4.95	1.47	1.34
25	f	101	BCR	C11-C12	4.97	1.47	1.34
25	a	608	BCR	C23-C22	4.99	1.56	1.45
25	C	514	BCR	C24-C23	5.02	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	515	BCR	C24-C23	5.04	1.48	1.33
25	c	515	BCR	C11-C12	5.06	1.47	1.34
25	B	618	BCR	C11-C12	5.07	1.47	1.34
25	K	101	BCR	C24-C23	5.07	1.48	1.33
25	A	609	BCR	C24-C23	5.08	1.48	1.33
25	c	516	BCR	C24-C23	5.09	1.48	1.33
25	k	101	BCR	C24-C23	5.10	1.48	1.33
25	K	101	BCR	C11-C12	5.10	1.47	1.34
25	A	609	BCR	C23-C22	5.11	1.57	1.45
23	b	615	CLA	C4A-NA	5.12	1.46	1.38
25	B	619	BCR	C17-C18	5.13	1.42	1.35
25	c	515	BCR	C23-C22	5.16	1.57	1.45
25	t	101	BCR	C24-C23	5.17	1.48	1.33
23	B	613	CLA	C4A-NA	5.19	1.46	1.38
25	b	622	BCR	C24-C23	5.19	1.49	1.33
25	f	101	BCR	C24-C23	5.19	1.49	1.33
25	f	101	BCR	C23-C22	5.20	1.57	1.45
25	a	608	BCR	C24-C23	5.20	1.49	1.33
25	B	620	BCR	C11-C12	5.21	1.47	1.34
23	a	605	CLA	C4A-NA	5.23	1.46	1.38
25	C	521	BCR	C11-C12	5.23	1.47	1.34
23	D	402	CLA	C4A-NA	5.24	1.46	1.38
33	E	102	HEM	C3D-C2D	5.25	1.53	1.37
25	C	515	BCR	C17-C18	5.25	1.42	1.35
25	c	522	BCR	C23-C22	5.25	1.57	1.45
25	C	521	BCR	C23-C22	5.25	1.57	1.45
25	B	620	BCR	C24-C23	5.25	1.49	1.33
25	B	619	BCR	C24-C23	5.27	1.49	1.33
23	D	403	CLA	C4A-NA	5.29	1.46	1.38
25	C	515	BCR	C23-C22	5.30	1.57	1.45
33	e	102	HEM	C3D-C2D	5.30	1.53	1.37
25	F	101	BCR	C24-C23	5.31	1.49	1.33
33	V	202	HEM	C3D-C2D	5.31	1.53	1.37
23	d	402	CLA	C4A-NA	5.31	1.46	1.38
25	b	622	BCR	C11-C12	5.32	1.48	1.34
23	b	605	CLA	C4A-NA	5.32	1.46	1.38
23	a	604	CLA	C4A-NA	5.32	1.46	1.38
25	B	618	BCR	C24-C23	5.33	1.49	1.33
25	H	101	BCR	C11-C12	5.33	1.48	1.34
23	A	606	CLA	C4A-NA	5.33	1.46	1.38
23	C	504	CLA	C4A-NA	5.33	1.46	1.38
23	B	612	CLA	C4A-NA	5.34	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	613	CLA	C4A-NA	5.35	1.46	1.38
23	A	605	CLA	C4A-NA	5.35	1.46	1.38
25	C	515	BCR	C11-C12	5.36	1.48	1.34
25	c	522	BCR	C24-C23	5.37	1.49	1.33
23	b	614	CLA	C4A-NA	5.37	1.46	1.38
25	C	521	BCR	C24-C23	5.38	1.49	1.33
25	k	101	BCR	C11-C12	5.38	1.48	1.34
23	b	606	CLA	C4A-NA	5.39	1.46	1.38
25	b	621	BCR	C23-C22	5.41	1.57	1.45
25	b	621	BCR	C24-C23	5.42	1.49	1.33
25	c	522	BCR	C11-C12	5.43	1.48	1.34
23	B	605	CLA	C4A-NA	5.43	1.46	1.38
23	d	403	CLA	C4A-NA	5.43	1.46	1.38
25	c	516	BCR	C23-C22	5.44	1.57	1.45
23	C	505	CLA	C4A-NA	5.44	1.46	1.38
23	c	510	CLA	C4A-NA	5.44	1.46	1.38
25	k	101	BCR	C23-C22	5.45	1.57	1.45
25	h	101	BCR	C23-C22	5.45	1.57	1.45
25	C	514	BCR	C23-C22	5.45	1.57	1.45
25	A	609	BCR	C11-C12	5.46	1.48	1.34
23	C	509	CLA	C4A-NA	5.46	1.46	1.38
23	B	603	CLA	C4A-NA	5.46	1.46	1.38
25	a	608	BCR	C11-C12	5.47	1.48	1.34
25	h	101	BCR	C11-C12	5.47	1.48	1.34
33	v	201	HEM	C3D-C2D	5.47	1.53	1.37
23	C	510	CLA	C4A-NA	5.48	1.46	1.38
23	c	506	CLA	C4A-NA	5.48	1.46	1.38
23	a	607	CLA	C4A-NA	5.49	1.46	1.38
23	c	503	CLA	C4A-NA	5.50	1.47	1.38
23	c	513	CLA	C4A-NA	5.50	1.47	1.38
23	c	505	CLA	C4A-NA	5.52	1.47	1.38
23	A	608	CLA	C4A-NA	5.52	1.47	1.38
25	T	101	BCR	C11-C12	5.53	1.48	1.34
23	B	617	CLA	C4A-NA	5.54	1.47	1.38
25	t	101	BCR	C11-C12	5.54	1.48	1.34
23	B	614	CLA	C4A-NA	5.54	1.47	1.38
23	C	503	CLA	C4A-NA	5.55	1.47	1.38
23	B	604	CLA	C4A-NA	5.56	1.47	1.38
23	b	619	CLA	C4A-NA	5.56	1.47	1.38
25	t	101	BCR	C23-C22	5.56	1.58	1.45
23	b	604	CLA	C4A-NA	5.56	1.47	1.38
25	K	101	BCR	C23-C22	5.57	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	501	CLA	C4A-NA	5.58	1.47	1.38
25	t	101	BCR	C38-C26	5.58	1.60	1.51
23	C	513	CLA	C4A-NA	5.59	1.47	1.38
25	B	618	BCR	C38-C26	5.59	1.60	1.51
23	b	608	CLA	C4A-NA	5.60	1.47	1.38
23	b	612	CLA	C4A-NA	5.60	1.47	1.38
25	c	516	BCR	C11-C12	5.60	1.48	1.34
25	c	515	BCR	C38-C26	5.61	1.60	1.51
23	b	611	CLA	C4A-NA	5.61	1.47	1.38
23	c	509	CLA	C4A-NA	5.62	1.47	1.38
25	T	101	BCR	C23-C22	5.63	1.58	1.45
25	T	101	BCR	C38-C26	5.63	1.60	1.51
23	B	610	CLA	C4A-NA	5.64	1.47	1.38
23	b	617	CLA	C4A-NA	5.65	1.47	1.38
23	c	514	CLA	C4A-NA	5.65	1.47	1.38
23	C	511	CLA	C4A-NA	5.65	1.47	1.38
23	c	511	CLA	C4A-NA	5.67	1.47	1.38
23	C	502	CLA	C4A-NA	5.67	1.47	1.38
23	c	504	CLA	C4A-NA	5.68	1.47	1.38
23	C	508	CLA	C4A-NA	5.68	1.47	1.38
23	B	607[A]	CLA	C4A-NA	5.68	1.47	1.38
23	b	609[A]	CLA	C4A-NA	5.68	1.47	1.38
23	c	512	CLA	C4A-NA	5.69	1.47	1.38
25	C	514	BCR	C38-C26	5.70	1.60	1.51
23	c	507	CLA	C4A-NA	5.70	1.47	1.38
23	c	508	CLA	C4A-NA	5.71	1.47	1.38
23	b	613	CLA	C4A-NA	5.71	1.47	1.38
25	b	620	BCR	C38-C26	5.71	1.60	1.51
23	b	618	CLA	C4A-NA	5.72	1.47	1.38
23	B	611	CLA	C4A-NA	5.73	1.47	1.38
23	B	615	CLA	C4A-NA	5.73	1.47	1.38
23	C	512	CLA	C4A-NA	5.74	1.47	1.38
23	B	607[B]	CLA	C4A-NA	5.74	1.47	1.38
23	b	609[B]	CLA	C4A-NA	5.75	1.47	1.38
23	B	602	CLA	C4A-NA	5.75	1.47	1.38
25	K	101	BCR	C38-C26	5.77	1.60	1.51
23	C	507	CLA	C4A-NA	5.77	1.47	1.38
23	b	616	CLA	C4A-NA	5.78	1.47	1.38
23	b	607	CLA	C4A-NA	5.79	1.47	1.38
23	B	606	CLA	C4A-NA	5.79	1.47	1.38
23	c	502	CLA	C4A-NA	5.83	1.47	1.38
23	B	608	CLA	C4A-NA	5.83	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	C4A-NA	5.84	1.47	1.38
23	B	616	CLA	C4A-NA	5.84	1.47	1.38
23	B	609	CLA	C4A-NA	5.84	1.47	1.38
25	b	622	BCR	C38-C26	5.85	1.60	1.51
25	B	620	BCR	C38-C26	5.88	1.60	1.51
25	k	101	BCR	C38-C26	5.88	1.60	1.51
23	C	506	CLA	C4A-NA	5.91	1.47	1.38
25	C	521	BCR	C38-C26	5.91	1.60	1.51
25	B	620	BCR	C23-C22	5.95	1.58	1.45
25	c	516	BCR	C38-C26	5.97	1.61	1.51
25	C	515	BCR	C38-C26	6.00	1.61	1.51
25	c	522	BCR	C38-C26	6.04	1.61	1.51
25	b	622	BCR	C23-C22	6.09	1.59	1.45
25	B	618	BCR	C23-C22	6.14	1.59	1.45
26	d	404	PL9	O2-C1	6.19	1.41	1.24
25	b	621	BCR	C38-C26	6.22	1.61	1.51
23	A	608	CLA	C4C-NC	6.24	1.46	1.37
23	b	610	CLA	C4A-NA	6.29	1.48	1.38
25	B	619	BCR	C38-C26	6.33	1.61	1.51
25	a	608	BCR	C38-C26	6.34	1.61	1.51
26	D	405	PL9	O2-C1	6.34	1.41	1.24
25	H	101	BCR	C38-C26	6.36	1.61	1.51
25	h	101	BCR	C38-C26	6.38	1.61	1.51
23	b	606	CLA	C4C-NC	6.43	1.46	1.37
25	A	609	BCR	C38-C26	6.46	1.61	1.51
26	A	610	PL9	O2-C1	6.47	1.41	1.24
23	a	607	CLA	C4C-NC	6.53	1.47	1.37
26	a	609	PL9	O2-C1	6.54	1.42	1.24
23	C	504	CLA	C4C-NC	6.57	1.47	1.37
23	C	509	CLA	C4C-NC	6.59	1.47	1.37
23	b	612	CLA	C4C-NC	6.59	1.47	1.37
23	b	616	CLA	C4C-NC	6.59	1.47	1.37
23	c	502	CLA	C4C-NC	6.62	1.47	1.37
23	B	604	CLA	C4C-NC	6.62	1.47	1.37
23	C	501	CLA	C4C-NC	6.63	1.47	1.37
25	F	101	BCR	C38-C26	6.63	1.62	1.51
23	b	617	CLA	C4C-NC	6.63	1.47	1.37
23	d	402	CLA	C4C-NC	6.64	1.47	1.37
23	b	614	CLA	C4C-NC	6.64	1.47	1.37
23	c	508	CLA	C4C-NC	6.64	1.47	1.37
23	B	607[B]	CLA	C4C-NC	6.64	1.47	1.37
23	A	606	CLA	C4C-NC	6.66	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C4C-NC	6.67	1.47	1.37
23	b	608	CLA	C4C-NC	6.67	1.47	1.37
23	B	607[A]	CLA	C4C-NC	6.68	1.47	1.37
23	C	507	CLA	C4C-NC	6.68	1.47	1.37
23	B	612	CLA	C4C-NC	6.69	1.47	1.37
23	C	506	CLA	C4C-NC	6.70	1.47	1.37
23	b	610	CLA	C4C-NC	6.71	1.47	1.37
23	B	610	CLA	C4C-NC	6.71	1.47	1.37
23	d	403	CLA	C4C-NC	6.72	1.47	1.37
23	D	404	CLA	C4C-NC	6.72	1.47	1.37
23	C	513	CLA	C4C-NC	6.74	1.47	1.37
23	C	510	CLA	C4C-NC	6.74	1.47	1.37
23	b	615	CLA	C4C-NC	6.74	1.47	1.37
23	B	613	CLA	C4C-NC	6.75	1.47	1.37
23	b	609[B]	CLA	C4C-NC	6.75	1.47	1.37
23	a	613	CLA	C4C-NC	6.75	1.47	1.37
23	C	502	CLA	C4C-NC	6.76	1.47	1.37
23	B	608	CLA	C4C-NC	6.76	1.47	1.37
23	B	615	CLA	C4C-NC	6.76	1.47	1.37
25	f	101	BCR	C38-C26	6.76	1.62	1.51
23	C	511	CLA	C4C-NC	6.77	1.47	1.37
23	c	503	CLA	C4C-NC	6.77	1.47	1.37
23	c	505	CLA	C4C-NC	6.78	1.47	1.37
23	c	512	CLA	C4C-NC	6.80	1.47	1.37
23	B	605	CLA	C4C-NC	6.81	1.47	1.37
23	D	402	CLA	C4C-NC	6.81	1.47	1.37
23	a	605	CLA	C4C-NC	6.82	1.47	1.37
23	A	605	CLA	C4C-NC	6.83	1.47	1.37
23	b	607	CLA	C4C-NC	6.84	1.47	1.37
23	c	511	CLA	C4C-NC	6.85	1.47	1.37
23	a	604	CLA	C4C-NC	6.85	1.47	1.37
23	b	619	CLA	C4C-NC	6.86	1.47	1.37
23	b	605	CLA	C4C-NC	6.86	1.47	1.37
23	D	403	CLA	C4C-NC	6.86	1.47	1.37
23	b	613	CLA	C4C-NC	6.87	1.47	1.37
23	c	510	CLA	C4C-NC	6.87	1.47	1.37
23	c	509	CLA	C4C-NC	6.90	1.47	1.37
23	c	507	CLA	C4C-NC	6.91	1.47	1.37
23	B	606	CLA	C4C-NC	6.91	1.47	1.37
23	b	604	CLA	C4C-NC	6.91	1.47	1.37
23	b	609[A]	CLA	C4C-NC	6.92	1.47	1.37
23	c	513	CLA	C4C-NC	6.92	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C4C-NC	6.93	1.47	1.37
23	c	514	CLA	C4C-NC	6.93	1.47	1.37
25	B	620	BCR	C8-C9	6.94	1.61	1.45
23	c	506	CLA	C4C-NC	6.94	1.47	1.37
25	C	514	BCR	C8-C9	6.97	1.61	1.45
23	C	508	CLA	C4C-NC	6.97	1.47	1.37
23	C	503	CLA	C4C-NC	6.98	1.47	1.37
23	C	512	CLA	C4C-NC	6.99	1.47	1.37
23	C	505	CLA	C4C-NC	7.00	1.47	1.37
25	B	618	BCR	C8-C9	7.01	1.61	1.45
23	B	617	CLA	C4C-NC	7.02	1.47	1.37
23	c	504	CLA	C4C-NC	7.04	1.47	1.37
25	b	620	BCR	C8-C9	7.04	1.61	1.45
23	b	611	CLA	C4C-NC	7.05	1.47	1.37
23	B	616	CLA	C4C-NC	7.05	1.47	1.37
25	c	515	BCR	C8-C9	7.07	1.61	1.45
23	b	618	CLA	C4C-NC	7.08	1.47	1.37
25	b	621	BCR	C8-C9	7.12	1.61	1.45
23	B	609	CLA	C4C-NC	7.14	1.48	1.37
23	B	603	CLA	C4C-NC	7.14	1.48	1.37
25	b	622	BCR	C8-C9	7.15	1.61	1.45
25	T	101	BCR	C26-C25	7.20	1.46	1.34
25	B	619	BCR	C8-C9	7.25	1.61	1.45
25	t	101	BCR	C26-C25	7.27	1.47	1.34
25	C	521	BCR	C8-C9	7.29	1.61	1.45
23	B	602	CLA	C4C-NC	7.31	1.48	1.37
25	H	101	BCR	C8-C9	7.37	1.61	1.45
25	F	101	BCR	C8-C9	7.37	1.61	1.45
25	c	515	BCR	C26-C25	7.42	1.47	1.34
25	k	101	BCR	C8-C9	7.42	1.62	1.45
25	h	101	BCR	C8-C9	7.44	1.62	1.45
26	a	609	PL9	O1-C4	7.46	1.39	1.23
25	K	101	BCR	C8-C9	7.48	1.62	1.45
26	A	610	PL9	O1-C4	7.50	1.39	1.23
25	T	101	BCR	C8-C9	7.53	1.62	1.45
25	t	101	BCR	C8-C9	7.60	1.62	1.45
25	C	515	BCR	C8-C9	7.60	1.62	1.45
25	C	514	BCR	C26-C25	7.62	1.47	1.34
25	f	101	BCR	C8-C9	7.62	1.62	1.45
25	c	522	BCR	C8-C9	7.64	1.62	1.45
25	B	618	BCR	C26-C25	7.65	1.47	1.34
25	K	101	BCR	C26-C25	7.73	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	516	BCR	C8-C9	7.74	1.62	1.45
25	B	620	BCR	C26-C25	7.76	1.47	1.34
25	C	521	BCR	C26-C25	7.80	1.47	1.34
26	D	405	PL9	C33-C34	7.83	1.52	1.33
25	b	622	BCR	C26-C25	7.85	1.48	1.34
25	c	522	BCR	C26-C25	7.85	1.48	1.34
26	d	404	PL9	O1-C4	7.86	1.40	1.23
26	d	404	PL9	C33-C34	7.87	1.52	1.33
26	D	405	PL9	O1-C4	7.89	1.40	1.23
25	a	608	BCR	C8-C9	7.89	1.63	1.45
25	C	515	BCR	C26-C25	7.90	1.48	1.34
26	a	609	PL9	C33-C34	7.93	1.52	1.33
25	k	101	BCR	C26-C25	7.93	1.48	1.34
25	A	609	BCR	C8-C9	7.97	1.63	1.45
26	A	610	PL9	C33-C34	8.05	1.52	1.33
25	c	516	BCR	C26-C25	8.05	1.48	1.34
26	a	609	PL9	C43-C44	8.17	1.53	1.33
26	D	405	PL9	C28-C29	8.18	1.53	1.33
26	A	610	PL9	C8-C9	8.19	1.53	1.33
25	b	620	BCR	C26-C25	8.23	1.48	1.34
26	a	609	PL9	C8-C9	8.27	1.53	1.33
26	d	404	PL9	C8-C9	8.28	1.53	1.33
26	D	405	PL9	C8-C9	8.28	1.53	1.33
26	A	610	PL9	C28-C29	8.33	1.53	1.33
26	A	610	PL9	C43-C44	8.38	1.53	1.33
26	a	609	PL9	C13-C14	8.38	1.53	1.33
26	d	404	PL9	C28-C29	8.45	1.53	1.33
26	a	609	PL9	C28-C29	8.46	1.53	1.33
26	d	404	PL9	C43-C44	8.47	1.53	1.33
26	D	405	PL9	C43-C44	8.47	1.53	1.33
26	A	610	PL9	C48-C49	8.48	1.56	1.32
26	A	610	PL9	C13-C14	8.56	1.54	1.33
26	d	404	PL9	C48-C49	8.64	1.57	1.32
25	h	101	BCR	C26-C25	8.65	1.49	1.34
26	d	404	PL9	C13-C14	8.70	1.54	1.33
25	H	101	BCR	C26-C25	8.70	1.49	1.34
26	D	405	PL9	C48-C49	8.72	1.57	1.32
26	D	405	PL9	C13-C14	8.72	1.54	1.33
26	a	609	PL9	C48-C49	8.79	1.57	1.32
25	b	621	BCR	C16-C17	8.89	1.70	1.43
25	C	514	BCR	C16-C17	9.10	1.71	1.43
25	F	101	BCR	C16-C17	9.11	1.71	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	f	101	BCR	C26-C25	9.15	1.50	1.34
25	B	620	BCR	C16-C17	9.16	1.71	1.43
25	k	101	BCR	C16-C17	9.20	1.71	1.43
25	a	608	BCR	C26-C25	9.24	1.50	1.34
25	A	609	BCR	C26-C25	9.29	1.50	1.34
25	B	619	BCR	C16-C17	9.31	1.72	1.43
26	a	609	PL9	C23-C24	9.32	1.56	1.33
25	K	101	BCR	C16-C17	9.32	1.72	1.43
25	F	101	BCR	C26-C25	9.36	1.50	1.34
25	c	515	BCR	C16-C17	9.39	1.72	1.43
25	C	515	BCR	C16-C17	9.44	1.72	1.43
25	H	101	BCR	C16-C17	9.46	1.72	1.43
26	a	609	PL9	C38-C39	9.47	1.56	1.33
25	c	516	BCR	C16-C17	9.47	1.72	1.43
26	A	610	PL9	C23-C24	9.48	1.56	1.33
25	A	609	BCR	C16-C17	9.51	1.72	1.43
26	d	404	PL9	C38-C39	9.54	1.56	1.33
25	b	622	BCR	C16-C17	9.55	1.72	1.43
26	D	405	PL9	C23-C24	9.55	1.56	1.33
26	A	610	PL9	C38-C39	9.56	1.56	1.33
26	d	404	PL9	C23-C24	9.61	1.56	1.33
25	c	522	BCR	C16-C17	9.67	1.73	1.43
26	D	405	PL9	C38-C39	9.67	1.56	1.33
25	a	608	BCR	C16-C17	9.68	1.73	1.43
25	B	618	BCR	C16-C17	9.73	1.73	1.43
25	h	101	BCR	C16-C17	9.75	1.73	1.43
25	t	101	BCR	C16-C17	9.77	1.73	1.43
25	f	101	BCR	C16-C17	9.82	1.73	1.43
25	b	620	BCR	C16-C17	9.85	1.73	1.43
25	b	621	BCR	C26-C25	9.87	1.51	1.34
25	C	521	BCR	C16-C17	9.96	1.74	1.43
25	B	619	BCR	C26-C25	10.18	1.52	1.34
25	H	101	BCR	C37-C22	10.22	1.73	1.50
25	F	101	BCR	C37-C22	10.30	1.73	1.50
26	d	404	PL9	C18-C19	10.32	1.58	1.33
26	D	405	PL9	C18-C19	10.33	1.58	1.33
26	A	610	PL9	C18-C19	10.34	1.58	1.33
25	T	101	BCR	C16-C17	10.35	1.75	1.43
25	B	620	BCR	C8-C7	10.39	1.65	1.33
26	a	609	PL9	C18-C19	10.39	1.58	1.33
25	C	521	BCR	C37-C22	10.43	1.73	1.50
25	C	514	BCR	C37-C22	10.50	1.73	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	522	BCR	C37-C22	10.52	1.73	1.50
25	c	515	BCR	C8-C7	10.55	1.65	1.33
25	C	514	BCR	C8-C7	10.56	1.65	1.33
25	b	622	BCR	C8-C7	10.59	1.65	1.33
25	h	101	BCR	C8-C7	10.61	1.65	1.33
25	C	521	BCR	C8-C7	10.67	1.65	1.33
25	H	101	BCR	C8-C7	10.70	1.66	1.33
25	T	101	BCR	C8-C7	10.71	1.66	1.33
25	B	619	BCR	C8-C7	10.80	1.66	1.33
25	b	621	BCR	C8-C7	10.83	1.66	1.33
25	c	522	BCR	C8-C7	10.85	1.66	1.33
25	f	101	BCR	C37-C22	10.87	1.74	1.50
25	b	620	BCR	C8-C7	10.91	1.66	1.33
25	B	618	BCR	C8-C7	10.93	1.66	1.33
25	t	101	BCR	C37-C22	10.94	1.74	1.50
25	k	101	BCR	C8-C7	10.95	1.66	1.33
25	K	101	BCR	C8-C7	10.96	1.66	1.33
25	a	608	BCR	C37-C22	10.96	1.74	1.50
25	C	515	BCR	C37-C22	10.97	1.74	1.50
25	H	101	BCR	C20-C21	10.97	1.77	1.43
25	F	101	BCR	C20-C21	11.00	1.77	1.43
25	C	515	BCR	C8-C7	11.01	1.66	1.33
25	t	101	BCR	C8-C7	11.02	1.66	1.33
25	b	620	BCR	C37-C22	11.02	1.74	1.50
25	A	609	BCR	C37-C22	11.08	1.75	1.50
25	F	101	BCR	C8-C7	11.08	1.67	1.33
25	a	608	BCR	C8-C7	11.11	1.67	1.33
25	B	619	BCR	C20-C21	11.12	1.77	1.43
25	c	515	BCR	C37-C22	11.12	1.75	1.50
25	f	101	BCR	C8-C7	11.15	1.67	1.33
25	k	101	BCR	C37-C22	11.16	1.75	1.50
25	C	521	BCR	C20-C21	11.17	1.77	1.43
25	A	609	BCR	C8-C7	11.21	1.67	1.33
25	C	515	BCR	C20-C21	11.24	1.77	1.43
25	c	516	BCR	C8-C7	11.26	1.67	1.33
25	c	515	BCR	C20-C21	11.27	1.78	1.43
25	c	516	BCR	C20-C21	11.30	1.78	1.43
25	K	101	BCR	C37-C22	11.32	1.75	1.50
25	c	516	BCR	C37-C22	11.35	1.75	1.50
25	B	620	BCR	C37-C22	11.42	1.75	1.50
25	h	101	BCR	C37-C22	11.42	1.75	1.50
25	b	620	BCR	C20-C21	11.43	1.78	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	522	BCR	C20-C21	11.44	1.78	1.43
25	C	514	BCR	C20-C21	11.49	1.78	1.43
25	b	621	BCR	C37-C22	11.51	1.76	1.50
25	h	101	BCR	C20-C21	11.57	1.78	1.43
25	B	620	BCR	C20-C21	11.61	1.79	1.43
25	T	101	BCR	C37-C22	11.61	1.76	1.50
25	k	101	BCR	C20-C21	11.66	1.79	1.43
25	A	609	BCR	C20-C21	11.67	1.79	1.43
25	b	622	BCR	C37-C22	11.71	1.76	1.50
25	f	101	BCR	C20-C21	11.72	1.79	1.43
25	b	621	BCR	C20-C21	11.73	1.79	1.43
25	b	622	BCR	C20-C21	11.85	1.79	1.43
25	t	101	BCR	C20-C21	11.87	1.79	1.43
25	a	608	BCR	C20-C21	11.90	1.79	1.43
25	B	619	BCR	C37-C22	11.90	1.76	1.50
25	B	618	BCR	C20-C21	11.90	1.79	1.43
25	T	101	BCR	C36-C18	12.01	1.77	1.50
25	K	101	BCR	C20-C21	12.04	1.80	1.43
25	F	101	BCR	C36-C18	12.09	1.77	1.50
25	K	101	BCR	C36-C18	12.10	1.77	1.50
25	T	101	BCR	C20-C21	12.14	1.80	1.43
25	b	621	BCR	C36-C18	12.18	1.77	1.50
25	B	618	BCR	C37-C22	12.30	1.77	1.50
25	h	101	BCR	C36-C18	12.31	1.77	1.50
25	B	618	BCR	C36-C18	12.57	1.78	1.50
25	B	620	BCR	C36-C18	12.67	1.78	1.50
25	b	621	BCR	C16-C15	12.75	1.68	1.35
25	C	514	BCR	C16-C15	12.77	1.68	1.35
25	b	620	BCR	C36-C18	12.84	1.78	1.50
25	c	515	BCR	C36-C18	12.87	1.78	1.50
25	B	619	BCR	C16-C15	12.88	1.69	1.35
25	t	101	BCR	C36-C18	12.89	1.79	1.50
25	A	609	BCR	C36-C18	12.90	1.79	1.50
25	c	516	BCR	C36-C18	12.92	1.79	1.50
25	f	101	BCR	C36-C18	12.93	1.79	1.50
25	B	620	BCR	C16-C15	12.94	1.69	1.35
25	F	101	BCR	C16-C15	12.96	1.69	1.35
25	c	515	BCR	C16-C15	13.01	1.69	1.35
25	C	515	BCR	C36-C18	13.03	1.79	1.50
25	C	515	BCR	C16-C15	13.03	1.69	1.35
25	k	101	BCR	C16-C15	13.04	1.69	1.35
25	c	522	BCR	C16-C15	13.06	1.69	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	521	BCR	C36-C18	13.07	1.79	1.50
25	c	522	BCR	C36-C18	13.09	1.79	1.50
25	a	608	BCR	C36-C18	13.10	1.79	1.50
25	H	101	BCR	C16-C15	13.12	1.69	1.35
25	c	516	BCR	C16-C15	13.14	1.69	1.35
25	k	101	BCR	C36-C18	13.14	1.79	1.50
25	b	622	BCR	C16-C15	13.19	1.70	1.35
25	f	101	BCR	C16-C15	13.20	1.70	1.35
25	b	620	BCR	C5-C6	13.22	1.57	1.34
25	a	608	BCR	C16-C15	13.31	1.70	1.35
25	h	101	BCR	C5-C6	13.31	1.57	1.34
25	b	622	BCR	C36-C18	13.33	1.79	1.50
25	B	618	BCR	C5-C6	13.33	1.57	1.34
25	b	620	BCR	C16-C15	13.36	1.70	1.35
25	C	514	BCR	C36-C18	13.39	1.80	1.50
25	H	101	BCR	C36-C18	13.42	1.80	1.50
25	H	101	BCR	C5-C6	13.43	1.57	1.34
25	A	609	BCR	C16-C15	13.47	1.70	1.35
25	h	101	BCR	C16-C15	13.48	1.70	1.35
25	F	101	BCR	C5-C6	13.52	1.57	1.34
25	B	618	BCR	C16-C15	13.53	1.70	1.35
25	f	101	BCR	C5-C6	13.56	1.57	1.34
25	t	101	BCR	C16-C15	13.58	1.71	1.35
25	K	101	BCR	C16-C15	13.60	1.71	1.35
25	a	608	BCR	C5-C6	13.72	1.58	1.34
25	C	521	BCR	C16-C15	13.73	1.71	1.35
25	A	609	BCR	C5-C6	13.74	1.58	1.34
25	C	521	BCR	C5-C6	13.76	1.58	1.34
25	c	522	BCR	C5-C6	13.76	1.58	1.34
25	T	101	BCR	C5-C6	13.80	1.58	1.34
25	c	516	BCR	C5-C6	13.87	1.58	1.34
25	C	515	BCR	C5-C6	13.89	1.58	1.34
25	T	101	BCR	C16-C15	14.11	1.72	1.35
25	B	620	BCR	C5-C6	14.11	1.58	1.34
25	K	101	BCR	C5-C6	14.13	1.58	1.34
25	k	101	BCR	C5-C6	14.21	1.59	1.34
25	B	619	BCR	C36-C18	14.24	1.81	1.50
25	b	622	BCR	C5-C6	14.40	1.59	1.34
25	c	515	BCR	C5-C6	14.54	1.59	1.34
25	t	101	BCR	C5-C6	14.55	1.59	1.34
25	C	514	BCR	C5-C6	14.64	1.59	1.34
25	b	621	BCR	C5-C6	14.80	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	619	BCR	C5-C6	14.82	1.60	1.34
25	H	101	BCR	C20-C19	15.31	1.73	1.34
25	C	521	BCR	C20-C19	15.31	1.73	1.34
25	h	101	BCR	C20-C19	15.41	1.73	1.34
25	F	101	BCR	C20-C19	15.42	1.73	1.34
25	B	619	BCR	C20-C19	15.52	1.73	1.34
25	c	515	BCR	C20-C19	15.56	1.74	1.34
25	C	515	BCR	C20-C19	15.56	1.74	1.34
25	c	522	BCR	C20-C19	15.60	1.74	1.34
25	b	620	BCR	C20-C19	15.82	1.74	1.34
25	c	516	BCR	C20-C19	15.82	1.74	1.34
25	A	609	BCR	C20-C19	15.83	1.74	1.34
25	f	101	BCR	C20-C19	15.85	1.74	1.34
25	B	620	BCR	C20-C19	15.85	1.74	1.34
25	a	608	BCR	C20-C19	15.90	1.74	1.34
25	b	621	BCR	C20-C19	15.92	1.74	1.34
25	k	101	BCR	C20-C19	15.95	1.75	1.34
25	t	101	BCR	C20-C19	15.98	1.75	1.34
25	T	101	BCR	C20-C19	16.05	1.75	1.34
25	b	622	BCR	C20-C19	16.19	1.75	1.34
25	C	514	BCR	C20-C19	16.23	1.75	1.34
25	K	101	BCR	C20-C19	16.23	1.75	1.34
25	B	618	BCR	C20-C19	16.41	1.76	1.34
25	b	620	BCR	C10-C9	19.75	1.62	1.35
25	B	618	BCR	C10-C9	19.86	1.62	1.35
25	B	619	BCR	C10-C9	20.01	1.62	1.35
25	b	621	BCR	C10-C9	20.08	1.62	1.35
25	C	514	BCR	C10-C9	20.21	1.62	1.35
25	F	101	BCR	C10-C9	20.44	1.62	1.35
25	H	101	BCR	C10-C9	20.47	1.62	1.35
25	K	101	BCR	C10-C9	20.47	1.62	1.35
25	f	101	BCR	C10-C9	20.49	1.62	1.35
25	c	515	BCR	C10-C9	20.54	1.63	1.35
25	C	515	BCR	C10-C9	20.61	1.63	1.35
25	C	521	BCR	C10-C9	20.66	1.63	1.35
25	B	620	BCR	C10-C9	20.68	1.63	1.35
25	k	101	BCR	C10-C9	20.98	1.63	1.35
25	h	101	BCR	C10-C9	20.98	1.63	1.35
25	c	516	BCR	C10-C9	21.00	1.63	1.35
25	a	608	BCR	C10-C9	21.04	1.63	1.35
25	c	522	BCR	C10-C9	21.10	1.63	1.35
25	T	101	BCR	C10-C9	21.12	1.63	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	t	101	BCR	C10-C9	21.20	1.63	1.35
25	b	622	BCR	C10-C9	21.23	1.63	1.35
25	A	609	BCR	C10-C9	21.24	1.63	1.35
25	c	515	BCR	C14-C13	25.64	1.69	1.35
25	C	514	BCR	C14-C13	25.68	1.69	1.35
25	B	619	BCR	C14-C13	26.07	1.70	1.35
25	B	618	BCR	C14-C13	26.17	1.70	1.35
25	f	101	BCR	C14-C13	26.45	1.70	1.35
25	h	101	BCR	C14-C13	26.49	1.70	1.35
25	b	620	BCR	C14-C13	26.51	1.70	1.35
25	b	621	BCR	C14-C13	26.52	1.70	1.35
25	B	620	BCR	C14-C13	26.55	1.71	1.35
25	H	101	BCR	C14-C13	26.65	1.71	1.35
25	k	101	BCR	C14-C13	26.65	1.71	1.35
25	K	101	BCR	C14-C13	26.69	1.71	1.35
25	b	622	BCR	C14-C13	26.87	1.71	1.35
25	c	516	BCR	C14-C13	27.24	1.71	1.35
25	F	101	BCR	C14-C13	27.27	1.71	1.35
25	c	522	BCR	C14-C13	27.28	1.71	1.35
25	T	101	BCR	C14-C13	27.32	1.72	1.35
25	C	515	BCR	C14-C13	27.41	1.72	1.35
25	t	101	BCR	C14-C13	27.47	1.72	1.35
25	C	521	BCR	C14-C13	27.51	1.72	1.35
25	a	608	BCR	C14-C13	27.64	1.72	1.35
25	A	609	BCR	C14-C13	27.78	1.72	1.35

All (2021) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	622	BCR	C38-C26-C25	-14.78	107.96	124.51
25	T	101	BCR	C33-C5-C6	-14.67	108.08	124.51
25	B	620	BCR	C38-C26-C25	-14.50	108.27	124.51
25	c	515	BCR	C38-C26-C25	-14.16	108.66	124.51
25	C	514	BCR	C38-C26-C25	-13.78	109.09	124.51
25	F	101	BCR	C33-C5-C6	-13.70	109.17	124.51
25	T	101	BCR	C38-C26-C25	-13.62	109.26	124.51
25	t	101	BCR	C38-C26-C25	-13.61	109.27	124.51
25	b	620	BCR	C33-C5-C6	-13.53	109.36	124.51
25	B	618	BCR	C38-C26-C25	-13.42	109.48	124.51
25	K	101	BCR	C38-C26-C25	-13.37	109.55	124.51
25	B	618	BCR	C33-C5-C6	-13.35	109.56	124.51
25	C	521	BCR	C33-C5-C6	-13.34	109.58	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	k	101	BCR	C38-C26-C25	-13.30	109.62	124.51
25	b	620	BCR	C15-C14-C13	-13.21	108.45	127.31
25	f	101	BCR	C33-C5-C6	-13.15	109.79	124.51
25	h	101	BCR	C33-C5-C6	-13.15	109.79	124.51
25	A	609	BCR	C33-C5-C6	-13.09	109.86	124.51
25	c	522	BCR	C33-C5-C6	-12.95	110.02	124.51
25	k	101	BCR	C33-C5-C6	-12.89	110.07	124.51
25	C	514	BCR	C16-C17-C18	-12.79	109.06	127.31
25	a	608	BCR	C33-C5-C6	-12.78	110.21	124.51
25	C	521	BCR	C38-C26-C25	-12.76	110.22	124.51
25	K	101	BCR	C33-C5-C6	-12.68	110.31	124.51
25	H	101	BCR	C33-C5-C6	-12.38	110.64	124.51
25	c	516	BCR	C33-C5-C6	-12.34	110.69	124.51
25	c	515	BCR	C16-C17-C18	-12.33	109.71	127.31
25	T	101	BCR	C24-C23-C22	-12.31	107.72	126.21
25	F	101	BCR	C16-C17-C18	-12.29	109.77	127.31
25	c	522	BCR	C38-C26-C25	-12.18	110.87	124.51
25	H	101	BCR	C16-C17-C18	-12.16	109.95	127.31
25	c	516	BCR	C38-C26-C25	-11.98	111.09	124.51
25	C	515	BCR	C38-C26-C25	-11.83	111.27	124.51
25	C	514	BCR	C24-C23-C22	-11.67	108.68	126.21
25	B	618	BCR	C11-C10-C9	-11.47	110.94	127.31
25	b	620	BCR	C11-C10-C9	-11.41	111.03	127.31
25	B	620	BCR	C16-C17-C18	-11.30	111.18	127.31
25	h	101	BCR	C16-C17-C18	-10.95	111.69	127.31
25	h	101	BCR	C38-C26-C25	-10.94	112.26	124.51
25	B	619	BCR	C16-C17-C18	-10.91	111.74	127.31
25	c	515	BCR	C24-C23-C22	-10.77	110.03	126.21
25	B	620	BCR	C33-C5-C6	-10.76	112.47	124.51
25	c	515	BCR	C33-C5-C6	-10.73	112.50	124.51
25	t	101	BCR	C33-C5-C6	-10.73	112.50	124.51
25	B	618	BCR	C15-C14-C13	-10.70	112.04	127.31
25	C	515	BCR	C33-C5-C6	-10.68	112.56	124.51
25	C	515	BCR	C24-C23-C22	-10.57	110.33	126.21
25	b	620	BCR	C38-C26-C25	-10.56	112.69	124.51
25	H	101	BCR	C38-C26-C25	-10.53	112.72	124.51
25	b	622	BCR	C33-C5-C6	-10.49	112.77	124.51
25	F	101	BCR	C24-C23-C22	-10.48	110.46	126.21
25	C	514	BCR	C33-C5-C6	-10.44	112.82	124.51
25	b	621	BCR	C33-C5-C6	-10.41	112.86	124.51
25	A	609	BCR	C38-C26-C25	-10.37	112.90	124.51
25	B	619	BCR	C11-C10-C9	-10.30	112.61	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	608	BCR	C38-C26-C25	-10.23	113.06	124.51
25	k	101	BCR	C16-C17-C18	-10.13	112.86	127.31
25	t	101	BCR	C24-C23-C22	-10.00	111.18	126.21
25	B	620	BCR	C15-C14-C13	-9.99	113.06	127.31
25	C	521	BCR	C16-C17-C18	-9.93	113.14	127.31
25	c	516	BCR	C24-C23-C22	-9.77	111.53	126.21
26	d	404	PL9	C7-C8-C9	-9.68	110.39	126.79
25	A	609	BCR	C16-C17-C18	-9.64	113.55	127.31
25	b	622	BCR	C24-C23-C22	-9.61	111.78	126.21
25	f	101	BCR	C30-C25-C26	-9.58	109.12	122.59
26	D	405	PL9	C7-C8-C9	-9.56	110.59	126.79
25	B	619	BCR	C33-C5-C6	-9.52	113.85	124.51
25	b	622	BCR	C15-C14-C13	-9.52	113.72	127.31
25	b	621	BCR	C24-C23-C22	-9.34	112.19	126.21
25	B	619	BCR	C24-C23-C22	-9.30	112.24	126.21
25	C	515	BCR	C7-C8-C9	-9.27	112.29	126.21
25	f	101	BCR	C11-C10-C9	-9.20	114.18	127.31
25	B	620	BCR	C8-C7-C6	-9.19	101.53	127.25
25	b	621	BCR	C16-C17-C18	-9.14	114.26	127.31
25	c	522	BCR	C24-C23-C22	-9.12	112.51	126.21
25	F	101	BCR	C7-C8-C9	-9.10	112.54	126.21
25	K	101	BCR	C11-C10-C9	-9.08	114.36	127.31
25	c	522	BCR	C16-C17-C18	-9.03	114.42	127.31
25	F	101	BCR	C30-C25-C26	-9.01	109.92	122.59
25	H	101	BCR	C15-C14-C13	-8.99	114.48	127.31
25	C	515	BCR	C4-C5-C6	-8.96	109.58	122.74
25	K	101	BCR	C16-C17-C18	-8.89	114.62	127.31
25	C	521	BCR	C24-C23-C22	-8.87	112.89	126.21
25	C	515	BCR	C11-C10-C9	-8.84	114.69	127.31
25	b	621	BCR	C15-C14-C13	-8.74	114.83	127.31
25	c	516	BCR	C16-C17-C18	-8.74	114.84	127.31
25	C	514	BCR	C8-C7-C6	-8.64	103.07	127.25
25	h	101	BCR	C24-C23-C22	-8.54	113.37	126.21
25	b	621	BCR	C11-C10-C9	-8.54	115.13	127.31
25	c	522	BCR	C20-C21-C22	-8.50	115.18	127.31
25	a	608	BCR	C16-C17-C18	-8.48	115.21	127.31
25	f	101	BCR	C16-C17-C18	-8.43	115.28	127.31
25	b	621	BCR	C38-C26-C25	-8.37	115.14	124.51
25	f	101	BCR	C24-C23-C22	-8.31	113.72	126.21
25	f	101	BCR	C7-C8-C9	-8.28	113.76	126.21
25	B	618	BCR	C7-C8-C9	-8.25	113.82	126.21
25	c	515	BCR	C15-C14-C13	-8.22	115.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	101	BCR	C30-C25-C26	-8.20	111.07	122.59
25	C	515	BCR	C27-C26-C25	-8.18	110.73	122.74
25	F	101	BCR	C38-C26-C25	-8.15	115.39	124.51
25	b	620	BCR	C7-C8-C9	-8.13	114.00	126.21
25	b	622	BCR	C8-C7-C6	-8.11	104.55	127.25
25	B	618	BCR	C20-C21-C22	-8.09	115.77	127.31
25	C	514	BCR	C15-C14-C13	-8.08	115.78	127.31
25	t	101	BCR	C30-C25-C26	-8.07	111.25	122.59
25	B	620	BCR	C24-C23-C22	-8.07	114.09	126.21
25	T	101	BCR	C7-C6-C5	-8.01	102.44	121.54
25	h	101	BCR	C15-C14-C13	-7.93	115.99	127.31
25	B	620	BCR	C8-C9-C10	-7.92	106.79	118.94
25	a	608	BCR	C11-C10-C9	-7.92	116.01	127.31
25	F	101	BCR	C11-C10-C9	-7.92	116.01	127.31
25	c	516	BCR	C4-C5-C6	-7.91	111.12	122.74
25	c	516	BCR	C27-C26-C25	-7.90	111.14	122.74
25	b	620	BCR	C4-C5-C6	-7.88	111.17	122.74
25	T	101	BCR	C30-C25-C26	-7.80	111.63	122.59
25	B	619	BCR	C15-C14-C13	-7.80	116.18	127.31
25	a	608	BCR	C24-C23-C22	-7.77	114.54	126.21
25	f	101	BCR	C15-C14-C13	-7.77	116.23	127.31
25	B	619	BCR	C7-C8-C9	-7.73	114.59	126.21
25	t	101	BCR	C11-C10-C9	-7.73	116.28	127.31
25	K	101	BCR	C27-C26-C25	-7.71	111.43	122.74
25	T	101	BCR	C27-C26-C25	-7.67	111.49	122.74
25	a	608	BCR	C1-C6-C5	-7.66	111.83	122.59
25	f	101	BCR	C38-C26-C25	-7.64	115.96	124.51
25	a	608	BCR	C4-C5-C6	-7.61	111.58	122.74
25	k	101	BCR	C30-C25-C26	-7.60	111.92	122.59
25	B	618	BCR	C4-C5-C6	-7.58	111.61	122.74
25	F	101	BCR	C20-C21-C22	-7.54	116.55	127.31
25	b	620	BCR	C1-C6-C5	-7.47	112.09	122.59
25	h	101	BCR	C4-C5-C6	-7.43	111.83	122.74
25	C	515	BCR	C1-C6-C5	-7.42	112.16	122.59
25	c	515	BCR	C11-C10-C9	-7.39	116.76	127.31
26	A	610	PL9	C37-C38-C39	-7.37	109.42	127.66
25	c	515	BCR	C30-C25-C26	-7.37	112.23	122.59
25	H	101	BCR	C4-C5-C6	-7.29	112.04	122.74
25	B	620	BCR	C30-C25-C26	-7.28	112.36	122.59
25	t	101	BCR	C27-C26-C25	-7.22	112.15	122.74
26	a	609	PL9	C7-C8-C9	-7.18	114.63	126.79
25	A	609	BCR	C1-C6-C5	-7.18	112.51	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	BCR	C4-C5-C6	-7.17	112.21	122.74
26	a	609	PL9	C37-C38-C39	-7.17	109.91	127.66
25	C	515	BCR	C16-C17-C18	-7.15	117.10	127.31
25	A	609	BCR	C24-C23-C22	-7.12	115.51	126.21
25	F	101	BCR	C36-C18-C17	-7.12	112.95	122.92
25	c	516	BCR	C1-C6-C5	-7.11	112.59	122.59
25	A	609	BCR	C11-C10-C9	-7.11	117.17	127.31
25	B	618	BCR	C1-C6-C5	-7.08	112.64	122.59
25	H	101	BCR	C24-C23-C22	-7.06	115.60	126.21
25	f	101	BCR	C27-C26-C25	-6.98	112.49	122.74
25	K	101	BCR	C15-C14-C13	-6.98	117.34	127.31
25	c	522	BCR	C30-C25-C26	-6.97	112.80	122.59
25	C	521	BCR	C30-C25-C26	-6.95	112.83	122.59
26	d	404	PL9	C32-C33-C34	-6.90	110.58	127.66
25	C	514	BCR	C8-C9-C10	-6.88	108.38	118.94
25	c	515	BCR	C27-C26-C25	-6.84	112.69	122.74
25	k	101	BCR	C27-C26-C25	-6.82	112.72	122.74
25	t	101	BCR	C15-C14-C13	-6.82	117.58	127.31
25	A	609	BCR	C15-C14-C13	-6.80	117.60	127.31
25	c	515	BCR	C8-C7-C6	-6.80	108.20	127.25
26	d	404	PL9	C12-C13-C14	-6.80	110.84	127.66
25	f	101	BCR	C1-C6-C5	-6.79	113.05	122.59
25	C	521	BCR	C20-C21-C22	-6.78	117.63	127.31
26	A	610	PL9	C27-C28-C29	-6.75	110.95	127.66
26	A	610	PL9	C7-C8-C9	-6.74	115.37	126.79
25	F	101	BCR	C4-C5-C6	-6.73	112.87	122.74
26	d	404	PL9	C27-C28-C29	-6.69	111.11	127.66
25	k	101	BCR	C15-C14-C13	-6.68	117.77	127.31
26	A	610	PL9	C16-C14-C13	-6.68	107.51	121.10
25	c	515	BCR	C7-C8-C9	-6.64	116.24	126.21
26	a	609	PL9	C16-C14-C13	-6.63	107.60	121.10
26	D	405	PL9	C27-C28-C29	-6.61	111.30	127.66
25	C	514	BCR	C30-C25-C26	-6.59	113.33	122.59
25	F	101	BCR	C1-C6-C5	-6.58	113.34	122.59
25	f	101	BCR	C4-C5-C6	-6.55	113.13	122.74
26	A	610	PL9	C42-C43-C44	-6.55	111.46	127.66
26	a	609	PL9	C27-C28-C29	-6.53	111.49	127.66
26	a	609	PL9	C42-C43-C44	-6.53	111.51	127.66
25	B	618	BCR	C30-C25-C26	-6.52	113.43	122.59
26	D	405	PL9	C16-C14-C13	-6.50	107.86	121.10
25	C	521	BCR	C15-C14-C13	-6.49	118.04	127.31
25	b	620	BCR	C23-C24-C25	-6.44	109.22	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	609	PL9	C22-C23-C24	-6.41	111.79	127.66
25	b	622	BCR	C30-C25-C26	-6.41	113.58	122.59
25	B	620	BCR	C4-C5-C6	-6.41	113.33	122.74
25	b	622	BCR	C8-C9-C10	-6.41	109.11	118.94
25	c	522	BCR	C27-C26-C25	-6.40	113.34	122.74
25	C	521	BCR	C8-C7-C6	-6.40	109.34	127.25
25	C	521	BCR	C11-C10-C9	-6.39	118.18	127.31
26	D	405	PL9	C32-C33-C34	-6.38	111.88	127.66
25	K	101	BCR	C34-C9-C10	-6.37	113.99	122.92
25	c	516	BCR	C11-C10-C9	-6.37	118.21	127.31
25	T	101	BCR	C11-C10-C9	-6.36	118.23	127.31
26	A	610	PL9	C17-C18-C19	-6.36	111.93	127.66
25	k	101	BCR	C34-C9-C10	-6.35	114.02	122.92
25	F	101	BCR	C27-C26-C25	-6.35	113.42	122.74
25	H	101	BCR	C1-C6-C5	-6.35	113.67	122.59
25	K	101	BCR	C24-C23-C22	-6.35	116.67	126.21
26	a	609	PL9	C17-C18-C19	-6.34	111.98	127.66
26	D	405	PL9	C12-C13-C14	-6.33	111.99	127.66
25	a	608	BCR	C20-C21-C22	-6.32	118.29	127.31
26	d	404	PL9	C16-C14-C13	-6.27	108.34	121.10
25	b	620	BCR	C38-C26-C27	-6.25	101.75	113.56
26	A	610	PL9	C22-C23-C24	-6.24	112.22	127.66
25	b	622	BCR	C16-C17-C18	-6.23	118.42	127.31
25	c	516	BCR	C30-C25-C26	-6.22	113.84	122.59
25	C	521	BCR	C4-C5-C6	-6.20	113.63	122.74
25	c	516	BCR	C7-C8-C9	-6.20	116.89	126.21
25	h	101	BCR	C1-C6-C5	-6.18	113.90	122.59
25	c	522	BCR	C4-C5-C6	-6.17	113.68	122.74
25	c	522	BCR	C8-C7-C6	-6.17	109.98	127.25
25	C	515	BCR	C30-C25-C26	-6.17	113.92	122.59
25	C	521	BCR	C27-C26-C25	-6.14	113.72	122.74
25	B	618	BCR	C24-C23-C22	-6.14	116.99	126.21
25	B	618	BCR	C27-C26-C25	-6.12	113.76	122.74
25	H	101	BCR	C7-C8-C9	-6.11	117.04	126.21
25	C	514	BCR	C27-C26-C25	-6.08	113.81	122.74
25	k	101	BCR	C1-C6-C5	-6.07	114.06	122.59
25	t	101	BCR	C16-C17-C18	-6.06	118.66	127.31
25	B	619	BCR	C38-C26-C27	-6.04	102.15	113.56
26	a	609	PL9	C11-C9-C8	-6.03	108.83	121.10
25	T	101	BCR	C20-C21-C22	-6.02	118.72	127.31
25	c	515	BCR	C20-C21-C22	-6.02	118.72	127.31
26	d	404	PL9	C17-C18-C19	-6.02	112.78	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	522	BCR	C11-C10-C9	-6.01	118.73	127.31
26	D	405	PL9	C11-C9-C8	-6.00	108.89	121.10
25	B	620	BCR	C27-C26-C25	-5.99	113.95	122.74
25	K	101	BCR	C8-C7-C6	-5.97	110.53	127.25
25	k	101	BCR	C8-C7-C6	-5.97	110.53	127.25
25	t	101	BCR	C8-C7-C6	-5.97	110.54	127.25
26	D	405	PL9	C17-C18-C19	-5.95	112.95	127.66
25	f	101	BCR	C36-C18-C17	-5.94	114.61	122.92
26	a	609	PL9	C45-C44-C43	-5.94	108.10	123.70
26	A	610	PL9	C11-C9-C8	-5.91	109.06	121.10
26	A	610	PL9	C45-C44-C43	-5.91	108.17	123.70
25	T	101	BCR	C7-C8-C9	-5.90	117.35	126.21
26	d	404	PL9	C22-C23-C24	-5.87	113.14	127.66
26	a	609	PL9	C12-C13-C14	-5.85	113.18	127.66
25	k	101	BCR	C11-C10-C9	-5.84	118.97	127.31
25	c	522	BCR	C36-C18-C17	-5.84	114.75	122.92
25	b	622	BCR	C4-C5-C6	-5.83	114.18	122.74
26	D	405	PL9	C22-C23-C24	-5.81	113.28	127.66
25	B	619	BCR	C38-C26-C25	-5.81	118.01	124.51
25	c	522	BCR	C7-C6-C5	-5.80	107.70	121.54
26	d	404	PL9	C46-C44-C43	-5.80	109.30	121.10
26	a	609	PL9	C40-C39-C38	-5.78	108.52	123.70
26	d	404	PL9	C11-C9-C8	-5.77	109.37	121.10
25	C	521	BCR	C7-C6-C5	-5.75	107.82	121.54
25	k	101	BCR	C24-C23-C22	-5.75	117.57	126.21
25	c	522	BCR	C1-C6-C5	-5.74	114.53	122.59
26	a	609	PL9	C32-C33-C34	-5.74	113.46	127.66
26	D	405	PL9	C37-C38-C39	-5.73	113.48	127.66
26	a	609	PL9	C26-C24-C23	-5.71	109.48	121.10
26	A	610	PL9	C10-C9-C8	-5.71	108.71	123.70
25	H	101	BCR	C11-C10-C9	-5.70	119.17	127.31
26	d	404	PL9	C21-C19-C18	-5.70	109.51	121.10
26	D	405	PL9	C30-C29-C28	-5.69	108.75	123.70
26	d	404	PL9	C42-C43-C44	-5.67	113.64	127.66
25	c	515	BCR	C24-C25-C26	-5.66	108.05	121.54
25	A	609	BCR	C30-C25-C26	-5.65	114.65	122.59
25	C	514	BCR	C16-C15-C14	-5.65	111.40	123.46
26	d	404	PL9	C37-C38-C39	-5.62	113.75	127.66
26	D	405	PL9	C21-C19-C18	-5.61	109.67	121.10
25	c	515	BCR	C4-C5-C6	-5.60	114.52	122.74
26	A	610	PL9	C12-C13-C14	-5.59	113.82	127.66
26	a	609	PL9	C25-C24-C23	-5.58	109.04	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	622	BCR	C20-C21-C22	-5.56	119.38	127.31
26	a	609	PL9	C46-C44-C43	-5.56	109.79	121.10
25	c	515	BCR	C7-C6-C5	-5.55	108.31	121.54
25	b	620	BCR	C27-C26-C25	-5.54	114.60	122.74
25	h	101	BCR	C8-C7-C6	-5.53	111.76	127.25
26	A	610	PL9	C26-C24-C23	-5.53	109.84	121.10
26	a	609	PL9	C10-C9-C8	-5.53	109.18	123.70
25	K	101	BCR	C7-C8-C9	-5.52	117.91	126.21
25	F	101	BCR	C15-C14-C13	-5.50	119.45	127.31
25	b	622	BCR	C27-C26-C25	-5.50	114.66	122.74
25	C	514	BCR	C11-C10-C9	-5.50	119.46	127.31
25	a	608	BCR	C30-C25-C26	-5.50	114.86	122.59
25	h	101	BCR	C23-C24-C25	-5.49	111.87	127.25
25	H	101	BCR	C27-C26-C25	-5.49	114.68	122.74
25	H	101	BCR	C7-C6-C5	-5.49	108.46	121.54
26	A	610	PL9	C40-C39-C38	-5.47	109.32	123.70
25	b	621	BCR	C12-C13-C14	-5.47	110.55	118.94
25	C	515	BCR	C20-C21-C22	-5.46	119.52	127.31
26	a	609	PL9	C15-C14-C13	-5.45	109.38	123.70
25	C	521	BCR	C36-C18-C17	-5.44	115.30	122.92
26	d	404	PL9	C10-C9-C8	-5.44	109.41	123.70
26	d	404	PL9	C30-C29-C28	-5.43	109.42	123.70
26	D	405	PL9	C42-C43-C44	-5.43	114.22	127.66
25	c	522	BCR	C15-C14-C13	-5.43	119.56	127.31
25	C	521	BCR	C1-C6-C5	-5.42	114.98	122.59
25	T	101	BCR	C4-C5-C6	-5.38	114.84	122.74
25	H	101	BCR	C23-C24-C25	-5.38	112.20	127.25
25	c	516	BCR	C15-C14-C13	-5.36	119.66	127.31
25	C	521	BCR	C7-C8-C9	-5.36	118.16	126.21
25	t	101	BCR	C7-C6-C5	-5.35	108.78	121.54
25	B	618	BCR	C37-C22-C21	-5.34	115.44	122.92
25	T	101	BCR	C15-C14-C13	-5.31	119.73	127.31
25	a	608	BCR	C15-C14-C13	-5.31	119.73	127.31
26	d	404	PL9	C15-C14-C13	-5.30	109.78	123.70
26	D	405	PL9	C46-C44-C43	-5.28	110.36	121.10
25	C	514	BCR	C20-C21-C22	-5.27	119.79	127.31
25	h	101	BCR	C27-C26-C25	-5.26	115.02	122.74
25	C	514	BCR	C24-C25-C26	-5.25	109.01	121.54
26	D	405	PL9	C45-C44-C43	-5.24	109.93	123.70
25	b	620	BCR	C11-C12-C13	-5.23	111.71	126.42
25	b	621	BCR	C38-C26-C27	-5.22	103.69	113.56
25	t	101	BCR	C4-C5-C6	-5.21	115.09	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	101	BCR	C1-C6-C5	-5.20	115.28	122.59
25	T	101	BCR	C23-C24-C25	-5.19	112.71	127.25
25	b	621	BCR	C1-C6-C5	-5.19	115.30	122.59
26	A	610	PL9	C25-C24-C23	-5.16	110.13	123.70
25	B	619	BCR	C1-C6-C5	-5.16	115.34	122.59
25	C	515	BCR	C15-C14-C13	-5.15	119.97	127.31
25	h	101	BCR	C7-C6-C5	-5.15	109.27	121.54
26	A	610	PL9	C30-C29-C28	-5.13	110.22	123.70
26	A	610	PL9	C15-C14-C13	-5.13	110.23	123.70
25	b	621	BCR	C7-C8-C9	-5.12	118.51	126.21
25	B	618	BCR	C8-C7-C6	-5.11	112.95	127.25
26	D	405	PL9	C15-C14-C13	-5.11	110.28	123.70
26	D	405	PL9	C10-C9-C8	-5.09	110.33	123.70
25	K	101	BCR	C23-C22-C21	-5.09	111.14	118.94
25	b	622	BCR	C7-C6-C5	-5.08	109.42	121.54
26	a	609	PL9	C35-C34-C33	-5.03	110.49	123.70
25	C	514	BCR	C7-C6-C5	-5.02	109.56	121.54
25	K	101	BCR	C7-C6-C5	-5.02	109.57	121.54
26	d	404	PL9	C45-C44-C43	-5.01	110.53	123.70
25	C	514	BCR	C23-C24-C25	-4.97	113.33	127.25
25	K	101	BCR	C4-C5-C6	-4.96	115.46	122.74
25	B	620	BCR	C7-C6-C5	-4.95	109.73	121.54
26	D	405	PL9	C31-C29-C28	-4.95	111.03	121.10
25	c	515	BCR	C34-C9-C10	-4.95	116.00	122.92
25	a	608	BCR	C7-C8-C9	-4.93	118.80	126.21
26	D	405	PL9	C25-C24-C23	-4.92	110.76	123.70
26	A	610	PL9	C32-C33-C34	-4.92	115.48	127.66
25	B	618	BCR	C23-C24-C25	-4.91	113.50	127.25
26	d	404	PL9	C41-C39-C38	-4.91	111.11	121.10
25	k	101	BCR	C7-C6-C5	-4.89	109.88	121.54
25	T	101	BCR	C8-C7-C6	-4.88	113.58	127.25
25	t	101	BCR	C24-C25-C26	-4.88	109.91	121.54
25	C	514	BCR	C4-C5-C6	-4.85	115.61	122.74
26	A	610	PL9	C21-C19-C18	-4.85	111.22	121.10
26	A	610	PL9	C46-C44-C43	-4.85	111.22	121.10
25	T	101	BCR	C37-C22-C21	-4.85	116.13	122.92
26	a	609	PL9	C20-C19-C18	-4.85	110.96	123.70
26	d	404	PL9	C40-C39-C38	-4.84	110.97	123.70
25	B	618	BCR	C7-C6-C5	-4.84	109.99	121.54
25	F	101	BCR	C12-C13-C14	-4.83	111.53	118.94
25	B	618	BCR	C38-C26-C27	-4.81	104.46	113.56
25	c	516	BCR	C38-C26-C27	-4.80	104.48	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	PL9	C20-C19-C18	-4.80	111.10	123.70
26	a	609	PL9	C41-C39-C38	-4.77	111.39	121.10
26	A	610	PL9	C20-C19-C18	-4.77	111.18	123.70
25	b	620	BCR	C30-C25-C26	-4.77	115.89	122.59
26	A	610	PL9	C35-C34-C33	-4.75	111.22	123.70
26	a	609	PL9	C30-C29-C28	-4.75	111.23	123.70
26	a	609	PL9	C21-C19-C18	-4.74	111.45	121.10
25	c	515	BCR	C23-C24-C25	-4.74	113.98	127.25
25	b	621	BCR	C34-C9-C10	-4.74	116.29	122.92
26	D	405	PL9	C35-C34-C33	-4.73	111.28	123.70
26	d	404	PL9	C25-C24-C23	-4.70	111.36	123.70
25	t	101	BCR	C23-C24-C25	-4.64	114.25	127.25
33	e	102	HEM	CBD-CAD-C3D	-4.64	103.62	112.47
25	a	608	BCR	C8-C7-C6	-4.63	114.30	127.25
25	k	101	BCR	C4-C5-C6	-4.60	115.99	122.74
25	b	620	BCR	C8-C7-C6	-4.58	114.43	127.25
26	d	404	PL9	C26-C24-C23	-4.57	111.79	121.10
25	B	620	BCR	C31-C1-C6	-4.57	102.89	110.31
25	c	522	BCR	C38-C26-C27	-4.56	104.93	113.56
25	b	622	BCR	C38-C26-C27	-4.56	104.94	113.56
25	b	620	BCR	C7-C6-C5	-4.55	110.69	121.54
26	D	405	PL9	C26-C24-C23	-4.55	111.85	121.10
26	d	404	PL9	C47-C48-C49	-4.54	112.07	127.84
25	H	101	BCR	C20-C21-C22	-4.52	120.86	127.31
25	h	101	BCR	C35-C13-C14	-4.51	116.60	122.92
25	A	609	BCR	C7-C6-C5	-4.51	110.78	121.54
25	F	101	BCR	C7-C6-C5	-4.50	110.80	121.54
25	B	619	BCR	C30-C25-C26	-4.49	116.28	122.59
26	A	610	PL9	C50-C49-C48	-4.48	109.40	122.65
25	k	101	BCR	C38-C26-C27	-4.48	105.10	113.56
25	T	101	BCR	C24-C25-C26	-4.47	110.87	121.54
26	d	404	PL9	C20-C19-C18	-4.46	111.98	123.70
26	D	405	PL9	C47-C48-C49	-4.46	112.37	127.84
23	b	605	CLA	C1B-CHB-C4A	-4.45	121.30	130.12
26	D	405	PL9	C40-C39-C38	-4.45	112.01	123.70
33	E	102	HEM	CBD-CAD-C3D	-4.45	103.98	112.47
25	B	620	BCR	C38-C26-C27	-4.45	105.16	113.56
26	D	405	PL9	C41-C39-C38	-4.44	112.07	121.10
25	B	618	BCR	C11-C12-C13	-4.43	113.97	126.42
25	a	608	BCR	C7-C6-C5	-4.43	110.97	121.54
25	C	515	BCR	C38-C26-C27	-4.43	105.19	113.56
25	h	101	BCR	C24-C25-C26	-4.42	110.99	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	BCR	C36-C18-C17	-4.41	116.74	122.92
25	B	620	BCR	C23-C24-C25	-4.40	114.92	127.25
25	k	101	BCR	C23-C24-C25	-4.40	114.94	127.25
25	H	101	BCR	C38-C26-C27	-4.39	105.26	113.56
25	h	101	BCR	C8-C9-C10	-4.38	112.22	118.94
23	B	603	CLA	C1B-CHB-C4A	-4.37	121.46	130.12
25	f	101	BCR	C7-C6-C5	-4.37	111.11	121.54
26	a	609	PL9	C36-C34-C33	-4.36	112.22	121.10
25	H	101	BCR	C24-C25-C26	-4.36	111.15	121.54
25	B	619	BCR	C4-C5-C6	-4.32	116.40	122.74
25	h	101	BCR	C20-C21-C22	-4.30	121.17	127.31
25	A	609	BCR	C7-C8-C9	-4.30	119.75	126.21
25	B	620	BCR	C37-C22-C21	-4.28	116.92	122.92
25	t	101	BCR	C20-C21-C22	-4.28	121.20	127.31
25	C	521	BCR	C24-C25-C26	-4.28	111.34	121.54
25	H	101	BCR	C34-C9-C10	-4.27	116.95	122.92
25	A	609	BCR	C8-C7-C6	-4.26	115.31	127.25
25	b	622	BCR	C31-C1-C6	-4.26	103.40	110.31
25	K	101	BCR	C38-C26-C27	-4.25	105.53	113.56
25	h	101	BCR	C38-C26-C27	-4.24	105.54	113.56
25	b	622	BCR	C35-C13-C14	-4.24	116.98	122.92
25	k	101	BCR	C35-C13-C14	-4.23	116.99	122.92
25	c	515	BCR	C31-C1-C6	-4.22	103.47	110.31
25	b	620	BCR	C24-C23-C22	-4.21	119.88	126.21
26	d	404	PL9	C31-C29-C28	-4.21	112.54	121.10
25	T	101	BCR	C1-C6-C5	-4.17	116.73	122.59
25	C	515	BCR	C37-C22-C21	-4.17	117.08	122.92
23	b	612	CLA	C1B-CHB-C4A	-4.16	121.88	130.12
25	C	521	BCR	C38-C26-C27	-4.16	105.71	113.56
26	a	609	PL9	C31-C29-C28	-4.13	112.69	121.10
25	c	522	BCR	C7-C8-C9	-4.13	120.01	126.21
26	A	610	PL9	C51-C49-C48	-4.10	110.55	122.65
23	C	506	CLA	C1B-CHB-C4A	-4.09	122.02	130.12
25	B	618	BCR	C24-C25-C26	-4.08	111.81	121.54
25	c	516	BCR	C7-C6-C5	-4.08	111.81	121.54
25	H	101	BCR	C8-C7-C6	-4.06	115.87	127.25
25	c	522	BCR	C24-C25-C26	-4.06	111.86	121.54
23	D	403	CLA	C1B-CHB-C4A	-4.06	122.08	130.12
26	A	610	PL9	C41-C39-C38	-4.04	112.88	121.10
25	c	516	BCR	C34-C9-C10	-4.04	117.27	122.92
26	a	609	PL9	C47-C48-C49	-4.03	113.84	127.84
25	b	621	BCR	C30-C25-C26	-4.02	116.94	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	514	BCR	C31-C1-C6	-4.02	103.78	110.31
23	b	607	CLA	C1C-NC-C4C	-4.01	104.79	107.05
25	c	515	BCR	C16-C15-C14	-3.94	115.04	123.46
26	A	610	PL9	C47-C48-C49	-3.94	114.16	127.84
25	B	620	BCR	C24-C25-C26	-3.93	112.16	121.54
23	a	613	CLA	C1B-CHB-C4A	-3.91	122.37	130.12
26	A	610	PL9	C36-C34-C33	-3.91	113.14	121.10
23	d	402	CLA	C1B-CHB-C4A	-3.90	122.39	130.12
26	D	405	PL9	C36-C34-C33	-3.90	113.17	121.10
23	b	614	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
25	C	515	BCR	C33-C5-C4	-3.89	106.21	113.56
25	F	101	BCR	C8-C7-C6	-3.89	116.37	127.25
25	B	620	BCR	C20-C21-C22	-3.88	121.77	127.31
23	B	611	CLA	C1B-CHB-C4A	-3.88	122.44	130.12
25	K	101	BCR	C23-C24-C25	-3.87	116.43	127.25
25	B	619	BCR	C36-C18-C17	-3.85	117.53	122.92
23	B	610	CLA	C1B-CHB-C4A	-3.85	122.50	130.12
25	F	101	BCR	C33-C5-C4	-3.84	106.31	113.56
23	B	605	CLA	C1C-NC-C4C	-3.84	104.89	107.05
25	b	622	BCR	C23-C24-C25	-3.83	116.52	127.25
25	h	101	BCR	C31-C1-C6	-3.83	104.09	110.31
25	b	621	BCR	C20-C21-C22	-3.82	121.86	127.31
25	h	101	BCR	C7-C8-C9	-3.81	120.48	126.21
25	C	521	BCR	C23-C24-C25	-3.81	116.59	127.25
23	C	505	CLA	C1B-CHB-C4A	-3.81	122.58	130.12
25	b	622	BCR	C24-C25-C26	-3.80	112.48	121.54
25	k	101	BCR	C24-C25-C26	-3.80	112.49	121.54
23	B	605	CLA	O1D-CGD-CBD	-3.79	117.55	124.58
33	v	201	HEM	CBA-CAA-C2A	-3.79	105.24	112.48
25	B	620	BCR	C11-C10-C9	-3.78	121.91	127.31
23	B	609	CLA	C1B-CHB-C4A	-3.78	122.63	130.12
23	b	613	CLA	C1B-CHB-C4A	-3.78	122.64	130.12
23	B	612	CLA	CMB-C2B-C1B	-3.77	122.66	128.46
25	b	621	BCR	C4-C5-C6	-3.77	117.21	122.74
23	c	509	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
23	A	605	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
26	d	404	PL9	C50-C49-C48	-3.76	111.53	122.65
25	k	101	BCR	C23-C22-C21	-3.76	113.17	118.94
23	C	504	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
23	c	507	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
23	c	506	CLA	C1B-CHB-C4A	-3.76	122.68	130.12
23	a	607	CLA	C1B-CHB-C4A	-3.74	122.70	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	516	BCR	C8-C7-C6	-3.74	116.78	127.25
23	c	504	CLA	C1B-CHB-C4A	-3.74	122.71	130.12
25	f	101	BCR	C8-C7-C6	-3.73	116.81	127.25
25	b	620	BCR	C20-C21-C22	-3.73	121.99	127.31
26	a	609	PL9	C40-C39-C41	-3.72	108.88	115.29
25	B	618	BCR	C34-C9-C10	-3.72	117.72	122.92
25	H	101	BCR	C33-C5-C4	-3.71	106.54	113.56
23	b	611	CLA	C1B-CHB-C4A	-3.71	122.76	130.12
25	H	101	BCR	C30-C25-C26	-3.71	117.38	122.59
26	A	610	PL9	C40-C39-C41	-3.71	108.89	115.29
26	A	610	PL9	C15-C14-C16	-3.71	108.89	115.29
25	K	101	BCR	C12-C13-C14	-3.70	113.27	118.94
25	c	515	BCR	C3-C4-C5	-3.69	107.51	113.99
26	d	404	PL9	C45-C44-C46	-3.69	108.92	115.29
23	c	505	CLA	C1B-CHB-C4A	-3.69	122.82	130.12
25	A	609	BCR	C23-C22-C21	-3.69	113.29	118.94
26	a	609	PL9	C50-C49-C48	-3.68	111.77	122.65
23	C	513	CLA	C1B-CHB-C4A	-3.68	122.82	130.12
25	B	619	BCR	C34-C9-C10	-3.68	117.77	122.92
25	B	619	BCR	C20-C19-C18	-3.68	116.08	126.42
23	c	508	CLA	C1C-NC-C4C	-3.68	104.98	107.05
23	c	509	CLA	C1B-CHB-C4A	-3.65	122.89	130.12
23	D	402	CLA	C1B-CHB-C4A	-3.64	122.90	130.12
26	a	609	PL9	C15-C14-C16	-3.63	109.03	115.29
23	B	607[B]	CLA	C1B-CHB-C4A	-3.63	122.94	130.12
25	h	101	BCR	C33-C5-C4	-3.62	106.71	113.56
23	B	613	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
23	b	619	CLA	C1C-NC-C4C	-3.62	105.01	107.05
23	B	606	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
23	c	507	CLA	CMB-C2B-C1B	-3.62	122.91	128.46
25	C	515	BCR	C16-C15-C14	-3.61	115.75	123.46
25	C	514	BCR	C10-C11-C12	-3.61	112.25	123.26
26	a	609	PL9	C45-C44-C46	-3.60	109.07	115.29
26	D	405	PL9	C45-C44-C46	-3.60	109.08	115.29
25	h	101	BCR	C11-C10-C9	-3.59	122.18	127.31
23	c	502	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
23	C	508	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	B	607[A]	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
23	B	612	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
23	c	512	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
23	a	605	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
26	D	405	PL9	C51-C49-C48	-3.57	112.10	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	515	BCR	C8-C7-C6	-3.57	117.26	127.25
26	D	405	PL9	C50-C49-C48	-3.57	112.11	122.65
23	b	616	CLA	C1C-NC-C4C	-3.57	105.04	107.05
26	d	404	PL9	C51-C49-C48	-3.57	112.11	122.65
23	c	506	CLA	C1C-NC-C4C	-3.56	105.04	107.05
23	C	506	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
23	b	609[A]	CLA	C1B-CHB-C4A	-3.55	123.08	130.12
25	C	514	BCR	C37-C22-C21	-3.55	117.95	122.92
23	C	507	CLA	C1B-CHB-C4A	-3.55	123.08	130.12
23	b	613	CLA	C1C-NC-C4C	-3.55	105.05	107.05
25	C	514	BCR	C38-C26-C27	-3.54	106.87	113.56
23	D	404	CLA	C1C-NC-C4C	-3.53	105.06	107.05
25	B	620	BCR	C11-C12-C13	-3.50	116.58	126.42
23	C	509	CLA	C1B-CHB-C4A	-3.49	123.20	130.12
33	V	202	HEM	C1D-C2D-C3D	-3.49	104.57	107.00
23	C	503	CLA	C1B-CHB-C4A	-3.49	123.22	130.12
25	b	620	BCR	C34-C9-C10	-3.48	118.04	122.92
25	C	514	BCR	C34-C9-C10	-3.48	118.05	122.92
23	a	604	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
23	A	606	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
25	a	608	BCR	C11-C12-C13	-3.47	116.66	126.42
23	b	606	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	B	620	BCR	C35-C13-C14	-3.47	118.07	122.92
23	b	608	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
26	D	405	PL9	C10-C9-C11	-3.46	109.33	115.29
23	b	617	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
23	B	617	CLA	C1C-NC-C4C	-3.45	105.10	107.05
23	c	503	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
23	B	604	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
25	B	619	BCR	C11-C12-C13	-3.45	116.73	126.42
25	H	101	BCR	C31-C1-C6	-3.44	104.73	110.31
25	B	618	BCR	C33-C5-C4	-3.44	107.06	113.56
25	a	608	BCR	C36-C18-C17	-3.43	118.11	122.92
23	b	614	CLA	C1C-NC-C4C	-3.42	105.12	107.05
23	B	602	CLA	C1B-CHB-C4A	-3.41	123.35	130.12
23	A	608	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
23	b	609[B]	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
23	b	611	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
23	B	608	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
25	F	101	BCR	C34-C9-C10	-3.40	118.16	122.92
23	c	514	CLA	C1B-CHB-C4A	-3.40	123.39	130.12
23	a	607	CLA	CHA-C1A-NA	-3.39	118.32	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	PL9	C30-C29-C31	-3.38	109.45	115.29
23	A	605	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
23	D	402	CLA	O1D-CGD-CBD	-3.38	118.31	124.58
23	c	510	CLA	C1C-NC-C4C	-3.38	105.15	107.05
25	b	620	BCR	C30-C25-C24	-3.37	106.26	115.73
23	b	619	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
25	T	101	BCR	C34-C9-C10	-3.36	118.22	122.92
25	a	608	BCR	C27-C26-C25	-3.35	117.82	122.74
26	A	610	PL9	C31-C29-C28	-3.35	114.28	121.10
25	C	515	BCR	C7-C6-C5	-3.35	113.55	121.54
25	b	622	BCR	C11-C10-C9	-3.35	122.53	127.31
26	d	404	PL9	C35-C34-C33	-3.33	114.94	123.70
23	C	511	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
26	a	609	PL9	C51-C49-C48	-3.33	112.80	122.65
23	C	501	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
25	c	516	BCR	C16-C15-C14	-3.33	116.36	123.46
23	a	605	CLA	O1D-CGD-CBD	-3.32	118.42	124.58
25	K	101	BCR	C24-C25-C26	-3.32	113.62	121.54
23	C	508	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
25	b	620	BCR	C24-C25-C26	-3.32	113.63	121.54
23	d	403	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
23	c	508	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
23	C	507	CLA	C1C-NC-C4C	-3.31	105.18	107.05
23	C	512	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
33	v	201	HEM	C1D-C2D-C3D	-3.31	104.69	107.00
23	C	512	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	h	101	BCR	C20-C19-C18	-3.31	117.13	126.42
25	t	101	BCR	C7-C8-C9	-3.31	121.24	126.21
27	A	611	SQD	C1-C2-C3	-3.30	103.06	109.98
25	H	101	BCR	C8-C9-C10	-3.30	113.88	118.94
27	a	610	SQD	C1-C2-C3	-3.30	103.08	109.98
23	c	511	CLA	C1B-CHB-C4A	-3.29	123.60	130.12
23	C	513	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
23	C	505	CLA	C1C-NC-C4C	-3.29	105.20	107.05
23	B	615	CLA	C1B-CHB-C4A	-3.29	123.61	130.12
23	b	616	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
23	C	502	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
23	B	610	CLA	C1C-NC-C4C	-3.28	105.20	107.05
25	C	514	BCR	C12-C13-C14	-3.27	113.92	118.94
25	T	101	BCR	C20-C19-C18	-3.27	117.24	126.42
26	A	610	PL9	C45-C44-C46	-3.26	109.67	115.29
23	B	609	CLA	CMB-C2B-C1B	-3.25	123.47	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	502	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
23	b	604	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
24	D	401	PHO	O2D-CGD-O1D	-3.24	117.39	123.82
25	f	101	BCR	C34-C9-C10	-3.24	118.39	122.92
23	D	404	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
23	b	614	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
23	a	604	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
25	a	608	BCR	C38-C26-C27	-3.22	107.47	113.56
25	t	101	BCR	C35-C13-C14	-3.22	118.42	122.92
23	B	614	CLA	C1C-NC-C4C	-3.21	105.24	107.05
23	B	617	CLA	C1B-CHB-C4A	-3.21	123.77	130.12
25	h	101	BCR	C11-C12-C13	-3.21	117.41	126.42
23	C	509	CLA	C1C-NC-C4C	-3.21	105.24	107.05
23	b	618	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
23	b	604	CLA	C1C-NC-C4C	-3.20	105.25	107.05
23	B	615	CLA	C1C-NC-C4C	-3.20	105.25	107.05
25	t	101	BCR	C34-C9-C10	-3.20	118.44	122.92
23	C	510	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
32	C	518	DGD	O3G-C3G-C2G	-3.19	103.40	110.99
23	B	616	CLA	C1C-NC-C4C	-3.19	105.25	107.05
23	A	606	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
23	B	611	CLA	C1C-NC-C4C	-3.18	105.25	107.05
23	B	604	CLA	C1C-NC-C4C	-3.18	105.26	107.05
23	D	402	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
23	c	510	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
25	h	101	BCR	C30-C25-C26	-3.17	118.13	122.59
25	K	101	BCR	C11-C12-C13	-3.17	117.51	126.42
23	b	615	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
25	c	522	BCR	C33-C5-C4	-3.16	107.58	113.56
23	a	605	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
25	C	521	BCR	C33-C5-C4	-3.15	107.60	113.56
25	C	515	BCR	C1-C6-C7	-3.15	106.88	115.73
23	B	605	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
25	C	515	BCR	C24-C25-C26	-3.14	114.04	121.54
25	H	101	BCR	C36-C18-C17	-3.14	118.53	122.92
25	c	516	BCR	C33-C5-C4	-3.13	107.64	113.56
25	b	622	BCR	C11-C12-C13	-3.13	117.63	126.42
25	A	609	BCR	C33-C5-C4	-3.13	107.65	113.56
23	c	513	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
23	B	609	CLA	C1C-NC-C4C	-3.11	105.30	107.05
25	H	101	BCR	C11-C12-C13	-3.11	117.68	126.42
25	t	101	BCR	C11-C12-C13	-3.11	117.68	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	620	BCR	C23-C22-C21	-3.10	114.18	118.94
26	d	404	PL9	C15-C14-C16	-3.10	109.94	115.29
25	H	101	BCR	C20-C19-C18	-3.10	117.71	126.42
23	b	611	CLA	O1D-CGD-CBD	-3.10	118.84	124.58
23	C	501	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
25	A	609	BCR	C27-C26-C25	-3.09	118.21	122.74
23	B	616	CLA	C1B-CHB-C4A	-3.09	124.01	130.12
25	F	101	BCR	C16-C15-C14	-3.08	116.88	123.46
25	c	516	BCR	C35-C13-C14	-3.08	118.61	122.92
23	b	610	CLA	C1C-NC-C4C	-3.08	105.32	107.05
25	h	101	BCR	C40-C30-C25	-3.08	105.32	110.31
23	C	509	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
23	b	606	CLA	O1D-CGD-CBD	-3.06	118.90	124.58
23	b	615	CLA	C1C-NC-C4C	-3.06	105.33	107.05
23	B	602	CLA	C1C-NC-C4C	-3.06	105.33	107.05
25	k	101	BCR	C8-C9-C10	-3.05	114.26	118.94
25	f	101	BCR	C35-C13-C14	-3.05	118.65	122.92
23	b	607	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
33	V	202	HEM	CBA-CAA-C2A	-3.05	106.66	112.48
25	f	101	BCR	C37-C22-C23	-3.04	113.25	118.10
23	B	615	CLA	O1D-CGD-CBD	-3.04	118.94	124.58
26	D	405	PL9	C15-C14-C16	-3.03	110.06	115.29
33	E	102	HEM	C1D-C2D-C3D	-3.03	104.89	107.00
25	c	516	BCR	C20-C21-C22	-3.03	122.98	127.31
23	b	607	CLA	O1D-CGD-CBD	-3.02	118.97	124.58
23	A	608	CLA	C1C-NC-C4C	-3.02	105.35	107.05
23	b	609[A]	CLA	O1D-CGD-CBD	-3.02	118.97	124.58
25	a	608	BCR	C33-C5-C4	-3.01	107.87	113.56
27	a	610	SQD	C45-O47-C7	-3.01	110.77	117.88
25	b	621	BCR	C23-C22-C21	-3.01	114.33	118.94
26	d	404	PL9	C10-C9-C11	-3.01	110.10	115.29
27	A	611	SQD	C45-O47-C7	-3.00	110.78	117.88
23	b	605	CLA	O1D-CGD-CBD	-3.00	119.01	124.58
25	b	620	BCR	C33-C5-C4	-3.00	107.89	113.56
25	h	101	BCR	C16-C15-C14	-3.00	117.06	123.46
23	c	512	CLA	O1D-CGD-CBD	-2.99	119.03	124.58
25	B	619	BCR	C27-C26-C25	-2.99	118.35	122.74
23	B	604	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
23	b	611	CLA	O2D-CGD-O1D	-2.99	117.89	123.82
23	C	510	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
25	c	522	BCR	C23-C24-C25	-2.99	118.89	127.25
25	c	516	BCR	C23-C24-C25	-2.97	118.92	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	O2D-CGD-O1D	-2.97	117.92	123.82
23	D	404	CLA	CHA-C1A-NA	-2.97	119.28	126.18
25	b	621	BCR	C7-C6-C5	-2.97	114.47	121.54
25	T	101	BCR	C38-C26-C27	-2.96	107.96	113.56
23	B	614	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	k	101	BCR	C37-C22-C21	-2.96	118.78	122.92
32	c	519	DGD	O3G-C3G-C2G	-2.96	103.96	110.99
23	A	608	CLA	CHA-C1A-NA	-2.95	119.32	126.18
23	a	613	CLA	C1C-NC-C4C	-2.95	105.39	107.05
23	c	510	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
23	b	610	CLA	O1D-CGD-CBD	-2.95	119.11	124.58
25	b	621	BCR	C8-C7-C6	-2.94	119.01	127.25
23	D	402	CLA	O2D-CGD-O1D	-2.94	117.98	123.82
25	t	101	BCR	C38-C26-C27	-2.94	108.00	113.56
23	c	513	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
25	b	621	BCR	C10-C11-C12	-2.94	114.31	123.26
23	b	617	CLA	C1C-NC-C4C	-2.93	105.40	107.05
25	b	621	BCR	C37-C22-C21	-2.93	118.82	122.92
25	C	515	BCR	C23-C24-C25	-2.93	119.05	127.25
25	k	101	BCR	C33-C5-C4	-2.93	108.02	113.56
25	K	101	BCR	C33-C5-C4	-2.93	108.03	113.56
25	c	515	BCR	C20-C19-C18	-2.92	118.20	126.42
23	C	505	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
25	C	514	BCR	C11-C12-C13	-2.92	118.21	126.42
23	b	609[B]	CLA	O1D-CGD-CBD	-2.91	119.18	124.58
23	C	502	CLA	C1C-NC-C4C	-2.91	105.41	107.05
25	B	620	BCR	C10-C11-C12	-2.91	114.41	123.26
25	H	101	BCR	C40-C30-C25	-2.90	105.60	110.31
23	B	612	CLA	O1D-CGD-CBD	-2.90	119.19	124.58
23	c	506	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
23	a	613	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
23	c	508	CLA	O1D-CGD-CBD	-2.90	119.20	124.58
31	b	624	LHG	C5-O7-C7	-2.90	111.03	117.88
25	c	522	BCR	C34-C9-C10	-2.90	118.86	122.92
23	d	403	CLA	CHA-C1A-NA	-2.90	119.45	126.18
25	B	620	BCR	C16-C15-C14	-2.89	117.29	123.46
23	b	611	CLA	C1C-NC-C4C	-2.88	105.42	107.05
23	B	609	CLA	O1D-CGD-CBD	-2.88	119.24	124.58
25	c	515	BCR	C12-C13-C14	-2.88	114.53	118.94
23	B	606	CLA	C1C-NC-C4C	-2.88	105.43	107.05
23	c	511	CLA	CMB-C2B-C1B	-2.88	124.05	128.46
24	A	607	PHO	O2D-CGD-O1D	-2.87	118.12	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	606	CLA	CHA-C1A-NA	-2.87	119.51	126.18
23	C	511	CLA	O1D-CGD-CBD	-2.87	119.26	124.58
23	b	606	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
25	A	609	BCR	C38-C26-C27	-2.87	108.14	113.56
23	b	617	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
23	b	617	CLA	O2D-CGD-O1D	-2.86	118.14	123.82
23	A	608	CLA	O1D-CGD-CBD	-2.86	119.27	124.58
25	f	101	BCR	C33-C5-C4	-2.86	108.15	113.56
23	A	606	CLA	C1C-NC-C4C	-2.86	105.44	107.05
33	e	102	HEM	C1D-C2D-C3D	-2.86	105.01	107.00
23	B	607[A]	CLA	O1D-CGD-CBD	-2.85	119.29	124.58
23	b	607	CLA	CMB-C2B-C1B	-2.84	124.09	128.46
23	C	509	CLA	O1D-CGD-CBD	-2.84	119.31	124.58
25	A	609	BCR	C34-C9-C10	-2.84	118.95	122.92
23	C	507	CLA	O2D-CGD-O1D	-2.84	118.19	123.82
25	A	609	BCR	C11-C12-C13	-2.83	118.46	126.42
25	b	622	BCR	C33-C5-C4	-2.82	108.23	113.56
31	B	622	LHG	C5-O7-C7	-2.82	111.22	117.88
23	c	513	CLA	C1C-NC-C4C	-2.82	105.46	107.05
25	C	515	BCR	C20-C19-C18	-2.82	118.50	126.42
23	b	609[A]	CLA	C1C-NC-C4C	-2.81	105.47	107.05
23	c	506	CLA	O1D-CGD-CBD	-2.81	119.38	124.58
25	C	521	BCR	C37-C22-C21	-2.81	118.99	122.92
23	C	503	CLA	C1C-NC-C4C	-2.80	105.47	107.05
23	a	613	CLA	O1D-CGD-CBD	-2.80	119.39	124.58
23	C	510	CLA	C1C-NC-C4C	-2.80	105.47	107.05
32	c	519	DGD	C2G-O2G-C1B	-2.79	111.28	117.88
23	b	618	CLA	O1D-CGD-CBD	-2.79	119.41	124.58
23	b	617	CLA	O1D-CGD-CBD	-2.79	119.41	124.58
23	b	608	CLA	C1C-NC-C4C	-2.79	105.48	107.05
23	b	614	CLA	O1D-CGD-CBD	-2.78	119.43	124.58
23	C	505	CLA	O1D-CGD-CBD	-2.77	119.44	124.58
25	c	516	BCR	C24-C25-C26	-2.77	114.93	121.54
25	b	621	BCR	C16-C15-C14	-2.77	117.55	123.46
25	t	101	BCR	C33-C5-C4	-2.77	108.33	113.56
23	b	612	CLA	C1C-NC-C4C	-2.77	105.49	107.05
23	c	503	CLA	C1C-NC-C4C	-2.76	105.49	107.05
25	F	101	BCR	C10-C11-C12	-2.76	114.85	123.26
23	b	615	CLA	O2D-CGD-O1D	-2.76	118.34	123.82
23	c	508	CLA	O2D-CGD-O1D	-2.76	118.34	123.82
23	c	509	CLA	O2D-CGD-O1D	-2.76	118.35	123.82
27	A	611	SQD	C44-O6-C1	-2.75	108.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	O1D-CGD-CBD	-2.75	119.49	124.58
25	t	101	BCR	C36-C18-C17	-2.74	119.08	122.92
25	A	609	BCR	C16-C15-C14	-2.74	117.62	123.46
27	a	610	SQD	C44-O6-C1	-2.73	108.32	113.80
26	d	404	PL9	C30-C29-C31	-2.73	110.58	115.29
25	c	515	BCR	C38-C26-C27	-2.73	108.41	113.56
25	h	101	BCR	C10-C11-C12	-2.73	114.95	123.26
23	b	610	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
24	d	401	PHO	CMB-C2B-C1B	-2.72	120.84	125.05
25	A	609	BCR	C24-C25-C26	-2.72	115.06	121.54
23	D	404	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
23	b	609[B]	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
23	A	606	CLA	O1D-CGD-CBD	-2.71	119.55	124.58
23	B	607[B]	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
25	h	101	BCR	C34-C9-C10	-2.71	119.13	122.92
23	b	609[A]	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
23	B	614	CLA	O1D-CGD-CBD	-2.70	119.58	124.58
23	B	608	CLA	C1-C2-C3	-2.69	121.00	125.96
23	b	610	CLA	C1-C2-C3	-2.69	121.00	125.96
25	B	620	BCR	C20-C19-C18	-2.69	118.86	126.42
23	b	606	CLA	C1C-NC-C4C	-2.69	105.53	107.05
23	C	507	CLA	O1D-CGD-CBD	-2.69	119.60	124.58
23	a	604	CLA	C1C-NC-C4C	-2.69	105.54	107.05
23	a	613	CLA	CHA-C1A-NA	-2.68	119.95	126.18
23	B	604	CLA	CHB-C4A-NA	-2.68	120.80	124.51
23	c	504	CLA	C1C-NC-C4C	-2.68	105.54	107.05
24	d	401	PHO	O2D-CGD-O1D	-2.68	118.51	123.82
23	B	612	CLA	C1C-NC-C4C	-2.67	105.54	107.05
24	D	401	PHO	CMB-C2B-C1B	-2.66	120.93	125.05
23	b	618	CLA	C1C-NC-C4C	-2.66	105.55	107.05
23	b	610	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
23	B	612	CLA	C1-C2-C3	-2.66	121.06	125.96
23	B	607[A]	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
23	b	614	CLA	C1-C2-C3	-2.66	121.06	125.96
23	D	402	CLA	CHA-C1A-NA	-2.65	120.02	126.18
23	C	513	CLA	CHA-C1A-NA	-2.65	120.02	126.18
23	a	605	CLA	CHA-C1A-NA	-2.65	120.02	126.18
23	B	612	CLA	CHA-C1A-NA	-2.65	120.02	126.18
25	b	620	BCR	C36-C18-C17	-2.65	119.21	122.92
25	b	620	BCR	C37-C22-C21	-2.65	119.21	122.92
25	f	101	BCR	C16-C15-C14	-2.64	117.82	123.46
33	V	202	HEM	CBD-CAD-C3D	-2.64	107.42	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	h	101	BCR	C37-C22-C21	-2.64	119.22	122.92
25	f	101	BCR	C11-C12-C13	-2.64	118.99	126.42
23	B	606	CLA	O1D-CGD-CBD	-2.64	119.69	124.58
26	A	610	PL9	C25-C24-C26	-2.64	110.73	115.29
23	a	607	CLA	C1C-NC-C4C	-2.64	105.56	107.05
23	b	609[B]	CLA	C1C-NC-C4C	-2.63	105.57	107.05
23	B	605	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
25	K	101	BCR	C35-C13-C14	-2.63	119.24	122.92
23	c	504	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
23	B	608	CLA	C1C-NC-C4C	-2.62	105.57	107.05
23	C	512	CLA	O1D-CGD-CBD	-2.62	119.72	124.58
23	B	608	CLA	CHB-C4A-NA	-2.62	120.89	124.51
23	C	501	CLA	CHA-C1A-NA	-2.62	120.10	126.18
25	f	101	BCR	C1-C6-C7	-2.62	108.38	115.73
25	b	621	BCR	C27-C26-C25	-2.61	118.90	122.74
23	a	613	CLA	CHC-C1C-C2C	-2.61	119.48	126.75
23	C	506	CLA	O1D-CGD-CBD	-2.61	119.74	124.58
32	C	518	DGD	C2G-O2G-C1B	-2.61	111.71	117.88
23	c	510	CLA	O1D-CGD-CBD	-2.61	119.74	124.58
23	B	613	CLA	O1D-CGD-CBD	-2.61	119.74	124.58
23	C	511	CLA	C1C-NC-C4C	-2.61	105.58	107.05
23	c	506	CLA	O2D-CGD-O1D	-2.61	118.65	123.82
25	T	101	BCR	C16-C17-C18	-2.60	123.59	127.31
23	b	616	CLA	O2D-CGD-O1D	-2.60	118.66	123.82
23	A	605	CLA	C1C-NC-C4C	-2.60	105.58	107.05
23	b	610	CLA	CHC-C1C-C2C	-2.60	119.52	126.75
25	K	101	BCR	C37-C22-C23	-2.59	113.97	118.10
26	D	405	PL9	C7-C3-C2	-2.59	119.85	123.27
23	b	606	CLA	CHB-C4A-NA	-2.59	120.93	124.51
25	B	620	BCR	C1-C6-C5	-2.59	118.96	122.59
23	B	603	CLA	O2D-CGD-O1D	-2.58	118.70	123.82
25	B	618	BCR	C35-C13-C14	-2.58	119.31	122.92
25	C	521	BCR	C10-C11-C12	-2.58	115.41	123.26
25	H	101	BCR	C1-C6-C7	-2.58	108.49	115.73
25	F	101	BCR	C37-C22-C21	-2.58	119.31	122.92
24	a	606	PHO	O2D-CGD-O1D	-2.58	118.71	123.82
25	B	619	BCR	C16-C15-C14	-2.57	117.97	123.46
25	c	515	BCR	C11-C12-C13	-2.57	119.20	126.42
23	B	613	CLA	CMB-C2B-C1B	-2.56	124.53	128.46
23	c	507	CLA	C1C-NC-C4C	-2.56	105.61	107.05
23	c	503	CLA	O2D-CGD-O1D	-2.56	118.74	123.82
23	C	501	CLA	O1D-CGD-CBD	-2.56	119.83	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C1C-NC-C4C	-2.56	105.61	107.05
23	B	617	CLA	O1D-CGD-CBD	-2.55	119.85	124.58
23	d	403	CLA	CMB-C2B-C1B	-2.55	124.55	128.46
23	D	403	CLA	C1C-NC-C4C	-2.54	105.62	107.05
23	D	404	CLA	O1D-CGD-CBD	-2.54	119.87	124.58
25	B	619	BCR	C20-C21-C22	-2.54	123.69	127.31
23	B	602	CLA	O1D-CGD-CBD	-2.54	119.88	124.58
25	T	101	BCR	C11-C12-C13	-2.54	119.29	126.42
23	b	619	CLA	CHA-C1A-NA	-2.53	120.29	126.18
25	c	515	BCR	C10-C11-C12	-2.53	115.54	123.26
25	A	609	BCR	C20-C21-C22	-2.53	123.70	127.31
27	A	611	SQD	C1-O5-C5	-2.53	108.72	113.71
25	B	618	BCR	C30-C25-C24	-2.53	108.62	115.73
23	B	610	CLA	O1D-CGD-CBD	-2.53	119.89	124.58
25	b	622	BCR	C10-C11-C12	-2.53	115.56	123.26
23	a	607	CLA	O1D-CGD-CBD	-2.53	119.89	124.58
23	B	607[B]	CLA	O1D-CGD-CBD	-2.52	119.91	124.58
23	B	607[B]	CLA	C1C-NC-C4C	-2.52	105.63	107.05
23	a	605	CLA	C1C-NC-C4C	-2.52	105.63	107.05
23	C	512	CLA	C1C-NC-C4C	-2.52	105.63	107.05
25	T	101	BCR	C8-C9-C10	-2.51	115.08	118.94
23	B	615	CLA	O2D-CGD-O1D	-2.51	118.84	123.82
25	F	101	BCR	C1-C6-C7	-2.51	108.69	115.73
23	C	504	CLA	O1D-CGD-CBD	-2.51	119.93	124.58
26	a	609	PL9	C35-C34-C36	-2.51	110.96	115.29
24	A	607	PHO	CMB-C2B-C1B	-2.50	121.18	125.05
27	a	610	SQD	C1-O5-C5	-2.50	108.78	113.71
32	c	519	DGD	C3G-C2G-C1G	-2.50	106.22	111.86
23	B	616	CLA	O1D-CGD-CBD	-2.50	119.95	124.58
23	c	503	CLA	CHA-C1A-NA	-2.50	120.38	126.18
23	c	509	CLA	C1C-NC-C4C	-2.50	105.64	107.05
23	b	608	CLA	O1D-CGD-CBD	-2.50	119.95	124.58
24	d	401	PHO	C1-C2-C3	-2.49	121.36	125.96
23	b	619	CLA	CHC-C1C-C2C	-2.49	119.81	126.75
23	B	605	CLA	CHC-C1C-C2C	-2.49	119.83	126.75
23	b	609[B]	CLA	O2D-CGD-O1D	-2.48	118.89	123.82
23	b	607	CLA	O2D-CGD-O1D	-2.48	118.89	123.82
25	c	522	BCR	C8-C9-C10	-2.48	115.13	118.94
25	C	521	BCR	C8-C9-C10	-2.48	115.13	118.94
23	b	615	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
23	C	508	CLA	O1D-CGD-CBD	-2.48	119.98	124.58
23	C	513	CLA	C1C-NC-C4C	-2.48	105.65	107.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	O1D-CGD-CBD	-2.48	119.99	124.58
23	b	604	CLA	O1D-CGD-CBD	-2.48	119.99	124.58
23	c	507	CLA	O1D-CGD-CBD	-2.47	119.99	124.58
23	b	614	CLA	CHC-C1C-C2C	-2.47	119.87	126.75
25	B	618	BCR	C37-C22-C23	-2.47	114.17	118.10
23	C	504	CLA	C1C-NC-C4C	-2.47	105.66	107.05
23	C	510	CLA	O2D-CGD-O1D	-2.46	118.93	123.82
23	B	609	CLA	O2D-CGD-O1D	-2.46	118.94	123.82
28	J	101	LMG	C6-C5-C4	-2.46	107.18	112.99
23	b	619	CLA	O1D-CGD-CBD	-2.46	120.02	124.58
24	a	606	PHO	CBD-CHA-C4D	-2.46	105.77	108.54
23	c	511	CLA	C1C-NC-C4C	-2.45	105.67	107.05
25	c	515	BCR	C35-C13-C14	-2.45	119.49	122.92
25	a	608	BCR	C16-C15-C14	-2.45	118.23	123.46
23	b	606	CLA	O2D-CGD-O1D	-2.45	118.96	123.82
23	d	402	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
23	C	501	CLA	C1C-NC-C4C	-2.45	105.67	107.05
25	h	101	BCR	C36-C18-C17	-2.45	119.50	122.92
25	B	618	BCR	C16-C17-C18	-2.45	123.82	127.31
25	C	521	BCR	C34-C9-C10	-2.44	119.50	122.92
23	B	607[B]	CLA	C1-C2-C3	-2.44	121.46	125.96
23	B	604	CLA	O1D-CGD-CBD	-2.44	120.06	124.58
23	b	609[B]	CLA	C1-C2-C3	-2.44	121.47	125.96
23	B	617	CLA	CHC-C1C-C2C	-2.44	119.97	126.75
26	a	609	PL9	C25-C24-C26	-2.43	111.09	115.29
23	b	607	CLA	CHA-C1A-NA	-2.43	120.53	126.18
23	B	608	CLA	CHC-C1C-C2C	-2.43	120.00	126.75
25	a	608	BCR	C24-C25-C26	-2.43	115.76	121.54
24	A	607	PHO	CBD-CHA-C4D	-2.42	105.81	108.54
32	D	406	DGD	O2G-C1B-O1B	-2.42	117.71	123.69
23	C	502	CLA	O2D-CGD-O1D	-2.42	119.02	123.82
32	d	405	DGD	O2G-C1B-O1B	-2.42	117.72	123.69
23	b	616	CLA	CMB-C2B-C1B	-2.42	124.75	128.46
25	C	514	BCR	C33-C5-C4	-2.42	109.00	113.56
23	c	513	CLA	O1D-CGD-CBD	-2.41	120.11	124.58
25	c	516	BCR	C20-C19-C18	-2.41	119.64	126.42
26	a	609	PL9	C20-C19-C21	-2.41	111.13	115.29
25	C	515	BCR	C34-C9-C10	-2.41	119.55	122.92
25	B	619	BCR	C7-C6-C5	-2.41	115.80	121.54
23	B	603	CLA	O1D-CGD-CBD	-2.41	120.11	124.58
25	b	622	BCR	C1-C6-C5	-2.41	119.21	122.59
23	b	616	CLA	O1D-CGD-CBD	-2.41	120.12	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	514	CLA	O1D-CGD-CBD	-2.40	120.12	124.58
23	c	512	CLA	O2D-CGD-O1D	-2.40	119.05	123.82
23	c	510	CLA	CHC-C1C-C2C	-2.40	120.06	126.75
23	b	607	CLA	CHC-C1C-C2C	-2.40	120.07	126.75
25	c	522	BCR	C10-C11-C12	-2.40	115.96	123.26
23	c	505	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
25	H	101	BCR	C10-C11-C12	-2.39	115.97	123.26
25	B	620	BCR	C1-C6-C7	-2.39	109.01	115.73
25	C	514	BCR	C30-C25-C24	-2.39	109.01	115.73
25	b	620	BCR	C10-C11-C12	-2.39	115.98	123.26
25	b	622	BCR	C36-C18-C17	-2.38	119.58	122.92
26	D	405	PL9	C20-C19-C21	-2.38	111.18	115.29
23	B	604	CLA	CHA-C1A-NA	-2.38	120.66	126.18
23	c	508	CLA	CHC-C1C-C2C	-2.37	120.14	126.75
23	c	513	CLA	CHA-C1A-NA	-2.37	120.67	126.18
23	b	609[A]	CLA	O2D-CGD-O1D	-2.37	119.11	123.82
25	b	620	BCR	C35-C13-C14	-2.37	119.60	122.92
23	C	505	CLA	O2D-CGD-O1D	-2.37	119.12	123.82
23	b	612	CLA	O1D-CGD-CBD	-2.37	120.19	124.58
23	b	605	CLA	CHB-C4A-NA	-2.37	121.24	124.51
28	Z	101	LMG	O2-C2-C3	-2.37	104.82	110.34
32	c	518	DGD	O6D-C5D-C4D	-2.37	105.34	109.69
23	b	618	CLA	O2D-CGD-O1D	-2.36	119.13	123.82
23	c	513	CLA	C1-C2-C3	-2.36	121.61	125.96
26	A	610	PL9	C51-C49-C50	-2.36	109.28	114.59
23	C	512	CLA	C1-C2-C3	-2.35	121.62	125.96
23	D	403	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
23	c	514	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
32	c	518	DGD	C1E-O6E-C5E	-2.35	109.08	113.71
23	c	505	CLA	O1D-CGD-CBD	-2.35	120.23	124.58
23	D	403	CLA	O1D-CGD-CBD	-2.34	120.23	124.58
23	c	511	CLA	O2D-CGD-O1D	-2.34	119.18	123.82
25	B	619	BCR	C8-C7-C6	-2.34	120.71	127.25
23	D	402	CLA	C1C-NC-C4C	-2.33	105.73	107.05
26	A	610	PL9	C30-C29-C31	-2.33	111.26	115.29
23	D	403	CLA	CHA-C1A-NA	-2.33	120.76	126.18
25	t	101	BCR	C37-C22-C21	-2.33	119.66	122.92
25	T	101	BCR	C30-C25-C24	-2.33	109.19	115.73
23	C	513	CLA	O1D-CGD-CBD	-2.33	120.26	124.58
31	D	407	LHG	C5-O7-C7	-2.33	112.38	117.88
25	C	515	BCR	C35-C13-C14	-2.32	119.67	122.92
31	a	614	LHG	C5-O7-C7	-2.32	112.39	117.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	620	BCR	C33-C5-C4	-2.32	109.17	113.56
23	B	603	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
31	d	406	LHG	C5-O7-C7	-2.32	112.40	117.88
24	D	401	PHO	C1-C2-C3	-2.32	121.69	125.96
23	B	616	CLA	CHC-C1C-C2C	-2.31	120.30	126.75
23	b	606	CLA	CHA-C1A-NA	-2.31	120.80	126.18
23	C	503	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
25	t	101	BCR	C1-C6-C5	-2.31	119.34	122.59
25	f	101	BCR	C30-C25-C24	-2.31	109.25	115.73
26	d	404	PL9	C20-C19-C21	-2.31	111.31	115.29
32	C	518	DGD	O1G-C1A-O1A	-2.31	117.95	123.58
23	c	504	CLA	O1D-CGD-CBD	-2.30	120.31	124.58
23	C	509	CLA	CHA-C1A-NA	-2.30	120.83	126.18
25	c	515	BCR	C8-C9-C10	-2.30	115.41	118.94
23	b	604	CLA	CHA-C1A-NA	-2.30	120.84	126.18
25	B	619	BCR	C12-C13-C14	-2.30	115.41	118.94
23	C	509	CLA	CHC-C1C-C2C	-2.29	120.37	126.75
23	B	607[A]	CLA	C1C-NC-C4C	-2.29	105.76	107.05
27	X	101	SQD	O48-C23-O10	-2.28	118.01	123.58
25	f	101	BCR	C37-C22-C21	-2.28	119.73	122.92
23	c	507	CLA	CHB-C4A-NA	-2.28	121.36	124.51
23	C	510	CLA	CHA-C1A-NA	-2.28	120.89	126.18
23	D	402	CLA	CHC-C1C-C2C	-2.28	120.41	126.75
26	d	404	PL9	C7-C3-C2	-2.28	120.26	123.27
27	x	101	SQD	O48-C23-O10	-2.28	118.03	123.58
23	C	506	CLA	C1C-NC-C4C	-2.28	105.77	107.05
23	b	605	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
23	C	504	CLA	CHC-C1C-C2C	-2.27	120.42	126.75
23	B	607[A]	CLA	O2D-CGD-O1D	-2.27	119.31	123.82
25	B	619	BCR	C10-C11-C12	-2.27	116.35	123.26
23	b	612	CLA	C1-C2-C3	-2.27	121.78	125.96
23	a	605	CLA	CHC-C1C-C2C	-2.27	120.44	126.75
23	c	502	CLA	O1D-CGD-CBD	-2.26	120.38	124.58
23	C	507	CLA	CHC-C1C-C2C	-2.26	120.45	126.75
25	f	101	BCR	C20-C19-C18	-2.26	120.06	126.42
27	A	611	SQD	O48-C23-O10	-2.25	118.08	123.58
27	a	610	SQD	O48-C23-O10	-2.25	118.08	123.58
23	c	512	CLA	C1C-NC-C4C	-2.25	105.78	107.05
23	b	609[A]	CLA	C1-C2-C3	-2.25	121.81	125.96
25	h	101	BCR	C1-C6-C7	-2.25	109.41	115.73
25	b	622	BCR	C1-C6-C7	-2.25	109.41	115.73
23	D	403	CLA	CHB-C4A-NA	-2.25	121.40	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
23	d	403	CLA	O1D-CGD-CBD	-2.25	120.41	124.58
23	B	610	CLA	CHC-C1C-C2C	-2.25	120.50	126.75
23	B	607[B]	CLA	CHC-C1C-C2C	-2.25	120.50	126.75
23	B	616	CLA	CHA-C1A-NA	-2.24	120.97	126.18
26	A	610	PL9	C7-C3-C2	-2.24	120.31	123.27
23	B	610	CLA	C1-C2-C3	-2.24	121.83	125.96
23	B	607[A]	CLA	C1-C2-C3	-2.24	121.84	125.96
28	z	101	LMG	O2-C2-C3	-2.23	105.12	110.34
24	a	606	PHO	CMB-C2B-C1B	-2.23	121.60	125.05
23	b	611	CLA	CHA-C1A-NA	-2.23	121.00	126.18
23	C	508	CLA	O2D-CGD-O1D	-2.23	119.39	123.82
23	C	511	CLA	CHC-C1C-C2C	-2.23	120.54	126.75
23	B	612	CLA	CHC-C1C-C2C	-2.23	120.55	126.75
25	B	619	BCR	C31-C1-C6	-2.23	106.70	110.31
26	A	610	PL9	C10-C9-C11	-2.22	111.45	115.29
23	c	513	CLA	O2D-CGD-O1D	-2.22	119.41	123.82
25	b	621	BCR	C8-C9-C10	-2.22	115.53	118.94
23	b	605	CLA	CHA-C1A-NA	-2.22	121.02	126.18
25	c	522	BCR	C37-C22-C21	-2.22	119.81	122.92
25	C	515	BCR	C23-C22-C21	-2.22	115.53	118.94
23	c	509	CLA	O1D-CGD-CBD	-2.22	120.46	124.58
23	b	615	CLA	CHC-C1C-C2C	-2.22	120.57	126.75
27	b	601	SQD	C5-C6-S	-2.22	111.25	114.34
25	T	101	BCR	C33-C5-C4	-2.22	109.37	113.56
23	A	606	CLA	CHC-C1C-C2C	-2.21	120.60	126.75
23	C	507	CLA	CHA-C1A-NA	-2.21	121.05	126.18
23	A	605	CLA	O2D-CGD-O1D	-2.21	119.44	123.82
25	C	515	BCR	C11-C12-C13	-2.20	120.22	126.42
25	A	609	BCR	C20-C19-C18	-2.20	120.23	126.42
25	c	515	BCR	C1-C6-C7	-2.20	109.54	115.73
23	C	510	CLA	O1D-CGD-CBD	-2.20	120.50	124.58
25	B	618	BCR	C36-C18-C17	-2.20	119.84	122.92
23	B	617	CLA	CHA-C1A-NA	-2.20	121.07	126.18
27	a	612	SQD	C5-C6-S	-2.20	111.27	114.34
25	B	620	BCR	C23-C22-C21	-2.20	115.57	118.94
23	B	613	CLA	O2D-CGD-O1D	-2.20	119.46	123.82
23	B	611	CLA	CHA-C1A-NA	-2.20	121.08	126.18
23	B	607[B]	CLA	O2D-CGD-O1D	-2.20	119.46	123.82
23	a	604	CLA	CHC-C1C-C2C	-2.20	120.63	126.75
23	a	605	CLA	O2D-CGD-O1D	-2.19	119.47	123.82
23	b	606	CLA	CHC-C1C-C2C	-2.19	120.64	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C35-C13-C14	-2.19	119.86	122.92
25	H	101	BCR	C37-C22-C21	-2.19	119.86	122.92
25	A	609	BCR	C37-C22-C21	-2.19	119.86	122.92
23	b	614	CLA	CHA-C1A-NA	-2.19	121.10	126.18
32	c	517	DGD	C2G-O2G-C1B	-2.19	112.71	117.88
23	b	615	CLA	CHA-C1A-NA	-2.18	121.11	126.18
23	B	603	CLA	C1-C2-C3	-2.18	121.94	125.96
23	b	611	CLA	C11-C12-C13	-2.18	108.58	115.73
25	b	621	BCR	C11-C12-C13	-2.18	120.29	126.42
23	b	613	CLA	CHA-C1A-NA	-2.18	121.12	126.18
23	B	605	CLA	CHA-C1A-NA	-2.18	121.12	126.18
23	C	502	CLA	O1D-CGD-CBD	-2.18	120.54	124.58
23	C	510	CLA	CHC-C1C-C2C	-2.18	120.69	126.75
23	C	502	CLA	CHC-C1C-C2C	-2.18	120.69	126.75
23	b	609[B]	CLA	CHA-C1A-NA	-2.18	121.12	126.18
23	c	508	CLA	CHA-C1A-NA	-2.18	121.12	126.18
23	b	608	CLA	O2D-CGD-O1D	-2.17	119.51	123.82
25	c	516	BCR	C30-C25-C24	-2.17	109.62	115.73
23	C	507	CLA	CHB-C4A-NA	-2.17	121.51	124.51
23	b	613	CLA	CHC-C1C-C2C	-2.17	120.70	126.75
23	C	511	CLA	O2D-CGD-O1D	-2.17	119.51	123.82
25	A	609	BCR	C35-C13-C14	-2.17	119.88	122.92
23	a	607	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
31	B	622	LHG	O7-C7-O9	-2.17	118.33	123.69
23	b	605	CLA	C1-C2-C3	-2.17	121.96	125.96
25	b	622	BCR	C20-C19-C18	-2.17	120.33	126.42
23	B	614	CLA	O2D-CGD-O1D	-2.17	119.52	123.82
23	b	609[B]	CLA	CHC-C1C-C2C	-2.17	120.72	126.75
25	c	515	BCR	C30-C25-C24	-2.17	109.64	115.73
23	c	505	CLA	CHC-C1C-C2C	-2.17	120.72	126.75
23	B	609	CLA	C11-C12-C13	-2.17	108.62	115.73
25	B	620	BCR	C34-C9-C10	-2.17	119.89	122.92
23	B	616	CLA	O2D-CGD-O1D	-2.17	119.52	123.82
23	B	613	CLA	CHC-C1C-C2C	-2.16	120.73	126.75
23	C	503	CLA	O1D-CGD-CBD	-2.16	120.57	124.58
32	C	518	DGD	C3G-C2G-C1G	-2.16	106.98	111.86
23	C	508	CLA	C1C-NC-C4C	-2.16	105.83	107.05
25	a	608	BCR	C34-C9-C10	-2.16	119.90	122.92
25	H	101	BCR	C16-C15-C14	-2.16	118.86	123.46
23	B	608	CLA	O1D-CGD-CBD	-2.16	120.58	124.58
23	B	607[A]	CLA	CHA-C1A-NA	-2.16	121.17	126.18
25	K	101	BCR	C31-C1-C6	-2.15	106.81	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	CHC-C1C-C2C	-2.15	120.75	126.75
25	k	101	BCR	C7-C8-C9	-2.15	122.98	126.21
25	c	516	BCR	C1-C6-C7	-2.15	109.68	115.73
23	c	510	CLA	O2D-CGD-O1D	-2.15	119.55	123.82
25	T	101	BCR	C31-C1-C6	-2.15	106.82	110.31
25	b	622	BCR	C19-C18-C17	-2.15	115.64	118.94
23	d	403	CLA	C1C-NC-C4C	-2.15	105.84	107.05
23	B	611	CLA	CHC-C1C-C2C	-2.14	120.78	126.75
27	a	610	SQD	C5-C6-S	-2.14	111.35	114.34
23	C	503	CLA	CHA-C1A-NA	-2.14	121.21	126.18
23	b	616	CLA	CHC-C1C-C2C	-2.14	120.80	126.75
23	B	615	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
25	k	101	BCR	C11-C12-C13	-2.14	120.42	126.42
23	b	618	CLA	CHC-C1C-C2C	-2.14	120.80	126.75
25	f	101	BCR	C28-C27-C26	-2.13	110.25	113.99
25	h	101	BCR	C30-C25-C24	-2.13	109.73	115.73
23	c	508	CLA	CHB-C4A-NA	-2.13	121.56	124.51
23	B	611	CLA	O1D-CGD-CBD	-2.13	120.63	124.58
23	C	506	CLA	CHC-C1C-C2C	-2.13	120.82	126.75
23	C	503	CLA	CHC-C1C-C2C	-2.13	120.82	126.75
23	c	513	CLA	O2A-CGA-O1A	-2.13	118.39	123.58
23	d	402	CLA	O1D-CGD-CBD	-2.13	120.63	124.58
23	A	605	CLA	C4A-NA-C1A	-2.13	103.58	106.32
23	B	608	CLA	CMB-C2B-C1B	-2.13	125.20	128.46
25	a	608	BCR	C35-C13-C14	-2.12	119.95	122.92
25	c	522	BCR	C11-C12-C13	-2.12	120.45	126.42
23	B	603	CLA	CHC-C1C-C2C	-2.12	120.84	126.75
23	b	604	CLA	CHC-C1C-C2C	-2.12	120.84	126.75
23	B	607[A]	CLA	CHC-C1C-C2C	-2.12	120.85	126.75
23	A	605	CLA	CHC-C1C-C2C	-2.12	120.85	126.75
23	c	503	CLA	CHC-C1C-C2C	-2.12	120.86	126.75
32	C	517	DGD	C1E-O6E-C5E	-2.12	109.54	113.71
23	c	514	CLA	C1C-NC-C4C	-2.12	105.86	107.05
25	k	101	BCR	C10-C11-C12	-2.12	116.82	123.26
25	c	515	BCR	C36-C18-C17	-2.11	119.96	122.92
23	b	618	CLA	CHA-C1A-NA	-2.11	121.27	126.18
23	C	512	CLA	CHA-C1A-NA	-2.11	121.28	126.18
23	b	609[A]	CLA	CHC-C1C-C2C	-2.11	120.88	126.75
26	A	610	PL9	C20-C19-C21	-2.11	111.65	115.29
25	F	101	BCR	C30-C25-C24	-2.11	109.81	115.73
25	b	620	BCR	C37-C22-C23	-2.11	114.74	118.10
23	b	609[A]	CLA	CHA-C1A-NA	-2.11	121.29	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
27	A	611	SQD	C5-C6-S	-2.10	111.41	114.34
23	C	505	CLA	CHA-C1A-NA	-2.10	121.30	126.18
23	B	602	CLA	CHC-C1C-C2C	-2.10	120.91	126.75
23	B	603	CLA	CHB-C4A-NA	-2.10	121.61	124.51
23	b	612	CLA	CHB-C4A-NA	-2.10	121.61	124.51
23	C	505	CLA	CHB-C4A-NA	-2.10	121.61	124.51
23	C	508	CLA	CHC-C1C-C2C	-2.09	120.92	126.75
23	b	610	CLA	O2D-CGD-O1D	-2.09	119.67	123.82
23	A	605	CLA	O1D-CGD-CBD	-2.09	120.71	124.58
25	b	622	BCR	C30-C25-C24	-2.09	109.86	115.73
23	B	607[B]	CLA	CHA-C1A-NA	-2.09	121.33	126.18
23	d	403	CLA	CHC-C1C-C2C	-2.08	120.94	126.75
25	C	514	BCR	C20-C19-C18	-2.08	120.56	126.42
23	c	509	CLA	CHC-C1C-C2C	-2.08	120.95	126.75
28	j	101	LMG	C6-C5-C4	-2.08	108.07	112.99
27	B	623	SQD	O5-C1-C2	-2.08	105.88	110.34
31	D	408	LHG	O8-C23-O10	-2.08	118.51	123.58
27	b	602	SQD	O47-C7-O49	-2.08	118.57	123.69
27	b	602	SQD	O5-C1-C2	-2.07	105.89	110.34
23	c	513	CLA	CHC-C1C-C2C	-2.07	120.98	126.75
23	B	614	CLA	CHC-C1C-C2C	-2.07	120.98	126.75
23	A	608	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
27	B	623	SQD	O47-C7-O49	-2.07	118.58	123.69
23	b	612	CLA	CHC-C1C-C2C	-2.07	120.99	126.75
23	C	508	CLA	CHA-C1A-NA	-2.07	121.38	126.18
23	D	404	CLA	CHC-C1C-C2C	-2.06	121.00	126.75
23	C	501	CLA	O2D-CGD-O1D	-2.06	119.73	123.82
23	d	402	CLA	CHA-C1A-NA	-2.06	121.39	126.18
31	L	101	LHG	C5-O7-C7	-2.06	113.00	117.88
23	a	604	CLA	C4A-NA-C1A	-2.06	103.67	106.32
23	C	502	CLA	CHA-C1A-NA	-2.06	121.39	126.18
23	b	619	CLA	O2D-CGD-O1D	-2.06	119.74	123.82
31	D	408	LHG	C5-O7-C7	-2.06	113.01	117.88
23	B	615	CLA	CHA-C1A-NA	-2.06	121.40	126.18
25	C	515	BCR	C12-C13-C14	-2.06	115.79	118.94
23	c	512	CLA	CHC-C1C-C2C	-2.05	121.03	126.75
33	V	202	HEM	CAD-CBD-CGD	-2.05	109.16	112.66
23	c	511	CLA	CHA-C1A-NA	-2.05	121.42	126.18
23	B	613	CLA	CHA-C1A-NA	-2.05	121.42	126.18
25	C	514	BCR	C3-C4-C5	-2.05	110.39	113.99
26	d	404	PL9	C25-C24-C26	-2.05	111.75	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
23	c	505	CLA	C1C-NC-C4C	-2.05	105.89	107.05
23	c	511	CLA	CHC-C1C-C2C	-2.05	121.05	126.75
23	c	505	CLA	C7-C6-C5	-2.05	107.60	113.17
23	b	616	CLA	CHA-C1A-NA	-2.05	121.42	126.18
23	B	604	CLA	O2D-CGD-O1D	-2.04	119.76	123.82
23	a	604	CLA	O2D-CGD-O1D	-2.04	119.77	123.82
23	B	611	CLA	O2D-CGD-O1D	-2.04	119.77	123.82
23	c	509	CLA	CHA-C1A-NA	-2.04	121.44	126.18
25	b	621	BCR	C20-C19-C18	-2.04	120.69	126.42
23	b	617	CLA	CHC-C1C-C2C	-2.04	121.08	126.75
23	C	504	CLA	C7-C6-C5	-2.04	107.63	113.17
23	B	609	CLA	CHC-C1C-C2C	-2.04	121.08	126.75
23	b	605	CLA	O2D-CGD-O1D	-2.04	119.78	123.82
23	C	501	CLA	CHC-C1C-C2C	-2.03	121.09	126.75
31	l	101	LHG	C5-O7-C7	-2.03	113.07	117.88
23	b	614	CLA	O2D-CGD-O1D	-2.03	119.79	123.82
23	c	505	CLA	CHA-C1A-NA	-2.03	121.46	126.18
31	B	622	LHG	O8-C23-O10	-2.03	118.62	123.58
25	H	101	BCR	C30-C25-C24	-2.03	110.03	115.73
23	c	507	CLA	CBA-CAA-C2A	-2.03	107.80	113.82
32	C	516	DGD	O1G-C1A-O1A	-2.03	118.63	123.58
23	C	505	CLA	O2A-CGA-O1A	-2.02	118.65	123.58
28	J	101	LMG	C8-O7-C10	-2.02	113.10	117.88
23	a	607	CLA	O2D-CGD-O1D	-2.02	119.81	123.82
23	c	504	CLA	O2D-CGD-O1D	-2.02	119.82	123.82
23	B	602	CLA	CHA-C1A-NA	-2.02	121.50	126.18
23	B	614	CLA	C1-C2-C3	-2.01	122.25	125.96
23	c	504	CLA	CHC-C1C-C2C	-2.01	121.14	126.75
27	A	611	SQD	O5-C1-C2	-2.01	106.02	110.34
31	E	101	LHG	O7-C7-O9	-2.01	118.72	123.69
23	B	604	CLA	CHC-C1C-C2C	-2.01	121.15	126.75
25	c	516	BCR	C31-C1-C6	-2.01	107.05	110.31
23	b	611	CLA	C11-C10-C8	-2.01	109.14	115.73
23	a	613	CLA	O2D-CGD-O1D	-2.01	119.84	123.82
23	B	603	CLA	CHA-C1A-NA	-2.01	121.52	126.18
25	b	621	BCR	C33-C5-C4	-2.01	109.77	113.56
23	B	613	CLA	CHB-C4A-NA	-2.00	121.74	124.51
23	b	616	CLA	C1-C2-C3	-2.00	122.27	125.96
25	B	619	BCR	C23-C22-C21	-2.00	115.87	118.94
23	a	605	CLA	C1-O2A-CGA	2.00	121.38	116.77
25	B	618	BCR	C29-C28-C27	2.01	115.97	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C1-O2A-CGA	2.01	121.40	116.77
32	H	102	DGD	O6E-C5E-C6E	2.01	111.49	106.43
23	C	504	CLA	O2A-CGA-CBA	2.01	117.74	111.92
23	C	510	CLA	C4-C3-C5	2.02	118.77	115.29
23	b	605	CLA	C1-O2A-CGA	2.02	121.42	116.77
23	c	510	CLA	C4-C3-C5	2.02	118.77	115.29
23	C	501	CLA	CMB-C2B-C3B	2.02	128.56	124.88
32	d	405	DGD	O6D-C5D-C6D	2.02	110.68	106.64
23	b	610	CLA	CED-O2D-CGD	2.02	120.63	115.97
23	B	606	CLA	CED-O2D-CGD	2.03	120.64	115.97
23	C	509	CLA	C4-C3-C5	2.03	118.79	115.29
32	C	516	DGD	O6D-C5D-C6D	2.03	110.70	106.64
23	B	617	CLA	C4-C3-C5	2.04	118.80	115.29
32	c	518	DGD	O6E-C5E-C6E	2.04	111.55	106.43
25	F	101	BCR	C3-C4-C5	2.04	117.57	113.99
23	C	508	CLA	CMB-C2B-C3B	2.04	128.60	124.88
28	z	101	LMG	C4-C3-C2	2.04	114.41	110.83
25	b	622	BCR	C34-C9-C8	2.05	121.36	118.10
23	c	511	CLA	C1-O2A-CGA	2.05	121.48	116.77
23	C	513	CLA	CED-O2D-CGD	2.05	120.69	115.97
23	b	619	CLA	C4-C3-C5	2.05	118.82	115.29
27	x	101	SQD	C3-C4-C5	2.06	113.92	110.24
23	C	502	CLA	C1-O2A-CGA	2.07	121.53	116.77
27	X	101	SQD	C3-C4-C5	2.07	113.94	110.24
23	b	608	CLA	CED-O2D-CGD	2.07	120.74	115.97
23	D	402	CLA	CHD-C4C-C3C	2.07	127.94	124.88
23	C	505	CLA	CMD-C2D-C3D	2.07	128.65	124.88
25	a	608	BCR	C34-C9-C8	2.07	121.40	118.10
28	C	520	LMG	O6-C5-C4	2.07	113.49	109.69
23	c	507	CLA	CED-O2D-CGD	2.07	120.75	115.97
23	a	605	CLA	CMB-C2B-C3B	2.07	128.66	124.88
23	b	613	CLA	CED-O2D-CGD	2.08	120.77	115.97
32	C	517	DGD	C3E-C4E-C5E	2.09	113.98	110.24
32	h	102	DGD	O6E-C5E-C6E	2.09	111.69	106.43
25	B	620	BCR	C34-C9-C8	2.09	121.43	118.10
23	c	502	CLA	C4-C3-C5	2.10	118.91	115.29
32	C	517	DGD	C4E-C3E-C2E	2.10	114.51	110.83
23	C	501	CLA	C4-C3-C5	2.10	118.91	115.29
23	c	506	CLA	CMD-C2D-C3D	2.10	128.70	124.88
32	d	405	DGD	C3E-C4E-C5E	2.11	114.02	110.24
23	B	609	CLA	CHD-C4C-C3C	2.12	128.01	124.88
25	b	621	BCR	C2-C3-C4	2.12	116.22	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	604	CLA	CMB-C2B-C3B	2.12	128.75	124.88
23	C	508	CLA	O2A-CGA-CBA	2.13	118.06	111.92
23	C	512	CLA	CMB-C2B-C3B	2.13	128.75	124.88
25	C	515	BCR	C19-C18-C17	2.13	122.22	118.94
23	b	611	CLA	CMB-C2B-C3B	2.13	128.77	124.88
23	a	605	CLA	O2A-CGA-CBA	2.14	118.09	111.92
23	c	509	CLA	O2A-CGA-CBA	2.14	118.10	111.92
32	c	517	DGD	O1G-C1A-C2A	2.14	118.10	111.92
23	b	616	CLA	O2A-CGA-CBA	2.14	118.11	111.92
23	A	608	CLA	CED-O2D-CGD	2.14	120.90	115.97
33	e	102	HEM	CMC-C2C-C3C	2.14	128.78	124.88
23	C	513	CLA	C1-O2A-CGA	2.15	121.73	116.77
23	b	614	CLA	O2A-CGA-CBA	2.15	118.15	111.92
23	D	402	CLA	CMB-C2B-C3B	2.15	128.80	124.88
23	a	613	CLA	CHD-C4C-C3C	2.16	128.07	124.88
23	B	608	CLA	CHD-C4C-C3C	2.16	128.08	124.88
23	b	604	CLA	C1-O2A-CGA	2.18	121.78	116.77
23	B	608	CLA	O2A-CGA-CBA	2.18	118.22	111.92
23	B	608	CLA	C1-O2A-CGA	2.18	121.80	116.77
23	b	606	CLA	C1-O2A-CGA	2.19	121.81	116.77
23	C	509	CLA	CED-O2D-CGD	2.19	121.01	115.97
23	a	604	CLA	C4-C3-C5	2.19	119.07	115.29
32	c	517	DGD	O6D-C5D-C6D	2.20	111.03	106.64
23	c	507	CLA	CMB-C2B-C3B	2.20	128.89	124.88
23	C	512	CLA	C1-O2A-CGA	2.21	121.85	116.77
23	A	605	CLA	CMB-C2B-C3B	2.21	128.90	124.88
23	B	609	CLA	CMB-C2B-C3B	2.21	128.91	124.88
25	H	101	BCR	C35-C13-C12	2.21	121.63	118.10
23	C	513	CLA	CMB-C2B-C3B	2.22	128.92	124.88
23	B	609	CLA	C4-C3-C5	2.22	119.11	115.29
23	B	610	CLA	C1-O2A-CGA	2.22	121.88	116.77
25	h	101	BCR	C2-C3-C4	2.22	116.45	111.36
23	A	605	CLA	C4-C3-C5	2.22	119.12	115.29
23	b	611	CLA	C4-C3-C5	2.23	119.13	115.29
25	B	619	BCR	C2-C3-C4	2.23	116.46	111.36
25	c	522	BCR	C40-C30-C25	2.24	113.94	110.31
33	e	102	HEM	CMB-C2B-C3B	2.24	128.96	124.88
23	C	512	CLA	CED-O2D-CGD	2.24	121.14	115.97
28	A	612	LMG	O8-C28-C29	2.24	118.41	111.92
28	j	101	LMG	O6-C5-C4	2.26	113.83	109.69
32	d	405	DGD	C1E-C2E-C3E	2.26	114.70	109.98
23	C	506	CLA	CMB-C2B-C3B	2.26	129.00	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	601	SQD	C3-C4-C5	2.26	114.29	110.24
28	c	521	LMG	C3-C4-C5	2.27	114.30	110.24
25	h	101	BCR	C34-C9-C8	2.27	121.71	118.10
33	V	202	HEM	CMB-C2B-C3B	2.27	129.01	124.88
31	l	101	LHG	O8-C23-C24	2.27	118.49	111.92
23	c	508	CLA	C1-O2A-CGA	2.28	122.01	116.77
27	a	612	SQD	C3-C4-C5	2.28	114.32	110.24
25	b	621	BCR	C40-C30-C25	2.28	114.01	110.31
23	B	605	CLA	C1-O2A-CGA	2.30	122.06	116.77
23	C	506	CLA	CED-O2D-CGD	2.30	121.26	115.97
28	a	611	LMG	O8-C28-C29	2.30	118.56	111.92
23	b	609[B]	CLA	O2A-CGA-CBA	2.30	118.58	111.92
23	c	504	CLA	O2A-CGA-CBA	2.31	118.59	111.92
23	C	510	CLA	O2A-CGA-CBA	2.31	118.61	111.92
23	a	607	CLA	C1-O2A-CGA	2.32	122.11	116.77
32	h	102	DGD	O6D-C5D-C6D	2.32	111.27	106.64
23	B	614	CLA	O2A-CGA-CBA	2.32	118.63	111.92
31	L	101	LHG	O8-C23-C24	2.32	118.63	111.92
23	B	607[B]	CLA	O2A-CGA-CBA	2.32	118.63	111.92
23	B	612	CLA	O2A-CGA-CBA	2.33	118.65	111.92
23	b	611	CLA	O2A-CGA-CBA	2.34	118.68	111.92
32	d	405	DGD	C4E-C3E-C2E	2.34	114.93	110.83
23	C	507	CLA	C1-O2A-CGA	2.34	122.16	116.77
33	v	201	HEM	CMD-C2D-C3D	2.35	129.37	124.94
33	E	102	HEM	CMB-C2B-C3B	2.35	129.15	124.88
25	b	621	BCR	C29-C30-C25	2.35	114.16	110.48
23	B	608	CLA	CED-O2D-CGD	2.36	121.40	115.97
23	B	609	CLA	CAC-C3C-C4C	2.36	128.07	124.82
23	C	502	CLA	O2A-CGA-CBA	2.36	118.75	111.92
23	c	509	CLA	CMB-C2B-C3B	2.37	129.20	124.88
32	D	406	DGD	O6D-C5D-C6D	2.37	111.38	106.64
23	C	513	CLA	C4-C3-C5	2.37	119.38	115.29
23	D	404	CLA	O2A-CGA-CBA	2.38	118.79	111.92
23	c	514	CLA	C4-C3-C5	2.38	119.39	115.29
26	D	405	PL9	C53-C6-C1	2.38	119.90	114.87
23	b	612	CLA	O2A-CGA-CBA	2.39	118.83	111.92
23	c	513	CLA	C1-O2A-CGA	2.39	122.28	116.77
23	A	608	CLA	CHC-C1C-NC	2.39	128.32	124.17
23	b	609[A]	CLA	O2A-CGA-CBA	2.39	118.84	111.92
27	a	610	SQD	O48-C23-C24	2.40	118.84	111.92
23	b	607	CLA	C1-O2A-CGA	2.40	122.30	116.77
23	c	505	CLA	C1-O2A-CGA	2.40	122.31	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	j	101	LMG	O8-C28-C29	2.40	118.87	111.92
27	A	611	SQD	O48-C23-C24	2.41	118.88	111.92
23	c	506	CLA	CHC-C1C-NC	2.41	128.35	124.17
23	B	603	CLA	O2A-CGA-CBA	2.42	118.92	111.92
23	C	505	CLA	CHC-C1C-NC	2.43	128.39	124.17
23	d	403	CLA	C4-C3-C5	2.44	119.49	115.29
23	A	608	CLA	O2A-CGA-CBA	2.44	118.96	111.92
23	c	503	CLA	O2A-CGA-CBA	2.44	118.98	111.92
23	D	404	CLA	C4-C3-C5	2.44	119.50	115.29
23	b	613	CLA	C4-C3-C5	2.44	119.50	115.29
23	B	615	CLA	CHC-C1C-NC	2.44	128.41	124.17
28	J	101	LMG	O8-C28-C29	2.44	118.99	111.92
23	b	616	CLA	C1-O2A-CGA	2.45	122.41	116.77
23	B	606	CLA	C1-O2A-CGA	2.46	122.44	116.77
33	v	201	HEM	CMB-C2B-C3B	2.46	129.36	124.88
33	V	202	HEM	C4A-C3A-C2A	2.47	108.71	107.00
23	B	604	CLA	O2A-CGA-CBA	2.47	119.05	111.92
25	H	101	BCR	C36-C18-C19	2.47	122.03	118.10
23	B	611	CLA	C4-C3-C5	2.47	119.55	115.29
23	B	603	CLA	C1-O2A-CGA	2.48	122.48	116.77
23	B	607[A]	CLA	O2A-CGA-CBA	2.48	119.09	111.92
28	C	520	LMG	O8-C28-C29	2.48	119.09	111.92
23	B	615	CLA	C1-O2A-CGA	2.48	122.49	116.77
32	C	516	DGD	O1G-C1A-C2A	2.48	119.10	111.92
23	C	511	CLA	O2A-CGA-CBA	2.48	119.10	111.92
23	c	510	CLA	C1-O2A-CGA	2.49	122.50	116.77
23	c	503	CLA	C1-O2A-CGA	2.49	122.51	116.77
28	C	520	LMG	C3-C4-C5	2.50	114.71	110.24
23	b	611	CLA	CHC-C1C-NC	2.50	128.51	124.17
23	b	610	CLA	C1-O2A-CGA	2.50	122.52	116.77
23	B	614	CLA	C4-C3-C5	2.50	119.60	115.29
23	b	616	CLA	C4-C3-C5	2.50	119.61	115.29
23	C	502	CLA	C4-C3-C5	2.51	119.61	115.29
23	b	610	CLA	O2A-CGA-CBA	2.51	119.18	111.92
28	B	621	LMG	O8-C28-C29	2.51	119.19	111.92
23	B	616	CLA	C4-C3-C5	2.51	119.62	115.29
23	c	511	CLA	O2A-CGA-CBA	2.52	119.19	111.92
23	A	605	CLA	O2A-CGA-CBA	2.52	119.19	111.92
23	C	509	CLA	C1-O2A-CGA	2.52	122.58	116.77
23	C	503	CLA	O2A-CGA-CBA	2.52	119.21	111.92
23	B	615	CLA	O2A-CGA-CBA	2.52	119.22	111.92
23	c	512	CLA	C4-C3-C5	2.53	119.64	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	CHC-C1C-NC	2.53	128.56	124.17
23	b	618	CLA	C4-C3-C5	2.53	119.65	115.29
25	F	101	BCR	C36-C18-C19	2.53	122.13	118.10
23	C	511	CLA	C4-C3-C5	2.53	119.65	115.29
23	c	503	CLA	C4-C3-C5	2.53	119.65	115.29
27	a	612	SQD	O8-S-C6	2.53	109.78	105.74
23	D	403	CLA	CHC-C1C-NC	2.53	128.57	124.17
23	b	606	CLA	O2A-CGA-CBA	2.53	119.24	111.92
23	b	614	CLA	C1-O2A-CGA	2.54	122.61	116.77
26	d	404	PL9	C53-C6-C1	2.54	120.23	114.87
23	a	607	CLA	CHC-C1C-NC	2.54	128.58	124.17
31	E	101	LHG	O8-C23-C24	2.54	119.26	111.92
27	b	601	SQD	O8-S-C6	2.56	109.81	105.74
23	b	608	CLA	CHC-C1C-NC	2.56	128.61	124.17
25	C	514	BCR	C34-C9-C8	2.57	122.19	118.10
23	c	510	CLA	O2A-CGA-CBA	2.58	119.38	111.92
23	d	402	CLA	C4-C3-C5	2.59	119.75	115.29
23	D	403	CLA	C4-C3-C5	2.60	119.77	115.29
23	b	605	CLA	O2A-CGA-CBA	2.60	119.44	111.92
24	A	607	PHO	O1D-CGD-CBD	2.61	129.42	124.58
25	C	521	BCR	C40-C30-C25	2.61	114.54	110.31
23	d	403	CLA	O2A-CGA-CBA	2.61	119.47	111.92
31	e	101	LHG	O8-C23-C24	2.61	119.47	111.92
23	C	503	CLA	C4-C3-C5	2.61	119.79	115.29
23	B	606	CLA	CHC-C1C-NC	2.61	128.71	124.17
23	D	404	CLA	CHC-C1C-NC	2.62	128.72	124.17
23	B	614	CLA	CHC-C1C-NC	2.62	128.72	124.17
28	b	623	LMG	O8-C28-C29	2.62	119.50	111.92
23	c	504	CLA	C4-C3-C5	2.62	119.81	115.29
23	C	513	CLA	CHC-C1C-NC	2.62	128.72	124.17
31	d	406	LHG	O8-C23-C24	2.62	119.51	111.92
24	a	606	PHO	O1D-CGD-CBD	2.64	129.48	124.58
27	b	602	SQD	C4-C3-C2	2.65	115.47	110.83
23	c	514	CLA	CHC-C1C-NC	2.66	128.78	124.17
24	d	401	PHO	O1D-CGD-CBD	2.66	129.52	124.58
25	b	622	BCR	C36-C18-C19	2.66	122.34	118.10
27	B	623	SQD	C4-C3-C2	2.66	115.49	110.83
23	b	609[B]	CLA	C1-O2A-CGA	2.67	122.91	116.77
23	C	504	CLA	C1-O2A-CGA	2.67	122.91	116.77
23	B	605	CLA	C4-C3-C5	2.67	119.89	115.29
23	b	613	CLA	CHC-C1C-NC	2.67	128.80	124.17
32	D	406	DGD	O1G-C1A-C2A	2.67	119.64	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C4-C3-C5	2.67	119.90	115.29
23	c	509	CLA	C4-C3-C5	2.68	119.90	115.29
27	B	623	SQD	O9-S-C6	2.68	110.12	106.94
23	b	618	CLA	O2A-CGA-CBA	2.69	119.69	111.92
23	B	607[B]	CLA	C1-O2A-CGA	2.69	122.97	116.77
23	b	607	CLA	C4-C3-C5	2.69	119.93	115.29
28	c	521	LMG	O8-C28-C29	2.69	119.71	111.92
23	B	602	CLA	CHC-C1C-NC	2.70	128.85	124.17
26	d	404	PL9	C7-C3-C4	2.70	119.07	116.88
27	b	602	SQD	O9-S-C6	2.70	110.15	106.94
23	d	402	CLA	CHC-C1C-NC	2.70	128.86	124.17
23	B	609	CLA	O2A-CGA-CBA	2.71	119.74	111.92
32	d	405	DGD	O1G-C1A-C2A	2.71	119.75	111.92
23	c	514	CLA	O2A-CGA-CBA	2.71	119.76	111.92
23	a	604	CLA	O2A-CGA-CBA	2.71	119.76	111.92
23	B	609	CLA	CHC-C1C-NC	2.71	128.88	124.17
23	c	504	CLA	CHC-C1C-NC	2.72	128.89	124.17
32	D	406	DGD	C3E-C4E-C5E	2.72	115.11	110.24
23	c	512	CLA	O2A-CGA-CBA	2.73	119.81	111.92
23	b	604	CLA	CHC-C1C-NC	2.73	128.91	124.17
26	A	610	PL9	C53-C6-C1	2.74	120.65	114.87
23	b	610	CLA	C4-C3-C5	2.74	120.02	115.29
23	b	619	CLA	O2A-CGA-CBA	2.74	119.85	111.92
23	C	501	CLA	CHC-C1C-NC	2.75	128.94	124.17
25	c	522	BCR	C29-C28-C27	2.75	117.66	111.36
26	a	609	PL9	C53-C6-C1	2.75	120.68	114.87
23	c	507	CLA	CHC-C1C-NC	2.76	128.97	124.17
23	b	617	CLA	CHC-C1C-NC	2.77	128.97	124.17
23	B	611	CLA	CHC-C1C-NC	2.77	128.97	124.17
23	D	402	CLA	O2A-CGA-CBA	2.77	119.92	111.92
23	B	608	CLA	C4-C3-C5	2.77	120.07	115.29
28	J	101	LMG	O6-C5-C4	2.77	114.78	109.69
23	B	607[A]	CLA	C1-O2A-CGA	2.77	123.16	116.77
23	B	613	CLA	O2A-CGA-CBA	2.78	119.94	111.92
32	h	102	DGD	O1G-C1A-C2A	2.78	119.95	111.92
23	a	613	CLA	C4-C3-C5	2.78	120.09	115.29
23	D	402	CLA	C4-C3-C5	2.79	120.10	115.29
23	b	609[A]	CLA	C1-O2A-CGA	2.79	123.20	116.77
23	b	616	CLA	CHC-C1C-NC	2.79	129.02	124.17
23	c	511	CLA	CHC-C1C-NC	2.80	129.02	124.17
23	b	612	CLA	CHC-C1C-NC	2.80	129.03	124.17
23	A	605	CLA	CHC-C1C-NC	2.81	129.04	124.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609[A]	CLA	C4-C3-C5	2.81	120.13	115.29
23	C	509	CLA	O2A-CGA-CBA	2.81	120.04	111.92
23	B	605	CLA	O2A-CGA-CBA	2.81	120.05	111.92
25	f	101	BCR	C2-C3-C4	2.82	117.82	111.36
23	C	507	CLA	CHC-C1C-NC	2.82	129.07	124.17
24	D	401	PHO	O1D-CGD-CBD	2.83	129.84	124.58
32	H	102	DGD	O1G-C1A-C2A	2.83	120.11	111.92
23	D	403	CLA	O2A-CGA-CBA	2.84	120.13	111.92
23	C	510	CLA	CHC-C1C-NC	2.84	129.10	124.17
23	b	606	CLA	CHC-C1C-NC	2.84	129.10	124.17
23	B	607[A]	CLA	C4-C3-C5	2.84	120.19	115.29
23	B	617	CLA	O2A-CGA-CBA	2.84	120.14	111.92
23	C	501	CLA	O2A-CGA-CBA	2.84	120.14	111.92
23	c	502	CLA	CHC-C1C-NC	2.85	129.11	124.17
28	z	101	LMG	O1-C1-C2	2.85	112.84	108.24
23	b	609[A]	CLA	CHC-C1C-NC	2.85	129.11	124.17
23	b	615	CLA	O2A-CGA-CBA	2.85	120.16	111.92
23	C	512	CLA	O2A-CGA-CBA	2.85	120.17	111.92
31	D	408	LHG	O8-C23-C24	2.85	120.17	111.92
23	C	511	CLA	C1-O2A-CGA	2.85	123.34	116.77
23	C	509	CLA	CHC-C1C-NC	2.85	129.13	124.17
23	a	604	CLA	CHC-C1C-NC	2.86	129.13	124.17
23	B	607[B]	CLA	C4-C3-C5	2.86	120.22	115.29
23	c	513	CLA	CHC-C1C-NC	2.86	129.13	124.17
23	b	609[B]	CLA	C4-C3-C5	2.86	120.22	115.29
23	C	507	CLA	O2A-CGA-CBA	2.86	120.19	111.92
25	B	618	BCR	C2-C3-C4	2.86	117.92	111.36
23	c	509	CLA	CHC-C1C-NC	2.87	129.16	124.17
25	F	101	BCR	C23-C22-C21	2.88	123.36	118.94
23	d	402	CLA	O2A-CGA-CBA	2.88	120.25	111.92
23	c	503	CLA	CHC-C1C-NC	2.88	129.17	124.17
23	a	607	CLA	O2A-CGA-CBA	2.88	120.25	111.92
23	B	608	CLA	O2D-CGD-CBD	2.88	116.39	111.28
31	b	624	LHG	O8-C23-C24	2.88	120.26	111.92
31	D	407	LHG	O8-C23-C24	2.89	120.27	111.92
23	b	607	CLA	CHC-C1C-NC	2.89	129.19	124.17
23	c	502	CLA	O2A-CGA-CBA	2.89	120.28	111.92
23	c	512	CLA	CHC-C1C-NC	2.90	129.20	124.17
23	B	611	CLA	O2A-CGA-CBA	2.90	120.29	111.92
23	b	613	CLA	O2A-CGA-CBA	2.90	120.30	111.92
23	A	606	CLA	CHC-C1C-NC	2.90	129.21	124.17
31	B	622	LHG	O8-C23-C24	2.91	120.32	111.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CHC-C1C-NC	2.91	129.22	124.17
23	b	615	CLA	CHC-C1C-NC	2.92	129.25	124.17
23	B	607[A]	CLA	CHC-C1C-NC	2.92	129.25	124.17
23	c	513	CLA	O2A-CGA-CBA	2.93	120.38	111.92
28	c	520	LMG	O8-C28-C29	2.93	120.38	111.92
23	A	606	CLA	O2A-CGA-CBA	2.93	120.38	111.92
23	c	505	CLA	C4-C3-C5	2.93	120.34	115.29
23	d	403	CLA	CHC-C1C-NC	2.93	129.26	124.17
23	D	402	CLA	CHC-C1C-NC	2.93	129.26	124.17
23	B	612	CLA	CHC-C1C-NC	2.93	129.27	124.17
23	c	508	CLA	CHC-C1C-NC	2.94	129.28	124.17
23	b	606	CLA	C4-C3-C5	2.94	120.36	115.29
23	a	613	CLA	O2A-CGA-CBA	2.94	120.42	111.92
23	C	503	CLA	CHC-C1C-NC	2.94	129.28	124.17
27	b	602	SQD	O48-C23-C24	2.95	120.44	111.92
23	C	511	CLA	CHC-C1C-NC	2.95	129.29	124.17
32	D	406	DGD	C1E-C2E-C3E	2.95	116.14	109.98
23	B	612	CLA	C1-O2A-CGA	2.95	123.56	116.77
23	C	504	CLA	C4-C3-C5	2.95	120.38	115.29
23	C	506	CLA	CHC-C1C-NC	2.96	129.30	124.17
27	B	623	SQD	O48-C23-C24	2.96	120.47	111.92
23	c	508	CLA	O2A-CGA-CBA	2.96	120.47	111.92
23	B	610	CLA	CHC-C1C-NC	2.96	129.31	124.17
23	b	605	CLA	CHC-C1C-NC	2.96	129.31	124.17
28	C	519	LMG	O8-C28-C29	2.96	120.48	111.92
23	B	616	CLA	O2A-CGA-CBA	2.96	120.48	111.92
23	B	604	CLA	C4-C3-C5	2.96	120.39	115.29
23	C	508	CLA	CHC-C1C-NC	2.96	129.31	124.17
32	c	518	DGD	O1G-C1A-C2A	2.97	120.50	111.92
31	a	614	LHG	O8-C23-C24	2.97	120.50	111.92
23	b	617	CLA	C1-O2A-CGA	2.98	123.62	116.77
32	C	517	DGD	O1G-C1A-C2A	2.98	120.53	111.92
23	C	512	CLA	CHC-C1C-NC	2.98	129.35	124.17
23	a	605	CLA	CHC-C1C-NC	2.98	129.35	124.17
23	C	507	CLA	C4-C3-C5	2.98	120.43	115.29
23	b	607	CLA	O2A-CGA-CBA	2.98	120.55	111.92
23	B	613	CLA	CHC-C1C-NC	2.98	129.35	124.17
23	b	609[B]	CLA	CHC-C1C-NC	3.00	129.37	124.17
27	b	601	SQD	O6-C1-C2	3.01	113.10	108.24
23	c	507	CLA	C4-C3-C5	3.01	120.49	115.29
23	c	508	CLA	C4-C3-C5	3.02	120.49	115.29
27	a	612	SQD	O6-C1-C2	3.02	113.13	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CHC-C1C-NC	3.02	129.42	124.17
23	c	505	CLA	CHC-C1C-NC	3.03	129.42	124.17
23	A	606	CLA	C4-C3-C5	3.04	120.53	115.29
23	D	403	CLA	C2A-C1A-CHA	3.04	129.27	123.92
23	C	506	CLA	C4-C3-C5	3.04	120.54	115.29
23	a	605	CLA	C4-C3-C5	3.05	120.54	115.29
23	b	605	CLA	C4-C3-C5	3.05	120.54	115.29
25	F	101	BCR	C2-C3-C4	3.07	118.40	111.36
23	B	605	CLA	CHC-C1C-NC	3.07	129.51	124.17
27	x	101	SQD	O9-S-C6	3.08	110.60	106.94
27	X	101	SQD	O9-S-C6	3.09	110.61	106.94
23	B	603	CLA	C4-C3-C5	3.09	120.62	115.29
25	B	618	BCR	C36-C18-C19	3.10	123.03	118.10
23	b	618	CLA	CHC-C1C-NC	3.12	129.59	124.17
23	C	513	CLA	O2A-CGA-CBA	3.13	120.97	111.92
23	B	616	CLA	CHC-C1C-NC	3.13	129.61	124.17
23	c	510	CLA	CHC-C1C-NC	3.15	129.63	124.17
23	b	615	CLA	C4-C3-C5	3.16	120.73	115.29
23	B	613	CLA	C4-C3-C5	3.16	120.74	115.29
27	X	101	SQD	O7-S-C6	3.17	110.71	106.94
27	b	601	SQD	O48-C23-C24	3.17	121.09	111.92
23	B	607[B]	CLA	CHC-C1C-NC	3.17	129.68	124.17
27	x	101	SQD	O7-S-C6	3.18	110.71	106.94
25	T	101	BCR	C2-C1-C6	3.18	115.44	110.48
27	x	101	SQD	O48-C23-C24	3.18	121.12	111.92
23	b	614	CLA	CHC-C1C-NC	3.19	129.70	124.17
27	a	612	SQD	O48-C23-C24	3.19	121.14	111.92
27	X	101	SQD	O48-C23-C24	3.19	121.16	111.92
23	B	608	CLA	CHC-C1C-NC	3.20	129.72	124.17
23	b	604	CLA	O2A-CGA-CBA	3.21	121.19	111.92
23	c	513	CLA	C4-C3-C5	3.21	120.82	115.29
23	c	513	CLA	C2A-C1A-CHA	3.22	129.57	123.92
23	C	512	CLA	C4-C3-C5	3.22	120.84	115.29
23	a	613	CLA	CHC-C1C-NC	3.23	129.78	124.17
23	B	603	CLA	CHC-C1C-NC	3.24	129.79	124.17
23	b	619	CLA	CHC-C1C-NC	3.24	129.80	124.17
23	B	617	CLA	CHC-C1C-NC	3.25	129.81	124.17
25	B	619	BCR	C32-C1-C6	3.30	115.65	110.31
32	c	518	DGD	O2G-C1B-C2B	3.30	118.50	111.55
25	b	620	BCR	C2-C3-C4	3.32	118.97	111.36
27	a	610	SQD	O8-S-C6	3.34	111.07	105.74
23	B	615	CLA	C4-C3-C5	3.35	121.06	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	611	SQD	O8-S-C6	3.35	111.07	105.74
23	b	617	CLA	C4-C3-C5	3.35	121.06	115.29
23	b	608	CLA	C1-O2A-CGA	3.36	124.50	116.77
23	B	602	CLA	O2A-CGA-CBA	3.36	121.63	111.92
32	D	406	DGD	C4E-C3E-C2E	3.37	116.73	110.83
27	a	612	SQD	O9-S-C6	3.40	110.97	106.94
28	Z	101	LMG	O1-C1-C2	3.40	113.75	108.24
27	b	601	SQD	O47-C7-C8	3.41	118.74	111.55
32	d	405	DGD	O2G-C1B-C2B	3.41	118.75	111.55
23	B	611	CLA	O2D-CGD-CBD	3.42	117.35	111.28
27	a	612	SQD	O47-C7-C8	3.43	118.77	111.55
23	b	610	CLA	CHC-C1C-NC	3.43	130.12	124.17
27	b	601	SQD	O9-S-C6	3.44	111.03	106.94
23	b	618	CLA	C2A-C1A-CHA	3.45	129.99	123.92
23	A	608	CLA	C4-C3-C5	3.47	121.27	115.29
28	B	621	LMG	O7-C10-C11	3.47	118.87	111.55
32	H	102	DGD	O2G-C1B-C2B	3.48	118.89	111.55
23	a	607	CLA	C4-C3-C5	3.49	121.30	115.29
28	j	101	LMG	O7-C10-C11	3.49	118.91	111.55
23	d	403	CLA	C1-O2A-CGA	3.50	124.82	116.77
28	J	101	LMG	O7-C10-C11	3.51	118.94	111.55
23	C	512	CLA	C2A-C1A-CHA	3.52	130.10	123.92
23	b	610	CLA	C2A-C1A-CHA	3.53	130.13	123.92
31	E	101	LHG	O7-C7-C8	3.54	119.02	111.55
26	D	405	PL9	C7-C3-C4	3.55	119.76	116.88
28	b	623	LMG	O7-C10-C11	3.58	119.10	111.55
32	D	406	DGD	O2G-C1B-C2B	3.59	119.12	111.55
23	A	605	CLA	C3A-C2A-C1A	3.60	106.74	101.34
23	A	608	CLA	C1-O2A-CGA	3.63	125.12	116.77
28	C	520	LMG	O7-C10-C11	3.67	119.28	111.55
32	C	516	DGD	O2G-C1B-C2B	3.68	119.31	111.55
31	L	101	LHG	O7-C7-C8	3.70	119.35	111.55
32	C	518	DGD	O2G-C1B-C2B	3.71	119.37	111.55
23	D	404	CLA	C1-O2A-CGA	3.72	125.34	116.77
23	c	512	CLA	O2D-CGD-CBD	3.72	117.88	111.28
32	C	517	DGD	O2G-C1B-C2B	3.72	119.40	111.55
31	D	407	LHG	O7-C7-C8	3.74	119.44	111.55
28	z	101	LMG	O7-C10-C11	3.75	119.45	111.55
23	b	619	CLA	C2A-C1A-CHA	3.75	130.52	123.92
23	B	616	CLA	C2A-C1A-CHA	3.77	130.54	123.92
25	B	619	BCR	C29-C30-C25	3.77	116.37	110.48
31	d	406	LHG	O7-C7-C8	3.79	119.55	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	623	SQD	C3-C4-C5	3.79	117.03	110.24
23	b	608	CLA	C4-C3-C5	3.80	121.85	115.29
25	B	620	BCR	C2-C1-C6	3.80	116.43	110.48
27	b	602	SQD	C3-C4-C5	3.81	117.06	110.24
27	X	101	SQD	O47-C7-C8	3.82	119.60	111.55
27	x	101	SQD	O47-C7-C8	3.82	119.61	111.55
23	B	606	CLA	C4-C3-C5	3.82	121.88	115.29
23	b	613	CLA	O2D-CGD-CBD	3.84	118.09	111.28
27	B	623	SQD	O7-S-C6	3.84	111.50	106.94
28	A	612	LMG	O7-C10-C11	3.84	119.66	111.55
23	b	610	CLA	O2D-CGD-CBD	3.85	118.11	111.28
25	a	608	BCR	C39-C30-C25	3.85	116.55	110.31
23	B	610	CLA	C2A-C1A-CHA	3.85	130.69	123.92
23	A	605	CLA	C2A-C3A-C4A	3.85	108.09	101.87
23	b	608	CLA	C2A-C1A-CHA	3.87	130.73	123.92
25	h	101	BCR	C2-C1-C6	3.88	116.54	110.48
23	A	605	CLA	O2D-CGD-CBD	3.88	118.16	111.28
23	a	607	CLA	C2A-C1A-CHA	3.88	130.75	123.92
27	b	602	SQD	O7-S-C6	3.88	111.56	106.94
23	d	402	CLA	C2A-C1A-CHA	3.90	130.78	123.92
23	C	510	CLA	C2A-C1A-CHA	3.91	130.79	123.92
23	b	615	CLA	C2A-C1A-CHA	3.93	130.83	123.92
23	B	605	CLA	O2D-CGD-CBD	3.95	118.28	111.28
32	c	517	DGD	O2G-C1B-C2B	3.96	119.90	111.55
28	c	521	LMG	O7-C10-C11	3.96	119.91	111.55
23	b	608	CLA	O2D-CGD-CBD	3.98	118.33	111.28
31	l	101	LHG	O7-C7-C8	3.99	119.96	111.55
28	c	520	LMG	O7-C10-C11	3.99	119.96	111.55
31	D	408	LHG	O7-C7-C8	3.99	119.97	111.55
23	B	617	CLA	C2A-C1A-CHA	3.99	130.94	123.92
23	c	502	CLA	C2A-C1A-CHA	4.00	130.96	123.92
23	a	604	CLA	C3A-C2A-C1A	4.00	107.34	101.34
31	B	622	LHG	O7-C7-C8	4.01	120.00	111.55
25	H	101	BCR	C2-C1-C6	4.02	116.76	110.48
31	e	101	LHG	O7-C7-C8	4.02	120.03	111.55
25	A	609	BCR	C39-C30-C25	4.02	116.83	110.31
23	c	511	CLA	O2D-CGD-CBD	4.03	118.42	111.28
27	b	602	SQD	O47-C7-C8	4.03	120.04	111.55
27	x	101	SQD	O6-C1-C2	4.03	114.75	108.24
27	X	101	SQD	O6-C1-C2	4.03	114.75	108.24
23	b	606	CLA	O2D-CGD-CBD	4.03	118.43	111.28
27	B	623	SQD	O47-C7-C8	4.03	120.05	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C2A-C1A-CHA	4.06	131.06	123.92
23	b	612	CLA	O2D-CGD-CBD	4.06	118.49	111.28
25	b	622	BCR	C2-C1-C6	4.07	116.84	110.48
23	C	502	CLA	C2A-C1A-CHA	4.07	131.08	123.92
28	Z	101	LMG	O7-C10-C11	4.08	120.16	111.55
25	b	621	BCR	C32-C1-C6	4.10	116.96	110.31
31	b	624	LHG	O7-C7-C8	4.11	120.21	111.55
23	B	615	CLA	C2A-C1A-CHA	4.11	131.15	123.92
23	C	505	CLA	C2A-C1A-CHA	4.11	131.15	123.92
23	b	617	CLA	C2A-C1A-CHA	4.12	131.16	123.92
23	b	612	CLA	C2A-C1A-CHA	4.13	131.17	123.92
28	C	519	LMG	O7-C10-C11	4.13	120.25	111.55
28	a	611	LMG	O7-C10-C11	4.13	120.25	111.55
26	a	609	PL9	C7-C3-C4	4.13	120.23	116.88
23	b	605	CLA	C2A-C1A-CHA	4.13	131.19	123.92
27	b	602	SQD	O6-C1-C2	4.14	114.93	108.24
23	a	604	CLA	C2A-C3A-C4A	4.14	108.55	101.87
23	b	617	CLA	O2D-CGD-CBD	4.14	118.62	111.28
27	B	623	SQD	O6-C1-C2	4.14	114.94	108.24
23	C	508	CLA	C2A-C1A-CHA	4.15	131.21	123.92
23	c	505	CLA	O2D-CGD-CBD	4.15	118.64	111.28
23	B	602	CLA	O2D-CGD-CBD	4.15	118.65	111.28
23	C	511	CLA	C2A-C1A-CHA	4.16	131.23	123.92
23	c	512	CLA	C2A-C1A-CHA	4.16	131.24	123.92
23	b	604	CLA	O2D-CGD-CBD	4.16	118.66	111.28
23	a	604	CLA	C2A-C1A-CHA	4.16	131.24	123.92
23	D	402	CLA	O2D-CGD-CBD	4.16	118.67	111.28
23	B	602	CLA	C2A-C1A-CHA	4.19	131.29	123.92
25	C	514	BCR	C2-C1-C6	4.19	117.04	110.48
23	b	614	CLA	C2A-C1A-CHA	4.20	131.31	123.92
23	B	606	CLA	O2D-CGD-CBD	4.22	118.76	111.28
23	c	504	CLA	O2D-CGD-CBD	4.23	118.78	111.28
23	c	503	CLA	C2A-C1A-CHA	4.25	131.40	123.92
23	c	506	CLA	C2A-C1A-CHA	4.26	131.41	123.92
23	C	510	CLA	O2D-CGD-CBD	4.26	118.84	111.28
23	A	608	CLA	C2A-C1A-CHA	4.26	131.42	123.92
32	h	102	DGD	O2G-C1B-C2B	4.27	120.55	111.55
23	b	611	CLA	C2A-C1A-CHA	4.27	131.43	123.92
23	B	612	CLA	C2A-C1A-CHA	4.27	131.43	123.92
23	c	511	CLA	C2A-C1A-CHA	4.28	131.44	123.92
23	d	402	CLA	O2D-CGD-CBD	4.28	118.86	111.28
23	D	403	CLA	O2D-CGD-CBD	4.28	118.87	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	O2D-CGD-CBD	4.29	118.88	111.28
25	t	101	BCR	C2-C1-C6	4.31	117.21	110.48
23	C	509	CLA	C2A-C1A-CHA	4.31	131.50	123.92
27	A	611	SQD	O9-S-C6	4.31	112.07	106.94
23	b	616	CLA	C2A-C1A-CHA	4.32	131.52	123.92
23	B	609	CLA	C2A-C1A-CHA	4.33	131.53	123.92
23	C	513	CLA	C2A-C1A-CHA	4.33	131.53	123.92
27	a	610	SQD	O9-S-C6	4.33	112.08	106.94
23	D	404	CLA	O2D-CGD-CBD	4.34	118.97	111.28
32	c	519	DGD	O2G-C1B-C2B	4.35	120.72	111.55
23	c	504	CLA	C2A-C1A-CHA	4.39	131.64	123.92
23	C	503	CLA	C2A-C1A-CHA	4.39	131.64	123.92
23	B	606	CLA	C2A-C1A-CHA	4.40	131.65	123.92
23	c	514	CLA	C2A-C1A-CHA	4.40	131.65	123.92
27	a	610	SQD	O47-C7-C8	4.40	120.82	111.55
23	c	510	CLA	C2A-C1A-CHA	4.40	131.65	123.92
25	c	515	BCR	C2-C1-C6	4.40	117.36	110.48
27	A	611	SQD	O47-C7-C8	4.41	120.84	111.55
26	A	610	PL9	C7-C3-C4	4.44	120.49	116.88
23	b	604	CLA	C2A-C1A-CHA	4.45	131.74	123.92
23	C	503	CLA	O2D-CGD-CBD	4.45	119.17	111.28
23	C	502	CLA	O2D-CGD-CBD	4.45	119.17	111.28
23	a	604	CLA	O2D-CGD-CBD	4.46	119.18	111.28
23	B	615	CLA	O2D-CGD-CBD	4.46	119.18	111.28
23	C	511	CLA	O2D-CGD-CBD	4.46	119.19	111.28
23	B	605	CLA	C2A-C1A-CHA	4.46	131.77	123.92
23	c	509	CLA	C2A-C1A-CHA	4.47	131.78	123.92
23	d	403	CLA	C2A-C1A-CHA	4.48	131.79	123.92
23	b	607	CLA	C2A-C1A-CHA	4.48	131.80	123.92
23	B	608	CLA	C2A-C1A-CHA	4.49	131.82	123.92
23	B	607[B]	CLA	C2A-C1A-CHA	4.50	131.84	123.92
23	B	614	CLA	O2D-CGD-CBD	4.51	119.28	111.28
31	a	614	LHG	O7-C7-C8	4.51	121.06	111.55
23	d	403	CLA	O2D-CGD-CBD	4.52	119.29	111.28
23	b	611	CLA	C2A-C3A-C4A	4.53	109.19	101.87
23	b	609[B]	CLA	O2D-CGD-CBD	4.53	119.32	111.28
23	c	505	CLA	C2A-C1A-CHA	4.53	131.89	123.92
27	A	611	SQD	O6-C1-C2	4.54	115.58	108.24
27	a	610	SQD	O6-C1-C2	4.56	115.61	108.24
23	c	511	CLA	C2A-C3A-C4A	4.56	109.23	101.87
23	C	504	CLA	O2D-CGD-CBD	4.56	119.37	111.28
23	b	609[B]	CLA	C2A-C1A-CHA	4.56	131.94	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	C2A-C1A-CHA	4.57	131.95	123.92
23	b	613	CLA	C2A-C1A-CHA	4.57	131.95	123.92
23	c	507	CLA	O2D-CGD-CBD	4.57	119.38	111.28
23	a	605	CLA	C2A-C1A-CHA	4.57	131.96	123.92
23	b	609[A]	CLA	O2D-CGD-CBD	4.57	119.39	111.28
23	b	609[A]	CLA	C2A-C1A-CHA	4.57	131.96	123.92
23	C	513	CLA	O2D-CGD-CBD	4.59	119.41	111.28
23	b	605	CLA	C2A-C3A-C4A	4.59	109.28	101.87
23	B	614	CLA	C2A-C1A-CHA	4.59	131.99	123.92
23	C	511	CLA	C2A-C3A-C4A	4.59	109.28	101.87
23	b	613	CLA	C2A-C3A-C4A	4.59	109.29	101.87
23	C	509	CLA	O2D-CGD-CBD	4.59	119.42	111.28
23	C	508	CLA	O2D-CGD-CBD	4.60	119.43	111.28
23	C	504	CLA	C2A-C1A-CHA	4.60	132.02	123.92
23	c	508	CLA	C2A-C1A-CHA	4.61	132.03	123.92
23	B	607[A]	CLA	O2D-CGD-CBD	4.62	119.47	111.28
23	c	507	CLA	C2A-C1A-CHA	4.63	132.07	123.92
23	B	604	CLA	O2D-CGD-CBD	4.64	119.50	111.28
23	a	613	CLA	O2D-CGD-CBD	4.64	119.50	111.28
23	C	507	CLA	C2A-C1A-CHA	4.64	132.08	123.92
23	B	607[A]	CLA	C2A-C1A-CHA	4.65	132.09	123.92
23	c	514	CLA	O2D-CGD-CBD	4.66	119.54	111.28
23	B	610	CLA	O2D-CGD-CBD	4.68	119.58	111.28
23	d	402	CLA	C2A-C3A-C4A	4.68	109.43	101.87
23	B	613	CLA	O2D-CGD-CBD	4.68	119.58	111.28
23	C	506	CLA	O2D-CGD-CBD	4.68	119.59	111.28
23	a	607	CLA	C2A-C3A-C4A	4.69	109.45	101.87
23	C	503	CLA	C2A-C3A-C4A	4.70	109.46	101.87
23	B	611	CLA	C2A-C1A-CHA	4.71	132.20	123.92
23	C	512	CLA	O2D-CGD-CBD	4.72	119.64	111.28
23	b	616	CLA	O2D-CGD-CBD	4.72	119.65	111.28
23	A	605	CLA	C2A-C1A-CHA	4.72	132.22	123.92
23	B	609	CLA	C2A-C3A-C4A	4.72	109.50	101.87
23	B	607[B]	CLA	O2D-CGD-CBD	4.73	119.67	111.28
23	b	611	CLA	O2D-CGD-CBD	4.73	119.67	111.28
23	B	604	CLA	C2A-C1A-CHA	4.74	132.25	123.92
23	B	603	CLA	C2A-C3A-C4A	4.75	109.55	101.87
23	c	514	CLA	C2A-C3A-C4A	4.76	109.55	101.87
23	B	603	CLA	C3A-C2A-C1A	4.76	108.46	101.34
23	c	503	CLA	O2D-CGD-CBD	4.76	119.71	111.28
23	B	603	CLA	C2A-C1A-CHA	4.76	132.28	123.92
23	c	502	CLA	O2D-CGD-CBD	4.76	119.72	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2A-C3A-C4A	4.76	109.56	101.87
23	d	403	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	c	512	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	C	510	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	C	512	CLA	C2A-C3A-C4A	4.77	109.57	101.87
23	C	506	CLA	C2A-C1A-CHA	4.80	132.36	123.92
23	D	402	CLA	C2A-C1A-CHA	4.80	132.37	123.92
23	A	608	CLA	O2D-CGD-CBD	4.80	119.80	111.28
23	b	616	CLA	C2A-C3A-C4A	4.82	109.65	101.87
23	c	510	CLA	O2D-CGD-CBD	4.82	119.83	111.28
23	C	504	CLA	C3A-C2A-C1A	4.83	108.57	101.34
23	D	403	CLA	C2A-C3A-C4A	4.83	109.67	101.87
25	h	101	BCR	C29-C30-C25	4.83	118.03	110.48
23	C	506	CLA	C2A-C3A-C4A	4.84	109.69	101.87
23	a	605	CLA	O2D-CGD-CBD	4.84	119.87	111.28
23	C	505	CLA	C2A-C3A-C4A	4.85	109.70	101.87
23	a	613	CLA	C2A-C3A-C4A	4.85	109.70	101.87
23	B	609	CLA	O2D-CGD-CBD	4.87	119.92	111.28
23	D	404	CLA	C2A-C1A-CHA	4.88	132.50	123.92
23	B	612	CLA	O2D-CGD-CBD	4.89	119.96	111.28
23	c	513	CLA	C2A-C3A-C4A	4.90	109.78	101.87
23	A	608	CLA	C2A-C3A-C4A	4.90	109.79	101.87
23	B	617	CLA	C2A-C3A-C4A	4.92	109.81	101.87
23	a	613	CLA	C2A-C1A-CHA	4.92	132.58	123.92
23	B	604	CLA	C3A-C2A-C1A	4.92	108.72	101.34
23	c	502	CLA	C2A-C3A-C4A	4.93	109.83	101.87
23	A	606	CLA	C2A-C1A-CHA	4.93	132.58	123.92
23	B	615	CLA	C2A-C3A-C4A	4.94	109.85	101.87
23	c	506	CLA	C2A-C3A-C4A	4.95	109.87	101.87
23	b	617	CLA	C2A-C3A-C4A	4.95	109.87	101.87
23	b	619	CLA	C2A-C3A-C4A	4.96	109.88	101.87
23	B	614	CLA	C2A-C3A-C4A	4.96	109.88	101.87
23	c	509	CLA	O2D-CGD-CBD	4.97	120.09	111.28
23	A	606	CLA	O2D-CGD-CBD	4.98	120.10	111.28
23	D	402	CLA	C3A-C2A-C1A	4.98	108.81	101.34
23	A	606	CLA	C3A-C2A-C1A	5.00	108.82	101.34
23	b	614	CLA	C2A-C3A-C4A	5.00	109.94	101.87
23	B	617	CLA	O2D-CGD-CBD	5.00	120.14	111.28
23	d	403	CLA	C3A-C2A-C1A	5.02	108.86	101.34
23	C	502	CLA	C2A-C3A-C4A	5.03	109.99	101.87
23	b	619	CLA	O2D-CGD-CBD	5.04	120.21	111.28
23	C	513	CLA	C2A-C3A-C4A	5.04	110.01	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	607	CLA	O2D-CGD-CBD	5.06	120.26	111.28
23	c	504	CLA	C2A-C3A-C4A	5.07	110.06	101.87
23	d	402	CLA	C3A-C2A-C1A	5.08	108.94	101.34
23	b	607	CLA	C2A-C3A-C4A	5.09	110.09	101.87
23	c	505	CLA	C3A-C2A-C1A	5.10	108.98	101.34
23	D	402	CLA	C2A-C3A-C4A	5.10	110.11	101.87
23	c	510	CLA	C2A-C3A-C4A	5.10	110.11	101.87
23	c	513	CLA	O2D-CGD-CBD	5.11	120.33	111.28
23	a	605	CLA	C2A-C3A-C4A	5.11	110.12	101.87
23	B	608	CLA	C3A-C2A-C1A	5.11	109.00	101.34
23	c	509	CLA	C2A-C3A-C4A	5.12	110.14	101.87
23	C	507	CLA	C3A-C2A-C1A	5.12	109.02	101.34
23	D	404	CLA	C2A-C3A-C4A	5.13	110.15	101.87
23	b	606	CLA	C2A-C1A-CHA	5.13	132.95	123.92
23	b	614	CLA	O2D-CGD-CBD	5.14	120.39	111.28
23	C	501	CLA	O2D-CGD-CBD	5.15	120.41	111.28
23	b	615	CLA	C2A-C3A-C4A	5.16	110.20	101.87
23	c	508	CLA	C3A-C2A-C1A	5.17	109.08	101.34
25	H	101	BCR	C29-C30-C25	5.18	118.58	110.48
23	B	613	CLA	C3A-C2A-C1A	5.20	109.12	101.34
23	B	602	CLA	C2A-C3A-C4A	5.21	110.28	101.87
23	B	616	CLA	O2D-CGD-CBD	5.21	120.53	111.28
23	a	605	CLA	C3A-C2A-C1A	5.22	109.16	101.34
23	b	604	CLA	C2A-C3A-C4A	5.22	110.30	101.87
23	B	605	CLA	C2A-C3A-C4A	5.22	110.30	101.87
23	D	403	CLA	C3A-C2A-C1A	5.23	109.17	101.34
23	B	611	CLA	C3A-C2A-C1A	5.23	109.17	101.34
23	C	501	CLA	C2A-C3A-C4A	5.23	110.31	101.87
23	D	404	CLA	C3A-C2A-C1A	5.24	109.19	101.34
23	c	503	CLA	C2A-C3A-C4A	5.24	110.34	101.87
23	b	609[A]	CLA	C2A-C3A-C4A	5.25	110.36	101.87
23	B	612	CLA	C2A-C3A-C4A	5.26	110.36	101.87
23	C	509	CLA	C2A-C3A-C4A	5.26	110.37	101.87
23	B	607[A]	CLA	C2A-C3A-C4A	5.27	110.38	101.87
23	b	612	CLA	C2A-C3A-C4A	5.27	110.38	101.87
23	b	606	CLA	C2A-C3A-C4A	5.27	110.38	101.87
23	B	616	CLA	C3A-C2A-C1A	5.29	109.26	101.34
23	C	510	CLA	C3A-C2A-C1A	5.29	109.26	101.34
23	c	505	CLA	C2A-C3A-C4A	5.29	110.42	101.87
23	B	604	CLA	C2A-C3A-C4A	5.31	110.44	101.87
23	B	613	CLA	C2A-C3A-C4A	5.31	110.44	101.87
23	A	606	CLA	C2A-C3A-C4A	5.31	110.45	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	C2A-C3A-C4A	5.32	110.47	101.87
23	C	508	CLA	C2A-C3A-C4A	5.33	110.47	101.87
23	b	605	CLA	C3A-C2A-C1A	5.33	109.32	101.34
23	B	607[B]	CLA	C2A-C3A-C4A	5.33	110.47	101.87
23	b	618	CLA	O2D-CGD-CBD	5.33	120.73	111.28
23	b	607	CLA	C3A-C2A-C1A	5.33	109.33	101.34
23	a	613	CLA	C3A-C2A-C1A	5.34	109.34	101.34
23	b	608	CLA	C3A-C2A-C1A	5.35	109.35	101.34
23	B	609	CLA	C3A-C2A-C1A	5.36	109.36	101.34
23	b	610	CLA	C3A-C2A-C1A	5.37	109.38	101.34
23	c	503	CLA	C3A-C2A-C1A	5.38	109.39	101.34
23	c	506	CLA	O2D-CGD-CBD	5.38	120.82	111.28
23	A	608	CLA	C3A-C2A-C1A	5.39	109.41	101.34
23	C	504	CLA	C2A-C3A-C4A	5.39	110.58	101.87
23	B	612	CLA	C3A-C2A-C1A	5.41	109.45	101.34
23	a	607	CLA	C3A-C2A-C1A	5.42	109.46	101.34
23	b	615	CLA	O2D-CGD-CBD	5.43	120.92	111.28
23	B	606	CLA	C3A-C2A-C1A	5.44	109.48	101.34
23	b	613	CLA	C3A-C2A-C1A	5.44	109.48	101.34
23	c	510	CLA	C3A-C2A-C1A	5.45	109.50	101.34
23	b	615	CLA	C3A-C2A-C1A	5.45	109.51	101.34
23	b	606	CLA	C3A-C2A-C1A	5.46	109.51	101.34
23	B	603	CLA	O2D-CGD-CBD	5.46	120.95	111.28
23	b	604	CLA	C3A-C2A-C1A	5.47	109.53	101.34
23	c	514	CLA	C3A-C2A-C1A	5.48	109.54	101.34
23	C	509	CLA	C3A-C2A-C1A	5.49	109.56	101.34
23	b	609[B]	CLA	C2A-C3A-C4A	5.50	110.76	101.87
23	c	507	CLA	C2A-C3A-C4A	5.50	110.76	101.87
23	b	610	CLA	C2A-C3A-C4A	5.51	110.77	101.87
23	C	505	CLA	O2D-CGD-CBD	5.52	121.06	111.28
23	B	617	CLA	C3A-C2A-C1A	5.52	109.61	101.34
23	c	513	CLA	C3A-C2A-C1A	5.53	109.62	101.34
23	b	618	CLA	C3A-C2A-C1A	5.53	109.62	101.34
23	c	508	CLA	C2A-C3A-C4A	5.54	110.82	101.87
23	b	611	CLA	C3A-C2A-C1A	5.54	109.64	101.34
23	c	511	CLA	C3A-C2A-C1A	5.55	109.65	101.34
23	b	619	CLA	C3A-C2A-C1A	5.56	109.67	101.34
23	C	502	CLA	C3A-C2A-C1A	5.56	109.67	101.34
23	b	617	CLA	C3A-C2A-C1A	5.56	109.67	101.34
23	b	609[A]	CLA	C3A-C2A-C1A	5.58	109.69	101.34
23	b	605	CLA	O2D-CGD-CBD	5.58	121.17	111.28
23	b	608	CLA	C2A-C3A-C4A	5.58	110.88	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C3A-C2A-C1A	5.58	109.70	101.34
23	C	508	CLA	C3A-C2A-C1A	5.58	109.70	101.34
23	B	606	CLA	C2A-C3A-C4A	5.59	110.89	101.87
23	B	615	CLA	C3A-C2A-C1A	5.59	109.72	101.34
23	b	609[B]	CLA	C3A-C2A-C1A	5.62	109.76	101.34
23	B	602	CLA	C3A-C2A-C1A	5.63	109.77	101.34
23	C	507	CLA	C2A-C3A-C4A	5.65	110.99	101.87
23	b	618	CLA	C2A-C3A-C4A	5.65	111.00	101.87
23	B	616	CLA	C2A-C3A-C4A	5.66	111.02	101.87
23	C	501	CLA	C3A-C2A-C1A	5.67	109.83	101.34
23	b	614	CLA	C3A-C2A-C1A	5.67	109.83	101.34
23	B	608	CLA	C2A-C3A-C4A	5.68	111.04	101.87
23	B	607[A]	CLA	C3A-C2A-C1A	5.70	109.87	101.34
23	c	507	CLA	C3A-C2A-C1A	5.71	109.90	101.34
23	C	506	CLA	C3A-C2A-C1A	5.73	109.92	101.34
23	b	616	CLA	C3A-C2A-C1A	5.74	109.93	101.34
23	C	503	CLA	C3A-C2A-C1A	5.74	109.94	101.34
23	c	509	CLA	C3A-C2A-C1A	5.75	109.94	101.34
23	B	610	CLA	C3A-C2A-C1A	5.78	110.00	101.34
23	C	512	CLA	C3A-C2A-C1A	5.78	110.00	101.34
23	B	614	CLA	C3A-C2A-C1A	5.81	110.05	101.34
23	B	607[B]	CLA	C3A-C2A-C1A	5.85	110.09	101.34
23	B	605	CLA	C3A-C2A-C1A	5.88	110.14	101.34
23	c	502	CLA	C3A-C2A-C1A	5.89	110.17	101.34
23	c	504	CLA	C3A-C2A-C1A	5.92	110.21	101.34
23	C	511	CLA	C3A-C2A-C1A	6.00	110.33	101.34
23	c	512	CLA	C3A-C2A-C1A	6.01	110.34	101.34
23	b	612	CLA	C3A-C2A-C1A	6.01	110.34	101.34
23	C	507	CLA	O2D-CGD-CBD	6.11	122.12	111.28
23	c	508	CLA	O2D-CGD-CBD	6.25	122.37	111.28
23	c	506	CLA	C3A-C2A-C1A	6.37	110.88	101.34
23	C	505	CLA	C3A-C2A-C1A	6.58	111.19	101.34
25	B	619	BCR	C21-C20-C19	13.79	165.28	123.26
25	k	101	BCR	C21-C20-C19	16.36	173.12	123.26
25	T	101	BCR	C21-C20-C19	16.40	173.22	123.26
25	B	618	BCR	C21-C20-C19	16.56	173.72	123.26
25	F	101	BCR	C21-C20-C19	16.79	174.43	123.26
25	K	101	BCR	C21-C20-C19	17.03	175.16	123.26
25	b	622	BCR	C21-C20-C19	17.29	175.94	123.26
25	f	101	BCR	C21-C20-C19	17.35	176.11	123.26
25	c	522	BCR	C21-C20-C19	17.45	176.43	123.26
25	H	101	BCR	C21-C20-C19	17.45	176.44	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	609	BCR	C21-C20-C19	17.56	176.77	123.26
25	t	101	BCR	C21-C20-C19	17.73	177.28	123.26
25	a	608	BCR	C21-C20-C19	17.75	177.34	123.26
25	b	621	BCR	C21-C20-C19	17.89	177.78	123.26
25	C	515	BCR	C21-C20-C19	17.93	177.89	123.26
25	h	101	BCR	C21-C20-C19	17.98	178.05	123.26
25	C	521	BCR	C21-C20-C19	18.05	178.26	123.26
25	b	620	BCR	C21-C20-C19	18.10	178.41	123.26
25	B	620	BCR	C21-C20-C19	18.17	178.62	123.26
25	C	514	BCR	C21-C20-C19	18.21	178.74	123.26
25	c	515	BCR	C21-C20-C19	18.24	178.82	123.26
25	c	516	BCR	C21-C20-C19	18.50	179.63	123.26
25	b	620	BCR	C15-C16-C17	21.12	168.55	123.46
25	H	101	BCR	C15-C16-C17	22.45	171.38	123.46
25	h	101	BCR	C15-C16-C17	22.65	171.81	123.46
25	C	521	BCR	C15-C16-C17	22.99	172.53	123.46
25	B	618	BCR	C15-C16-C17	22.99	172.54	123.46
25	k	101	BCR	C15-C16-C17	23.32	173.24	123.46
25	f	101	BCR	C15-C16-C17	23.49	173.60	123.46
25	B	620	BCR	C15-C16-C17	23.49	173.61	123.46
25	C	514	BCR	C15-C16-C17	23.50	173.62	123.46
25	b	622	BCR	C15-C16-C17	23.53	173.69	123.46
25	c	522	BCR	C15-C16-C17	23.56	173.74	123.46
25	B	619	BCR	C15-C16-C17	23.60	173.84	123.46
25	c	516	BCR	C15-C16-C17	23.67	173.98	123.46
25	t	101	BCR	C15-C16-C17	23.92	174.52	123.46
25	K	101	BCR	C15-C16-C17	23.92	174.52	123.46
25	F	101	BCR	C15-C16-C17	23.93	174.55	123.46
25	C	515	BCR	C15-C16-C17	24.12	174.94	123.46
25	a	608	BCR	C15-C16-C17	24.22	175.17	123.46
25	A	609	BCR	C15-C16-C17	24.23	175.18	123.46
25	T	101	BCR	C15-C16-C17	24.31	175.34	123.46
25	c	515	BCR	C15-C16-C17	24.40	175.54	123.46
25	b	621	BCR	C15-C16-C17	25.22	177.29	123.46

All (200) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	609[B]	CLA	NA
23	b	609[B]	CLA	NC
23	b	609[B]	CLA	ND
23	c	514	CLA	NC

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Mol	Chain	Res	Type	Atom
23	c	514	CLA	ND
23	B	607[A]	CLA	NA
23	B	607[A]	CLA	NC
23	B	607[A]	CLA	ND
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	D	404	CLA	NA
23	D	404	CLA	NC
23	D	404	CLA	ND
23	D	402	CLA	NC
23	D	402	CLA	ND
23	D	402	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	618	CLA	NC
23	b	618	CLA	ND
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	A	605	CLA	NC
23	A	605	CLA	ND
23	C	506	CLA	NC
23	C	506	CLA	ND
23	C	506	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	b	611	CLA	NA
23	b	611	CLA	NC

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Mol	Chain	Res	Type	Atom
23	b	611	CLA	ND
23	b	608	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	B	612	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	B	617	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	c	502	CLA	NC
23	c	502	CLA	ND
23	A	606	CLA	NC
23	A	606	CLA	ND
23	A	606	CLA	NA
23	a	604	CLA	NC
23	a	604	CLA	ND
23	D	403	CLA	NC
23	D	403	CLA	ND
23	D	403	CLA	NA
23	b	617	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	ND
23	C	503	CLA	NC
23	C	503	CLA	ND
23	b	609[A]	CLA	NC
23	b	609[A]	CLA	ND
23	b	609[A]	CLA	NA
23	B	611	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	609	CLA	NC
23	B	609	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	609	CLA	NA
23	B	607[B]	CLA	NA
23	B	607[B]	CLA	NC
23	B	607[B]	CLA	ND
23	B	615	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	b	607	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	a	605	CLA	NC
23	a	605	CLA	ND
23	a	605	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	d	402	CLA	NC
23	d	402	CLA	ND
23	d	402	CLA	NA
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	505	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	A	608	CLA	NA
23	A	608	CLA	NC
23	A	608	CLA	ND
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	616	CLA	NA
23	d	403	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	C	511	CLA	NC
23	C	511	CLA	ND
23	c	503	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	612	CLA	NC
23	b	612	CLA	ND
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA
23	C	507	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	a	607	CLA	NC
23	a	607	CLA	ND
23	a	607	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	C	501	CLA	NA
23	C	501	CLA	NC
23	C	501	CLA	ND
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	c	510	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	c	509	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	604	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	b	610	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	b	613	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	616	CLA	NC
23	b	616	CLA	ND
23	a	613	CLA	NC
23	a	613	CLA	ND
23	a	613	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	k	101	BCR	C10-C11-C12-C13
25	t	101	BCR	C21-C20-C19-C18
25	b	621	BCR	C16-C17-C18-C19
25	c	522	BCR	C21-C20-C19-C18
25	B	618	BCR	C21-C20-C19-C18
25	a	608	BCR	C21-C20-C19-C18
25	K	101	BCR	C17-C16-C15-C14
25	A	609	BCR	C17-C16-C15-C14
25	C	515	BCR	C17-C16-C15-C14
25	T	101	BCR	C17-C16-C15-C14

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Mol	Chain	Res	Type	Atoms
25	b	621	BCR	C16-C17-C18-C36
25	b	621	BCR	C20-C21-C22-C37
25	k	101	BCR	C16-C17-C18-C19
25	B	619	BCR	C16-C17-C18-C36
25	C	515	BCR	C21-C20-C19-C18
25	b	621	BCR	C21-C20-C19-C18
25	h	101	BCR	C10-C11-C12-C13
28	Z	101	LMG	C8-O7-C10-C11
28	z	101	LMG	C8-O7-C10-C11

There are no ring outliers.

73 monomers are involved in 543 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	601	OEX	1	0
23	A	605	CLA	8	0
23	A	606	CLA	6	0
24	A	607	PHO	1	0
23	A	608	CLA	7	0
25	A	609	BCR	16	0
26	A	610	PL9	15	0
27	A	611	SQD	4	0
28	A	612	LMG	2	0
23	B	602	CLA	5	0
23	B	603	CLA	2	0
23	B	604	CLA	15	0
23	B	605	CLA	10	0
23	B	606	CLA	16	0
23	B	607[A]	CLA	1	0
23	B	607[B]	CLA	4	0
23	B	608	CLA	12	0
23	B	609	CLA	1	0
23	B	610	CLA	5	0
23	B	611	CLA	3	0
23	B	612	CLA	8	0
23	B	613	CLA	9	0
23	B	614	CLA	6	0
23	B	615	CLA	8	0
23	B	616	CLA	5	0
23	B	617	CLA	14	0
25	B	618	BCR	27	0
25	B	619	BCR	28	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	620	BCR	36	0
28	B	621	LMG	4	0
31	B	622	LHG	3	0
27	B	623	SQD	9	0
23	C	501	CLA	8	0
23	C	502	CLA	12	0
23	C	503	CLA	12	0
23	C	504	CLA	10	0
23	C	505	CLA	8	0
23	C	506	CLA	11	0
23	C	507	CLA	12	0
23	C	508	CLA	7	0
23	C	509	CLA	6	0
23	C	510	CLA	9	0
23	C	511	CLA	10	0
23	C	512	CLA	6	0
23	C	513	CLA	4	0
25	C	514	BCR	11	0
25	C	515	BCR	22	0
32	C	516	DGD	2	0
32	C	517	DGD	2	0
32	C	518	DGD	7	0
28	C	519	LMG	1	0
28	C	520	LMG	1	0
25	C	521	BCR	15	0
24	D	401	PHO	11	0
23	D	402	CLA	9	0
23	D	403	CLA	6	0
23	D	404	CLA	3	0
26	D	405	PL9	7	0
32	D	406	DGD	1	0
31	D	407	LHG	1	0
31	D	408	LHG	10	0
31	E	101	LHG	4	0
33	E	102	HEM	5	0
25	F	101	BCR	29	0
25	H	101	BCR	21	0
32	H	102	DGD	5	0
28	J	101	LMG	5	0
25	K	101	BCR	30	0
31	L	101	LHG	4	0
25	T	101	BCR	38	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	V	202	HEM	3	0
27	X	101	SQD	4	0
28	Z	101	LMG	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.31	3 (0%) 84 77	57, 63, 84, 93	0
1	a	334/334 (100%)	-0.22	2 (0%) 89 84	78, 84, 104, 114	0
2	B	504/504 (100%)	-0.19	4 (0%) 86 79	59, 68, 89, 111	0
2	b	504/504 (100%)	-0.11	7 (1%) 75 66	80, 88, 110, 131	0
3	C	451/451 (100%)	-0.05	9 (1%) 65 56	61, 72, 85, 97	0
3	c	451/451 (100%)	-0.18	6 (1%) 77 68	82, 93, 105, 118	0
4	D	342/342 (100%)	-0.28	1 (0%) 93 90	57, 64, 80, 102	0
4	d	342/342 (100%)	-0.21	5 (1%) 73 64	78, 85, 101, 123	0
5	E	81/81 (100%)	-0.12	0 100 100	68, 81, 98, 104	0
5	e	81/81 (100%)	0.10	1 (1%) 79 70	89, 102, 119, 125	0
6	F	34/34 (100%)	-0.30	1 (2%) 51 40	68, 74, 99, 102	0
6	f	34/34 (100%)	-0.23	1 (2%) 51 40	89, 95, 120, 122	0
7	H	65/65 (100%)	0.25	6 (9%) 9 8	64, 74, 81, 99	0
7	h	65/65 (100%)	0.38	4 (6%) 20 16	85, 95, 102, 120	0
8	I	38/38 (100%)	-0.24	0 100 100	70, 74, 105, 109	0
8	i	38/38 (100%)	-0.10	1 (2%) 56 45	90, 95, 126, 130	0
9	J	38/38 (100%)	-0.17	1 (2%) 56 45	66, 78, 109, 112	0
9	j	38/38 (100%)	-0.18	1 (2%) 56 45	87, 99, 129, 133	0
10	K	37/37 (100%)	-0.56	0 100 100	74, 79, 86, 88	0
10	k	37/37 (100%)	-0.03	1 (2%) 54 44	94, 100, 107, 108	0
11	L	37/37 (100%)	0.03	5 (13%) 3 3	58, 62, 90, 99	0
11	l	37/37 (100%)	-0.04	2 (5%) 26 21	79, 83, 111, 120	0
12	M	34/34 (100%)	-0.64	0 100 100	62, 64, 77, 93	0
12	m	34/34 (100%)	-0.45	0 100 100	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%)	-0.25	0 100 100	59, 73, 95, 111	0
13	o	243/243 (100%)	0.03	5 (2%) 63 54	79, 94, 116, 132	0
14	T	30/30 (100%)	-0.12	3 (10%) 7 6	60, 64, 85, 93	0
14	t	30/30 (100%)	-0.43	0 100 100	80, 85, 105, 114	0
15	U	97/97 (100%)	-0.10	1 (1%) 82 74	64, 71, 89, 90	0
15	u	97/97 (100%)	-0.20	1 (1%) 82 74	84, 92, 110, 111	0
16	V	137/137 (100%)	-0.31	1 (0%) 87 82	64, 69, 80, 88	0
16	v	137/137 (100%)	-0.23	3 (2%) 62 52	84, 89, 101, 109	0
17	Y	29/29 (100%)	-0.14	1 (3%) 45 35	82, 89, 115, 118	0
17	y	29/29 (100%)	-0.31	0 100 100	103, 110, 136, 138	0
18	X	39/39 (100%)	0.07	6 (15%) 2 2	74, 80, 107, 108	0
18	x	39/39 (100%)	-0.12	3 (7%) 13 11	95, 101, 127, 129	0
19	Z	62/62 (100%)	-0.31	1 (1%) 72 63	80, 89, 109, 112	0
19	z	62/62 (100%)	-0.15	2 (3%) 47 36	101, 110, 129, 133	0
All	All	5264/5264 (100%)	-0.17	88 (1%) 70 61	57, 83, 107, 138	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	L	2	GLU	4.6
7	H	2	ALA	4.3
11	L	3	PRO	4.2
7	h	2	ALA	4.2
18	X	2	THR	3.9
3	C	138	GLU	3.6
6	F	12	SER	3.6
5	e	84	LYS	3.5
9	J	3	SER	3.5
9	j	3	SER	3.5
18	X	38	GLN	3.5
13	o	189	ARG	3.4
7	h	3	ARG	3.3
4	D	12	ARG	3.3
11	L	1	MET	3.3
18	X	37	VAL	3.3
15	U	9	LEU	3.3
13	o	25	THR	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	137	PRO	3.2
11	l	1	MET	3.2
17	Y	43	ARG	3.1
18	X	33	GLN	3.1
6	f	12	SER	3.0
2	b	117	TYR	3.0
4	d	260	ALA	2.8
4	d	98	GLN	2.8
16	v	105	ARG	2.8
2	B	505	ARG	2.8
3	C	145[A]	SER	2.7
7	H	64	ALA	2.7
18	x	2	THR	2.7
3	c	142	GLU	2.7
11	L	5	PRO	2.6
7	h	4	ARG	2.6
8	i	38	GLU	2.6
3	c	200	THR	2.6
1	a	11	ALA	2.6
18	X	39	ARG	2.6
7	H	3	ARG	2.5
11	l	8	GLN	2.5
18	X	36	LYS	2.5
16	v	106	ASN	2.5
7	h	23	PRO	2.5
2	b	491	VAL	2.5
2	b	187	PRO	2.5
2	b	497	GLN	2.5
2	b	119	ASP	2.5
4	d	11	GLU	2.5
4	d	99	GLY	2.5
3	C	25	ASN	2.5
18	x	3	ILE	2.5
3	c	198	VAL	2.4
7	H	56	ASP	2.4
1	A	11	ALA	2.4
18	x	40	SER	2.4
3	C	200	THR	2.4
19	Z	35	ARG	2.4
14	T	28	ARG	2.4
10	k	46	ARG	2.4
2	B	218	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	121	GLU	2.3
3	c	145[A]	SER	2.3
1	A	74	GLY	2.3
3	C	266	TRP	2.3
3	C	183	GLY	2.2
16	V	14	SER	2.2
2	B	70	GLY	2.2
7	H	27	THR	2.2
1	A	13	LEU	2.2
14	T	26	PRO	2.1
14	T	30	THR	2.1
3	c	201	ASN	2.1
7	H	16	SER	2.1
15	u	9	LEU	2.1
1	a	222	SER	2.1
13	o	164	LEU	2.1
3	c	25	ASN	2.1
13	o	58	ASN	2.1
3	C	24	THR	2.1
19	z	1	MET	2.1
19	z	38	GLN	2.0
13	o	87	VAL	2.0
2	B	498	LYS	2.0
2	b	482	ILE	2.0
11	L	6	ASN	2.0
4	d	349	GLY	2.0
3	C	199	ILE	2.0
16	v	90	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
21	CL	u	201	1/1	0.08	0.16	112,112,112,112	0
30	CA	B	601	1/1	0.20	1.13	117,117,117,117	0
30	CA	b	603	1/1	0.20	0.56	137,137,137,137	0
21	CL	V	201	1/1	0.21	0.33	91,91,91,91	0
26	PL9	A	610	55/55	0.47	0.36	93,109,118,119	0
25	BCR	h	101	40/40	0.51	0.62	87,94,103,104	0
32	DGD	d	405	62/66	0.58	0.48	138,151,164,165	0
25	BCR	c	522	40/40	0.58	0.39	91,95,98,99	0
26	PL9	a	609	55/55	0.59	0.45	113,130,139,140	0
25	BCR	a	608	40/40	0.62	0.64	83,89,93,94	0
25	BCR	H	101	40/40	0.62	0.56	67,74,83,83	0
28	LMG	C	520	51/55	0.64	0.55	83,117,122,123	0
21	CL	a	602	1/1	0.64	0.16	86,86,86,86	0
26	PL9	d	404	55/55	0.67	0.30	80,84,91,93	0
32	DGD	D	406	62/66	0.69	0.44	118,130,143,144	0
27	SQD	a	610	54/54	0.69	0.50	110,119,128,128	0
25	BCR	T	101	40/40	0.70	0.40	65,78,85,86	0
25	BCR	C	521	40/40	0.70	0.30	70,74,78,78	0
25	BCR	b	622	40/40	0.71	0.55	89,94,100,101	0
31	LHG	E	101	42/49	0.72	0.38	110,124,127,127	0
23	CLA	C	513	65/65	0.72	0.47	80,85,105,105	0
27	SQD	x	101	43/54	0.73	0.49	128,136,140,140	0
31	LHG	e	101	42/49	0.74	0.40	131,145,147,148	0
23	CLA	B	617	65/65	0.74	0.45	63,69,118,119	0
28	LMG	c	521	51/55	0.74	0.51	104,137,142,143	0
23	CLA	b	609[B]	65/65	0.75	0.46	83,87,93,95	65
27	SQD	A	611	54/54	0.75	0.41	90,98,107,108	0
25	BCR	b	621	40/40	0.75	0.40	83,89,101,101	0
25	BCR	C	515	40/40	0.75	0.34	71,78,81,82	0
25	BCR	f	101	40/40	0.75	0.35	87,91,109,110	0
23	CLA	C	512	65/65	0.75	0.41	78,82,103,104	0
23	CLA	b	609[A]	65/65	0.75	0.46	85,90,102,103	65
25	BCR	C	514	40/40	0.76	0.39	78,84,87,88	0
23	CLA	C	507	65/65	0.76	0.41	70,74,92,94	0
27	SQD	b	602	54/54	0.76	0.42	99,107,121,121	0
23	CLA	b	604	65/65	0.76	0.72	94,102,127,128	0
23	CLA	c	502	65/65	0.76	0.35	90,93,106,108	0
25	BCR	b	620	40/40	0.77	0.60	84,88,90,90	0
25	BCR	F	101	40/40	0.77	0.33	66,71,88,90	0
25	BCR	A	609	40/40	0.77	0.56	63,68,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
28	LMG	z	101	37/55	0.77	0.51	117,145,149,150	0
23	CLA	c	513	65/65	0.77	0.41	99,102,124,124	0
25	BCR	t	101	40/40	0.78	0.36	86,99,106,106	0
23	CLA	b	618	65/65	0.78	0.39	86,89,107,108	0
28	LMG	c	520	51/55	0.78	0.38	92,118,134,135	0
27	SQD	B	623	54/54	0.78	0.30	119,127,141,142	0
30	CA	f	102	1/1	0.79	0.38	118,118,118,118	0
28	LMG	C	519	51/55	0.79	0.41	72,98,113,114	0
23	CLA	B	607[A]	65/65	0.80	0.40	65,69,81,82	65
30	CA	F	102	1/1	0.80	0.61	97,97,97,97	0
23	CLA	c	504	65/65	0.80	0.29	89,93,96,97	0
21	CL	A	602	1/1	0.80	0.23	65,65,65,65	0
28	LMG	b	623	51/55	0.80	0.39	91,100,112,116	0
23	CLA	B	607[B]	65/65	0.80	0.40	63,67,72,75	65
27	SQD	X	101	43/54	0.80	0.39	108,115,119,119	0
25	BCR	K	101	40/40	0.80	0.37	75,78,79,80	0
25	BCR	c	515	40/40	0.80	0.44	99,105,108,108	0
29	FE2	a	615	1/1	0.80	0.17	88,88,88,88	0
23	CLA	B	602	65/65	0.80	0.41	73,82,107,107	0
28	LMG	J	101	51/55	0.80	0.34	66,76,106,108	0
23	CLA	c	503	65/65	0.81	0.36	85,87,101,103	0
23	CLA	c	508	65/65	0.81	0.32	91,94,113,115	0
25	BCR	B	620	40/40	0.81	0.40	68,74,80,80	0
28	LMG	Z	101	37/55	0.81	0.40	96,124,129,129	0
31	LHG	l	101	49/49	0.81	0.30	84,92,104,106	0
27	SQD	b	601	54/54	0.81	0.32	91,103,109,109	0
23	CLA	C	511	65/65	0.81	0.33	70,75,78,79	0
25	BCR	c	516	40/40	0.82	0.27	92,98,102,102	0
25	BCR	B	618	40/40	0.82	0.37	63,68,69,70	0
23	CLA	b	619	65/65	0.82	0.43	83,90,139,139	0
32	DGD	c	519	62/66	0.82	0.47	83,93,113,117	0
23	CLA	b	617	65/65	0.82	0.37	82,86,121,122	0
23	CLA	a	605	65/65	0.83	0.33	80,83,124,126	0
23	CLA	B	616	65/65	0.83	0.35	65,68,86,87	0
23	CLA	C	506	65/65	0.83	0.30	72,79,115,115	0
23	CLA	a	607	65/65	0.84	0.42	83,85,133,133	0
24	PHO	D	401	64/64	0.84	0.31	59,63,69,73	0
23	CLA	d	403	65/65	0.84	0.33	86,89,126,128	0
28	LMG	B	621	51/55	0.85	0.34	70,80,92,95	0
27	SQD	a	612	54/54	0.85	0.31	111,124,129,130	0
34	MG	j	102	1/1	0.85	0.18	89,89,89,89	0
32	DGD	C	518	62/66	0.85	0.35	62,72,93,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	CLA	a	604	65/65	0.85	0.30	77,80,87,95	0
23	CLA	c	507	65/65	0.85	0.30	93,100,136,136	0
23	CLA	C	505	65/65	0.85	0.30	69,71,85,85	0
28	LMG	A	612	51/55	0.85	0.30	94,100,105,105	0
23	CLA	B	608	65/65	0.85	0.35	58,61,73,74	0
28	LMG	a	611	51/55	0.86	0.27	114,121,126,126	0
31	LHG	a	614	49/49	0.86	0.35	87,94,124,125	0
23	CLA	c	514	65/65	0.86	0.30	101,106,125,126	0
32	DGD	c	517	62/66	0.86	0.26	84,94,122,124	0
29	FE2	A	613	1/1	0.86	0.29	67,67,67,67	0
31	LHG	D	408	49/49	0.86	0.35	67,74,103,104	0
26	PL9	D	405	55/55	0.86	0.21	60,64,70,72	0
23	CLA	b	612	65/65	0.86	0.28	85,90,92,93	0
23	CLA	c	510	65/65	0.86	0.26	91,93,108,108	0
23	CLA	b	613	65/65	0.86	0.44	82,86,94,98	0
25	BCR	k	101	40/40	0.86	0.32	95,99,100,100	0
23	CLA	D	404	65/65	0.87	0.34	65,68,106,107	0
24	PHO	d	401	64/64	0.87	0.28	80,84,90,94	0
23	CLA	C	509	65/65	0.87	0.24	70,72,87,88	0
23	CLA	b	615	65/65	0.87	0.35	81,85,91,92	0
24	PHO	a	606	64/64	0.88	0.33	78,83,86,87	0
31	LHG	d	406	49/49	0.88	0.35	85,89,98,102	0
23	CLA	B	610	65/65	0.88	0.30	64,69,72,73	0
23	CLA	B	615	65/65	0.88	0.27	61,65,101,102	0
23	CLA	b	606	65/65	0.88	0.28	79,84,92,96	0
23	CLA	C	508	65/65	0.88	0.30	66,70,95,99	0
31	LHG	b	624	49/49	0.88	0.25	91,96,102,102	0
32	DGD	C	517	62/66	0.88	0.32	63,75,103,104	0
33	HEM	e	102	43/43	0.88	0.45	101,103,107,108	0
32	DGD	c	518	62/66	0.88	0.30	84,96,124,124	0
23	CLA	C	501	65/65	0.88	0.35	69,73,85,87	0
28	LMG	j	101	51/55	0.88	0.24	87,96,126,129	0
23	CLA	b	616	65/65	0.88	0.31	80,84,106,108	0
25	BCR	B	619	40/40	0.88	0.30	62,69,81,81	0
23	CLA	c	512	65/65	0.88	0.25	90,95,99,99	0
23	CLA	A	608	65/65	0.89	0.34	62,65,112,113	0
22	BCT	a	603	4/4	0.89	0.49	100,101,101,103	0
23	CLA	A	606	65/65	0.89	0.31	60,62,104,106	0
32	DGD	C	516	62/66	0.89	0.22	64,73,102,103	0
23	CLA	B	611	65/65	0.89	0.27	62,65,73,77	0
32	DGD	h	102	62/66	0.89	0.25	87,93,99,101	0
23	CLA	b	608	65/65	0.89	0.27	80,84,95,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	LHG	B	622	49/49	0.89	0.25	70,75,81,82	0
32	DGD	H	102	62/66	0.89	0.23	66,72,79,81	0
23	CLA	C	504	65/65	0.89	0.29	66,68,95,95	0
23	CLA	b	605	65/65	0.89	0.24	85,88,93,94	0
23	CLA	b	610	65/65	0.90	0.32	79,82,94,95	0
23	CLA	B	606	65/65	0.90	0.23	59,64,75,76	0
23	CLA	c	506	65/65	0.90	0.22	89,92,106,106	0
23	CLA	b	611	65/65	0.90	0.26	82,86,92,93	0
33	HEM	E	102	43/43	0.90	0.28	80,82,86,87	0
23	CLA	c	509	65/65	0.91	0.27	87,90,115,119	0
23	CLA	C	502	65/65	0.91	0.33	65,67,80,83	0
23	CLA	B	614	65/65	0.91	0.26	60,63,85,87	0
31	LHG	D	407	49/49	0.91	0.21	64,69,78,81	0
23	CLA	D	403	65/65	0.91	0.28	54,59,75,76	0
23	CLA	B	604	65/65	0.91	0.25	58,63,72,76	0
23	CLA	C	503	65/65	0.91	0.34	68,72,76,77	0
23	CLA	B	605	65/65	0.91	0.25	60,63,91,91	0
34	MG	J	102	1/1	0.91	0.47	68,68,68,68	0
23	CLA	B	613	65/65	0.91	0.30	61,64,71,72	0
23	CLA	B	603	65/65	0.91	0.23	64,67,72,73	0
23	CLA	a	613	65/65	0.91	0.34	75,79,91,96	0
33	HEM	v	201	43/43	0.91	0.30	84,86,88,90	0
23	CLA	b	614	65/65	0.92	0.29	80,83,94,96	0
23	CLA	D	402	65/65	0.92	0.28	54,59,70,76	0
31	LHG	L	101	49/49	0.92	0.23	63,72,83,85	0
21	CL	A	603	1/1	0.92	0.20	62,62,62,62	0
23	CLA	B	609	65/65	0.92	0.24	61,65,71,72	0
23	CLA	A	605	65/65	0.92	0.25	56,59,66,75	0
23	CLA	b	607	65/65	0.93	0.24	81,84,111,112	0
23	CLA	c	505	65/65	0.93	0.26	86,89,115,116	0
23	CLA	c	511	65/65	0.93	0.24	86,90,96,99	0
24	PHO	A	607	64/64	0.93	0.26	57,62,65,67	0
23	CLA	d	402	65/65	0.94	0.26	75,80,95,96	0
20	OEX	A	601	10/10	0.94	0.31	63,64,67,67	0
23	CLA	B	612	65/65	0.94	0.24	60,62,73,75	0
33	HEM	V	202	43/43	0.94	0.26	63,65,68,69	0
21	CL	c	501	1/1	0.95	0.19	83,83,83,83	0
23	CLA	C	510	65/65	0.95	0.23	65,69,76,78	0
30	CA	o	301	1/1	0.96	0.24	110,110,110,110	0
20	OEX	a	601	10/10	0.96	0.32	83,84,87,88	0
22	BCT	A	604	4/4	0.97	0.21	79,80,81,82	0
30	CA	O	301	1/1	0.97	0.17	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.