



wwPDB EM Map/Model Validation Report ⓘ

Jun 2, 2016 – 09:45 AM EDT

PDB ID : 3JCU
EMDB ID: : EMD-6617
Title : Cryo-EM structure of spinach PSII-LHCII supercomplex at 3.2 Angstrom resolution
Authors : Wei, X.P.; Zhang, X.Z.; Su, X.D.; Cao, P.; Liu, X.Y.; Li, M.; Chang, W.R.; Liu, Z.F.
Deposited on : 2016-03-10
Resolution : 3.20 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027674

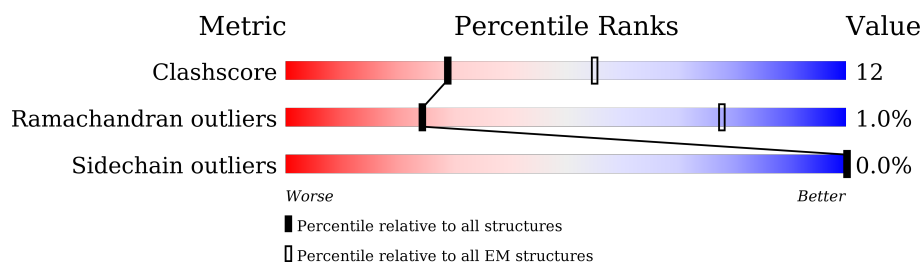
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



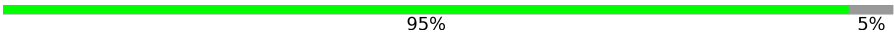









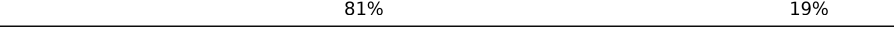
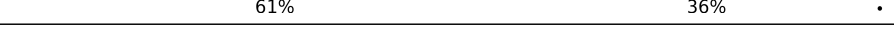
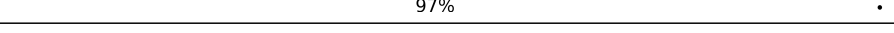


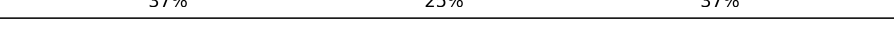


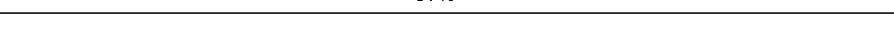






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	344	58% 39% .
1	a	344	97% .
2	B	508	54% 41% .
2	b	508	95% . .
3	C	473	54% 40% 5%
3	c	473	95% 5%
4	D	353	54% 42% .
4	d	353	96% .
5	E	83	66% 29% 5%

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Mol	Chain	Length	Quality of chain
5	e	83	 95% 5%
6	F	39	 64% 18% 18%
6	f	39	 82% 18%
7	G	267	 46% 35% 18%
7	N	267	 48% 34% 18%
7	Y	267	 52% 29% 18%
7	g	267	 81% 18%
7	n	267	 81% 18%
7	y	267	 81% 18%
8	H	73	 47% 34% 19%
8	h	73	 81% 19%
9	I	36	 61% 36% .
9	i	36	 97% .
10	J	40	 55% 30% 15%
10	j	40	 85% 15%
11	K	59	 37% 25% 37%
11	k	59	 63% 37%
12	L	38	 79% 18% .
12	l	38	 97% .
13	M	34	 65% 32% .
13	m	34	 97% .
14	O	332	 33% 39% . 27%
14	o	332	 72% . 27%
15	P	267	 33% 31% 36%
15	p	267	 64% . 36%

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Mol	Chain	Length	Quality of chain
16	Q	232	
16	q	232	
17	R	243	
17	r	243	
18	S	295	
18	s	295	
19	T	33	
19	t	33	
20	U	99	
20	u	99	
21	W	137	
21	w	137	
22	X	117	
22	x	117	
23	Z	62	
23	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
27	CLA	A	405	X	-	-	-
27	CLA	A	406	X	-	-	-
27	CLA	A	407	X	-	-	-
27	CLA	A	410	X	-	-	-
27	CLA	B	602	X	-	-	-
27	CLA	B	603	X	-	-	-
27	CLA	B	604	X	-	-	-
27	CLA	B	605	X	-	-	-
27	CLA	B	606	X	-	-	-
27	CLA	B	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	B	608	X	-	-	-
27	CLA	B	609	X	-	-	-
27	CLA	B	610	X	-	-	-
27	CLA	B	611	X	-	-	-
27	CLA	B	612	X	-	-	-
27	CLA	B	613	X	-	-	-
27	CLA	B	614	X	-	-	-
27	CLA	B	615	X	-	-	-
27	CLA	B	616	X	-	-	-
27	CLA	B	617	X	-	-	-
27	CLA	C	501	X	-	-	-
27	CLA	C	502	X	-	-	-
27	CLA	C	503	X	-	-	-
27	CLA	C	504	X	-	-	-
27	CLA	C	505	X	-	-	-
27	CLA	C	506	X	-	-	-
27	CLA	C	507	X	-	-	-
27	CLA	C	508	X	-	-	-
27	CLA	C	509	X	-	-	-
27	CLA	C	510	X	-	-	-
27	CLA	C	511	X	-	-	-
27	CLA	C	512	X	-	-	-
27	CLA	C	513	X	-	-	-
27	CLA	D	402	X	-	-	-
27	CLA	D	403	X	-	-	-
27	CLA	G	602	X	-	-	-
27	CLA	G	603	X	-	-	-
27	CLA	G	604	X	-	-	-
27	CLA	G	610	X	-	-	-
27	CLA	G	611	X	-	-	-
27	CLA	G	612	X	-	-	-
27	CLA	G	613	X	-	-	-
27	CLA	G	614	X	-	-	-
27	CLA	N	602	X	-	-	-
27	CLA	N	603	X	-	-	-
27	CLA	N	604	X	-	-	-
27	CLA	N	610	X	-	-	-
27	CLA	N	611	X	-	-	-
27	CLA	N	612	X	-	-	-
27	CLA	N	613	X	-	-	-
27	CLA	N	614	X	-	-	-
27	CLA	R	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	R	602	X	-	-	-
27	CLA	R	603	X	-	-	-
27	CLA	R	604	X	-	-	-
27	CLA	R	609	X	-	-	-
27	CLA	R	610	X	-	-	-
27	CLA	R	611	X	-	-	-
27	CLA	R	612	X	-	-	-
27	CLA	R	613	X	-	-	-
27	CLA	R	616	X	-	-	-
27	CLA	S	602	X	-	-	-
27	CLA	S	603	X	-	-	-
27	CLA	S	604	X	-	-	-
27	CLA	S	609	X	-	-	-
27	CLA	S	610	X	-	-	-
27	CLA	S	611	X	-	-	-
27	CLA	S	612	X	-	-	-
27	CLA	S	613	X	-	-	-
27	CLA	S	614	X	-	-	-
27	CLA	Y	602	X	-	-	-
27	CLA	Y	603	X	-	-	-
27	CLA	Y	604	X	-	-	-
27	CLA	Y	610	X	-	-	-
27	CLA	Y	611	X	-	-	-
27	CLA	Y	612	X	-	-	-
27	CLA	Y	613	X	-	-	-
27	CLA	Y	614	X	-	-	-
27	CLA	a	405	X	-	-	-
27	CLA	a	406	X	-	-	-
27	CLA	a	407	X	-	-	-
27	CLA	a	410	X	-	-	-
27	CLA	b	602	X	-	-	-
27	CLA	b	603	X	-	-	-
27	CLA	b	604	X	-	-	-
27	CLA	b	605	X	-	-	-
27	CLA	b	606	X	-	-	-
27	CLA	b	607	X	-	-	-
27	CLA	b	608	X	-	-	-
27	CLA	b	609	X	-	-	-
27	CLA	b	610	X	-	-	-
27	CLA	b	611	X	-	-	-
27	CLA	b	612	X	-	-	-
27	CLA	b	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	b	614	X	-	-	-
27	CLA	b	615	X	-	-	-
27	CLA	b	616	X	-	-	-
27	CLA	b	617	X	-	-	-
27	CLA	c	501	X	-	-	-
27	CLA	c	502	X	-	-	-
27	CLA	c	503	X	-	-	-
27	CLA	c	504	X	-	-	-
27	CLA	c	505	X	-	-	-
27	CLA	c	506	X	-	-	-
27	CLA	c	507	X	-	-	-
27	CLA	c	508	X	-	-	-
27	CLA	c	509	X	-	-	-
27	CLA	c	510	X	-	-	-
27	CLA	c	511	X	-	-	-
27	CLA	c	512	X	-	-	-
27	CLA	c	513	X	-	-	-
27	CLA	d	402	X	-	-	-
27	CLA	d	403	X	-	-	-
27	CLA	g	602	X	-	-	-
27	CLA	g	603	X	-	-	-
27	CLA	g	604	X	-	-	-
27	CLA	g	610	X	-	-	-
27	CLA	g	611	X	-	-	-
27	CLA	g	612	X	-	-	-
27	CLA	g	613	X	-	-	-
27	CLA	g	614	X	-	-	-
27	CLA	n	602	X	-	-	-
27	CLA	n	603	X	-	-	-
27	CLA	n	604	X	-	-	-
27	CLA	n	610	X	-	-	-
27	CLA	n	611	X	-	-	-
27	CLA	n	612	X	-	-	-
27	CLA	n	613	X	-	-	-
27	CLA	n	614	X	-	-	-
27	CLA	r	601	X	-	-	-
27	CLA	r	602	X	-	-	-
27	CLA	r	603	X	-	-	-
27	CLA	r	604	X	-	-	-
27	CLA	r	609	X	-	-	-
27	CLA	r	610	X	-	-	-
27	CLA	r	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	CLA	r	612	X	-	-	-
27	CLA	r	613	X	-	-	-
27	CLA	r	616	X	-	-	-
27	CLA	s	602	X	-	-	-
27	CLA	s	603	X	-	-	-
27	CLA	s	604	X	-	-	-
27	CLA	s	609	X	-	-	-
27	CLA	s	610	X	-	-	-
27	CLA	s	611	X	-	-	-
27	CLA	s	612	X	-	-	-
27	CLA	s	613	X	-	-	-
27	CLA	s	614	X	-	-	-
27	CLA	y	602	X	-	-	-
27	CLA	y	603	X	-	-	-
27	CLA	y	604	X	-	-	-
27	CLA	y	610	X	-	-	-
27	CLA	y	611	X	-	-	-
27	CLA	y	612	X	-	-	-
27	CLA	y	613	X	-	-	-
27	CLA	y	614	X	-	-	-
33	BCT	D	401	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 75994 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		
1	a	334	Total	C	N	O	S	0	0
			2614	1707	430	464	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		
2	b	487	Total	C	N	O	S	0	0
			3820	2501	640	667	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		
3	c	449	Total	C	N	O	S	0	0
			3475	2284	581	599	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		
4	d	340	Total	C	N	O	S	0	0
			2703	1786	443	462	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	79	Total	C	N	O	0	0
			636	412	104	120		
5	e	79	Total	C	N	O	0	0
			636	412	104	120		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	32	Total	C	N	O	S	0	0
			257	174	43	39	1		
6	f	32	Total	C	N	O	S	0	0
			257	174	43	39	1		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	N	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	Y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	g	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	n	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		
7	y	218	Total	C	N	O	S	0	0
			1661	1079	270	305	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			434	288	65	78	3		
8	h	59	Total	C	N	O	S	0	0
			434	288	65	78	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	35	Total	C	N	O	S	0	0
			286	195	44	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	34	Total	C	N	O		0	0
			247	168	38	41			
10	j	34	Total	C	N	O		0	0
			247	168	38	41			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	37	Total	C	N	O	S	0	0
			307	217	43	46	1		
11	k	37	Total	C	N	O	S	0	0
			307	217	43	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	37	Total	C	N	O		0	0
			311	205	49	57			
12	l	37	Total	C	N	O		0	0
			311	205	49	57			

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	33	Total	C	N	O		0	0
			258	176	37	45			
13	m	33	Total	C	N	O		0	0
			258	176	37	45			

- Molecule 14 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		
14	o	243	Total	C	N	O	S	0	0
			1844	1164	301	376	3		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		
15	p	172	Total	C	N	O	S	0	0
			1324	841	215	266	2		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	148	Total	C	N	O		0	0
			1162	736	202	224			
16	q	148	Total	C	N	O		0	0
			1162	736	202	224			

- Molecule 17 is a protein called Chlorophyll A-B Binding protein 29 kD (CP29).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		
17	r	232	Total	C	N	O	S	0	0
			1806	1170	293	339	4		

- Molecule 18 is a protein called Chlorophyll A-B Binding protein 26 kD (CP26).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		
18	s	214	Total	C	N	O	S	0	0
			1653	1080	269	299	5		

- Molecule 19 is a protein called Photosystem II Reaction Center protein Tc.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			245	171	34	39	1		
19	t	30	Total	C	N	O	S	0	0
			245	171	34	39	1		

- Molecule 20 is a protein called Photosystem II Reaction Center Tn protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total	C	N	O	S	0	0
			193	123	35	32	3		
20	u	25	Total	C	N	O	S	0	0
			193	123	35	32	3		

- Molecule 21 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	54	Total	C	N	O	S	0	0
			419	276	61	81	1		
21	w	54	Total	C	N	O	S	0	0
			419	276	61	81	1		

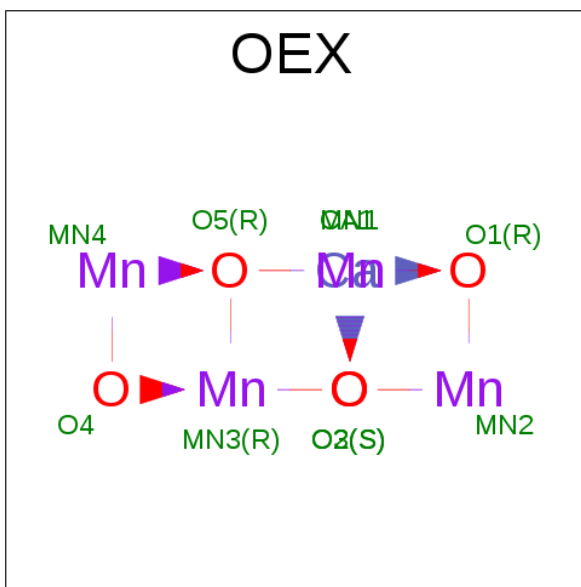
- Molecule 22 is a protein called Photosystem II Reaction Center X protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	35	Total	C	N	O	0	0
			246	163	38	45		
22	x	35	Total	C	N	O	0	0
			246	163	38	45		

- Molecule 23 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	61	Total	C	N	O	0	0
			454	306	68	80		
23	z	61	Total	C	N	O	0	0
			454	306	68	80		

- Molecule 24 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

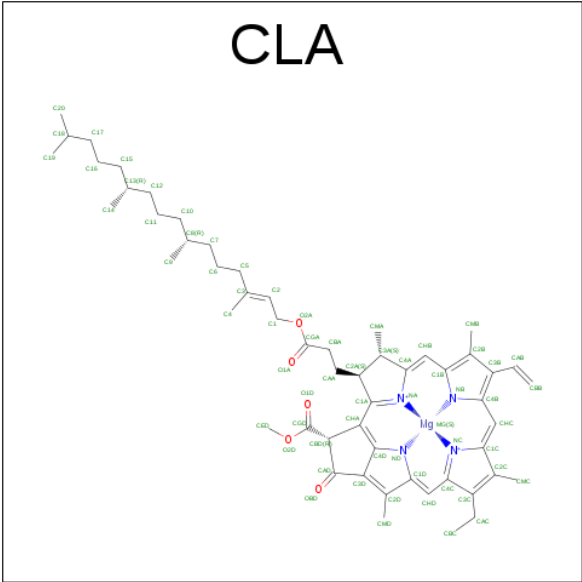
- Molecule 25 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	Fe	0
			1	1	
25	a	1	Total	Fe	0
			1	1	

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
26	A	2	Total	Cl	0
			2	2	
26	a	2	Total	Cl	0
			2	2	

- Molecule 27 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	C	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	G	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	N	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	R	1	Total 522	C 422	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	R	1	Total	C	Mg	N	O	0
			522	422	10	40	50	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	S	1	Total	C	Mg	N	O	0
			441	351	9	36	45	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
27	Y	1	Total	C	Mg	N	O	0
			472	392	8	32	40	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
27	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	c	1	Total	C	Mg	N	O	0
			829	699	13	52	65	
27	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	
27	g	1	Total	C	Mg	N	O	0
			424	344	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	g	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	n	1	Total 424	C 344	Mg 8	N 32	O 40	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	r	1	Total 522	C 422	Mg 10	N 40	O 50	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0

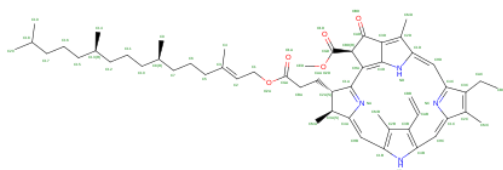
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Mol	Chain	Residues	Atoms					AltConf
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	s	1	Total 441	C 351	Mg 9	N 36	O 45	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0
27	y	1	Total 472	C 392	Mg 8	N 32	O 40	0

- Molecule 28 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).

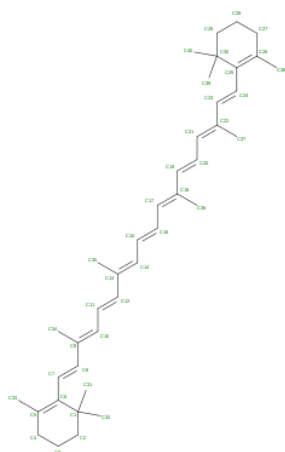
PHO



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	N	O	0
			128	110	8	10	
28	A	1	Total	C	N	O	0
			128	110	8	10	
28	a	1	Total	C	N	O	0
			128	110	8	10	
28	a	1	Total	C	N	O	0
			128	110	8	10	

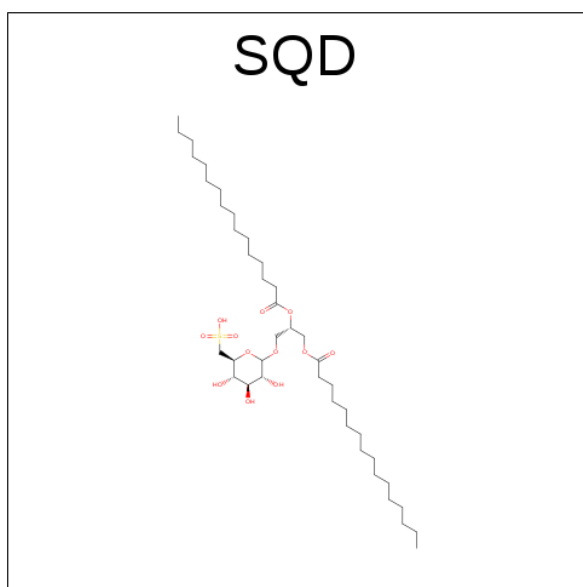
- Molecule 29 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

BCR



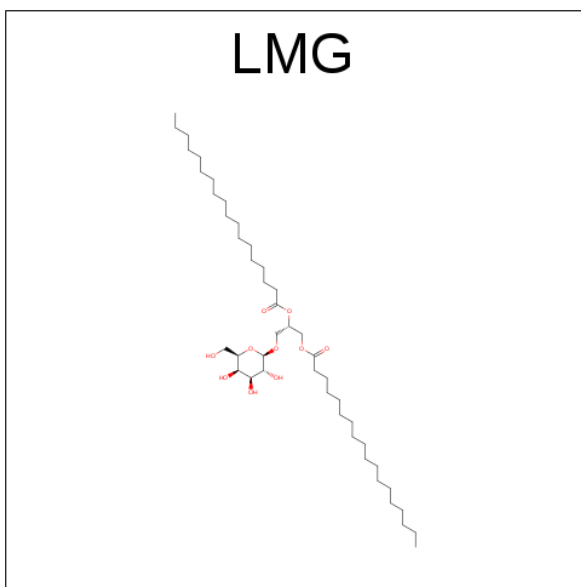
Mol	Chain	Residues	Atoms	AltConf
29	A	1	Total C 40 40	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	B	1	Total C 120 120	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	C	1	Total C 160 160	0
29	D	1	Total C 40 40	0
29	H	1	Total C 40 40	0
29	a	1	Total C 40 40	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	b	1	Total C 120 120	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	c	1	Total C 160 160	0
29	d	1	Total C 40 40	0
29	h	1	Total C 40 40	0

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



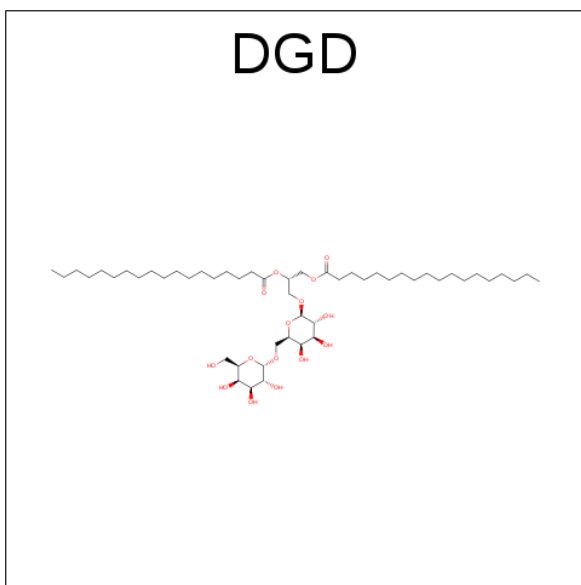
Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	O	S	0
			108	82	24	2	
30	A	1	Total	C	O	S	0
			108	82	24	2	
30	B	1	Total	C	O	S	0
			54	41	12	1	
30	a	1	Total	C	O	S	0
			108	82	24	2	
30	a	1	Total	C	O	S	0
			108	82	24	2	
30	b	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



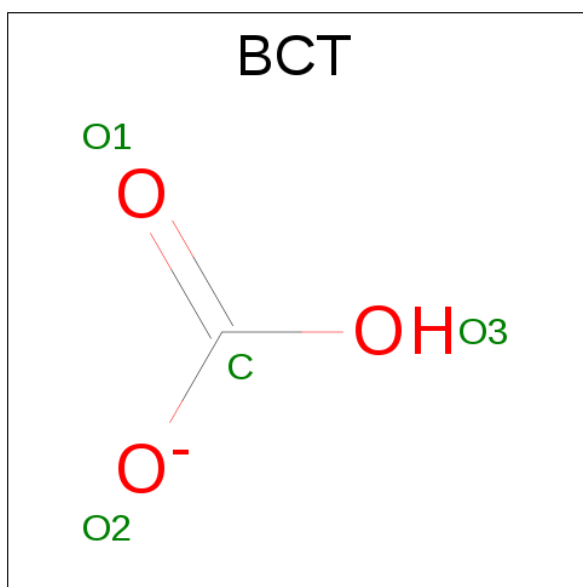
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			48	38	10	
31	B	1	Total	C	O	0
			51	41	10	
31	C	1	Total	C	O	0
			51	41	10	
31	D	1	Total	C	O	0
			46	36	10	
31	Z	1	Total	C	O	0
			51	41	10	
31	a	1	Total	C	O	0
			48	38	10	
31	b	1	Total	C	O	0
			51	41	10	
31	c	1	Total	C	O	0
			51	41	10	
31	d	1	Total	C	O	0
			46	36	10	
31	z	1	Total	C	O	0
			51	41	10	

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



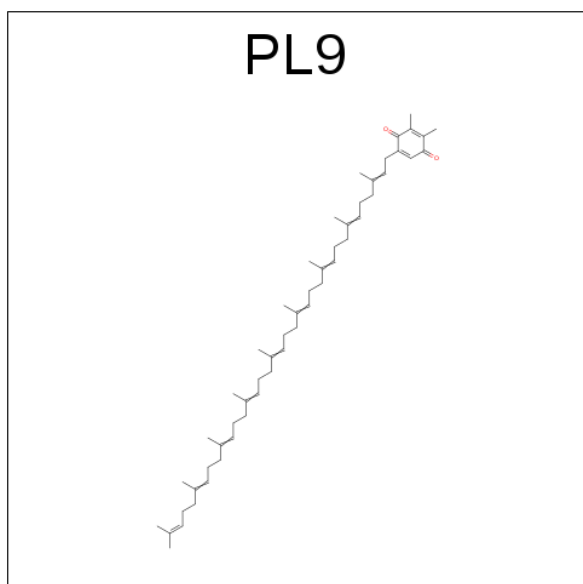
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total	C	O	0
			179	134	45	
32	C	1	Total	C	O	0
			179	134	45	
32	C	1	Total	C	O	0
			179	134	45	
32	H	1	Total	C	O	0
			62	47	15	
32	c	1	Total	C	O	0
			179	134	45	
32	c	1	Total	C	O	0
			179	134	45	
32	c	1	Total	C	O	0
			179	134	45	
32	h	1	Total	C	O	0
			62	47	15	

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



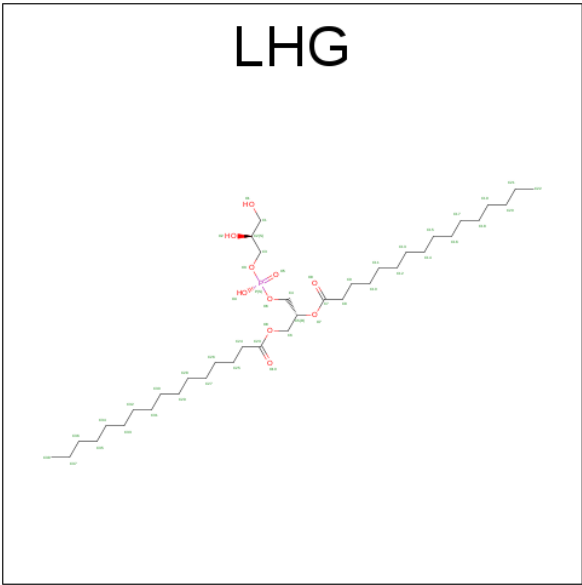
Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	d	1	Total	C	O	0
			4	1	3	

- Molecule 34 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			AltConf
34	D	1	Total	C	O	0
			55	53	2	
34	d	1	Total	C	O	0
			55	53	2	

- Molecule 35 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



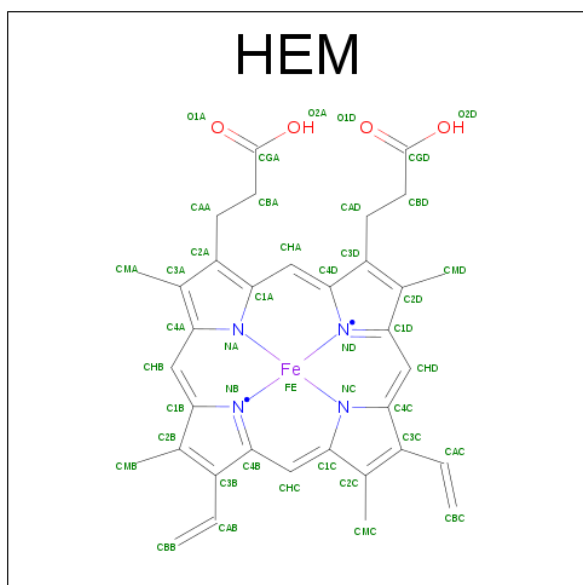
Mol	Chain	Residues	Atoms				AltConf
35	D	1	Total	C	O	P	0
			129	96	30	3	
35	D	1	Total	C	O	P	0
			129	96	30	3	
35	D	1	Total	C	O	P	0
			129	96	30	3	
35	G	1	Total	C	O	P	0
			49	38	10	1	
35	L	1	Total	C	O	P	0
			49	38	10	1	
35	N	1	Total	C	O	P	0
			49	38	10	1	
35	R	1	Total	C	O	P	0
			49	38	10	1	
35	S	1	Total	C	O	P	0
			49	38	10	1	
35	Y	1	Total	C	O	P	0
			49	38	10	1	

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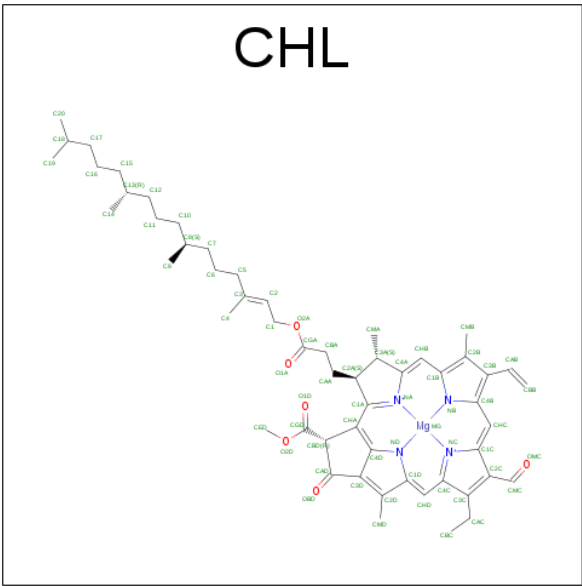
Mol	Chain	Residues	Atoms				AltConf
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	d	1	Total	C	O	P	0
			129	96	30	3	
35	g	1	Total	C	O	P	0
			49	38	10	1	
35	l	1	Total	C	O	P	0
			49	38	10	1	
35	n	1	Total	C	O	P	0
			49	38	10	1	
35	r	1	Total	C	O	P	0
			49	38	10	1	
35	s	1	Total	C	O	P	0
			49	38	10	1	
35	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
36	F	1	Total 43	C 34	Fe 1	N 4	O 4	0
36	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 37 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
37	G	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
			314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
37	G	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
			314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
37	G	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
			314	248	6	24	36	
	G	1	Total	C	Mg	N	O	
37	N	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
			314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
37	N	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
			314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
37	N	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
			314	248	6	24	36	
	N	1	Total	C	Mg	N	O	
37	R	1	Total	C	Mg	N	O	0
			150	117	3	12	18	

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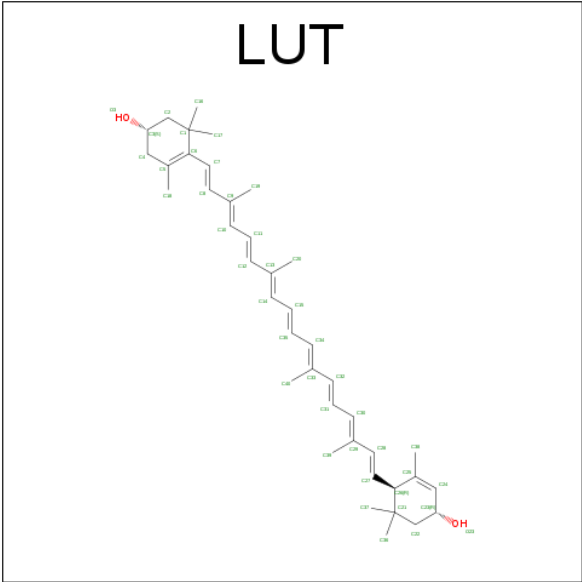
Mol	Chain	Residues	Atoms					AltConf
37	R	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	R	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	S	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	Y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	g	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	n	1	Total	C	Mg	N	O	0
			314	248	6	24	36	
37	r	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	r	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	r	1	Total	C	Mg	N	O	0
			150	117	3	12	18	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	s	1	Total	C	Mg	N	O	0
			201	157	4	16	24	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	
37	y	1	Total	C	Mg	N	O	0
			330	264	6	24	36	

- Molecule 38 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



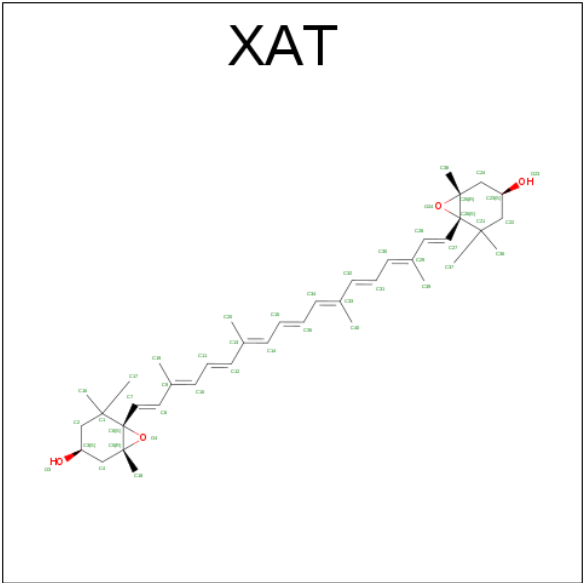
Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			84	80	4	
38	G	1	Total	C	O	0
			84	80	4	
38	N	1	Total	C	O	0
			84	80	4	
38	N	1	Total	C	O	0
			84	80	4	
38	R	1	Total	C	O	0
			42	40	2	
38	S	1	Total	C	O	0
			84	80	4	
38	S	1	Total	C	O	0
			84	80	4	
38	Y	1	Total	C	O	0
			84	80	4	
38	Y	1	Total	C	O	0
			84	80	4	
38	g	1	Total	C	O	0
			84	80	4	
38	g	1	Total	C	O	0
			84	80	4	
38	n	1	Total	C	O	0
			84	80	4	
38	n	1	Total	C	O	0
			84	80	4	
38	r	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
38	s	1	Total	C	O	0
			84	80	4	
38	s	1	Total	C	O	0
			84	80	4	
38	y	1	Total	C	O	0
			84	80	4	
38	y	1	Total	C	O	0
			84	80	4	

- Molecule 39 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



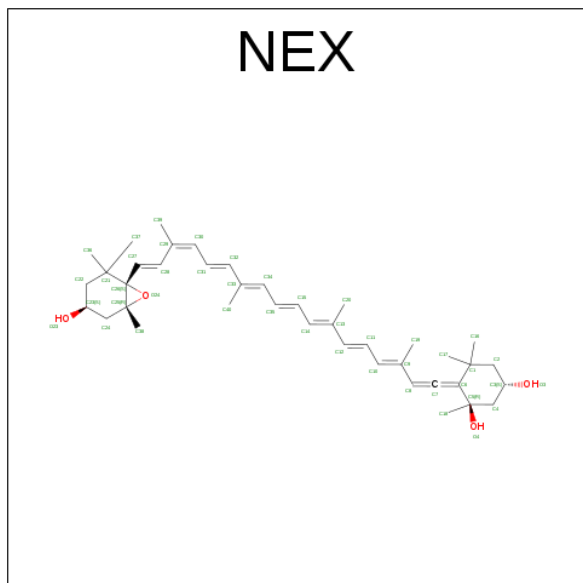
Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			44	40	4	
39	N	1	Total	C	O	0
			44	40	4	
39	R	1	Total	C	O	0
			44	40	4	
39	Y	1	Total	C	O	0
			44	40	4	
39	g	1	Total	C	O	0
			44	40	4	
39	n	1	Total	C	O	0
			44	40	4	
39	r	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
39	y	1	Total	C	O	0
			44	40	4	

- Molecule 40 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
40	G	1	Total	C	O	0
			44	40	4	
40	N	1	Total	C	O	0
			44	40	4	
40	R	1	Total	C	O	0
			44	40	4	
40	S	1	Total	C	O	0
			44	40	4	
40	Y	1	Total	C	O	0
			44	40	4	
40	g	1	Total	C	O	0
			44	40	4	
40	n	1	Total	C	O	0
			44	40	4	
40	r	1	Total	C	O	0
			44	40	4	
40	s	1	Total	C	O	0
			44	40	4	

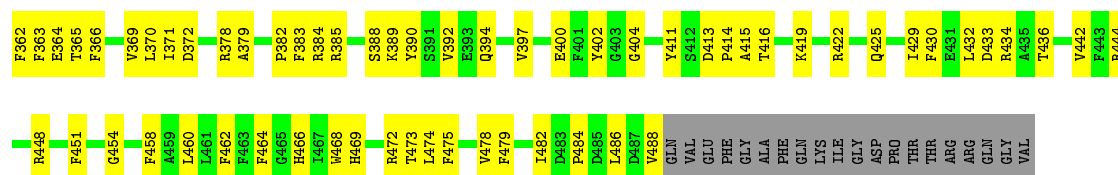
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
40	y	1	44	40	4	0

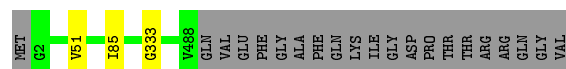
- Molecule 1: Photosystem II protein D1





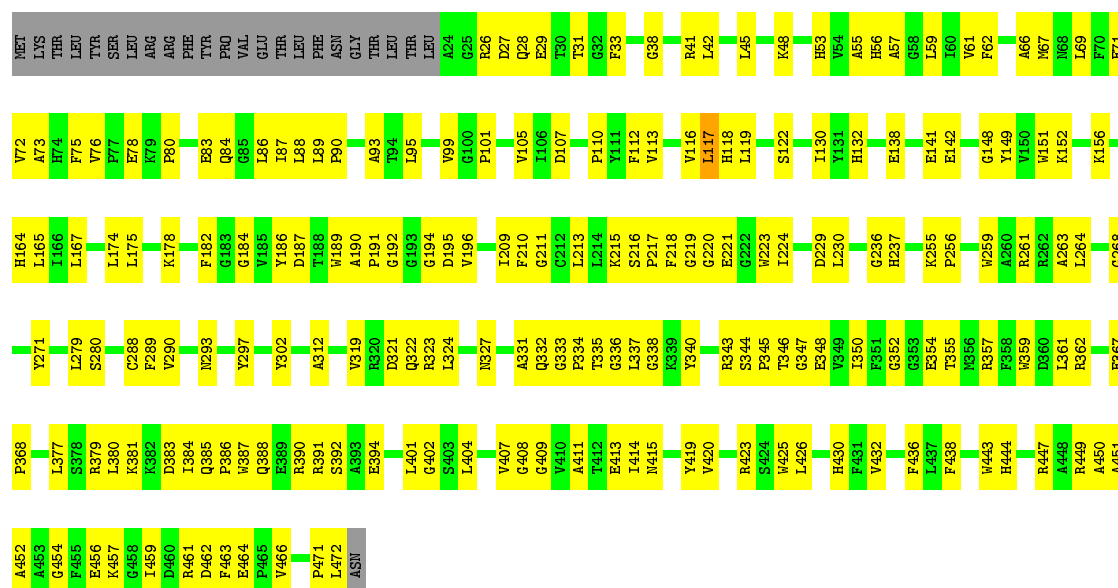
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  95%



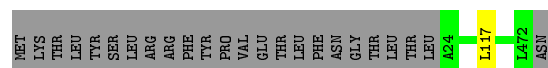
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  54% 40% 5%



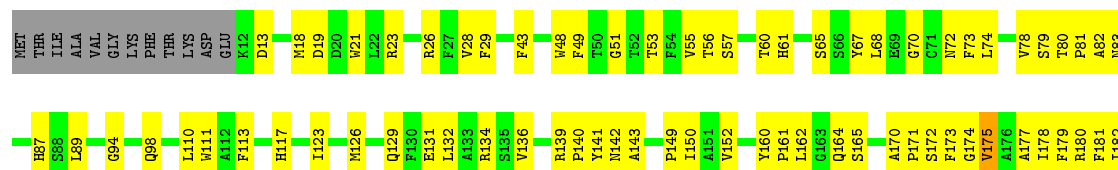
• Molecule 3: Photosystem II CP43 reaction center protein

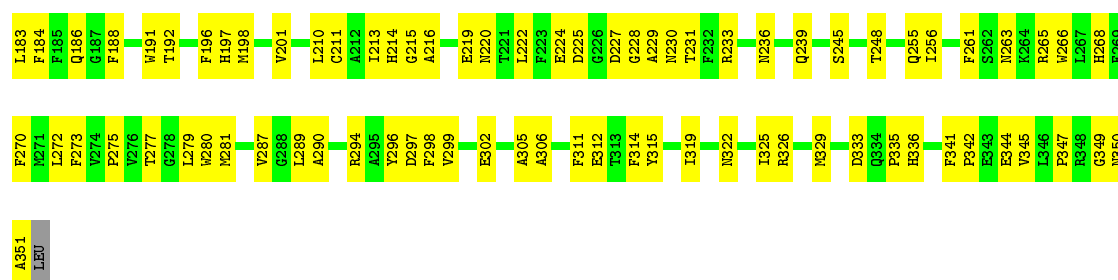
Chain c:  95% 5%



• Molecule 4: Photosystem II D2 protein

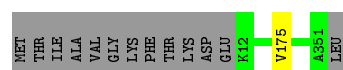
Chain D:  54% 42%





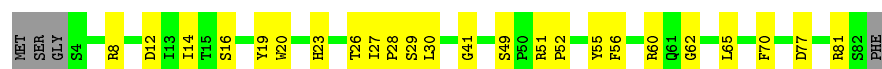
• Molecule 4: Photosystem II D2 protein

Chain d: 96%



• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 66%



• Molecule 5: Cytochrome b559 subunit alpha

Chain e: 95%



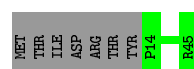
• Molecule 6: Cytochrome b559 subunit beta

Chain F: 64%



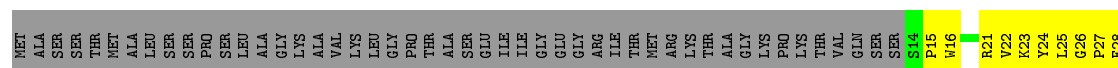
• Molecule 6: Cytochrome b559 subunit beta

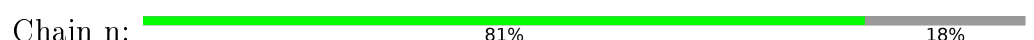
Chain f: 82%

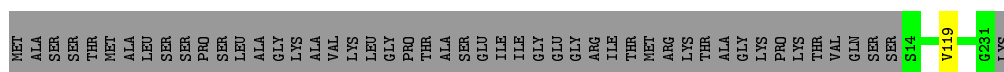


• Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain G: 46%

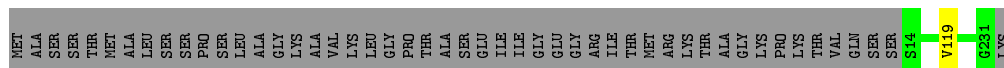






- Molecule 7: Chlorophyll a-b binding protein, chloroplastic

Chain y: 81% 18%



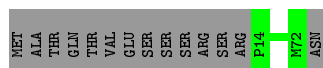
- Molecule 8: Photosystem II reaction center protein H

Chain H: 47% 34% 19%



- Molecule 8: Photosystem II reaction center protein H

Chain h: 81% 19%



- Molecule 9: Protein Photosystem II reaction center protein I

Chain I: 61% 36% .



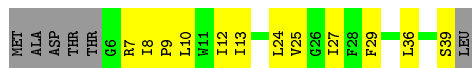
- Molecule 9: Protein Photosystem II reaction center protein I

Chain i: 97% .



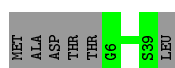
- Molecule 10: Photosystem II reaction center protein J

Chain J: 55% 30% 15%

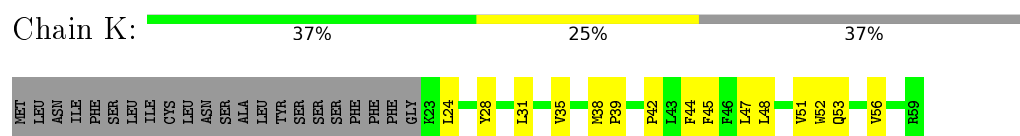


- Molecule 10: Photosystem II reaction center protein J

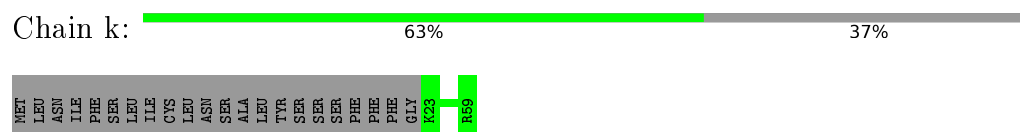
Chain j: 85% 15%



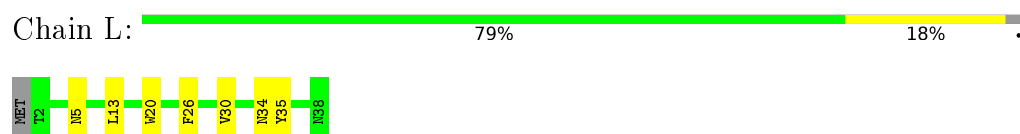
- Molecule 11: Photosystem II reaction center protein K



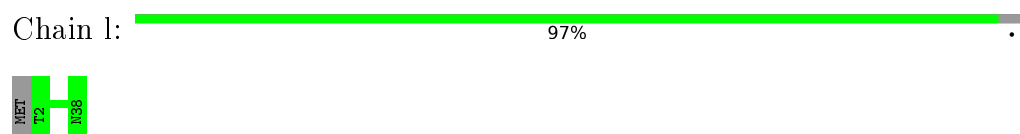
- Molecule 11: Photosystem II reaction center protein K



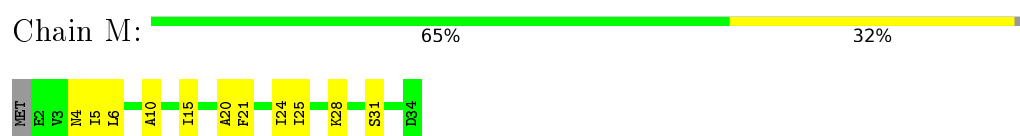
- Molecule 12: Protein Photosystem II reaction center protein L



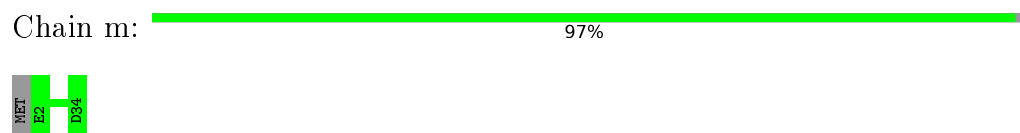
- Molecule 12: Protein Photosystem II reaction center protein L



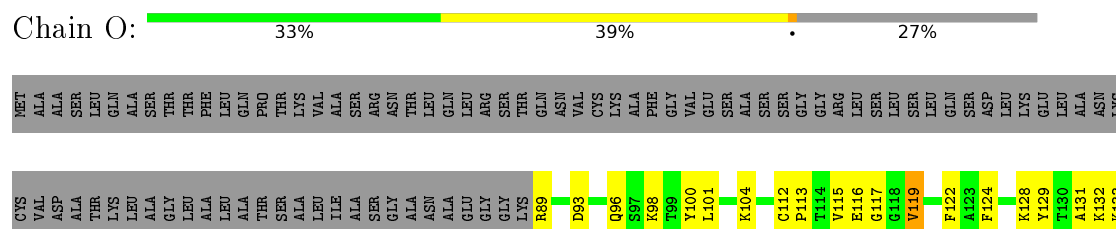
- Molecule 13: Photosystem II reaction center protein M

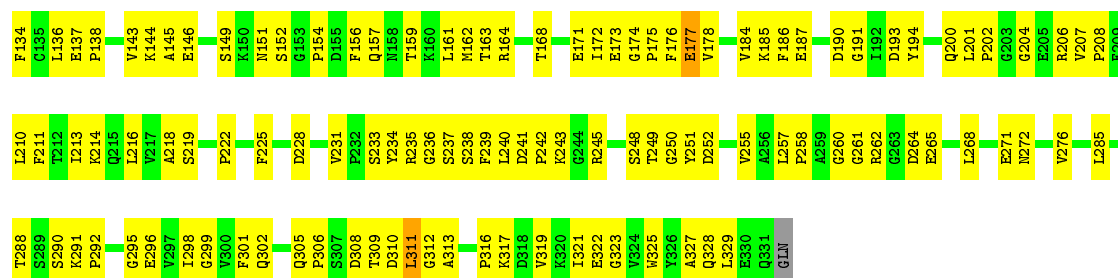


- Molecule 13: Photosystem II reaction center protein M



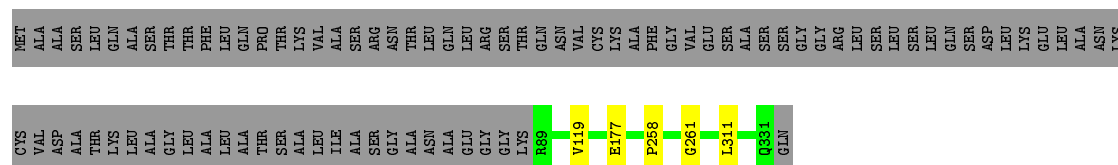
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic





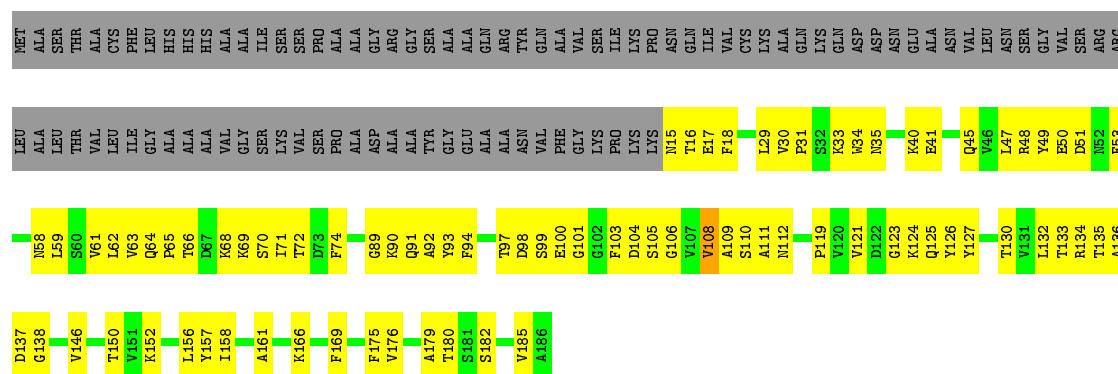
- Molecule 14: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 72% 27%



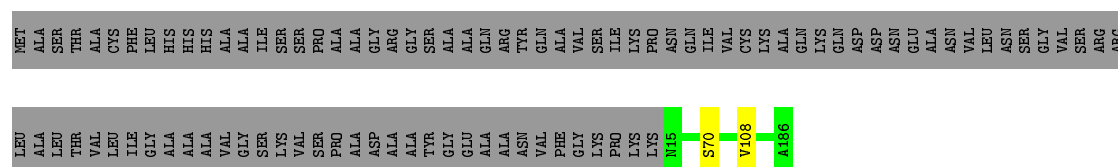
- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P: 33% 31% 36%



- Molecule 15: Oxygen-evolving enhancer protein 2, chloroplastic

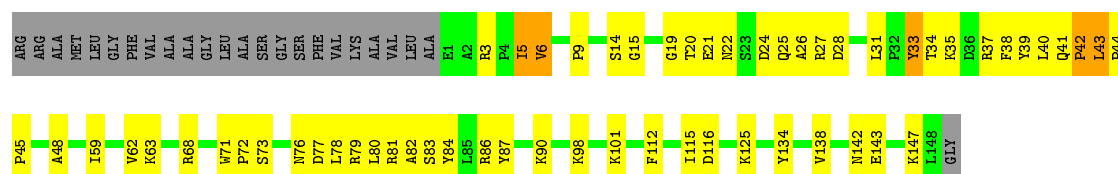
Chain p: 64% 36%



- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

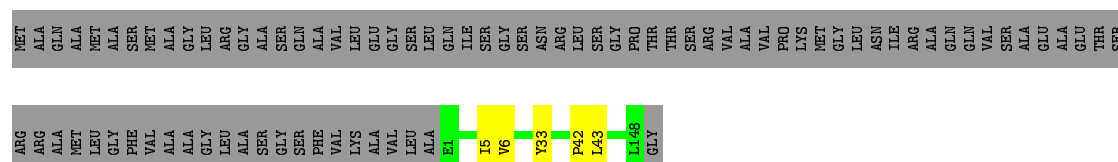
Chain Q: 38% 23% 36%





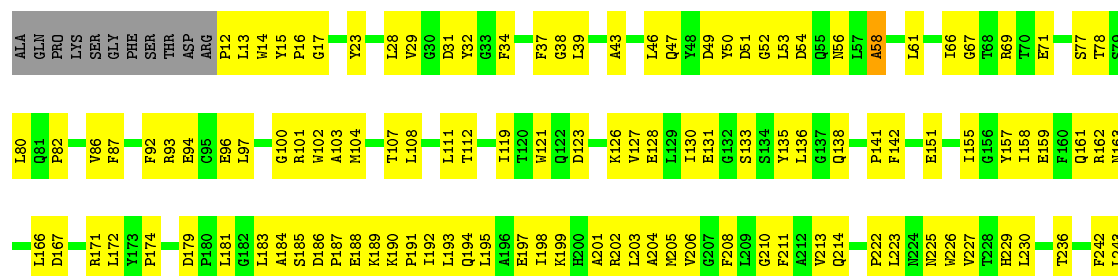
- Molecule 16: Oxygen-evolving enhancer protein 3, chloroplastic

Chain q: 62% 36%



- Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)

Chain R: 47% 48% 5%



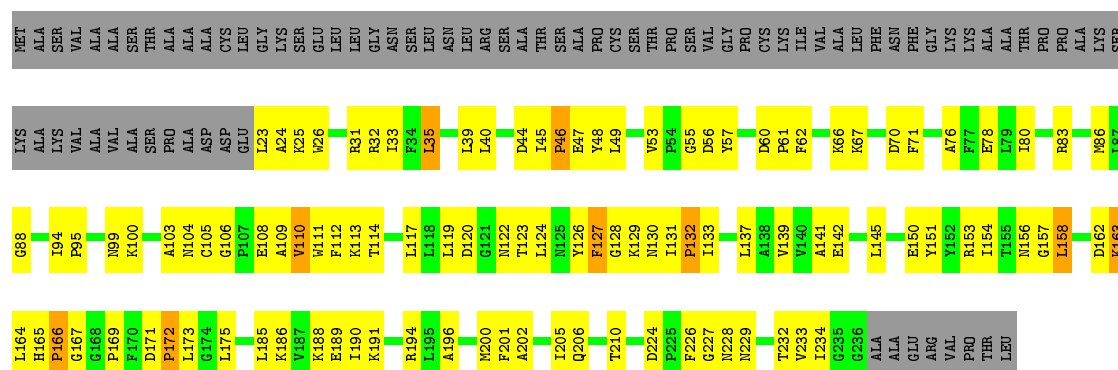
- Molecule 17: Chlorophyll A-B Binding protein 29 kD (CP29)

Chain r: 92% 5%



- Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

Chain S: 36% 33% 27%



- Molecule 18: Chlorophyll A-B Binding protein 26 kD (CP26)

Chain s: 

MET ALA SER VAL ALA SER THR ALA ALA ASP CYS GLY LYS GLU LEU LEU GLY ASN SER LEU ASN LEU ARG SER ALA THR SER ALA PRO CYS SER THR PRO VAL GLY PRO CYS LYS ILE VAL ALA LEU PHE ASN PHE GLY LYS LYS ALA THR PRO ALA LYS SER


LYS ALA LYS VAL ALA VAL ALA SER PRO ALA ASP ASP GLU L23 L35 P46 V110 F127 P132 L158 K163 P166 P172 G236 ALA ALA GLU ARG VAL PRO THR LEU

- Molecule 19: Photosystem II Reaction Center protein Tc

Chain T: 

H1 Y6 L9 L10 T13 I16 I17 K28 L29 S30 THR LYS

- Molecule 19: Photosystem II Reaction Center protein Tc

Chain t: 

H1 S30 THR LYS

- Molecule 20: Photosystem II Reaction Center Tn protein

Chain U: 

MET ALA SER ILE THR MET THR ALA ALA PHE LEU GLY THR VAL SER LYS GLN PRO PRO THR HIS HIS K10 K11 K12 Y13 R24 I25 K28

ALA CYS SER VAL ARG ALA MET MET ALA ALA PHE LEU GLU PRO LYS R4 G5 T6 P7 E8 A9 K10 K11 K12 Y13 R24 I25 K28

- Molecule 20: Photosystem II Reaction Center Tn protein

Chain u: 

MET ALA SER ILE THR MET THR ALA ALA PHE LEU GLY THR VAL SER LYS GLN PRO PRO THR HIS HIS K10 K11 K12 Y13 R24 I25 K28

ALA CYS SER VAL ARG ALA MET MET ALA ALA PHE LEU GLU PRO LYS R4 P7 K28

- Molecule 21: Photosystem II reaction center W protein, chloroplastic

Chain W: 

MET THR THR THR SER SER SER SER LEU VAL ALA ARG ALA SER LEU VAL HIS ASN SER ARG VAL VAL SER SER SER PRO ILE LEU GLY LEU PRO SER MET THR LYS ARG SER LYS THR CYS THR SER ILE GLU ASN LYS PRO SER THR THR THR THR THR THR THR



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	109042	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	59000	Depositor
Image detector	OTHER	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, OEX, LUT, DGD, CL, CHL, XAT, CLA, PL9, FE2, NEX, HEM, BCT, PHO, 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 >2	RMSZ	# Z >2
1	A	0.60	0/2695	0.59	0/3674
1	a	0.60	0/2695	0.59	0/3674
10	J	0.28	0/253	0.45	0/343
10	j	0.29	0/253	0.45	0/343
11	K	0.49	0/320	0.49	0/436
11	k	0.49	0/320	0.49	0/436
12	L	0.60	0/319	0.49	0/434
12	l	0.60	0/319	0.49	0/434
13	M	0.52	0/262	0.55	0/359
13	m	0.52	0/262	0.55	0/359
14	O	0.39	0/1880	0.51	0/2541
14	o	0.39	0/1880	0.51	0/2541
15	P	0.28	0/1353	0.49	0/1828
15	p	0.28	0/1353	0.49	0/1828
16	Q	0.28	0/1186	0.57	2/1609 (0.1%)
16	q	0.28	0/1186	0.57	2/1609 (0.1%)
17	R	0.41	0/1853	0.55	0/2522
17	r	0.41	0/1853	0.55	0/2522
18	S	0.39	0/1700	0.62	0/2310
18	s	0.39	0/1700	0.62	0/2310
19	T	0.56	0/252	0.55	0/341
19	t	0.56	0/252	0.55	0/341
2	B	0.59	0/3951	0.55	0/5379
2	b	0.59	0/3951	0.55	0/5379
20	U	0.44	0/197	0.55	0/264
20	u	0.44	0/197	0.55	0/264
21	W	0.49	0/429	0.60	0/582
21	w	0.49	0/429	0.60	0/582
22	X	0.42	0/250	0.50	0/342
22	x	0.43	0/250	0.50	0/342
23	Z	0.38	0/464	0.53	0/636

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
23	z	0.38	0/464	0.53	0/636
3	C	0.56	0/3589	0.55	0/4891
3	c	0.56	0/3589	0.55	0/4891
4	D	0.62	0/2796	0.56	0/3811
4	d	0.62	0/2796	0.56	0/3811
5	E	0.42	0/654	0.48	0/889
5	e	0.42	0/654	0.48	0/889
6	F	0.42	0/265	0.48	0/358
6	f	0.43	0/265	0.48	0/358
7	G	0.42	0/1713	0.49	0/2333
7	N	0.42	0/1713	0.49	0/2333
7	Y	0.51	0/1713	0.51	0/2333
7	g	0.42	0/1713	0.49	0/2333
7	n	0.41	0/1713	0.49	0/2333
7	y	0.51	0/1713	0.51	0/2333
8	H	0.49	0/444	0.53	0/605
8	h	0.49	0/444	0.53	0/605
9	I	0.62	0/294	0.57	0/397
9	i	0.62	0/294	0.58	0/397
All	All	0.50	0/61090	0.54	4/83100 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	a	0	1
18	S	0	1
18	s	0	1
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	q	42	PRO	CA-C-N	5.67	129.68	117.20
16	Q	42	PRO	CA-C-N	5.67	129.67	117.20
16	Q	42	PRO	C-N-CA	5.03	134.26	121.70
16	q	42	PRO	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	PRO	Peptide
18	S	35	LEU	Peptide
1	a	141	PRO	Peptide
18	s	35	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2614	0	2521	160	0
1	a	2614	0	2521	0	0
2	B	3820	0	3690	207	0
2	b	3820	0	3690	0	0
3	C	3475	0	3416	199	0
3	c	3475	0	3416	0	0
4	D	2703	0	2592	152	0
4	d	2703	0	2592	0	0
5	E	636	0	612	19	0
5	e	636	0	612	0	0
6	F	257	0	267	9	0
6	f	257	0	267	0	0
7	G	1661	0	1592	100	0
7	N	1661	0	1592	90	0
7	Y	1661	0	1592	79	0
7	g	1661	0	1592	0	0
7	n	1661	0	1592	0	0
7	y	1661	0	1592	0	0
8	H	434	0	459	24	0
8	h	434	0	459	0	0
9	I	286	0	295	12	0
9	i	286	0	295	0	0
10	J	247	0	258	9	0
10	j	247	0	258	0	0
11	K	307	0	310	18	0
11	k	307	0	310	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	311	0	299	10	0
12	l	311	0	299	0	0
13	M	258	0	277	10	0
13	m	258	0	277	0	0
14	O	1844	0	1812	122	0
14	o	1844	0	1812	0	0
15	P	1324	0	1283	76	0
15	p	1324	0	1283	0	0
16	Q	1162	0	1190	65	0
16	q	1162	0	1190	0	0
17	R	1806	0	1784	128	0
17	r	1806	0	1784	0	0
18	S	1653	0	1620	124	0
18	s	1653	0	1620	0	0
19	T	245	0	260	9	0
19	t	245	0	260	0	0
20	U	193	0	205	10	0
20	u	193	0	205	0	0
21	W	419	0	401	30	0
21	w	419	0	401	0	0
22	X	246	0	256	7	0
22	x	246	0	256	0	0
23	Z	454	0	479	20	0
23	z	454	0	479	0	0
24	A	10	0	0	2	0
24	a	10	0	0	0	0
25	A	1	0	0	0	0
25	a	1	0	0	0	0
26	A	2	0	0	1	0
26	a	2	0	0	0	0
27	A	239	0	242	34	0
27	B	1040	0	1152	109	0
27	C	829	0	903	73	0
27	D	130	0	144	16	0
27	G	424	0	378	44	0
27	N	424	0	378	31	0
27	R	522	0	456	59	0
27	S	441	0	351	39	0
27	Y	472	0	477	45	0
27	a	239	0	242	0	0
27	b	1040	0	1152	0	0
27	c	829	0	903	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	d	130	0	144	0	0
27	g	424	0	378	0	0
27	n	424	0	378	0	0
27	r	522	0	456	0	0
27	s	441	0	351	0	0
27	y	472	0	477	0	0
28	A	128	0	148	10	0
28	a	128	0	148	0	0
29	A	40	0	56	6	0
29	B	120	0	168	20	0
29	C	160	0	224	31	0
29	D	40	0	56	5	0
29	H	40	0	56	7	0
29	a	40	0	56	0	0
29	b	120	0	168	0	0
29	c	160	0	224	0	0
29	d	40	0	56	0	0
29	h	40	0	56	0	0
30	A	108	0	155	6	0
30	B	54	0	77	3	0
30	a	108	0	154	0	0
30	b	54	0	77	0	0
31	A	48	0	66	8	0
31	B	51	0	72	10	0
31	C	51	0	72	5	0
31	D	46	0	62	3	0
31	Z	51	0	72	6	0
31	a	48	0	66	0	0
31	b	51	0	72	0	0
31	c	51	0	72	0	0
31	d	46	0	62	0	0
31	z	51	0	72	0	0
32	C	179	0	232	31	0
32	H	62	0	82	10	0
32	c	179	0	232	0	0
32	h	62	0	82	0	0
33	D	4	0	0	5	0
33	d	4	0	0	0	0
34	D	55	0	80	9	0
34	d	55	0	80	0	0
35	D	129	0	177	14	0
35	G	49	0	74	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	L	49	0	74	7	0
35	N	49	0	74	7	0
35	R	49	0	74	3	0
35	S	49	0	74	3	0
35	Y	49	0	74	8	0
35	d	129	0	177	0	0
35	g	49	0	74	0	0
35	l	49	0	74	0	0
35	n	49	0	74	0	0
35	r	49	0	74	0	0
35	s	49	0	74	0	0
35	y	49	0	74	0	0
36	F	43	0	30	5	0
36	f	43	0	30	0	0
37	G	314	0	251	38	0
37	N	314	0	251	40	0
37	R	150	0	111	21	0
37	S	201	0	147	13	0
37	Y	330	0	284	30	0
37	g	314	0	251	0	0
37	n	314	0	251	0	0
37	r	150	0	111	0	0
37	s	201	0	147	0	0
37	y	330	0	284	0	0
38	G	84	0	112	16	0
38	N	84	0	112	18	0
38	R	42	0	56	13	0
38	S	84	0	112	19	0
38	Y	84	0	112	17	0
38	g	84	0	112	0	0
38	n	84	0	112	0	0
38	r	42	0	56	0	0
38	s	84	0	112	0	0
38	y	84	0	112	0	0
39	G	44	0	56	8	0
39	N	44	0	56	8	0
39	R	44	0	56	8	0
39	Y	44	0	56	10	0
39	g	44	0	56	0	0
39	n	44	0	56	0	0
39	r	44	0	56	0	0
39	y	44	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	G	44	0	56	3	0
40	N	44	0	56	3	0
40	R	44	0	56	6	0
40	S	44	0	56	5	0
40	Y	44	0	56	5	0
40	g	44	0	56	0	0
40	n	44	0	56	0	0
40	r	44	0	56	0	0
40	s	44	0	56	0	0
40	y	44	0	56	0	0
All	All	75994	0	75847	1874	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 12.

All (1874) 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)
27:G:611:CLA:NB	35:G:2630:LHG:O4	1.78	1.15
1:A:317:TRP:HE3	4:D:180:ARG:HD3	1.26	0.98
1:A:303:ASN:O	3:C:415:ASN:ND2	2.05	0.90
17:R:158:ILE:HD11	40:R:623:NEX:H34	1.53	0.90
2:B:277:GLN:HB3	20:U:24:ARG:HG3	1.55	0.89
2:B:382:PRO:O	2:B:385:ARG:NH2	2.07	0.87
18:S:205:ILE:HG21	27:S:613:CLA:HAC2	1.57	0.86
3:C:345:PRO:HB3	14:O:164:ARG:HE	1.41	0.85
4:D:180:ARG:NH2	4:D:333:ASP:OD1	2.09	0.85
17:R:208:PHE:HA	17:R:211:PHE:HD2	1.42	0.84
15:P:99:SER:H	15:P:106:GLY:H	1.23	0.84
14:O:200:GLN:HE21	14:O:204:GLY:HA2	1.42	0.84
14:O:225:PHE:HB2	14:O:285:LEU:HB2	1.60	0.83
14:O:89:ARG:NH1	14:O:137:GLU:OE2	2.12	0.83
1:A:48:PHE:HE2	34:D:405:PL9:H48	1.43	0.82
2:B:187:VAL:HG13	27:B:602:CLA:HMD3	1.62	0.82
1:A:82:ILE:HD11	1:A:111:PRO:HB2	1.61	0.81
37:N:601:CHL:HHC	37:N:601:CHL:HBB1	1.63	0.81
1:A:317:TRP:CE3	4:D:180:ARG:HD3	2.16	0.80
3:C:78:GLU:HB2	16:Q:33:TYR:HA	1.64	0.80
18:S:99:ASN:ND2	18:S:108:GLU:OE2	2.14	0.79
3:C:332:GLN:HB3	15:P:101:GLY:H	1.47	0.79
3:C:31:THR:HG23	3:C:33:PHE:H	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:404:CL:CL	3:C:354:GLU:N	2.53	0.78
7:G:41:PRO:HB2	7:G:181:ILE:HD12	1.64	0.78
37:N:609:CHL:HBB1	37:Y:601:CHL:H51	1.65	0.78
7:N:94:GLU:H	7:N:103:GLN:HE21	1.32	0.77
3:C:331:ALA:O	14:O:194:TYR:OH	2.02	0.77
1:A:333:GLU:OE2	24:A:401:OEX:O5	2.03	0.77
27:B:613:CLA:H13	27:B:614:CLA:HAB	1.67	0.77
7:G:220:ASN:HB2	27:G:614:CLA:HED3	1.68	0.76
27:G:602:CLA:H2	38:G:1621:LUT:H26	1.68	0.76
17:R:97:LEU:HD23	17:R:172:LEU:HD22	1.68	0.76
3:C:76:VAL:O	3:C:84:GLN:NE2	2.18	0.76
7:G:182:LYS:NZ	35:G:2630:LHG:O5	2.19	0.76
18:S:57:TYR:OH	18:S:191:LYS:NZ	2.16	0.76
39:N:1622:XAT:H393	35:Y:2630:LHG:H101	1.68	0.76
2:B:389:LYS:NZ	15:P:41:GLU:OE2	2.19	0.75
1:A:29:TYR:O	1:A:129:ARG:NH2	2.17	0.75
2:B:385:ARG:HD2	15:P:93:TYR:H	1.51	0.75
4:D:26:ARG:HG3	4:D:28:VAL:H	1.51	0.75
37:N:606:CHL:HBB1	37:N:606:CHL:HHC	1.69	0.74
3:C:148:GLY:O	3:C:156:LYS:NZ	2.21	0.74
7:Y:126:ALA:HB3	37:Y:605:CHL:HMC	1.70	0.74
1:A:64:ARG:HH21	14:O:163:THR:HB	1.53	0.74
3:C:189:TRP:O	16:Q:79:ARG:NH1	2.21	0.74
28:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.70	0.74
2:B:422:ARG:HD3	14:O:262:ARG:HE	1.53	0.74
16:Q:112:PHE:HA	16:Q:115:ILE:HG22	1.70	0.73
16:Q:42:PRO:HB2	16:Q:43:LEU:HB2	1.70	0.73
29:B:618:BCR:HC31	31:B:622:LMG:H291	1.71	0.73
7:Y:94:GLU:H	7:Y:103:GLN:HE21	1.36	0.73
2:B:22:VAL:HG13	27:B:615:CLA:HMB3	1.71	0.72
2:B:260:SER:HG	2:B:262:THR:HG1	1.38	0.72
14:O:296:GLU:HG2	14:O:328:GLN:HG2	1.70	0.72
1:A:259:ILE:HG22	1:A:260:PHE:H	1.55	0.72
1:A:301:ASN:HB3	3:C:407:VAL:HG21	1.72	0.72
27:B:602:CLA:H93	29:H:101:BCR:H402	1.72	0.72
17:R:94:GLU:HA	17:R:172:LEU:HD21	1.70	0.72
18:S:189:GLU:OE1	27:S:610:CLA:NA	2.24	0.71
1:A:153:ALA:HB1	27:A:405:CLA:HED1	1.73	0.71
2:B:53:ASP:OD2	2:B:58:GLN:NE2	2.23	0.71
3:C:45:LEU:HD22	3:C:138:GLU:HB3	1.73	0.71
27:C:504:CLA:H71	32:C:520:DGD:HBW2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:225:ALA:HA	39:Y:1622:XAT:H22	1.72	0.71
14:O:276:VAL:HG22	14:O:311:LEU:HD11	1.73	0.71
15:P:108:VAL:HG23	15:P:109:ALA:H	1.55	0.71
7:G:52:SER:HB3	7:G:58:PHE:HD1	1.56	0.71
7:G:118:LEU:O	7:G:120:HIS:N	2.24	0.71
17:R:229:HIS:ND1	17:R:236:THR:OG1	2.20	0.71
23:Z:26:VAL:HG13	23:Z:36:ASN:HB3	1.72	0.71
32:C:519:DGD:HA31	31:C:521:LMG:H331	1.73	0.71
14:O:178:VAL:HA	14:O:184:VAL:HG22	1.73	0.71
14:O:302:GLN:HG2	14:O:322:GLU:HG2	1.73	0.71
3:C:95:LEU:O	3:C:178:LYS:NZ	2.20	0.70
37:N:608:CHL:HBB1	37:N:608:CHL:HHC	1.72	0.70
18:S:164:LEU:HB3	18:S:165:HIS:HB3	1.72	0.70
7:N:211:ASP:O	7:N:219:ASN:ND2	2.24	0.70
37:S:606:CHL:HHC	37:S:606:CHL:HBB1	1.72	0.70
10:J:7:ARG:HG3	10:J:8:ILE:HD12	1.74	0.70
29:D:404:BCR:H401	10:J:25:VAL:HG22	1.74	0.70
1:A:296:ASN:HB3	3:C:401:LEU:HA	1.73	0.70
1:A:85:THR:HG22	1:A:168:PHE:HB2	1.74	0.70
37:N:607:CHL:H142	37:Y:601:CHL:H18	1.74	0.70
3:C:297:TYR:O	3:C:423:ARG:NH2	2.25	0.70
1:A:195:HIS:HD2	1:A:196:PRO:HD2	1.57	0.70
12:L:30:VAL:O	12:L:34:ASN:ND2	2.25	0.70
37:Y:607:CHL:HBB1	37:Y:607:CHL:HHC	1.74	0.69
14:O:132:LYS:HG3	14:O:133:LYS:H	1.58	0.69
20:U:5:GLY:O	20:U:10:LYS:NZ	2.25	0.69
3:C:261:ARG:NH2	21:W:131:GLU:OE1	2.25	0.69
7:Y:24:TYR:CG	7:Y:46:TRP:HB2	2.28	0.69
3:C:332:GLN:HG3	3:C:336:GLY:HA2	1.72	0.69
7:G:179:LYS:HD3	27:G:612:CLA:HAA2	1.73	0.69
37:R:606:CHL:HMB1	27:R:609:CLA:HBC2	1.74	0.69
2:B:157:HIS:HE1	27:B:607:CLA:NA	1.89	0.69
27:Y:602:CLA:H92	27:Y:603:CLA:HMA1	1.74	0.69
29:D:404:BCR:H14C	6:F:33:PHE:CD2	2.28	0.69
17:R:29:VAL:HG21	17:R:194:GLN:HE21	1.57	0.69
13:M:5:ILE:HG23	13:M:5:ILE:HG23	0.00	0.68
7:Y:21:ARG:NH2	7:Y:36:LEU:O	2.26	0.68
4:D:57:SER:OG	4:D:65:SER:OG	2.08	0.68
1:A:221:SER:HA	4:D:139:ARG:HB2	1.76	0.68
27:G:610:CLA:H2	38:G:1620:LUT:H28	1.75	0.68
37:R:608:CHL:H12	38:R:620:LUT:H383	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:31:SER:OG	13:M:31:SER:OG	0.00	0.68
14:O:164:ARG:HA	21:W:88:ARG:HH22	1.58	0.68
7:Y:52:SER:OG	7:Y:61:ASN:ND2	2.26	0.68
27:Y:602:CLA:HAB	38:Y:1621:LUT:H32	1.76	0.68
15:P:68:LYS:HA	15:P:69:LYS:HB2	1.75	0.68
17:R:96:GLU:OE2	17:R:202:ARG:NE	2.27	0.68
35:D:408:LHG:H101	35:D:408:LHG:H351	1.76	0.68
27:G:602:CLA:HBA1	38:G:1621:LUT:H382	1.76	0.67
17:R:93:ARG:HH12	27:R:602:CLA:HED1	1.58	0.67
7:Y:212:HIS:CG	27:Y:613:CLA:HAA2	2.29	0.67
23:Z:33:TRP:O	23:Z:37:LYS:N	2.27	0.67
4:D:186:GLN:HB2	27:D:402:CLA:HBC1	1.76	0.67
18:S:35:LEU:HD13	18:S:39:LEU:HB3	1.77	0.67
27:B:615:CLA:H102	35:L:101:LHG:H372	1.75	0.67
1:A:82:ILE:HG22	1:A:174:LEU:HB2	1.76	0.67
7:N:99:LYS:HA	37:N:607:CHL:HED2	1.77	0.67
27:B:603:CLA:HBD	27:B:603:CLA:HBA2	1.76	0.67
15:P:30:VAL:HG13	15:P:59:LEU:HD21	1.76	0.67
17:R:191:PRO:O	17:R:194:GLN:HG2	1.95	0.67
18:S:123:THR:HG23	18:S:130:ASN:HD21	1.60	0.67
5:E:19:TYR:O	5:E:23:HIS:ND1	2.24	0.67
14:O:143:VAL:HG22	14:O:319:VAL:HG22	1.77	0.67
3:C:387:TRP:NE1	16:Q:80:LEU:O	2.26	0.67
1:A:196:PRO:HA	1:A:199:MET:HG3	1.77	0.67
1:A:57:PRO:O	14:O:206:ARG:NH1	2.25	0.66
3:C:66:ALA:HB1	11:K:38:MET:HB3	1.78	0.66
18:S:145:LEU:HD22	37:S:606:CHL:HMA2	1.77	0.66
24:A:401:OEX:O4	3:C:357:ARG:NH2	2.28	0.66
2:B:370:LEU:HB2	2:B:379:ALA:HB3	1.76	0.66
4:D:192:THR:HG23	27:D:402:CLA:HBC2	1.78	0.66
37:N:606:CHL:HBA2	37:N:606:CHL:HBD	1.76	0.66
1:A:199:MET:HG2	32:C:520:DGD:HAE2	1.76	0.66
14:O:124:PHE:HE2	14:O:329:LEU:HD12	1.60	0.66
18:S:46:PRO:HB2	18:S:49:LEU:HB2	1.77	0.66
21:W:97:PRO:HG2	21:W:100:LEU:HD12	1.76	0.66
1:A:257:ARG:HH21	4:D:136:VAL:HG22	1.60	0.66
27:S:613:CLA:H2	27:S:614:CLA:HMD1	1.76	0.66
16:Q:138:VAL:O	16:Q:142:ASN:ND2	2.27	0.66
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.78	0.66
15:P:111:ALA:HA	15:P:133:THR:HA	1.78	0.66
2:B:71:ILE:HD13	2:B:96:VAL:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:256:PRO:HA	27:C:506:CLA:HED3	1.78	0.66
1:A:246:TYR:CE2	1:A:248:ILE:HG22	2.31	0.66
1:A:149:ALA:HB2	1:A:280:VAL:HG13	1.78	0.66
7:G:26:GLY:O	7:G:29:SER:OG	2.12	0.66
2:B:227:LYS:O	2:B:230:ARG:NH1	2.29	0.66
3:C:464:GLU:OE2	4:D:248:THR:OG1	2.14	0.66
14:O:241:ASP:OD1	14:O:245:ARG:N	2.29	0.66
17:R:222:PRO:HA	17:R:225:ASN:HD22	1.61	0.66
18:S:234:ILE:HG13	23:Z:60:LEU:HD21	1.77	0.66
27:B:604:CLA:H192	27:B:610:CLA:H91	1.78	0.65
29:B:618:BCR:H322	31:B:622:LMG:H111	1.77	0.65
3:C:110:PRO:HB3	31:Z:101:LMG:H142	1.78	0.65
28:A:408:PHO:H41	30:A:418:SQD:H192	1.79	0.65
4:D:139:ARG:NH2	4:D:141:TYR:OH	2.30	0.65
7:G:21:ARG:NH2	7:G:36:LEU:O	2.29	0.65
18:S:139:VAL:HG22	37:S:607:CHL:HBC1	1.77	0.65
3:C:26:ARG:O	3:C:41:ARG:NH1	2.29	0.65
4:D:19:ASP:OD2	4:D:23:ARG:NH2	2.26	0.65
14:O:173:GLU:N	14:O:190:ASP:O	2.28	0.65
3:C:42:LEU:HD21	27:C:511:CLA:H2A	1.77	0.65
28:A:409:PHO:OBD	4:D:129:GLN:NE2	2.29	0.65
6:F:24:HIS:NE2	36:F:101:HEM:NA	2.45	0.65
2:B:254:GLY:HA3	32:H:102:DGD:HB61	1.78	0.65
17:R:208:PHE:HA	17:R:211:PHE:CD2	2.30	0.65
18:S:127:PHE:HB3	18:S:129:LYS:H	1.61	0.65
2:B:212:ALA:HB2	27:B:610:CLA:HMC3	1.79	0.65
3:C:459:ILE:HG22	3:C:461:ARG:H	1.62	0.65
3:C:409:GLY:HA3	3:C:413:GLU:HG2	1.79	0.65
29:D:404:BCR:H14C	6:F:33:PHE:CE2	2.32	0.65
7:Y:179:LYS:HD3	27:Y:612:CLA:HAA2	1.79	0.65
37:Y:601:CHL:HHC	37:Y:601:CHL:HBB1	1.78	0.65
18:S:210:THR:HG22	18:S:233:VAL:HG11	1.79	0.65
7:N:213:LEU:HD21	27:N:614:CLA:HMC3	1.79	0.64
17:R:127:VAL:O	17:R:131:GLU:HG2	1.97	0.64
3:C:264:LEU:HD11	29:C:515:BCR:H322	1.79	0.64
7:G:63:GLU:HA	7:G:155:LEU:HD21	1.79	0.64
1:A:323:ARG:NH1	15:P:53:PHE:O	2.31	0.64
2:B:469:HIS:HE1	27:B:612:CLA:NA	1.96	0.64
14:O:310:ASP:O	14:O:313:ALA:N	2.25	0.64
1:A:61:ASP:HB2	1:A:63:ILE:HG12	1.78	0.64
18:S:153:ARG:HB2	37:S:608:CHL:CHD	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:O	4:D:255:GLN:NE2	2.28	0.64
16:Q:40:LEU:HD13	16:Q:41:GLN:HG3	1.79	0.64
1:A:246:TYR:OH	33:D:401:BCT:O2	2.16	0.64
15:P:146:VAL:HG12	15:P:180:THR:HG21	1.80	0.64
2:B:383:PHE:O	14:O:250:GLY:N	2.31	0.64
18:S:78:GLU:OE2	18:S:194:ARG:NE	2.30	0.64
27:B:603:CLA:H171	32:H:102:DGD:HAF2	1.80	0.63
18:S:31:ARG:NE	18:S:56:ASP:OD2	2.31	0.63
18:S:53:VAL:HG21	18:S:71:PHE:HE2	1.63	0.63
37:Y:608:CHL:HBB1	37:Y:608:CHL:HHC	1.80	0.63
3:C:38:GLY:HA3	27:C:511:CLA:HMD3	1.80	0.63
3:C:333:GLY:H	15:P:101:GLY:HA2	1.63	0.63
2:B:392:VAL:HG13	2:B:397:VAL:HB	1.81	0.63
35:G:2630:LHG:H102	35:G:2630:LHG:H282	1.80	0.63
4:D:141:TYR:OH	35:D:408:LHG:O4	2.10	0.63
14:O:144:LYS:HA	14:O:156:PHE:HA	1.80	0.63
18:S:157:GLY:HA2	18:S:158:LEU:HB3	1.81	0.63
14:O:235:ARG:HB2	14:O:311:LEU:HD13	1.81	0.63
3:C:86:LEU:HD13	3:C:89:LEU:HD12	1.80	0.63
14:O:291:LYS:O	14:O:295:GLY:N	2.30	0.63
15:P:48:ARG:HH12	15:P:50:GLU:HB3	1.64	0.63
1:A:183:MET:HA	27:A:405:CLA:HMD2	1.80	0.63
7:N:163:PRO:HD2	38:N:1620:LUT:H23	1.81	0.63
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.17	0.63
7:N:63:GLU:HA	7:N:155:LEU:HD21	1.81	0.63
14:O:124:PHE:CE2	14:O:329:LEU:HD12	2.34	0.63
14:O:149:SER:HB3	14:O:154:PRO:HG3	1.81	0.63
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.34	0.63
14:O:146:GLU:HG2	14:O:317:LYS:HE3	1.81	0.63
3:C:387:TRP:HA	3:C:390:ARG:HG3	1.81	0.62
37:S:601:CHL:HHC	37:S:601:CHL:HBB1	1.82	0.62
7:Y:217:VAL:O	7:Y:220:ASN:ND2	2.32	0.62
7:Y:99:LYS:HA	37:Y:607:CHL:HED2	1.81	0.62
1:A:136:ARG:NH1	9:I:27:ASP:OD1	2.29	0.62
27:C:503:CLA:HMA1	31:Z:101:LMG:H191	1.81	0.62
7:G:211:ASP:O	7:G:219:ASN:ND2	2.27	0.62
7:N:182:LYS:HZ1	35:N:2630:LHG:P	2.23	0.62
14:O:211:PHE:HA	14:O:305:GLN:HE22	1.64	0.62
7:G:193:GLY:O	7:G:197:GLN:HB2	2.00	0.62
7:N:118:LEU:HD23	37:N:605:CHL:HED2	1.81	0.62
7:N:135:MET:HA	7:N:138:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:83:ARG:NH2	18:S:189:GLU:OE2	2.32	0.62
2:B:233:ASN:O	2:B:236:THR:HG22	2.00	0.62
2:B:347:ARG:NH1	2:B:400:GLU:OE1	2.32	0.62
18:S:60:ASP:OD1	38:S:1621:LUT:O23	2.18	0.62
7:N:21:ARG:NH2	7:N:36:LEU:O	2.32	0.62
18:S:26:TRP:HZ3	18:S:57:TYR:HH	1.47	0.62
5:E:8:ARG:NH2	5:E:12:ASP:O	2.33	0.62
37:N:608:CHL:H12	38:N:1620:LUT:H383	1.82	0.62
1:A:100:ALA:HB2	21:W:88:ARG:HD3	1.82	0.61
27:B:612:CLA:HMB1	27:B:612:CLA:HBB1	1.82	0.61
7:Y:94:GLU:N	7:Y:103:GLN:HE21	1.97	0.61
7:N:212:HIS:HB2	27:N:613:CLA:HAA2	1.83	0.61
1:A:220:THR:HA	1:A:223:LEU:HD13	1.82	0.61
34:D:405:PL9:H122	35:D:409:LHG:HC92	1.82	0.61
1:A:77:ILE:HD11	19:T:6:TYR:HB3	1.83	0.61
7:Y:182:LYS:NZ	27:Y:611:CLA:O1D	2.27	0.61
29:C:516:BCR:HC7	23:Z:20:LEU:HD11	1.82	0.61
32:C:520:DGD:HAT1	4:D:74:LEU:HD22	1.82	0.61
17:R:195:LEU:HD21	17:R:199:LYS:HE3	1.83	0.61
31:C:521:LMG:H311	31:C:521:LMG:H212	1.83	0.61
1:A:140:ARG:HH21	1:A:142:TRP:HZ3	1.49	0.61
14:O:134:PHE:HB3	14:O:172:ILE:HB	1.83	0.61
14:O:129:TYR:HB2	14:O:176:PHE:HB3	1.83	0.61
2:B:125:ASP:OD2	2:B:128:THR:N	2.34	0.61
3:C:319:VAL:HG22	3:C:384:ILE:HD13	1.83	0.61
3:C:209:ILE:HG23	29:C:515:BCR:H403	1.83	0.61
17:R:181:LEU:HD12	38:R:620:LUT:H222	1.83	0.61
18:S:123:THR:O	18:S:130:ASN:ND2	2.34	0.61
1:A:302:PHE:HE2	4:D:74:LEU:HD12	1.66	0.60
27:G:610:CLA:H2	38:G:1620:LUT:H26	1.83	0.60
37:G:608:CHL:H12	38:G:1620:LUT:H383	1.84	0.60
7:N:180:GLU:HB2	27:N:610:CLA:C1B	2.31	0.60
27:N:614:CLA:O1A	27:N:614:CLA:H3A	2.01	0.60
14:O:175:PRO:HG2	14:O:187:GLU:HB2	1.82	0.60
15:P:41:GLU:HB3	15:P:45:GLN:HE22	1.66	0.60
2:B:311:PHE:O	2:B:317:ASN:ND2	2.35	0.60
14:O:131:ALA:HB2	14:O:186:PHE:HE1	1.67	0.60
27:R:611:CLA:HBC3	35:R:2630:LHG:HC62	1.83	0.60
3:C:346:THR:OG1	3:C:348:GLU:OE1	2.15	0.60
3:C:464:GLU:OE2	4:D:245:SER:OG	2.18	0.60
27:D:403:CLA:HBB1	27:D:403:CLA:HMB1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:16:SER:HB2	23:Z:47:TRP:HE1	1.67	0.60
27:B:613:CLA:H151	27:B:614:CLA:HBB2	1.84	0.60
14:O:143:VAL:HB	14:O:201:LEU:HD21	1.84	0.60
18:S:78:GLU:HB2	27:S:602:CLA:C1B	2.32	0.60
7:G:213:LEU:HD21	27:G:614:CLA:HMC3	1.84	0.60
7:G:215:ASP:OD2	7:G:218:ASN:ND2	2.31	0.60
7:N:70:ARG:NE	7:N:180:GLU:OE2	2.34	0.60
18:S:171:ASP:OD1	38:S:1620:LUT:O23	2.20	0.60
4:D:18:MET:HE1	22:X:106:VAL:HA	1.83	0.60
3:C:132:HIS:CE1	27:C:513:CLA:NA	2.70	0.60
7:N:118:LEU:O	7:N:120:HIS:N	2.35	0.60
7:N:164:LEU:HD12	38:N:1620:LUT:H222	1.82	0.60
2:B:340:TRP:HA	2:B:430:PHE:HD1	1.67	0.60
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.84	0.60
2:B:216:HIS:CE1	27:B:610:CLA:NA	2.70	0.59
4:D:72:ASN:HA	31:D:411:LMG:HC1	1.83	0.59
32:C:519:DGD:HA41	10:J:29:PHE:HD2	1.67	0.59
3:C:377:LEU:HD11	3:C:381:LYS:HE3	1.84	0.59
7:G:24:TYR:CG	7:G:46:TRP:HB2	2.37	0.59
2:B:15:ASP:OD2	12:L:5:ASN:ND2	2.35	0.59
7:N:126:ALA:HB3	37:N:605:CHL:HMC	1.85	0.59
16:Q:33:TYR:HB3	16:Q:35:LYS:HG2	1.84	0.59
17:R:87:PHE:HA	17:R:92:PHE:CE2	2.38	0.59
1:A:106:LEU:HD11	29:A:411:BCR:H402	1.84	0.59
7:Y:24:TYR:CD1	7:Y:46:TRP:HB2	2.37	0.59
3:C:107:ASP:OD2	31:Z:101:LMG:O2	2.20	0.59
1:A:305:SER:HA	10:J:39:SER:HB3	1.85	0.59
27:C:502:CLA:H12	27:C:503:CLA:H42	1.85	0.59
16:Q:43:LEU:HD22	16:Q:45:PRO:HD3	1.84	0.59
2:B:357:ARG:NH1	2:B:358:ARG:O	2.36	0.59
32:C:518:DGD:O4E	32:C:518:DGD:O5E	2.19	0.59
4:D:350:ASN:OD1	4:D:351:ALA:N	2.36	0.59
27:D:403:CLA:H152	22:X:91:ILE:HG22	1.85	0.59
7:Y:63:GLU:HA	7:Y:155:LEU:HD21	1.85	0.59
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.85	0.59
2:B:394:GLN:HE21	15:P:90:LYS:HB2	1.68	0.59
3:C:216:SER:HB3	3:C:221:GLU:OE1	2.02	0.59
7:G:24:TYR:CD1	7:G:46:TRP:HB2	2.37	0.59
14:O:138:PRO:HA	14:O:323:GLY:HA3	1.85	0.59
16:Q:76:ASN:OD1	16:Q:77:ASP:N	2.36	0.59
2:B:46:ASP:HB3	2:B:58:GLN:HE22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:CZ3	27:C:505:CLA:HAA2	2.38	0.58
7:Y:182:LYS:HZ3	27:Y:611:CLA:CGD	2.16	0.58
27:B:604:CLA:H143	27:B:609:CLA:HAC1	1.85	0.58
14:O:238:SER:HB2	15:P:137:ASP:H	1.68	0.58
15:P:35:ASN:N	15:P:50:GLU:O	2.36	0.58
28:A:409:PHO:HBB1	28:A:409:PHO:HMB1	1.86	0.58
27:R:601:CLA:HBC3	27:R:601:CLA:HHD	1.85	0.58
17:R:87:PHE:HA	17:R:92:PHE:HE2	1.69	0.58
1:A:207:GLY:HA3	1:A:278:TRP:NE1	2.19	0.58
2:B:388:SER:O	2:B:394:GLN:NE2	2.27	0.58
3:C:116:VAL:HG11	29:C:514:BCR:HC32	1.86	0.58
2:B:208:LEU:HD12	27:B:603:CLA:HMC1	1.85	0.58
7:G:121:ALA:HA	37:G:605:CHL:C1C	2.34	0.58
14:O:145:ALA:HB2	14:O:157:GLN:HE22	1.69	0.58
18:S:142:GLU:HG2	37:S:606:CHL:CHB	2.34	0.58
3:C:48:LYS:HE2	3:C:138:GLU:HG2	1.85	0.58
1:A:302:PHE:CE2	4:D:74:LEU:HD12	2.39	0.58
17:R:162:ARG:HA	37:R:608:CHL:HBC2	1.85	0.58
1:A:27:ARG:NH1	1:A:27:ARG:O	2.37	0.58
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.39	0.58
2:B:46:ASP:HB3	2:B:58:GLN:NE2	2.18	0.58
2:B:150:CYS:HB2	27:B:604:CLA:HMC3	1.86	0.58
27:C:511:CLA:HBA1	29:C:517:BCR:H271	1.86	0.58
7:G:163:PRO:HD2	38:G:1620:LUT:H23	1.85	0.58
1:A:135:PHE:CZ	9:I:31:ASN:HB3	2.39	0.58
17:R:208:PHE:CZ	39:R:622:XAT:H10	2.39	0.58
7:Y:131:GLN:OE1	37:Y:607:CHL:HMC	2.04	0.58
4:D:149:PRO:HB3	27:D:402:CLA:H41	1.86	0.58
37:N:607:CHL:HBB1	37:N:607:CHL:HHC	1.85	0.58
16:Q:80:LEU:HD12	16:Q:81:ARG:HG3	1.86	0.58
5:E:27:ILE:HG12	36:F:101:HEM:HMC3	1.86	0.57
37:G:606:CHL:HMB1	37:G:609:CHL:HAC1	1.85	0.57
37:R:606:CHL:HBA2	40:R:623:NEX:H403	1.86	0.57
7:Y:139:GLU:HG3	37:Y:609:CHL:C4B	2.34	0.57
1:A:267:ASN:OD1	1:A:269:ARG:N	2.37	0.57
7:N:24:TYR:CD1	7:N:46:TRP:HB2	2.39	0.57
14:O:164:ARG:HA	21:W:88:ARG:NH2	2.19	0.57
16:Q:40:LEU:HB2	16:Q:41:GLN:HG3	1.86	0.57
1:A:63:ILE:HB	3:C:335:THR:HG21	1.86	0.57
4:D:270:PHE:HZ	34:D:405:PL9:H203	1.69	0.57
7:G:180:GLU:HB2	27:G:610:CLA:C1B	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:405:CLA:HMB1	27:A:405:CLA:HBB1	1.86	0.57
1:A:93:PHE:HZ	27:A:410:CLA:HAA1	1.69	0.57
7:G:92:PHE:HE1	7:G:113:LEU:HA	1.69	0.57
7:G:119:VAL:N	37:G:605:CHL:O1D	2.37	0.57
27:N:610:CLA:HBB1	27:N:610:CLA:H51	1.85	0.57
2:B:155:ALA:O	2:B:159:THR:OG1	2.22	0.57
27:B:605:CLA:HBA1	27:B:605:CLA:HBD	1.87	0.57
27:A:410:CLA:H13	27:C:506:CLA:H152	1.86	0.57
3:C:71:GLU:O	3:C:75:PHE:N	2.38	0.57
1:A:63:ILE:HA	3:C:337:LEU:HD13	1.86	0.57
17:R:101:ARG:NE	17:R:197:GLU:OE2	2.38	0.57
7:Y:118:LEU:O	7:Y:120:HIS:N	2.38	0.57
2:B:332:ASN:ND2	31:B:622:LMG:O4	2.38	0.57
7:N:87:ARG:HH21	7:N:207:GLU:HA	1.70	0.57
27:Y:613:CLA:H112	35:Y:2630:LHG:H322	1.86	0.57
2:B:422:ARG:NH2	14:O:252:ASP:OD1	2.38	0.57
17:R:210:GLY:O	17:R:214:GLN:HG2	2.05	0.57
2:B:282:GLN:HE22	20:U:24:ARG:HB2	1.69	0.57
29:B:618:BCR:H282	30:B:621:SQD:H82	1.87	0.57
29:C:516:BCR:H373	11:K:47:LEU:HB3	1.87	0.57
7:G:66:VAL:HB	7:G:155:LEU:HD22	1.87	0.57
14:O:310:ASP:O	14:O:312:GLY:N	2.38	0.57
27:Y:602:CLA:HBA1	38:Y:1621:LUT:H382	1.87	0.57
7:G:162:ASP:OD1	38:G:1620:LUT:O23	2.23	0.56
1:A:341:LEU:HD11	15:P:169:PHE:HZ	1.69	0.56
1:A:140:ARG:NH1	4:D:222:LEU:HD12	2.20	0.56
37:N:601:CHL:HED3	35:N:2630:LHG:H142	1.87	0.56
17:R:92:PHE:HB3	27:R:602:CLA:HHB	1.87	0.56
17:R:211:PHE:CZ	38:R:620:LUT:H8	2.40	0.56
17:R:47:GLN:HB3	17:R:66:ILE:HB	1.88	0.56
7:Y:135:MET:HA	7:Y:138:VAL:HG22	1.86	0.56
39:N:1622:XAT:H22	7:Y:225:ALA:HA	1.87	0.56
1:A:254:TYR:HE2	4:D:142:ASN:HD22	1.53	0.56
3:C:113:VAL:O	3:C:117:LEU:HG	2.05	0.56
3:C:151:TRP:HB2	21:W:137:LEU:HD23	1.87	0.56
18:S:123:THR:HG23	18:S:130:ASN:ND2	2.20	0.56
2:B:112:ILE:HG21	29:B:620:BCR:H272	1.85	0.56
9:I:28:PRO:HB3	21:W:135:LEU:HD12	1.87	0.56
15:P:99:SER:HB2	15:P:108:VAL:H	1.71	0.56
16:Q:78:LEU:HD11	16:Q:115:ILE:HD11	1.87	0.56
40:S:1623:NEX:H192	40:S:1623:NEX:H183	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:92:PHE:CE1	7:Y:113:LEU:HA	2.40	0.56
27:A:410:CLA:HMB1	27:A:410:CLA:HBB1	1.87	0.56
18:S:32:ARG:NH1	35:S:2630:LHG:O1	2.39	0.56
18:S:78:GLU:OE1	27:S:602:CLA:C4A	2.50	0.56
1:A:85:THR:HA	1:A:109:GLY:HA3	1.87	0.56
7:G:52:SER:OG	7:G:61:ASN:ND2	2.36	0.56
17:R:96:GLU:HB2	27:R:602:CLA:C1B	2.36	0.56
3:C:152:LYS:HZ2	21:W:137:LEU:HD11	1.70	0.56
27:A:407:CLA:HED1	4:D:175:VAL:HG22	1.88	0.56
7:N:188:MET:SD	27:N:602:CLA:HBB1	2.45	0.56
17:R:119:ILE:HD13	17:R:127:VAL:HG21	1.87	0.56
7:Y:173:PHE:CE2	7:Y:177:LYS:HE3	2.41	0.56
3:C:271:TYR:CE1	27:C:507:CLA:HAC2	2.41	0.56
4:D:315:TYR:CE2	4:D:319:ILE:HD11	2.41	0.56
27:G:611:CLA:C1B	35:G:2630:LHG:O4	2.53	0.56
15:P:169:PHE:HB2	16:Q:28:ASP:HB3	1.88	0.56
17:R:138:GLN:HE21	37:Y:605:CHL:HHB	148.08	0.56
18:S:122:ASN:HB2	18:S:132:PRO:HB2	1.87	0.56
18:S:202:ALA:O	18:S:206:GLN:HG2	2.06	0.56
3:C:255:LYS:NZ	21:W:132:GLU:OE2	2.39	0.56
7:N:173:PHE:CE2	7:N:177:LYS:HE3	2.41	0.56
15:P:74:PHE:HB2	15:P:127:TYR:HE2	1.71	0.56
27:C:513:CLA:HBB1	27:C:513:CLA:HMB1	1.88	0.56
16:Q:86:ARG:O	16:Q:90:LYS:HG2	2.06	0.56
37:G:601:CHL:HED3	35:G:2630:LHG:H121	1.89	0.55
4:D:13:ASP:OD2	8:H:37:TRP:NE1	2.38	0.55
7:N:145:GLY:HA2	37:N:608:CHL:HAC1	1.88	0.55
17:R:159:GLU:OE1	27:R:609:CLA:NA	2.39	0.55
37:G:601:CHL:H122	35:G:2630:LHG:H212	1.89	0.55
12:L:30:VAL:HG22	19:T:9:LEU:HB3	1.88	0.55
2:B:464:PHE:HD2	27:B:612:CLA:HAC2	1.71	0.55
3:C:141:GLU:OE2	3:C:149:TYR:N	2.39	0.55
4:D:216:ALA:O	4:D:220:ASN:ND2	2.29	0.55
7:G:24:TYR:CE2	7:G:25:LEU:HG	2.42	0.55
27:G:611:CLA:C4B	35:G:2630:LHG:O4	2.53	0.55
7:G:71:TRP:CD1	37:G:609:CHL:HMD3	2.41	0.55
14:O:234:TYR:H	14:O:308:ASP:CG	2.09	0.55
17:R:126:LYS:HB2	37:R:607:CHL:CGD	2.37	0.55
35:D:409:LHG:H302	19:T:17:ILE:HG23	1.87	0.55
7:Y:103:GLN:HE22	27:Y:604:CLA:HED3	1.71	0.55
1:A:43:THR:HG23	29:A:411:BCR:H362	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLU:OE1	2:B:63:ILE:HG12	2.07	0.55
3:C:211:GLY:O	3:C:215:LYS:HG3	2.06	0.55
7:G:97:TRP:HE1	7:G:205:PRO:HD3	1.72	0.55
14:O:159:THR:HG22	14:O:201:LEU:HD23	1.89	0.55
7:Y:136:GLY:HA2	37:Y:609:CHL:HAB	1.88	0.55
1:A:47:VAL:HG13	1:A:115:ILE:HG12	1.89	0.55
27:C:505:CLA:HMB1	27:C:505:CLA:HBB1	1.88	0.55
3:C:59:LEU:HD13	27:C:510:CLA:HMD2	1.87	0.55
21:W:100:LEU:O	21:W:101:SER:OG	2.21	0.55
1:A:202:VAL:HG11	27:A:407:CLA:C3D	2.37	0.55
1:A:47:VAL:HG11	1:A:114:LEU:HD22	1.88	0.55
27:C:503:CLA:H2	27:C:501:CLA:C2D	2.37	0.55
7:G:131:GLN:OE1	37:G:607:CHL:HMC	2.07	0.55
17:R:121:TRP:HE1	17:R:222:PRO:HG2	1.71	0.55
18:S:55:GLY:HA3	18:S:190:ILE:HD11	1.89	0.55
1:A:140:ARG:HH12	4:D:222:LEU:HD12	1.71	0.55
2:B:222:PRO:HG2	2:B:225:LEU:HD12	1.89	0.55
2:B:256:MET:O	2:B:448:ARG:NH1	2.39	0.55
4:D:188:PHE:CD1	4:D:326:ARG:HG2	2.42	0.55
9:I:13:ILE:HD13	21:W:109:LEU:HA	1.89	0.55
37:N:607:CHL:HBC2	7:Y:222:TRP:CH2	2.41	0.55
15:P:34:TRP:HA	15:P:51:ASP:HA	1.89	0.55
18:S:162:ASP:HB2	18:S:164:LEU:HD13	1.88	0.55
18:S:189:GLU:HB2	27:S:610:CLA:C1B	2.37	0.55
2:B:12:VAL:HB	27:B:613:CLA:HMC2	1.88	0.55
4:D:83:ASN:HD22	4:D:336:HIS:CD2	2.25	0.55
7:G:94:GLU:O	7:G:103:GLN:NE2	2.40	0.55
17:R:14:TRP:CD2	17:R:34:PHE:HD1	2.25	0.55
27:S:611:CLA:H3A	27:S:611:CLA:CGA	2.37	0.55
7:Y:180:GLU:OE1	27:Y:610:CLA:C4A	2.54	0.55
3:C:263:ALA:HB2	9:I:24:LEU:HD23	1.89	0.55
3:C:29:GLU:HA	4:D:233:ARG:HH12	1.72	0.55
7:N:70:ARG:NH1	37:N:608:CHL:OBD	2.33	0.55
7:N:71:TRP:CD1	37:N:609:CHL:HMD3	2.42	0.55
17:R:179:ASP:HA	38:R:620:LUT:H24	1.88	0.55
17:R:208:PHE:CD2	39:R:622:XAT:H12	2.42	0.55
18:S:47:GLU:N	18:S:48:TYR:HB2	2.22	0.55
7:N:162:ASP:OD1	38:N:1620:LUT:O23	2.25	0.55
37:S:606:CHL:HBA2	37:S:606:CHL:HBD	1.89	0.55
27:B:609:CLA:H172	27:B:610:CLA:H192	1.89	0.54
29:C:516:BCR:H19C	11:K:51:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:PRO:HD2	10:J:12:ILE:HD12	1.89	0.54
18:S:172:PRO:HD2	38:S:1620:LUT:H23	1.89	0.54
18:S:206:GLN:NE2	38:S:1620:LUT:H42	2.22	0.54
28:A:409:PHO:H3A	27:D:402:CLA:H121	1.89	0.54
2:B:30:VAL:HG11	27:B:613:CLA:H112	1.89	0.54
2:B:245:VAL:HG21	27:B:613:CLA:HED3	1.90	0.54
11:K:28:TYR:O	11:K:31:LEU:HG	2.08	0.54
17:R:127:VAL:HG23	17:R:128:GLU:HG3	1.90	0.54
17:R:214:GLN:HG3	38:R:620:LUT:H42	1.88	0.54
18:S:154:ILE:HD11	27:S:609:CLA:HMA1	1.89	0.54
17:R:179:ASP:OD1	38:R:620:LUT:O23	2.23	0.54
7:Y:104:ILE:HG21	7:Y:124:ILE:HD13	1.88	0.54
3:C:362:ARG:HD2	14:O:101:LEU:HD21	1.89	0.54
14:O:309:THR:HG22	14:O:316:PRO:HD3	1.90	0.54
17:R:195:LEU:O	17:R:198:ILE:HG22	2.07	0.54
7:Y:70:ARG:NE	7:Y:180:GLU:OE2	2.37	0.54
1:A:201:GLY:HA3	1:A:286:THR:HG23	1.90	0.54
2:B:366:PHE:HD2	2:B:425:GLN:HE21	1.55	0.54
2:B:61:PHE:HB2	27:B:608:CLA:HMA3	1.90	0.54
3:C:345:PRO:HB3	14:O:164:ARG:NE	2.19	0.54
4:D:294:ARG:HG3	4:D:296:TYR:HB2	1.88	0.54
4:D:61:HIS:CD2	4:D:79:SER:HB3	2.43	0.54
13:M:28:LYS:HG3	13:M:31:SER:HB3	6.07	0.54
7:N:203:LYS:HB2	7:N:208:ASN:HD21	1.72	0.54
17:R:96:GLU:OE1	27:R:602:CLA:C4A	2.54	0.54
4:D:335:PRO:HB2	5:E:65:LEU:HD22	1.89	0.54
14:O:128:LYS:HG2	14:O:177:GLU:HG2	1.89	0.54
14:O:299:GLY:HA3	14:O:325:TRP:CE2	2.43	0.54
17:R:163:ASN:HD22	27:R:616:CLA:HBC3	1.73	0.54
17:R:214:GLN:OE1	27:R:613:CLA:C4D	2.38	0.54
3:C:450:ALA:O	3:C:454:GLY:N	2.40	0.54
7:G:83:GLU:HB3	7:G:206:LEU:HD12	1.89	0.54
1:A:322:ASN:HD21	15:P:53:PHE:HE1	1.56	0.54
27:S:610:CLA:HBB1	27:S:610:CLA:HMB1	1.89	0.54
2:B:64:PRO:HA	2:B:67:THR:HG22	1.90	0.54
3:C:407:VAL:HG13	3:C:415:ASN:HA	1.90	0.54
27:C:506:CLA:H12	29:C:515:BCR:H323	1.90	0.54
1:A:312:ARG:HA	15:P:33:LYS:HA	1.89	0.54
3:C:368:PRO:HG3	16:Q:79:ARG:HB2	1.90	0.54
7:Y:188:MET:HE3	27:Y:602:CLA:HMC3	1.89	0.54
2:B:30:VAL:HG12	27:B:606:CLA:HHD	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:610:CLA:CBB	38:N:1620:LUT:H32	2.38	0.54
7:N:71:TRP:CE2	37:N:608:CHL:HED2	2.43	0.54
17:R:205:MET:SD	27:R:602:CLA:HMC3	2.48	0.54
31:A:413:LMG:HC61	21:W:99:GLY:HA2	1.90	0.54
27:B:605:CLA:HMD2	27:B:613:CLA:H202	1.90	0.54
27:C:511:CLA:H141	23:Z:20:LEU:HD22	1.89	0.54
8:H:50:PHE:HB2	29:H:101:BCR:C10	2.38	0.54
17:R:31:ASP:HA	27:R:602:CLA:HED2	1.89	0.54
19:T:10:LEU:O	19:T:13:THR:OG1	2.21	0.54
7:G:173:PHE:CE2	7:G:177:LYS:HE3	2.43	0.53
17:R:214:GLN:HE22	27:R:613:CLA:C1A	2.21	0.53
27:R:602:CLA:HAB	39:R:622:XAT:H32	1.89	0.53
27:S:604:CLA:C1C	40:S:1623:NEX:H222	2.38	0.53
1:A:191:ASN:HB2	3:C:411:ALA:HB1	1.91	0.53
7:G:27:PRO:HD2	37:G:601:CHL:HBB1	1.91	0.53
27:N:611:CLA:O1A	27:N:611:CLA:H3A	2.08	0.53
3:C:56:HIS:HB2	27:C:509:CLA:HMB2	1.90	0.53
14:O:235:ARG:HD2	14:O:239:PHE:CG	2.44	0.53
16:Q:80:LEU:HD12	16:Q:81:ARG:H	1.74	0.53
17:R:14:TRP:CD2	17:R:16:PRO:HD3	2.44	0.53
29:C:514:BCR:HC21	23:Z:58:ASN:HD22	1.74	0.53
2:B:355:PHE:N	2:B:371:ILE:O	2.37	0.53
3:C:189:TRP:HZ3	3:C:367:GLU:HG3	1.74	0.53
27:N:611:CLA:O1D	27:N:611:CLA:H2A	2.08	0.53
17:R:204:ALA:O	17:R:208:PHE:N	2.37	0.53
17:R:184:ALA:HB3	27:R:610:CLA:HAA2	1.91	0.53
18:S:94:ILE:HG21	27:S:604:CLA:HAC2	1.90	0.53
7:Y:196:VAL:HB	27:Y:613:CLA:HAC2	1.91	0.53
3:C:350:ILE:HG21	3:C:359:TRP:HB2	1.90	0.53
11:K:35:VAL:HA	11:K:38:MET:HG2	1.91	0.53
37:N:606:CHL:HMB1	37:N:609:CHL:HAC1	1.91	0.53
15:P:161:ALA:HB3	15:P:176:VAL:HG13	1.91	0.53
1:A:43:THR:O	1:A:47:VAL:HG12	2.08	0.53
5:E:41:GLY:O	5:E:51:ARG:NH2	2.42	0.53
7:N:94:GLU:N	7:N:103:GLN:HE21	2.04	0.53
31:D:411:LMG:O6	6:F:41:GLN:NE2	2.40	0.53
2:B:137:LYS:HD2	8:H:26:LEU:O	2.09	0.53
21:W:102:ASN:HB3	21:W:105:LEU:HD13	1.90	0.53
2:B:462:PHE:HE2	27:B:614:CLA:HMB3	1.74	0.53
3:C:321:ASP:OD2	3:C:340:TYR:OH	2.17	0.53
8:H:25:PRO:HG2	17:R:78:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:610:CLA:H2A	27:N:610:CLA:O1D	2.09	0.53
3:C:394:GLU:HB2	16:Q:27:ARG:NE	2.24	0.53
3:C:78:GLU:O	16:Q:34:THR:N	2.42	0.53
17:R:213:VAL:HG12	27:R:613:CLA:HMD3	1.90	0.53
2:B:388:SER:C	2:B:394:GLN:HE22	2.11	0.53
27:N:610:CLA:H2	38:N:1620:LUT:H28	1.91	0.53
16:Q:31:LEU:O	16:Q:37:ARG:NH2	2.42	0.53
18:S:158:LEU:HG	18:S:163:LYS:HG2	1.91	0.53
1:A:64:ARG:HH11	3:C:337:LEU:HD11	1.74	0.52
2:B:45:PHE:HD1	2:B:60:MET:HG3	1.74	0.52
4:D:325:ILE:O	4:D:329:MET:HG2	2.09	0.52
14:O:268:LEU:O	14:O:272:ASN:N	2.40	0.52
1:A:26:ASN:OD1	30:A:418:SQD:O3	2.18	0.52
2:B:120:LEU:HB2	2:B:123:PHE:CE2	2.44	0.52
2:B:105:GLY:HA3	29:B:619:BCR:H282	1.92	0.52
27:C:511:CLA:H161	29:C:517:BCR:H19C	1.91	0.52
7:G:188:MET:SD	27:G:602:CLA:HMC3	2.49	0.52
7:Y:44:TYR:HB2	27:Y:602:CLA:HMD1	1.92	0.52
1:A:290:ILE:HG13	27:A:405:CLA:HED3	1.92	0.52
3:C:457:LYS:HB3	4:D:224:GLU:HG2	1.91	0.52
7:G:138:VAL:O	7:G:142:ARG:HG3	2.09	0.52
7:N:87:ARG:NH2	7:N:207:GLU:HA	2.24	0.52
27:R:609:CLA:HMA2	27:R:616:CLA:HMD2	1.90	0.52
7:Y:164:LEU:HD12	38:Y:1620:LUT:H222	1.92	0.52
1:A:199:MET:CG	32:C:520:DGD:HA92	2.39	0.52
2:B:394:GLN:NE2	15:P:90:LYS:HB2	2.24	0.52
3:C:466:VAL:HG21	4:D:248:THR:HG23	1.92	0.52
4:D:182:ILE:HA	27:D:402:CLA:HMD2	1.92	0.52
37:G:601:CHL:HMA1	39:G:1622:XAT:H403	1.92	0.52
31:B:622:LMG:O10	13:M:4:ASN:ND2	2.43	0.52
7:N:131:GLN:OE1	37:N:607:CHL:HMC	2.10	0.52
14:O:237:SER:HA	14:O:276:VAL:HG21	1.92	0.52
18:S:142:GLU:OE2	37:S:607:CHL:HMC	2.09	0.52
27:B:609:CLA:H62	27:B:610:CLA:H121	1.92	0.52
31:B:622:LMG:H351	13:M:10:ALA:HB1	1.91	0.52
5:E:8:ARG:HE	5:E:12:ASP:HB3	1.75	0.52
14:O:119:VAL:HB	14:O:290:SER:O	2.10	0.52
18:S:76:ALA:O	18:S:80:ILE:HG12	2.10	0.52
20:U:5:GLY:HA3	20:U:28:LYS:HA	1.92	0.52
7:Y:73:MET:SD	27:Y:610:CLA:HAB	2.50	0.52
1:A:131:TRP:CZ2	3:C:449:ARG:HG2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:ARG:HD3	14:O:262:ARG:NE	2.23	0.52
27:B:615:CLA:H2	30:B:621:SQD:H121	1.92	0.52
29:C:517:BCR:H312	11:K:31:LEU:HD22	1.92	0.52
7:N:16:TRP:HZ3	7:N:44:TYR:HH	2.67	0.52
16:Q:80:LEU:HD12	16:Q:81:ARG:N	2.25	0.52
9:I:9:TYR:OH	21:W:99:GLY:HA3	2.10	0.52
1:A:36:LEU:HD22	1:A:125:CYS:SG	2.50	0.52
1:A:32:TRP:O	1:A:35:VAL:HG22	2.10	0.52
7:G:221:ALA:N	27:G:613:CLA:O1A	2.43	0.52
14:O:245:ARG:HD2	14:O:272:ASN:HA	1.91	0.52
14:O:310:ASP:HB3	14:O:313:ALA:HB3	1.92	0.52
17:R:102:TRP:CE2	37:R:608:CHL:HED2	2.45	0.52
18:S:162:ASP:O	18:S:164:LEU:HA	2.10	0.52
27:C:511:CLA:H8	23:Z:24:PRO:HB3	1.92	0.52
7:N:92:PHE:HE1	7:N:113:LEU:HA	1.75	0.52
14:O:241:ASP:OD2	14:O:245:ARG:HB2	2.10	0.52
21:W:107:TRP:HH2	7:Y:84:LEU:HD21	1.75	0.52
7:Y:71:TRP:CD1	37:Y:609:CHL:HMD3	2.45	0.52
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.91	0.52
2:B:458:PHE:CE2	31:B:622:LMG:H212	2.45	0.52
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.92	0.52
39:N:1622:XAT:H363	35:Y:2630:LHG:HC41	1.92	0.52
14:O:257:LEU:O	14:O:262:ARG:HG2	2.10	0.52
17:R:159:GLU:OE1	17:R:162:ARG:NH2	2.43	0.52
3:C:119:LEU:O	3:C:122:SER:OG	2.20	0.52
32:C:520:DGD:HAW2	4:D:74:LEU:CD2	2.40	0.52
15:P:74:PHE:HE2	15:P:156:LEU:HD21	1.75	0.52
16:Q:79:ARG:O	16:Q:83:SER:HB3	2.10	0.52
3:C:178:LYS:NZ	3:C:184:GLY:O	2.43	0.51
14:O:235:ARG:HD2	14:O:239:PHE:CD2	2.45	0.51
15:P:47:LEU:HB3	15:P:61:VAL:HB	1.93	0.51
16:Q:42:PRO:CB	16:Q:43:LEU:HB2	2.39	0.51
14:O:93:ASP:OD1	16:Q:68:ARG:NH2	2.43	0.51
17:R:12:PRO:N	17:R:15:TYR:HH	2.08	0.51
29:B:619:BCR:H333	31:B:622:LMG:H382	1.93	0.51
27:C:504:CLA:H72	32:C:519:DGD:HB1	1.92	0.51
3:C:73:ALA:HA	11:K:24:LEU:HG	1.92	0.51
7:N:24:TYR:CE2	7:N:25:LEU:HG	2.45	0.51
14:O:211:PHE:HD1	14:O:321:ILE:HD13	1.74	0.51
15:P:31:PRO:HD3	15:P:179:ALA:HB2	1.92	0.51
16:Q:22:ASN:O	16:Q:26:ALA:N	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:42:PRO:HB2	16:Q:43:LEU:CB	2.40	0.51
17:R:100:GLY:HA3	17:R:201:ALA:HB1	1.92	0.51
23:Z:12:LEU:HD13	23:Z:50:LEU:HB2	1.92	0.51
1:A:199:MET:SD	32:C:520:DGD:HA92	2.50	0.51
29:C:517:BCR:H313	11:K:31:LEU:HD13	1.93	0.51
37:N:609:CHL:HAA2	7:Y:48:THR:HG21	1.91	0.51
14:O:144:LYS:HB2	14:O:156:PHE:HB3	1.93	0.51
17:R:133:SER:HB2	37:R:606:CHL:HMD3	1.92	0.51
18:S:83:ARG:HD3	27:S:610:CLA:HAC2	1.92	0.51
7:Y:119:VAL:N	37:Y:605:CHL:O1D	2.40	0.51
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.92	0.51
1:A:197:PHE:CZ	32:C:520:DGD:HBH1	2.46	0.51
7:G:71:TRP:CE2	37:G:608:CHL:HED2	2.46	0.51
37:N:601:CHL:HHD	35:N:2630:LHG:HC41	1.92	0.51
1:A:340:PRO:HB2	15:P:166:LYS:HB2	1.92	0.51
4:D:48:TRP:NE1	4:D:173:PHE:O	2.28	0.51
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.46	0.51
7:N:220:ASN:OD1	7:N:223:ASN:N	2.44	0.51
17:R:158:ILE:HD13	37:R:608:CHL:HMA1	1.93	0.51
27:A:406:CLA:H203	28:A:408:PHO:H101	1.93	0.51
27:B:604:CLA:H192	27:B:610:CLA:H112	1.93	0.51
7:G:119:VAL:HA	37:G:605:CHL:C4D	2.40	0.51
14:O:176:PHE:CZ	14:O:184:VAL:HG11	2.46	0.51
15:P:71:ILE:HD12	15:P:150:THR:HA	1.93	0.51
17:R:112:THR:HG21	27:R:604:CLA:HAC2	1.92	0.51
18:S:189:GLU:OE1	27:S:610:CLA:C4A	2.59	0.51
2:B:472:ARG:HA	2:B:479:PHE:CE2	2.46	0.51
29:D:404:BCR:H16C	6:F:33:PHE:HD2	1.76	0.51
17:R:101:ARG:HA	17:R:104:MET:HE3	2.91	0.51
7:Y:27:PRO:HD2	37:Y:601:CHL:HBB1	1.93	0.51
37:Y:601:CHL:HMA3	35:Y:2630:LHG:H121	1.93	0.51
39:G:1622:XAT:H10	35:G:2630:LHG:H212	1.93	0.51
37:G:601:CHL:HAC2	35:G:2630:LHG:HC41	1.93	0.51
14:O:184:VAL:HB	14:O:225:PHE:CE1	2.46	0.51
3:C:338:GLY:HA2	14:O:194:TYR:OH	2.11	0.51
17:R:39:LEU:HD13	27:R:602:CLA:H42	1.93	0.51
18:S:119:LEU:HD22	37:S:607:CHL:HMD1	1.93	0.51
21:W:121:PHE:CE2	27:Y:612:CLA:H11	2.46	0.51
2:B:157:HIS:HE1	27:B:607:CLA:C1A	2.24	0.51
2:B:121:GLU:OE1	8:H:14:PRO:HB2	2.11	0.51
18:S:188:LYS:HD3	27:S:612:CLA:HAA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:618:BCR:H383	30:B:621:SQD:H101	1.93	0.51
3:C:290:VAL:O	3:C:423:ARG:NH1	2.43	0.51
3:C:443:TRP:HH2	35:D:410:LHG:HC61	1.76	0.51
7:G:70:ARG:NE	7:G:180:GLU:OE2	2.43	0.51
15:P:103:PHE:CE2	15:P:136:ALA:HB2	2.46	0.51
17:R:202:ARG:HH22	27:R:602:CLA:CED	2.23	0.51
18:S:49:LEU:HD21	27:S:602:CLA:HBD	1.93	0.51
3:C:368:PRO:O	16:Q:76:ASN:HB2	2.11	0.50
3:C:456:GLU:N	3:C:456:GLU:OE1	2.38	0.50
27:C:506:CLA:HMB1	27:C:506:CLA:HBB1	1.93	0.50
36:F:101:HEM:HBC2	36:F:101:HEM:HMC1	1.93	0.50
14:O:193:ASP:OD2	14:O:214:LYS:HG2	2.11	0.50
7:Y:71:TRP:CE2	37:Y:608:CHL:HED2	2.47	0.50
1:A:82:ILE:CG2	1:A:174:LEU:HB2	2.41	0.50
37:G:607:CHL:H43	7:N:230:PRO:HB3	1.93	0.50
7:G:73:MET:HE3	27:G:610:CLA:HMC3	1.97	0.50
11:K:42:PRO:HA	11:K:45:PHE:HD2	1.76	0.50
17:R:185:SER:HB2	17:R:186:ASP:HB3	1.93	0.50
23:Z:15:THR:HA	23:Z:18:ILE:HD12	1.93	0.50
2:B:323:GLY:N	2:B:326:ARG:HD2	2.27	0.50
27:B:606:CLA:H193	27:B:610:CLA:HBB2	1.93	0.50
2:B:96:VAL:HG11	27:B:606:CLA:HMA3	1.92	0.50
3:C:279:LEU:HD11	27:C:507:CLA:HBA1	1.92	0.50
29:C:514:BCR:HC21	23:Z:58:ASN:ND2	2.27	0.50
7:N:136:GLY:HA2	37:N:609:CHL:HAB	1.93	0.50
15:P:47:LEU:HD11	15:P:49:TYR:CE2	2.46	0.50
18:S:206:GLN:OE1	27:S:613:CLA:C4D	2.47	0.50
39:N:1622:XAT:H221	35:Y:2630:LHG:HC32	1.93	0.50
1:A:121:LEU:HD21	27:A:410:CLA:HMB3	1.93	0.50
2:B:71:ILE:HG13	27:B:607:CLA:HMA2	1.94	0.50
3:C:80:PRO:HD2	3:C:83:GLU:OE1	2.11	0.50
11:K:39:PRO:O	11:K:42:PRO:HD2	2.11	0.50
17:R:155:ILE:HG13	37:R:606:CHL:HMB3	1.93	0.50
1:A:82:ILE:HD13	1:A:115:ILE:HD12	1.93	0.50
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.47	0.50
2:B:247:PHE:CE1	27:B:603:CLA:H8	2.46	0.50
14:O:122:PHE:CZ	14:O:124:PHE:HB2	2.46	0.50
17:R:163:ASN:OD1	27:R:616:CLA:HMD3	2.12	0.50
18:S:150:GLU:O	18:S:153:ARG:HG2	2.12	0.50
7:G:46:TRP:O	38:G:1621:LUT:H24	2.11	0.50
18:S:62:PHE:HD2	38:S:1621:LUT:H222	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.42	0.50
1:A:217:SER:HB2	4:D:142:ASN:HA	1.94	0.50
1:A:264:SER:OG	1:A:265:PHE:N	2.44	0.50
2:B:475:PHE:O	2:B:478:VAL:HG22	2.12	0.50
2:B:474:LEU:HD11	27:B:609:CLA:HAA2	1.94	0.50
27:C:510:CLA:HMB1	27:C:510:CLA:HBB1	1.93	0.50
12:L:26:PHE:O	12:L:30:VAL:HG23	2.12	0.50
7:Y:173:PHE:CZ	7:Y:177:LYS:HE3	2.47	0.50
37:Y:601:CHL:H43	37:Y:601:CHL:HMA2	1.94	0.50
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.94	0.50
1:A:42:LEU:HB3	29:A:411:BCR:H353	1.94	0.50
2:B:251:VAL:HG22	27:B:603:CLA:H92	1.94	0.50
27:B:616:CLA:H71	27:B:617:CLA:H162	1.94	0.50
1:A:48:PHE:CE2	34:D:405:PL9:H48	2.35	0.50
7:N:121:ALA:HA	37:N:605:CHL:CHC	2.42	0.50
2:B:19:LEU:HD11	2:B:23:HIS:CE1	2.47	0.50
2:B:462:PHE:CE2	27:B:614:CLA:HMB3	2.46	0.50
17:R:28:LEU:HB3	17:R:93:ARG:HH11	1.77	0.50
14:O:131:ALA:N	14:O:174:GLY:O	2.44	0.49
15:P:126:TYR:CD1	15:P:150:THR:HB	2.47	0.49
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.93	0.49
2:B:204:ALA:O	2:B:207:THR:OG1	2.21	0.49
7:G:63:GLU:O	7:G:67:ILE:HG12	2.12	0.49
3:C:130:ILE:HD12	23:Z:27:PHE:HE2	1.77	0.49
3:C:28:GLN:HE21	4:D:230:ASN:ND2	2.11	0.49
4:D:227:ASP:OD2	4:D:233:ARG:NH1	2.45	0.49
4:D:322:ASN:O	4:D:326:ARG:HG3	2.12	0.49
36:F:101:HEM:HBB2	36:F:101:HEM:HMB1	1.95	0.49
7:G:118:LEU:HD23	37:G:605:CHL:HED2	1.94	0.49
34:D:405:PL9:H472	19:T:10:LEU:HD22	1.94	0.49
1:A:341:LEU:HB3	1:A:343:LEU:HG	1.94	0.49
27:B:608:CLA:C4A	27:B:608:CLA:HBA2	2.43	0.49
3:C:430:HIS:CD2	27:C:502:CLA:ND	2.80	0.49
30:A:412:SQD:H301	29:C:516:BCR:H291	1.95	0.49
7:G:96:VAL:HG12	7:G:99:LYS:H	1.78	0.49
12:L:26:PHE:CD2	19:T:16:ILE:HD11	2.47	0.49
7:N:189:PHE:CD1	27:N:602:CLA:H201	2.47	0.49
16:Q:63:LYS:HB2	16:Q:134:TYR:CZ	2.47	0.49
7:Y:211:ASP:O	7:Y:219:ASN:ND2	2.42	0.49
7:G:175:GLU:HG3	27:G:611:CLA:HED1	1.95	0.49
27:G:604:CLA:HMB3	37:G:606:CHL:HBB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:222:PRO:HA	14:O:225:PHE:CE1	2.48	0.49
15:P:49:TYR:HB2	15:P:59:LEU:HG	1.95	0.49
17:R:211:PHE:HZ	38:R:620:LUT:H8	1.78	0.49
18:S:111:TRP:O	18:S:114:THR:HG22	2.12	0.49
7:Y:180:GLU:HB2	27:Y:610:CLA:C1B	2.42	0.49
1:A:56:PRO:HA	1:A:73:TYR:CE2	2.48	0.49
2:B:366:PHE:O	2:B:425:GLN:NE2	2.30	0.49
4:D:94:GLY:O	4:D:98:GLN:N	2.41	0.49
7:G:44:TYR:CD2	37:G:601:CHL:HMD2	2.47	0.49
12:L:13:LEU:HA	35:L:101:LHG:HC11	1.94	0.49
7:N:24:TYR:CE1	7:N:46:TRP:HB2	2.48	0.49
37:R:608:CHL:HHC	37:R:608:CHL:HBB1	1.94	0.49
2:B:18:ARG:NH1	12:L:5:ASN:HD22	2.11	0.49
1:A:135:PHE:CE1	3:C:449:ARG:HG3	2.48	0.49
2:B:475:PHE:HD2	4:D:140:PRO:HD3	1.77	0.49
35:D:409:LHG:H192	19:T:17:ILE:HD11	1.95	0.49
14:O:162:MET:HE3	14:O:200:GLN:HB2	1.93	0.49
17:R:163:ASN:O	17:R:171:ARG:NH2	2.46	0.49
17:R:197:GLU:OE1	27:R:610:CLA:NA	2.46	0.49
18:S:165:HIS:CD2	18:S:186:LYS:HE2	2.48	0.49
3:C:348:GLU:OE1	3:C:348:GLU:N	2.42	0.49
37:N:607:CHL:H142	37:Y:601:CHL:H161	1.95	0.49
14:O:143:VAL:HG21	14:O:207:VAL:HG11	1.95	0.49
31:A:413:LMG:H321	31:A:413:LMG:H292	1.59	0.49
2:B:173:GLY:HA3	2:B:265:ILE:HD11	1.95	0.49
5:E:26:THR:O	5:E:29:SER:OG	2.22	0.49
7:G:69:CYS:HB3	7:G:184:GLY:HA3	1.95	0.49
12:L:26:PHE:HE1	13:M:15:ILE:HG23	1.78	0.49
16:Q:40:LEU:HB2	16:Q:41:GLN:CG	2.42	0.49
21:W:121:PHE:CD2	27:Y:612:CLA:H42	2.48	0.49
7:Y:73:MET:HE3	27:Y:610:CLA:HMC3	1.96	0.49
2:B:167:TRP:CD1	2:B:264:PRO:HG2	2.47	0.49
3:C:213:LEU:O	3:C:223:TRP:NE1	2.46	0.49
3:C:319:VAL:O	3:C:323:ARG:HG2	2.13	0.49
37:N:601:CHL:C1D	35:N:2630:LHG:HC82	2.42	0.49
14:O:96:GLN:OE1	16:Q:68:ARG:NE	2.32	0.49
15:P:17:GLU:HG3	15:P:18:PHE:CD2	2.48	0.49
16:Q:19:GLY:HA2	16:Q:20:THR:HA	1.54	0.49
18:S:66:LYS:HG3	18:S:67:LYS:H	1.78	0.49
2:B:390:TYR:HB2	4:D:344:GLU:OE2	2.13	0.48
3:C:408:GLY:HA3	3:C:419:TYR:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:SER:OG	4:D:211:CYS:HB2	2.13	0.48
4:D:236:ASN:O	4:D:239:GLN:HG2	2.13	0.48
4:D:56:THR:HB	5:E:49:SER:HA	1.95	0.48
7:G:44:TYR:N	27:G:602:CLA:OBD	2.46	0.48
7:N:178:VAL:O	7:N:181:ILE:HG22	2.13	0.48
27:N:613:CLA:H2	27:N:614:CLA:HMD1	1.95	0.48
14:O:255:VAL:HG13	14:O:262:ARG:HD3	1.95	0.48
15:P:130:THR:HG22	15:P:146:VAL:HG13	1.95	0.48
18:S:112:PHE:CE2	18:S:113:LYS:HE2	2.48	0.48
18:S:26:TRP:HZ2	27:S:611:CLA:HMA3	1.78	0.48
7:Y:163:PRO:HD2	38:Y:1620:LUT:H23	1.95	0.48
3:C:130:ILE:HD12	23:Z:27:PHE:CE2	2.48	0.48
27:G:610:CLA:O1D	27:G:610:CLA:H2A	2.14	0.48
7:G:65:GLU:OE2	7:G:185:ARG:NE	2.46	0.48
7:N:73:MET:HE3	27:N:610:CLA:HMC3	1.95	0.48
14:O:245:ARG:HA	14:O:251:TYR:O	2.13	0.48
17:R:223:LEU:O	17:R:227:VAL:HG23	2.13	0.48
7:Y:15:PRO:HG2	7:Y:16:TRP:CD1	2.48	0.48
27:B:605:CLA:CHA	27:B:605:CLA:HBA1	2.43	0.48
3:C:61:VAL:HG12	3:C:118:HIS:O	2.13	0.48
3:C:343:ARG:NH1	3:C:347:GLY:O	2.45	0.48
27:C:505:CLA:HMD3	27:C:507:CLA:HAB	1.95	0.48
8:H:17:THR:O	8:H:21:ALA:N	2.45	0.48
35:N:2630:LHG:H211	39:Y:1622:XAT:H10	1.95	0.48
16:Q:22:ASN:HA	16:Q:25:GLN:HB3	1.96	0.48
16:Q:59:ILE:O	16:Q:62:VAL:HG22	2.13	0.48
18:S:156:ASN:O	18:S:158:LEU:HB3	2.13	0.48
7:G:222:TRP:CH2	37:Y:607:CHL:HBC2	2.48	0.48
27:Y:611:CLA:NA	35:Y:2630:LHG:O4	2.46	0.48
1:A:187:GLN:NE2	1:A:191:ASN:HA	2.28	0.48
27:A:407:CLA:O2D	32:C:520:DGD:HAH2	2.13	0.48
27:B:608:CLA:HBB1	27:B:608:CLA:HMB1	1.96	0.48
2:B:61:PHE:CE1	27:B:608:CLA:HMB3	2.48	0.48
2:B:475:PHE:CE1	4:D:134:ARG:HB2	2.49	0.48
37:G:601:CHL:HBA2	37:Y:609:CHL:HBA1	1.96	0.48
27:G:610:CLA:CHA	27:G:610:CLA:HBA1	2.40	0.48
27:G:610:CLA:HBB1	27:G:610:CLA:HMB1	1.96	0.48
4:D:306:ALA:HA	14:O:243:LYS:HG3	1.95	0.48
15:P:74:PHE:CE2	15:P:156:LEU:HD21	2.49	0.48
2:B:383:PHE:CG	4:D:347:PRO:HA	2.49	0.48
2:B:383:PHE:HD1	14:O:251:TYR:CE1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:ARG:NH1	14:O:260:GLY:HA2	2.29	0.48
27:B:607:CLA:H102	27:B:607:CLA:H61	1.56	0.48
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.95	0.48
2:B:254:GLY:HA2	32:H:102:DGD:HBW1	1.94	0.48
7:N:185:ARG:HA	7:N:188:MET:HE2	1.94	0.48
14:O:116:GLU:HA	14:O:117:GLY:HA2	1.51	0.48
21:W:129:GLU:HB3	21:W:130:ASP:HB2	1.95	0.48
7:Y:24:TYR:CE2	7:Y:25:LEU:HG	2.49	0.48
2:B:383:PHE:CD2	4:D:347:PRO:HA	2.49	0.48
37:G:601:CHL:HHC	37:G:601:CHL:HBB1	1.96	0.48
7:N:209:LEU:HA	27:N:613:CLA:HMA2	1.95	0.48
14:O:157:GLN:HE21	14:O:201:LEU:HD22	1.79	0.48
35:N:2630:LHG:HC81	39:Y:1622:XAT:H361	1.96	0.48
1:A:207:GLY:HA3	1:A:278:TRP:HE1	1.78	0.48
2:B:345:ILE:HD12	2:B:402:TYR:CE2	2.49	0.48
2:B:39:LEU:HG	2:B:97:ALA:HB1	1.96	0.48
7:G:54:ASP:O	7:G:58:PHE:N	2.44	0.48
15:P:104:ASP:OD1	15:P:105:SER:N	2.45	0.48
16:Q:73:SER:HA	16:Q:76:ASN:ND2	2.29	0.48
38:S:1620:LUT:H401	38:S:1620:LUT:H35	1.70	0.48
18:S:114:THR:HG21	38:S:1621:LUT:O3	2.14	0.48
18:S:165:HIS:HE1	27:S:610:CLA:HMA3	1.79	0.48
1:A:197:PHE:HB3	1:A:285:PHE:O	2.13	0.48
7:G:44:TYR:HB2	27:G:602:CLA:HMD1	1.96	0.48
8:H:65:VAL:HG12	8:H:67:LEU:HG	1.95	0.48
27:N:610:CLA:HMB1	27:N:612:CLA:HAA1	1.96	0.48
3:C:327:ASN:HD21	14:O:190:ASP:HB3	1.79	0.48
14:O:218:ALA:HB1	14:O:225:PHE:HB3	1.96	0.48
14:O:255:VAL:HA	14:O:262:ARG:HD3	1.96	0.48
17:R:47:GLN:HB3	17:R:67:GLY:H	1.79	0.48
1:A:230:ASN:O	2:B:3:LEU:HD23	2.14	0.48
1:A:63:ILE:HG21	1:A:336:ALA:HA	1.96	0.48
29:A:411:BCR:H15C	29:A:411:BCR:H351	1.71	0.48
2:B:255:THR:HG21	27:B:603:CLA:HED1	1.96	0.48
2:B:36:SER:OG	29:B:619:BCR:H362	2.14	0.48
3:C:280:SER:OG	3:C:438:PHE:HB2	2.14	0.48
27:C:504:CLA:C3D	32:C:519:DGD:HB21	2.44	0.48
4:D:229:ALA:O	35:D:410:LHG:O1	2.25	0.48
7:G:180:GLU:OE1	27:G:610:CLA:C4A	2.59	0.48
9:I:5:LYS:HE2	9:I:9:TYR:HE2	1.79	0.48
14:O:245:ARG:NE	14:O:271:GLU:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:GLY:HA2	16:Q:82:ALA:O	2.14	0.48
27:R:601:CLA:HBC2	35:R:2630:LHG:O7	2.14	0.48
17:R:29:VAL:HG21	17:R:194:GLN:NE2	2.27	0.48
2:B:166:ILE:HG22	2:B:167:TRP:O	2.14	0.48
2:B:371:ILE:HG22	2:B:372:ASP:O	2.14	0.48
3:C:132:HIS:HE1	27:C:513:CLA:NA	2.11	0.48
40:G:1623:NEX:H191	40:G:1623:NEX:H11	1.71	0.48
8:H:20:GLY:O	8:H:24:LYS:HG3	2.14	0.48
13:M:31:SER:HG	13:M:31:SER:HG	0.00	0.48
27:Y:603:CLA:C3D	37:Y:609:CHL:H2	2.44	0.48
2:B:16:PRO:HB2	2:B:123:PHE:CD1	2.49	0.47
2:B:364:GLU:HG2	4:D:296:TYR:CE2	2.49	0.47
2:B:365:THR:OG1	4:D:326:ARG:NH2	2.34	0.47
1:A:224:ILE:HG23	2:B:484:PRO:HA	1.96	0.47
3:C:186:TYR:HA	3:C:196:VAL:HA	1.96	0.47
3:C:344:SER:OG	3:C:348:GLU:OE1	2.31	0.47
4:D:342:PRO:O	4:D:345:VAL:HG22	2.14	0.47
5:E:60:ARG:NH1	5:E:62:GLY:O	2.47	0.47
7:G:74:LEU:HD11	27:G:610:CLA:HBC1	1.96	0.47
27:S:610:CLA:HMB1	27:S:612:CLA:HAA1	1.96	0.47
27:B:613:CLA:HMB1	27:B:613:CLA:HBB1	1.95	0.47
3:C:288:CYS:SG	32:C:518:DGD:HB22	2.54	0.47
3:C:452:ALA:HB1	21:W:135:LEU:HB3	1.96	0.47
2:B:442:VAL:HG21	4:D:299:VAL:HG22	1.97	0.47
7:G:16:TRP:HZ2	27:G:611:CLA:HMA3	1.79	0.47
14:O:98:LYS:O	16:Q:72:PRO:HG3	2.14	0.47
29:C:516:BCR:C7	23:Z:20:LEU:HD11	2.44	0.47
2:B:311:PHE:HA	2:B:430:PHE:HZ	1.79	0.47
27:B:603:CLA:H42	32:H:102:DGD:HB22	1.96	0.47
3:C:444:HIS:CE1	27:C:508:CLA:NA	2.82	0.47
30:A:412:SQD:H322	29:C:516:BCR:H391	1.96	0.47
4:D:273:PHE:HZ	35:D:408:LHG:H122	1.78	0.47
4:D:70:GLY:HA3	10:J:36:LEU:HB3	1.96	0.47
15:P:136:ALA:HA	15:P:137:ASP:OD1	2.14	0.47
3:C:182:PHE:CZ	27:S:614:CLA:HBB1	2.50	0.47
1:A:140:ARG:NH1	4:D:231:THR:HG21	2.30	0.47
1:A:246:TYR:CE1	33:D:401:BCT:O1	2.68	0.47
28:A:408:PHO:HBC2	28:A:408:PHO:HHD	1.96	0.47
2:B:454:GLY:HA2	31:B:622:LMG:H211	1.96	0.47
5:E:23:HIS:NE2	36:F:101:HEM:ND	2.63	0.47
27:G:611:CLA:HBA1	27:G:611:CLA:H3A	1.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:81:PHE:HB3	7:G:82:PRO:HD3	1.96	0.47
9:I:19:PHE:CE1	9:I:23:PHE:HE2	2.32	0.47
10:J:24:LEU:O	10:J:27:ILE:HG22	2.15	0.47
7:N:52:SER:HB3	7:N:58:PHE:HD1	1.80	0.47
14:O:132:LYS:HG3	14:O:133:LYS:N	2.29	0.47
15:P:97:THR:OG1	15:P:98:ASP:HB3	2.15	0.47
3:C:391:ARG:NE	16:Q:84:TYR:OH	2.48	0.47
1:A:321:ILE:HG12	4:D:180:ARG:HB3	1.97	0.47
14:O:237:SER:HB3	15:P:98:ASP:O	2.14	0.47
15:P:152:LYS:HD2	15:P:185:VAL:HG11	1.97	0.47
15:P:45:GLN:HA	15:P:62:LEU:HA	1.96	0.47
3:C:101:PRO:HB3	16:Q:86:ARG:HB3	1.97	0.47
17:R:188:GLU:O	17:R:190:LYS:N	2.48	0.47
37:Y:607:CHL:HBB2	37:Y:609:CHL:HBC1	1.97	0.47
23:Z:3:ILE:H	23:Z:61:ILE:HG21	1.79	0.47
2:B:434:ARG:NH2	14:O:264:ASP:OD2	2.48	0.47
27:B:602:CLA:H91	27:B:602:CLA:C2D	2.45	0.47
3:C:41:ARG:NH1	27:C:511:CLA:HMD1	2.29	0.47
4:D:188:PHE:HD1	4:D:326:ARG:HG2	1.79	0.47
5:E:14:ILE:O	5:E:20:TRP:NE1	2.42	0.47
5:E:30:LEU:HD13	6:F:28:VAL:HG13	1.96	0.47
27:G:604:CLA:C2B	40:G:1623:NEX:H383	2.45	0.47
2:B:61:PHE:CE2	27:B:605:CLA:HMA1	2.50	0.47
27:C:509:CLA:H3A	27:C:509:CLA:HBA1	1.54	0.47
1:A:276:ALA:HB2	4:D:215:GLY:C	2.35	0.47
7:G:81:PHE:CE2	7:G:85:LEU:HD11	2.50	0.47
40:N:1623:NEX:H401	40:N:1623:NEX:H35	1.77	0.47
17:R:183:LEU:HB2	27:R:610:CLA:O1A	2.15	0.47
27:S:604:CLA:O1D	27:S:604:CLA:H2A	2.15	0.47
27:S:613:CLA:CHB	27:S:614:CLA:HMD3	2.45	0.47
2:B:25:MET:HE2	29:B:618:BCR:H393	1.97	0.47
27:B:602:CLA:H143	27:B:602:CLA:H161	1.65	0.47
2:B:142:HIS:HB3	27:B:611:CLA:H101	1.97	0.47
3:C:27:ASP:O	3:C:31:THR:HG22	2.15	0.47
1:A:131:TRP:HZ2	3:C:449:ARG:HG2	1.79	0.47
3:C:87:ILE:C	3:C:90:PRO:HD2	2.35	0.47
4:D:78:VAL:O	4:D:111:TRP:HD1	1.98	0.47
40:N:1623:NEX:H11	40:N:1623:NEX:H191	1.72	0.47
14:O:210:LEU:HD23	14:O:234:TYR:HA	1.96	0.47
40:Y:1623:NEX:H183	40:Y:1623:NEX:H192	1.96	0.47
7:Y:185:ARG:HD3	27:Y:602:CLA:CHD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Y:601:CHL:H102	37:Y:601:CHL:H61	1.46	0.47
2:B:167:TRP:HD1	2:B:264:PRO:HG2	1.80	0.47
27:C:513:CLA:HMD1	18:S:39:LEU:HD11	1.96	0.47
7:N:128:TRP:O	7:N:132:VAL:HG23	2.15	0.47
38:N:1620:LUT:H201	38:N:1620:LUT:H15	1.77	0.47
7:Y:169:ASP:O	7:Y:173:PHE:N	2.41	0.47
28:A:409:PHO:HAC1	4:D:275:PRO:HB2	1.97	0.47
3:C:379:ARG:O	3:C:383:ASP:N	2.45	0.47
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.97	0.47
3:C:132:HIS:HE1	27:C:513:CLA:C1A	2.28	0.47
7:G:157:PRO:HB3	37:G:608:CHL:HBC2	1.96	0.47
7:G:156:TYR:HB3	27:G:610:CLA:HED2	1.97	0.47
7:N:191:MET:HE2	38:N:1621:LUT:H10	1.96	0.47
7:G:64:LEU:HD11	7:N:49:ALA:HA	1.97	0.47
27:R:616:CLA:HBA1	27:R:616:CLA:H12	1.44	0.47
18:S:67:LYS:HB2	18:S:70:ASP:H	1.80	0.47
7:Y:213:LEU:HD21	27:Y:614:CLA:HMC3	1.95	0.47
7:Y:52:SER:HB3	7:Y:58:PHE:HD1	1.79	0.47
1:A:173:PRO:HB2	1:A:178:GLY:HA3	1.96	0.47
7:G:128:TRP:CD1	7:N:222:TRP:HZ2	2.33	0.47
7:G:173:PHE:HE1	27:G:610:CLA:H2A	1.80	0.47
27:N:602:CLA:HBA1	38:N:1621:LUT:H382	1.96	0.47
37:R:608:CHL:HBC3	37:R:608:CHL:HHD	1.97	0.47
18:S:105:CYS:HA	27:S:604:CLA:HED1	1.96	0.47
7:Y:109:GLY:HA3	7:Y:122:GLN:NE2	2.30	0.47
1:A:198:HIS:CE1	27:A:405:CLA:NB	2.83	0.46
1:A:239:PHE:HE2	19:T:29:ILE:HG13	1.80	0.46
2:B:384:ARG:HG3	14:O:249:THR:HG22	1.97	0.46
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.97	0.46
5:E:70:PHE:HD2	20:U:28:LYS:HD2	1.80	0.46
14:O:161:LEU:HD23	21:W:88:ARG:NH2	2.30	0.46
15:P:92:ALA:HA	15:P:94:PHE:N	2.30	0.46
27:S:609:CLA:H3A	27:S:609:CLA:HBA2	1.37	0.46
27:Y:602:CLA:H41	27:Y:603:CLA:HBA1	1.97	0.46
1:A:197:PHE:CE2	32:C:520:DGD:HBN2	2.50	0.46
3:C:462:ASP:OD1	3:C:463:PHE:N	2.49	0.46
27:C:503:CLA:H2	27:C:501:CLA:C3D	2.46	0.46
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.15	0.46
4:D:298:PHE:O	4:D:302:GLU:HG2	2.15	0.46
27:G:602:CLA:H92	27:G:602:CLA:H62	1.77	0.46
27:G:604:CLA:H2	37:G:606:CHL:CAD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:G:613:CLA:C4B	38:G:1620:LUT:H183	2.46	0.46
7:N:139:GLU:HG3	37:N:609:CHL:C4B	2.46	0.46
7:N:197:GLN:NE2	38:N:1620:LUT:O3	2.49	0.46
15:P:121:VAL:O	15:P:123:GLY:N	2.46	0.46
27:R:611:CLA:H3A	27:R:611:CLA:HBA2	1.45	0.46
1:A:198:HIS:HA	1:A:286:THR:HG22	1.98	0.46
2:B:366:PHE:HD2	2:B:425:GLN:NE2	2.13	0.46
27:B:602:CLA:H92	27:B:602:CLA:H61	1.78	0.46
27:B:607:CLA:O1D	27:B:607:CLA:H2A	2.16	0.46
3:C:178:LYS:HB2	27:C:502:CLA:H203	1.98	0.46
32:C:520:DGD:HAW2	4:D:74:LEU:HD22	1.96	0.46
34:D:405:PL9:H401	34:D:405:PL9:H422	1.70	0.46
4:D:49:PHE:HE1	31:D:411:LMG:H321	1.80	0.46
37:G:607:CHL:HHC	37:G:607:CHL:HBB1	1.97	0.46
7:G:212:HIS:CG	27:G:613:CLA:HAA2	2.51	0.46
37:N:601:CHL:CHC	37:N:601:CHL:HBB1	2.42	0.46
37:N:607:CHL:H111	37:N:607:CHL:H152	1.52	0.46
15:P:31:PRO:HG3	15:P:175:PHE:HB3	1.98	0.46
17:R:126:LYS:O	17:R:130:ILE:HG12	2.15	0.46
17:R:13:LEU:HB2	17:R:15:TYR:CE1	2.51	0.46
18:S:224:ASP:HB3	18:S:227:GLY:HA3	1.96	0.46
21:W:105:LEU:O	21:W:108:ILE:HG13	2.16	0.46
7:Y:192:PHE:HD2	27:Y:613:CLA:HMC1	1.80	0.46
1:A:184:ILE:HG23	1:A:328:MET:SD	2.55	0.46
2:B:475:PHE:CD1	4:D:134:ARG:HD3	2.51	0.46
3:C:223:TRP:CG	3:C:224:ILE:N	2.82	0.46
27:C:502:CLA:H193	18:S:226:PHE:HE2	1.80	0.46
7:G:197:GLN:HG3	27:G:613:CLA:C1D	2.46	0.46
14:O:233:SER:N	15:P:100:GLU:OE2	2.48	0.46
17:R:210:GLY:O	17:R:214:GLN:N	2.41	0.46
35:Y:2630:LHG:H272	35:Y:2630:LHG:H242	1.54	0.46
2:B:236:THR:HB	2:B:473:THR:HG21	1.98	0.46
2:B:45:PHE:CD1	2:B:60:MET:HG3	2.50	0.46
27:B:613:CLA:H18	27:B:613:CLA:H151	1.69	0.46
27:B:613:CLA:HBA2	27:B:613:CLA:H3A	1.32	0.46
27:C:502:CLA:H161	27:C:502:CLA:H141	1.61	0.46
27:C:508:CLA:HBC3	27:C:510:CLA:H92	1.97	0.46
27:C:509:CLA:H161	27:C:509:CLA:H141	1.58	0.46
27:A:407:CLA:HED2	32:C:520:DGD:HAE1	1.98	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
5:E:8:ARG:HH22	5:E:16:SER:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:94:GLU:HB3	7:G:103:GLN:HE21	1.81	0.46
37:G:609:CHL:HAA2	7:N:48:THR:HG21	1.97	0.46
7:G:63:GLU:HA	7:G:155:LEU:HD11	1.97	0.46
4:D:89:LEU:HG	8:H:62:ASN:ND2	2.31	0.46
14:O:162:MET:CE	14:O:200:GLN:HB2	2.46	0.46
40:R:623:NEX:H15	40:R:623:NEX:H201	1.68	0.46
7:G:49:ALA:HA	7:Y:64:LEU:HD11	1.98	0.46
2:B:324:LEU:HD21	4:D:196:PHE:HE2	1.81	0.46
3:C:451:ALA:HA	3:C:456:GLU:OE1	2.16	0.46
1:A:246:TYR:HE1	33:D:401:BCT:O1	1.99	0.46
37:G:607:CHL:HBC2	7:N:222:TRP:CH2	2.51	0.46
17:R:197:GLU:OE1	27:R:610:CLA:NB	2.49	0.46
2:B:486:LEU:HD23	2:B:488:VAL:H	1.80	0.46
3:C:213:LEU:HD23	3:C:224:ILE:HG21	1.98	0.46
1:A:92:HIS:CE1	3:C:220:GLY:HA3	2.51	0.46
3:C:425:TRP:HB3	27:C:504:CLA:HHB	1.98	0.46
4:D:79:SER:O	4:D:111:TRP:HB2	2.16	0.46
4:D:152:VAL:HG22	27:D:402:CLA:HED3	1.97	0.46
7:G:197:GLN:O	7:G:201:THR:OG1	2.17	0.46
27:G:602:CLA:H111	27:G:602:CLA:H93	1.67	0.46
7:N:121:ALA:HA	37:N:605:CHL:C1C	2.46	0.46
7:N:58:PHE:O	7:N:62:ARG:HG3	2.15	0.46
15:P:62:LEU:HD11	15:P:158:ILE:HD12	1.98	0.46
17:R:141:PRO:HD3	7:Y:117:SER:HB3	132.91	0.46
17:R:151:GLU:OE1	37:R:607:CHL:HMC	2.15	0.46
27:R:613:CLA:HMB3	38:R:620:LUT:H162	1.96	0.46
18:S:114:THR:HA	18:S:117:LEU:HD23	1.98	0.46
18:S:124:LEU:HG	18:S:128:GLY:HA2	1.97	0.46
7:Y:208:ASN:HB3	27:Y:613:CLA:O1D	2.16	0.46
3:C:210:PHE:HD1	3:C:213:LEU:HD12	1.81	0.46
1:A:312:ARG:HD2	5:E:56:PHE:CE2	2.51	0.46
7:G:131:GLN:HE21	37:G:609:CHL:HMC	1.81	0.46
7:G:135:MET:HA	7:G:138:VAL:HG22	1.98	0.46
32:H:102:DGD:HB62	32:H:102:DGD:HB91	1.70	0.46
17:R:93:ARG:HH12	27:R:602:CLA:CED	2.26	0.46
18:S:133:ILE:HD13	18:S:137:LEU:HB3	1.98	0.46
18:S:66:LYS:HG3	18:S:67:LYS:N	2.31	0.46
27:Y:610:CLA:H52	38:Y:1620:LUT:H30	1.98	0.46
39:G:1622:XAT:H201	39:G:1622:XAT:H15	1.68	0.46
37:G:607:CHL:HAA2	39:Y:1622:XAT:H41	1.98	0.46
18:S:194:ARG:NH2	27:S:602:CLA:O2D	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:229:ASN:N	18:S:232:THR:OG1	2.49	0.46
27:S:603:CLA:HBB1	27:S:603:CLA:HMB1	1.96	0.46
27:Y:602:CLA:H52	38:Y:1621:LUT:H28	1.98	0.46
1:A:331:MET:SD	4:D:347:PRO:HB2	2.56	0.46
2:B:411:TYR:CD1	2:B:416:THR:HG21	2.51	0.46
2:B:103:PHE:CE2	27:B:606:CLA:HMC3	2.51	0.46
32:C:520:DGD:HB32	32:C:520:DGD:HB61	1.65	0.46
4:D:266:TRP:CH2	35:L:101:LHG:HC82	2.51	0.46
7:G:201:THR:HG22	7:G:224:PHE:HE2	1.82	0.46
7:N:105:PHE:HE2	37:N:607:CHL:HMD1	1.81	0.46
17:R:101:ARG:HA	17:R:104:MET:HE2	1.98	0.46
17:R:190:LYS:HB3	17:R:193:LEU:HG	1.98	0.46
18:S:44:ASP:OD1	18:S:44:ASP:N	2.49	0.46
37:S:608:CHL:H2A	37:S:608:CHL:HED3	1.99	0.46
2:B:167:TRP:HA	2:B:178:VAL:HA	1.98	0.45
2:B:246:PHE:HB3	2:B:462:PHE:HB2	1.98	0.45
3:C:290:VAL:HG21	3:C:426:LEU:HB2	1.98	0.45
3:C:334:PRO:HB3	15:P:137:ASP:HB2	1.98	0.45
1:A:288:LEU:HD13	3:C:432:VAL:HG13	1.98	0.45
27:C:502:CLA:H111	27:C:502:CLA:H152	1.86	0.45
7:G:128:TRP:O	7:G:132:VAL:HG23	2.16	0.45
39:G:1622:XAT:H391	39:G:1622:XAT:H31	1.83	0.45
8:H:61:TYR:CE1	32:H:102:DGD:HB31	2.51	0.45
17:R:23:TYR:OH	17:R:38:GLY:HA2	2.15	0.45
27:S:603:CLA:HMD2	27:S:609:CLA:ND	2.31	0.45
7:Y:64:LEU:HD13	27:Y:603:CLA:HAA2	1.98	0.45
27:Y:611:CLA:H122	27:Y:612:CLA:H143	1.98	0.45
1:A:131:TRP:CH2	27:C:505:CLA:HAA2	2.52	0.45
1:A:217:SER:HA	4:D:272:LEU:HD12	1.99	0.45
1:A:339:PHE:HB3	1:A:340:PRO:HD2	1.98	0.45
1:A:56:PRO:HB2	14:O:206:ARG:NH2	2.30	0.45
2:B:256:MET:HA	2:B:263:THR:HG21	1.99	0.45
3:C:256:PRO:O	3:C:261:ARG:NH1	2.49	0.45
29:C:517:BCR:H15C	29:C:517:BCR:H351	1.73	0.45
29:C:517:BCR:H371	29:C:517:BCR:H24C	1.71	0.45
4:D:21:TRP:CZ2	22:X:108:VAL:HG11	2.52	0.45
1:A:237:TYR:CD2	4:D:263:ASN:HA	2.51	0.45
37:G:605:CHL:H3A	37:G:605:CHL:HBA2	1.73	0.45
7:N:180:GLU:OE1	27:N:610:CLA:C4A	2.64	0.45
15:P:15:ASN:HA	15:P:16:THR:HA	1.61	0.45
16:Q:14:SER:HA	16:Q:15:GLY:HA3	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:206:VAL:HG23	27:R:602:CLA:HMC1	1.98	0.45
37:R:606:CHL:H43	40:R:623:NEX:H402	1.98	0.45
18:S:158:LEU:HB2	37:S:608:CHL:HAC1	1.98	0.45
18:S:224:ASP:O	18:S:228:ASN:N	2.38	0.45
21:W:129:GLU:HA	21:W:130:ASP:HA	1.76	0.45
39:Y:1622:XAT:H31	39:Y:1622:XAT:H391	1.78	0.45
7:Y:215:ASP:OD2	7:Y:218:ASN:ND2	2.39	0.45
7:Y:63:GLU:HA	7:Y:155:LEU:HD11	1.98	0.45
7:Y:66:VAL:HG21	7:Y:155:LEU:HD13	1.98	0.45
3:C:167:LEU:HD13	27:C:512:CLA:HBA2	1.98	0.45
3:C:236:GLY:C	29:C:515:BCR:H383	2.37	0.45
29:C:516:BCR:H351	29:C:516:BCR:H15C	1.83	0.45
27:A:407:CLA:O1D	32:C:520:DGD:HAH2	2.16	0.45
31:C:521:LMG:H182	31:C:521:LMG:H291	1.99	0.45
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.51	0.45
7:G:92:PHE:CE1	7:G:113:LEU:HA	2.50	0.45
32:H:102:DGD:O4D	32:H:102:DGD:O5D	2.20	0.45
14:O:231:VAL:HG21	14:O:306:PRO:HD2	1.99	0.45
38:R:620:LUT:H15	38:R:620:LUT:H201	1.80	0.45
7:Y:81:PHE:HB3	7:Y:82:PRO:HD3	1.98	0.45
2:B:298:PHE:HB2	2:B:402:TYR:CD1	2.51	0.45
2:B:166:ILE:HD13	27:B:604:CLA:HED1	1.98	0.45
27:C:508:CLA:H61	27:C:508:CLA:H92	1.78	0.45
27:C:510:CLA:H61	27:C:510:CLA:H2	1.65	0.45
4:D:261:PHE:HD2	34:D:405:PL9:HC72	1.82	0.45
32:H:102:DGD:HB62	32:H:102:DGD:HB32	1.75	0.45
31:B:622:LMG:HC92	13:M:6:LEU:HD12	1.98	0.45
39:N:1622:XAT:H15	39:N:1622:XAT:H201	1.75	0.45
18:S:109:ALA:HA	18:S:110:VAL:O	2.17	0.45
27:Y:610:CLA:H2	38:Y:1620:LUT:H28	1.98	0.45
7:Y:118:LEU:HD23	37:Y:605:CHL:HED2	1.98	0.45
2:B:340:TRP:HB2	2:B:430:PHE:HE1	1.81	0.45
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.83	0.45
1:A:269:ARG:HE	4:D:222:LEU:HD13	1.82	0.45
7:G:23:LYS:HG3	7:G:29:SER:HB3	1.98	0.45
17:R:185:SER:HA	17:R:186:ASP:HA	1.71	0.45
17:R:128:GLU:OE2	27:R:604:CLA:HAA1	2.16	0.45
18:S:119:LEU:HD12	18:S:120:ASP:OD1	2.16	0.45
20:U:8:GLU:HA	20:U:11:LYS:NZ	2.32	0.45
39:Y:1622:XAT:H35	39:Y:1622:XAT:H401	1.68	0.45
7:Y:42:GLY:O	7:Y:185:ARG:NH1	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:27:PHE:HE1	23:Z:33:TRP:CZ3	2.35	0.45
1:A:227:THR:HB	1:A:231:GLU:HG3	1.98	0.45
27:A:405:CLA:H72	27:A:405:CLA:H111	1.69	0.45
2:B:299:SER:O	2:B:303:SER:OG	2.24	0.45
3:C:69:LEU:HA	3:C:72:VAL:HG12	1.98	0.45
4:D:349:GLY:HA2	4:D:350:ASN:HA	1.62	0.45
29:H:101:BCR:H371	29:H:101:BCR:H24C	1.79	0.45
37:N:607:CHL:HMA1	37:N:607:CHL:H43	1.99	0.45
14:O:207:VAL:HA	14:O:208:PRO:HD2	1.70	0.45
17:R:213:VAL:HG21	27:R:613:CLA:HAC2	1.99	0.45
18:S:49:LEU:HB3	18:S:56:ASP:OD1	2.17	0.45
2:B:201:HIS:HE1	27:B:603:CLA:C1D	2.30	0.45
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.52	0.45
3:C:361:LEU:HD12	32:C:518:DGD:O3E	2.17	0.45
32:C:519:DGD:HB81	31:C:521:LMG:H421	1.98	0.45
7:N:104:ILE:HG21	7:N:124:ILE:HD13	1.97	0.45
7:N:191:MET:CE	38:N:1621:LUT:H10	2.47	0.45
38:S:1621:LUT:H401	38:S:1621:LUT:H35	1.77	0.45
18:S:88:GLY:HA2	38:S:1621:LUT:H181	1.98	0.45
18:S:94:ILE:HG22	18:S:95:PRO:HD3	1.99	0.45
8:H:56:ILE:HG12	22:X:87:PHE:CE2	2.52	0.45
7:Y:146:GLY:N	37:Y:608:CHL:HMC	2.32	0.45
2:B:14:ASN:OD1	17:R:53:LEU:HB2	2.17	0.45
2:B:247:PHE:HB2	27:B:609:CLA:HBC1	1.98	0.45
2:B:283:GLU:OE2	2:B:286:ARG:NH2	2.50	0.45
3:C:187:ASP:HB3	3:C:190:ALA:HB2	1.99	0.45
3:C:390:ARG:NH1	16:Q:40:LEU:O	2.50	0.45
27:C:510:CLA:H122	27:C:510:CLA:HMA3	1.99	0.45
3:C:93:ALA:HB1	3:C:99:VAL:HG11	1.99	0.45
7:G:112:TYR:HD2	7:G:118:LEU:HD13	1.81	0.45
38:N:1620:LUT:H35	38:N:1620:LUT:H401	1.78	0.45
27:N:610:CLA:H92	27:N:610:CLA:H61	1.78	0.45
15:P:119:PRO:HD2	15:P:126:TYR:O	2.17	0.45
15:P:136:ALA:HA	15:P:137:ASP:HA	1.67	0.45
27:R:601:CLA:C4C	35:R:2630:LHG:HC82	2.47	0.45
18:S:62:PHE:CD2	38:S:1621:LUT:H222	2.52	0.45
22:X:110:ASN:O	22:X:113:PRO:HD3	2.17	0.45
1:A:267:ASN:OD1	1:A:268:SER:N	2.50	0.45
2:B:181:VAL:CG1	2:B:196:GLY:HA2	2.47	0.45
3:C:142:GLU:OE1	3:C:142:GLU:N	2.50	0.45
31:A:413:LMG:H411	32:C:518:DGD:HB72	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:G:1622:XAT:H373	39:G:1622:XAT:H23	1.76	0.45
7:G:59:ALA:HA	7:G:62:ARG:NH1	2.32	0.45
4:D:266:TRP:HH2	35:L:101:LHG:HC82	1.81	0.45
15:P:109:ALA:HA	15:P:135:THR:HA	1.99	0.45
3:C:390:ARG:HG2	16:Q:39:TYR:C	2.37	0.45
17:R:108:LEU:O	17:R:112:THR:HG22	2.17	0.45
1:A:225:ARG:HD3	17:R:58:ALA:HB1	1.98	0.45
18:S:86:MET:HE3	27:S:610:CLA:HMC3	2.05	0.45
7:Y:111:ASP:OD1	7:Y:120:HIS:ND1	2.40	0.45
27:A:406:CLA:H162	27:A:406:CLA:H203	1.74	0.45
2:B:341:LEU:HD12	2:B:429:ILE:HG22	1.99	0.45
27:B:614:CLA:H161	29:B:619:BCR:H312	1.99	0.45
3:C:377:LEU:HB3	14:O:171:GLU:OE1	2.18	0.45
4:D:174:GLY:O	4:D:178:ILE:HG12	2.17	0.45
27:D:402:CLA:H143	27:D:402:CLA:H161	1.77	0.45
5:E:77:ASP:O	5:E:81:ARG:HG3	2.17	0.45
13:M:20:ALA:O	13:M:24:ILE:HG13	2.17	0.45
14:O:137:GLU:HA	14:O:168:THR:HG22	1.99	0.45
4:D:305:ALA:HB3	14:O:243:LYS:HD3	1.98	0.45
3:C:368:PRO:HA	16:Q:76:ASN:HB2	1.99	0.45
21:W:131:GLU:HA	21:W:132:GLU:HA	1.54	0.45
27:Y:613:CLA:H152	27:Y:613:CLA:H111	1.71	0.45
7:Y:92:PHE:HE1	7:Y:113:LEU:HA	1.81	0.45
1:A:259:ILE:HG22	1:A:260:PHE:N	2.29	0.44
30:A:412:SQD:H351	30:A:412:SQD:H382	1.69	0.44
27:B:613:CLA:H61	27:B:613:CLA:H102	1.68	0.44
2:B:80:ILE:HG13	2:B:81:THR:N	2.32	0.44
27:C:506:CLA:H162	27:C:506:CLA:H122	1.82	0.44
27:C:505:CLA:CMD	27:C:507:CLA:HAB	2.47	0.44
32:C:520:DGD:HB51	32:C:520:DGD:HBW1	1.99	0.44
27:A:407:CLA:CED	4:D:175:VAL:HG13	2.47	0.44
1:A:130:GLU:HG2	4:D:256:ILE:HG21	1.98	0.44
27:D:402:CLA:H91	27:D:402:CLA:H112	1.82	0.44
2:B:468:TRP:CH2	35:D:408:LHG:HC42	2.53	0.44
7:G:127:ILE:HG12	37:G:605:CHL:HAC1	1.99	0.44
7:G:70:ARG:NH1	37:G:608:CHL:OBD	2.37	0.44
16:Q:42:PRO:O	16:Q:87:TYR:OH	2.28	0.44
18:S:157:GLY:HA2	18:S:158:LEU:O	2.17	0.44
18:S:61:PRO:HD2	38:S:1621:LUT:H23	1.99	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.52	0.44
1:A:140:ARG:NH2	1:A:142:TRP:HZ3	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:406:CLA:HBB1	28:A:408:PHO:H141	1.99	0.44
31:A:413:LMG:H342	3:C:217:PRO:HD3	2.00	0.44
3:C:387:TRP:CE3	16:Q:84:TYR:HE2	2.36	0.44
3:C:55:ALA:HB1	29:C:517:BCR:H373	1.99	0.44
4:D:117:HIS:CE1	27:D:403:CLA:NA	2.85	0.44
4:D:80:THR:HG21	4:D:170:ALA:O	2.18	0.44
40:G:1623:NEX:H15	40:G:1623:NEX:H201	1.63	0.44
7:G:52:SER:HB3	7:G:58:PHE:CD1	2.46	0.44
14:O:164:ARG:HA	21:W:88:ARG:HH12	1.82	0.44
1:A:121:LEU:CD2	27:A:410:CLA:HMB3	2.47	0.44
2:B:150:CYS:HB2	27:B:604:CLA:CMC	2.47	0.44
2:B:85:ILE:HD11	14:O:202:PRO:HD3	66.03	0.44
3:C:195:ASP:HB2	16:Q:86:ARG:HD3	2.00	0.44
4:D:311:PHE:O	14:O:242:PRO:HG2	2.18	0.44
11:K:44:PHE:O	11:K:48:LEU:N	2.47	0.44
14:O:100:TYR:CE2	14:O:104:LYS:HD2	2.53	0.44
14:O:248:SER:OG	14:O:249:THR:N	2.50	0.44
15:P:97:THR:HA	15:P:98:ASP:HA	1.67	0.44
18:S:151:TYR:HA	18:S:154:ILE:HD12	2.00	0.44
35:S:2630:LHG:H361	35:S:2630:LHG:H331	1.59	0.44
40:Y:1623:NEX:H35	40:Y:1623:NEX:H401	1.80	0.44
2:B:278:GLY:O	2:B:282:GLN:HG3	2.16	0.44
29:C:515:BCR:H15C	29:C:515:BCR:H351	1.69	0.44
29:C:516:BCR:HC41	11:K:38:MET:SD	2.58	0.44
4:D:297:ASP:HA	4:D:315:TYR:OH	2.18	0.44
7:G:16:TRP:HZ3	7:G:44:TYR:HH	1.65	0.44
35:D:409:LHG:O1	35:L:101:LHG:O4	2.24	0.44
7:N:24:TYR:HB3	7:N:44:TYR:HB3	2.00	0.44
7:N:64:LEU:HD11	7:Y:49:ALA:HA	1.99	0.44
15:P:99:SER:N	15:P:106:GLY:H	2.03	0.44
15:P:45:GLN:HG2	15:P:62:LEU:HB3	2.00	0.44
18:S:122:ASN:HB2	18:S:132:PRO:HG2	2.00	0.44
18:S:165:HIS:NE2	27:S:610:CLA:HED3	2.33	0.44
2:B:282:GLN:NE2	20:U:25:ILE:HG12	2.33	0.44
29:A:411:BCR:H20C	29:A:411:BCR:H361	1.83	0.44
2:B:167:TRP:HZ2	2:B:266:GLU:OE1	2.00	0.44
27:C:510:CLA:H192	27:C:510:CLA:H162	1.78	0.44
3:C:57:ALA:O	3:C:61:VAL:HG23	2.18	0.44
7:G:222:TRP:HB3	7:Y:105:PHE:HZ	1.82	0.44
35:D:408:LHG:O1	35:L:101:LHG:O5	2.33	0.44
17:R:102:TRP:CD1	27:R:609:CLA:HMD3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:80:LEU:HD22	27:R:616:CLA:CHC	2.48	0.44
18:S:83:ARG:HD2	37:S:608:CHL:OBD	2.17	0.44
22:X:87:PHE:O	22:X:90:SER:HB3	2.18	0.44
1:A:187:GLN:HB2	27:A:405:CLA:CAC	2.48	0.44
1:A:197:PHE:HD2	1:A:289:GLY:HA2	1.83	0.44
2:B:18:ARG:HG3	2:B:118:TRP:HB3	2.00	0.44
2:B:415:ALA:HB1	2:B:419:LYS:NZ	2.32	0.44
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.00	0.44
2:B:460:LEU:HG	4:D:280:TRP:HZ3	1.82	0.44
4:D:349:GLY:HA3	14:O:240:LEU:HD11	1.99	0.44
9:I:17:SER:HB2	21:W:116:ILE:HD12	1.99	0.44
7:N:136:GLY:CA	37:N:609:CHL:HAB	2.48	0.44
31:Z:101:LMG:HC1	31:Z:101:LMG:HC8	1.87	0.44
1:A:45:THR:HG23	27:A:406:CLA:H201	2.00	0.44
2:B:141:ILE:HD13	27:B:616:CLA:HBB1	2.00	0.44
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.53	0.44
2:B:343:HIS:HA	2:B:344:PRO:HD2	1.85	0.44
27:C:508:CLA:H62	27:C:508:CLA:H41	1.72	0.44
27:C:509:CLA:H192	27:C:512:CLA:HMD2	2.00	0.44
1:A:181:ASN:HD22	4:D:314:PHE:HD1	1.66	0.44
37:G:601:CHL:HHD	35:G:2630:LHG:HC41	2.00	0.44
17:R:103:ALA:O	17:R:107:THR:HG23	2.18	0.44
17:R:167:ASP:O	17:R:171:ARG:HG3	2.18	0.44
17:R:211:PHE:HD1	17:R:222:PRO:CB	2.30	0.44
18:S:169:PRO:O	18:S:172:PRO:HD3	2.18	0.44
18:S:44:ASP:O	18:S:45:ILE:HG13	2.17	0.44
38:Y:1620:LUT:H401	38:Y:1620:LUT:H35	1.85	0.44
2:B:281:GLN:OE1	2:B:358:ARG:NH1	2.51	0.44
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.00	0.44
2:B:74:SER:OG	2:B:94:GLU:OE2	2.36	0.44
27:C:504:CLA:H193	27:C:510:CLA:H93	1.99	0.44
27:C:511:CLA:HMB1	27:C:511:CLA:HBB1	2.00	0.44
3:C:67:MET:HB3	3:C:88:LEU:HD11	2.00	0.44
4:D:197:HIS:O	4:D:201:VAL:HG23	2.18	0.44
5:E:52:PRO:HA	5:E:55:TYR:CE2	2.53	0.44
3:C:195:ASP:CB	16:Q:86:ARG:HD3	2.48	0.44
18:S:166:PRO:HB2	18:S:167:GLY:H	1.64	0.44
18:S:175:LEU:HD13	27:S:610:CLA:H11	1.99	0.44
18:S:33:ILE:HG21	18:S:40:LEU:HD21	2.00	0.44
27:B:617:CLA:H142	27:B:617:CLA:H112	1.85	0.44
29:B:620:BCR:H351	29:B:620:BCR:H15C	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:HIS:CD2	27:C:509:CLA:NA	2.86	0.44
4:D:171:PRO:HG3	4:D:181:PHE:CD1	2.53	0.44
8:H:50:PHE:HB2	29:H:101:BCR:H10C	2.00	0.44
7:N:173:PHE:HE1	27:N:610:CLA:H2A	1.83	0.44
14:O:124:PHE:HE1	14:O:292:PRO:HA	1.83	0.44
18:S:200:MET:HE2	38:S:1621:LUT:H12	2.00	0.44
31:A:413:LMG:H331	31:A:413:LMG:H361	1.70	0.43
4:D:179:PHE:O	4:D:182:ILE:HB	2.18	0.43
7:G:15:PRO:O	7:G:21:ARG:HA	2.18	0.43
7:G:142:ARG:HG2	37:G:608:CHL:C1D	2.48	0.43
13:M:21:PHE:CZ	13:M:25:ILE:HD11	2.53	0.43
7:N:225:ALA:HB1	39:Y:1622:XAT:H183	2.00	0.43
14:O:162:MET:HE3	14:O:206:ARG:HG2	2.05	0.43
27:Y:613:CLA:H2	27:Y:613:CLA:H61	1.73	0.43
27:A:406:CLA:HED2	4:D:198:MET:SD	2.59	0.43
27:B:609:CLA:H161	27:B:609:CLA:H141	1.64	0.43
3:C:322:GLN:NE2	3:C:380:LEU:O	2.47	0.43
27:C:505:CLA:HBA2	27:C:505:CLA:C4A	2.48	0.43
4:D:160:TYR:O	4:D:164:GLN:HG2	2.18	0.43
4:D:277:THR:O	4:D:281:MET:HG2	2.18	0.43
4:D:123:ILE:HD11	32:H:102:DGD:HAH1	2.00	0.43
11:K:52:TRP:O	11:K:56:VAL:HG22	2.18	0.43
7:N:144:ALA:HB2	7:Y:28:PHE:O	2.18	0.43
7:N:188:MET:HE3	27:N:602:CLA:HMC3	1.99	0.43
7:N:101:GLY:HA2	37:N:606:CHL:HAC2	2.00	0.43
37:N:607:CHL:H8	37:N:607:CHL:H121	1.82	0.43
2:B:384:ARG:HA	14:O:249:THR:HA	2.00	0.43
2:B:378:ARG:HE	15:P:40:LYS:NZ	2.16	0.43
20:U:13:TYR:CB	20:U:25:ILE:HD12	2.48	0.43
38:Y:1620:LUT:H201	38:Y:1620:LUT:H15	1.86	0.43
27:Y:610:CLA:H92	27:Y:610:CLA:H61	1.66	0.43
27:Y:611:CLA:C1D	27:Y:612:CLA:HMD2	2.49	0.43
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.53	0.43
1:A:45:THR:OG1	28:A:408:PHO:H62	2.17	0.43
3:C:436:PHE:O	27:C:508:CLA:HMC1	2.19	0.43
29:C:516:BCR:H20C	29:C:516:BCR:H361	1.83	0.43
27:A:407:CLA:CGD	32:C:520:DGD:HAH2	2.48	0.43
27:D:403:CLA:H91	8:H:48:ALA:HB1	1.99	0.43
15:P:72:THR:HG23	15:P:125:GLN:HE21	1.84	0.43
15:P:66:THR:HG21	15:P:156:LEU:HG	2.01	0.43
3:C:368:PRO:HB3	16:Q:80:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:214:GLN:OE1	27:R:613:CLA:C1D	2.48	0.43
38:R:620:LUT:H31	38:R:620:LUT:H391	1.87	0.43
37:Y:607:CHL:HHC	37:Y:607:CHL:CBB	2.47	0.43
1:A:100:ALA:HB2	21:W:88:ARG:CD	2.48	0.43
2:B:5:TRP:HA	2:B:8:VAL:HG13	2.00	0.43
2:B:216:HIS:HE1	27:B:610:CLA:C1A	2.32	0.43
27:B:611:CLA:H102	27:B:616:CLA:HAA1	2.01	0.43
31:B:622:LMG:H152	31:B:622:LMG:H121	1.74	0.43
3:C:387:TRP:CE2	3:C:388:GLN:HG3	2.54	0.43
4:D:43:PHE:HB3	4:D:113:PHE:CZ	2.54	0.43
4:D:80:THR:HG22	4:D:111:TRP:CE2	2.53	0.43
7:N:63:GLU:HA	7:N:155:LEU:HD11	2.00	0.43
14:O:185:LYS:HA	14:O:219:SER:HA	2.00	0.43
14:O:288:THR:OG1	14:O:298:ILE:HG23	2.18	0.43
17:R:86:VAL:HG22	27:R:616:CLA:CGA	2.48	0.43
7:G:28:PHE:HA	7:Y:144:ALA:HB2	2.01	0.43
27:Y:602:CLA:H2	38:Y:1621:LUT:H26	2.00	0.43
37:Y:609:CHL:H112	37:Y:609:CHL:H152	1.30	0.43
2:B:97:ALA:O	2:B:101:ILE:HG12	2.18	0.43
27:B:605:CLA:H193	27:B:605:CLA:H162	1.69	0.43
3:C:210:PHE:CD1	3:C:213:LEU:HD12	2.54	0.43
3:C:344:SER:OG	3:C:348:GLU:N	2.51	0.43
4:D:117:HIS:HE1	27:D:403:CLA:C4D	2.31	0.43
8:H:15:LYS:HA	8:H:16:PRO:HD2	1.90	0.43
7:N:205:PRO:HB3	38:N:1620:LUT:H41	2.01	0.43
7:N:46:TRP:CD1	7:N:48:THR:HG23	2.53	0.43
38:Y:1621:LUT:H201	38:Y:1621:LUT:H15	1.80	0.43
27:Y:611:CLA:H142	27:Y:611:CLA:H111	1.80	0.43
1:A:85:THR:CG2	1:A:168:PHE:HB2	2.47	0.43
1:A:21:ILE:HD13	1:A:35:VAL:HG11	2.00	0.43
2:B:164:PRO:HG3	27:B:607:CLA:O1D	2.19	0.43
2:B:415:ALA:O	2:B:419:LYS:HG3	2.18	0.43
1:A:92:HIS:HE1	3:C:220:GLY:HA3	1.84	0.43
3:C:312:ALA:HB1	3:C:392:SER:HA	2.01	0.43
27:C:505:CLA:H71	27:C:505:CLA:H112	1.78	0.43
29:C:514:BCR:H15C	29:C:514:BCR:H351	1.74	0.43
2:B:385:ARG:HB3	15:P:93:TYR:N	2.34	0.43
18:S:108:GLU:N	18:S:117:LEU:HD22	2.34	0.43
18:S:206:GLN:HE22	38:S:1620:LUT:H42	1.84	0.43
18:S:104:ASN:HB2	27:S:604:CLA:HMD1	2.01	0.43
29:B:619:BCR:H341	29:B:619:BCR:H11C	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:368:PRO:HG3	16:Q:79:ARG:CB	2.48	0.43
3:C:62:PHE:HE2	11:K:42:PRO:HD3	1.84	0.43
7:G:25:LEU:O	37:G:601:CHL:HBB1	2.19	0.43
7:G:27:PRO:HD2	37:G:601:CHL:CBB	2.49	0.43
14:O:136:LEU:HG	14:O:325:TRP:HB3	2.01	0.43
15:P:124:LYS:HG3	15:P:152:LYS:HE2	2.01	0.43
16:Q:27:ARG:NH1	16:Q:38:PHE:HD1	2.17	0.43
15:P:112:ASN:HA	16:Q:9:PRO:O	2.19	0.43
17:R:142:PHE:CE2	37:R:606:CHL:HED3	2.53	0.43
17:R:14:TRP:HB2	27:R:601:CLA:C1D	2.49	0.43
18:S:45:ILE:N	18:S:46:PRO:HD3	2.34	0.43
18:S:165:HIS:CE1	27:S:610:CLA:HMA3	2.54	0.43
2:B:337:ALA:HA	2:B:432:LEU:HD23	2.01	0.43
1:A:223:LEU:O	2:B:482:ILE:HG12	2.19	0.43
27:A:405:CLA:HMB2	27:D:402:CLA:HMB2	2.01	0.43
4:D:60:THR:HA	4:D:82:ALA:HB2	2.01	0.43
27:G:610:CLA:C2	38:G:1620:LUT:H26	2.49	0.43
38:G:1620:LUT:H401	38:G:1620:LUT:H35	1.76	0.43
8:H:52:VAL:O	8:H:56:ILE:HG13	2.19	0.43
2:B:325:PHE:CG	12:L:35:TYR:HB3	2.54	0.43
15:P:49:TYR:O	15:P:58:ASN:HB2	2.19	0.43
17:R:14:TRP:HA	27:R:601:CLA:C4C	2.49	0.43
27:R:613:CLA:O2D	27:R:613:CLA:H2A	2.18	0.43
18:S:175:LEU:HD12	38:S:1620:LUT:H221	2.01	0.43
27:S:602:CLA:HMC2	38:S:1621:LUT:C31	2.49	0.43
7:Y:115:ASN:HA	7:Y:116:PRO:HD3	1.87	0.43
3:C:297:TYR:HD1	3:C:302:TYR:CZ	2.37	0.43
29:C:515:BCR:H11C	29:C:515:BCR:H341	1.78	0.43
3:C:95:LEU:HD23	3:C:95:LEU:HA	1.84	0.43
29:H:101:BCR:H351	29:H:101:BCR:H15C	1.87	0.43
7:N:229:VAL:HA	7:N:230:PRO:HD2	1.92	0.43
7:N:81:PHE:HB3	7:N:82:PRO:HD3	2.01	0.43
15:P:63:VAL:HG22	15:P:157:TYR:CD1	2.54	0.43
15:P:64:GLN:HA	15:P:65:PRO:HD3	1.88	0.43
17:R:14:TRP:HD1	17:R:32:TYR:O	2.02	0.43
18:S:119:LEU:HA	18:S:120:ASP:HA	1.78	0.43
18:S:57:TYR:CD2	37:S:601:CHL:HMD2	2.54	0.43
27:A:410:CLA:H12	31:A:413:LMG:H112	2.00	0.43
2:B:218:SER:OG	2:B:219:VAL:N	2.52	0.43
7:G:187:ALA:O	7:G:191:MET:HG2	2.19	0.43
7:N:22:VAL:HB	37:N:601:CHL:HBC1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:N:602:CLA:H172	27:N:602:CLA:H13	1.82	0.43
27:R:610:CLA:H143	27:R:610:CLA:H111	1.77	0.43
1:A:246:TYR:HH	33:D:401:BCT:C	2.31	0.42
2:B:475:PHE:CE1	4:D:134:ARG:HD3	2.54	0.42
29:B:619:BCR:H20C	29:B:619:BCR:H361	1.88	0.42
3:C:348:GLU:OE2	14:O:104:LYS:HA	2.19	0.42
27:C:503:CLA:CHB	31:Z:101:LMG:H212	2.49	0.42
27:C:503:CLA:H101	27:C:503:CLA:H62	1.86	0.42
32:C:520:DGD:HB71	32:C:520:DGD:HBT1	1.65	0.42
4:D:188:PHE:HE1	4:D:326:ARG:HA	1.84	0.42
4:D:214:HIS:HA	34:D:405:PL9:O2	2.19	0.42
3:C:461:ARG:NH1	4:D:225:ASP:OD2	2.46	0.42
38:G:1620:LUT:H15	38:G:1620:LUT:H201	1.87	0.42
7:N:153:ASP:OD2	7:N:156:TYR:HB2	2.19	0.42
38:N:1621:LUT:H35	38:N:1621:LUT:H401	1.81	0.42
15:P:34:TRP:CD1	15:P:51:ASP:HA	2.54	0.42
16:Q:44:PRO:HG2	16:Q:48:ALA:N	2.34	0.42
18:S:108:GLU:HG3	18:S:110:VAL:HG22	2.01	0.42
38:S:1621:LUT:H15	38:S:1621:LUT:H201	1.91	0.42
27:S:604:CLA:HBA2	27:S:604:CLA:H3A	1.54	0.42
21:W:130:ASP:HB3	21:W:133:SER:HB2	2.01	0.42
39:Y:1622:XAT:H11	39:Y:1622:XAT:H191	1.84	0.42
7:Y:220:ASN:HB2	27:Y:614:CLA:HED1	2.00	0.42
27:A:410:CLA:H93	27:A:410:CLA:H112	1.83	0.42
2:B:383:PHE:HE2	4:D:349:GLY:H	1.67	0.42
3:C:229:ASP:OD1	3:C:230:LEU:N	2.52	0.42
32:C:520:DGD:HAH1	4:D:73:PHE:HE2	1.84	0.42
38:N:1621:LUT:H15	38:N:1621:LUT:H201	1.77	0.42
40:N:1623:NEX:H201	40:N:1623:NEX:H15	1.74	0.42
15:P:110:SER:N	15:P:134:ARG:O	2.46	0.42
16:Q:40:LEU:CD1	16:Q:41:GLN:HG3	2.48	0.42
38:S:1620:LUT:H201	38:S:1620:LUT:H15	1.90	0.42
18:S:162:ASP:O	18:S:163:LYS:HB2	2.20	0.42
35:S:2630:LHG:H292	35:S:2630:LHG:H262	1.81	0.42
38:Y:1621:LUT:H401	38:Y:1621:LUT:H35	1.81	0.42
2:B:127:ARG:HH11	17:R:69:ARG:HD2	1.84	0.42
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.02	0.42
2:B:8:VAL:HG23	2:B:9:HIS:CD2	2.54	0.42
3:C:387:TRP:O	3:C:390:ARG:HB2	2.19	0.42
3:C:165:LEU:HD21	27:C:506:CLA:CAB	2.49	0.42
3:C:259:TRP:HH2	27:C:507:CLA:H201	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:404:BCR:H11C	29:D:404:BCR:H341	1.76	0.42
7:N:14:SER:HA	7:N:15:PRO:HD2	1.88	0.42
14:O:249:THR:HG21	15:P:138:GLY:HA3	2.01	0.42
17:R:198:ILE:HD12	17:R:198:ILE:HA	1.96	0.42
17:R:242:PHE:CD2	17:R:243:LEU:HG	2.54	0.42
18:S:103:ALA:HB1	18:S:104:ASN:HA	2.01	0.42
18:S:141:ALA:O	18:S:145:LEU:HB2	2.20	0.42
27:Y:602:CLA:H111	27:Y:602:CLA:H93	1.81	0.42
1:A:84:PRO:HD2	4:D:314:PHE:HZ	1.85	0.42
27:B:607:CLA:H142	27:B:607:CLA:H111	1.86	0.42
27:B:610:CLA:H2	8:H:47:MET:HE3	2.10	0.42
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.55	0.42
2:B:383:PHE:CZ	14:O:250:GLY:HA2	2.54	0.42
15:P:121:VAL:HG21	15:P:126:TYR:CE2	2.55	0.42
37:Y:601:CHL:H92	37:Y:601:CHL:H112	1.69	0.42
23:Z:40:VAL:O	23:Z:44:THR:N	2.51	0.42
1:A:223:LEU:O	2:B:482:ILE:N	2.40	0.42
2:B:46:ASP:HA	2:B:47:PRO:HD2	1.80	0.42
27:B:617:CLA:H11	27:B:617:CLA:H51	1.81	0.42
3:C:219:GLY:HA2	32:C:518:DGD:C2D	2.49	0.42
29:C:514:BCR:H361	29:C:514:BCR:H20C	1.86	0.42
8:H:59:GLU:HB3	8:H:64:SER:HB2	2.02	0.42
27:A:410:CLA:HMC2	9:I:11:VAL:HG11	2.01	0.42
7:N:83:GLU:CD	7:N:206:LEU:HB2	2.40	0.42
17:R:174:PRO:HD2	27:R:610:CLA:OBD	2.20	0.42
39:R:622:XAT:H15	39:R:622:XAT:H201	1.92	0.42
27:A:406:CLA:H141	27:A:406:CLA:H161	1.81	0.42
27:B:603:CLA:HBA1	8:H:57:ILE:HB	2.01	0.42
27:B:606:CLA:H18	27:B:606:CLA:H152	1.82	0.42
27:B:606:CLA:H41	27:B:606:CLA:H61	1.93	0.42
27:C:505:CLA:H92	27:C:505:CLA:H62	1.81	0.42
37:G:601:CHL:HBA1	37:G:601:CHL:H3A	1.77	0.42
37:G:608:CHL:HBA2	37:G:608:CHL:C4A	2.49	0.42
7:G:176:LEU:C	27:G:610:CLA:HMA1	2.40	0.42
16:Q:71:TRP:CD1	16:Q:125:LYS:HB2	2.55	0.42
38:S:1620:LUT:H11	38:S:1620:LUT:H191	1.92	0.42
27:Y:610:CLA:H141	27:Y:610:CLA:H162	1.81	0.42
1:A:300:PHE:HE2	32:C:520:DGD:HA71	1.85	0.42
2:B:160:GLY:HA2	2:B:163:GLY:O	2.19	0.42
2:B:70:GLY:HA2	2:B:178:VAL:CG2	2.49	0.42
3:C:164:HIS:HA	3:C:167:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:404:LEU:HD21	32:C:520:DGD:HB51	2.02	0.42
27:C:511:CLA:HMD2	11:K:53:GLN:HE22	1.84	0.42
7:N:42:GLY:O	7:N:185:ARG:NH1	2.50	0.42
27:N:602:CLA:H2	38:N:1621:LUT:H26	2.02	0.42
14:O:115:VAL:HG22	14:O:296:GLU:HB3	2.01	0.42
14:O:193:ASP:HB2	14:O:213:ILE:O	2.20	0.42
14:O:216:LEU:HA	14:O:228:ASP:O	2.20	0.42
17:R:49:ASP:OD1	17:R:50:TYR:N	2.53	0.42
17:R:197:GLU:HB2	27:R:610:CLA:C1B	2.50	0.42
20:U:6:THR:HG22	20:U:10:LYS:HZ3	1.85	0.42
7:Y:226:THR:O	7:Y:229:VAL:HG23	2.19	0.42
1:A:304:GLN:NE2	1:A:313:VAL:HG21	2.35	0.42
2:B:185:TRP:HB3	27:B:602:CLA:HMA3	2.02	0.42
27:B:612:CLA:HBB2	27:B:614:CLA:HMB2	2.02	0.42
29:B:618:BCR:H11C	29:B:618:BCR:H341	1.78	0.42
29:B:619:BCR:H15C	29:B:619:BCR:H351	1.74	0.42
3:C:182:PHE:CD2	27:C:502:CLA:H201	2.55	0.42
3:C:387:TRP:HZ2	16:Q:80:LEU:HA	1.85	0.42
7:N:169:ASP:HA	7:N:170:PRO:HD3	1.89	0.42
7:N:24:TYR:O	37:N:601:CHL:C1C	2.39	0.42
14:O:190:ASP:HA	14:O:191:GLY:HA2	1.80	0.42
14:O:133:LYS:NZ	14:O:328:GLN:OE1	2.36	0.42
15:P:89:GLY:O	16:Q:6:VAL:HG23	2.19	0.42
17:R:135:TYR:HD1	27:R:604:CLA:HBA1	1.85	0.42
17:R:66:ILE:HG21	17:R:69:ARG:NH1	2.35	0.42
40:S:1623:NEX:H401	40:S:1623:NEX:H35	1.88	0.42
27:Y:604:CLA:HBA2	27:Y:604:CLA:C4A	2.49	0.42
7:Y:119:VAL:HA	37:Y:605:CHL:C4D	2.50	0.42
1:A:187:GLN:HB2	27:A:405:CLA:HAC2	2.02	0.42
2:B:342:GLY:N	2:B:404:GLY:HA3	2.35	0.42
27:B:606:CLA:H92	27:B:606:CLA:H61	1.86	0.42
3:C:112:PHE:HE2	29:C:514:BCR:HC31	1.85	0.42
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.55	0.42
7:G:91:LYS:O	7:G:114:GLY:HA3	2.20	0.42
37:G:601:CHL:C1D	35:G:2630:LHG:HC82	2.50	0.42
14:O:136:LEU:HD23	14:O:301:PHE:CZ	2.55	0.42
15:P:112:ASN:O	15:P:132:LEU:N	2.43	0.42
17:R:37:PHE:CD2	39:R:622:XAT:H372	2.55	0.42
17:R:123:ASP:HA	37:R:607:CHL:HED2	2.02	0.42
37:R:608:CHL:HBA2	37:R:608:CHL:H3A	1.85	0.42
17:R:193:LEU:HD22	27:R:612:CLA:HBA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:109:ALA:HB3	27:S:604:CLA:HED3	2.02	0.42
18:S:25:LYS:O	18:S:31:ARG:HA	2.20	0.42
18:S:44:ASP:C	18:S:45:ILE:HG13	2.41	0.42
3:C:152:LYS:HG2	21:W:136:SER:HB3	2.02	0.42
23:Z:23:VAL:HB	23:Z:24:PRO:HD3	2.02	0.42
2:B:20:ILE:O	2:B:24:ILE:HG13	2.20	0.42
27:B:611:CLA:H202	27:B:611:CLA:H161	1.77	0.42
2:B:237:VAL:HG12	27:B:613:CLA:HMD1	2.02	0.42
27:C:504:CLA:H62	27:C:504:CLA:H92	1.81	0.42
7:G:186:LEU:HA	35:G:2630:LHG:H261	2.02	0.42
7:G:68:HIS:CE1	27:G:603:CLA:ND	2.87	0.42
7:G:69:CYS:N	7:G:188:MET:HE2	2.34	0.42
27:B:602:CLA:HAC1	29:H:101:BCR:H383	2.02	0.42
32:H:102:DGD:HBW2	32:H:102:DGD:HB91	1.76	0.42
35:N:2630:LHG:H211	39:Y:1622:XAT:H12	2.02	0.42
37:N:605:CHL:H11	18:S:100:LYS:HD2	2.02	0.42
14:O:151:ASN:CG	14:O:152:SER:H	2.23	0.42
14:O:236:GLY:HA2	15:P:100:GLU:OE1	2.20	0.42
17:R:112:THR:HG21	27:R:604:CLA:CAC	2.50	0.42
17:R:136:LEU:O	17:R:136:LEU:HD23	2.20	0.42
17:R:157:TYR:O	17:R:161:GLN:HG2	2.20	0.42
17:R:203:LEU:HD13	27:R:611:CLA:HBC1	2.02	0.42
1:A:230:ASN:HB2	17:R:56:ASN:HA	2.02	0.42
40:Y:1623:NEX:H191	40:Y:1623:NEX:H11	1.72	0.42
7:Y:81:PHE:CD2	27:Y:604:CLA:HAC2	2.55	0.42
2:B:340:TRP:HA	2:B:430:PHE:CD1	2.51	0.41
3:C:352:GLY:O	3:C:355:THR:HG22	2.20	0.41
4:D:172:SER:HB2	4:D:177:ALA:CB	2.49	0.41
4:D:43:PHE:CE2	27:D:403:CLA:C2C	3.03	0.41
38:G:1621:LUT:H201	38:G:1621:LUT:H15	1.88	0.41
27:G:603:CLA:HBB1	38:G:1621:LUT:C14	2.50	0.41
7:G:96:VAL:HB	7:G:99:LYS:HB2	2.02	0.41
27:C:511:CLA:HMD2	11:K:53:GLN:NE2	2.35	0.41
27:N:602:CLA:HBB2	38:N:1621:LUT:H34	2.03	0.41
7:N:117:SER:O	37:N:605:CHL:HMA2	2.20	0.41
18:S:126:TYR:CG	18:S:127:PHE:N	2.88	0.41
18:S:162:ASP:C	18:S:164:LEU:HA	2.40	0.41
18:S:44:ASP:OD1	18:S:46:PRO:HD3	2.20	0.41
1:A:238:ARG:NH1	19:T:28:LYS:O	2.31	0.41
38:Y:1620:LUT:H11	38:Y:1620:LUT:H191	1.93	0.41
23:Z:50:LEU:O	23:Z:54:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:HA	1:A:294:ALA:CB	2.50	0.41
1:A:193:LEU:HD21	27:A:405:CLA:HMC3	2.02	0.41
27:A:406:CLA:HBB1	27:A:406:CLA:HMB1	2.02	0.41
1:A:95:PRO:HG2	1:A:98:GLU:HG2	2.01	0.41
27:B:603:CLA:H93	27:B:603:CLA:H61	1.69	0.41
2:B:462:PHE:CE2	27:B:605:CLA:HAC2	2.56	0.41
27:B:608:CLA:HBC2	29:B:618:BCR:H321	2.02	0.41
3:C:268:GLY:HA2	3:C:271:TYR:CD2	2.55	0.41
3:C:118:HIS:HE1	27:C:503:CLA:C4A	2.33	0.41
7:G:16:TRP:CZ2	27:G:611:CLA:HMA3	2.55	0.41
3:C:80:PRO:HD3	16:Q:37:ARG:NH1	2.34	0.41
17:R:161:GLN:HB3	37:R:608:CHL:CMC	2.51	0.41
8:H:25:PRO:CG	17:R:78:THR:HG21	2.50	0.41
18:S:131:ILE:HB	18:S:133:ILE:H	1.85	0.41
40:S:1623:NEX:H11	40:S:1623:NEX:H191	1.82	0.41
18:S:172:PRO:HA	18:S:173:LEU:HA	1.86	0.41
1:A:196:PRO:HG3	1:A:300:PHE:HE2	1.85	0.41
27:A:405:CLA:H92	27:A:405:CLA:H62	1.81	0.41
2:B:26:HIS:O	2:B:30:VAL:HG23	2.20	0.41
1:A:93:PHE:HB2	3:C:218:PHE:CB	2.50	0.41
3:C:344:SER:N	3:C:348:GLU:O	2.38	0.41
1:A:304:GLN:HG3	3:C:414:ILE:HG22	2.03	0.41
3:C:459:ILE:O	4:D:224:GLU:N	2.37	0.41
27:C:502:CLA:HBB2	27:C:510:CLA:H151	2.01	0.41
7:N:24:TYR:O	37:N:601:CHL:C4C	2.47	0.41
3:C:390:ARG:HG2	16:Q:39:TYR:O	2.20	0.41
27:R:602:CLA:H141	27:R:602:CLA:H161	1.83	0.41
3:C:221:GLU:HG3	21:W:93:GLY:HA2	2.03	0.41
38:Y:1621:LUT:H391	38:Y:1621:LUT:H31	1.90	0.41
1:A:93:PHE:HB2	3:C:218:PHE:CG	2.55	0.41
2:B:369:VAL:HG21	4:D:341:PHE:CE1	2.55	0.41
27:B:613:CLA:H162	27:B:613:CLA:H122	1.75	0.41
29:B:618:BCR:H24C	29:B:618:BCR:H371	1.90	0.41
3:C:289:PHE:HB3	3:C:297:TYR:CE2	2.55	0.41
32:C:519:DGD:HA81	32:C:519:DGD:HAE2	1.88	0.41
4:D:126:MET:HE3	4:D:143:ALA:O	2.22	0.41
5:E:70:PHE:CZ	8:H:66:LEU:HD21	2.56	0.41
39:G:1622:XAT:H173	39:G:1622:XAT:H3	1.83	0.41
27:G:610:CLA:H62	27:G:610:CLA:H41	1.87	0.41
7:N:24:TYR:CD2	7:N:25:LEU:HG	2.56	0.41
37:G:609:CHL:HMB2	37:N:601:CHL:H3A	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:143:GLU:O	16:Q:147:LYS:HG2	2.21	0.41
18:S:23:LEU:HA	18:S:24:ALA:HA	1.70	0.41
1:A:102:VAL:O	1:A:106:LEU:HG	2.20	0.41
1:A:89:ILE:HD11	1:A:108:ASN:HB3	2.03	0.41
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.86	0.41
1:A:245:THR:OG1	4:D:265:ARG:NE	2.38	0.41
1:A:246:TYR:OH	33:D:401:BCT:C	2.68	0.41
2:B:252:VAL:HG12	27:B:604:CLA:O1A	2.20	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.56	0.41
2:B:352:ARG:CD	2:B:378:ARG:HH12	2.34	0.41
2:B:345:ILE:HD12	2:B:402:TYR:CD2	2.55	0.41
2:B:466:HIS:CE1	27:B:609:CLA:ND	2.88	0.41
27:B:605:CLA:HBA1	27:B:605:CLA:CBD	2.50	0.41
2:B:61:PHE:CZ	27:B:605:CLA:HMA1	2.56	0.41
27:B:608:CLA:HMD2	29:B:618:BCR:H323	2.02	0.41
3:C:289:PHE:HD1	3:C:293:ASN:HD22	1.67	0.41
39:G:1622:XAT:H393	35:G:2630:LHG:HC92	2.03	0.41
8:H:59:GLU:O	8:H:64:SER:N	2.53	0.41
7:N:115:ASN:HA	7:N:116:PRO:HD2	1.90	0.41
27:N:602:CLA:H101	38:N:1621:LUT:H371	2.02	0.41
39:N:1622:XAT:H391	39:N:1622:XAT:H31	1.88	0.41
27:N:602:CLA:H161	27:N:602:CLA:H193	1.83	0.41
17:R:158:ILE:HG21	37:R:608:CHL:HMA3	2.02	0.41
27:S:610:CLA:HBB1	27:S:612:CLA:HAA1	2.03	0.41
7:Y:68:HIS:CE1	27:Y:603:CLA:ND	2.88	0.41
27:B:604:CLA:H61	27:B:604:CLA:H41	1.74	0.41
2:B:458:PHE:HB3	27:B:605:CLA:HBC2	2.03	0.41
27:B:609:CLA:HBB1	27:B:609:CLA:HMB1	2.02	0.41
29:B:618:BCR:H351	29:B:618:BCR:H15C	1.79	0.41
3:C:324:LEU:HD13	15:P:134:ARG:NH2	2.36	0.41
29:C:516:BCR:H332	11:K:38:MET:HE1	2.06	0.41
4:D:43:PHE:HE2	27:D:403:CLA:C2C	2.34	0.41
7:G:22:VAL:HG23	7:G:44:TYR:HE1	1.85	0.41
27:B:616:CLA:H161	8:H:19:VAL:HG11	2.02	0.41
14:O:134:PHE:HD1	14:O:327:ALA:HB2	1.85	0.41
17:R:34:PHE:CD2	39:R:622:XAT:H383	2.55	0.41
17:R:51:ASP:N	17:R:52:GLY:HA2	2.36	0.41
18:S:163:LYS:HB2	18:S:164:LEU:HA	2.02	0.41
18:S:196:ALA:O	18:S:200:MET:HG2	2.21	0.41
2:B:282:GLN:NE2	20:U:25:ILE:H	2.18	0.41
18:S:226:PHE:HB3	31:Z:101:LMG:H132	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:411:BCR:H11C	29:A:411:BCR:H341	1.82	0.41
31:A:413:LMG:H332	3:C:223:TRP:NE1	2.36	0.41
2:B:296:GLN:HE22	2:B:304:LYS:NZ	2.19	0.41
2:B:363:PHE:HB3	2:B:365:THR:O	2.21	0.41
2:B:333:GLY:HA2	2:B:444:ARG:HH11	1.86	0.41
2:B:256:MET:HG2	2:B:451:PHE:CD2	2.56	0.41
27:B:603:CLA:CB D	27:B:603:CLA:HBA2	2.48	0.41
31:C:521:LMG:H211	31:C:521:LMG:H181	1.90	0.41
4:D:29:PHE:CG	4:D:132:LEU:HD21	2.56	0.41
7:G:112:TYR:HB3	7:G:118:LEU:HB3	2.03	0.41
27:G:611:CLA:C4C	35:G:2630:LHG:HC62	2.51	0.41
15:P:29:LEU:HB3	15:P:182:SER:HB3	2.03	0.41
3:C:191:PRO:HD2	16:Q:116:ASP:OD1	2.21	0.41
37:R:608:CHL:HBD	37:R:608:CHL:HAA1	2.03	0.41
18:S:106:GLY:O	18:S:124:LEU:HB2	2.21	0.41
27:S:603:CLA:HMD2	27:S:609:CLA:C4D	2.51	0.41
22:X:92:ALA:O	22:X:96:VAL:HG23	2.20	0.41
2:B:208:LEU:HA	2:B:208:LEU:HD23	1.94	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.96	0.41
27:B:615:CLA:HBA2	27:B:615:CLA:H11	1.66	0.41
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.56	0.41
2:B:460:LEU:HD22	4:D:287:VAL:HG21	2.03	0.41
4:D:219:GLU:HG2	35:D:410:LHG:C23	2.51	0.41
9:I:12:VAL:O	9:I:16:VAL:HG23	2.21	0.41
11:K:35:VAL:HA	11:K:38:MET:CG	2.50	0.41
12:L:20:TRP:CE3	35:L:101:LHG:H132	2.56	0.41
7:N:104:ILE:HD12	7:N:104:ILE:HA	1.91	0.41
7:N:64:LEU:HD13	27:N:603:CLA:HBA1	2.01	0.41
14:O:265:GLU:OE1	14:O:265:GLU:N	2.54	0.41
27:R:609:CLA:HHC	27:R:609:CLA:HBB1	2.02	0.41
27:R:613:CLA:H3A	27:R:613:CLA:HBA2	1.82	0.41
39:R:622:XAT:H35	39:R:622:XAT:H401	1.90	0.41
40:R:623:NEX:H11	40:R:623:NEX:H191	1.77	0.41
27:S:614:CLA:H12	27:S:614:CLA:C4D	2.50	0.41
37:G:601:CHL:HMB2	37:Y:609:CHL:HMB1	2.01	0.41
1:A:127:MET:HB2	1:A:147:TYR:HD2	1.85	0.41
30:A:418:SQD:H161	30:A:418:SQD:H191	1.76	0.41
2:B:318:ASN:HA	2:B:319:PRO:HD2	1.86	0.41
27:B:610:CLA:C3D	8:H:43:MET:HB2	2.51	0.41
27:B:616:CLA:H152	27:B:616:CLA:H112	1.92	0.41
27:B:616:CLA:H91	27:B:616:CLA:H112	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:LEU:HD11	27:C:512:CLA:H61	2.02	0.41
2:B:273:TYR:HE1	4:D:165:SER:HA	1.86	0.41
1:A:68:SER:N	4:D:312:GLU:O	2.54	0.41
4:D:53:THR:HA	4:D:67:TYR:CD2	2.56	0.41
7:N:98:PHE:CE1	7:N:99:LYS:HE3	2.56	0.41
17:R:197:GLU:CD	27:R:610:CLA:NB	2.74	0.41
18:S:123:THR:O	18:S:124:LEU:HD12	2.21	0.41
18:S:127:PHE:HB3	18:S:129:LYS:HB3	2.03	0.41
40:S:1623:NEX:H201	40:S:1623:NEX:H15	1.67	0.41
7:Y:98:PHE:CD1	7:Y:99:LYS:HG3	2.56	0.41
1:A:142:TRP:HZ2	3:C:447:ARG:HB2	1.86	0.41
2:B:413:ASP:N	2:B:413:ASP:OD1	2.52	0.41
27:B:614:CLA:HMD3	29:B:619:BCR:H341	2.03	0.41
27:B:615:CLA:H41	27:B:615:CLA:H62	1.87	0.41
3:C:216:SER:OG	3:C:218:PHE:HD2	2.04	0.41
27:C:501:CLA:H193	27:C:506:CLA:C1B	2.51	0.41
29:C:517:BCR:H11C	29:C:517:BCR:H341	1.88	0.41
4:D:181:PHE:O	4:D:184:PHE:HB3	2.21	0.41
7:G:54:ASP:HB3	7:G:57:THR:HB	2.03	0.41
27:N:610:CLA:H143	27:N:610:CLA:H111	1.87	0.41
7:N:65:GLU:OE2	7:N:185:ARG:NE	2.53	0.41
15:P:91:GLN:HB3	16:Q:3:ARG:O	2.21	0.41
27:R:602:CLA:H41	27:R:602:CLA:H62	1.90	0.41
17:R:202:ARG:HH22	27:R:602:CLA:HED3	1.86	0.41
27:R:610:CLA:H52	38:R:620:LUT:H30	2.03	0.41
17:R:77:SER:HA	17:R:166:LEU:HD21	2.03	0.41
18:S:185:LEU:C	27:S:610:CLA:HMA1	2.41	0.41
7:Y:66:VAL:HB	7:Y:155:LEU:HD22	2.03	0.41
1:A:317:TRP:HZ2	4:D:79:SER:OG	2.04	0.41
1:A:317:TRP:HZ3	4:D:180:ARG:NH1	2.19	0.41
2:B:362:PHE:CE2	4:D:184:PHE:HZ	2.39	0.41
2:B:8:VAL:HG22	27:B:612:CLA:H11	2.03	0.41
3:C:354:GLU:O	3:C:357:ARG:HG2	2.21	0.41
34:D:405:PL9:H101	34:D:405:PL9:H121	1.66	0.41
1:A:276:ALA:HB1	35:D:410:LHG:H262	2.03	0.41
4:D:80:THR:HA	4:D:81:PRO:HD3	1.85	0.41
6:F:45:ARG:HB3	10:J:36:LEU:HD23	2.03	0.41
7:G:155:LEU:HA	7:G:155:LEU:HD23	1.88	0.41
39:G:1622:XAT:H401	39:G:1622:XAT:H35	1.82	0.41
7:G:35:TYR:OH	7:G:47:ASP:OD2	2.27	0.41
16:Q:134:TYR:O	16:Q:138:VAL:HG23	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:111:LEU:HD11	17:R:211:PHE:CZ	2.56	0.41
27:R:604:CLA:CHC	40:R:623:NEX:H222	2.51	0.41
7:Y:180:GLU:HB2	27:Y:610:CLA:CHB	2.51	0.41
2:B:321:LYS:HD3	2:B:321:LYS:HA	1.89	0.40
2:B:120:LEU:HD13	27:B:617:CLA:HMD2	2.03	0.40
3:C:415:ASN:O	32:C:520:DGD:O3E	2.26	0.40
27:C:503:CLA:H151	27:C:510:CLA:HBB2	2.04	0.40
4:D:126:MET:SD	4:D:150:ILE:HD12	2.62	0.40
4:D:164:GLN:HE21	4:D:290:ALA:HA	1.86	0.40
3:C:443:TRP:CH2	35:D:410:LHG:HC61	2.55	0.40
7:G:191:MET:CE	38:G:1621:LUT:H10	2.52	0.40
38:G:1621:LUT:H35	38:G:1621:LUT:H401	1.83	0.40
27:G:614:CLA:H3A	27:G:614:CLA:HBA1	1.86	0.40
10:J:10:LEU:HA	10:J:13:ILE:HD12	2.03	0.40
16:Q:98:LYS:O	16:Q:101:LYS:HG2	2.21	0.40
16:Q:21:GLU:HB2	16:Q:24:ASP:HB2	2.02	0.40
37:R:608:CHL:C3D	27:R:610:CLA:HMD3	2.52	0.40
7:Y:46:TRP:CE3	38:Y:1621:LUT:H383	2.56	0.40
27:B:604:CLA:H141	27:B:610:CLA:H8	2.03	0.40
2:B:73:ASN:HB3	2:B:88:PRO:HA	2.03	0.40
2:B:42:LEU:HD11	2:B:93:TYR:HB3	2.02	0.40
3:C:112:PHE:CE2	29:C:514:BCR:HC31	2.56	0.40
3:C:379:ARG:NH2	16:Q:73:SER:OG	2.54	0.40
3:C:385:GLN:HB3	3:C:386:PRO:HD2	2.02	0.40
3:C:408:GLY:HA2	3:C:419:TYR:O	2.21	0.40
27:C:502:CLA:H161	27:C:502:CLA:H192	1.82	0.40
27:C:506:CLA:H41	27:C:506:CLA:H62	1.71	0.40
3:C:457:LYS:HE3	4:D:228:GLY:HA3	2.03	0.40
7:G:16:TRP:NE1	27:G:611:CLA:HED3	2.37	0.40
39:N:1622:XAT:H191	39:N:1622:XAT:H11	1.86	0.40
39:N:1622:XAT:H3	39:N:1622:XAT:H173	1.89	0.40
7:N:52:SER:O	7:N:58:PHE:HB2	2.20	0.40
27:N:610:CLA:H43	27:N:612:CLA:HBA1	2.03	0.40
14:O:112:CYS:HA	14:O:113:PRO:HD3	1.98	0.40
1:A:64:ARG:NH2	14:O:163:THR:HB	2.29	0.40
17:R:214:GLN:HE22	27:R:613:CLA:CHA	2.34	0.40
37:R:607:CHL:HBB1	37:R:607:CHL:HHC	2.04	0.40
27:R:610:CLA:H41	27:R:610:CLA:H62	1.83	0.40
38:R:620:LUT:H11	38:R:620:LUT:H191	1.95	0.40
38:R:620:LUT:H35	38:R:620:LUT:H401	1.95	0.40
17:R:121:TRP:HE3	39:R:622:XAT:H173	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:200:MET:CE	38:S:1621:LUT:H10	2.52	0.40
18:S:201:PHE:O	18:S:205:ILE:HG22	2.22	0.40
18:S:224:ASP:O	18:S:227:GLY:N	2.55	0.40
38:Y:1620:LUT:H391	38:Y:1620:LUT:H31	1.90	0.40
23:Z:5:PHE:HD1	23:Z:57:LEU:HB2	1.87	0.40
2:B:275:TRP:CZ2	2:B:315:ILE:HB	2.57	0.40
27:B:609:CLA:H142	27:B:609:CLA:H91	2.02	0.40
27:B:616:CLA:H3A	27:B:616:CLA:HBA1	1.84	0.40
3:C:471:PRO:O	3:C:472:LEU:HB2	2.21	0.40
4:D:191:TRP:NE1	4:D:197:HIS:CD2	2.90	0.40
4:D:68:LEU:HB2	6:F:40:MET:HE1	2.07	0.40
27:G:602:CLA:H41	27:G:602:CLA:H61	1.83	0.40
9:I:5:LYS:HE2	9:I:9:TYR:CE2	2.57	0.40
7:N:115:ASN:HB3	7:N:118:LEU:HD12	2.03	0.40
14:O:133:LYS:HZ1	14:O:328:GLN:CD	2.20	0.40
15:P:90:LYS:HG2	16:Q:5:ILE:HG13	2.03	0.40
38:Y:1621:LUT:H191	38:Y:1621:LUT:H11	1.92	0.40
39:Y:1622:XAT:H3	39:Y:1622:XAT:H173	1.86	0.40
40:Y:1623:NEX:H201	40:Y:1623:NEX:H15	1.73	0.40
7:Y:167:ALA:HA	7:Y:173:PHE:HB2	2.03	0.40
27:Y:611:CLA:CHD	35:Y:2630:LHG:HC62	2.52	0.40
2:B:18:ARG:HD3	2:B:115:TRP:CH2	2.57	0.40
2:B:264:PRO:HD2	2:B:267:LEU:HD12	2.04	0.40
27:B:613:CLA:CMB	27:B:615:CLA:HBB1	2.52	0.40
2:B:87:ASP:HA	2:B:88:PRO:HD2	1.94	0.40
3:C:187:ASP:O	3:C:194:GLY:HA2	2.22	0.40
4:D:29:PHE:HZ	4:D:131:GLU:HG2	1.86	0.40
4:D:183:LEU:HD23	4:D:183:LEU:HA	1.93	0.40
7:G:22:VAL:HG23	7:G:44:TYR:CE1	2.57	0.40
29:H:101:BCR:H20C	29:H:101:BCR:H361	1.90	0.40
27:N:611:CLA:C1D	27:N:612:CLA:HMD2	2.52	0.40
17:R:192:ILE:O	17:R:195:LEU:HB3	2.21	0.40
17:R:201:ALA:O	17:R:205:MET:HB2	2.22	0.40
17:R:69:ARG:O	17:R:71:GLU:HG3	2.22	0.40
31:A:413:LMG:HC62	21:W:96:LEU:HB2	2.02	0.40
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.03	0.40
1:A:183:MET:SD	27:A:406:CLA:HMD3	2.61	0.40
2:B:150:CYS:O	2:B:202:HIS:HB3	2.22	0.40
2:B:382:PRO:HG2	2:B:385:ARG:HH21	1.87	0.40
27:B:604:CLA:H152	8:H:50:PHE:HE2	1.87	0.40
27:B:610:CLA:H93	27:B:610:CLA:H62	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:143:ILE:O	7:N:151:VAL:HG21	2.21	0.40
7:N:189:PHE:HD1	27:N:602:CLA:H201	1.87	0.40
17:R:226:TRP:CH2	17:R:230:LEU:HD22	2.57	0.40
27:R:611:CLA:HBA1	27:R:611:CLA:H12	1.79	0.40
18:S:109:ALA:HA	18:S:110:VAL:C	2.42	0.40
27:Y:604:CLA:O2A	40:Y:1623:NEX:H241	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
1	a	332/344 (96%)	321 (97%)	11 (3%)	0	100	100
2	B	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	30	75
2	b	485/508 (96%)	469 (97%)	13 (3%)	3 (1%)	30	75
3	C	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
3	c	447/473 (94%)	424 (95%)	23 (5%)	0	100	100
4	D	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	46	85
4	d	338/353 (96%)	317 (94%)	20 (6%)	1 (0%)	46	85
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
6	F	30/39 (77%)	30 (100%)	0	0	100	100
6	f	30/39 (77%)	30 (100%)	0	0	100	100
7	G	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	34	78
7	N	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	34	78
7	Y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	34	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	g	216/267 (81%)	208 (96%)	7 (3%)	1 (0%)	34	78
7	n	216/267 (81%)	210 (97%)	5 (2%)	1 (0%)	34	78
7	y	216/267 (81%)	205 (95%)	10 (5%)	1 (0%)	34	78
8	H	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
8	h	57/73 (78%)	56 (98%)	1 (2%)	0	100	100
9	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
9	i	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
10	J	32/40 (80%)	32 (100%)	0	0	100	100
10	j	32/40 (80%)	32 (100%)	0	0	100	100
11	K	35/59 (59%)	35 (100%)	0	0	100	100
11	k	35/59 (59%)	35 (100%)	0	0	100	100
12	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
12	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
13	M	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
13	m	31/34 (91%)	30 (97%)	1 (3%)	0	100	100
14	O	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	9	46
14	o	241/332 (73%)	210 (87%)	26 (11%)	5 (2%)	9	46
15	P	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	16	60
15	p	170/267 (64%)	148 (87%)	20 (12%)	2 (1%)	16	60
16	Q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	6	39
16	q	146/232 (63%)	134 (92%)	8 (6%)	4 (3%)	6	39
17	R	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	4	28
17	r	230/243 (95%)	211 (92%)	10 (4%)	9 (4%)	4	28
18	S	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	4	28
18	s	212/295 (72%)	187 (88%)	17 (8%)	8 (4%)	4	28
19	T	28/33 (85%)	28 (100%)	0	0	100	100
19	t	28/33 (85%)	28 (100%)	0	0	100	100
20	U	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	3	25
20	u	23/99 (23%)	21 (91%)	1 (4%)	1 (4%)	3	25
21	W	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	10	50
21	w	52/137 (38%)	46 (88%)	5 (10%)	1 (2%)	10	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	X	33/117 (28%)	33 (100%)	0	0	100	100
22	x	33/117 (28%)	33 (100%)	0	0	100	100
23	Z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
23	z	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
All	All	7548/9396 (80%)	7100 (94%)	374 (5%)	74 (1%)	24	65

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	85	ILE
14	O	258	PRO
14	O	311	LEU
15	P	108	VAL
18	S	110	VAL
18	S	163	LYS
2	b	85	ILE
14	o	258	PRO
14	o	311	LEU
15	p	108	VAL
18	s	110	VAL
18	s	163	LYS
7	G	119	VAL
14	O	261	GLY
16	Q	5	ILE
17	R	43	ALA
17	R	58	ALA
18	S	166	PRO
21	W	86	ASP
7	g	119	VAL
14	o	261	GLY
16	q	5	ILE
17	r	43	ALA
17	r	58	ALA
18	s	166	PRO
21	w	86	ASP
2	B	51	VAL
17	R	17	GLY
17	R	189	LYS
18	S	127	PHE
2	b	51	VAL
17	r	17	GLY

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Mol	Chain	Res	Type
17	r	189	LYS
18	s	127	PHE
14	O	119	VAL
15	P	70	SER
17	R	54	ASP
17	R	61	LEU
18	S	158	LEU
14	o	119	VAL
15	p	70	SER
17	r	54	ASP
17	r	61	LEU
18	s	158	LEU
2	B	333	GLY
7	N	119	VAL
14	O	177	GLU
16	Q	33	TYR
17	R	46	LEU
17	R	82	PRO
18	S	46	PRO
18	S	132	PRO
2	b	333	GLY
7	n	119	VAL
16	q	33	TYR
17	r	46	LEU
17	r	82	PRO
18	s	46	PRO
18	s	132	PRO
17	R	187	PRO
7	Y	119	VAL
14	o	177	GLU
17	r	187	PRO
7	y	119	VAL
4	D	175	VAL
16	Q	43	LEU
4	d	175	VAL
16	q	43	LEU
16	Q	6	VAL
18	S	172	PRO
20	U	7	PRO
16	q	6	VAL
18	s	172	PRO
20	u	7	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	270/279 (97%)	270 (100%)	0	100	100
1	a	270/279 (97%)	270 (100%)	0	100	100
2	B	389/406 (96%)	389 (100%)	0	100	100
2	b	389/406 (96%)	389 (100%)	0	100	100
3	C	351/374 (94%)	350 (100%)	1 (0%)	94	98
3	c	351/374 (94%)	350 (100%)	1 (0%)	94	98
4	D	272/283 (96%)	272 (100%)	0	100	100
4	d	272/283 (96%)	272 (100%)	0	100	100
5	E	70/73 (96%)	70 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	27/34 (79%)	27 (100%)	0	100	100
6	f	27/34 (79%)	27 (100%)	0	100	100
7	G	168/206 (82%)	168 (100%)	0	100	100
7	N	168/206 (82%)	168 (100%)	0	100	100
7	Y	168/206 (82%)	168 (100%)	0	100	100
7	g	168/206 (82%)	168 (100%)	0	100	100
7	n	168/206 (82%)	168 (100%)	0	100	100
7	y	168/206 (82%)	168 (100%)	0	100	100
8	H	48/61 (79%)	48 (100%)	0	100	100
8	h	48/61 (79%)	48 (100%)	0	100	100
9	I	32/33 (97%)	32 (100%)	0	100	100
9	i	32/33 (97%)	32 (100%)	0	100	100
10	J	25/30 (83%)	25 (100%)	0	100	100
10	j	25/30 (83%)	25 (100%)	0	100	100
11	K	32/52 (62%)	32 (100%)	0	100	100
11	k	32/52 (62%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	35/36 (97%)	35 (100%)	0	100	100
12	l	35/36 (97%)	35 (100%)	0	100	100
13	M	29/30 (97%)	29 (100%)	0	100	100
13	m	29/30 (97%)	29 (100%)	0	100	100
14	O	202/269 (75%)	202 (100%)	0	100	100
14	o	202/269 (75%)	202 (100%)	0	100	100
15	P	144/212 (68%)	144 (100%)	0	100	100
15	p	144/212 (68%)	144 (100%)	0	100	100
16	Q	129/187 (69%)	129 (100%)	0	100	100
16	q	129/187 (69%)	129 (100%)	0	100	100
17	R	189/198 (96%)	189 (100%)	0	100	100
17	r	189/198 (96%)	189 (100%)	0	100	100
18	S	167/226 (74%)	167 (100%)	0	100	100
18	s	167/226 (74%)	167 (100%)	0	100	100
19	T	27/30 (90%)	27 (100%)	0	100	100
19	t	27/30 (90%)	27 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/110 (40%)	44 (100%)	0	100	100
21	w	44/110 (40%)	44 (100%)	0	100	100
22	X	26/90 (29%)	26 (100%)	0	100	100
22	x	26/90 (29%)	26 (100%)	0	100	100
23	Z	52/53 (98%)	52 (100%)	0	100	100
23	z	52/53 (98%)	52 (100%)	0	100	100
All	All	6170/7528 (82%)	6168 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	117	LEU
3	c	117	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	157	HIS
2	B	179	GLN
2	B	216	HIS
2	B	282	GLN
2	B	296	GLN
2	B	332	ASN
2	B	343	HIS
3	C	68	ASN
3	C	201	ASN
3	C	327	ASN
3	C	332	GLN
3	C	418	ASN
4	D	83	ASN
4	D	142	ASN
4	D	164	GLN
4	D	230	ASN
7	G	61	ASN
7	G	103	GLN
8	H	62	ASN
11	K	53	GLN
13	M	32	GLN
7	N	103	GLN
7	N	208	ASN
14	O	305	GLN
14	O	331	GLN
15	P	35	ASN
15	P	112	ASN
16	Q	75	GLN
17	R	55	GLN
17	R	138	GLN
17	R	194	GLN
17	R	235	HIS
18	S	81	HIS
18	S	104	ASN
7	Y	103	GLN
7	Y	208	ASN
23	Z	58	ASN
1	a	304	GLN
2	b	179	GLN
2	b	216	HIS
2	b	282	GLN
2	b	296	GLN
2	b	332	ASN

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Mol	Chain	Res	Type
2	b	343	HIS
3	c	68	ASN
3	c	201	ASN
3	c	327	ASN
3	c	332	GLN
3	c	418	ASN
4	d	83	ASN
4	d	142	ASN
4	d	164	GLN
4	d	230	ASN
7	g	61	ASN
7	g	103	GLN
8	h	62	ASN
11	k	53	GLN
13	m	32	GLN
7	n	103	GLN
7	n	208	ASN
14	o	305	GLN
14	o	331	GLN
15	p	35	ASN
15	p	112	ASN
16	q	75	GLN
17	r	55	GLN
17	r	138	GLN
17	r	194	GLN
17	r	235	HIS
18	s	81	HIS
18	s	104	ASN
7	y	103	GLN
7	y	208	ASN
23	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 322 ligands modelled in this entry, 6 are monoatomic - leaving 316 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	$\# Z > 2$
24	OEX	A	401	1,3	0,15,15	0.00	-	0,32,32	0.00	-
27	CLA	A	405	-	57,73,73	1.24	7 (12%)	61,113,113	1.24	6 (9%)
27	CLA	A	406	-	57,73,73	1.19	7 (12%)	61,113,113	1.24	5 (8%)
27	CLA	A	407	-	41,57,73	1.36	7 (17%)	43,93,113	1.39	6 (13%)
28	PHO	A	408	-	67,69,69	1.20	10 (14%)	86,99,99	1.15	10 (11%)
28	PHO	A	409	-	67,69,69	1.20	10 (14%)	86,99,99	1.12	6 (6%)
27	CLA	A	410	-	52,68,73	1.25	8 (15%)	55,107,113	1.29	6 (10%)
29	BCR	A	411	-	41,41,41	0.92	3 (7%)	56,56,56	2.07	17 (30%)
30	SQD	A	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.72	10 (16%)
31	LMG	A	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
30	SQD	A	418	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	9 (14%)
27	CLA	B	602	-	57,73,73	1.15	8 (14%)	61,113,113	1.17	5 (8%)
27	CLA	B	603	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	9 (14%)
27	CLA	B	604	-	57,73,73	1.22	8 (14%)	61,113,113	1.26	6 (9%)
27	CLA	B	605	-	57,73,73	1.20	7 (12%)	61,113,113	1.40	11 (18%)
27	CLA	B	606	-	57,73,73	1.21	8 (14%)	61,113,113	1.15	5 (8%)
27	CLA	B	607	-	57,73,73	1.18	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	B	608	-	57,73,73	1.14	8 (14%)	61,113,113	1.22	5 (8%)
27	CLA	B	609	-	57,73,73	1.14	7 (12%)	61,113,113	1.25	6 (9%)
27	CLA	B	610	-	57,73,73	1.15	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	B	611	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	7 (11%)
27	CLA	B	612	-	57,73,73	1.22	7 (12%)	61,113,113	1.35	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	B	613	-	57,73,73	1.20	8 (14%)	61,113,113	1.33	9 (14%)
27	CLA	B	614	-	57,73,73	1.19	8 (14%)	61,113,113	1.16	5 (8%)
27	CLA	B	615	-	57,73,73	1.20	8 (14%)	61,113,113	1.17	8 (13%)
27	CLA	B	616	-	57,73,73	1.19	7 (12%)	61,113,113	1.18	6 (9%)
27	CLA	B	617	-	57,73,73	1.19	7 (12%)	61,113,113	1.23	6 (9%)
29	BCR	B	618	-	41,41,41	0.91	3 (7%)	56,56,56	2.21	18 (32%)
29	BCR	B	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.07	17 (30%)
29	BCR	B	620	-	41,41,41	0.96	2 (4%)	56,56,56	2.13	17 (30%)
30	SQD	B	621	-	53,54,54	0.95	5 (9%)	62,65,65	1.96	9 (14%)
31	LMG	B	622	-	51,51,55	0.78	2 (3%)	59,59,63	1.45	8 (13%)
27	CLA	C	501	-	57,73,73	1.18	8 (14%)	61,113,113	1.25	8 (13%)
27	CLA	C	502	-	57,73,73	1.16	7 (12%)	61,113,113	1.26	5 (8%)
27	CLA	C	503	-	57,73,73	1.18	8 (14%)	61,113,113	1.25	10 (16%)
27	CLA	C	504	-	57,73,73	1.17	7 (12%)	61,113,113	1.20	5 (8%)
27	CLA	C	505	-	57,73,73	1.20	7 (12%)	61,113,113	1.35	7 (11%)
27	CLA	C	506	-	57,73,73	1.17	8 (14%)	61,113,113	1.30	7 (11%)
27	CLA	C	507	-	57,73,73	1.22	8 (14%)	61,113,113	1.15	6 (9%)
27	CLA	C	508	-	57,73,73	1.25	8 (14%)	61,113,113	1.34	9 (14%)
27	CLA	C	509	-	57,73,73	1.21	8 (14%)	61,113,113	1.34	10 (16%)
27	CLA	C	510	-	57,73,73	1.17	7 (12%)	61,113,113	1.29	6 (9%)
27	CLA	C	511	3	57,73,73	1.17	7 (12%)	61,113,113	1.28	6 (9%)
27	CLA	C	512	-	57,73,73	1.15	7 (12%)	61,113,113	1.23	8 (13%)
27	CLA	C	513	-	41,57,73	1.37	7 (17%)	43,93,113	1.44	7 (16%)
29	BCR	C	514	-	41,41,41	0.90	1 (2%)	56,56,56	2.01	19 (33%)
29	BCR	C	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	19 (33%)
29	BCR	C	516	-	41,41,41	0.79	0	56,56,56	2.30	18 (32%)
29	BCR	C	517	-	41,41,41	0.96	2 (4%)	56,56,56	2.32	16 (28%)
32	DGD	C	518	-	56,56,67	1.13	8 (14%)	70,70,81	1.72	16 (22%)
32	DGD	C	519	-	63,63,67	0.97	4 (6%)	77,77,81	1.53	14 (18%)
32	DGD	C	520	-	63,63,67	0.96	4 (6%)	77,77,81	1.53	12 (15%)
31	LMG	C	521	-	51,51,55	0.73	0	59,59,63	1.39	8 (13%)
33	BCT	D	401	-	0,3,3	0.00	-	0,3,3	0.00	-
27	CLA	D	402	-	57,73,73	1.25	7 (12%)	61,113,113	1.28	7 (11%)
27	CLA	D	403	-	57,73,73	1.14	6 (10%)	61,113,113	1.30	7 (11%)
29	BCR	D	404	-	41,41,41	0.80	0	56,56,56	2.19	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PL9	D	405	-	54,55,55	1.60	9 (16%)	68,69,69	1.57	15 (22%)
35	LHG	D	408	-	42,42,48	0.76	1 (2%)	43,48,54	1.29	5 (11%)
35	LHG	D	409	-	48,48,48	0.74	1 (2%)	49,54,54	1.37	8 (16%)
35	LHG	D	410	-	36,36,48	0.70	0	37,42,54	1.28	4 (10%)
31	LMG	D	411	-	46,46,55	0.83	4 (8%)	54,54,63	1.42	6 (11%)
36	HEM	F	101	5,6	24,50,50	2.33	6 (25%)	16,82,82	1.42	3 (18%)
38	LUT	G	1620	-	42,43,43	1.00	2 (4%)	49,60,60	1.91	15 (30%)
38	LUT	G	1621	-	42,43,43	1.04	2 (4%)	49,60,60	1.86	17 (34%)
39	XAT	G	1622	-	47,47,47	1.38	3 (6%)	40,74,74	1.82	8 (20%)
40	NEX	G	1623	-	42,46,46	1.25	2 (4%)	40,70,70	1.96	11 (27%)
35	LHG	G	2630	27	48,48,48	0.61	1 (2%)	49,54,54	1.29	7 (14%)
37	CHL	G	601	7	64,74,74	4.13	26 (40%)	47,114,114	2.08	16 (34%)
27	CLA	G	602	7	57,73,73	1.18	8 (14%)	61,113,113	1.27	7 (11%)
27	CLA	G	603	-	41,57,73	1.33	7 (17%)	43,93,113	1.37	6 (13%)
27	CLA	G	604	-	41,57,73	1.34	7 (17%)	43,93,113	1.32	7 (16%)
37	CHL	G	605	7	46,56,74	4.71	26 (56%)	28,92,114	2.52	15 (53%)
37	CHL	G	606	-	48,58,74	4.72	26 (54%)	29,94,114	2.51	14 (48%)
37	CHL	G	607	-	48,58,74	4.69	26 (54%)	29,94,114	2.31	12 (41%)
37	CHL	G	608	-	48,58,74	4.68	25 (52%)	29,94,114	2.35	13 (44%)
37	CHL	G	609	7	48,58,74	4.72	27 (56%)	29,94,114	2.36	12 (41%)
27	CLA	G	610	7	57,73,73	1.14	6 (10%)	61,113,113	1.23	5 (8%)
27	CLA	G	611	35	41,57,73	1.32	7 (17%)	43,93,113	1.34	6 (13%)
27	CLA	G	612	7	41,57,73	1.35	7 (17%)	43,93,113	1.32	6 (13%)
27	CLA	G	613	7	41,57,73	1.32	7 (17%)	43,93,113	1.41	8 (18%)
27	CLA	G	614	-	41,57,73	1.32	5 (12%)	43,93,113	1.31	5 (11%)
29	BCR	H	101	-	41,41,41	0.86	1 (2%)	56,56,56	2.00	19 (33%)
32	DGD	H	102	-	63,63,67	0.98	3 (4%)	77,77,81	1.49	10 (12%)
35	LHG	L	101	-	48,48,48	0.71	1 (2%)	49,54,54	1.32	7 (14%)
38	LUT	N	1620	-	42,43,43	0.98	3 (7%)	49,60,60	2.01	16 (32%)
38	LUT	N	1621	-	42,43,43	1.02	3 (7%)	49,60,60	1.82	13 (26%)
39	XAT	N	1622	-	47,47,47	1.38	3 (6%)	40,74,74	2.25	14 (35%)
40	NEX	N	1623	-	42,46,46	1.26	2 (4%)	40,70,70	1.99	9 (22%)
35	LHG	N	2630	27	48,48,48	0.60	1 (2%)	49,54,54	1.29	7 (14%)
37	CHL	N	601	7	48,58,74	4.68	24 (50%)	29,94,114	2.48	14 (48%)
27	CLA	N	602	7	57,73,73	1.17	7 (12%)	61,113,113	1.16	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	N	603	-	41,57,73	1.35	7 (17%)	43,93,113	1.35	6 (13%)
27	CLA	N	604	-	41,57,73	1.33	7 (17%)	43,93,113	1.38	6 (13%)
37	CHL	N	605	7	46,56,74	4.84	26 (56%)	28,92,114	2.60	15 (53%)
37	CHL	N	606	-	48,58,74	4.70	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	N	607	-	64,74,74	4.13	26 (40%)	47,114,114	1.96	15 (31%)
37	CHL	N	608	-	48,58,74	4.74	26 (54%)	29,94,114	2.39	12 (41%)
37	CHL	N	609	7	48,58,74	4.81	26 (54%)	29,94,114	2.44	13 (44%)
27	CLA	N	610	7	57,73,73	1.16	6 (10%)	61,113,113	1.22	7 (11%)
27	CLA	N	611	35	41,57,73	1.29	6 (14%)	43,93,113	1.38	8 (18%)
27	CLA	N	612	7	41,57,73	1.34	7 (17%)	43,93,113	1.36	7 (16%)
27	CLA	N	613	7	41,57,73	1.33	7 (17%)	43,93,113	1.35	5 (11%)
27	CLA	N	614	-	41,57,73	1.27	4 (9%)	43,93,113	1.35	7 (16%)
35	LHG	R	2630	27	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
27	CLA	R	601	17	41,57,73	1.29	5 (12%)	43,93,113	1.45	8 (18%)
27	CLA	R	602	17	57,73,73	1.17	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	R	603	-	41,57,73	1.33	7 (17%)	43,93,113	1.33	7 (16%)
27	CLA	R	604	-	41,57,73	1.32	6 (14%)	43,93,113	1.46	6 (13%)
37	CHL	R	606	-	48,58,74	4.71	26 (54%)	29,94,114	2.42	12 (41%)
37	CHL	R	607	-	48,58,74	4.72	25 (52%)	29,94,114	2.38	13 (44%)
37	CHL	R	608	-	48,58,74	4.73	26 (54%)	29,94,114	2.30	12 (41%)
27	CLA	R	609	17	41,57,73	1.32	7 (17%)	43,93,113	1.29	5 (11%)
27	CLA	R	610	17	57,73,73	1.16	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	R	611	35	41,57,73	1.30	5 (12%)	43,93,113	1.29	6 (13%)
27	CLA	R	612	-	41,57,73	1.31	7 (17%)	43,93,113	1.28	5 (11%)
27	CLA	R	613	17	41,57,73	1.30	5 (12%)	43,93,113	1.34	5 (11%)
27	CLA	R	616	17	41,57,73	1.32	6 (14%)	43,93,113	1.32	6 (13%)
38	LUT	R	620	-	42,43,43	0.95	2 (4%)	49,60,60	1.70	15 (30%)
39	XAT	R	622	-	47,47,47	1.37	2 (4%)	40,74,74	1.91	13 (32%)
40	NEX	R	623	-	42,46,46	1.30	2 (4%)	40,70,70	1.85	12 (30%)
38	LUT	S	1620	-	42,43,43	0.99	3 (7%)	49,60,60	2.07	16 (32%)
38	LUT	S	1621	-	42,43,43	0.97	3 (7%)	49,60,60	1.82	16 (32%)
40	NEX	S	1623	-	42,46,46	1.21	3 (7%)	40,70,70	1.89	9 (22%)
35	LHG	S	2630	27	48,48,48	0.64	1 (2%)	49,54,54	1.28	6 (12%)
37	CHL	S	601	18	50,60,74	4.63	25 (50%)	29,97,114	2.51	13 (44%)
27	CLA	S	602	18	41,57,73	1.38	6 (14%)	43,93,113	1.37	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	S	603	-	41,57,73	1.30	5 (12%)	43,93,113	1.38	5 (11%)
27	CLA	S	604	-	41,57,73	1.32	6 (14%)	43,93,113	1.40	8 (18%)
37	CHL	S	606	-	48,58,74	4.65	25 (52%)	29,94,114	2.33	12 (41%)
37	CHL	S	607	-	48,58,74	4.61	24 (50%)	29,94,114	2.66	13 (44%)
37	CHL	S	608	-	47,57,74	4.59	23 (48%)	28,93,114	2.58	12 (42%)
27	CLA	S	609	18	41,57,73	1.34	4 (9%)	43,93,113	1.29	4 (9%)
27	CLA	S	610	18	41,57,73	1.32	5 (12%)	43,93,113	1.38	6 (13%)
27	CLA	S	611	35	41,57,73	1.33	6 (14%)	43,93,113	1.36	5 (11%)
27	CLA	S	612	18	41,57,73	1.33	7 (17%)	43,93,113	1.34	7 (16%)
27	CLA	S	613	18	41,57,73	1.32	7 (17%)	43,93,113	1.41	6 (13%)
27	CLA	S	614	-	41,57,73	1.36	7 (17%)	43,93,113	1.32	6 (13%)
38	LUT	Y	1620	-	42,43,43	1.05	3 (7%)	49,60,60	1.90	17 (34%)
38	LUT	Y	1621	-	42,43,43	1.12	4 (9%)	49,60,60	1.89	17 (34%)
39	XAT	Y	1622	-	47,47,47	1.35	2 (4%)	40,74,74	1.99	11 (27%)
40	NEX	Y	1623	-	42,46,46	1.28	2 (4%)	40,70,70	2.00	10 (25%)
35	LHG	Y	2630	27	48,48,48	0.74	2 (4%)	49,54,54	1.31	7 (14%)
37	CHL	Y	601	7	64,74,74	4.11	27 (42%)	47,114,114	2.08	15 (31%)
27	CLA	Y	602	7	57,73,73	1.20	8 (14%)	61,113,113	1.28	8 (13%)
27	CLA	Y	603	-	41,57,73	1.36	7 (17%)	43,93,113	1.35	7 (16%)
27	CLA	Y	604	-	41,57,73	1.39	8 (19%)	43,93,113	1.38	6 (13%)
37	CHL	Y	605	7	46,56,74	4.80	26 (56%)	28,92,114	2.41	11 (39%)
37	CHL	Y	606	-	48,58,74	4.77	26 (54%)	29,94,114	2.50	12 (41%)
37	CHL	Y	607	-	48,58,74	4.78	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	Y	608	-	48,58,74	4.76	27 (56%)	29,94,114	2.30	11 (37%)
37	CHL	Y	609	7	64,74,74	4.14	26 (40%)	47,114,114	2.13	14 (29%)
27	CLA	Y	610	7	57,73,73	1.17	7 (12%)	61,113,113	1.25	7 (11%)
27	CLA	Y	611	35	57,73,73	1.15	7 (12%)	61,113,113	1.22	7 (11%)
27	CLA	Y	612	7	57,73,73	1.17	8 (14%)	61,113,113	1.23	7 (11%)
27	CLA	Y	613	7	57,73,73	1.18	8 (14%)	61,113,113	1.20	6 (9%)
27	CLA	Y	614	-	41,57,73	1.35	7 (17%)	43,93,113	1.34	7 (16%)
31	LMG	Z	101	-	51,51,55	0.71	0	59,59,63	1.35	7 (11%)
24	OEX	a	401	1,3	0,15,15	0.00	-	0,32,32	0.00	-
27	CLA	a	405	-	57,73,73	1.24	7 (12%)	61,113,113	1.24	6 (9%)
27	CLA	a	406	-	57,73,73	1.19	7 (12%)	61,113,113	1.24	5 (8%)
27	CLA	a	407	-	41,57,73	1.36	7 (17%)	43,93,113	1.39	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	PHO	a	408	-	67,69,69	1.20	10 (14%)	86,99,99	1.15	10 (11%)
28	PHO	a	409	-	67,69,69	1.20	10 (14%)	86,99,99	1.12	6 (6%)
27	CLA	a	410	-	52,68,73	1.25	8 (15%)	55,107,113	1.29	6 (10%)
29	BCR	a	411	-	41,41,41	0.91	3 (7%)	56,56,56	2.08	16 (28%)
30	SQD	a	412	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	10 (16%)
31	LMG	a	413	-	48,48,55	0.81	1 (2%)	56,56,63	1.56	13 (23%)
30	SQD	a	418	-	53,54,54	0.97	5 (9%)	62,65,65	1.73	10 (16%)
27	CLA	b	602	-	57,73,73	1.15	8 (14%)	61,113,113	1.17	5 (8%)
27	CLA	b	603	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	9 (14%)
27	CLA	b	604	-	57,73,73	1.22	8 (14%)	61,113,113	1.25	6 (9%)
27	CLA	b	605	-	57,73,73	1.20	7 (12%)	61,113,113	1.40	11 (18%)
27	CLA	b	606	-	57,73,73	1.21	8 (14%)	61,113,113	1.15	5 (8%)
27	CLA	b	607	-	57,73,73	1.18	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	b	608	-	57,73,73	1.14	8 (14%)	61,113,113	1.22	5 (8%)
27	CLA	b	609	-	57,73,73	1.14	7 (12%)	61,113,113	1.25	6 (9%)
27	CLA	b	610	-	57,73,73	1.16	8 (14%)	61,113,113	1.23	8 (13%)
27	CLA	b	611	-	57,73,73	1.19	8 (14%)	61,113,113	1.25	7 (11%)
27	CLA	b	612	-	57,73,73	1.22	7 (12%)	61,113,113	1.34	8 (13%)
27	CLA	b	613	-	57,73,73	1.20	8 (14%)	61,113,113	1.33	9 (14%)
27	CLA	b	614	-	57,73,73	1.19	8 (14%)	61,113,113	1.16	5 (8%)
27	CLA	b	615	-	57,73,73	1.20	8 (14%)	61,113,113	1.17	8 (13%)
27	CLA	b	616	-	57,73,73	1.19	7 (12%)	61,113,113	1.18	7 (11%)
27	CLA	b	617	-	57,73,73	1.18	7 (12%)	61,113,113	1.23	6 (9%)
29	BCR	b	618	-	41,41,41	0.91	3 (7%)	56,56,56	2.21	18 (32%)
29	BCR	b	619	-	41,41,41	0.92	3 (7%)	56,56,56	2.07	17 (30%)
29	BCR	b	620	-	41,41,41	0.96	3 (7%)	56,56,56	2.13	17 (30%)
30	SQD	b	621	-	53,54,54	0.94	5 (9%)	62,65,65	1.96	9 (14%)
31	LMG	b	622	-	51,51,55	0.78	2 (3%)	59,59,63	1.45	7 (11%)
27	CLA	c	501	-	57,73,73	1.18	7 (12%)	61,113,113	1.25	8 (13%)
27	CLA	c	502	-	57,73,73	1.16	7 (12%)	61,113,113	1.26	6 (9%)
27	CLA	c	503	-	57,73,73	1.18	8 (14%)	61,113,113	1.25	10 (16%)
27	CLA	c	504	-	57,73,73	1.17	6 (10%)	61,113,113	1.20	5 (8%)
27	CLA	c	505	-	57,73,73	1.20	7 (12%)	61,113,113	1.35	6 (9%)
27	CLA	c	506	-	57,73,73	1.17	8 (14%)	61,113,113	1.30	7 (11%)
27	CLA	c	507	-	57,73,73	1.22	8 (14%)	61,113,113	1.15	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	c	508	-	57,73,73	1.24	8 (14%)	61,113,113	1.35	9 (14%)
27	CLA	c	509	-	57,73,73	1.21	8 (14%)	61,113,113	1.34	9 (14%)
27	CLA	c	510	-	57,73,73	1.17	7 (12%)	61,113,113	1.29	6 (9%)
27	CLA	c	511	3	57,73,73	1.17	7 (12%)	61,113,113	1.28	6 (9%)
27	CLA	c	512	-	57,73,73	1.15	7 (12%)	61,113,113	1.23	8 (13%)
27	CLA	c	513	-	41,57,73	1.37	8 (19%)	43,93,113	1.45	7 (16%)
29	BCR	c	514	-	41,41,41	0.89	1 (2%)	56,56,56	2.01	19 (33%)
29	BCR	c	515	-	41,41,41	0.90	1 (2%)	56,56,56	2.15	19 (33%)
29	BCR	c	516	-	41,41,41	0.78	0	56,56,56	2.29	18 (32%)
29	BCR	c	517	-	41,41,41	0.96	2 (4%)	56,56,56	2.32	16 (28%)
32	DGD	c	518	-	56,56,67	1.13	8 (14%)	70,70,81	1.73	16 (22%)
32	DGD	c	519	-	63,63,67	0.96	4 (6%)	77,77,81	1.54	14 (18%)
32	DGD	c	520	-	63,63,67	0.96	4 (6%)	77,77,81	1.53	11 (14%)
31	LMG	c	521	-	51,51,55	0.73	0	59,59,63	1.39	8 (13%)
33	BCT	d	401	-	0,3,3	0.00	-	0,3,3	0.00	-
27	CLA	d	402	-	57,73,73	1.25	8 (14%)	61,113,113	1.27	7 (11%)
27	CLA	d	403	-	57,73,73	1.14	6 (10%)	61,113,113	1.30	7 (11%)
29	BCR	d	404	-	41,41,41	0.81	0	56,56,56	2.19	14 (25%)
34	PL9	d	405	-	54,55,55	1.60	9 (16%)	68,69,69	1.57	15 (22%)
35	LHG	d	408	-	42,42,48	0.76	1 (2%)	43,48,54	1.29	5 (11%)
35	LHG	d	409	-	48,48,48	0.74	1 (2%)	49,54,54	1.37	8 (16%)
35	LHG	d	410	-	36,36,48	0.70	0	37,42,54	1.28	4 (10%)
31	LMG	d	411	-	46,46,55	0.83	4 (8%)	54,54,63	1.42	6 (11%)
36	HEM	f	101	5,6	24,50,50	2.32	6 (25%)	16,82,82	1.42	3 (18%)
38	LUT	g	1620	-	42,43,43	0.99	2 (4%)	49,60,60	1.92	15 (30%)
38	LUT	g	1621	-	42,43,43	1.03	2 (4%)	49,60,60	1.87	17 (34%)
39	XAT	g	1622	-	47,47,47	1.38	3 (6%)	40,74,74	1.82	8 (20%)
40	NEX	g	1623	-	42,46,46	1.26	3 (7%)	40,70,70	1.96	10 (25%)
35	LHG	g	2630	27	48,48,48	0.60	0	49,54,54	1.29	7 (14%)
37	CHL	g	601	7	64,74,74	4.13	26 (40%)	47,114,114	2.08	16 (34%)
27	CLA	g	602	7	57,73,73	1.18	8 (14%)	61,113,113	1.27	7 (11%)
27	CLA	g	603	-	41,57,73	1.33	6 (14%)	43,93,113	1.37	6 (13%)
27	CLA	g	604	-	41,57,73	1.34	6 (14%)	43,93,113	1.32	7 (16%)
37	CHL	g	605	7	46,56,74	4.70	26 (56%)	28,92,114	2.52	15 (53%)
37	CHL	g	606	-	48,58,74	4.71	26 (54%)	29,94,114	2.51	14 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	g	607	-	48,58,74	4.68	26 (54%)	29,94,114	2.31	12 (41%)
37	CHL	g	608	-	48,58,74	4.69	25 (52%)	29,94,114	2.35	13 (44%)
37	CHL	g	609	7	48,58,74	4.71	26 (54%)	29,94,114	2.36	12 (41%)
27	CLA	g	610	7	57,73,73	1.14	6 (10%)	61,113,113	1.22	5 (8%)
27	CLA	g	611	35	41,57,73	1.32	7 (17%)	43,93,113	1.35	6 (13%)
27	CLA	g	612	7	41,57,73	1.35	7 (17%)	43,93,113	1.32	6 (13%)
27	CLA	g	613	7	41,57,73	1.32	8 (19%)	43,93,113	1.41	8 (18%)
27	CLA	g	614	-	41,57,73	1.32	5 (12%)	43,93,113	1.31	5 (11%)
29	BCR	h	101	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	19 (33%)
32	DGD	h	102	-	63,63,67	0.97	3 (4%)	77,77,81	1.49	10 (12%)
35	LHG	l	101	-	48,48,48	0.71	1 (2%)	49,54,54	1.32	7 (14%)
38	LUT	n	1620	-	42,43,43	0.97	2 (4%)	49,60,60	2.01	16 (32%)
38	LUT	n	1621	-	42,43,43	1.01	3 (7%)	49,60,60	1.82	13 (26%)
39	XAT	n	1622	-	47,47,47	1.38	3 (6%)	40,74,74	2.24	14 (35%)
40	NEX	n	1623	-	42,46,46	1.26	2 (4%)	40,70,70	1.99	9 (22%)
35	LHG	n	2630	27	48,48,48	0.60	1 (2%)	49,54,54	1.29	7 (14%)
37	CHL	n	601	7	48,58,74	4.68	24 (50%)	29,94,114	2.48	14 (48%)
27	CLA	n	602	7	57,73,73	1.17	7 (12%)	61,113,113	1.16	5 (8%)
27	CLA	n	603	-	41,57,73	1.35	7 (17%)	43,93,113	1.35	6 (13%)
27	CLA	n	604	-	41,57,73	1.32	6 (14%)	43,93,113	1.38	6 (13%)
37	CHL	n	605	7	46,56,74	4.85	26 (56%)	28,92,114	2.60	15 (53%)
37	CHL	n	606	-	48,58,74	4.70	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	n	607	-	64,74,74	4.12	26 (40%)	47,114,114	1.96	15 (31%)
37	CHL	n	608	-	48,58,74	4.74	26 (54%)	29,94,114	2.39	12 (41%)
37	CHL	n	609	7	48,58,74	4.81	26 (54%)	29,94,114	2.44	13 (44%)
27	CLA	n	610	7	57,73,73	1.16	7 (12%)	61,113,113	1.22	7 (11%)
27	CLA	n	611	35	41,57,73	1.29	6 (14%)	43,93,113	1.39	8 (18%)
27	CLA	n	612	7	41,57,73	1.34	6 (14%)	43,93,113	1.35	7 (16%)
27	CLA	n	613	7	41,57,73	1.32	7 (17%)	43,93,113	1.35	5 (11%)
27	CLA	n	614	-	41,57,73	1.27	4 (9%)	43,93,113	1.35	7 (16%)
35	LHG	r	2630	27	48,48,48	0.60	0	49,54,54	1.25	6 (12%)
27	CLA	r	601	17	41,57,73	1.29	5 (12%)	43,93,113	1.45	8 (18%)
27	CLA	r	602	17	57,73,73	1.16	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	r	603	-	41,57,73	1.34	7 (17%)	43,93,113	1.33	6 (13%)
27	CLA	r	604	-	41,57,73	1.31	5 (12%)	43,93,113	1.45	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	CHL	r	606	-	48,58,74	4.70	26 (54%)	29,94,114	2.42	12 (41%)
37	CHL	r	607	-	48,58,74	4.72	25 (52%)	29,94,114	2.38	12 (41%)
37	CHL	r	608	-	48,58,74	4.73	26 (54%)	29,94,114	2.30	12 (41%)
27	CLA	r	609	17	41,57,73	1.32	7 (17%)	43,93,113	1.29	5 (11%)
27	CLA	r	610	17	57,73,73	1.16	7 (12%)	61,113,113	1.17	6 (9%)
27	CLA	r	611	35	41,57,73	1.30	5 (12%)	43,93,113	1.29	6 (13%)
27	CLA	r	612	-	41,57,73	1.32	7 (17%)	43,93,113	1.29	5 (11%)
27	CLA	r	613	17	41,57,73	1.30	5 (12%)	43,93,113	1.35	5 (11%)
27	CLA	r	616	17	41,57,73	1.32	5 (12%)	43,93,113	1.31	6 (13%)
38	LUT	r	620	-	42,43,43	0.94	2 (4%)	49,60,60	1.70	15 (30%)
39	XAT	r	622	-	47,47,47	1.37	3 (6%)	40,74,74	1.91	13 (32%)
40	NEX	r	623	-	42,46,46	1.30	2 (4%)	40,70,70	1.85	13 (32%)
38	LUT	s	1620	-	42,43,43	0.98	3 (7%)	49,60,60	2.06	16 (32%)
38	LUT	s	1621	-	42,43,43	0.98	3 (7%)	49,60,60	1.81	15 (30%)
40	NEX	s	1623	-	42,46,46	1.21	3 (7%)	40,70,70	1.89	9 (22%)
35	LHG	s	2630	27	48,48,48	0.63	1 (2%)	49,54,54	1.28	6 (12%)
37	CHL	s	601	18	50,60,74	4.62	25 (50%)	29,97,114	2.51	13 (44%)
27	CLA	s	602	18	41,57,73	1.37	6 (14%)	43,93,113	1.37	7 (16%)
27	CLA	s	603	-	41,57,73	1.30	5 (12%)	43,93,113	1.37	6 (13%)
27	CLA	s	604	-	41,57,73	1.32	7 (17%)	43,93,113	1.40	8 (18%)
37	CHL	s	606	-	48,58,74	4.64	25 (52%)	29,94,114	2.32	12 (41%)
37	CHL	s	607	-	48,58,74	4.61	24 (50%)	29,94,114	2.65	13 (44%)
37	CHL	s	608	-	47,57,74	4.59	23 (48%)	28,93,114	2.58	12 (42%)
27	CLA	s	609	18	41,57,73	1.33	5 (12%)	43,93,113	1.29	4 (9%)
27	CLA	s	610	18	41,57,73	1.32	5 (12%)	43,93,113	1.39	6 (13%)
27	CLA	s	611	35	41,57,73	1.32	7 (17%)	43,93,113	1.36	5 (11%)
27	CLA	s	612	18	41,57,73	1.33	7 (17%)	43,93,113	1.34	7 (16%)
27	CLA	s	613	18	41,57,73	1.32	7 (17%)	43,93,113	1.42	6 (13%)
27	CLA	s	614	-	41,57,73	1.37	7 (17%)	43,93,113	1.31	6 (13%)
38	LUT	y	1620	-	42,43,43	1.05	3 (7%)	49,60,60	1.90	17 (34%)
38	LUT	y	1621	-	42,43,43	1.12	4 (9%)	49,60,60	1.90	17 (34%)
39	XAT	y	1622	-	47,47,47	1.35	2 (4%)	40,74,74	1.98	11 (27%)
40	NEX	y	1623	-	42,46,46	1.28	2 (4%)	40,70,70	2.00	10 (25%)
35	LHG	y	2630	27	48,48,48	0.73	1 (2%)	49,54,54	1.31	7 (14%)
37	CHL	y	601	7	64,74,74	4.12	27 (42%)	47,114,114	2.08	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CLA	y	602	7	57,73,73	1.20	8 (14%)	61,113,113	1.28	8 (13%)
27	CLA	y	603	-	41,57,73	1.36	7 (17%)	43,93,113	1.35	7 (16%)
27	CLA	y	604	-	41,57,73	1.38	8 (19%)	43,93,113	1.38	6 (13%)
37	CHL	y	605	7	46,56,74	4.80	26 (56%)	28,92,114	2.41	11 (39%)
37	CHL	y	606	-	48,58,74	4.77	26 (54%)	29,94,114	2.50	13 (44%)
37	CHL	y	607	-	48,58,74	4.78	26 (54%)	29,94,114	2.37	13 (44%)
37	CHL	y	608	-	48,58,74	4.76	27 (56%)	29,94,114	2.30	11 (37%)
37	CHL	y	609	7	64,74,74	4.14	26 (40%)	47,114,114	2.12	14 (29%)
27	CLA	y	610	7	57,73,73	1.17	7 (12%)	61,113,113	1.25	7 (11%)
27	CLA	y	611	35	57,73,73	1.15	7 (12%)	61,113,113	1.22	7 (11%)
27	CLA	y	612	7	57,73,73	1.17	8 (14%)	61,113,113	1.23	7 (11%)
27	CLA	y	613	7	57,73,73	1.18	8 (14%)	61,113,113	1.20	7 (11%)
27	CLA	y	614	-	41,57,73	1.35	6 (14%)	43,93,113	1.33	7 (16%)
31	LMG	z	101	-	51,51,55	0.71	0	59,59,63	1.36	8 (13%)

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
24	OEX	A	401	1,3	-	0/0/68/68	0/0/6/6
27	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	A	406	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	A	407	-	3/3/16/25	0/18/116/135	0/0/9/9
28	PHO	A	408	-	-	0/53/103/103	0/1/6/6
28	PHO	A	409	-	-	0/53/103/103	0/1/6/6
27	CLA	A	410	-	3/3/19/25	0/31/129/135	0/0/9/9
29	BCR	A	411	-	-	0/29/63/63	0/2/2/2
30	SQD	A	412	-	-	0/49/69/69	0/1/1/1
31	LMG	A	413	-	-	0/43/63/70	0/1/1/1
30	SQD	A	418	-	-	0/49/69/69	0/1/1/1
27	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	B	618	-	-	0/29/63/63	0/2/2/2
29	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	BCR	B	620	-	-	0/29/63/63	0/2/2/2
30	SQD	B	621	-	-	0/49/69/69	0/1/1/1
31	LMG	B	622	-	-	0/46/66/70	0/1/1/1
27	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	C	513	-	3/3/16/25	0/18/116/135	0/0/9/9
29	BCR	C	514	-	-	0/29/63/63	0/2/2/2
29	BCR	C	515	-	-	0/29/63/63	0/2/2/2
29	BCR	C	516	-	-	0/29/63/63	0/2/2/2
29	BCR	C	517	-	-	0/29/63/63	0/2/2/2
32	DGD	C	518	-	-	0/44/84/95	0/2/2/2
32	DGD	C	519	-	-	0/51/91/95	0/2/2/2
32	DGD	C	520	-	-	0/51/91/95	0/2/2/2
31	LMG	C	521	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCT	D	401	-	-	0/0/0/0	0/0/0/0
27	CLA	D	402	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	D	404	-	-	0/29/63/63	0/2/2/2
34	PL9	D	405	-	-	0/53/73/73	0/1/1/1
35	LHG	D	408	-	-	0/47/47/53	0/0/0/0
35	LHG	D	409	-	-	0/53/53/53	0/0/0/0
35	LHG	D	410	-	-	0/41/41/53	0/0/0/0
31	LMG	D	411	-	-	0/41/61/70	0/1/1/1
36	HEM	F	101	5,6	-	0/6/54/54	0/0/8/8
38	LUT	G	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	G	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	G	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	G	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	G	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	G	601	7	-	0/41/177/177	0/0/9/9
27	CLA	G	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	G	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	G	605	7	-	0/20/156/177	0/0/9/9
37	CHL	G	606	-	-	0/22/158/177	0/0/9/9
37	CHL	G	607	-	-	0/22/158/177	0/0/9/9
37	CHL	G	608	-	-	0/22/158/177	0/0/9/9
37	CHL	G	609	7	-	0/22/158/177	0/0/9/9
27	CLA	G	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	G	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	G	614	-	3/3/16/25	0/18/116/135	0/0/9/9
29	BCR	H	101	-	-	0/29/63/63	0/2/2/2
32	DGD	H	102	-	-	0/51/91/95	0/2/2/2
35	LHG	L	101	-	-	0/53/53/53	0/0/0/0
38	LUT	N	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	N	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	N	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	N	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	N	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	N	601	7	-	0/22/158/177	0/0/9/9
27	CLA	N	602	7	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	CLA	N	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	N	605	7	-	0/20/156/177	0/0/9/9
37	CHL	N	606	-	-	0/22/158/177	0/0/9/9
37	CHL	N	607	-	-	0/41/177/177	0/0/9/9
37	CHL	N	608	-	-	0/22/158/177	0/0/9/9
37	CHL	N	609	7	-	0/22/158/177	0/0/9/9
27	CLA	N	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	N	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	N	614	-	3/3/16/25	0/18/116/135	0/0/9/9
35	LHG	R	2630	27	-	0/53/53/53	0/0/0/0
27	CLA	R	601	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	602	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	R	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	R	606	-	-	0/22/158/177	0/0/9/9
37	CHL	R	607	-	-	0/22/158/177	0/0/9/9
37	CHL	R	608	-	-	0/22/158/177	0/0/9/9
27	CLA	R	609	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	610	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	R	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	612	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	613	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	R	616	17	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	R	620	-	-	0/29/67/67	0/2/2/2
39	XAT	R	622	-	-	0/31/93/93	0/2/4/4
40	NEX	R	623	-	-	0/27/83/83	0/2/3/3
38	LUT	S	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
40	NEX	S	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	S	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	S	601	18	-	0/25/161/177	0/0/9/9
27	CLA	S	602	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	603	-	2/2/16/25	0/18/116/135	0/0/9/9
27	CLA	S	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	S	606	-	-	0/22/158/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	S	607	-	-	0/22/158/177	0/0/9/9
37	CHL	S	608	-	-	0/21/157/177	0/0/9/9
27	CLA	S	609	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	610	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	612	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	613	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	S	614	-	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	Y	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	Y	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	Y	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	Y	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	Y	601	7	-	0/41/177/177	0/0/9/9
27	CLA	Y	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	Y	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	Y	605	7	-	0/20/156/177	0/0/9/9
37	CHL	Y	606	-	-	0/22/158/177	0/0/9/9
37	CHL	Y	607	-	-	0/22/158/177	0/0/9/9
37	CHL	Y	608	-	-	0/22/158/177	0/0/9/9
37	CHL	Y	609	7	-	0/41/177/177	0/0/9/9
27	CLA	Y	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	611	35	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	612	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	613	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	Y	614	-	3/3/16/25	0/18/116/135	0/0/9/9
31	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
24	OEX	a	401	1,3	-	0/0/68/68	0/0/6/6
27	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	a	407	-	3/3/16/25	0/18/116/135	0/0/9/9
28	PHO	a	408	-	-	0/53/103/103	0/1/6/6
28	PHO	a	409	-	-	0/53/103/103	0/1/6/6
27	CLA	a	410	-	3/3/19/25	0/31/129/135	0/0/9/9
29	BCR	a	411	-	-	0/29/63/63	0/2/2/2
30	SQD	a	412	-	-	0/49/69/69	0/1/1/1
31	LMG	a	413	-	-	0/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	SQD	a	418	-	-	0/49/69/69	0/1/1/1
27	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	b	618	-	-	0/29/63/63	0/2/2/2
29	BCR	b	619	-	-	0/29/63/63	0/2/2/2
29	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	SQD	b	621	-	-	0/49/69/69	0/1/1/1
31	LMG	b	622	-	-	0/46/66/70	0/1/1/1
27	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	c	513	-	3/3/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	BCR	c	514	-	-	0/29/63/63	0/2/2/2
29	BCR	c	515	-	-	0/29/63/63	0/2/2/2
29	BCR	c	516	-	-	0/29/63/63	0/2/2/2
29	BCR	c	517	-	-	0/29/63/63	0/2/2/2
32	DGD	c	518	-	-	0/44/84/95	0/2/2/2
32	DGD	c	519	-	-	0/51/91/95	0/2/2/2
32	DGD	c	520	-	-	0/51/91/95	0/2/2/2
31	LMG	c	521	-	-	0/46/66/70	0/1/1/1
33	BCT	d	401	-	-	0/0/0/0	0/0/0/0
27	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
29	BCR	d	404	-	-	0/29/63/63	0/2/2/2
34	PL9	d	405	-	-	0/53/73/73	0/1/1/1
35	LHG	d	408	-	-	0/47/47/53	0/0/0/0
35	LHG	d	409	-	-	0/53/53/53	0/0/0/0
35	LHG	d	410	-	-	0/41/41/53	0/0/0/0
31	LMG	d	411	-	-	0/41/61/70	0/1/1/1
36	HEM	f	101	5,6	-	0/6/54/54	0/0/8/8
38	LUT	g	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	g	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	g	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	g	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	g	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	g	601	7	-	0/41/177/177	0/0/9/9
27	CLA	g	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	g	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	g	605	7	-	0/20/156/177	0/0/9/9
37	CHL	g	606	-	-	0/22/158/177	0/0/9/9
37	CHL	g	607	-	-	0/22/158/177	0/0/9/9
37	CHL	g	608	-	-	0/22/158/177	0/0/9/9
37	CHL	g	609	7	-	0/22/158/177	0/0/9/9
27	CLA	g	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	g	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	g	614	-	3/3/16/25	0/18/116/135	0/0/9/9
29	BCR	h	101	-	-	0/29/63/63	0/2/2/2
32	DGD	h	102	-	-	0/51/91/95	0/2/2/2
35	LHG	l	101	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	n	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	n	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	n	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	n	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	n	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	n	601	7	-	0/22/158/177	0/0/9/9
27	CLA	n	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	n	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	n	605	7	-	0/20/156/177	0/0/9/9
37	CHL	n	606	-	-	0/22/158/177	0/0/9/9
37	CHL	n	607	-	-	0/41/177/177	0/0/9/9
37	CHL	n	608	-	-	0/22/158/177	0/0/9/9
37	CHL	n	609	7	-	0/22/158/177	0/0/9/9
27	CLA	n	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	n	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	612	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	613	7	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	n	614	-	3/3/16/25	0/18/116/135	0/0/9/9
35	LHG	r	2630	27	-	0/53/53/53	0/0/0/0
27	CLA	r	601	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	602	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	r	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	r	606	-	-	0/22/158/177	0/0/9/9
37	CHL	r	607	-	-	0/22/158/177	0/0/9/9
37	CHL	r	608	-	-	0/22/158/177	0/0/9/9
27	CLA	r	609	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	610	17	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	r	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	612	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	613	17	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	r	616	17	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	r	620	-	-	0/29/67/67	0/2/2/2
39	XAT	r	622	-	-	0/31/93/93	0/2/4/4
40	NEX	r	623	-	-	0/27/83/83	0/2/3/3
38	LUT	s	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	s	1621	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	NEX	s	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	s	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	s	601	18	-	0/25/161/177	0/0/9/9
27	CLA	s	602	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	603	-	2/2/16/25	0/18/116/135	0/0/9/9
27	CLA	s	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	s	606	-	-	0/22/158/177	0/0/9/9
37	CHL	s	607	-	-	0/22/158/177	0/0/9/9
37	CHL	s	608	-	-	0/21/157/177	0/0/9/9
27	CLA	s	609	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	610	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	611	35	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	612	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	613	18	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	s	614	-	3/3/16/25	0/18/116/135	0/0/9/9
38	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
38	LUT	y	1621	-	-	0/29/67/67	0/2/2/2
39	XAT	y	1622	-	-	0/31/93/93	0/2/4/4
40	NEX	y	1623	-	-	0/27/83/83	0/2/3/3
35	LHG	y	2630	27	-	0/53/53/53	0/0/0/0
37	CHL	y	601	7	-	0/41/177/177	0/0/9/9
27	CLA	y	602	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	603	-	3/3/16/25	0/18/116/135	0/0/9/9
27	CLA	y	604	-	3/3/16/25	0/18/116/135	0/0/9/9
37	CHL	y	605	7	-	0/20/156/177	0/0/9/9
37	CHL	y	606	-	-	0/22/158/177	0/0/9/9
37	CHL	y	607	-	-	0/22/158/177	0/0/9/9
37	CHL	y	608	-	-	0/22/158/177	0/0/9/9
37	CHL	y	609	7	-	0/41/177/177	0/0/9/9
27	CLA	y	610	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	611	35	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	612	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	613	7	3/3/20/25	0/37/135/135	0/0/9/9
27	CLA	y	614	-	3/3/16/25	0/18/116/135	0/0/9/9
31	LMG	z	101	-	-	0/46/66/70	0/1/1/1

All (2657) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	601	CHL	C3D-C4D	-20.31	1.32	1.54
37	g	601	CHL	C3D-C4D	-20.27	1.32	1.54
37	R	608	CHL	C3D-C4D	-20.19	1.32	1.54
37	r	608	CHL	C3D-C4D	-20.19	1.32	1.54
37	Y	608	CHL	C3D-C4D	-20.18	1.32	1.54
37	Y	601	CHL	C3D-C4D	-20.18	1.32	1.54
37	y	601	CHL	C3D-C4D	-20.17	1.32	1.54
37	n	605	CHL	C3D-C4D	-20.15	1.32	1.54
37	y	608	CHL	C3D-C4D	-20.14	1.32	1.54
37	y	609	CHL	C3D-C4D	-20.13	1.32	1.54
37	y	606	CHL	C3D-C4D	-20.11	1.32	1.54
37	n	608	CHL	C3D-C4D	-20.11	1.32	1.54
37	g	608	CHL	C3D-C4D	-20.11	1.32	1.54
37	Y	606	CHL	C3D-C4D	-20.09	1.32	1.54
37	Y	609	CHL	C3D-C4D	-20.09	1.32	1.54
37	N	607	CHL	C3D-C4D	-20.07	1.32	1.54
37	n	607	CHL	C3D-C4D	-20.05	1.32	1.54
37	n	609	CHL	C3D-C4D	-20.05	1.32	1.54
37	N	609	CHL	C3D-C4D	-20.05	1.32	1.54
37	N	608	CHL	C3D-C4D	-20.04	1.32	1.54
37	Y	607	CHL	C3D-C4D	-20.04	1.32	1.54
37	y	607	CHL	C3D-C4D	-20.03	1.32	1.54
37	N	605	CHL	C3D-C4D	-20.02	1.32	1.54
37	G	608	CHL	C3D-C4D	-19.99	1.32	1.54
37	G	609	CHL	C3D-C4D	-19.99	1.32	1.54
37	S	601	CHL	C3D-C4D	-19.98	1.32	1.54
37	G	606	CHL	C3D-C4D	-19.97	1.32	1.54
37	N	601	CHL	C3D-C4D	-19.96	1.32	1.54
37	n	601	CHL	C3D-C4D	-19.95	1.32	1.54
37	g	609	CHL	C3D-C4D	-19.94	1.32	1.54
37	s	601	CHL	C3D-C4D	-19.91	1.32	1.54
37	g	606	CHL	C3D-C4D	-19.91	1.32	1.54
37	R	607	CHL	C3D-C4D	-19.89	1.32	1.54
37	r	607	CHL	C3D-C4D	-19.89	1.32	1.54
37	S	606	CHL	C3D-C4D	-19.89	1.32	1.54
37	s	606	CHL	C3D-C4D	-19.89	1.32	1.54
37	N	606	CHL	C3D-C4D	-19.88	1.32	1.54
37	n	606	CHL	C3D-C4D	-19.81	1.33	1.54
37	R	606	CHL	C3D-C4D	-19.80	1.33	1.54
37	S	607	CHL	C3D-C4D	-19.75	1.33	1.54
37	s	607	CHL	C3D-C4D	-19.72	1.33	1.54
37	S	608	CHL	C3D-C4D	-19.69	1.33	1.54
37	s	608	CHL	C3D-C4D	-19.69	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	r	606	CHL	C3D-C4D	-19.69	1.33	1.54
37	y	605	CHL	C3D-C4D	-19.61	1.33	1.54
37	G	607	CHL	C3D-C4D	-19.58	1.33	1.54
37	G	605	CHL	C3D-C4D	-19.58	1.33	1.54
37	g	607	CHL	C3D-C4D	-19.58	1.33	1.54
37	Y	605	CHL	C3D-C4D	-19.58	1.33	1.54
37	g	605	CHL	C3D-C4D	-19.54	1.33	1.54
37	g	606	CHL	CHB-C4A	-8.36	1.31	1.52
37	Y	607	CHL	CHB-C4A	-8.35	1.31	1.52
37	G	606	CHL	CHB-C4A	-8.34	1.31	1.52
37	y	607	CHL	CHB-C4A	-8.31	1.31	1.52
37	N	607	CHL	CHB-C4A	-8.23	1.32	1.52
37	y	606	CHL	CHB-C4A	-8.22	1.32	1.52
37	Y	606	CHL	CHB-C4A	-8.22	1.32	1.52
37	n	607	CHL	CHB-C4A	-8.22	1.32	1.52
37	N	608	CHL	CHB-C4A	-8.21	1.32	1.52
37	s	601	CHL	CHB-C4A	-8.21	1.32	1.52
37	S	601	CHL	CHB-C4A	-8.21	1.32	1.52
37	n	609	CHL	CHB-C4A	-8.21	1.32	1.52
37	N	609	CHL	CHB-C4A	-8.21	1.32	1.52
37	N	606	CHL	CHB-C4A	-8.20	1.32	1.52
37	n	608	CHL	CHB-C4A	-8.19	1.32	1.52
37	y	608	CHL	CHB-C4A	-8.19	1.32	1.52
37	Y	608	CHL	CHB-C4A	-8.18	1.32	1.52
37	n	606	CHL	CHB-C4A	-8.18	1.32	1.52
37	R	607	CHL	CHB-C4A	-8.15	1.32	1.52
37	r	607	CHL	CHB-C4A	-8.15	1.32	1.52
37	G	607	CHL	CHB-C4A	-8.15	1.32	1.52
37	g	607	CHL	CHB-C4A	-8.12	1.32	1.52
37	G	608	CHL	CHB-C4A	-8.09	1.32	1.52
37	y	601	CHL	CHB-C4A	-8.08	1.32	1.52
37	Y	609	CHL	CHB-C4A	-8.07	1.32	1.52
37	y	609	CHL	CHB-C4A	-8.07	1.32	1.52
37	r	606	CHL	CHB-C4A	-8.07	1.32	1.52
37	n	605	CHL	CHB-C4A	-8.06	1.32	1.52
37	g	608	CHL	CHB-C4A	-8.05	1.32	1.52
37	R	606	CHL	CHB-C4A	-8.05	1.32	1.52
37	N	605	CHL	CHB-C4A	-8.04	1.32	1.52
37	Y	601	CHL	CHB-C4A	-8.04	1.32	1.52
37	S	606	CHL	CHB-C4A	-8.04	1.32	1.52
37	s	606	CHL	CHB-C4A	-8.04	1.32	1.52
37	g	601	CHL	CHB-C4A	-8.02	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	601	CHL	CHB-C4A	-8.00	1.32	1.52
37	r	608	CHL	CHB-C4A	-7.97	1.32	1.52
37	R	608	CHL	CHB-C4A	-7.97	1.32	1.52
37	s	607	CHL	CHB-C4A	-7.92	1.32	1.52
37	S	607	CHL	CHB-C4A	-7.92	1.32	1.52
37	y	605	CHL	CHB-C4A	-7.92	1.32	1.52
37	Y	605	CHL	CHB-C4A	-7.92	1.32	1.52
37	N	601	CHL	CHB-C4A	-7.91	1.32	1.52
37	g	609	CHL	CHB-C4A	-7.90	1.32	1.52
37	G	609	CHL	CHB-C4A	-7.90	1.32	1.52
37	n	601	CHL	CHB-C4A	-7.90	1.32	1.52
37	g	605	CHL	CHB-C4A	-7.89	1.32	1.52
37	G	605	CHL	CHB-C4A	-7.89	1.32	1.52
37	R	606	CHL	C3B-C2B	-7.74	1.45	1.55
37	r	606	CHL	C3B-C2B	-7.69	1.45	1.55
37	Y	607	CHL	C1B-NB	-7.62	1.33	1.50
37	y	607	CHL	C1B-NB	-7.61	1.34	1.50
37	s	608	CHL	CHB-C4A	-7.58	1.33	1.52
37	y	606	CHL	C3B-C2B	-7.57	1.45	1.55
37	y	607	CHL	C3B-C2B	-7.57	1.45	1.55
37	Y	607	CHL	C3B-C2B	-7.56	1.45	1.55
37	S	608	CHL	CHB-C4A	-7.55	1.33	1.52
37	n	609	CHL	C4B-NB	-7.55	1.34	1.50
37	Y	606	CHL	C3B-C2B	-7.52	1.46	1.55
37	N	609	CHL	C3B-C2B	-7.52	1.46	1.55
37	N	609	CHL	C4B-NB	-7.51	1.34	1.50
37	n	609	CHL	C3B-C2B	-7.49	1.46	1.55
37	R	608	CHL	C1B-NB	-7.47	1.34	1.50
37	n	606	CHL	C3B-C2B	-7.47	1.46	1.55
37	N	606	CHL	C3B-C2B	-7.47	1.46	1.55
37	R	608	CHL	C1D-ND	-7.47	1.34	1.50
37	r	608	CHL	C1D-ND	-7.47	1.34	1.50
37	y	605	CHL	C3B-C2B	-7.46	1.46	1.55
37	Y	605	CHL	C3B-C2B	-7.46	1.46	1.55
37	n	609	CHL	C1B-NB	-7.45	1.34	1.50
37	N	609	CHL	C1B-NB	-7.45	1.34	1.50
37	Y	608	CHL	C3B-C2B	-7.45	1.46	1.55
37	g	601	CHL	C3B-C2B	-7.45	1.46	1.55
37	Y	609	CHL	C1B-NB	-7.45	1.34	1.50
37	n	608	CHL	C3B-C2B	-7.44	1.46	1.55
37	r	608	CHL	C1B-NB	-7.43	1.34	1.50
37	y	609	CHL	C1B-NB	-7.42	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	y	608	CHL	C3B-C2B	-7.42	1.46	1.55
37	y	601	CHL	C1B-NB	-7.42	1.34	1.50
37	N	605	CHL	C3B-C2B	-7.42	1.46	1.55
37	Y	609	CHL	C3B-C2B	-7.41	1.46	1.55
37	y	609	CHL	C3B-C2B	-7.40	1.46	1.55
37	N	608	CHL	C3B-C2B	-7.40	1.46	1.55
37	G	601	CHL	C3B-C2B	-7.40	1.46	1.55
37	Y	601	CHL	C1B-NB	-7.39	1.34	1.50
37	g	609	CHL	C1B-NB	-7.39	1.34	1.50
37	Y	608	CHL	C1B-NB	-7.39	1.34	1.50
37	n	607	CHL	C1B-NB	-7.38	1.34	1.50
37	G	609	CHL	C1B-NB	-7.38	1.34	1.50
37	y	608	CHL	C1D-ND	-7.37	1.34	1.50
37	N	607	CHL	C1B-NB	-7.37	1.34	1.50
37	Y	608	CHL	C1D-ND	-7.37	1.34	1.50
37	G	607	CHL	C1B-NB	-7.36	1.34	1.50
37	R	606	CHL	C1B-NB	-7.36	1.34	1.50
37	y	607	CHL	C1D-ND	-7.36	1.34	1.50
37	Y	607	CHL	C1D-ND	-7.36	1.34	1.50
37	g	609	CHL	C4B-NB	-7.36	1.34	1.50
37	y	606	CHL	C1D-ND	-7.36	1.34	1.50
37	Y	606	CHL	C1D-ND	-7.36	1.34	1.50
37	N	607	CHL	C4B-NB	-7.36	1.34	1.50
37	n	607	CHL	C4B-NB	-7.36	1.34	1.50
37	G	607	CHL	C3B-C2B	-7.36	1.46	1.55
37	y	608	CHL	C1B-NB	-7.36	1.34	1.50
37	s	606	CHL	C1B-NB	-7.35	1.34	1.50
37	s	607	CHL	C1B-NB	-7.35	1.34	1.50
37	S	607	CHL	C1B-NB	-7.35	1.34	1.50
37	n	605	CHL	C3B-C2B	-7.34	1.46	1.55
37	y	601	CHL	C1D-ND	-7.34	1.34	1.50
37	g	607	CHL	C1B-NB	-7.34	1.34	1.50
37	R	606	CHL	C1D-ND	-7.33	1.34	1.50
37	r	606	CHL	C1D-ND	-7.33	1.34	1.50
37	n	607	CHL	C1D-ND	-7.33	1.34	1.50
37	R	607	CHL	C1D-ND	-7.33	1.34	1.50
37	r	607	CHL	C1D-ND	-7.33	1.34	1.50
37	R	607	CHL	C1B-NB	-7.33	1.34	1.50
37	r	607	CHL	C1B-NB	-7.33	1.34	1.50
37	g	607	CHL	C3B-C2B	-7.33	1.46	1.55
37	S	601	CHL	C3B-C2B	-7.33	1.46	1.55
37	Y	601	CHL	C3B-C2B	-7.32	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	y	601	CHL	C3B-C2B	-7.32	1.46	1.55
37	y	606	CHL	C1B-NB	-7.32	1.34	1.50
37	Y	606	CHL	C1B-NB	-7.32	1.34	1.50
37	G	609	CHL	C4B-NB	-7.32	1.34	1.50
37	n	601	CHL	C1B-NB	-7.32	1.34	1.50
37	N	601	CHL	C1B-NB	-7.32	1.34	1.50
37	r	606	CHL	C1B-NB	-7.31	1.34	1.50
37	N	607	CHL	C1D-ND	-7.31	1.34	1.50
37	G	601	CHL	C4B-NB	-7.31	1.34	1.50
37	g	601	CHL	C4B-NB	-7.31	1.34	1.50
37	Y	607	CHL	C4B-NB	-7.31	1.34	1.50
37	n	608	CHL	C1B-NB	-7.31	1.34	1.50
37	S	606	CHL	C1B-NB	-7.31	1.34	1.50
37	Y	601	CHL	C1D-ND	-7.31	1.34	1.50
37	s	607	CHL	C4B-NB	-7.30	1.34	1.50
37	S	607	CHL	C4B-NB	-7.30	1.34	1.50
37	Y	605	CHL	C4B-NB	-7.30	1.34	1.50
37	G	608	CHL	C1B-NB	-7.30	1.34	1.50
37	g	608	CHL	C1B-NB	-7.30	1.34	1.50
37	s	607	CHL	C1D-ND	-7.30	1.34	1.50
37	S	607	CHL	C1D-ND	-7.30	1.34	1.50
37	N	608	CHL	C1B-NB	-7.29	1.34	1.50
37	g	606	CHL	C3B-C2B	-7.29	1.46	1.55
37	n	605	CHL	C4B-NB	-7.28	1.34	1.50
37	N	605	CHL	C4B-NB	-7.28	1.34	1.50
37	G	606	CHL	C3B-C2B	-7.28	1.46	1.55
37	y	605	CHL	C4B-NB	-7.27	1.34	1.50
37	Y	609	CHL	C4B-NB	-7.27	1.34	1.50
37	g	608	CHL	C4B-NB	-7.27	1.34	1.50
37	y	609	CHL	C4B-NB	-7.27	1.34	1.50
37	S	601	CHL	C1D-ND	-7.27	1.34	1.50
37	n	607	CHL	C3B-C2B	-7.26	1.46	1.55
37	N	601	CHL	C4B-NB	-7.26	1.34	1.50
37	y	607	CHL	C4B-NB	-7.26	1.34	1.50
37	S	608	CHL	C1D-ND	-7.26	1.34	1.50
37	s	608	CHL	C1D-ND	-7.26	1.34	1.50
37	G	601	CHL	C1B-NB	-7.26	1.34	1.50
37	S	606	CHL	C3B-C2B	-7.26	1.46	1.55
37	s	606	CHL	C3B-C2B	-7.26	1.46	1.55
37	n	609	CHL	C1D-ND	-7.26	1.34	1.50
37	Y	609	CHL	C1D-ND	-7.26	1.34	1.50
37	G	601	CHL	C1D-ND	-7.26	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	r	607	CHL	C4B-NB	-7.25	1.34	1.50
37	y	609	CHL	C1D-ND	-7.25	1.34	1.50
37	s	601	CHL	C3B-C2B	-7.25	1.46	1.55
37	n	601	CHL	C4B-NB	-7.25	1.34	1.50
37	R	607	CHL	C4B-NB	-7.25	1.34	1.50
37	y	605	CHL	C1B-NB	-7.25	1.34	1.50
37	Y	601	CHL	C4B-NB	-7.25	1.34	1.50
37	N	609	CHL	C1D-ND	-7.25	1.34	1.50
37	s	601	CHL	C1D-ND	-7.25	1.34	1.50
37	G	606	CHL	C1D-ND	-7.25	1.34	1.50
37	g	606	CHL	C1D-ND	-7.25	1.34	1.50
37	G	606	CHL	C1B-NB	-7.25	1.34	1.50
37	N	601	CHL	C1D-ND	-7.24	1.34	1.50
37	g	606	CHL	C1B-NB	-7.24	1.34	1.50
37	G	608	CHL	C4B-NB	-7.24	1.34	1.50
37	g	607	CHL	C1D-ND	-7.23	1.34	1.50
37	N	607	CHL	C3B-C2B	-7.23	1.46	1.55
37	N	606	CHL	C1D-ND	-7.23	1.34	1.50
37	n	606	CHL	C1D-ND	-7.23	1.34	1.50
37	g	606	CHL	C4B-NB	-7.23	1.34	1.50
37	g	605	CHL	C4B-NB	-7.23	1.34	1.50
37	n	601	CHL	C1D-ND	-7.23	1.34	1.50
37	g	605	CHL	C1B-NB	-7.23	1.34	1.50
37	n	605	CHL	C1D-ND	-7.22	1.34	1.50
37	Y	605	CHL	C1B-NB	-7.22	1.34	1.50
37	G	606	CHL	C4B-NB	-7.22	1.34	1.50
37	G	605	CHL	C1B-NB	-7.22	1.34	1.50
37	y	601	CHL	C4B-NB	-7.22	1.34	1.50
37	g	601	CHL	C1B-NB	-7.21	1.34	1.50
37	n	605	CHL	C1B-NB	-7.21	1.34	1.50
37	N	605	CHL	C1B-NB	-7.21	1.34	1.50
37	S	608	CHL	C4B-NB	-7.21	1.34	1.50
37	G	607	CHL	C1D-ND	-7.21	1.34	1.50
37	Y	605	CHL	C1D-ND	-7.21	1.34	1.50
37	s	608	CHL	C4B-NB	-7.21	1.34	1.50
37	y	606	CHL	C4B-NB	-7.21	1.34	1.50
37	s	601	CHL	C1B-NB	-7.21	1.34	1.50
37	S	601	CHL	C1B-NB	-7.21	1.34	1.50
37	N	606	CHL	C1B-NB	-7.20	1.34	1.50
37	n	606	CHL	C1B-NB	-7.20	1.34	1.50
37	N	605	CHL	C1D-ND	-7.20	1.34	1.50
37	Y	606	CHL	C4B-NB	-7.20	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	605	CHL	C4B-NB	-7.20	1.34	1.50
37	s	601	CHL	C4B-NB	-7.19	1.34	1.50
37	S	601	CHL	C4B-NB	-7.19	1.34	1.50
37	g	601	CHL	C1D-ND	-7.19	1.34	1.50
37	S	606	CHL	C1D-ND	-7.17	1.34	1.50
37	s	606	CHL	C1D-ND	-7.17	1.34	1.50
37	y	608	CHL	C4B-NB	-7.17	1.34	1.50
37	y	605	CHL	C1D-ND	-7.16	1.34	1.50
37	S	608	CHL	C1B-NB	-7.15	1.35	1.50
37	s	608	CHL	C1B-NB	-7.15	1.35	1.50
37	r	607	CHL	C3B-C2B	-7.14	1.46	1.55
37	R	607	CHL	C3B-C2B	-7.14	1.46	1.55
37	N	608	CHL	C4B-NB	-7.14	1.35	1.50
37	g	607	CHL	C4B-NB	-7.13	1.35	1.50
37	G	605	CHL	C1D-ND	-7.12	1.35	1.50
37	G	609	CHL	C1D-ND	-7.12	1.35	1.50
37	g	609	CHL	C1D-ND	-7.12	1.35	1.50
37	G	607	CHL	C4B-NB	-7.12	1.35	1.50
37	n	608	CHL	C4B-NB	-7.11	1.35	1.50
37	S	606	CHL	C4B-NB	-7.11	1.35	1.50
37	r	608	CHL	C4B-NB	-7.11	1.35	1.50
37	Y	608	CHL	C4B-NB	-7.11	1.35	1.50
37	s	606	CHL	C4B-NB	-7.10	1.35	1.50
37	g	605	CHL	C1D-ND	-7.09	1.35	1.50
37	R	606	CHL	C4B-NB	-7.09	1.35	1.50
37	G	608	CHL	C1D-ND	-7.07	1.35	1.50
37	r	606	CHL	C4B-NB	-7.07	1.35	1.50
37	N	608	CHL	C1D-ND	-7.06	1.35	1.50
37	n	608	CHL	C1D-ND	-7.06	1.35	1.50
37	G	608	CHL	C3B-C2B	-7.06	1.46	1.55
37	n	606	CHL	C4B-NB	-7.06	1.35	1.50
37	R	608	CHL	C4B-NB	-7.05	1.35	1.50
37	g	608	CHL	C1D-ND	-7.05	1.35	1.50
37	R	608	CHL	C3B-C2B	-7.04	1.46	1.55
37	N	606	CHL	C4B-NB	-7.03	1.35	1.50
37	g	608	CHL	C3B-C2B	-7.02	1.46	1.55
37	r	608	CHL	C3B-C2B	-6.98	1.46	1.55
37	g	605	CHL	C3B-C2B	-6.91	1.46	1.55
37	G	605	CHL	C3B-C2B	-6.91	1.46	1.55
37	G	609	CHL	C3B-C2B	-6.85	1.46	1.55
37	g	609	CHL	C3B-C2B	-6.76	1.46	1.55
37	r	608	CHL	C4D-ND	-6.75	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	S	607	CHL	C3B-C2B	-6.73	1.47	1.55
37	y	606	CHL	C4D-ND	-6.73	1.35	1.50
37	Y	606	CHL	C4D-ND	-6.73	1.35	1.50
37	R	608	CHL	C4D-ND	-6.71	1.35	1.50
37	n	601	CHL	C3B-C2B	-6.70	1.47	1.55
37	N	601	CHL	C3B-C2B	-6.69	1.47	1.55
37	s	607	CHL	C3B-C2B	-6.66	1.47	1.55
37	g	609	CHL	C4D-ND	-6.61	1.36	1.50
37	G	609	CHL	C4D-ND	-6.61	1.36	1.50
37	N	608	CHL	C4D-ND	-6.60	1.36	1.50
37	n	608	CHL	C4D-ND	-6.60	1.36	1.50
37	N	606	CHL	C4D-ND	-6.60	1.36	1.50
37	Y	609	CHL	C4D-ND	-6.59	1.36	1.50
37	y	608	CHL	C4D-ND	-6.58	1.36	1.50
37	Y	608	CHL	C4D-ND	-6.57	1.36	1.50
37	Y	601	CHL	C4D-ND	-6.57	1.36	1.50
37	y	609	CHL	C4D-ND	-6.57	1.36	1.50
37	n	606	CHL	C4D-ND	-6.56	1.36	1.50
37	y	601	CHL	C4D-ND	-6.56	1.36	1.50
37	Y	609	CHL	C3B-C4B	-6.54	1.47	1.54
37	g	606	CHL	C4D-ND	-6.54	1.36	1.50
37	N	607	CHL	C4D-ND	-6.53	1.36	1.50
37	s	601	CHL	C4D-ND	-6.53	1.36	1.50
37	S	601	CHL	C4D-ND	-6.53	1.36	1.50
37	n	607	CHL	C4D-ND	-6.53	1.36	1.50
37	n	609	CHL	C4D-ND	-6.53	1.36	1.50
37	N	609	CHL	C4D-ND	-6.53	1.36	1.50
37	n	601	CHL	C4D-ND	-6.52	1.36	1.50
37	N	601	CHL	C4D-ND	-6.52	1.36	1.50
37	y	609	CHL	C3B-C4B	-6.51	1.47	1.54
37	G	606	CHL	C4D-ND	-6.51	1.36	1.50
37	N	605	CHL	C4D-ND	-6.49	1.36	1.50
37	G	601	CHL	C4D-ND	-6.49	1.36	1.50
37	g	601	CHL	C4D-ND	-6.49	1.36	1.50
37	n	605	CHL	C4D-ND	-6.48	1.36	1.50
37	y	605	CHL	C4D-ND	-6.48	1.36	1.50
37	R	607	CHL	C4D-ND	-6.47	1.36	1.50
37	r	607	CHL	C4D-ND	-6.47	1.36	1.50
37	Y	605	CHL	C4D-ND	-6.44	1.36	1.50
37	S	608	CHL	C4D-ND	-6.44	1.36	1.50
37	G	607	CHL	C4D-ND	-6.44	1.36	1.50
37	g	607	CHL	C4D-ND	-6.43	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	y	607	CHL	C4D-ND	-6.43	1.36	1.50
37	Y	607	CHL	C4D-ND	-6.43	1.36	1.50
37	s	608	CHL	C4D-ND	-6.42	1.36	1.50
37	g	608	CHL	C4D-ND	-6.41	1.36	1.50
37	G	608	CHL	C4D-ND	-6.41	1.36	1.50
37	n	609	CHL	C3B-C4B	-6.39	1.47	1.54
37	S	606	CHL	C4D-ND	-6.37	1.36	1.50
37	N	609	CHL	C3B-C4B	-6.37	1.47	1.54
37	s	606	CHL	C4D-ND	-6.35	1.36	1.50
37	S	607	CHL	C4D-ND	-6.33	1.36	1.50
37	s	607	CHL	C4D-ND	-6.31	1.36	1.50
37	R	606	CHL	C4D-ND	-6.29	1.36	1.50
37	r	606	CHL	C4D-ND	-6.28	1.36	1.50
37	g	605	CHL	C4D-ND	-6.25	1.36	1.50
37	G	605	CHL	C4D-ND	-6.23	1.36	1.50
37	g	609	CHL	C3B-C4B	-6.16	1.47	1.54
37	G	609	CHL	C3B-C4B	-6.15	1.47	1.54
37	S	608	CHL	C3B-C2B	-6.12	1.47	1.55
37	s	608	CHL	C3B-C2B	-6.12	1.47	1.55
34	D	405	PL9	C3-C4	-5.89	1.39	1.49
34	d	405	PL9	C3-C4	-5.87	1.39	1.49
37	y	605	CHL	C3B-C4B	-5.84	1.47	1.54
37	Y	605	CHL	C3B-C4B	-5.82	1.47	1.54
37	r	606	CHL	C3B-C4B	-5.72	1.48	1.54
37	R	606	CHL	C3B-C4B	-5.69	1.48	1.54
37	g	607	CHL	C3B-C4B	-5.64	1.48	1.54
37	R	607	CHL	C3B-C4B	-5.61	1.48	1.54
37	y	607	CHL	C3B-C4B	-5.60	1.48	1.54
37	Y	607	CHL	C3B-C4B	-5.59	1.48	1.54
37	r	607	CHL	C3B-C4B	-5.59	1.48	1.54
37	G	607	CHL	C3B-C4B	-5.59	1.48	1.54
37	n	605	CHL	C3B-C4B	-5.55	1.48	1.54
37	n	607	CHL	C3B-C4B	-5.55	1.48	1.54
37	N	605	CHL	C3B-C4B	-5.55	1.48	1.54
37	N	607	CHL	C3B-C4B	-5.54	1.48	1.54
37	Y	601	CHL	C3B-C4B	-5.48	1.48	1.54
37	y	601	CHL	C3B-C4B	-5.48	1.48	1.54
37	s	607	CHL	C3B-C4B	-5.45	1.48	1.54
37	S	607	CHL	C3B-C4B	-5.45	1.48	1.54
37	G	601	CHL	C3B-C4B	-5.39	1.48	1.54
37	s	601	CHL	C3B-C4B	-5.36	1.48	1.54
37	g	601	CHL	C3B-C4B	-5.34	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	608	CHL	C3B-C4B	-5.31	1.48	1.54
37	g	605	CHL	C3B-C4B	-5.30	1.48	1.54
37	G	605	CHL	C3B-C4B	-5.30	1.48	1.54
37	G	608	CHL	C3B-C4B	-5.27	1.48	1.54
37	S	601	CHL	C3B-C4B	-5.27	1.48	1.54
37	r	608	CHL	C3B-C4B	-5.24	1.48	1.54
37	n	605	CHL	C1A-CHA	-5.21	1.46	1.54
37	Y	608	CHL	C3B-C4B	-5.21	1.48	1.54
37	n	601	CHL	C3B-C4B	-5.21	1.48	1.54
37	y	606	CHL	C3B-C4B	-5.21	1.48	1.54
37	n	608	CHL	C3B-C4B	-5.19	1.48	1.54
37	N	601	CHL	C3B-C4B	-5.19	1.48	1.54
37	N	605	CHL	C1A-CHA	-5.18	1.46	1.54
37	g	608	CHL	C3B-C4B	-5.17	1.48	1.54
37	y	608	CHL	C3B-C4B	-5.16	1.48	1.54
37	N	608	CHL	C3B-C4B	-5.14	1.48	1.54
37	s	601	CHL	C1A-CHA	-5.11	1.46	1.54
37	Y	606	CHL	C3B-C4B	-5.11	1.48	1.54
37	G	606	CHL	C1A-CHA	-5.11	1.46	1.54
37	g	606	CHL	C1A-CHA	-5.11	1.46	1.54
37	s	608	CHL	C3B-C4B	-5.08	1.48	1.54
37	S	608	CHL	C3B-C4B	-5.08	1.48	1.54
37	y	606	CHL	C1A-CHA	-5.06	1.46	1.54
37	Y	606	CHL	C1A-CHA	-5.06	1.46	1.54
37	S	601	CHL	C1A-CHA	-5.04	1.46	1.54
37	r	607	CHL	C1A-CHA	-5.00	1.47	1.54
37	G	606	CHL	C3B-C4B	-5.00	1.48	1.54
37	g	606	CHL	C3B-C4B	-5.00	1.48	1.54
37	G	601	CHL	C1A-CHA	-5.00	1.47	1.54
36	F	101	HEM	C3B-C2B	-4.98	1.34	1.40
37	N	606	CHL	C3B-C4B	-4.96	1.48	1.54
37	g	609	CHL	C1A-CHA	-4.96	1.47	1.54
37	G	609	CHL	C1A-CHA	-4.96	1.47	1.54
37	g	601	CHL	C1A-CHA	-4.96	1.47	1.54
36	f	101	HEM	C3B-C2B	-4.95	1.34	1.40
37	R	607	CHL	C1A-CHA	-4.95	1.47	1.54
36	f	101	HEM	C3C-C2C	-4.94	1.34	1.40
36	F	101	HEM	C3C-C2C	-4.94	1.34	1.40
37	y	601	CHL	C1A-CHA	-4.92	1.47	1.54
37	Y	601	CHL	C1A-CHA	-4.90	1.47	1.54
37	n	606	CHL	C1A-CHA	-4.90	1.47	1.54
37	N	606	CHL	C1A-CHA	-4.90	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	609	CHL	C1A-CHA	-4.89	1.47	1.54
37	n	606	CHL	C3B-C4B	-4.88	1.48	1.54
37	n	608	CHL	C1A-CHA	-4.88	1.47	1.54
37	n	609	CHL	C1A-CHA	-4.87	1.47	1.54
37	N	609	CHL	C1A-CHA	-4.87	1.47	1.54
37	y	609	CHL	C1A-CHA	-4.82	1.47	1.54
37	Y	607	CHL	CHB-C1B	-4.82	1.45	1.53
37	y	607	CHL	CHB-C1B	-4.81	1.45	1.53
37	y	606	CHL	CHD-C1D	-4.80	1.45	1.53
37	R	608	CHL	CHD-C1D	-4.80	1.45	1.53
37	n	606	CHL	CHD-C1D	-4.80	1.45	1.53
37	N	606	CHL	CHD-C1D	-4.80	1.45	1.53
37	n	601	CHL	C1A-CHA	-4.80	1.47	1.54
37	N	601	CHL	C1A-CHA	-4.80	1.47	1.54
37	N	608	CHL	C1A-CHA	-4.80	1.47	1.54
37	S	606	CHL	C3B-C4B	-4.79	1.49	1.54
37	Y	606	CHL	CHD-C1D	-4.77	1.45	1.53
37	N	608	CHL	CHD-C1D	-4.75	1.45	1.53
37	n	608	CHL	CHD-C1D	-4.75	1.45	1.53
37	s	606	CHL	C3B-C4B	-4.75	1.49	1.54
37	r	608	CHL	CHD-C1D	-4.74	1.45	1.53
37	N	607	CHL	C4A-C3A	-4.73	1.48	1.53
37	r	606	CHL	CHD-C1D	-4.70	1.45	1.53
37	R	606	CHL	C1A-CHA	-4.69	1.47	1.54
37	n	607	CHL	C4A-C3A	-4.69	1.48	1.53
37	y	608	CHL	C1A-CHA	-4.67	1.47	1.54
37	n	608	CHL	CHB-C1B	-4.66	1.46	1.53
37	y	608	CHL	CHB-C1B	-4.65	1.46	1.53
37	Y	608	CHL	CHB-C1B	-4.65	1.46	1.53
37	y	606	CHL	CHB-C1B	-4.65	1.46	1.53
37	N	608	CHL	CHB-C1B	-4.65	1.46	1.53
37	G	607	CHL	CHB-C1B	-4.64	1.46	1.53
37	r	606	CHL	C1A-CHA	-4.63	1.47	1.54
37	Y	606	CHL	CHB-C1B	-4.63	1.46	1.53
37	y	609	CHL	CHD-C1D	-4.63	1.46	1.53
37	g	601	CHL	CHD-C1D	-4.63	1.46	1.53
37	Y	608	CHL	C1A-CHA	-4.63	1.47	1.54
37	R	606	CHL	CHD-C1D	-4.63	1.46	1.53
37	N	607	CHL	CHD-C1D	-4.62	1.46	1.53
37	g	607	CHL	CHB-C1B	-4.62	1.46	1.53
37	Y	609	CHL	CHD-C1D	-4.61	1.46	1.53
37	G	607	CHL	CHD-C1D	-4.61	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	607	CHL	CHD-C1D	-4.61	1.46	1.53
37	Y	605	CHL	C1A-CHA	-4.61	1.47	1.54
37	G	601	CHL	CHD-C1D	-4.61	1.46	1.53
37	y	607	CHL	CHD-C1D	-4.60	1.46	1.53
37	Y	607	CHL	CHD-C1D	-4.60	1.46	1.53
37	y	608	CHL	CHD-C1D	-4.59	1.46	1.53
37	Y	608	CHL	CHD-C1D	-4.59	1.46	1.53
37	n	609	CHL	CHB-C1B	-4.59	1.46	1.53
37	N	609	CHL	CHB-C1B	-4.59	1.46	1.53
37	S	606	CHL	C1A-CHA	-4.59	1.47	1.54
37	G	608	CHL	C1A-CHA	-4.55	1.47	1.54
37	g	608	CHL	C1A-CHA	-4.55	1.47	1.54
37	n	607	CHL	CHB-C1B	-4.55	1.46	1.53
37	y	605	CHL	C1A-CHA	-4.54	1.47	1.54
37	n	609	CHL	C4A-C3A	-4.54	1.48	1.53
37	y	601	CHL	CHD-C1D	-4.53	1.46	1.53
37	s	601	CHL	CHB-C1B	-4.52	1.46	1.53
37	S	601	CHL	CHB-C1B	-4.52	1.46	1.53
37	n	607	CHL	CHD-C1D	-4.52	1.46	1.53
37	N	607	CHL	CHB-C1B	-4.52	1.46	1.53
37	y	605	CHL	CHD-C1D	-4.52	1.46	1.53
37	Y	605	CHL	CHD-C1D	-4.52	1.46	1.53
37	Y	607	CHL	C1A-CHA	-4.51	1.47	1.54
37	G	607	CHL	CHC-C4B	-4.51	1.46	1.53
37	s	601	CHL	CHD-C1D	-4.51	1.46	1.53
37	S	601	CHL	CHD-C1D	-4.51	1.46	1.53
37	n	607	CHL	C1A-CHA	-4.50	1.47	1.54
37	Y	601	CHL	CHD-C1D	-4.50	1.46	1.53
37	r	606	CHL	CHB-C1B	-4.50	1.46	1.53
37	R	606	CHL	CHB-C1B	-4.50	1.46	1.53
37	s	606	CHL	C1A-CHA	-4.50	1.47	1.54
37	g	606	CHL	CHB-C1B	-4.49	1.46	1.53
37	N	609	CHL	C4A-C3A	-4.49	1.48	1.53
37	g	607	CHL	CHC-C4B	-4.49	1.46	1.53
37	N	607	CHL	C1A-CHA	-4.48	1.47	1.54
37	R	607	CHL	CHD-C1D	-4.48	1.46	1.53
37	r	607	CHL	CHD-C1D	-4.48	1.46	1.53
37	y	607	CHL	C1A-CHA	-4.48	1.47	1.54
37	n	606	CHL	CHB-C1B	-4.47	1.46	1.53
37	r	608	CHL	C1A-CHA	-4.47	1.47	1.54
37	Y	608	CHL	CHC-C4B	-4.47	1.46	1.53
37	R	608	CHL	C1A-CHA	-4.46	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	R	607	CHL	CHB-C1B	-4.46	1.46	1.53
37	r	607	CHL	CHB-C1B	-4.46	1.46	1.53
37	G	606	CHL	CHB-C1B	-4.45	1.46	1.53
37	n	605	CHL	CHB-C1B	-4.44	1.46	1.53
37	N	606	CHL	CHB-C1B	-4.44	1.46	1.53
37	N	605	CHL	CHB-C1B	-4.44	1.46	1.53
37	g	608	CHL	CHB-C1B	-4.44	1.46	1.53
37	N	609	CHL	CHD-C1D	-4.44	1.46	1.53
37	y	607	CHL	C4A-C3A	-4.42	1.48	1.53
37	Y	607	CHL	C4A-C3A	-4.42	1.48	1.53
37	y	605	CHL	CHB-C1B	-4.42	1.46	1.53
37	y	605	CHL	CHC-C4B	-4.41	1.46	1.53
37	G	608	CHL	CHB-C1B	-4.41	1.46	1.53
37	Y	605	CHL	CHC-C4B	-4.41	1.46	1.53
37	n	609	CHL	CHD-C1D	-4.40	1.46	1.53
37	Y	609	CHL	CHB-C1B	-4.40	1.46	1.53
37	y	609	CHL	CHB-C1B	-4.40	1.46	1.53
37	Y	605	CHL	CHB-C1B	-4.39	1.46	1.53
37	g	601	CHL	CHB-C1B	-4.39	1.46	1.53
37	y	608	CHL	CHC-C4B	-4.39	1.46	1.53
37	G	601	CHL	CHB-C1B	-4.39	1.46	1.53
37	Y	601	CHL	CHB-C1B	-4.38	1.46	1.53
37	G	607	CHL	C1A-CHA	-4.38	1.47	1.54
37	g	607	CHL	C1A-CHA	-4.38	1.47	1.54
37	n	601	CHL	CHD-C1D	-4.36	1.46	1.53
37	N	601	CHL	CHD-C1D	-4.36	1.46	1.53
37	Y	609	CHL	CHC-C4B	-4.36	1.46	1.53
37	Y	607	CHL	CHC-C4B	-4.36	1.46	1.53
37	y	607	CHL	CHC-C4B	-4.36	1.46	1.53
37	y	601	CHL	CHB-C1B	-4.35	1.46	1.53
37	N	605	CHL	CHD-C1D	-4.34	1.46	1.53
37	N	607	CHL	CHC-C4B	-4.34	1.46	1.53
37	g	601	CHL	C4A-C3A	-4.34	1.48	1.53
37	y	609	CHL	CHC-C4B	-4.33	1.46	1.53
37	N	609	CHL	CHC-C4B	-4.33	1.46	1.53
37	n	605	CHL	CHD-C1D	-4.33	1.46	1.53
37	g	601	CHL	CHC-C4B	-4.33	1.46	1.53
37	G	601	CHL	C4A-C3A	-4.31	1.48	1.53
37	g	606	CHL	CHD-C1D	-4.30	1.46	1.53
37	G	608	CHL	CHC-C4B	-4.30	1.46	1.53
37	n	609	CHL	CHC-C4B	-4.28	1.46	1.53
37	g	608	CHL	CHD-C1D	-4.27	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	r	607	CHL	CHC-C4B	-4.27	1.46	1.53
37	G	606	CHL	CHD-C1D	-4.27	1.46	1.53
37	R	607	CHL	CHC-C4B	-4.26	1.46	1.53
37	n	607	CHL	CHC-C4B	-4.26	1.46	1.53
37	G	601	CHL	CHC-C4B	-4.26	1.46	1.53
37	g	609	CHL	CHD-C1D	-4.25	1.46	1.53
37	G	609	CHL	CHD-C1D	-4.25	1.46	1.53
37	N	605	CHL	C4A-C3A	-4.25	1.48	1.53
37	G	609	CHL	CHC-C4B	-4.25	1.46	1.53
37	S	601	CHL	C4A-C3A	-4.25	1.48	1.53
37	s	601	CHL	C4A-C3A	-4.25	1.48	1.53
37	g	608	CHL	CHC-C4B	-4.24	1.46	1.53
37	Y	601	CHL	C4A-C3A	-4.24	1.48	1.53
37	S	601	CHL	CHC-C4B	-4.24	1.46	1.53
34	D	405	PL9	C6-C1	-4.23	1.40	1.48
37	y	601	CHL	C4A-C3A	-4.22	1.48	1.53
37	n	608	CHL	CHC-C4B	-4.22	1.46	1.53
37	g	609	CHL	CHC-C4B	-4.22	1.46	1.53
37	r	608	CHL	CHC-C4B	-4.22	1.46	1.53
37	S	607	CHL	C4A-C3A	-4.22	1.48	1.53
34	d	405	PL9	C6-C1	-4.21	1.40	1.48
37	S	606	CHL	CHB-C1B	-4.20	1.46	1.53
37	s	601	CHL	CHC-C4B	-4.19	1.46	1.53
37	s	607	CHL	CHB-C1B	-4.19	1.46	1.53
37	S	607	CHL	CHB-C1B	-4.19	1.46	1.53
37	Y	601	CHL	CHC-C4B	-4.18	1.46	1.53
37	y	601	CHL	CHC-C4B	-4.18	1.46	1.53
37	s	608	CHL	CHD-C1D	-4.18	1.46	1.53
37	n	605	CHL	CHC-C4B	-4.18	1.46	1.53
37	N	605	CHL	CHC-C4B	-4.18	1.46	1.53
37	G	608	CHL	CHD-C1D	-4.17	1.46	1.53
37	n	605	CHL	C4A-C3A	-4.17	1.48	1.53
37	G	605	CHL	CHD-C1D	-4.17	1.46	1.53
37	R	608	CHL	CHC-C4B	-4.16	1.46	1.53
37	g	605	CHL	CHB-C1B	-4.16	1.46	1.53
37	s	608	CHL	C1A-CHA	-4.16	1.48	1.54
37	s	607	CHL	C4A-C3A	-4.16	1.48	1.53
37	r	606	CHL	CHC-C4B	-4.15	1.46	1.53
37	S	608	CHL	CHD-C1D	-4.15	1.46	1.53
37	N	608	CHL	CHC-C4B	-4.15	1.46	1.53
37	R	606	CHL	CHC-C4B	-4.15	1.46	1.53
37	g	605	CHL	CHD-C1D	-4.14	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	605	CHL	CHB-C1B	-4.13	1.46	1.53
37	G	609	CHL	CHB-C1B	-4.13	1.46	1.53
37	s	607	CHL	C1A-CHA	-4.13	1.48	1.54
37	S	607	CHL	C1A-CHA	-4.13	1.48	1.54
37	g	605	CHL	C1A-CHA	-4.13	1.48	1.54
37	G	605	CHL	C1A-CHA	-4.13	1.48	1.54
37	y	606	CHL	C4A-C3A	-4.13	1.48	1.53
37	Y	606	CHL	C4A-C3A	-4.13	1.48	1.53
37	s	606	CHL	CHB-C1B	-4.12	1.46	1.53
37	g	609	CHL	CHB-C1B	-4.10	1.46	1.53
37	S	608	CHL	C1A-CHA	-4.09	1.48	1.54
37	r	608	CHL	CHB-C1B	-4.09	1.46	1.53
37	g	608	CHL	C4A-C3A	-4.08	1.48	1.53
37	Y	609	CHL	C4A-C3A	-4.08	1.48	1.53
37	y	609	CHL	C4A-C3A	-4.08	1.48	1.53
37	n	601	CHL	CHB-C1B	-4.06	1.47	1.53
37	N	601	CHL	CHB-C1B	-4.06	1.47	1.53
37	r	608	CHL	C4A-C3A	-4.06	1.48	1.53
37	G	606	CHL	C4A-C3A	-4.05	1.48	1.53
37	g	606	CHL	C4A-C3A	-4.05	1.48	1.53
37	S	606	CHL	C4A-C3A	-4.05	1.48	1.53
37	s	606	CHL	C4A-C3A	-4.05	1.48	1.53
37	Y	608	CHL	C4A-C3A	-4.04	1.48	1.53
37	r	606	CHL	C4A-C3A	-4.02	1.49	1.53
37	R	608	CHL	CHB-C1B	-4.02	1.47	1.53
37	y	608	CHL	C4A-C3A	-4.01	1.49	1.53
37	G	608	CHL	C4A-C3A	-4.00	1.49	1.53
37	R	608	CHL	C4A-C3A	-3.98	1.49	1.53
37	n	606	CHL	C4A-C3A	-3.97	1.49	1.53
37	N	606	CHL	C4A-C3A	-3.97	1.49	1.53
37	y	607	CHL	CHC-C1C	-3.97	1.46	1.53
37	Y	607	CHL	CHC-C1C	-3.97	1.46	1.53
37	g	601	CHL	C1A-C2A	-3.97	1.49	1.53
37	R	607	CHL	C4A-C3A	-3.96	1.49	1.53
37	Y	605	CHL	C4A-C3A	-3.94	1.49	1.53
37	G	605	CHL	CHC-C4B	-3.94	1.47	1.53
37	r	607	CHL	C4A-C3A	-3.93	1.49	1.53
37	S	606	CHL	CHD-C1D	-3.93	1.47	1.53
37	G	605	CHL	C4A-C3A	-3.92	1.49	1.53
37	g	605	CHL	CHC-C4B	-3.92	1.47	1.53
40	Y	1623	NEX	C7-C8	-3.92	1.25	1.31
37	R	606	CHL	C4A-C3A	-3.91	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	601	CHL	C1A-C2A	-3.91	1.49	1.53
37	N	601	CHL	C4A-C3A	-3.91	1.49	1.53
37	s	607	CHL	CHD-C1D	-3.90	1.47	1.53
37	Y	601	CHL	C1A-C2A	-3.89	1.49	1.53
37	N	608	CHL	C4A-C3A	-3.89	1.49	1.53
37	g	607	CHL	C4A-C3A	-3.89	1.49	1.53
37	s	606	CHL	CHD-C1D	-3.88	1.47	1.53
37	y	605	CHL	CHC-C1C	-3.88	1.46	1.53
37	y	606	CHL	CHC-C4B	-3.87	1.47	1.53
37	Y	606	CHL	CHC-C4B	-3.87	1.47	1.53
37	y	605	CHL	C4A-C3A	-3.87	1.49	1.53
37	s	607	CHL	CHC-C4B	-3.87	1.47	1.53
37	S	607	CHL	CHC-C4B	-3.87	1.47	1.53
37	G	609	CHL	C4A-C3A	-3.86	1.49	1.53
37	S	607	CHL	CHD-C1D	-3.86	1.47	1.53
37	n	601	CHL	C4A-C3A	-3.86	1.49	1.53
37	g	605	CHL	C4A-C3A	-3.85	1.49	1.53
40	y	1623	NEX	C7-C8	-3.84	1.25	1.31
37	n	608	CHL	C4A-C3A	-3.84	1.49	1.53
37	S	606	CHL	CHC-C4B	-3.83	1.47	1.53
37	N	601	CHL	CHC-C4B	-3.83	1.47	1.53
37	Y	605	CHL	CHC-C1C	-3.83	1.46	1.53
37	y	608	CHL	CHC-C1C	-3.82	1.46	1.53
37	Y	608	CHL	CHC-C1C	-3.82	1.46	1.53
37	g	609	CHL	C4A-C3A	-3.81	1.49	1.53
37	s	606	CHL	CHC-C4B	-3.81	1.47	1.53
37	G	607	CHL	C4A-C3A	-3.81	1.49	1.53
37	n	606	CHL	CHC-C4B	-3.81	1.47	1.53
37	G	607	CHL	CHC-C1C	-3.81	1.46	1.53
37	y	601	CHL	C1A-C2A	-3.81	1.49	1.53
37	G	606	CHL	CHC-C4B	-3.79	1.47	1.53
37	n	601	CHL	CHC-C4B	-3.79	1.47	1.53
37	g	606	CHL	CHC-C4B	-3.78	1.47	1.53
37	g	607	CHL	CHC-C1C	-3.78	1.46	1.53
37	Y	601	CHL	CHC-C1C	-3.76	1.46	1.53
37	y	601	CHL	CHC-C1C	-3.75	1.46	1.53
37	N	606	CHL	CHC-C4B	-3.74	1.47	1.53
37	S	608	CHL	CHB-C1B	-3.72	1.47	1.53
37	n	609	CHL	CHC-C1C	-3.72	1.46	1.53
37	N	609	CHL	CHC-C1C	-3.72	1.46	1.53
37	S	601	CHL	C1A-C2A	-3.70	1.49	1.53
37	n	607	CHL	CHC-C1C	-3.70	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	606	CHL	C1A-C2A	-3.69	1.49	1.53
37	g	606	CHL	C1A-C2A	-3.69	1.49	1.53
37	N	608	CHL	CHC-C1C	-3.69	1.46	1.53
37	s	601	CHL	C1A-C2A	-3.69	1.49	1.53
40	R	623	NEX	C7-C8	-3.67	1.25	1.31
37	G	601	CHL	CHC-C1C	-3.66	1.46	1.53
37	n	608	CHL	CHC-C1C	-3.66	1.46	1.53
40	r	623	NEX	C7-C8	-3.65	1.25	1.31
37	s	608	CHL	CHB-C1B	-3.64	1.47	1.53
37	N	607	CHL	CHC-C1C	-3.64	1.46	1.53
37	g	609	CHL	CHC-C1C	-3.63	1.46	1.53
37	g	601	CHL	CHC-C1C	-3.62	1.46	1.53
37	r	608	CHL	CHC-C1C	-3.59	1.46	1.53
37	R	608	CHL	CHC-C1C	-3.59	1.46	1.53
37	G	609	CHL	CHC-C1C	-3.57	1.46	1.53
37	y	609	CHL	CHC-C1C	-3.57	1.46	1.53
37	S	601	CHL	CHC-C1C	-3.56	1.46	1.53
37	s	601	CHL	CHC-C1C	-3.56	1.46	1.53
37	Y	609	CHL	CHC-C1C	-3.53	1.47	1.53
37	y	608	CHL	C3D-C2D	-3.51	1.45	1.55
37	R	607	CHL	CHC-C1C	-3.51	1.47	1.53
37	y	606	CHL	CHD-C4C	-3.51	1.47	1.53
37	r	607	CHL	CHC-C1C	-3.50	1.47	1.53
37	Y	606	CHL	C3D-C2D	-3.50	1.45	1.55
37	N	608	CHL	C3D-C2D	-3.50	1.45	1.55
37	n	608	CHL	C3D-C2D	-3.50	1.45	1.55
37	n	601	CHL	C1A-C2A	-3.50	1.49	1.53
37	N	601	CHL	C1A-C2A	-3.50	1.49	1.53
27	C	508	CLA	CMB-C2B	-3.50	1.44	1.51
37	Y	607	CHL	CHD-C4C	-3.49	1.47	1.53
27	C	507	CLA	C3B-C2B	-3.49	1.35	1.40
37	Y	608	CHL	C3D-C2D	-3.49	1.45	1.55
37	Y	606	CHL	CHD-C4C	-3.48	1.47	1.53
37	s	608	CHL	CHC-C4B	-3.48	1.48	1.53
37	y	607	CHL	CHD-C4C	-3.48	1.47	1.53
27	c	508	CLA	CMB-C2B	-3.48	1.44	1.51
37	G	608	CHL	CHC-C1C	-3.48	1.47	1.53
37	g	608	CHL	CHC-C1C	-3.48	1.47	1.53
37	N	605	CHL	C1A-C2A	-3.46	1.49	1.53
37	r	606	CHL	CHC-C1C	-3.46	1.47	1.53
37	y	606	CHL	C3D-C2D	-3.45	1.45	1.55
37	R	606	CHL	CHC-C1C	-3.43	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	605	CHL	C1A-C2A	-3.43	1.49	1.53
37	g	601	CHL	C3D-C2D	-3.42	1.45	1.55
37	S	608	CHL	CHC-C4B	-3.42	1.48	1.53
27	c	507	CLA	C3B-C2B	-3.42	1.36	1.40
37	G	601	CHL	C3D-C2D	-3.42	1.46	1.55
37	n	606	CHL	CHC-C1C	-3.41	1.47	1.53
37	R	608	CHL	C3D-C2D	-3.41	1.46	1.55
40	g	1623	NEX	C7-C8	-3.40	1.26	1.31
37	n	607	CHL	CHD-C4C	-3.40	1.47	1.53
37	y	606	CHL	C1A-C2A	-3.40	1.49	1.53
37	Y	606	CHL	C1A-C2A	-3.40	1.49	1.53
40	N	1623	NEX	C7-C8	-3.40	1.26	1.31
37	R	608	CHL	CHD-C4C	-3.39	1.47	1.53
40	G	1623	NEX	C7-C8	-3.39	1.26	1.31
37	Y	606	CHL	CHC-C1C	-3.39	1.47	1.53
37	Y	605	CHL	CHD-C4C	-3.39	1.47	1.53
37	r	608	CHL	C3D-C2D	-3.39	1.46	1.55
37	R	606	CHL	CHD-C4C	-3.39	1.47	1.53
37	y	607	CHL	C3D-C2D	-3.38	1.46	1.55
37	Y	607	CHL	C3D-C2D	-3.38	1.46	1.55
37	r	608	CHL	CHD-C4C	-3.37	1.47	1.53
37	r	606	CHL	C1A-C2A	-3.37	1.49	1.53
37	r	606	CHL	CHD-C4C	-3.37	1.47	1.53
37	N	606	CHL	CHC-C1C	-3.37	1.47	1.53
37	g	608	CHL	C3D-C2D	-3.37	1.46	1.55
37	N	607	CHL	CHD-C4C	-3.37	1.47	1.53
37	G	608	CHL	C3D-C2D	-3.36	1.46	1.55
40	n	1623	NEX	C7-C8	-3.36	1.26	1.31
37	n	606	CHL	C3D-C2D	-3.35	1.46	1.55
37	n	605	CHL	CHC-C1C	-3.35	1.47	1.53
37	N	605	CHL	CHC-C1C	-3.35	1.47	1.53
37	y	605	CHL	CHD-C4C	-3.34	1.47	1.53
37	S	606	CHL	CHC-C1C	-3.33	1.47	1.53
37	N	607	CHL	C3D-C2D	-3.32	1.46	1.55
37	n	607	CHL	C3D-C2D	-3.32	1.46	1.55
37	N	606	CHL	C3D-C2D	-3.32	1.46	1.55
37	y	606	CHL	CHC-C1C	-3.32	1.47	1.53
37	g	607	CHL	CHD-C4C	-3.32	1.47	1.53
38	N	1620	LUT	C21-C26	-3.32	1.52	1.56
38	n	1620	LUT	C21-C26	-3.32	1.52	1.56
37	G	607	CHL	CHD-C4C	-3.30	1.47	1.53
37	s	606	CHL	CHC-C1C	-3.30	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	609	CHL	C1A-C2A	-3.30	1.49	1.53
37	y	609	CHL	C1A-C2A	-3.30	1.49	1.53
37	Y	605	CHL	C3D-C2D	-3.30	1.46	1.55
37	R	606	CHL	C1A-C2A	-3.30	1.49	1.53
37	n	606	CHL	CHD-C4C	-3.30	1.47	1.53
37	N	606	CHL	CHD-C4C	-3.30	1.47	1.53
35	d	409	LHG	O7-C5	-3.29	1.37	1.46
35	D	409	LHG	O7-C5	-3.29	1.37	1.46
37	n	601	CHL	CHC-C1C	-3.29	1.47	1.53
37	r	606	CHL	C3D-C2D	-3.29	1.46	1.55
37	Y	609	CHL	C3D-C2D	-3.28	1.46	1.55
37	y	609	CHL	C3D-C2D	-3.28	1.46	1.55
37	N	601	CHL	CHC-C1C	-3.28	1.47	1.53
27	b	604	CLA	CMB-C2B	-3.28	1.44	1.51
27	b	612	CLA	CMC-C2C	-3.28	1.43	1.50
37	y	605	CHL	C3D-C2D	-3.27	1.46	1.55
38	Y	1620	LUT	C21-C26	-3.27	1.52	1.56
37	n	609	CHL	C3D-C2D	-3.27	1.46	1.55
37	N	609	CHL	C3D-C2D	-3.27	1.46	1.55
37	R	606	CHL	C3D-C2D	-3.26	1.46	1.55
38	y	1620	LUT	C21-C26	-3.26	1.52	1.56
37	G	601	CHL	CHD-C4C	-3.26	1.47	1.53
27	B	612	CLA	CMC-C2C	-3.26	1.43	1.50
38	g	1620	LUT	C21-C26	-3.25	1.52	1.56
37	Y	609	CHL	CHD-C4C	-3.24	1.47	1.53
37	y	609	CHL	CHD-C4C	-3.24	1.47	1.53
37	g	609	CHL	C1A-C2A	-3.24	1.49	1.53
37	g	605	CHL	CHC-C1C	-3.24	1.47	1.53
27	B	604	CLA	CMB-C2B	-3.22	1.45	1.51
37	n	609	CHL	C1A-C2A	-3.22	1.49	1.53
37	N	609	CHL	C1A-C2A	-3.22	1.49	1.53
37	G	609	CHL	C1A-C2A	-3.22	1.49	1.53
37	g	606	CHL	C3D-C2D	-3.21	1.46	1.55
37	g	601	CHL	CHD-C4C	-3.21	1.47	1.53
38	G	1620	LUT	C21-C26	-3.21	1.52	1.56
37	s	601	CHL	CHD-C4C	-3.21	1.47	1.53
37	y	608	CHL	CHD-C4C	-3.21	1.47	1.53
37	Y	608	CHL	CHD-C4C	-3.21	1.47	1.53
38	Y	1621	LUT	C21-C26	-3.20	1.52	1.56
32	c	518	DGD	O1G-C1G	-3.20	1.38	1.45
37	N	608	CHL	CHD-C4C	-3.20	1.47	1.53
27	c	506	CLA	CMB-C2B	-3.19	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	518	DGD	O1G-C1G	-3.19	1.38	1.45
37	R	607	CHL	C3D-C2D	-3.19	1.46	1.55
37	r	607	CHL	C3D-C2D	-3.19	1.46	1.55
37	N	605	CHL	C3D-C2D	-3.19	1.46	1.55
37	G	607	CHL	C3D-C2D	-3.19	1.46	1.55
27	B	612	CLA	CMB-C2B	-3.19	1.45	1.51
37	S	608	CHL	C4A-C3A	-3.18	1.49	1.53
37	G	605	CHL	CHC-C1C	-3.18	1.47	1.53
37	n	609	CHL	CHD-C4C	-3.18	1.47	1.53
37	S	601	CHL	CHD-C4C	-3.18	1.47	1.53
37	G	609	CHL	C3D-C2D	-3.18	1.46	1.55
37	N	609	CHL	CHD-C4C	-3.17	1.47	1.53
37	n	605	CHL	C3D-C2D	-3.17	1.46	1.55
37	g	607	CHL	C3D-C2D	-3.17	1.46	1.55
32	h	102	DGD	O1G-C1G	-3.17	1.38	1.45
32	H	102	DGD	O1G-C1G	-3.17	1.38	1.45
37	s	607	CHL	CHC-C1C	-3.17	1.47	1.53
37	n	601	CHL	C3D-C2D	-3.17	1.46	1.55
37	s	608	CHL	C4A-C3A	-3.17	1.49	1.53
37	g	609	CHL	C3D-C2D	-3.17	1.46	1.55
37	G	606	CHL	C3D-C2D	-3.16	1.46	1.55
37	n	608	CHL	CHD-C4C	-3.16	1.47	1.53
37	y	601	CHL	C3D-C2D	-3.16	1.46	1.55
37	G	606	CHL	CHC-C1C	-3.16	1.47	1.53
37	g	606	CHL	CHC-C1C	-3.16	1.47	1.53
27	b	612	CLA	CMB-C2B	-3.16	1.45	1.51
38	y	1621	LUT	C21-C26	-3.15	1.52	1.56
37	N	601	CHL	C3D-C2D	-3.15	1.46	1.55
37	Y	601	CHL	C3D-C2D	-3.15	1.46	1.55
37	S	606	CHL	C3D-C2D	-3.14	1.46	1.55
27	C	506	CLA	CMB-C2B	-3.14	1.45	1.51
37	R	607	CHL	CHD-C4C	-3.14	1.47	1.53
37	s	606	CHL	C3D-C2D	-3.13	1.46	1.55
37	S	608	CHL	C1A-C2A	-3.13	1.50	1.53
37	S	607	CHL	CHC-C1C	-3.13	1.47	1.53
37	s	601	CHL	C3D-C2D	-3.13	1.46	1.55
37	r	607	CHL	CHD-C4C	-3.13	1.47	1.53
38	S	1621	LUT	C21-C26	-3.12	1.52	1.56
37	y	601	CHL	CHD-C4C	-3.12	1.47	1.53
37	s	608	CHL	C1A-C2A	-3.11	1.50	1.53
37	S	601	CHL	C3D-C2D	-3.10	1.46	1.55
27	b	615	CLA	C3B-C2B	-3.09	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	s	1623	NEX	C7-C8	-3.09	1.26	1.31
38	G	1621	LUT	C21-C26	-3.08	1.52	1.56
38	g	1621	LUT	C21-C26	-3.08	1.52	1.56
38	s	1621	LUT	C21-C26	-3.08	1.52	1.56
38	R	620	LUT	C21-C26	-3.08	1.52	1.56
37	n	608	CHL	C1A-C2A	-3.07	1.50	1.53
40	S	1623	NEX	C7-C8	-3.07	1.26	1.31
34	d	405	PL9	C52-C5	-3.07	1.44	1.50
27	B	606	CLA	C3B-C2B	-3.06	1.36	1.40
34	D	405	PL9	C52-C5	-3.06	1.44	1.50
27	C	508	CLA	C3B-C2B	-3.06	1.36	1.40
27	Y	610	CLA	CMB-C2B	-3.05	1.45	1.51
27	b	604	CLA	C3B-C2B	-3.05	1.36	1.40
27	B	604	CLA	C3B-C2B	-3.05	1.36	1.40
37	Y	601	CHL	CHD-C4C	-3.05	1.47	1.53
37	N	608	CHL	C1A-C2A	-3.05	1.50	1.53
27	B	615	CLA	C3B-C2B	-3.05	1.36	1.40
37	g	605	CHL	C3D-C2D	-3.04	1.47	1.55
27	D	402	CLA	CMD-C2D	-3.04	1.44	1.51
37	g	609	CHL	CHD-C4C	-3.04	1.47	1.53
37	G	609	CHL	CHD-C4C	-3.04	1.47	1.53
37	G	605	CHL	C3D-C2D	-3.04	1.47	1.55
37	r	608	CHL	C1A-C2A	-3.04	1.50	1.53
37	y	605	CHL	C1A-C2A	-3.04	1.50	1.53
27	y	610	CLA	CMB-C2B	-3.04	1.45	1.51
27	Y	604	CLA	CMB-C2B	-3.03	1.45	1.51
27	y	604	CLA	CMB-C2B	-3.02	1.45	1.51
38	G	1621	LUT	C22-C21	-3.02	1.51	1.54
29	B	620	BCR	C1-C6	-3.01	1.49	1.53
34	d	405	PL9	C53-C6	-3.01	1.44	1.50
37	n	606	CHL	C1A-C2A	-3.01	1.50	1.53
37	N	606	CHL	C1A-C2A	-3.01	1.50	1.53
37	G	606	CHL	CHD-C4C	-3.01	1.47	1.53
37	g	606	CHL	CHD-C4C	-3.01	1.47	1.53
27	d	402	CLA	CMD-C2D	-3.00	1.45	1.51
38	r	620	LUT	C21-C26	-3.00	1.52	1.56
27	b	607	CLA	C3B-C2B	-3.00	1.36	1.40
27	B	607	CLA	C3B-C2B	-3.00	1.36	1.40
37	Y	605	CHL	C1A-C2A	-3.00	1.50	1.53
27	Y	613	CLA	C3B-C2B	-2.99	1.36	1.40
27	y	613	CLA	C3B-C2B	-2.99	1.36	1.40
27	B	616	CLA	C3B-C2B	-2.99	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	620	BCR	C1-C6	-2.99	1.49	1.53
27	c	508	CLA	C3B-C2B	-2.99	1.36	1.40
27	c	505	CLA	CMD-C2D	-2.98	1.45	1.51
27	b	605	CLA	CMB-C2B	-2.98	1.45	1.51
27	B	605	CLA	CMB-C2B	-2.98	1.45	1.51
27	b	612	CLA	C3B-C2B	-2.98	1.36	1.40
27	A	410	CLA	CMB-C2B	-2.98	1.45	1.51
27	a	410	CLA	CMB-C2B	-2.98	1.45	1.51
37	R	608	CHL	C1A-C2A	-2.97	1.50	1.53
37	y	608	CHL	C1A-C2A	-2.97	1.50	1.53
34	D	405	PL9	C53-C6	-2.97	1.44	1.50
27	b	606	CLA	CMB-C2B	-2.97	1.45	1.51
27	C	505	CLA	CMD-C2D	-2.96	1.45	1.51
27	B	613	CLA	CMD-C2D	-2.96	1.45	1.51
27	C	507	CLA	CMB-C2B	-2.96	1.45	1.51
27	b	606	CLA	C3B-C2B	-2.96	1.36	1.40
37	Y	608	CHL	C1A-C2A	-2.95	1.50	1.53
38	g	1621	LUT	C22-C21	-2.95	1.51	1.54
27	b	613	CLA	CMD-C2D	-2.94	1.45	1.51
32	C	519	DGD	O2G-C2G	-2.94	1.38	1.46
37	n	601	CHL	CHD-C4C	-2.94	1.48	1.53
27	c	507	CLA	CMB-C2B	-2.94	1.45	1.51
27	B	612	CLA	C3B-C2B	-2.94	1.36	1.40
27	c	509	CLA	CMB-C2B	-2.94	1.45	1.51
37	S	606	CHL	C1A-C2A	-2.94	1.50	1.53
37	N	601	CHL	CHD-C4C	-2.93	1.48	1.53
37	s	608	CHL	C3D-C2D	-2.92	1.47	1.55
27	A	405	CLA	CMD-C2D	-2.92	1.45	1.51
32	c	519	DGD	O2G-C2G	-2.91	1.38	1.46
35	d	408	LHG	O7-C5	-2.91	1.38	1.46
37	s	606	CHL	C1A-C2A	-2.91	1.50	1.53
37	S	608	CHL	C3D-C2D	-2.90	1.47	1.55
38	N	1621	LUT	C21-C26	-2.90	1.52	1.56
38	n	1621	LUT	C21-C26	-2.90	1.52	1.56
27	B	606	CLA	CMB-C2B	-2.90	1.45	1.51
27	D	402	CLA	CMB-C2B	-2.89	1.45	1.51
27	d	402	CLA	CMB-C2B	-2.89	1.45	1.51
27	B	614	CLA	CMB-C2B	-2.89	1.45	1.51
37	s	607	CHL	C3D-C2D	-2.89	1.47	1.55
27	C	509	CLA	CMB-C2B	-2.89	1.45	1.51
27	c	504	CLA	CMB-C2B	-2.89	1.45	1.51
27	C	504	CLA	CMB-C2B	-2.89	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	607	CHL	CBD-CAD	-2.89	1.48	1.53
35	D	408	LHG	O7-C5	-2.89	1.38	1.46
37	y	607	CHL	CBD-CAD	-2.89	1.48	1.53
27	b	616	CLA	C3B-C2B	-2.88	1.36	1.40
37	G	608	CHL	C1A-C2A	-2.88	1.50	1.53
37	g	608	CHL	C1A-C2A	-2.88	1.50	1.53
27	n	604	CLA	CMB-C2B	-2.88	1.45	1.51
38	S	1620	LUT	C21-C26	-2.88	1.52	1.56
27	A	406	CLA	CMD-C2D	-2.88	1.45	1.51
27	y	613	CLA	CMB-C2B	-2.88	1.45	1.51
27	n	610	CLA	CMB-C2B	-2.88	1.45	1.51
37	S	607	CHL	C3D-C2D	-2.88	1.47	1.55
27	a	405	CLA	CMD-C2D	-2.88	1.45	1.51
27	C	502	CLA	CMB-C2B	-2.88	1.45	1.51
27	a	406	CLA	CMD-C2D	-2.88	1.45	1.51
27	b	614	CLA	CMB-C2B	-2.88	1.45	1.51
37	r	607	CHL	C1A-C2A	-2.87	1.50	1.53
27	c	501	CLA	C3B-C2B	-2.87	1.36	1.40
27	a	407	CLA	CMB-C2B	-2.86	1.45	1.51
37	G	608	CHL	CHD-C4C	-2.86	1.48	1.53
27	c	502	CLA	CMB-C2B	-2.86	1.45	1.51
37	N	609	CHL	C2A-C3A	-2.85	1.49	1.55
27	b	615	CLA	CMB-C2B	-2.85	1.45	1.51
27	C	501	CLA	CMB-C2B	-2.84	1.45	1.51
27	N	610	CLA	CMB-C2B	-2.84	1.45	1.51
27	N	604	CLA	CMB-C2B	-2.84	1.45	1.51
27	c	501	CLA	CMB-C2B	-2.84	1.45	1.51
37	N	607	CHL	CBD-CAD	-2.84	1.48	1.53
27	B	615	CLA	CMB-C2B	-2.84	1.45	1.51
27	Y	602	CLA	CMB-C2B	-2.84	1.45	1.51
37	n	609	CHL	C2A-C3A	-2.84	1.49	1.55
37	R	607	CHL	C1A-C2A	-2.84	1.50	1.53
27	c	503	CLA	CMB-C2B	-2.84	1.45	1.51
27	s	604	CLA	CMB-C2B	-2.84	1.45	1.51
27	C	501	CLA	C3B-C2B	-2.84	1.36	1.40
27	b	603	CLA	C3B-C2B	-2.83	1.36	1.40
27	a	405	CLA	CMB-C2B	-2.83	1.45	1.51
27	y	602	CLA	CMB-C2B	-2.83	1.45	1.51
37	y	605	CHL	CBD-CAD	-2.83	1.49	1.53
27	S	604	CLA	CMB-C2B	-2.82	1.45	1.51
27	b	611	CLA	CMB-C2B	-2.82	1.45	1.51
27	Y	613	CLA	CMB-C2B	-2.82	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	608	CHL	CHD-C4C	-2.82	1.48	1.53
27	c	510	CLA	CMB-C2B	-2.82	1.45	1.51
27	b	607	CLA	CMB-C2B	-2.82	1.45	1.51
27	B	617	CLA	CMD-C2D	-2.82	1.45	1.51
27	b	617	CLA	CMD-C2D	-2.82	1.45	1.51
37	g	605	CHL	C1A-C2A	-2.82	1.50	1.53
27	B	613	CLA	CMB-C2B	-2.81	1.45	1.51
27	b	610	CLA	CMB-C2B	-2.81	1.45	1.51
27	B	607	CLA	CMB-C2B	-2.81	1.45	1.51
37	n	607	CHL	CBD-CAD	-2.81	1.49	1.53
27	A	407	CLA	CMB-C2B	-2.81	1.45	1.51
37	Y	605	CHL	CBD-CAD	-2.80	1.49	1.53
27	C	510	CLA	CMB-C2B	-2.80	1.45	1.51
37	Y	606	CHL	C3B-CAB	-2.80	1.48	1.50
27	b	616	CLA	CMB-C2B	-2.80	1.45	1.51
27	G	602	CLA	CMD-C2D	-2.80	1.45	1.51
27	b	613	CLA	CMB-C2B	-2.79	1.46	1.51
27	Y	604	CLA	C3B-C2B	-2.79	1.36	1.40
27	B	616	CLA	CMB-C2B	-2.79	1.46	1.51
27	g	612	CLA	CMB-C2B	-2.79	1.46	1.51
27	A	405	CLA	CMB-C2B	-2.79	1.46	1.51
27	Y	603	CLA	CMB-C2B	-2.78	1.46	1.51
27	g	602	CLA	CMD-C2D	-2.78	1.45	1.51
27	B	611	CLA	CMB-C2B	-2.78	1.46	1.51
37	n	609	CHL	C3B-CAB	-2.78	1.48	1.50
35	l	101	LHG	O7-C5	-2.78	1.39	1.46
27	y	603	CLA	CMB-C2B	-2.78	1.46	1.51
27	B	603	CLA	CMB-C2B	-2.78	1.46	1.51
37	y	606	CHL	CBD-CAD	-2.78	1.49	1.53
37	Y	606	CHL	CBD-CAD	-2.78	1.49	1.53
35	L	101	LHG	O7-C5	-2.77	1.39	1.46
27	A	410	CLA	CMD-C2D	-2.77	1.45	1.51
27	a	410	CLA	CMD-C2D	-2.77	1.45	1.51
27	R	603	CLA	CMB-C2B	-2.77	1.46	1.51
27	r	603	CLA	CMB-C2B	-2.77	1.46	1.51
27	B	610	CLA	CMB-C2B	-2.77	1.46	1.51
27	C	501	CLA	CMD-C2D	-2.77	1.45	1.51
27	c	501	CLA	CMD-C2D	-2.77	1.45	1.51
27	y	604	CLA	C3B-C2B	-2.77	1.36	1.40
37	N	605	CHL	CHD-C4C	-2.77	1.48	1.53
37	n	605	CHL	CHD-C4C	-2.77	1.48	1.53
38	s	1620	LUT	C21-C26	-2.77	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	s	606	CHL	CHD-C4C	-2.77	1.48	1.53
37	G	605	CHL	C1A-C2A	-2.77	1.50	1.53
27	A	407	CLA	CMD-C2D	-2.77	1.45	1.51
37	y	608	CHL	CBD-CAD	-2.76	1.49	1.53
37	Y	608	CHL	CBD-CAD	-2.76	1.49	1.53
27	B	603	CLA	C3B-C2B	-2.76	1.36	1.40
27	C	503	CLA	CMB-C2B	-2.76	1.46	1.51
27	N	602	CLA	CMB-C2B	-2.76	1.46	1.51
27	n	602	CLA	CMB-C2B	-2.76	1.46	1.51
27	Y	602	CLA	CMD-C2D	-2.76	1.45	1.51
37	N	609	CHL	C3B-CAB	-2.76	1.48	1.50
37	Y	609	CHL	C3B-CAB	-2.75	1.48	1.50
37	y	609	CHL	C3B-CAB	-2.75	1.48	1.50
27	s	610	CLA	CMB-C2B	-2.75	1.46	1.51
27	G	613	CLA	CMB-C2B	-2.75	1.46	1.51
28	A	408	PHO	C1C-NC	-2.74	1.32	1.38
27	B	617	CLA	CMB-C2B	-2.74	1.46	1.51
27	b	617	CLA	CMB-C2B	-2.74	1.46	1.51
37	S	606	CHL	CHD-C4C	-2.74	1.48	1.53
27	B	608	CLA	CMB-C2B	-2.74	1.46	1.51
37	N	608	CHL	C3D-CAD	-2.74	1.46	1.51
27	a	407	CLA	CMD-C2D	-2.74	1.45	1.51
27	g	604	CLA	CMB-C2B	-2.74	1.46	1.51
27	G	604	CLA	CMB-C2B	-2.74	1.46	1.51
27	y	602	CLA	CMD-C2D	-2.74	1.45	1.51
37	N	606	CHL	CBD-CAD	-2.74	1.49	1.53
27	B	609	CLA	CMB-C2B	-2.73	1.46	1.51
27	b	609	CLA	CMB-C2B	-2.73	1.46	1.51
37	n	606	CHL	CBD-CAD	-2.73	1.49	1.53
27	y	614	CLA	CMB-C2B	-2.73	1.46	1.51
27	S	614	CLA	CMD-C2D	-2.73	1.45	1.51
27	s	614	CLA	CMD-C2D	-2.73	1.45	1.51
27	c	511	CLA	CMB-C2B	-2.72	1.46	1.51
27	G	602	CLA	CMB-C2B	-2.72	1.46	1.51
27	g	602	CLA	CMB-C2B	-2.72	1.46	1.51
27	C	505	CLA	CMB-C2B	-2.72	1.46	1.51
27	c	505	CLA	CMB-C2B	-2.72	1.46	1.51
27	G	612	CLA	CMB-C2B	-2.72	1.46	1.51
27	b	603	CLA	CMB-C2B	-2.72	1.46	1.51
27	Y	603	CLA	C3B-C2B	-2.72	1.36	1.40
27	B	602	CLA	CMB-C2B	-2.72	1.46	1.51
27	b	602	CLA	CMB-C2B	-2.72	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	408	PHO	C1C-NC	-2.71	1.32	1.38
37	y	606	CHL	C3B-CAB	-2.71	1.48	1.50
27	b	608	CLA	CMB-C2B	-2.71	1.46	1.51
27	c	509	CLA	CMD-C2D	-2.71	1.45	1.51
27	S	610	CLA	CMB-C2B	-2.71	1.46	1.51
37	n	608	CHL	C3D-CAD	-2.71	1.46	1.51
27	g	613	CLA	CMB-C2B	-2.70	1.46	1.51
37	y	607	CHL	C1A-C2A	-2.70	1.50	1.53
37	Y	607	CHL	C1A-C2A	-2.70	1.50	1.53
27	c	506	CLA	CMD-C2D	-2.70	1.45	1.51
27	y	603	CLA	C3B-C2B	-2.70	1.36	1.40
27	c	512	CLA	CMB-C2B	-2.70	1.46	1.51
27	C	512	CLA	CMB-C2B	-2.70	1.46	1.51
37	r	608	CHL	C3D-CAD	-2.70	1.46	1.51
27	C	509	CLA	CMD-C2D	-2.70	1.45	1.51
32	C	518	DGD	O5D-C6D	-2.70	1.38	1.43
27	g	611	CLA	CMB-C2B	-2.70	1.46	1.51
27	C	511	CLA	CMD-C2D	-2.70	1.45	1.51
27	G	611	CLA	CMB-C2B	-2.70	1.46	1.51
27	s	614	CLA	CMB-C2B	-2.69	1.46	1.51
27	S	613	CLA	CMB-C2B	-2.69	1.46	1.51
27	s	613	CLA	CMB-C2B	-2.69	1.46	1.51
27	C	507	CLA	CMD-C2D	-2.69	1.45	1.51
27	c	513	CLA	CMD-C2D	-2.69	1.45	1.51
27	C	513	CLA	CMD-C2D	-2.69	1.45	1.51
37	g	607	CHL	C1A-C2A	-2.69	1.50	1.53
27	b	604	CLA	CMD-C2D	-2.69	1.45	1.51
27	B	604	CLA	CMD-C2D	-2.69	1.45	1.51
27	r	609	CLA	CMB-C2B	-2.69	1.46	1.51
27	R	609	CLA	CMB-C2B	-2.69	1.46	1.51
37	S	606	CHL	C2B-C1B	-2.69	1.47	1.53
27	Y	614	CLA	CMB-C2B	-2.69	1.46	1.51
27	C	504	CLA	CMD-C2D	-2.68	1.45	1.51
37	S	607	CHL	CHD-C4C	-2.68	1.48	1.53
37	g	605	CHL	CHD-C4C	-2.68	1.48	1.53
27	s	602	CLA	CMD-C2D	-2.68	1.45	1.51
27	A	406	CLA	CMB-C2B	-2.68	1.46	1.51
27	N	613	CLA	CMB-C2B	-2.68	1.46	1.51
37	n	608	CHL	CBD-CAD	-2.68	1.49	1.53
27	C	511	CLA	CMB-C2B	-2.68	1.46	1.51
38	N	1621	LUT	C22-C21	-2.68	1.51	1.54
27	b	607	CLA	CMD-C2D	-2.68	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	n	607	CHL	C1A-C2A	-2.67	1.50	1.53
27	c	504	CLA	C3B-C2B	-2.67	1.37	1.40
38	y	1621	LUT	C22-C21	-2.67	1.51	1.54
27	C	508	CLA	CMD-C2D	-2.67	1.45	1.51
27	c	508	CLA	CMD-C2D	-2.67	1.45	1.51
27	N	611	CLA	CMB-C2B	-2.67	1.46	1.51
27	B	609	CLA	CMD-C2D	-2.67	1.45	1.51
37	R	608	CHL	C3D-CAD	-2.66	1.46	1.51
27	Y	612	CLA	CMB-C2B	-2.66	1.46	1.51
27	y	612	CLA	CMB-C2B	-2.66	1.46	1.51
38	Y	1621	LUT	C22-C21	-2.66	1.51	1.54
27	d	403	CLA	CMB-C2B	-2.66	1.46	1.51
27	C	506	CLA	CMD-C2D	-2.66	1.45	1.51
27	C	513	CLA	CMB-C2B	-2.66	1.46	1.51
27	b	616	CLA	CMD-C2D	-2.66	1.45	1.51
27	c	511	CLA	CMD-C2D	-2.66	1.45	1.51
37	S	608	CHL	CHC-C1C	-2.66	1.48	1.53
37	G	607	CHL	C1A-C2A	-2.66	1.50	1.53
27	c	504	CLA	CMD-C2D	-2.66	1.45	1.51
37	s	606	CHL	C2B-C1B	-2.66	1.48	1.53
27	S	611	CLA	CMB-C2B	-2.66	1.46	1.51
27	s	611	CLA	CMB-C2B	-2.66	1.46	1.51
27	c	510	CLA	CMD-C2D	-2.65	1.45	1.51
37	Y	606	CHL	C2B-C1B	-2.65	1.48	1.53
27	c	507	CLA	CMD-C2D	-2.65	1.45	1.51
27	c	513	CLA	CMB-C2B	-2.65	1.46	1.51
37	n	605	CHL	C2A-C3A	-2.65	1.49	1.55
37	y	607	CHL	C2A-C3A	-2.65	1.49	1.55
27	G	614	CLA	CMB-C2B	-2.65	1.46	1.51
27	S	612	CLA	CMB-C2B	-2.65	1.46	1.51
27	b	609	CLA	CMD-C2D	-2.65	1.45	1.51
27	r	602	CLA	CMB-C2B	-2.65	1.46	1.51
27	R	602	CLA	CMB-C2B	-2.65	1.46	1.51
27	D	403	CLA	CMB-C2B	-2.65	1.46	1.51
27	s	612	CLA	CMB-C2B	-2.65	1.46	1.51
27	c	508	CLA	CMC-C2C	-2.64	1.45	1.50
27	N	603	CLA	CMB-C2B	-2.64	1.46	1.51
27	n	603	CLA	CMB-C2B	-2.64	1.46	1.51
27	R	604	CLA	CMB-C2B	-2.64	1.46	1.51
27	r	604	CLA	CMB-C2B	-2.64	1.46	1.51
27	S	614	CLA	CMB-C2B	-2.64	1.46	1.51
27	b	614	CLA	CMD-C2D	-2.64	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	614	CLA	CMD-C2D	-2.64	1.45	1.51
37	Y	606	CHL	C2A-C3A	-2.64	1.49	1.55
27	N	612	CLA	CMB-C2B	-2.64	1.46	1.51
27	D	403	CLA	CMD-C2D	-2.64	1.45	1.51
35	Y	2630	LHG	O7-C5	-2.64	1.39	1.46
35	y	2630	LHG	O7-C5	-2.64	1.39	1.46
37	G	605	CHL	CHD-C4C	-2.64	1.48	1.53
37	s	608	CHL	CHC-C1C	-2.63	1.48	1.53
37	Y	609	CHL	CBD-CAD	-2.63	1.49	1.53
37	y	609	CHL	CBD-CAD	-2.63	1.49	1.53
27	B	607	CLA	CMD-C2D	-2.63	1.45	1.51
27	C	503	CLA	C3B-C2B	-2.63	1.37	1.40
37	y	606	CHL	C2B-C1B	-2.63	1.48	1.53
38	n	1621	LUT	C22-C21	-2.63	1.51	1.54
37	G	606	CHL	C2A-C3A	-2.63	1.49	1.55
27	S	602	CLA	CMD-C2D	-2.63	1.45	1.51
27	g	610	CLA	CMB-C2B	-2.63	1.46	1.51
27	B	616	CLA	CMD-C2D	-2.63	1.45	1.51
37	R	606	CHL	C3B-CAB	-2.63	1.48	1.50
37	s	607	CHL	CHD-C4C	-2.63	1.48	1.53
37	y	601	CHL	CBD-CAD	-2.63	1.49	1.53
27	n	611	CLA	CMB-C2B	-2.63	1.46	1.51
27	g	614	CLA	CMB-C2B	-2.63	1.46	1.51
27	C	512	CLA	CMD-C2D	-2.63	1.45	1.51
27	B	610	CLA	CMD-C2D	-2.63	1.45	1.51
37	N	607	CHL	C1A-C2A	-2.63	1.50	1.53
27	b	610	CLA	CMD-C2D	-2.62	1.45	1.51
27	a	406	CLA	CMB-C2B	-2.62	1.46	1.51
37	Y	609	CHL	C2A-C3A	-2.62	1.49	1.55
37	y	609	CHL	C2A-C3A	-2.62	1.49	1.55
32	c	518	DGD	O5D-C6D	-2.62	1.38	1.43
27	b	611	CLA	CMD-C2D	-2.62	1.45	1.51
27	Y	611	CLA	CMB-C2B	-2.62	1.46	1.51
27	y	611	CLA	CMB-C2B	-2.62	1.46	1.51
37	y	607	CHL	C2B-C1B	-2.62	1.48	1.53
37	Y	607	CHL	C2B-C1B	-2.62	1.48	1.53
27	g	603	CLA	CMB-C2B	-2.62	1.46	1.51
38	Y	1621	LUT	C1-C6	-2.62	1.50	1.53
38	y	1621	LUT	C1-C6	-2.62	1.50	1.53
37	g	601	CHL	CBD-CAD	-2.62	1.49	1.53
27	Y	603	CLA	CMD-C2D	-2.62	1.45	1.51
27	n	610	CLA	CMD-C2D	-2.62	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	607	CHL	C2A-C3A	-2.62	1.49	1.55
37	r	606	CHL	C3B-CAB	-2.61	1.48	1.50
27	G	610	CLA	CMB-C2B	-2.61	1.46	1.51
27	n	613	CLA	CMB-C2B	-2.61	1.46	1.51
27	r	612	CLA	CMB-C2B	-2.61	1.46	1.51
27	r	610	CLA	CMB-C2B	-2.61	1.46	1.51
37	G	601	CHL	CBD-CAD	-2.61	1.49	1.53
27	b	605	CLA	CMD-C2D	-2.61	1.45	1.51
27	B	605	CLA	CMD-C2D	-2.61	1.45	1.51
37	N	605	CHL	C2A-C3A	-2.61	1.49	1.55
27	y	614	CLA	CMD-C2D	-2.61	1.45	1.51
27	n	610	CLA	C3B-C2B	-2.61	1.37	1.40
27	R	612	CLA	CMB-C2B	-2.61	1.46	1.51
37	y	606	CHL	C2A-C3A	-2.61	1.49	1.55
32	c	518	DGD	O2G-C2G	-2.60	1.39	1.46
32	C	518	DGD	O2G-C2G	-2.60	1.39	1.46
37	N	608	CHL	CBD-CAD	-2.60	1.49	1.53
27	B	615	CLA	CMD-C2D	-2.60	1.45	1.51
27	Y	612	CLA	CMD-C2D	-2.60	1.45	1.51
27	b	615	CLA	CMD-C2D	-2.60	1.45	1.51
27	y	612	CLA	CMD-C2D	-2.60	1.45	1.51
27	C	508	CLA	CMC-C2C	-2.60	1.45	1.50
27	b	612	CLA	CMD-C2D	-2.60	1.45	1.51
27	Y	614	CLA	CMD-C2D	-2.60	1.45	1.51
27	G	603	CLA	CMB-C2B	-2.60	1.46	1.51
37	g	606	CHL	C2A-C3A	-2.60	1.50	1.55
27	n	612	CLA	CMB-C2B	-2.60	1.46	1.51
37	G	606	CHL	C2B-C1B	-2.60	1.48	1.53
27	B	611	CLA	CMD-C2D	-2.60	1.45	1.51
37	N	608	CHL	C2B-C1B	-2.60	1.48	1.53
37	n	608	CHL	C2B-C1B	-2.60	1.48	1.53
37	n	607	CHL	C3B-CAB	-2.60	1.48	1.50
27	n	603	CLA	C3B-C2B	-2.60	1.37	1.40
27	N	603	CLA	C3B-C2B	-2.60	1.37	1.40
27	c	512	CLA	CMD-C2D	-2.60	1.45	1.51
27	d	403	CLA	CMD-C2D	-2.60	1.45	1.51
27	C	510	CLA	CMD-C2D	-2.59	1.45	1.51
27	B	612	CLA	CMD-C2D	-2.59	1.45	1.51
27	R	610	CLA	CMB-C2B	-2.59	1.46	1.51
27	b	606	CLA	CMD-C2D	-2.59	1.45	1.51
37	g	606	CHL	C2B-C1B	-2.59	1.48	1.53
27	r	603	CLA	C3B-C2B	-2.59	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	y	608	CHL	C3D-CAD	-2.59	1.46	1.51
37	N	607	CHL	C3B-CAB	-2.59	1.48	1.50
32	C	520	DGD	O5D-C6D	-2.59	1.39	1.43
27	B	606	CLA	CMD-C2D	-2.58	1.45	1.51
27	n	602	CLA	CMD-C2D	-2.58	1.45	1.51
27	S	609	CLA	CMB-C2B	-2.58	1.46	1.51
37	Y	601	CHL	CBD-CAD	-2.58	1.49	1.53
37	R	608	CHL	CBD-CAD	-2.58	1.49	1.53
37	G	607	CHL	C2A-C3A	-2.58	1.50	1.55
37	g	607	CHL	C2A-C3A	-2.58	1.50	1.55
27	C	504	CLA	C3B-C2B	-2.58	1.37	1.40
37	G	606	CHL	C3B-CAB	-2.58	1.48	1.50
27	y	603	CLA	CMD-C2D	-2.57	1.46	1.51
27	S	611	CLA	CMD-C2D	-2.57	1.46	1.51
27	s	611	CLA	CMD-C2D	-2.57	1.46	1.51
27	n	604	CLA	CMD-C2D	-2.57	1.46	1.51
37	Y	608	CHL	C3D-CAD	-2.57	1.46	1.51
27	g	610	CLA	CMD-C2D	-2.57	1.46	1.51
27	B	614	CLA	C3B-C2B	-2.57	1.37	1.40
32	c	520	DGD	O5D-C6D	-2.57	1.39	1.43
27	N	610	CLA	CMD-C2D	-2.56	1.46	1.51
27	N	614	CLA	CMB-C2B	-2.56	1.46	1.51
27	n	614	CLA	CMB-C2B	-2.56	1.46	1.51
27	r	616	CLA	CMB-C2B	-2.56	1.46	1.51
27	B	617	CLA	C3B-C2B	-2.56	1.37	1.40
27	b	617	CLA	C3B-C2B	-2.56	1.37	1.40
28	a	409	PHO	C1C-NC	-2.56	1.32	1.38
27	N	602	CLA	CMD-C2D	-2.56	1.46	1.51
27	G	612	CLA	C3B-C2B	-2.56	1.37	1.40
27	N	604	CLA	CMD-C2D	-2.56	1.46	1.51
27	R	616	CLA	CMB-C2B	-2.56	1.46	1.51
27	G	610	CLA	CMD-C2D	-2.56	1.46	1.51
27	b	602	CLA	CMD-C2D	-2.56	1.46	1.51
27	Y	610	CLA	CMD-C2D	-2.56	1.46	1.51
37	g	606	CHL	C3B-CAB	-2.56	1.48	1.50
27	c	513	CLA	CMC-C2C	-2.56	1.45	1.50
31	A	413	LMG	O8-C9	-2.56	1.39	1.45
37	N	601	CHL	CBD-CAD	-2.55	1.49	1.53
27	y	610	CLA	CMD-C2D	-2.55	1.46	1.51
37	r	606	CHL	C2B-C1B	-2.55	1.48	1.53
37	n	606	CHL	C2B-C1B	-2.55	1.48	1.53
37	N	606	CHL	C2B-C1B	-2.55	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	603	CLA	CMD-C2D	-2.55	1.46	1.51
27	Y	611	CLA	CMD-C2D	-2.55	1.46	1.51
27	C	506	CLA	C3B-C2B	-2.55	1.37	1.40
27	R	610	CLA	CMD-C2D	-2.55	1.46	1.51
27	C	513	CLA	CMC-C2C	-2.54	1.45	1.50
31	a	413	LMG	O8-C9	-2.54	1.39	1.45
37	R	606	CHL	CBD-CAD	-2.54	1.49	1.53
27	b	614	CLA	C3B-C2B	-2.54	1.37	1.40
37	r	606	CHL	CBD-CAD	-2.54	1.49	1.53
37	S	601	CHL	CBD-CAD	-2.54	1.49	1.53
28	A	409	PHO	C1C-NC	-2.54	1.32	1.38
37	r	608	CHL	CBD-CAD	-2.54	1.49	1.53
27	B	608	CLA	CMD-C2D	-2.54	1.46	1.51
27	c	503	CLA	C3B-C2B	-2.53	1.37	1.40
27	b	603	CLA	CMD-C2D	-2.53	1.46	1.51
27	D	402	CLA	C3B-C2B	-2.53	1.37	1.40
27	r	616	CLA	CMD-C2D	-2.53	1.46	1.51
27	R	609	CLA	CMD-C2D	-2.53	1.46	1.51
27	c	509	CLA	C4D-ND	-2.53	1.31	1.37
27	r	613	CLA	CMB-C2B	-2.53	1.46	1.51
37	n	601	CHL	CBD-CAD	-2.53	1.49	1.53
27	c	503	CLA	CMD-C2D	-2.53	1.46	1.51
27	Y	613	CLA	CMD-C2D	-2.53	1.46	1.51
27	R	611	CLA	CMB-C2B	-2.53	1.46	1.51
27	r	611	CLA	CMB-C2B	-2.53	1.46	1.51
32	c	520	DGD	O6D-C5D	-2.53	1.38	1.44
27	B	611	CLA	C3B-C2B	-2.53	1.37	1.40
27	b	611	CLA	C3B-C2B	-2.53	1.37	1.40
27	b	608	CLA	CMD-C2D	-2.53	1.46	1.51
27	r	610	CLA	CMD-C2D	-2.53	1.46	1.51
27	s	613	CLA	CMD-C2D	-2.53	1.46	1.51
27	B	602	CLA	CMD-C2D	-2.52	1.46	1.51
27	Y	612	CLA	C3B-C2B	-2.52	1.37	1.40
27	y	612	CLA	C3B-C2B	-2.52	1.37	1.40
27	R	603	CLA	C3B-C2B	-2.52	1.37	1.40
27	s	602	CLA	CMB-C2B	-2.52	1.46	1.51
27	S	602	CLA	CMB-C2B	-2.52	1.46	1.51
34	d	405	PL9	C36-C34	-2.52	1.45	1.51
34	D	405	PL9	C36-C34	-2.52	1.45	1.51
37	n	608	CHL	C2A-C3A	-2.52	1.50	1.55
37	n	605	CHL	CBD-CAD	-2.52	1.49	1.53
37	N	605	CHL	CBD-CAD	-2.52	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	s	609	CLA	CMB-C2B	-2.52	1.46	1.51
27	S	613	CLA	CMD-C2D	-2.52	1.46	1.51
27	y	611	CLA	CMD-C2D	-2.52	1.46	1.51
37	n	606	CHL	C2A-C3A	-2.52	1.50	1.55
37	N	606	CHL	C2A-C3A	-2.52	1.50	1.55
27	R	616	CLA	CMD-C2D	-2.52	1.46	1.51
27	y	613	CLA	CMD-C2D	-2.52	1.46	1.51
27	B	617	CLA	CMC-C2C	-2.51	1.45	1.50
27	N	610	CLA	C3B-C2B	-2.51	1.37	1.40
37	n	609	CHL	CBD-CAD	-2.51	1.49	1.53
37	N	609	CHL	CBD-CAD	-2.51	1.49	1.53
27	B	603	CLA	CMD-C2D	-2.51	1.46	1.51
27	A	410	CLA	C3B-C2B	-2.51	1.37	1.40
32	C	520	DGD	O6D-C5D	-2.51	1.38	1.44
27	n	603	CLA	CMD-C2D	-2.51	1.46	1.51
27	c	506	CLA	C3B-C2B	-2.51	1.37	1.40
37	y	601	CHL	C2B-C1B	-2.51	1.48	1.53
37	y	609	CHL	C2B-C1B	-2.51	1.48	1.53
37	Y	601	CHL	C2B-C1B	-2.51	1.48	1.53
27	g	612	CLA	C3B-C2B	-2.51	1.37	1.40
27	C	503	CLA	CMD-C2D	-2.51	1.46	1.51
27	r	609	CLA	CMD-C2D	-2.51	1.46	1.51
27	y	604	CLA	CMD-C2D	-2.51	1.46	1.51
27	g	604	CLA	CMD-C2D	-2.50	1.46	1.51
37	n	609	CHL	C2B-C1B	-2.50	1.48	1.53
37	N	609	CHL	C2B-C1B	-2.50	1.48	1.53
37	y	605	CHL	C2A-C3A	-2.50	1.50	1.55
27	G	603	CLA	C3B-C2B	-2.50	1.37	1.40
27	g	603	CLA	CMD-C2D	-2.50	1.46	1.51
27	G	603	CLA	CMD-C2D	-2.50	1.46	1.51
27	r	604	CLA	CMD-C2D	-2.50	1.46	1.51
27	b	617	CLA	CMC-C2C	-2.50	1.45	1.50
27	C	509	CLA	C4D-ND	-2.50	1.31	1.37
27	r	613	CLA	CMD-C2D	-2.49	1.46	1.51
37	Y	607	CHL	C3B-CAB	-2.49	1.48	1.50
37	Y	609	CHL	C2B-C1B	-2.49	1.48	1.53
37	G	606	CHL	CBD-CAD	-2.49	1.49	1.53
27	y	602	CLA	C3B-C2B	-2.49	1.37	1.40
32	c	519	DGD	O1G-C1G	-2.49	1.39	1.45
28	a	408	PHO	CMC-C2C	-2.49	1.45	1.50
37	N	608	CHL	C3B-CAB	-2.48	1.48	1.50
27	c	502	CLA	CMD-C2D	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	r	607	CHL	CBD-CAD	-2.48	1.49	1.53
37	Y	605	CHL	C2A-C3A	-2.48	1.50	1.55
27	c	512	CLA	C3B-C2B	-2.48	1.37	1.40
37	R	607	CHL	CBD-CAD	-2.48	1.49	1.53
27	R	613	CLA	CMD-C2D	-2.48	1.46	1.51
27	a	410	CLA	C3B-C2B	-2.48	1.37	1.40
32	C	519	DGD	O1G-C1G	-2.48	1.39	1.45
37	y	608	CHL	C2B-C1B	-2.48	1.48	1.53
27	G	604	CLA	CMD-C2D	-2.48	1.46	1.51
37	y	607	CHL	C3B-CAB	-2.48	1.48	1.50
29	c	515	BCR	C30-C25	-2.48	1.50	1.53
37	N	608	CHL	C2A-C3A	-2.48	1.50	1.55
27	N	614	CLA	CMD-C2D	-2.47	1.46	1.51
27	S	611	CLA	C3B-C2B	-2.47	1.37	1.40
27	R	603	CLA	CMD-C2D	-2.47	1.46	1.51
27	R	613	CLA	CMB-C2B	-2.47	1.46	1.51
27	Y	604	CLA	CMD-C2D	-2.47	1.46	1.51
27	R	602	CLA	CMD-C2D	-2.47	1.46	1.51
27	C	502	CLA	CMD-C2D	-2.47	1.46	1.51
27	a	405	CLA	CMC-C2C	-2.47	1.45	1.50
29	C	515	BCR	C30-C25	-2.47	1.50	1.53
27	b	613	CLA	CMC-C2C	-2.47	1.45	1.50
28	A	408	PHO	CMC-C2C	-2.47	1.45	1.50
37	R	606	CHL	C2B-C1B	-2.46	1.48	1.53
27	N	602	CLA	C3B-C2B	-2.46	1.37	1.40
27	n	602	CLA	C3B-C2B	-2.46	1.37	1.40
27	R	604	CLA	CMD-C2D	-2.46	1.46	1.51
27	d	402	CLA	C3B-C2B	-2.46	1.37	1.40
27	r	603	CLA	CMD-C2D	-2.46	1.46	1.51
27	b	606	CLA	CMC-C2C	-2.46	1.45	1.50
27	B	606	CLA	CMC-C2C	-2.46	1.45	1.50
37	R	606	CHL	C2A-C3A	-2.46	1.50	1.55
37	Y	608	CHL	C2A-C3A	-2.46	1.50	1.55
37	s	601	CHL	C2A-C3A	-2.45	1.50	1.55
38	Y	1620	LUT	C22-C21	-2.45	1.51	1.54
37	s	601	CHL	CBD-CAD	-2.45	1.49	1.53
27	b	605	CLA	C3B-C2B	-2.45	1.37	1.40
27	B	605	CLA	C3B-C2B	-2.45	1.37	1.40
27	B	610	CLA	C3B-C2B	-2.45	1.37	1.40
37	g	608	CHL	C2B-C1B	-2.45	1.48	1.53
38	N	1621	LUT	C1-C6	-2.45	1.50	1.53
37	n	606	CHL	C3B-CAB	-2.44	1.48	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	606	CHL	C3B-CAB	-2.44	1.48	1.50
27	g	603	CLA	C3B-C2B	-2.44	1.37	1.40
27	A	405	CLA	CMC-C2C	-2.44	1.45	1.50
27	r	601	CLA	CMB-C2B	-2.44	1.46	1.51
37	Y	601	CHL	C2A-C3A	-2.44	1.50	1.55
37	y	601	CHL	C2A-C3A	-2.44	1.50	1.55
32	C	520	DGD	O2G-C2G	-2.44	1.40	1.46
27	G	613	CLA	C3B-C2B	-2.44	1.37	1.40
27	g	613	CLA	C3B-C2B	-2.44	1.37	1.40
27	s	604	CLA	CMD-C2D	-2.44	1.46	1.51
31	D	411	LMG	O8-C9	-2.44	1.39	1.45
31	d	411	LMG	O8-C9	-2.44	1.39	1.45
27	G	614	CLA	CMD-C2D	-2.44	1.46	1.51
27	R	612	CLA	CMD-C2D	-2.44	1.46	1.51
27	s	611	CLA	C3B-C2B	-2.43	1.37	1.40
32	c	520	DGD	O2G-C2G	-2.43	1.40	1.46
27	g	612	CLA	CMD-C2D	-2.43	1.46	1.51
27	B	613	CLA	CMC-C2C	-2.43	1.45	1.50
37	r	606	CHL	C2A-C3A	-2.43	1.50	1.55
27	r	602	CLA	CMD-C2D	-2.43	1.46	1.51
27	R	601	CLA	CMB-C2B	-2.43	1.46	1.51
27	b	607	CLA	CMC-C2C	-2.43	1.45	1.50
37	N	601	CHL	C2B-C1B	-2.43	1.48	1.53
27	s	612	CLA	CMD-C2D	-2.43	1.46	1.51
27	S	604	CLA	CMD-C2D	-2.43	1.46	1.51
37	Y	608	CHL	C2B-C1B	-2.43	1.48	1.53
27	s	603	CLA	CMD-C2D	-2.42	1.46	1.51
37	G	608	CHL	C2B-C1B	-2.42	1.48	1.53
37	g	606	CHL	CBD-CAD	-2.42	1.49	1.53
37	g	605	CHL	CBD-CAD	-2.42	1.49	1.53
37	G	605	CHL	CBD-CAD	-2.42	1.49	1.53
27	Y	602	CLA	C3B-C2B	-2.42	1.37	1.40
37	n	601	CHL	C2B-C1B	-2.42	1.48	1.53
27	G	613	CLA	CMD-C2D	-2.42	1.46	1.51
27	g	613	CLA	CMD-C2D	-2.42	1.46	1.51
27	s	609	CLA	CMD-C2D	-2.42	1.46	1.51
37	y	601	CHL	C3D-CAD	-2.41	1.47	1.51
27	A	407	CLA	C3B-C2B	-2.41	1.37	1.40
27	g	614	CLA	CMD-C2D	-2.41	1.46	1.51
37	n	607	CHL	C2B-C1B	-2.41	1.48	1.53
27	S	612	CLA	CMD-C2D	-2.41	1.46	1.51
37	y	608	CHL	C2A-C3A	-2.41	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	C	520	DGD	O1G-C1G	-2.41	1.39	1.45
32	c	520	DGD	O1G-C1G	-2.41	1.39	1.45
27	S	603	CLA	CMD-C2D	-2.41	1.46	1.51
27	n	614	CLA	CMD-C2D	-2.41	1.46	1.51
27	N	613	CLA	CMD-C2D	-2.41	1.46	1.51
37	N	607	CHL	C2A-C3A	-2.41	1.50	1.55
27	b	614	CLA	CMC-C2C	-2.41	1.45	1.50
37	G	601	CHL	C2A-C3A	-2.41	1.50	1.55
37	g	601	CHL	C2A-C3A	-2.41	1.50	1.55
27	N	611	CLA	CMD-C2D	-2.40	1.46	1.51
27	n	611	CLA	CMD-C2D	-2.40	1.46	1.51
37	n	609	CHL	C3D-CAD	-2.40	1.47	1.51
37	N	609	CHL	C3D-CAD	-2.40	1.47	1.51
27	A	405	CLA	C4D-ND	-2.40	1.32	1.37
27	a	405	CLA	C4D-ND	-2.40	1.32	1.37
37	Y	605	CHL	C3B-CAB	-2.40	1.48	1.50
27	r	612	CLA	CMD-C2D	-2.40	1.46	1.51
27	G	612	CLA	CMD-C2D	-2.40	1.46	1.51
37	n	608	CHL	C3B-CAB	-2.40	1.48	1.50
27	B	607	CLA	CMC-C2C	-2.39	1.45	1.50
37	N	607	CHL	C2B-C1B	-2.39	1.48	1.53
27	R	611	CLA	CMD-C2D	-2.39	1.46	1.51
34	d	405	PL9	C31-C29	-2.39	1.45	1.51
28	a	409	PHO	CMC-C2C	-2.39	1.45	1.50
37	g	609	CHL	CBD-CAD	-2.39	1.49	1.53
37	G	609	CHL	CBD-CAD	-2.39	1.49	1.53
29	C	517	BCR	C1-C6	-2.39	1.50	1.53
27	b	610	CLA	C3B-C2B	-2.39	1.37	1.40
27	g	611	CLA	CMD-C2D	-2.39	1.46	1.51
27	S	609	CLA	CMD-C2D	-2.39	1.46	1.51
27	Y	610	CLA	CMC-C2C	-2.39	1.45	1.50
27	y	610	CLA	CMC-C2C	-2.39	1.45	1.50
37	g	609	CHL	C2A-C3A	-2.38	1.50	1.55
27	C	512	CLA	C3B-C2B	-2.38	1.37	1.40
28	A	409	PHO	CMC-C2C	-2.38	1.45	1.50
38	y	1620	LUT	C22-C21	-2.38	1.52	1.54
37	G	601	CHL	C3D-CAD	-2.38	1.47	1.51
27	B	614	CLA	CMC-C2C	-2.38	1.45	1.50
38	n	1621	LUT	C1-C6	-2.38	1.50	1.53
27	G	611	CLA	CMD-C2D	-2.38	1.46	1.51
37	s	601	CHL	C2B-C1B	-2.38	1.48	1.53
27	c	511	CLA	CMC-C2C	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	S	601	CHL	C2A-C3A	-2.37	1.50	1.55
37	n	607	CHL	C2A-C3A	-2.37	1.50	1.55
27	B	604	CLA	CMC-C2C	-2.37	1.45	1.50
27	B	608	CLA	C3B-C2B	-2.37	1.37	1.40
27	s	603	CLA	CMB-C2B	-2.37	1.46	1.51
27	D	402	CLA	C4D-ND	-2.37	1.32	1.37
27	d	402	CLA	C4D-ND	-2.37	1.32	1.37
27	r	611	CLA	CMD-C2D	-2.37	1.46	1.51
27	g	611	CLA	C3B-C2B	-2.37	1.37	1.40
27	G	611	CLA	C3B-C2B	-2.37	1.37	1.40
37	Y	601	CHL	C3D-CAD	-2.37	1.47	1.51
27	S	603	CLA	CMB-C2B	-2.36	1.46	1.51
34	D	405	PL9	C31-C29	-2.36	1.45	1.51
37	N	607	CHL	C3D-CAD	-2.36	1.47	1.51
37	y	606	CHL	C3D-CAD	-2.36	1.47	1.51
35	n	2630	LHG	O7-C5	-2.36	1.40	1.46
27	Y	602	CLA	CMC-C2C	-2.36	1.45	1.50
27	b	613	CLA	C4D-ND	-2.36	1.32	1.37
28	a	408	PHO	CHC-C4B	-2.36	1.34	1.40
28	A	408	PHO	CHC-C4B	-2.36	1.34	1.40
37	S	606	CHL	CBD-CAD	-2.36	1.49	1.53
27	b	605	CLA	CMC-C2C	-2.35	1.45	1.50
27	N	612	CLA	CMD-C2D	-2.35	1.46	1.51
27	C	511	CLA	CMC-C2C	-2.35	1.45	1.50
37	y	605	CHL	C3B-CAB	-2.35	1.48	1.50
37	s	606	CHL	CBD-CAD	-2.35	1.49	1.53
27	C	513	CLA	C4D-ND	-2.35	1.32	1.37
27	B	605	CLA	CMC-C2C	-2.35	1.45	1.50
27	r	601	CLA	CMD-C2D	-2.35	1.46	1.51
27	C	506	CLA	C4D-ND	-2.35	1.32	1.37
37	R	607	CHL	C2A-C3A	-2.35	1.50	1.55
37	g	601	CHL	C3D-CAD	-2.35	1.47	1.51
37	G	609	CHL	C2A-C3A	-2.35	1.50	1.55
27	R	601	CLA	CMD-C2D	-2.35	1.46	1.51
27	s	610	CLA	CMD-C2D	-2.35	1.46	1.51
32	C	518	DGD	O3E-C3E	-2.34	1.37	1.43
37	n	607	CHL	C3D-CAD	-2.34	1.47	1.51
27	B	613	CLA	C4D-ND	-2.34	1.32	1.37
27	y	602	CLA	CMC-C2C	-2.34	1.45	1.50
32	h	102	DGD	O5D-C6D	-2.34	1.39	1.43
27	n	613	CLA	CMD-C2D	-2.34	1.46	1.51
37	s	607	CHL	C1A-C2A	-2.34	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	S	607	CHL	C1A-C2A	-2.34	1.50	1.53
27	g	604	CLA	C3B-C2B	-2.34	1.37	1.40
35	N	2630	LHG	O7-C5	-2.34	1.40	1.46
37	s	608	CHL	CHD-C4C	-2.34	1.49	1.53
27	b	604	CLA	CMC-C2C	-2.34	1.45	1.50
27	C	511	CLA	C4D-ND	-2.34	1.32	1.37
27	b	603	CLA	C4D-ND	-2.34	1.32	1.37
27	B	603	CLA	C4D-ND	-2.34	1.32	1.37
29	c	517	BCR	C1-C6	-2.34	1.50	1.53
27	N	610	CLA	CMC-C2C	-2.34	1.45	1.50
29	C	514	BCR	C30-C25	-2.34	1.50	1.53
37	r	607	CHL	C2A-C3A	-2.34	1.50	1.55
27	b	608	CLA	C3B-C2B	-2.34	1.37	1.40
27	d	402	CLA	CMC-C2C	-2.33	1.45	1.50
37	S	608	CHL	CHD-C4C	-2.33	1.49	1.53
37	R	608	CHL	C2A-C3A	-2.33	1.50	1.55
37	r	608	CHL	C2A-C3A	-2.33	1.50	1.55
37	n	606	CHL	C3D-CAD	-2.33	1.47	1.51
37	N	606	CHL	C3D-CAD	-2.33	1.47	1.51
37	G	608	CHL	C3D-CAD	-2.33	1.47	1.51
37	S	601	CHL	C2B-C1B	-2.33	1.48	1.53
27	D	402	CLA	CMC-C2C	-2.33	1.45	1.50
27	B	616	CLA	CMC-C2C	-2.33	1.45	1.50
27	b	616	CLA	CMC-C2C	-2.33	1.45	1.50
28	a	408	PHO	CMB-C2B	-2.33	1.45	1.50
28	A	408	PHO	CMB-C2B	-2.33	1.45	1.50
37	R	607	CHL	C3B-CAB	-2.33	1.48	1.50
27	C	511	CLA	C3B-C2B	-2.32	1.37	1.40
27	C	509	CLA	C3B-C2B	-2.32	1.37	1.40
27	c	506	CLA	C4D-ND	-2.32	1.32	1.37
27	n	612	CLA	C3B-C2B	-2.32	1.37	1.40
32	c	519	DGD	O6D-C5D	-2.32	1.38	1.44
37	r	607	CHL	C3B-CAB	-2.32	1.48	1.50
31	D	411	LMG	O7-C8	-2.32	1.40	1.46
31	d	411	LMG	O7-C8	-2.32	1.40	1.46
29	b	620	BCR	C30-C25	-2.32	1.50	1.53
27	r	602	CLA	CMC-C2C	-2.32	1.45	1.50
27	S	612	CLA	C3B-C2B	-2.32	1.37	1.40
27	a	407	CLA	C3B-C2B	-2.32	1.37	1.40
32	C	519	DGD	O6D-C5D	-2.32	1.38	1.44
27	Y	611	CLA	C3B-C2B	-2.32	1.37	1.40
27	y	611	CLA	C3B-C2B	-2.32	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	s	607	CHL	C3B-CAB	-2.32	1.48	1.50
37	S	607	CHL	C3B-CAB	-2.32	1.48	1.50
29	B	620	BCR	C30-C25	-2.31	1.50	1.53
37	Y	606	CHL	C3D-CAD	-2.31	1.47	1.51
27	b	610	CLA	C4D-ND	-2.31	1.32	1.37
27	c	511	CLA	C4D-ND	-2.31	1.32	1.37
27	S	610	CLA	CMD-C2D	-2.31	1.46	1.51
27	c	513	CLA	C4D-ND	-2.31	1.32	1.37
29	a	411	BCR	C1-C6	-2.31	1.50	1.53
37	r	607	CHL	C2B-C1B	-2.31	1.48	1.53
37	G	608	CHL	CBD-CAD	-2.31	1.49	1.53
37	g	608	CHL	CBD-CAD	-2.31	1.49	1.53
38	G	1620	LUT	C1-C6	-2.31	1.50	1.53
38	g	1620	LUT	C1-C6	-2.31	1.50	1.53
27	R	602	CLA	CMC-C2C	-2.31	1.46	1.50
32	H	102	DGD	O5D-C6D	-2.31	1.39	1.43
32	c	518	DGD	O3E-C3E	-2.31	1.37	1.43
27	c	509	CLA	C3B-C2B	-2.31	1.37	1.40
27	N	604	CLA	C3B-C2B	-2.31	1.37	1.40
37	g	608	CHL	C3D-CAD	-2.30	1.47	1.51
27	B	612	CLA	C4D-ND	-2.30	1.32	1.37
27	b	607	CLA	C3B-CAB	-2.30	1.42	1.47
27	B	607	CLA	C3B-CAB	-2.30	1.42	1.47
37	R	607	CHL	C2B-C1B	-2.30	1.48	1.53
37	y	605	CHL	C2B-C1B	-2.30	1.48	1.53
27	s	612	CLA	C3B-C2B	-2.30	1.37	1.40
37	n	605	CHL	C2B-C1B	-2.30	1.48	1.53
37	N	605	CHL	C2B-C1B	-2.30	1.48	1.53
27	a	406	CLA	CMC-C2C	-2.30	1.46	1.50
37	G	607	CHL	C2B-C1B	-2.30	1.48	1.53
37	g	607	CHL	C2B-C1B	-2.30	1.48	1.53
37	Y	605	CHL	C3D-CAD	-2.30	1.47	1.51
27	c	504	CLA	CMC-C2C	-2.30	1.46	1.50
27	b	615	CLA	CMC-C2C	-2.30	1.46	1.50
27	Y	611	CLA	CMC-C2C	-2.29	1.46	1.50
29	h	101	BCR	C1-C6	-2.29	1.50	1.53
32	h	102	DGD	O2G-C2G	-2.29	1.40	1.46
29	c	514	BCR	C30-C25	-2.29	1.50	1.53
27	B	611	CLA	C4D-ND	-2.29	1.32	1.37
27	b	611	CLA	C4D-ND	-2.29	1.32	1.37
27	n	612	CLA	CMD-C2D	-2.29	1.46	1.51
38	N	1620	LUT	C22-C21	-2.29	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y	602	CLA	C3B-CAB	-2.29	1.42	1.47
27	G	604	CLA	C3B-C2B	-2.29	1.37	1.40
27	B	615	CLA	CMC-C2C	-2.29	1.46	1.50
37	G	601	CHL	C2B-C1B	-2.29	1.48	1.53
27	c	511	CLA	C3B-C2B	-2.29	1.37	1.40
37	y	607	CHL	C3D-CAD	-2.29	1.47	1.51
37	Y	607	CHL	C3D-CAD	-2.29	1.47	1.51
37	G	607	CHL	CBD-CAD	-2.29	1.49	1.53
27	B	610	CLA	C4D-ND	-2.29	1.32	1.37
35	S	2630	LHG	O7-C5	-2.29	1.40	1.46
29	C	517	BCR	C30-C25	-2.29	1.50	1.53
27	B	602	CLA	C3B-C2B	-2.29	1.37	1.40
27	b	602	CLA	C3B-C2B	-2.29	1.37	1.40
29	A	411	BCR	C1-C6	-2.28	1.50	1.53
37	g	609	CHL	C3B-CAB	-2.28	1.48	1.50
27	G	602	CLA	CMC-C2C	-2.28	1.46	1.50
27	g	602	CLA	CMC-C2C	-2.28	1.46	1.50
29	c	517	BCR	C30-C25	-2.28	1.50	1.53
27	n	610	CLA	CMC-C2C	-2.28	1.46	1.50
37	S	607	CHL	C2B-C1B	-2.28	1.48	1.53
32	H	102	DGD	O2G-C2G	-2.28	1.40	1.46
27	A	406	CLA	CMC-C2C	-2.28	1.46	1.50
27	C	510	CLA	CMC-C2C	-2.28	1.46	1.50
27	c	510	CLA	CMC-C2C	-2.28	1.46	1.50
27	Y	604	CLA	CMC-C2C	-2.28	1.46	1.50
27	D	403	CLA	C4D-ND	-2.28	1.32	1.37
27	d	403	CLA	C4D-ND	-2.28	1.32	1.37
37	y	605	CHL	C3D-CAD	-2.28	1.47	1.51
38	S	1620	LUT	C1-C6	-2.27	1.50	1.53
38	s	1620	LUT	C1-C6	-2.27	1.50	1.53
37	S	606	CHL	C2A-C3A	-2.27	1.50	1.55
37	Y	609	CHL	C3D-CAD	-2.27	1.47	1.51
37	y	609	CHL	C3D-CAD	-2.27	1.47	1.51
27	c	509	CLA	CMC-C2C	-2.27	1.46	1.50
27	C	509	CLA	CMC-C2C	-2.27	1.46	1.50
27	S	614	CLA	C3B-C2B	-2.27	1.37	1.40
27	b	603	CLA	CMC-C2C	-2.27	1.46	1.50
27	B	603	CLA	CMC-C2C	-2.27	1.46	1.50
38	n	1620	LUT	C22-C21	-2.27	1.52	1.54
27	Y	612	CLA	C4D-ND	-2.27	1.32	1.37
37	s	606	CHL	C2A-C3A	-2.27	1.50	1.55
27	y	603	CLA	CMC-C2C	-2.27	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	G	601	CHL	C3B-CAB	-2.27	1.48	1.50
37	r	608	CHL	C2B-C1B	-2.27	1.48	1.53
27	C	507	CLA	C3B-CAB	-2.27	1.43	1.47
27	b	612	CLA	C4D-ND	-2.26	1.32	1.37
27	C	505	CLA	C4D-ND	-2.26	1.32	1.37
27	c	505	CLA	CMC-C2C	-2.26	1.46	1.50
37	s	607	CHL	C2B-C1B	-2.26	1.48	1.53
27	N	603	CLA	C4D-ND	-2.26	1.32	1.37
27	C	507	CLA	C4D-ND	-2.26	1.32	1.37
27	c	505	CLA	C4D-ND	-2.26	1.32	1.37
27	c	507	CLA	C4D-ND	-2.26	1.32	1.37
29	b	618	BCR	C30-C25	-2.26	1.50	1.53
35	s	2630	LHG	O7-C5	-2.26	1.40	1.46
37	R	608	CHL	C2B-C1B	-2.26	1.48	1.53
28	A	408	PHO	CMD-C2D	-2.26	1.46	1.50
27	A	407	CLA	C4D-ND	-2.26	1.32	1.37
27	a	407	CLA	C4D-ND	-2.26	1.32	1.37
37	Y	605	CHL	C2B-C1B	-2.26	1.48	1.53
27	C	505	CLA	CMC-C2C	-2.26	1.46	1.50
27	C	512	CLA	CMC-C2C	-2.26	1.46	1.50
27	y	611	CLA	CMC-C2C	-2.26	1.46	1.50
27	S	602	CLA	CMC-C2C	-2.26	1.46	1.50
37	g	607	CHL	CBD-CAD	-2.25	1.49	1.53
37	g	601	CHL	C2B-C1B	-2.25	1.48	1.53
31	b	622	LMG	O7-C8	-2.25	1.40	1.46
31	B	622	LMG	O7-C8	-2.25	1.40	1.46
27	b	603	CLA	C3B-CAB	-2.25	1.43	1.47
27	B	603	CLA	C3B-CAB	-2.25	1.43	1.47
37	g	609	CHL	C2B-C1B	-2.25	1.48	1.53
27	y	612	CLA	C4D-ND	-2.25	1.32	1.37
27	n	611	CLA	C3B-C2B	-2.25	1.37	1.40
27	y	602	CLA	C3B-CAB	-2.25	1.43	1.47
34	d	405	PL9	C7-C8	-2.25	1.47	1.50
34	D	405	PL9	C7-C8	-2.25	1.47	1.50
27	c	503	CLA	CMC-C2C	-2.25	1.46	1.50
37	g	601	CHL	C3B-CAB	-2.25	1.48	1.50
37	y	608	CHL	C3B-CAB	-2.24	1.48	1.50
37	Y	608	CHL	C3B-CAB	-2.24	1.48	1.50
27	Y	613	CLA	C4D-ND	-2.24	1.32	1.37
27	y	613	CLA	C4D-ND	-2.24	1.32	1.37
27	C	502	CLA	C4D-ND	-2.24	1.32	1.37
27	C	502	CLA	C3B-C2B	-2.24	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y	603	CLA	CMC-C2C	-2.24	1.46	1.50
38	R	620	LUT	C22-C21	-2.24	1.52	1.54
27	A	410	CLA	CMC-C2C	-2.24	1.46	1.50
27	a	410	CLA	CMC-C2C	-2.24	1.46	1.50
27	a	410	CLA	C4D-ND	-2.24	1.32	1.37
32	C	518	DGD	O3D-C3D	-2.24	1.37	1.43
28	A	409	PHO	CMD-C2D	-2.24	1.46	1.50
27	C	504	CLA	CMC-C2C	-2.24	1.46	1.50
27	c	508	CLA	C4D-ND	-2.24	1.32	1.37
29	H	101	BCR	C1-C6	-2.24	1.50	1.53
27	s	614	CLA	C3B-C2B	-2.24	1.37	1.40
28	a	409	PHO	CMD-C2D	-2.24	1.46	1.50
37	G	609	CHL	C2B-C1B	-2.24	1.48	1.53
27	r	610	CLA	CMC-C2C	-2.24	1.46	1.50
27	R	610	CLA	CMC-C2C	-2.24	1.46	1.50
27	c	507	CLA	C3B-CAB	-2.24	1.43	1.47
27	N	612	CLA	C3B-C2B	-2.23	1.37	1.40
37	G	608	CHL	C2A-C3A	-2.23	1.50	1.55
37	g	608	CHL	C2A-C3A	-2.23	1.50	1.55
32	c	518	DGD	O3D-C3D	-2.23	1.37	1.43
27	B	615	CLA	C3B-CAB	-2.23	1.43	1.47
27	b	615	CLA	C3B-CAB	-2.23	1.43	1.47
27	a	406	CLA	C4D-ND	-2.23	1.32	1.37
27	b	604	CLA	C3B-CAB	-2.23	1.43	1.47
27	b	609	CLA	C3B-C2B	-2.23	1.37	1.40
27	B	611	CLA	CMC-C2C	-2.23	1.46	1.50
27	b	611	CLA	CMC-C2C	-2.23	1.46	1.50
27	A	405	CLA	C3B-C2B	-2.23	1.37	1.40
27	n	603	CLA	C4D-ND	-2.23	1.32	1.37
29	b	619	BCR	C1-C6	-2.23	1.50	1.53
27	c	507	CLA	CMC-C2C	-2.23	1.46	1.50
27	C	503	CLA	CMC-C2C	-2.22	1.46	1.50
27	c	512	CLA	CMC-C2C	-2.22	1.46	1.50
28	a	408	PHO	CMD-C2D	-2.22	1.46	1.50
27	n	604	CLA	C3B-C2B	-2.22	1.37	1.40
27	y	604	CLA	CMC-C2C	-2.22	1.46	1.50
27	n	602	CLA	CMC-C2C	-2.22	1.46	1.50
37	G	609	CHL	C3B-CAB	-2.22	1.48	1.50
27	B	604	CLA	C3B-CAB	-2.21	1.43	1.47
27	c	503	CLA	C4D-ND	-2.21	1.32	1.37
37	y	608	CHL	CBD-CGD	-2.21	1.48	1.52
37	Y	608	CHL	CBD-CGD	-2.21	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	407	CLA	CMC-C2C	-2.21	1.46	1.50
27	c	502	CLA	C4D-ND	-2.21	1.32	1.37
29	B	618	BCR	C30-C25	-2.21	1.50	1.53
27	n	603	CLA	CMC-C2C	-2.21	1.46	1.50
27	Y	614	CLA	C4D-ND	-2.21	1.32	1.37
27	A	406	CLA	C4D-ND	-2.21	1.32	1.37
37	g	605	CHL	C3B-CAB	-2.21	1.48	1.50
37	G	605	CHL	C3B-CAB	-2.21	1.48	1.50
27	A	410	CLA	C4D-ND	-2.21	1.32	1.37
27	r	609	CLA	CMC-C2C	-2.20	1.46	1.50
27	C	508	CLA	C3B-CAB	-2.20	1.43	1.47
27	c	508	CLA	C3B-CAB	-2.20	1.43	1.47
27	c	512	CLA	C4D-ND	-2.20	1.32	1.37
27	C	512	CLA	C4D-ND	-2.20	1.32	1.37
31	D	411	LMG	O4-C4	-2.20	1.37	1.43
31	d	411	LMG	O4-C4	-2.20	1.37	1.43
27	S	613	CLA	CMC-C2C	-2.20	1.46	1.50
27	C	507	CLA	CMC-C2C	-2.20	1.46	1.50
27	Y	612	CLA	C3B-CAB	-2.20	1.43	1.47
27	C	508	CLA	C4D-ND	-2.20	1.32	1.37
27	Y	613	CLA	CMC-C2C	-2.20	1.46	1.50
27	C	501	CLA	CMC-C2C	-2.20	1.46	1.50
30	B	621	SQD	O2-C2	-2.20	1.37	1.43
37	s	607	CHL	CBD-CAD	-2.20	1.49	1.53
37	S	607	CHL	CBD-CAD	-2.20	1.49	1.53
27	s	613	CLA	CMC-C2C	-2.20	1.46	1.50
27	s	602	CLA	CMC-C2C	-2.20	1.46	1.50
37	s	601	CHL	C3B-CAB	-2.20	1.48	1.50
37	n	605	CHL	C3B-CAB	-2.20	1.48	1.50
27	B	608	CLA	CMC-C2C	-2.20	1.46	1.50
38	r	620	LUT	C22-C21	-2.19	1.52	1.54
27	c	502	CLA	CMC-C2C	-2.19	1.46	1.50
27	C	502	CLA	CMC-C2C	-2.19	1.46	1.50
27	C	510	CLA	C4D-ND	-2.19	1.32	1.37
37	Y	601	CHL	C3B-CAB	-2.19	1.48	1.50
37	y	601	CHL	C3B-CAB	-2.19	1.48	1.50
27	B	610	CLA	CMC-C2C	-2.19	1.46	1.50
27	S	613	CLA	C4D-ND	-2.19	1.32	1.37
27	s	612	CLA	CMC-C2C	-2.19	1.46	1.50
27	y	612	CLA	C3B-CAB	-2.19	1.43	1.47
27	G	602	CLA	C4D-ND	-2.19	1.32	1.37
27	b	614	CLA	C3B-CAB	-2.19	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	g	609	CHL	C3D-CAD	-2.19	1.47	1.51
37	G	609	CHL	C3D-CAD	-2.19	1.47	1.51
27	N	603	CLA	CMC-C2C	-2.19	1.46	1.50
37	r	608	CHL	C3B-CAB	-2.19	1.48	1.50
30	A	412	SQD	O2-C2	-2.19	1.37	1.43
30	a	412	SQD	O2-C2	-2.19	1.37	1.43
27	R	603	CLA	C4D-ND	-2.19	1.32	1.37
27	r	603	CLA	C4D-ND	-2.19	1.32	1.37
27	B	609	CLA	CMC-C2C	-2.19	1.46	1.50
27	b	608	CLA	CMC-C2C	-2.19	1.46	1.50
27	b	610	CLA	CMC-C2C	-2.19	1.46	1.50
29	B	619	BCR	C1-C6	-2.18	1.50	1.53
37	R	606	CHL	C3D-CAD	-2.18	1.47	1.51
27	b	604	CLA	C4D-ND	-2.18	1.32	1.37
37	S	601	CHL	C3B-CAB	-2.18	1.48	1.50
37	s	606	CHL	C3B-CAB	-2.18	1.48	1.50
27	c	501	CLA	CMC-C2C	-2.18	1.46	1.50
27	c	502	CLA	C3B-C2B	-2.18	1.37	1.40
27	N	602	CLA	CMC-C2C	-2.18	1.46	1.50
28	a	409	PHO	CHC-C4B	-2.18	1.35	1.40
27	S	604	CLA	CMC-C2C	-2.18	1.46	1.50
27	a	406	CLA	C3B-C2B	-2.18	1.37	1.40
27	C	506	CLA	CMC-C2C	-2.18	1.46	1.50
27	d	403	CLA	C3B-C2B	-2.18	1.37	1.40
27	y	613	CLA	CMC-C2C	-2.18	1.46	1.50
27	b	605	CLA	C4D-ND	-2.17	1.32	1.37
27	B	605	CLA	C4D-ND	-2.17	1.32	1.37
27	B	611	CLA	C3B-CAB	-2.17	1.43	1.47
27	B	609	CLA	C3B-C2B	-2.17	1.37	1.40
27	C	503	CLA	C4D-ND	-2.17	1.32	1.37
27	Y	612	CLA	CMC-C2C	-2.17	1.46	1.50
27	y	612	CLA	CMC-C2C	-2.17	1.46	1.50
27	S	612	CLA	CMC-C2C	-2.17	1.46	1.50
27	a	407	CLA	CMC-C2C	-2.17	1.46	1.50
27	A	406	CLA	C3B-C2B	-2.17	1.37	1.40
30	b	621	SQD	O2-C2	-2.17	1.37	1.43
27	G	612	CLA	CMC-C2C	-2.17	1.46	1.50
29	b	619	BCR	C30-C25	-2.17	1.50	1.53
37	r	606	CHL	C3D-CAD	-2.17	1.47	1.51
27	B	614	CLA	C4D-ND	-2.17	1.32	1.37
27	R	609	CLA	CMC-C2C	-2.17	1.46	1.50
27	b	614	CLA	C4D-ND	-2.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	604	CLA	C4D-ND	-2.16	1.32	1.37
28	a	409	PHO	CAA-C2A	-2.16	1.49	1.54
27	S	614	CLA	C4D-ND	-2.16	1.32	1.37
27	c	510	CLA	C4D-ND	-2.16	1.32	1.37
27	s	614	CLA	C4D-ND	-2.16	1.32	1.37
27	s	613	CLA	C4D-ND	-2.16	1.32	1.37
27	G	613	CLA	C4D-ND	-2.16	1.32	1.37
27	g	613	CLA	C4D-ND	-2.16	1.32	1.37
27	b	611	CLA	C3B-CAB	-2.16	1.43	1.47
27	N	604	CLA	CMC-C2C	-2.16	1.46	1.50
27	a	405	CLA	C3B-C2B	-2.16	1.37	1.40
27	Y	610	CLA	C3B-C2B	-2.16	1.37	1.40
27	G	610	CLA	CMC-C2C	-2.16	1.46	1.50
27	b	613	CLA	C3B-C2B	-2.16	1.37	1.40
27	N	611	CLA	C3B-C2B	-2.16	1.37	1.40
27	B	614	CLA	C3B-CAB	-2.15	1.43	1.47
27	Y	602	CLA	C4D-ND	-2.15	1.32	1.37
27	y	602	CLA	C4D-ND	-2.15	1.32	1.37
27	g	602	CLA	C4D-ND	-2.15	1.32	1.37
28	A	409	PHO	CHC-C4B	-2.15	1.35	1.40
39	n	1622	XAT	O4-C5	-2.15	1.43	1.46
27	y	613	CLA	C3B-CAB	-2.15	1.43	1.47
27	s	610	CLA	CMC-C2C	-2.15	1.46	1.50
27	s	614	CLA	CMC-C2C	-2.15	1.46	1.50
27	B	607	CLA	C4D-ND	-2.15	1.32	1.37
27	n	604	CLA	CMC-C2C	-2.15	1.46	1.50
27	s	604	CLA	C3B-C2B	-2.15	1.37	1.40
27	s	604	CLA	CMC-C2C	-2.15	1.46	1.50
37	g	605	CHL	C2B-C1B	-2.15	1.49	1.53
37	G	605	CHL	C2B-C1B	-2.15	1.49	1.53
27	C	509	CLA	C3B-CAB	-2.15	1.43	1.47
27	g	613	CLA	CMC-C2C	-2.15	1.46	1.50
27	R	604	CLA	CMC-C2C	-2.15	1.46	1.50
27	g	610	CLA	CMC-C2C	-2.15	1.46	1.50
27	a	410	CLA	C3B-CAB	-2.15	1.43	1.47
27	y	614	CLA	C4D-ND	-2.14	1.32	1.37
27	g	603	CLA	CMC-C2C	-2.14	1.46	1.50
27	G	603	CLA	CMC-C2C	-2.14	1.46	1.50
27	C	503	CLA	C3B-CAB	-2.14	1.43	1.47
27	Y	613	CLA	C3B-CAB	-2.14	1.43	1.47
27	c	506	CLA	CMC-C2C	-2.14	1.46	1.50
27	b	609	CLA	CMC-C2C	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	619	BCR	C30-C25	-2.14	1.50	1.53
27	c	503	CLA	C3B-CAB	-2.14	1.43	1.47
27	B	602	CLA	CMC-C2C	-2.14	1.46	1.50
27	b	602	CLA	CMC-C2C	-2.14	1.46	1.50
27	G	613	CLA	CMC-C2C	-2.14	1.46	1.50
30	b	621	SQD	O3-C3	-2.14	1.37	1.43
27	b	606	CLA	C4D-ND	-2.14	1.32	1.37
28	A	409	PHO	CAA-C2A	-2.14	1.50	1.54
27	D	403	CLA	C3B-C2B	-2.14	1.37	1.40
30	a	418	SQD	O4-C4	-2.14	1.37	1.43
27	b	607	CLA	C4D-ND	-2.14	1.32	1.37
27	S	604	CLA	C3B-C2B	-2.13	1.37	1.40
27	n	613	CLA	C3B-C2B	-2.13	1.37	1.40
27	R	602	CLA	C3B-C2B	-2.13	1.37	1.40
27	r	612	CLA	C3B-C2B	-2.13	1.37	1.40
27	S	610	CLA	CMC-C2C	-2.13	1.46	1.50
30	B	621	SQD	O3-C3	-2.13	1.37	1.43
32	C	519	DGD	O5D-C6D	-2.13	1.39	1.43
40	S	1623	NEX	C1-C6	-2.13	1.51	1.54
27	B	608	CLA	C4D-ND	-2.13	1.32	1.37
27	b	608	CLA	C4D-ND	-2.13	1.32	1.37
32	C	518	DGD	O2E-C2E	-2.13	1.37	1.43
38	s	1620	LUT	C22-C21	-2.13	1.52	1.54
27	Y	611	CLA	C4D-ND	-2.13	1.32	1.37
27	y	603	CLA	C4D-ND	-2.12	1.32	1.37
27	Y	603	CLA	C4D-ND	-2.12	1.32	1.37
39	N	1622	XAT	O4-C5	-2.12	1.43	1.46
37	N	605	CHL	C3B-CAB	-2.12	1.48	1.50
28	a	408	PHO	CAA-C2A	-2.12	1.50	1.54
27	y	610	CLA	C3B-C2B	-2.12	1.37	1.40
27	N	613	CLA	CMC-C2C	-2.12	1.46	1.50
27	B	613	CLA	C3B-CAB	-2.12	1.43	1.47
30	A	418	SQD	O4-C4	-2.12	1.38	1.43
40	s	1623	NEX	C1-C6	-2.12	1.51	1.54
27	y	611	CLA	C4D-ND	-2.12	1.32	1.37
27	S	614	CLA	CMC-C2C	-2.12	1.46	1.50
30	a	418	SQD	O2-C2	-2.11	1.38	1.43
27	A	410	CLA	C3B-CAB	-2.11	1.43	1.47
29	B	618	BCR	C21-C22	-2.11	1.33	1.35
29	b	618	BCR	C21-C22	-2.11	1.33	1.35
27	B	617	CLA	C4D-ND	-2.11	1.32	1.37
27	b	617	CLA	C4D-ND	-2.11	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	G	1622	XAT	O4-C5	-2.11	1.43	1.46
29	b	618	BCR	C1-C6	-2.11	1.50	1.53
38	S	1620	LUT	C22-C21	-2.11	1.52	1.54
27	B	616	CLA	C4D-ND	-2.11	1.32	1.37
27	b	616	CLA	C4D-ND	-2.11	1.32	1.37
37	G	605	CHL	C2A-C3A	-2.11	1.50	1.55
30	A	412	SQD	O3-C3	-2.11	1.38	1.43
38	s	1621	LUT	C22-C21	-2.11	1.52	1.54
38	S	1621	LUT	C22-C21	-2.11	1.52	1.54
27	B	615	CLA	C4D-ND	-2.11	1.32	1.37
27	b	615	CLA	C4D-ND	-2.11	1.32	1.37
27	r	609	CLA	C3B-C2B	-2.10	1.37	1.40
27	N	613	CLA	C4D-ND	-2.10	1.32	1.37
27	B	606	CLA	C4D-ND	-2.10	1.32	1.37
27	b	609	CLA	C4D-ND	-2.10	1.32	1.37
27	y	610	CLA	C4D-ND	-2.10	1.32	1.37
27	S	603	CLA	CMC-C2C	-2.10	1.46	1.50
34	d	405	PL9	C46-C44	-2.10	1.46	1.51
27	N	611	CLA	CMC-C2C	-2.10	1.46	1.50
27	g	612	CLA	CMC-C2C	-2.10	1.46	1.50
27	n	611	CLA	CMC-C2C	-2.10	1.46	1.50
27	b	606	CLA	C3B-CAB	-2.10	1.43	1.47
32	c	518	DGD	O2E-C2E	-2.10	1.38	1.43
27	S	613	CLA	C3B-C2B	-2.10	1.37	1.40
27	s	613	CLA	C3B-C2B	-2.10	1.37	1.40
27	G	604	CLA	CMC-C2C	-2.10	1.46	1.50
37	n	601	CHL	C2A-C3A	-2.10	1.50	1.55
27	N	613	CLA	C3B-C2B	-2.10	1.37	1.40
27	c	509	CLA	C3B-CAB	-2.10	1.43	1.47
27	C	501	CLA	C4D-ND	-2.10	1.32	1.37
39	g	1622	XAT	O4-C5	-2.10	1.43	1.46
27	R	613	CLA	CMC-C2C	-2.09	1.46	1.50
27	B	606	CLA	C3B-CAB	-2.09	1.43	1.47
27	g	611	CLA	CMC-C2C	-2.09	1.46	1.50
27	r	603	CLA	CMC-C2C	-2.09	1.46	1.50
27	r	604	CLA	CMC-C2C	-2.09	1.46	1.50
27	B	609	CLA	C4D-ND	-2.09	1.32	1.37
30	A	418	SQD	O2-C2	-2.09	1.38	1.43
27	R	610	CLA	C3B-C2B	-2.09	1.37	1.40
27	g	611	CLA	C4D-ND	-2.09	1.32	1.37
27	G	611	CLA	C4D-ND	-2.09	1.32	1.37
27	s	603	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	r	610	CLA	C4D-ND	-2.09	1.32	1.37
27	r	602	CLA	C3B-C2B	-2.09	1.37	1.40
27	c	501	CLA	C4D-ND	-2.09	1.32	1.37
37	S	606	CHL	C3B-CAB	-2.09	1.48	1.50
27	g	604	CLA	CMC-C2C	-2.09	1.46	1.50
30	a	412	SQD	O4-C4	-2.08	1.38	1.43
27	c	506	CLA	C3B-CAB	-2.08	1.43	1.47
28	A	409	PHO	CMB-C2B	-2.08	1.46	1.50
27	R	612	CLA	C3B-C2B	-2.08	1.37	1.40
27	r	612	CLA	C4D-ND	-2.08	1.32	1.37
27	C	513	CLA	C3B-CAB	-2.08	1.43	1.47
32	c	519	DGD	O5D-C6D	-2.08	1.39	1.43
34	D	405	PL9	C46-C44	-2.08	1.46	1.51
31	b	622	LMG	O4-C4	-2.08	1.38	1.43
29	B	618	BCR	C1-C6	-2.08	1.51	1.53
27	R	603	CLA	CMC-C2C	-2.08	1.46	1.50
28	A	408	PHO	CAA-C2A	-2.08	1.50	1.54
34	D	405	PL9	C21-C19	-2.08	1.46	1.51
38	Y	1620	LUT	C1-C6	-2.07	1.51	1.53
38	y	1620	LUT	C1-C6	-2.07	1.51	1.53
27	R	609	CLA	C3B-C2B	-2.07	1.37	1.40
27	B	602	CLA	C4D-ND	-2.07	1.32	1.37
27	b	602	CLA	C4D-ND	-2.07	1.32	1.37
27	S	612	CLA	C4D-ND	-2.07	1.32	1.37
27	s	611	CLA	CMC-C2C	-2.07	1.46	1.50
27	C	506	CLA	C3B-CAB	-2.07	1.43	1.47
27	r	609	CLA	C4D-ND	-2.07	1.32	1.37
30	B	621	SQD	O4-C4	-2.07	1.38	1.43
27	S	611	CLA	CMC-C2C	-2.07	1.46	1.50
37	Y	601	CHL	CBD-CGD	-2.07	1.48	1.52
27	Y	604	CLA	C3B-CAB	-2.07	1.43	1.47
27	R	602	CLA	C4D-ND	-2.07	1.32	1.37
27	y	614	CLA	C3B-C2B	-2.07	1.37	1.40
37	y	601	CHL	CBD-CGD	-2.07	1.48	1.52
27	G	611	CLA	CMC-C2C	-2.07	1.46	1.50
27	n	613	CLA	CMC-C2C	-2.07	1.46	1.50
27	G	612	CLA	C4D-ND	-2.07	1.32	1.37
27	Y	610	CLA	C4D-ND	-2.07	1.32	1.37
37	g	605	CHL	C2A-C3A	-2.07	1.51	1.55
27	B	613	CLA	C3B-C2B	-2.07	1.37	1.40
27	B	610	CLA	C3B-CAB	-2.07	1.43	1.47
27	b	610	CLA	C3B-CAB	-2.07	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	613	CLA	C3B-CAB	-2.06	1.43	1.47
27	n	613	CLA	C4D-ND	-2.06	1.32	1.37
28	a	409	PHO	CMB-C2B	-2.06	1.46	1.50
27	R	616	CLA	C3B-C2B	-2.06	1.37	1.40
37	G	606	CHL	C3D-CAD	-2.06	1.47	1.51
27	R	609	CLA	C4D-ND	-2.06	1.32	1.37
27	S	602	CLA	C4D-ND	-2.06	1.32	1.37
30	A	412	SQD	O4-C4	-2.06	1.38	1.43
27	N	612	CLA	CMC-C2C	-2.06	1.46	1.50
27	c	513	CLA	C3B-CAB	-2.06	1.43	1.47
38	Y	1621	LUT	C10-C9	-2.06	1.33	1.35
38	y	1621	LUT	C10-C9	-2.06	1.33	1.35
30	a	412	SQD	O3-C3	-2.06	1.38	1.43
27	c	510	CLA	C3B-C2B	-2.06	1.37	1.40
27	y	604	CLA	C3B-CAB	-2.06	1.43	1.47
27	c	513	CLA	C3B-C2B	-2.06	1.37	1.40
38	s	1621	LUT	C1-C6	-2.05	1.51	1.53
38	S	1621	LUT	C1-C6	-2.05	1.51	1.53
27	s	612	CLA	C4D-ND	-2.05	1.32	1.37
27	G	610	CLA	C4D-ND	-2.05	1.32	1.37
27	Y	604	CLA	C4D-ND	-2.05	1.32	1.37
27	R	610	CLA	C4D-ND	-2.05	1.32	1.37
27	r	613	CLA	CMC-C2C	-2.05	1.46	1.50
27	g	610	CLA	C4D-ND	-2.05	1.32	1.37
27	R	611	CLA	C3B-C2B	-2.05	1.37	1.40
27	r	611	CLA	C3B-C2B	-2.05	1.37	1.40
31	B	622	LMG	O4-C4	-2.05	1.38	1.43
27	r	602	CLA	C4D-ND	-2.05	1.33	1.37
34	d	405	PL9	C21-C19	-2.05	1.46	1.51
27	R	612	CLA	C4D-ND	-2.05	1.33	1.37
37	R	608	CHL	C3B-CAB	-2.05	1.48	1.50
27	R	616	CLA	CMC-C2C	-2.05	1.46	1.50
27	B	602	CLA	C3B-CAB	-2.05	1.43	1.47
27	b	602	CLA	C3B-CAB	-2.05	1.43	1.47
27	s	609	CLA	C3B-C2B	-2.04	1.37	1.40
32	c	518	DGD	O6D-C5D	-2.04	1.39	1.44
32	C	518	DGD	O6D-C5D	-2.04	1.39	1.44
27	Y	614	CLA	C3B-C2B	-2.04	1.37	1.40
27	G	604	CLA	C3B-CAB	-2.04	1.43	1.47
27	C	510	CLA	C3B-C2B	-2.04	1.37	1.40
27	B	608	CLA	C3B-CAB	-2.04	1.43	1.47
27	b	608	CLA	C3B-CAB	-2.04	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	c	518	DGD	O2D-C2D	-2.04	1.38	1.43
27	g	612	CLA	C4D-ND	-2.04	1.33	1.37
27	n	602	CLA	C4D-ND	-2.04	1.33	1.37
27	r	616	CLA	CMC-C2C	-2.04	1.46	1.50
27	R	601	CLA	CMC-C2C	-2.04	1.46	1.50
37	N	601	CHL	C2A-C3A	-2.04	1.51	1.55
29	A	411	BCR	C30-C25	-2.04	1.51	1.53
27	r	612	CLA	CMC-C2C	-2.04	1.46	1.50
27	g	602	CLA	C3B-CAB	-2.03	1.43	1.47
37	N	605	CHL	C3D-CAD	-2.03	1.47	1.51
27	s	602	CLA	C4D-ND	-2.03	1.33	1.37
27	g	613	CLA	C3B-CAB	-2.03	1.43	1.47
38	N	1620	LUT	C1-C6	-2.03	1.51	1.53
27	N	612	CLA	C4D-ND	-2.03	1.33	1.37
27	n	610	CLA	C4D-ND	-2.03	1.33	1.37
29	A	411	BCR	C21-C22	-2.03	1.33	1.35
29	a	411	BCR	C21-C22	-2.03	1.33	1.35
27	N	604	CLA	C4D-ND	-2.03	1.33	1.37
32	C	518	DGD	O2D-C2D	-2.03	1.38	1.43
30	b	621	SQD	O4-C4	-2.03	1.38	1.43
37	G	607	CHL	C3B-CAB	-2.03	1.48	1.50
27	s	611	CLA	C4D-ND	-2.03	1.33	1.37
37	G	607	CHL	C3D-CAD	-2.03	1.47	1.51
27	n	612	CLA	C4D-ND	-2.03	1.33	1.37
35	Y	2630	LHG	C8-C7	-2.03	1.44	1.50
27	Y	614	CLA	CMC-C2C	-2.02	1.46	1.50
39	r	622	XAT	O4-C5	-2.02	1.43	1.46
37	g	607	CHL	C3B-CAB	-2.02	1.48	1.50
27	r	610	CLA	C3B-C2B	-2.02	1.37	1.40
27	y	604	CLA	C4D-ND	-2.02	1.33	1.37
27	C	505	CLA	C3B-C2B	-2.02	1.37	1.40
27	c	505	CLA	C3B-C2B	-2.02	1.37	1.40
27	s	604	CLA	C4D-ND	-2.02	1.33	1.37
27	R	612	CLA	CMC-C2C	-2.02	1.46	1.50
29	B	619	BCR	C10-C9	-2.02	1.33	1.35
29	b	619	BCR	C10-C9	-2.02	1.33	1.35
27	C	501	CLA	C3B-CAB	-2.02	1.43	1.47
27	r	601	CLA	CMC-C2C	-2.01	1.46	1.50
37	n	605	CHL	C3D-CAD	-2.01	1.47	1.51
31	d	411	LMG	O1-C7	-2.01	1.40	1.43
27	C	504	CLA	C4D-ND	-2.01	1.33	1.37
27	R	604	CLA	C3B-C2B	-2.01	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	G	2630	LHG	O7-C5	-2.01	1.41	1.46
37	g	606	CHL	C3D-CAD	-2.01	1.47	1.51
31	D	411	LMG	O1-C7	-2.01	1.40	1.43
27	g	614	CLA	C3B-C2B	-2.01	1.37	1.40
27	G	602	CLA	C3B-CAB	-2.01	1.43	1.47
27	G	602	CLA	C3B-C2B	-2.01	1.37	1.40
27	g	602	CLA	C3B-C2B	-2.01	1.37	1.40
29	b	620	BCR	C21-C22	-2.01	1.33	1.35
27	N	602	CLA	C4D-ND	-2.01	1.33	1.37
30	a	418	SQD	O3-C3	-2.01	1.38	1.43
27	G	603	CLA	C4D-ND	-2.00	1.33	1.37
37	S	608	CHL	C2B-C1B	-2.00	1.49	1.53
37	s	608	CHL	C2B-C1B	-2.00	1.49	1.53
27	G	614	CLA	CMC-C2C	-2.00	1.46	1.50
29	a	411	BCR	C30-C25	-2.00	1.51	1.53
37	g	607	CHL	C3D-CAD	-2.00	1.47	1.51
27	d	402	CLA	C3B-CAB	-2.00	1.43	1.47
30	A	418	SQD	O3-C3	-2.00	1.38	1.43
40	g	1623	NEX	O24-C25	-2.00	1.43	1.46
37	g	605	CHL	CMC-C2C	2.00	1.48	1.45
37	G	609	CHL	CMC-C2C	2.01	1.48	1.45
36	f	101	HEM	CAD-C3D	2.02	1.54	1.52
36	F	101	HEM	CAD-C3D	2.02	1.54	1.52
28	a	408	PHO	C1A-NA	2.02	1.41	1.37
28	A	408	PHO	C1A-NA	2.02	1.41	1.37
37	s	608	CHL	CMC-C2C	2.04	1.48	1.45
37	S	608	CHL	CMC-C2C	2.05	1.48	1.45
37	G	605	CHL	CMC-C2C	2.05	1.48	1.45
28	A	408	PHO	CHC-C1C	2.07	1.42	1.38
27	c	508	CLA	CHC-C1C	2.10	1.41	1.35
28	a	408	PHO	CHC-C1C	2.10	1.42	1.38
27	b	605	CLA	CHC-C1C	2.11	1.41	1.35
27	B	605	CLA	CHC-C1C	2.11	1.41	1.35
27	C	508	CLA	CHC-C1C	2.12	1.41	1.35
28	A	409	PHO	C1A-NA	2.18	1.42	1.37
28	a	409	PHO	C1A-NA	2.18	1.42	1.37
27	b	614	CLA	CHC-C1C	2.20	1.41	1.35
27	B	614	CLA	CHC-C1C	2.20	1.41	1.35
27	Y	613	CLA	CHC-C1C	2.21	1.41	1.35
27	y	613	CLA	CHC-C1C	2.21	1.41	1.35
27	C	513	CLA	CHC-C1C	2.21	1.41	1.35
27	c	512	CLA	CHC-C1C	2.22	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	513	CLA	CHC-C1C	2.22	1.41	1.35
27	A	410	CLA	CHC-C1C	2.23	1.41	1.35
27	a	410	CLA	CHC-C1C	2.24	1.41	1.35
27	S	604	CLA	CHC-C1C	2.24	1.41	1.35
27	s	604	CLA	CHC-C1C	2.24	1.41	1.35
27	B	616	CLA	CHC-C1C	2.25	1.41	1.35
27	b	616	CLA	CHC-C1C	2.25	1.41	1.35
27	A	405	CLA	CHC-C1C	2.25	1.41	1.35
27	a	405	CLA	CHC-C1C	2.25	1.41	1.35
27	B	611	CLA	CHC-C1C	2.25	1.41	1.35
27	b	611	CLA	CHC-C1C	2.25	1.41	1.35
27	a	406	CLA	CHC-C1C	2.25	1.41	1.35
27	n	613	CLA	CHC-C1C	2.25	1.41	1.35
27	C	512	CLA	CHC-C1C	2.26	1.41	1.35
27	g	613	CLA	CHC-C1C	2.26	1.41	1.35
27	N	613	CLA	CHC-C1C	2.27	1.42	1.35
27	C	507	CLA	CHC-C1C	2.28	1.42	1.35
27	c	507	CLA	CHC-C1C	2.28	1.42	1.35
27	A	406	CLA	CHC-C1C	2.28	1.42	1.35
27	c	503	CLA	CHC-C1C	2.29	1.42	1.35
27	c	504	CLA	CHC-C1C	2.29	1.42	1.35
27	C	504	CLA	CHC-C1C	2.29	1.42	1.35
27	y	602	CLA	CHC-C1C	2.30	1.42	1.35
27	G	613	CLA	CHC-C1C	2.30	1.42	1.35
27	C	503	CLA	CHC-C1C	2.30	1.42	1.35
27	Y	602	CLA	CHC-C1C	2.30	1.42	1.35
27	c	506	CLA	CHC-C1C	2.30	1.42	1.35
27	n	603	CLA	CHC-C1C	2.30	1.42	1.35
27	C	506	CLA	CHC-C1C	2.30	1.42	1.35
27	c	502	CLA	CHC-C1C	2.31	1.42	1.35
27	C	502	CLA	CHC-C1C	2.31	1.42	1.35
27	R	609	CLA	CHC-C1C	2.31	1.42	1.35
28	A	409	PHO	CHC-C1C	2.32	1.43	1.38
27	N	603	CLA	CHC-C1C	2.32	1.42	1.35
27	B	615	CLA	CHC-C1C	2.32	1.42	1.35
27	b	615	CLA	CHC-C1C	2.32	1.42	1.35
27	C	510	CLA	CHC-C1C	2.32	1.42	1.35
27	c	510	CLA	CHC-C1C	2.32	1.42	1.35
27	y	604	CLA	CHC-C1C	2.32	1.42	1.35
28	a	409	PHO	CHC-C1C	2.33	1.43	1.38
27	B	610	CLA	CHC-C1C	2.33	1.42	1.35
28	a	408	PHO	C4C-NC	2.33	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	407	CLA	CHC-C1C	2.33	1.42	1.35
27	B	602	CLA	CHC-C1C	2.33	1.42	1.35
27	b	602	CLA	CHC-C1C	2.33	1.42	1.35
27	b	603	CLA	CHC-C1C	2.33	1.42	1.35
27	B	603	CLA	CHC-C1C	2.33	1.42	1.35
27	N	612	CLA	CHC-C1C	2.33	1.42	1.35
27	D	403	CLA	CHC-C1C	2.33	1.42	1.35
27	d	403	CLA	CHC-C1C	2.33	1.42	1.35
27	C	511	CLA	CHC-C1C	2.34	1.42	1.35
27	d	402	CLA	CHC-C1C	2.34	1.42	1.35
27	b	613	CLA	CHC-C1C	2.34	1.42	1.35
27	B	613	CLA	CHC-C1C	2.34	1.42	1.35
27	Y	604	CLA	CHC-C1C	2.34	1.42	1.35
27	D	402	CLA	CHC-C1C	2.34	1.42	1.35
27	y	614	CLA	CHC-C1C	2.34	1.42	1.35
27	B	609	CLA	CHC-C1C	2.34	1.42	1.35
27	y	610	CLA	CHC-C1C	2.34	1.42	1.35
27	A	407	CLA	CHC-C1C	2.34	1.42	1.35
27	n	612	CLA	CHC-C1C	2.34	1.42	1.35
27	c	511	CLA	CHC-C1C	2.35	1.42	1.35
27	b	610	CLA	CHC-C1C	2.35	1.42	1.35
27	b	609	CLA	CHC-C1C	2.36	1.42	1.35
28	A	408	PHO	C4C-NC	2.36	1.42	1.36
27	Y	614	CLA	CHC-C1C	2.36	1.42	1.35
27	N	611	CLA	CHC-C1C	2.36	1.42	1.35
27	g	604	CLA	CHC-C1C	2.36	1.42	1.35
27	G	604	CLA	CHC-C1C	2.36	1.42	1.35
27	r	609	CLA	CHC-C1C	2.36	1.42	1.35
27	r	604	CLA	CHC-C1C	2.36	1.42	1.35
27	g	603	CLA	CHC-C1C	2.36	1.42	1.35
27	G	603	CLA	CHC-C1C	2.36	1.42	1.35
27	G	602	CLA	CHC-C1C	2.37	1.42	1.35
27	g	602	CLA	CHC-C1C	2.37	1.42	1.35
27	r	610	CLA	CHC-C1C	2.37	1.42	1.35
27	C	501	CLA	CHC-C1C	2.37	1.42	1.35
27	Y	612	CLA	CHC-C1C	2.37	1.42	1.35
27	y	612	CLA	CHC-C1C	2.37	1.42	1.35
27	c	501	CLA	CHC-C1C	2.37	1.42	1.35
27	Y	610	CLA	CHC-C1C	2.37	1.42	1.35
27	b	607	CLA	CHC-C1C	2.37	1.42	1.35
27	B	607	CLA	CHC-C1C	2.37	1.42	1.35
28	A	409	PHO	C4C-NC	2.38	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	604	CLA	CHC-C1C	2.38	1.42	1.35
28	a	409	PHO	C4C-NC	2.38	1.42	1.36
27	n	604	CLA	CHC-C1C	2.38	1.42	1.35
27	b	604	CLA	CHC-C1C	2.38	1.42	1.35
27	B	604	CLA	CHC-C1C	2.38	1.42	1.35
27	n	611	CLA	CHC-C1C	2.39	1.42	1.35
27	S	612	CLA	CHC-C1C	2.39	1.42	1.35
27	r	602	CLA	CHC-C1C	2.39	1.42	1.35
27	N	604	CLA	CHC-C1C	2.40	1.42	1.35
27	b	606	CLA	CHC-C1C	2.40	1.42	1.35
27	s	612	CLA	CHC-C1C	2.40	1.42	1.35
27	S	610	CLA	CHC-C1C	2.41	1.42	1.35
27	Y	603	CLA	CHC-C1C	2.41	1.42	1.35
27	y	603	CLA	CHC-C1C	2.41	1.42	1.35
27	r	616	CLA	CHC-C1C	2.41	1.42	1.35
27	R	610	CLA	CHC-C1C	2.42	1.42	1.35
27	s	613	CLA	CHC-C1C	2.42	1.42	1.35
27	R	602	CLA	CHC-C1C	2.42	1.42	1.35
27	Y	611	CLA	CHC-C1C	2.42	1.42	1.35
27	R	603	CLA	CHC-C1C	2.42	1.42	1.35
27	r	603	CLA	CHC-C1C	2.42	1.42	1.35
27	c	505	CLA	CHC-C1C	2.42	1.42	1.35
27	G	610	CLA	CHC-C1C	2.43	1.42	1.35
27	S	603	CLA	CHC-C1C	2.43	1.42	1.35
27	S	613	CLA	CHC-C1C	2.43	1.42	1.35
27	B	606	CLA	CHC-C1C	2.43	1.42	1.35
27	C	505	CLA	CHC-C1C	2.43	1.42	1.35
27	C	509	CLA	CHC-C1C	2.43	1.42	1.35
27	s	614	CLA	CHC-C1C	2.44	1.42	1.35
27	B	608	CLA	CHC-C1C	2.44	1.42	1.35
27	b	608	CLA	CHC-C1C	2.44	1.42	1.35
27	y	611	CLA	CHC-C1C	2.44	1.42	1.35
27	R	613	CLA	CHC-C1C	2.44	1.42	1.35
27	r	613	CLA	CHC-C1C	2.44	1.42	1.35
27	s	603	CLA	CHC-C1C	2.44	1.42	1.35
27	g	610	CLA	CHC-C1C	2.44	1.42	1.35
27	R	616	CLA	CHC-C1C	2.44	1.42	1.35
27	n	602	CLA	CHC-C1C	2.44	1.42	1.35
27	R	611	CLA	CHC-C1C	2.45	1.42	1.35
27	r	611	CLA	CHC-C1C	2.45	1.42	1.35
27	s	611	CLA	CHC-C1C	2.45	1.42	1.35
27	g	611	CLA	CHC-C1C	2.45	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	602	CLA	CHC-C1C	2.45	1.42	1.35
27	s	610	CLA	CHC-C1C	2.45	1.42	1.35
27	S	614	CLA	CHC-C1C	2.46	1.42	1.35
27	b	612	CLA	CHC-C1C	2.46	1.42	1.35
27	B	612	CLA	CHC-C1C	2.46	1.42	1.35
27	c	509	CLA	CHC-C1C	2.47	1.42	1.35
27	r	612	CLA	CHC-C1C	2.48	1.42	1.35
27	R	612	CLA	CHC-C1C	2.48	1.42	1.35
27	G	611	CLA	CHC-C1C	2.48	1.42	1.35
27	S	611	CLA	CHC-C1C	2.48	1.42	1.35
27	N	614	CLA	CHC-C1C	2.49	1.42	1.35
27	n	614	CLA	CHC-C1C	2.49	1.42	1.35
27	b	617	CLA	CHC-C1C	2.49	1.42	1.35
27	S	609	CLA	CHC-C1C	2.49	1.42	1.35
27	s	609	CLA	CHC-C1C	2.49	1.42	1.35
27	N	610	CLA	CHC-C1C	2.49	1.42	1.35
27	n	610	CLA	CHC-C1C	2.50	1.42	1.35
27	g	612	CLA	CHC-C1C	2.50	1.42	1.35
27	B	617	CLA	CHC-C1C	2.50	1.42	1.35
27	G	612	CLA	CHC-C1C	2.52	1.42	1.35
27	s	602	CLA	CHC-C1C	2.53	1.42	1.35
27	r	601	CLA	CHC-C1C	2.55	1.42	1.35
27	R	601	CLA	CHC-C1C	2.55	1.42	1.35
27	S	602	CLA	CHC-C1C	2.58	1.42	1.35
27	g	614	CLA	CHC-C1C	2.59	1.42	1.35
27	G	614	CLA	CHC-C1C	2.62	1.43	1.35
27	c	506	CLA	CHB-C4A	2.63	1.37	1.33
30	A	412	SQD	O47-C7	2.67	1.42	1.34
30	a	412	SQD	O47-C7	2.67	1.42	1.34
27	B	612	CLA	CHB-C4A	2.67	1.37	1.33
27	C	506	CLA	CHB-C4A	2.68	1.37	1.33
27	b	607	CLA	CHB-C4A	2.70	1.37	1.33
27	B	607	CLA	CHB-C4A	2.70	1.37	1.33
27	b	612	CLA	CHB-C4A	2.72	1.37	1.33
30	B	621	SQD	O47-C7	2.72	1.42	1.34
30	b	621	SQD	O47-C7	2.72	1.42	1.34
27	B	608	CLA	CHB-C4A	2.78	1.37	1.33
27	b	608	CLA	CHB-C4A	2.78	1.37	1.33
30	a	418	SQD	O47-C7	2.79	1.42	1.34
30	A	418	SQD	O47-C7	2.81	1.42	1.34
27	B	614	CLA	CHB-C4A	2.88	1.37	1.33
27	B	610	CLA	CHB-C4A	2.92	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	b	610	CLA	CHB-C4A	2.92	1.37	1.33
30	b	621	SQD	O48-C23	2.92	1.42	1.33
27	b	614	CLA	CHB-C4A	2.93	1.37	1.33
27	b	606	CLA	CHB-C4A	2.93	1.37	1.33
27	c	507	CLA	CHB-C4A	2.93	1.37	1.33
27	C	507	CLA	CHB-C4A	2.94	1.37	1.33
28	a	408	PHO	C3B-C4B	2.94	1.49	1.43
30	B	621	SQD	O48-C23	2.94	1.42	1.33
27	B	606	CLA	CHB-C4A	2.96	1.37	1.33
27	B	611	CLA	CHB-C4A	2.96	1.37	1.33
27	b	611	CLA	CHB-C4A	2.96	1.37	1.33
28	A	408	PHO	C3B-C4B	2.98	1.49	1.43
27	b	604	CLA	CHB-C4A	3.02	1.37	1.33
27	B	604	CLA	CHB-C4A	3.03	1.37	1.33
27	r	603	CLA	CHB-C4A	3.03	1.37	1.33
27	c	508	CLA	CHB-C4A	3.06	1.37	1.33
27	B	603	CLA	CHB-C4A	3.06	1.37	1.33
27	R	603	CLA	CHB-C4A	3.07	1.37	1.33
27	s	611	CLA	CHB-C4A	3.08	1.37	1.33
27	G	613	CLA	CHB-C4A	3.08	1.37	1.33
27	c	509	CLA	CHB-C4A	3.08	1.37	1.33
27	C	509	CLA	CHB-C4A	3.08	1.37	1.33
27	B	609	CLA	CHB-C4A	3.08	1.37	1.33
28	A	409	PHO	C3B-C4B	3.08	1.49	1.43
28	a	409	PHO	C3B-C4B	3.08	1.49	1.43
27	Y	613	CLA	CHB-C4A	3.11	1.37	1.33
27	y	613	CLA	CHB-C4A	3.11	1.37	1.33
27	S	611	CLA	CHB-C4A	3.11	1.37	1.33
27	C	508	CLA	CHB-C4A	3.12	1.37	1.33
27	C	511	CLA	CHB-C4A	3.13	1.37	1.33
27	Y	612	CLA	CHB-C4A	3.13	1.37	1.33
27	c	511	CLA	CHB-C4A	3.13	1.37	1.33
27	D	403	CLA	CHB-C4A	3.13	1.37	1.33
27	b	603	CLA	CHB-C4A	3.13	1.37	1.33
27	b	609	CLA	CHB-C4A	3.13	1.37	1.33
27	c	501	CLA	CHB-C4A	3.14	1.37	1.33
27	c	503	CLA	CHB-C4A	3.14	1.37	1.33
27	B	617	CLA	CHB-C4A	3.15	1.37	1.33
27	b	617	CLA	CHB-C4A	3.15	1.37	1.33
27	A	407	CLA	CHB-C4A	3.15	1.37	1.33
30	A	418	SQD	O48-C23	3.16	1.42	1.33
30	A	412	SQD	O48-C23	3.16	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	y	603	CLA	CHB-C4A	3.16	1.37	1.33
27	g	613	CLA	CHB-C4A	3.16	1.37	1.33
27	a	407	CLA	CHB-C4A	3.17	1.37	1.33
30	a	418	SQD	O48-C23	3.17	1.42	1.33
30	a	412	SQD	O48-C23	3.18	1.42	1.33
27	C	503	CLA	CHB-C4A	3.18	1.37	1.33
27	y	612	CLA	CHB-C4A	3.18	1.37	1.33
27	C	502	CLA	CHB-C4A	3.18	1.37	1.33
27	b	616	CLA	CHB-C4A	3.18	1.37	1.33
27	d	403	CLA	CHB-C4A	3.20	1.37	1.33
27	B	615	CLA	CHB-C4A	3.20	1.37	1.33
27	b	615	CLA	CHB-C4A	3.20	1.37	1.33
27	Y	603	CLA	CHB-C4A	3.20	1.37	1.33
27	C	501	CLA	CHB-C4A	3.21	1.37	1.33
27	n	603	CLA	CHB-C4A	3.21	1.37	1.33
27	N	603	CLA	CHB-C4A	3.21	1.37	1.33
27	B	613	CLA	CHB-C4A	3.22	1.37	1.33
27	a	410	CLA	CHB-C4A	3.22	1.37	1.33
27	A	410	CLA	CHB-C4A	3.22	1.37	1.33
27	c	502	CLA	CHB-C4A	3.22	1.37	1.33
27	C	512	CLA	CHB-C4A	3.24	1.37	1.33
27	r	609	CLA	CHB-C4A	3.24	1.37	1.33
27	R	609	CLA	CHB-C4A	3.24	1.37	1.33
27	B	616	CLA	CHB-C4A	3.25	1.37	1.33
27	n	604	CLA	CHB-C4A	3.25	1.37	1.33
27	A	406	CLA	CHB-C4A	3.27	1.37	1.33
27	c	504	CLA	CHB-C4A	3.27	1.37	1.33
27	C	504	CLA	CHB-C4A	3.27	1.37	1.33
27	b	613	CLA	CHB-C4A	3.27	1.37	1.33
27	S	613	CLA	CHB-C4A	3.27	1.37	1.33
27	s	613	CLA	CHB-C4A	3.27	1.37	1.33
27	C	505	CLA	CHB-C4A	3.30	1.38	1.33
27	n	610	CLA	CHB-C4A	3.31	1.38	1.33
27	c	512	CLA	CHB-C4A	3.32	1.38	1.33
27	C	510	CLA	CHB-C4A	3.32	1.38	1.33
27	c	510	CLA	CHB-C4A	3.32	1.38	1.33
27	n	611	CLA	CHB-C4A	3.33	1.38	1.33
27	G	611	CLA	CHB-C4A	3.34	1.38	1.33
27	c	505	CLA	CHB-C4A	3.35	1.38	1.33
27	c	513	CLA	CHB-C4A	3.35	1.38	1.33
27	C	513	CLA	CHB-C4A	3.35	1.38	1.33
27	G	612	CLA	CHB-C4A	3.35	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	614	CLA	CHB-C4A	3.36	1.38	1.33
27	n	614	CLA	CHB-C4A	3.36	1.38	1.33
27	N	604	CLA	CHB-C4A	3.36	1.38	1.33
27	a	406	CLA	CHB-C4A	3.36	1.38	1.33
27	N	610	CLA	CHB-C4A	3.36	1.38	1.33
27	g	612	CLA	CHB-C4A	3.38	1.38	1.33
27	g	611	CLA	CHB-C4A	3.38	1.38	1.33
27	N	611	CLA	CHB-C4A	3.39	1.38	1.33
27	G	603	CLA	CHB-C4A	3.40	1.38	1.33
27	y	604	CLA	CHB-C4A	3.42	1.38	1.33
27	Y	604	CLA	CHB-C4A	3.42	1.38	1.33
27	g	603	CLA	CHB-C4A	3.42	1.38	1.33
27	R	612	CLA	CHB-C4A	3.44	1.38	1.33
27	Y	611	CLA	CHB-C4A	3.46	1.38	1.33
36	f	101	HEM	C3B-CAB	3.46	1.55	1.47
27	r	613	CLA	CHB-C4A	3.47	1.38	1.33
27	y	611	CLA	CHB-C4A	3.48	1.38	1.33
27	s	603	CLA	CHB-C4A	3.49	1.38	1.33
27	S	614	CLA	CHB-C4A	3.49	1.38	1.33
27	s	614	CLA	CHB-C4A	3.49	1.38	1.33
27	n	613	CLA	CHB-C4A	3.49	1.38	1.33
27	S	603	CLA	CHB-C4A	3.49	1.38	1.33
27	R	616	CLA	CHB-C4A	3.49	1.38	1.33
27	r	616	CLA	CHB-C4A	3.49	1.38	1.33
27	r	612	CLA	CHB-C4A	3.50	1.38	1.33
36	F	101	HEM	C3B-CAB	3.51	1.55	1.47
27	y	602	CLA	CHB-C4A	3.51	1.38	1.33
36	f	101	HEM	C3C-CAC	3.52	1.55	1.47
27	S	604	CLA	CHB-C4A	3.52	1.38	1.33
27	s	604	CLA	CHB-C4A	3.52	1.38	1.33
27	N	613	CLA	CHB-C4A	3.53	1.38	1.33
36	F	101	HEM	C3C-CAC	3.53	1.55	1.47
27	R	613	CLA	CHB-C4A	3.54	1.38	1.33
27	Y	602	CLA	CHB-C4A	3.55	1.38	1.33
27	B	602	CLA	CHB-C4A	3.55	1.38	1.33
27	b	602	CLA	CHB-C4A	3.55	1.38	1.33
27	R	604	CLA	CHB-C4A	3.55	1.38	1.33
27	r	604	CLA	CHB-C4A	3.55	1.38	1.33
27	s	612	CLA	CHB-C4A	3.55	1.38	1.33
27	S	612	CLA	CHB-C4A	3.55	1.38	1.33
27	N	602	CLA	CHB-C4A	3.56	1.38	1.33
27	n	602	CLA	CHB-C4A	3.56	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	R	601	CLA	CHB-C4A	3.57	1.38	1.33
27	r	601	CLA	CHB-C4A	3.57	1.38	1.33
27	G	604	CLA	CHB-C4A	3.59	1.38	1.33
27	a	405	CLA	CHB-C4A	3.59	1.38	1.33
27	G	614	CLA	CHB-C4A	3.60	1.38	1.33
27	g	604	CLA	CHB-C4A	3.60	1.38	1.33
27	g	614	CLA	CHB-C4A	3.63	1.38	1.33
27	Y	610	CLA	CHB-C4A	3.63	1.38	1.33
27	s	610	CLA	CHB-C4A	3.63	1.38	1.33
27	g	602	CLA	CHB-C4A	3.64	1.38	1.33
27	y	614	CLA	CHB-C4A	3.65	1.38	1.33
27	A	405	CLA	CHB-C4A	3.66	1.38	1.33
27	N	612	CLA	CHB-C4A	3.66	1.38	1.33
27	G	602	CLA	CHB-C4A	3.66	1.38	1.33
27	n	612	CLA	CHB-C4A	3.66	1.38	1.33
37	r	608	CHL	OBD-CAD	3.67	1.27	1.21
27	S	610	CLA	CHB-C4A	3.68	1.38	1.33
27	G	610	CLA	CHB-C4A	3.68	1.38	1.33
37	R	608	CHL	OBD-CAD	3.68	1.27	1.21
27	y	610	CLA	CHB-C4A	3.68	1.38	1.33
27	s	609	CLA	CHB-C4A	3.69	1.38	1.33
27	Y	614	CLA	CHB-C4A	3.70	1.38	1.33
27	R	611	CLA	CHB-C4A	3.70	1.38	1.33
27	g	610	CLA	CHB-C4A	3.71	1.38	1.33
27	r	611	CLA	CHB-C4A	3.71	1.38	1.33
27	r	610	CLA	CHB-C4A	3.72	1.38	1.33
27	R	610	CLA	CHB-C4A	3.72	1.38	1.33
27	D	402	CLA	CHB-C4A	3.78	1.38	1.33
27	S	609	CLA	CHB-C4A	3.78	1.38	1.33
27	d	402	CLA	CHB-C4A	3.79	1.38	1.33
27	r	602	CLA	CHB-C4A	3.85	1.38	1.33
37	N	608	CHL	OBD-CAD	3.87	1.28	1.21
27	R	602	CLA	CHB-C4A	3.87	1.38	1.33
37	n	608	CHL	OBD-CAD	3.88	1.28	1.21
37	G	608	CHL	OBD-CAD	3.89	1.28	1.21
27	b	605	CLA	CHB-C4A	3.89	1.38	1.33
27	B	605	CLA	CHB-C4A	3.89	1.38	1.33
37	Y	601	CHL	OBD-CAD	3.89	1.28	1.21
37	y	605	CHL	OBD-CAD	3.91	1.28	1.21
37	Y	605	CHL	OBD-CAD	3.91	1.28	1.21
37	S	608	CHL	OBD-CAD	3.91	1.28	1.21
37	g	608	CHL	OBD-CAD	3.92	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	s	602	CLA	CHB-C4A	3.92	1.38	1.33
37	y	601	CHL	OBD-CAD	3.96	1.28	1.21
27	S	602	CLA	CHB-C4A	3.96	1.38	1.33
37	s	608	CHL	OBD-CAD	3.97	1.28	1.21
37	Y	608	CHL	OBD-CAD	3.99	1.28	1.21
37	Y	606	CHL	OBD-CAD	4.01	1.28	1.21
37	R	608	CHL	O2A-CGA	4.02	1.45	1.33
37	R	606	CHL	OBD-CAD	4.03	1.28	1.21
37	r	606	CHL	OBD-CAD	4.04	1.28	1.21
37	y	606	CHL	OBD-CAD	4.04	1.28	1.21
37	g	601	CHL	OBD-CAD	4.04	1.28	1.21
37	y	607	CHL	OBD-CAD	4.05	1.28	1.21
37	y	608	CHL	OBD-CAD	4.05	1.28	1.21
37	n	606	CHL	OBD-CAD	4.06	1.28	1.21
37	r	608	CHL	O2A-CGA	4.06	1.45	1.33
37	n	601	CHL	OBD-CAD	4.07	1.28	1.21
37	N	601	CHL	OBD-CAD	4.07	1.28	1.21
37	n	605	CHL	OBD-CAD	4.08	1.28	1.21
37	Y	607	CHL	OBD-CAD	4.08	1.28	1.21
37	S	601	CHL	OBD-CAD	4.08	1.28	1.21
37	G	601	CHL	OBD-CAD	4.08	1.28	1.21
37	N	607	CHL	OBD-CAD	4.09	1.28	1.21
37	s	601	CHL	OBD-CAD	4.11	1.28	1.21
37	N	605	CHL	OBD-CAD	4.11	1.28	1.21
37	n	607	CHL	OBD-CAD	4.11	1.28	1.21
37	g	609	CHL	OBD-CAD	4.11	1.28	1.21
37	G	609	CHL	OBD-CAD	4.11	1.28	1.21
37	N	606	CHL	OBD-CAD	4.12	1.28	1.21
37	g	606	CHL	OBD-CAD	4.13	1.28	1.21
37	Y	609	CHL	OBD-CAD	4.14	1.28	1.21
37	y	609	CHL	OBD-CAD	4.14	1.28	1.21
37	Y	601	CHL	O2A-CGA	4.16	1.45	1.33
37	y	601	CHL	O2A-CGA	4.16	1.45	1.33
37	n	605	CHL	O2A-CGA	4.16	1.45	1.33
37	N	605	CHL	O2A-CGA	4.16	1.45	1.33
37	r	606	CHL	O2A-CGA	4.16	1.45	1.33
37	G	608	CHL	O2A-CGA	4.16	1.45	1.33
37	R	606	CHL	O2A-CGA	4.17	1.45	1.33
37	g	601	CHL	O2A-CGA	4.17	1.45	1.33
37	n	609	CHL	OBD-CAD	4.17	1.28	1.21
37	N	609	CHL	OBD-CAD	4.17	1.28	1.21
37	G	606	CHL	OBD-CAD	4.18	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	609	CHL	O2A-CGA	4.18	1.45	1.33
37	y	609	CHL	O2A-CGA	4.18	1.45	1.33
37	g	608	CHL	O2A-CGA	4.19	1.45	1.33
37	G	601	CHL	O2A-CGA	4.20	1.45	1.33
37	y	605	CHL	O2A-CGA	4.20	1.45	1.33
37	G	606	CHL	O2A-CGA	4.20	1.45	1.33
37	g	606	CHL	O2A-CGA	4.20	1.45	1.33
37	s	601	CHL	O2A-CGA	4.21	1.45	1.33
37	n	608	CHL	O2A-CGA	4.21	1.45	1.33
37	S	601	CHL	O2A-CGA	4.21	1.45	1.33
37	S	607	CHL	OBD-CAD	4.21	1.28	1.21
37	N	601	CHL	O2A-CGA	4.22	1.45	1.33
37	Y	605	CHL	O2A-CGA	4.23	1.45	1.33
37	N	608	CHL	O2A-CGA	4.23	1.45	1.33
37	g	605	CHL	OBD-CAD	4.23	1.28	1.21
37	G	605	CHL	OBD-CAD	4.23	1.28	1.21
37	g	607	CHL	OBD-CAD	4.23	1.28	1.21
37	g	605	CHL	O2A-CGA	4.23	1.45	1.33
37	G	605	CHL	O2A-CGA	4.23	1.45	1.33
37	G	607	CHL	OBD-CAD	4.23	1.28	1.21
37	s	607	CHL	OBD-CAD	4.23	1.28	1.21
37	y	608	CHL	O2A-CGA	4.24	1.45	1.33
37	Y	608	CHL	O2A-CGA	4.24	1.45	1.33
37	n	601	CHL	O2A-CGA	4.24	1.45	1.33
37	N	606	CHL	O2A-CGA	4.25	1.46	1.33
37	s	608	CHL	O2A-CGA	4.25	1.46	1.33
37	R	607	CHL	O2A-CGA	4.26	1.46	1.33
37	S	607	CHL	O2A-CGA	4.26	1.46	1.33
37	n	606	CHL	O2A-CGA	4.26	1.46	1.33
37	Y	607	CHL	O2A-CGA	4.27	1.46	1.33
37	g	609	CHL	O2A-CGA	4.27	1.46	1.33
37	n	609	CHL	O2A-CGA	4.27	1.46	1.33
37	N	609	CHL	O2A-CGA	4.27	1.46	1.33
37	n	607	CHL	O2A-CGA	4.28	1.46	1.33
37	y	607	CHL	O2A-CGA	4.28	1.46	1.33
37	G	609	CHL	O2A-CGA	4.28	1.46	1.33
37	r	607	CHL	O2A-CGA	4.28	1.46	1.33
37	S	608	CHL	O2A-CGA	4.29	1.46	1.33
37	S	606	CHL	OBD-CAD	4.29	1.28	1.21
37	s	607	CHL	O2A-CGA	4.29	1.46	1.33
37	G	607	CHL	O2A-CGA	4.30	1.46	1.33
37	g	607	CHL	O2A-CGA	4.30	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	607	CHL	O2A-CGA	4.31	1.46	1.33
37	s	606	CHL	OBD-CAD	4.31	1.28	1.21
37	r	607	CHL	OBD-CAD	4.31	1.28	1.21
37	S	606	CHL	O2A-CGA	4.32	1.46	1.33
37	R	607	CHL	OBD-CAD	4.33	1.28	1.21
37	s	606	CHL	O2A-CGA	4.34	1.46	1.33
39	r	622	XAT	C6-C5	4.34	1.53	1.48
40	Y	1623	NEX	C26-C25	4.36	1.53	1.48
37	y	606	CHL	O2A-CGA	4.37	1.46	1.33
37	Y	606	CHL	O2A-CGA	4.37	1.46	1.33
39	N	1622	XAT	C26-C25	4.39	1.53	1.48
39	n	1622	XAT	C26-C25	4.39	1.53	1.48
39	R	622	XAT	C6-C5	4.41	1.53	1.48
40	y	1623	NEX	C26-C25	4.43	1.54	1.48
37	y	608	CHL	O2D-CGD	4.44	1.44	1.33
37	Y	608	CHL	O2D-CGD	4.44	1.44	1.33
37	Y	609	CHL	O2D-CGD	4.51	1.44	1.33
37	N	606	CHL	O2D-CGD	4.51	1.44	1.33
37	Y	607	CHL	O2D-CGD	4.51	1.44	1.33
37	y	607	CHL	O2D-CGD	4.51	1.44	1.33
37	N	608	CHL	O2D-CGD	4.51	1.44	1.33
37	R	606	CHL	O2D-CGD	4.51	1.44	1.33
37	y	609	CHL	O2D-CGD	4.52	1.44	1.33
37	n	608	CHL	O2D-CGD	4.53	1.44	1.33
37	r	606	CHL	O2D-CGD	4.53	1.44	1.33
37	n	606	CHL	O2D-CGD	4.53	1.44	1.33
40	s	1623	NEX	C26-C25	4.55	1.54	1.48
40	S	1623	NEX	C26-C25	4.55	1.54	1.48
39	r	622	XAT	C26-C25	4.57	1.54	1.48
37	n	607	CHL	O2D-CGD	4.58	1.45	1.33
37	N	607	CHL	O2D-CGD	4.59	1.45	1.33
39	n	1622	XAT	C6-C5	4.59	1.54	1.48
37	y	606	CHL	O2D-CGD	4.60	1.45	1.33
37	Y	606	CHL	O2D-CGD	4.60	1.45	1.33
40	R	623	NEX	C26-C25	4.61	1.54	1.48
37	n	601	CHL	O2D-CGD	4.62	1.45	1.33
37	n	609	CHL	O2D-CGD	4.63	1.45	1.33
37	N	609	CHL	O2D-CGD	4.63	1.45	1.33
37	y	605	CHL	O2D-CGD	4.63	1.45	1.33
37	N	605	CHL	O2D-CGD	4.64	1.45	1.33
37	N	601	CHL	O2D-CGD	4.64	1.45	1.33
39	R	622	XAT	C26-C25	4.64	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	Y	601	CHL	O2D-CGD	4.64	1.45	1.33
39	N	1622	XAT	C6-C5	4.65	1.54	1.48
37	G	601	CHL	O2D-CGD	4.66	1.45	1.33
40	N	1623	NEX	C26-C25	4.66	1.54	1.48
37	y	601	CHL	O2D-CGD	4.66	1.45	1.33
37	g	609	CHL	O2D-CGD	4.66	1.45	1.33
37	G	609	CHL	O2D-CGD	4.66	1.45	1.33
37	R	607	CHL	O2D-CGD	4.67	1.45	1.33
37	r	608	CHL	O2D-CGD	4.67	1.45	1.33
37	Y	605	CHL	O2D-CGD	4.67	1.45	1.33
40	n	1623	NEX	C26-C25	4.68	1.54	1.48
37	R	608	CHL	O2D-CGD	4.68	1.45	1.33
37	n	605	CHL	O2D-CGD	4.68	1.45	1.33
37	G	606	CHL	O2D-CGD	4.69	1.45	1.33
37	s	601	CHL	O2D-CGD	4.69	1.45	1.33
37	S	601	CHL	O2D-CGD	4.69	1.45	1.33
37	g	606	CHL	O2D-CGD	4.69	1.45	1.33
37	r	607	CHL	O2D-CGD	4.70	1.45	1.33
39	G	1622	XAT	C26-C25	4.71	1.54	1.48
39	g	1622	XAT	C26-C25	4.71	1.54	1.48
37	G	607	CHL	O2D-CGD	4.71	1.45	1.33
37	g	607	CHL	O2D-CGD	4.71	1.45	1.33
37	G	608	CHL	O2D-CGD	4.71	1.45	1.33
37	g	608	CHL	O2D-CGD	4.71	1.45	1.33
40	r	623	NEX	C26-C25	4.71	1.54	1.48
37	g	601	CHL	O2D-CGD	4.72	1.45	1.33
39	G	1622	XAT	C6-C5	4.73	1.54	1.48
37	g	605	CHL	O2D-CGD	4.76	1.45	1.33
37	s	606	CHL	O2D-CGD	4.78	1.45	1.33
39	y	1622	XAT	C26-C25	4.79	1.54	1.48
37	G	605	CHL	O2D-CGD	4.79	1.45	1.33
39	g	1622	XAT	C6-C5	4.80	1.54	1.48
37	S	606	CHL	O2D-CGD	4.81	1.45	1.33
39	Y	1622	XAT	C26-C25	4.81	1.54	1.48
37	s	607	CHL	O2D-CGD	4.81	1.45	1.33
37	S	607	CHL	O2D-CGD	4.81	1.45	1.33
37	s	608	CHL	O2D-CGD	4.83	1.45	1.33
40	G	1623	NEX	C26-C25	4.83	1.54	1.48
37	S	608	CHL	O2D-CGD	4.84	1.45	1.33
40	g	1623	NEX	C26-C25	4.85	1.54	1.48
39	y	1622	XAT	C6-C5	4.93	1.54	1.48
39	Y	1622	XAT	C6-C5	4.93	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	f	101	HEM	C3D-C2D	5.23	1.53	1.37
36	F	101	HEM	C3D-C2D	5.24	1.53	1.37
37	y	606	CHL	C3C-C2C	8.28	1.45	1.34
37	Y	606	CHL	C3C-C2C	8.28	1.45	1.34
37	y	609	CHL	C3C-C2C	8.31	1.45	1.34
37	Y	607	CHL	C3C-C2C	8.36	1.45	1.34
37	y	607	CHL	C3C-C2C	8.36	1.45	1.34
37	Y	609	CHL	C3C-C2C	8.41	1.45	1.34
37	Y	601	CHL	C3C-C2C	8.42	1.45	1.34
37	y	601	CHL	C3C-C2C	8.42	1.45	1.34
37	s	601	CHL	C3C-C2C	8.48	1.45	1.34
37	R	606	CHL	C3C-C2C	8.50	1.45	1.34
37	r	606	CHL	C3C-C2C	8.50	1.45	1.34
37	S	601	CHL	C3C-C2C	8.53	1.45	1.34
37	G	601	CHL	C3C-C2C	8.54	1.45	1.34
37	g	601	CHL	C3C-C2C	8.56	1.45	1.34
37	Y	608	CHL	C3C-C2C	8.63	1.45	1.34
37	y	608	CHL	C3C-C2C	8.66	1.45	1.34
37	n	607	CHL	C3C-C2C	8.68	1.45	1.34
37	N	607	CHL	C3C-C2C	8.70	1.45	1.34
37	n	609	CHL	C3C-C2C	8.72	1.45	1.34
37	N	609	CHL	C3C-C2C	8.72	1.45	1.34
37	n	606	CHL	C3C-C2C	8.77	1.45	1.34
37	N	606	CHL	C3C-C2C	8.77	1.45	1.34
37	n	608	CHL	C3C-C2C	8.77	1.45	1.34
37	S	606	CHL	C3C-C2C	8.80	1.45	1.34
37	s	606	CHL	C3C-C2C	8.80	1.45	1.34
37	Y	605	CHL	C3C-C2C	8.82	1.45	1.34
37	R	607	CHL	C3C-C2C	8.83	1.45	1.34
37	r	607	CHL	C3C-C2C	8.84	1.45	1.34
37	G	606	CHL	C3C-C2C	8.84	1.45	1.34
37	g	606	CHL	C3C-C2C	8.84	1.45	1.34
37	y	605	CHL	C3C-C2C	8.85	1.45	1.34
37	G	607	CHL	C3C-C2C	8.89	1.45	1.34
37	g	607	CHL	C3C-C2C	8.89	1.45	1.34
37	N	608	CHL	C3C-C2C	8.90	1.45	1.34
37	S	607	CHL	C3C-C2C	8.95	1.46	1.34
37	G	609	CHL	C3C-C2C	8.97	1.46	1.34
37	g	609	CHL	C3C-C2C	9.00	1.46	1.34
37	s	607	CHL	C3C-C2C	9.01	1.46	1.34
37	n	605	CHL	C3C-C2C	9.07	1.46	1.34
37	G	608	CHL	C3C-C2C	9.07	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	N	605	CHL	C3C-C2C	9.08	1.46	1.34
37	g	608	CHL	C3C-C2C	9.09	1.46	1.34
37	r	608	CHL	C3C-C2C	9.10	1.46	1.34
37	R	608	CHL	C3C-C2C	9.14	1.46	1.34
37	n	601	CHL	C3C-C2C	9.42	1.46	1.34
37	N	601	CHL	C3C-C2C	9.42	1.46	1.34
37	g	605	CHL	C3C-C2C	9.47	1.46	1.34
37	G	605	CHL	C3C-C2C	9.47	1.46	1.34
37	s	608	CHL	C3C-C2C	9.52	1.46	1.34
37	S	608	CHL	C3C-C2C	9.53	1.46	1.34

All (2930) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	N	1622	XAT	C31-C30-C29	-6.86	117.25	127.22
39	n	1622	XAT	C31-C30-C29	-6.85	117.26	127.22
29	C	516	BCR	C24-C23-C22	-6.56	116.30	126.21
29	c	516	BCR	C24-C23-C22	-6.54	116.33	126.21
29	D	404	BCR	C11-C10-C9	-6.39	117.94	127.22
29	d	404	BCR	C11-C10-C9	-6.39	117.94	127.22
29	C	517	BCR	C7-C8-C9	-6.37	116.58	126.21
29	c	517	BCR	C7-C8-C9	-6.37	116.59	126.21
39	Y	1622	XAT	C35-C34-C33	-6.34	118.01	127.22
29	C	516	BCR	C16-C17-C18	-6.31	118.05	127.22
39	y	1622	XAT	C35-C34-C33	-6.30	118.06	127.22
29	c	516	BCR	C16-C17-C18	-6.27	118.11	127.22
40	G	1623	NEX	C15-C14-C13	-5.81	118.78	127.22
40	g	1623	NEX	C15-C14-C13	-5.77	118.84	127.22
29	C	515	BCR	C15-C14-C13	-5.69	118.95	127.22
29	c	515	BCR	C15-C14-C13	-5.66	118.99	127.22
40	s	1623	NEX	C15-C14-C13	-5.66	119.00	127.22
40	S	1623	NEX	C15-C14-C13	-5.63	119.03	127.22
39	g	1622	XAT	C15-C14-C13	-5.62	119.05	127.22
39	G	1622	XAT	C15-C14-C13	-5.62	119.06	127.22
32	c	518	DGD	O3G-C3G-C2G	-5.61	97.65	110.99
32	C	518	DGD	O3G-C3G-C2G	-5.60	97.65	110.99
29	D	404	BCR	C7-C8-C9	-5.59	117.77	126.21
29	d	404	BCR	C7-C8-C9	-5.58	117.77	126.21
29	D	404	BCR	C24-C23-C22	-5.56	117.80	126.21
29	d	404	BCR	C24-C23-C22	-5.56	117.80	126.21
29	H	101	BCR	C16-C17-C18	-5.51	119.22	127.22
29	h	101	BCR	C16-C17-C18	-5.48	119.26	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	517	BCR	C11-C10-C9	-5.47	119.27	127.22
29	C	517	BCR	C11-C10-C9	-5.47	119.28	127.22
29	b	618	BCR	C28-C27-C26	-5.46	104.81	113.87
29	B	618	BCR	C28-C27-C26	-5.45	104.84	113.87
40	Y	1623	NEX	C15-C14-C13	-5.41	119.35	127.22
29	b	620	BCR	C16-C17-C18	-5.40	119.37	127.22
29	b	620	BCR	C7-C8-C9	-5.40	118.05	126.21
29	B	620	BCR	C7-C8-C9	-5.40	118.05	126.21
29	c	517	BCR	C15-C14-C13	-5.36	119.44	127.22
29	C	517	BCR	C15-C14-C13	-5.36	119.44	127.22
29	B	620	BCR	C16-C17-C18	-5.36	119.44	127.22
40	y	1623	NEX	C15-C14-C13	-5.35	119.44	127.22
40	r	623	NEX	C15-C14-C13	-5.32	119.49	127.22
40	R	623	NEX	C15-C14-C13	-5.32	119.49	127.22
29	c	517	BCR	C24-C23-C22	-5.32	118.18	126.21
29	C	517	BCR	C24-C23-C22	-5.32	118.18	126.21
40	G	1623	NEX	C11-C10-C9	-5.29	119.52	127.22
40	g	1623	NEX	C11-C10-C9	-5.29	119.52	127.22
29	b	619	BCR	C15-C14-C13	-5.25	119.59	127.22
29	B	619	BCR	C15-C14-C13	-5.25	119.59	127.22
29	a	411	BCR	C15-C14-C13	-5.24	119.60	127.22
29	A	411	BCR	C15-C14-C13	-5.24	119.61	127.22
29	b	618	BCR	C7-C8-C9	-5.15	118.43	126.21
29	c	515	BCR	C3-C4-C5	-5.14	105.36	113.87
39	n	1622	XAT	C15-C14-C13	-5.14	119.76	127.22
29	C	515	BCR	C3-C4-C5	-5.11	105.39	113.87
38	S	1620	LUT	C35-C34-C33	-5.11	119.79	127.22
29	B	618	BCR	C7-C8-C9	-5.10	118.50	126.21
38	s	1620	LUT	C35-C34-C33	-5.10	119.81	127.22
39	N	1622	XAT	C15-C14-C13	-5.08	119.83	127.22
38	S	1620	LUT	C7-C8-C9	-5.04	118.59	126.21
29	C	516	BCR	C20-C21-C22	-5.04	119.90	127.22
38	s	1620	LUT	C7-C8-C9	-5.01	118.64	126.21
40	n	1623	NEX	C11-C10-C9	-5.01	119.94	127.22
29	c	516	BCR	C20-C21-C22	-4.99	119.96	127.22
40	N	1623	NEX	C11-C10-C9	-4.99	119.96	127.22
29	c	514	BCR	C15-C14-C13	-4.97	119.99	127.22
29	C	514	BCR	C15-C14-C13	-4.93	120.05	127.22
32	c	519	DGD	O3G-C3G-C2G	-4.92	99.28	110.99
32	C	519	DGD	O3G-C3G-C2G	-4.90	99.33	110.99
29	c	516	BCR	C33-C5-C6	-4.86	119.44	124.62
29	C	516	BCR	C33-C5-C6	-4.86	119.44	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	411	BCR	C16-C17-C18	-4.82	120.22	127.22
29	A	411	BCR	C16-C17-C18	-4.80	120.25	127.22
32	c	520	DGD	O3G-C3G-C2G	-4.79	99.58	110.99
32	C	520	DGD	O3G-C3G-C2G	-4.78	99.61	110.99
29	c	515	BCR	C11-C10-C9	-4.76	120.30	127.22
29	C	515	BCR	C11-C10-C9	-4.73	120.35	127.22
29	b	618	BCR	C33-C5-C6	-4.73	119.59	124.62
29	B	618	BCR	C33-C5-C6	-4.72	119.60	124.62
40	N	1623	NEX	C35-C34-C33	-4.71	120.37	127.22
40	n	1623	NEX	C15-C14-C13	-4.70	120.39	127.22
29	C	514	BCR	C16-C17-C18	-4.68	120.41	127.22
37	Y	609	CHL	CBC-CAC-C3C	-4.67	106.33	113.16
37	y	609	CHL	CBC-CAC-C3C	-4.67	106.33	113.16
40	n	1623	NEX	C35-C34-C33	-4.66	120.44	127.22
29	c	514	BCR	C16-C17-C18	-4.66	120.44	127.22
30	B	621	SQD	O9-S-O7	-4.64	100.84	113.96
40	N	1623	NEX	C15-C14-C13	-4.64	120.47	127.22
37	y	606	CHL	CBA-CAA-C2A	-4.64	109.03	115.88
37	Y	606	CHL	CBA-CAA-C2A	-4.64	109.03	115.88
30	b	621	SQD	O9-S-O7	-4.64	100.86	113.96
30	a	418	SQD	O9-S-O7	-4.63	100.87	113.96
30	A	418	SQD	O9-S-O7	-4.63	100.88	113.96
37	G	606	CHL	CBA-CAA-C2A	-4.56	109.15	115.88
27	C	505	CLA	CMB-C2B-C1B	-4.55	120.58	128.31
27	c	505	CLA	CMB-C2B-C1B	-4.55	120.58	128.31
30	a	412	SQD	O9-S-O7	-4.54	101.13	113.96
37	g	606	CHL	CBA-CAA-C2A	-4.54	109.18	115.88
29	b	619	BCR	C24-C23-C22	-4.53	119.37	126.21
29	a	411	BCR	C33-C5-C6	-4.52	119.81	124.62
30	A	412	SQD	O9-S-O7	-4.51	101.22	113.96
38	n	1620	LUT	C15-C14-C13	-4.48	120.71	127.22
29	b	618	BCR	C11-C10-C9	-4.48	120.71	127.22
29	B	619	BCR	C24-C23-C22	-4.47	119.45	126.21
37	S	607	CHL	CBC-CAC-C3C	-4.47	106.64	113.16
29	A	411	BCR	C33-C5-C6	-4.46	119.87	124.62
29	B	618	BCR	C11-C10-C9	-4.46	120.74	127.22
37	s	607	CHL	CBC-CAC-C3C	-4.46	106.65	113.16
38	N	1620	LUT	C15-C14-C13	-4.46	120.74	127.22
29	B	618	BCR	C15-C14-C13	-4.45	120.75	127.22
29	b	618	BCR	C15-C14-C13	-4.45	120.75	127.22
38	G	1620	LUT	C35-C34-C33	-4.45	120.76	127.22
38	g	1620	LUT	C35-C34-C33	-4.44	120.76	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	515	BCR	C7-C8-C9	-4.44	119.50	126.21
29	c	517	BCR	C33-C5-C6	-4.42	119.91	124.62
29	c	515	BCR	C7-C8-C9	-4.42	119.53	126.21
40	Y	1623	NEX	C35-C34-C33	-4.40	120.83	127.22
40	y	1623	NEX	C35-C34-C33	-4.40	120.83	127.22
29	C	517	BCR	C33-C5-C6	-4.39	119.94	124.62
38	n	1620	LUT	C35-C34-C33	-4.38	120.85	127.22
38	s	1621	LUT	C35-C34-C33	-4.38	120.85	127.22
29	b	620	BCR	C15-C14-C13	-4.38	120.86	127.22
29	B	620	BCR	C15-C14-C13	-4.38	120.86	127.22
29	C	515	BCR	C24-C23-C22	-4.38	119.60	126.21
38	N	1620	LUT	C35-C34-C33	-4.36	120.89	127.22
29	c	515	BCR	C24-C23-C22	-4.35	119.63	126.21
37	N	605	CHL	C4A-C3A-C2A	-4.34	97.30	103.98
29	d	404	BCR	C33-C5-C6	-4.34	120.00	124.62
38	S	1621	LUT	C35-C34-C33	-4.33	120.93	127.22
29	d	404	BCR	C38-C26-C25	-4.33	120.01	124.62
29	b	619	BCR	C20-C21-C22	-4.33	120.93	127.22
29	B	619	BCR	C20-C21-C22	-4.32	120.94	127.22
37	n	605	CHL	C4A-C3A-C2A	-4.32	97.33	103.98
29	D	404	BCR	C38-C26-C25	-4.31	120.03	124.62
29	D	404	BCR	C33-C5-C6	-4.30	120.04	124.62
29	c	517	BCR	C20-C21-C22	-4.29	120.98	127.22
29	C	517	BCR	C20-C21-C22	-4.29	120.98	127.22
37	G	601	CHL	CBC-CAC-C3C	-4.29	106.90	113.16
29	b	618	BCR	C24-C23-C22	-4.26	119.77	126.21
27	Y	610	CLA	CMB-C2B-C1B	-4.26	121.07	128.31
38	Y	1621	LUT	C15-C14-C13	-4.24	121.05	127.22
38	y	1621	LUT	C15-C14-C13	-4.24	121.05	127.22
37	S	608	CHL	CBC-CAC-C3C	-4.24	106.96	113.16
37	g	601	CHL	CBC-CAC-C3C	-4.24	106.96	113.16
29	B	618	BCR	C24-C23-C22	-4.24	119.81	126.21
27	y	610	CLA	CMB-C2B-C1B	-4.23	121.11	128.31
37	s	608	CHL	CBC-CAC-C3C	-4.23	106.98	113.16
29	B	619	BCR	C16-C17-C18	-4.23	121.08	127.22
29	b	619	BCR	C16-C17-C18	-4.22	121.08	127.22
29	C	516	BCR	C7-C8-C9	-4.21	119.85	126.21
29	c	516	BCR	C7-C8-C9	-4.20	119.87	126.21
29	A	411	BCR	C7-C8-C9	-4.18	119.89	126.21
27	s	610	CLA	CMB-C2B-C1B	-4.18	121.20	128.31
37	r	606	CHL	CBA-CAA-C2A	-4.17	109.72	115.88
27	S	610	CLA	CMB-C2B-C1B	-4.17	121.23	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	403	CLA	CMB-C2B-C1B	-4.16	121.23	128.31
29	a	411	BCR	C7-C8-C9	-4.16	119.92	126.21
29	c	514	BCR	C11-C10-C9	-4.16	121.17	127.22
37	R	606	CHL	CBA-CAA-C2A	-4.15	109.76	115.88
29	C	514	BCR	C11-C10-C9	-4.14	121.20	127.22
27	D	403	CLA	CMB-C2B-C1B	-4.14	121.27	128.31
32	H	102	DGD	O3G-C3G-C2G	-4.13	101.16	110.99
32	h	102	DGD	O3G-C3G-C2G	-4.13	101.17	110.99
29	B	619	BCR	C33-C5-C6	-4.12	120.23	124.62
29	b	619	BCR	C33-C5-C6	-4.12	120.23	124.62
39	y	1622	XAT	C31-C30-C29	-4.11	121.25	127.22
39	Y	1622	XAT	C31-C30-C29	-4.09	121.28	127.22
38	N	1621	LUT	C15-C14-C13	-4.07	121.30	127.22
38	n	1621	LUT	C15-C14-C13	-4.07	121.31	127.22
38	Y	1620	LUT	C18-C5-C6	-4.07	120.29	124.62
38	y	1620	LUT	C18-C5-C6	-4.07	120.29	124.62
37	N	609	CHL	CBC-CAC-C3C	-4.06	107.23	113.16
37	y	609	CHL	CBA-CAA-C2A	-4.06	109.89	115.88
37	Y	609	CHL	CBA-CAA-C2A	-4.06	109.89	115.88
29	B	619	BCR	C11-C10-C9	-4.05	121.34	127.22
40	g	1623	NEX	C35-C34-C33	-4.04	121.34	127.22
29	C	517	BCR	C38-C26-C25	-4.04	120.32	124.62
39	G	1622	XAT	C31-C30-C29	-4.04	121.35	127.22
40	G	1623	NEX	C35-C34-C33	-4.03	121.36	127.22
37	s	607	CHL	OMC-CMC-C2C	-4.03	119.33	124.49
37	S	607	CHL	OMC-CMC-C2C	-4.03	119.33	124.49
29	b	619	BCR	C11-C10-C9	-4.03	121.36	127.22
37	n	609	CHL	CBC-CAC-C3C	-4.03	107.28	113.16
29	c	517	BCR	C38-C26-C25	-4.02	120.34	124.62
39	g	1622	XAT	C31-C30-C29	-4.00	121.40	127.22
27	C	508	CLA	CMB-C2B-C1B	-4.00	121.50	128.31
27	A	405	CLA	CMB-C2B-C1B	-3.99	121.53	128.31
27	c	508	CLA	CMB-C2B-C1B	-3.98	121.54	128.31
27	C	511	CLA	CMB-C2B-C1B	-3.98	121.54	128.31
27	a	405	CLA	CMB-C2B-C1B	-3.98	121.54	128.31
29	H	101	BCR	C24-C23-C22	-3.98	120.20	126.21
27	b	612	CLA	CMB-C2B-C1B	-3.97	121.55	128.31
27	B	612	CLA	CMB-C2B-C1B	-3.96	121.58	128.31
27	A	407	CLA	CMB-C2B-C1B	-3.95	121.60	128.31
29	h	101	BCR	C24-C23-C22	-3.94	120.25	126.21
27	c	511	CLA	CMB-C2B-C1B	-3.93	121.62	128.31
38	n	1621	LUT	C35-C34-C33	-3.93	121.51	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	407	CLA	CMB-C2B-C1B	-3.92	121.64	128.31
38	N	1621	LUT	C35-C34-C33	-3.92	121.52	127.22
27	c	506	CLA	CMB-C2B-C1B	-3.92	121.65	128.31
27	C	506	CLA	CMB-C2B-C1B	-3.91	121.66	128.31
37	Y	601	CHL	CBC-CAC-C3C	-3.89	107.47	113.16
29	h	101	BCR	C20-C21-C22	-3.89	121.56	127.22
29	B	618	BCR	C20-C21-C22	-3.88	121.58	127.22
29	b	618	BCR	C20-C21-C22	-3.88	121.58	127.22
29	H	101	BCR	C20-C21-C22	-3.88	121.59	127.22
29	D	404	BCR	C16-C17-C18	-3.87	121.60	127.22
29	h	101	BCR	C7-C8-C9	-3.86	120.37	126.21
29	H	101	BCR	C7-C8-C9	-3.86	120.37	126.21
29	b	620	BCR	C4-C5-C6	-3.86	118.48	122.73
29	B	620	BCR	C4-C5-C6	-3.86	118.48	122.73
37	y	601	CHL	CBC-CAC-C3C	-3.86	107.52	113.16
39	R	622	XAT	C35-C34-C33	-3.86	121.61	127.22
29	d	404	BCR	C16-C17-C18	-3.85	121.62	127.22
29	B	618	BCR	C27-C26-C25	-3.84	118.51	122.73
37	R	606	CHL	OMC-CMC-C2C	-3.83	119.59	124.49
39	Y	1622	XAT	C11-C10-C9	-3.83	121.66	127.22
37	n	609	CHL	CBA-CAA-C2A	-3.83	110.24	115.88
37	r	606	CHL	OMC-CMC-C2C	-3.82	119.60	124.49
37	N	609	CHL	CBA-CAA-C2A	-3.82	110.25	115.88
29	b	618	BCR	C27-C26-C25	-3.82	118.54	122.73
38	n	1621	LUT	C18-C5-C6	-3.81	120.56	124.62
39	r	622	XAT	C35-C34-C33	-3.81	121.68	127.22
27	C	510	CLA	CMB-C2B-C1B	-3.81	121.83	128.31
39	y	1622	XAT	C11-C10-C9	-3.81	121.69	127.22
38	N	1621	LUT	C18-C5-C6	-3.80	120.57	124.62
38	R	620	LUT	C15-C14-C13	-3.79	121.72	127.22
38	r	620	LUT	C15-C14-C13	-3.79	121.72	127.22
39	R	622	XAT	C35-C15-C14	-3.78	115.09	123.23
27	c	510	CLA	CMB-C2B-C1B	-3.77	121.89	128.31
29	a	411	BCR	C11-C10-C9	-3.77	121.73	127.22
39	r	622	XAT	C35-C15-C14	-3.77	115.10	123.23
27	G	610	CLA	CMB-C2B-C1B	-3.76	121.92	128.31
29	c	514	BCR	C24-C23-C22	-3.76	120.53	126.21
27	c	513	CLA	CMB-C2B-C1B	-3.76	121.92	128.31
27	B	604	CLA	CMB-C2B-C1B	-3.75	121.93	128.31
38	y	1621	LUT	C35-C34-C33	-3.75	121.78	127.22
27	b	604	CLA	CMB-C2B-C1B	-3.74	121.94	128.31
27	C	509	CLA	CMB-C2B-C1B	-3.74	121.94	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	617	CLA	CMB-C2B-C1B	-3.74	121.95	128.31
27	b	617	CLA	CMB-C2B-C1B	-3.74	121.95	128.31
29	C	514	BCR	C24-C23-C22	-3.74	120.56	126.21
27	C	513	CLA	CMB-C2B-C1B	-3.74	121.96	128.31
40	y	1623	NEX	C11-C10-C9	-3.73	121.80	127.22
40	Y	1623	NEX	C11-C10-C9	-3.73	121.80	127.22
37	n	608	CHL	CBC-CAC-C3C	-3.73	107.72	113.16
29	A	411	BCR	C38-C26-C25	-3.72	120.65	124.62
27	g	610	CLA	CMB-C2B-C1B	-3.72	121.98	128.31
38	Y	1621	LUT	C35-C34-C33	-3.72	121.81	127.22
29	A	411	BCR	C11-C10-C9	-3.72	121.81	127.22
29	H	101	BCR	C10-C11-C12	-3.72	111.62	123.11
29	h	101	BCR	C10-C11-C12	-3.71	111.65	123.11
37	N	608	CHL	CBC-CAC-C3C	-3.70	107.75	113.16
27	C	502	CLA	CMB-C2B-C1B	-3.70	122.02	128.31
27	c	509	CLA	CMB-C2B-C1B	-3.69	122.03	128.31
27	c	502	CLA	CMB-C2B-C1B	-3.69	122.04	128.31
37	S	607	CHL	CBA-CAA-C2A	-3.68	110.45	115.88
37	s	607	CHL	CBA-CAA-C2A	-3.68	110.45	115.88
29	c	517	BCR	C16-C17-C18	-3.68	121.87	127.22
40	s	1623	NEX	C11-C10-C9	-3.67	121.89	127.22
40	S	1623	NEX	C11-C10-C9	-3.67	121.89	127.22
38	N	1620	LUT	C8-C7-C6	-3.66	116.60	127.24
29	a	411	BCR	C38-C26-C25	-3.66	120.72	124.62
29	B	618	BCR	C16-C17-C18	-3.66	121.91	127.22
29	b	618	BCR	C16-C17-C18	-3.66	121.91	127.22
29	B	619	BCR	C8-C7-C6	-3.65	116.64	127.24
32	C	520	DGD	O6D-C1D-O3G	-3.65	101.23	109.99
38	n	1620	LUT	C8-C7-C6	-3.65	116.64	127.24
29	b	619	BCR	C8-C7-C6	-3.65	116.65	127.24
29	C	517	BCR	C16-C17-C18	-3.65	121.92	127.22
29	c	516	BCR	C15-C14-C13	-3.64	121.93	127.22
32	c	520	DGD	O6D-C1D-O3G	-3.64	101.25	109.99
29	c	516	BCR	C28-C27-C26	-3.64	107.83	113.87
40	r	623	NEX	C11-C10-C9	-3.64	121.93	127.22
29	C	516	BCR	C15-C14-C13	-3.62	121.95	127.22
37	Y	605	CHL	OMC-CMC-C2C	-3.62	119.86	124.49
29	C	516	BCR	C28-C27-C26	-3.62	107.87	113.87
27	A	410	CLA	CMB-C2B-C1B	-3.62	122.16	128.31
27	a	410	CLA	CMB-C2B-C1B	-3.62	122.16	128.31
38	G	1621	LUT	C35-C34-C33	-3.62	121.97	127.22
40	R	623	NEX	C11-C10-C9	-3.61	121.97	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	g	1621	LUT	C35-C34-C33	-3.61	121.98	127.22
27	a	406	CLA	CMB-C2B-C1B	-3.60	122.18	128.31
37	y	605	CHL	OMC-CMC-C2C	-3.60	119.88	124.49
27	B	603	CLA	CAA-C2A-C3A	-3.60	103.01	112.79
27	b	613	CLA	CMB-C2B-C1B	-3.59	122.20	128.31
27	A	406	CLA	CMB-C2B-C1B	-3.59	122.20	128.31
29	A	411	BCR	C20-C21-C22	-3.59	122.00	127.22
29	a	411	BCR	C20-C21-C22	-3.59	122.00	127.22
38	g	1620	LUT	C7-C8-C9	-3.59	120.78	126.21
38	G	1620	LUT	C7-C8-C9	-3.59	120.78	126.21
32	C	519	DGD	O6D-C1D-O3G	-3.59	101.39	109.99
27	g	602	CLA	CMB-C2B-C1B	-3.59	122.21	128.31
27	s	613	CLA	CMB-C2B-C1B	-3.58	122.22	128.31
32	C	520	DGD	O5D-C6D-C5D	-3.58	102.76	109.14
32	c	519	DGD	O6D-C1D-O3G	-3.58	101.40	109.99
27	b	603	CLA	CAA-C2A-C3A	-3.58	103.08	112.79
29	H	101	BCR	C28-C27-C26	-3.57	107.94	113.87
27	G	602	CLA	CMB-C2B-C1B	-3.57	122.24	128.31
37	y	606	CHL	CBC-CAC-C3C	-3.57	107.95	113.16
37	Y	606	CHL	CBC-CAC-C3C	-3.57	107.95	113.16
27	B	608	CLA	CMB-C2B-C1B	-3.57	122.24	128.31
27	S	613	CLA	CMB-C2B-C1B	-3.57	122.25	128.31
29	B	620	BCR	C24-C23-C22	-3.56	120.82	126.21
29	b	620	BCR	C24-C23-C22	-3.56	120.83	126.21
27	B	609	CLA	CMB-C2B-C1B	-3.56	122.26	128.31
29	h	101	BCR	C15-C14-C13	-3.56	122.05	127.22
29	H	101	BCR	C15-C14-C13	-3.56	122.05	127.22
29	h	101	BCR	C28-C27-C26	-3.55	107.98	113.87
27	B	613	CLA	CMB-C2B-C1B	-3.55	122.27	128.31
32	c	520	DGD	O5D-C6D-C5D	-3.55	102.83	109.14
38	G	1620	LUT	C18-C5-C6	-3.54	120.84	124.62
27	b	609	CLA	CMB-C2B-C1B	-3.54	122.28	128.31
38	g	1620	LUT	C18-C5-C6	-3.54	120.85	124.62
38	n	1621	LUT	C8-C7-C6	-3.54	116.97	127.24
29	b	620	BCR	C38-C26-C25	-3.53	120.86	124.62
29	B	620	BCR	C38-C26-C25	-3.53	120.86	124.62
27	y	604	CLA	CMB-C2B-C1B	-3.53	122.31	128.31
27	b	605	CLA	CAA-C2A-C3A	-3.53	103.22	112.79
27	B	605	CLA	CAA-C2A-C3A	-3.53	103.22	112.79
27	b	608	CLA	CMB-C2B-C1B	-3.53	122.32	128.31
37	Y	607	CHL	CBA-CAA-C2A	-3.52	110.69	115.88
38	S	1620	LUT	C11-C10-C9	-3.52	122.11	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	N	1621	LUT	C8-C7-C6	-3.51	117.04	127.24
38	Y	1620	LUT	C35-C34-C33	-3.51	122.12	127.22
38	y	1620	LUT	C35-C34-C33	-3.51	122.12	127.22
38	S	1620	LUT	C18-C5-C6	-3.50	120.89	124.62
38	y	1620	LUT	C7-C8-C9	-3.50	120.92	126.21
38	n	1620	LUT	C18-C5-C6	-3.50	120.89	124.62
38	s	1620	LUT	C18-C5-C6	-3.50	120.89	124.62
27	r	601	CLA	CMB-C2B-C1B	-3.50	122.36	128.31
27	Y	604	CLA	CMB-C2B-C1B	-3.50	122.36	128.31
27	R	601	CLA	CMB-C2B-C1B	-3.49	122.37	128.31
32	C	519	DGD	O3G-C1D-C2D	-3.49	103.70	108.00
32	c	519	DGD	O3G-C1D-C2D	-3.49	103.70	108.00
38	g	1621	LUT	C18-C5-C6	-3.49	120.90	124.62
37	y	607	CHL	CBA-CAA-C2A	-3.49	110.73	115.88
29	d	404	BCR	C20-C21-C22	-3.49	122.15	127.22
29	C	516	BCR	C38-C26-C25	-3.49	120.91	124.62
27	c	512	CLA	CMB-C2B-C1B	-3.49	122.38	128.31
29	c	514	BCR	C3-C4-C5	-3.48	108.09	113.87
38	Y	1620	LUT	C7-C8-C9	-3.48	120.95	126.21
27	C	512	CLA	CMB-C2B-C1B	-3.48	122.39	128.31
27	N	604	CLA	CMB-C2B-C1B	-3.47	122.41	128.31
27	S	603	CLA	CMB-C2B-C1B	-3.47	122.41	128.31
37	n	605	CHL	CBA-CAA-C2A	-3.47	110.76	115.88
38	s	1620	LUT	C11-C10-C9	-3.47	122.18	127.22
29	c	515	BCR	C28-C27-C26	-3.46	108.12	113.87
29	C	514	BCR	C3-C4-C5	-3.46	108.13	113.87
38	N	1620	LUT	C18-C5-C6	-3.46	120.93	124.62
29	c	514	BCR	C20-C21-C22	-3.46	122.19	127.22
29	c	516	BCR	C38-C26-C25	-3.46	120.94	124.62
38	G	1621	LUT	C18-C5-C6	-3.46	120.94	124.62
29	C	515	BCR	C28-C27-C26	-3.45	108.14	113.87
29	a	411	BCR	C24-C23-C22	-3.45	121.00	126.21
32	c	518	DGD	C3G-C2G-C1G	-3.45	104.05	112.08
32	C	518	DGD	C3G-C2G-C1G	-3.45	104.05	112.08
37	N	605	CHL	CBA-CAA-C2A	-3.45	110.79	115.88
27	n	604	CLA	CMB-C2B-C1B	-3.44	122.45	128.31
37	r	608	CHL	OMC-CMC-C2C	-3.44	120.08	124.49
29	D	404	BCR	C20-C21-C22	-3.44	122.22	127.22
29	C	514	BCR	C20-C21-C22	-3.44	122.22	127.22
27	s	603	CLA	CMB-C2B-C1B	-3.44	122.47	128.31
38	Y	1620	LUT	C15-C14-C13	-3.44	122.23	127.22
38	y	1620	LUT	C15-C14-C13	-3.44	122.23	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	411	BCR	C24-C23-C22	-3.43	121.03	126.21
31	D	411	LMG	C1-C2-C3	-3.43	103.19	109.98
31	d	411	LMG	C1-C2-C3	-3.42	103.20	109.98
29	c	515	BCR	C21-C20-C19	-3.42	112.55	123.11
29	B	620	BCR	C1-C6-C5	-3.41	117.94	122.50
27	n	611	CLA	O2D-CGD-O1D	-3.41	116.59	123.77
37	Y	608	CHL	CBC-CAC-C3C	-3.41	108.18	113.16
29	C	515	BCR	C21-C20-C19	-3.41	112.58	123.11
37	R	608	CHL	OMC-CMC-C2C	-3.41	120.13	124.49
29	b	620	BCR	C1-C6-C5	-3.40	117.95	122.50
27	N	611	CLA	O2D-CGD-O1D	-3.40	116.61	123.77
32	C	518	DGD	O6D-C1D-O3G	-3.40	101.85	109.99
27	s	604	CLA	CMB-C2B-C1B	-3.40	122.54	128.31
39	N	1622	XAT	C15-C35-C34	-3.39	115.92	123.23
29	c	516	BCR	C3-C4-C5	-3.39	108.26	113.87
37	y	608	CHL	CBC-CAC-C3C	-3.38	108.22	113.16
39	G	1622	XAT	C35-C34-C33	-3.38	122.31	127.22
32	c	518	DGD	O6D-C1D-O3G	-3.38	101.89	109.99
29	b	620	BCR	C33-C5-C6	-3.38	121.02	124.62
29	B	620	BCR	C33-C5-C6	-3.38	121.02	124.62
39	N	1622	XAT	C11-C10-C9	-3.37	122.32	127.22
27	r	604	CLA	CMB-C2B-C1B	-3.37	122.57	128.31
39	g	1622	XAT	C35-C34-C33	-3.36	122.33	127.22
29	C	516	BCR	C3-C4-C5	-3.36	108.30	113.87
27	b	605	CLA	CMB-C2B-C1B	-3.36	122.60	128.31
27	B	605	CLA	CMB-C2B-C1B	-3.36	122.60	128.31
27	S	604	CLA	CMB-C2B-C1B	-3.36	122.60	128.31
27	R	604	CLA	CMB-C2B-C1B	-3.35	122.61	128.31
27	B	610	CLA	CMB-C2B-C1B	-3.35	122.62	128.31
39	n	1622	XAT	C15-C35-C34	-3.35	116.02	123.23
38	y	1621	LUT	C10-C11-C12	-3.34	112.79	123.11
38	Y	1621	LUT	C10-C11-C12	-3.34	112.79	123.11
38	S	1621	LUT	C8-C7-C6	-3.34	117.54	127.24
27	c	504	CLA	CMB-C2B-C1B	-3.34	122.63	128.31
27	C	504	CLA	CMB-C2B-C1B	-3.34	122.63	128.31
37	g	601	CHL	CBA-CAA-C2A	-3.34	110.95	115.88
37	N	601	CHL	OMC-CMC-C2C	-3.34	120.22	124.49
38	s	1621	LUT	C8-C7-C6	-3.33	117.56	127.24
37	G	601	CHL	CBA-CAA-C2A	-3.33	110.97	115.88
27	R	610	CLA	CMB-C2B-C1B	-3.33	122.65	128.31
39	n	1622	XAT	C11-C10-C9	-3.32	122.39	127.22
27	b	610	CLA	CMB-C2B-C1B	-3.32	122.67	128.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	s	601	CHL	OMC-CMC-C2C	-3.32	120.25	124.49
27	N	614	CLA	CMB-C2B-C1B	-3.32	122.67	128.31
27	n	614	CLA	CMB-C2B-C1B	-3.32	122.67	128.31
27	n	610	CLA	CMB-C2B-C1B	-3.32	122.67	128.31
37	n	601	CHL	OMC-CMC-C2C	-3.31	120.25	124.49
37	S	601	CHL	OMC-CMC-C2C	-3.31	120.25	124.49
38	y	1621	LUT	C8-C7-C6	-3.31	117.63	127.24
27	r	610	CLA	CMB-C2B-C1B	-3.31	122.69	128.31
38	Y	1621	LUT	C8-C7-C6	-3.29	117.68	127.24
27	n	613	CLA	CMB-C2B-C1B	-3.29	122.72	128.31
27	y	611	CLA	CMB-C2B-C1B	-3.28	122.73	128.31
27	N	610	CLA	CMB-C2B-C1B	-3.28	122.73	128.31
37	s	601	CHL	CBA-CAA-C2A	-3.28	111.04	115.88
29	d	404	BCR	C3-C4-C5	-3.28	108.43	113.87
31	A	413	LMG	C1-C2-C3	-3.28	103.48	109.98
31	a	413	LMG	C1-C2-C3	-3.28	103.48	109.98
37	S	606	CHL	CBC-CAC-C3C	-3.27	108.38	113.16
27	s	602	CLA	CMB-C2B-C1B	-3.27	122.75	128.31
37	s	606	CHL	CBC-CAC-C3C	-3.27	108.38	113.16
29	D	404	BCR	C3-C4-C5	-3.27	108.45	113.87
37	n	601	CHL	CBA-CAA-C2A	-3.27	111.06	115.88
27	Y	611	CLA	CMB-C2B-C1B	-3.27	122.76	128.31
34	d	405	PL9	C27-C28-C29	-3.27	120.55	127.75
29	c	514	BCR	C28-C27-C26	-3.26	108.46	113.87
29	c	516	BCR	C16-C15-C14	-3.26	116.21	123.23
29	C	516	BCR	C16-C15-C14	-3.26	116.21	123.23
27	N	613	CLA	CMB-C2B-C1B	-3.26	122.77	128.31
38	R	620	LUT	C18-C5-C6	-3.25	121.16	124.62
38	r	620	LUT	C18-C5-C6	-3.25	121.16	124.62
37	S	601	CHL	CBA-CAA-C2A	-3.25	111.08	115.88
29	C	514	BCR	C28-C27-C26	-3.25	108.48	113.87
37	g	608	CHL	OMC-CMC-C2C	-3.25	120.34	124.49
27	S	612	CLA	CMB-C2B-C1B	-3.25	122.79	128.31
27	S	602	CLA	CMB-C2B-C1B	-3.24	122.80	128.31
34	D	405	PL9	C27-C28-C29	-3.24	120.59	127.75
29	B	619	BCR	C7-C8-C9	-3.24	121.31	126.21
29	b	619	BCR	C7-C8-C9	-3.24	121.31	126.21
38	G	1621	LUT	C8-C7-C6	-3.24	117.84	127.24
38	g	1621	LUT	C8-C7-C6	-3.23	117.86	127.24
37	G	608	CHL	OMC-CMC-C2C	-3.23	120.36	124.49
37	G	607	CHL	CBA-CAA-C2A	-3.23	111.11	115.88
37	N	601	CHL	CBA-CAA-C2A	-3.23	111.11	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	514	BCR	C33-C5-C6	-3.22	121.19	124.62
29	b	619	BCR	C28-C27-C26	-3.22	108.54	113.87
27	s	612	CLA	CMB-C2B-C1B	-3.22	122.84	128.31
38	g	1621	LUT	C15-C14-C13	-3.21	122.55	127.22
27	s	609	CLA	CMB-C2B-C1B	-3.21	122.85	128.31
27	S	609	CLA	CMB-C2B-C1B	-3.20	122.87	128.31
29	B	619	BCR	C28-C27-C26	-3.20	108.57	113.87
27	g	613	CLA	CMB-C2B-C1B	-3.19	122.89	128.31
27	S	611	CLA	CMB-C2B-C1B	-3.19	122.89	128.31
27	s	611	CLA	CMB-C2B-C1B	-3.19	122.89	128.31
29	H	101	BCR	C38-C26-C25	-3.19	121.23	124.62
38	G	1621	LUT	C15-C14-C13	-3.19	122.59	127.22
39	r	622	XAT	C15-C14-C13	-3.18	122.59	127.22
29	B	619	BCR	C15-C16-C17	-3.18	116.37	123.23
27	G	613	CLA	CMB-C2B-C1B	-3.18	122.90	128.31
37	g	607	CHL	CBA-CAA-C2A	-3.18	111.19	115.88
29	b	619	BCR	C15-C16-C17	-3.18	116.38	123.23
37	S	601	CHL	C4A-C3A-C2A	-3.18	99.09	103.98
27	B	607	CLA	O2D-CGD-O1D	-3.17	117.09	123.77
29	C	514	BCR	C33-C5-C6	-3.17	121.24	124.62
29	b	620	BCR	C11-C10-C9	-3.17	122.61	127.22
39	R	622	XAT	C15-C14-C13	-3.17	122.61	127.22
32	c	518	DGD	C1D-C2D-C3D	-3.17	103.69	109.98
27	r	613	CLA	CMB-C2B-C1B	-3.17	122.92	128.31
37	N	605	CHL	OMC-CMC-C2C	-3.17	120.44	124.49
32	C	518	DGD	C1D-C2D-C3D	-3.17	103.70	109.98
27	B	614	CLA	CMB-C2B-C1B	-3.17	122.93	128.31
29	c	517	BCR	C15-C16-C17	-3.16	116.41	123.23
38	y	1621	LUT	C18-C5-C6	-3.16	121.25	124.62
38	Y	1620	LUT	C10-C11-C12	-3.16	113.35	123.11
27	b	607	CLA	O2D-CGD-O1D	-3.16	117.12	123.77
27	R	604	CLA	O2D-CGD-O1D	-3.15	117.13	123.77
29	C	516	BCR	C11-C10-C9	-3.15	122.64	127.22
38	y	1620	LUT	C10-C11-C12	-3.15	113.37	123.11
38	S	1621	LUT	C15-C14-C13	-3.15	122.64	127.22
37	s	601	CHL	C4A-C3A-C2A	-3.15	99.12	103.98
38	Y	1621	LUT	C18-C5-C6	-3.15	121.26	124.62
27	R	602	CLA	CMB-C2B-C1B	-3.15	122.95	128.31
29	c	516	BCR	C11-C10-C9	-3.15	122.64	127.22
29	h	101	BCR	C38-C26-C25	-3.15	121.27	124.62
27	b	614	CLA	CMB-C2B-C1B	-3.15	122.96	128.31
29	C	517	BCR	C15-C16-C17	-3.15	116.45	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	620	BCR	C11-C10-C9	-3.15	122.65	127.22
27	R	613	CLA	CMB-C2B-C1B	-3.14	122.96	128.31
27	r	602	CLA	CMB-C2B-C1B	-3.14	122.97	128.31
38	s	1621	LUT	C15-C14-C13	-3.14	122.66	127.22
37	s	601	CHL	CBC-CAC-C3C	-3.13	108.58	113.16
37	Y	601	CHL	CBA-CAA-C2A	-3.13	111.26	115.88
37	y	601	CHL	CBA-CAA-C2A	-3.13	111.26	115.88
37	n	605	CHL	OMC-CMC-C2C	-3.13	120.48	124.49
27	g	611	CLA	CMB-C2B-C1B	-3.13	122.99	128.31
27	G	611	CLA	CMB-C2B-C1B	-3.12	123.00	128.31
27	r	604	CLA	O2D-CGD-O1D	-3.12	117.20	123.77
29	B	620	BCR	C3-C4-C5	-3.12	108.70	113.87
37	S	601	CHL	CBC-CAC-C3C	-3.12	108.60	113.16
27	y	612	CLA	CMB-C2B-C1B	-3.11	123.02	128.31
27	n	610	CLA	O2D-CGD-O1D	-3.11	117.22	123.77
27	N	610	CLA	O2D-CGD-O1D	-3.11	117.23	123.77
38	S	1620	LUT	C35-C15-C14	-3.11	116.53	123.23
32	h	102	DGD	O6D-C1D-O3G	-3.10	102.55	109.99
32	H	102	DGD	O6D-C1D-O3G	-3.10	102.55	109.99
27	Y	612	CLA	CMB-C2B-C1B	-3.10	123.04	128.31
32	H	102	DGD	C3G-C2G-C1G	-3.10	104.86	112.08
29	b	620	BCR	C3-C4-C5	-3.10	108.73	113.87
27	g	614	CLA	CMB-C2B-C1B	-3.10	123.04	128.31
37	Y	607	CHL	OMC-CMC-C2C	-3.10	120.53	124.49
27	B	602	CLA	CMB-C2B-C1B	-3.09	123.05	128.31
27	b	602	CLA	CMB-C2B-C1B	-3.09	123.05	128.31
27	S	614	CLA	CMB-C2B-C1B	-3.09	123.06	128.31
38	R	620	LUT	C8-C7-C6	-3.09	118.28	127.24
29	C	515	BCR	C15-C16-C17	-3.09	116.58	123.23
32	h	102	DGD	C3G-C2G-C1G	-3.08	104.90	112.08
38	y	1621	LUT	C11-C10-C9	-3.08	122.74	127.22
38	g	1620	LUT	C11-C10-C9	-3.08	122.74	127.22
38	r	620	LUT	C8-C7-C6	-3.08	118.30	127.24
29	d	404	BCR	C16-C15-C14	-3.08	116.59	123.23
27	B	611	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
27	G	614	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
27	y	602	CLA	CMB-C2B-C1B	-3.08	123.08	128.31
29	c	515	BCR	C15-C16-C17	-3.08	116.60	123.23
27	r	612	CLA	CMB-C2B-C1B	-3.07	123.08	128.31
27	c	508	CLA	O2D-CGD-O1D	-3.07	117.31	123.77
38	Y	1621	LUT	C11-C10-C9	-3.06	122.77	127.22
40	s	1623	NEX	C31-C30-C29	-3.06	122.77	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	d	405	PL9	C31-C32-C33	-3.06	103.58	111.61
38	s	1620	LUT	C35-C15-C14	-3.06	116.63	123.23
38	g	1620	LUT	C15-C14-C13	-3.06	122.77	127.22
34	D	405	PL9	C31-C32-C33	-3.06	103.58	111.61
27	r	609	CLA	CMB-C2B-C1B	-3.06	123.11	128.31
27	R	609	CLA	CMB-C2B-C1B	-3.06	123.11	128.31
37	R	607	CHL	OMC-CMC-C2C	-3.06	120.58	124.49
27	B	607	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
37	y	607	CHL	OMC-CMC-C2C	-3.05	120.59	124.49
27	C	508	CLA	O2D-CGD-O1D	-3.05	117.35	123.77
27	B	606	CLA	CMB-C2B-C1B	-3.05	123.12	128.31
27	R	611	CLA	CMB-C2B-C1B	-3.05	123.13	128.31
27	r	611	CLA	CMB-C2B-C1B	-3.05	123.13	128.31
27	b	611	CLA	CMB-C2B-C1B	-3.04	123.13	128.31
27	s	614	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
27	A	410	CLA	O2D-CGD-O1D	-3.04	117.36	123.77
27	a	410	CLA	O2D-CGD-O1D	-3.04	117.36	123.77
37	G	606	CHL	OMC-CMC-C2C	-3.04	120.60	124.49
40	S	1623	NEX	C31-C30-C29	-3.04	122.80	127.22
39	r	622	XAT	C10-C11-C12	-3.04	113.72	123.11
29	D	404	BCR	C16-C15-C14	-3.04	116.68	123.23
27	G	612	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
27	r	603	CLA	CMB-C2B-C1B	-3.04	123.14	128.31
38	S	1621	LUT	C10-C11-C12	-3.04	113.72	123.11
38	G	1620	LUT	C11-C10-C9	-3.04	122.81	127.22
38	s	1621	LUT	C10-C11-C12	-3.04	113.73	123.11
29	c	517	BCR	C21-C20-C19	-3.04	113.73	123.11
29	C	517	BCR	C21-C20-C19	-3.04	113.73	123.11
27	R	612	CLA	CMB-C2B-C1B	-3.03	123.15	128.31
39	R	622	XAT	C10-C11-C12	-3.03	113.74	123.11
38	R	620	LUT	C31-C30-C29	-3.03	122.82	127.22
27	b	607	CLA	CMB-C2B-C1B	-3.03	123.16	128.31
27	g	612	CLA	CMB-C2B-C1B	-3.03	123.17	128.31
37	r	607	CHL	OMC-CMC-C2C	-3.03	120.62	124.49
27	Y	602	CLA	CMB-C2B-C1B	-3.03	123.17	128.31
27	R	603	CLA	CMB-C2B-C1B	-3.02	123.17	128.31
38	G	1620	LUT	C15-C14-C13	-3.02	122.83	127.22
27	Y	614	CLA	CMB-C2B-C1B	-3.01	123.18	128.31
37	g	606	CHL	OMC-CMC-C2C	-3.00	120.65	124.49
27	b	606	CLA	CMB-C2B-C1B	-3.00	123.20	128.31
38	r	620	LUT	C31-C30-C29	-3.00	122.86	127.22
38	Y	1620	LUT	C11-C10-C9	-3.00	122.86	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	n	611	CLA	CMB-C2B-C1B	-3.00	123.21	128.31
38	y	1621	LUT	C7-C8-C9	-3.00	121.68	126.21
27	y	614	CLA	CMB-C2B-C1B	-3.00	123.21	128.31
27	N	612	CLA	CMB-C2B-C1B	-2.99	123.22	128.31
27	B	613	CLA	O2D-CGD-O1D	-2.99	117.48	123.77
38	y	1620	LUT	C11-C10-C9	-2.99	122.88	127.22
27	n	612	CLA	CMB-C2B-C1B	-2.99	123.23	128.31
29	B	620	BCR	C21-C20-C19	-2.99	113.88	123.11
37	N	608	CHL	OMC-CMC-C2C	-2.99	120.67	124.49
38	n	1620	LUT	C30-C31-C32	-2.98	113.89	123.11
29	b	620	BCR	C21-C20-C19	-2.98	113.89	123.11
29	h	101	BCR	C16-C15-C14	-2.98	116.80	123.23
29	H	101	BCR	C16-C15-C14	-2.98	116.80	123.23
27	y	603	CLA	CMB-C2B-C1B	-2.98	123.24	128.31
35	D	409	LHG	C11-C10-C9	-2.98	99.06	114.54
35	d	409	LHG	C11-C10-C9	-2.98	99.07	114.54
27	b	603	CLA	CMB-C2B-C1B	-2.98	123.25	128.31
38	Y	1621	LUT	C7-C8-C9	-2.97	121.72	126.21
34	d	405	PL9	C7-C8-C9	-2.97	121.64	126.70
34	D	405	PL9	C7-C8-C9	-2.97	121.64	126.70
27	b	615	CLA	O2D-CGD-O1D	-2.97	117.51	123.77
37	n	608	CHL	OMC-CMC-C2C	-2.97	120.69	124.49
27	B	603	CLA	CMB-C2B-C1B	-2.97	123.26	128.31
27	Y	603	CLA	CMB-C2B-C1B	-2.97	123.26	128.31
27	c	501	CLA	CMB-C2B-C1B	-2.96	123.27	128.31
40	G	1623	NEX	C31-C30-C29	-2.96	122.92	127.22
27	C	503	CLA	CMB-C2B-C1B	-2.96	123.28	128.31
27	B	615	CLA	O2D-CGD-O1D	-2.96	117.54	123.77
27	b	613	CLA	O2D-CGD-O1D	-2.96	117.55	123.77
27	C	501	CLA	CMB-C2B-C1B	-2.95	123.29	128.31
38	N	1620	LUT	C30-C31-C32	-2.95	113.99	123.11
38	y	1620	LUT	C30-C31-C32	-2.95	113.99	123.11
32	c	520	DGD	C3G-C2G-C1G	-2.95	105.21	112.08
32	c	519	DGD	O5D-C6D-C5D	-2.95	103.89	109.14
38	Y	1620	LUT	C30-C31-C32	-2.95	114.00	123.11
32	C	519	DGD	O5D-C6D-C5D	-2.95	103.90	109.14
31	c	521	LMG	O6-C1-O1	-2.95	102.93	109.99
27	N	611	CLA	CMB-C2B-C1B	-2.94	123.30	128.31
32	C	520	DGD	C3G-C2G-C1G	-2.94	105.22	112.08
27	g	604	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
27	G	604	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
31	C	521	LMG	O6-C1-O1	-2.94	102.93	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	616	CLA	CMB-C2B-C1B	-2.94	123.31	128.31
32	c	518	DGD	C4E-C3E-C2E	-2.94	105.37	110.79
32	C	518	DGD	C4E-C3E-C2E	-2.94	105.37	110.79
37	y	607	CHL	CBC-CAC-C3C	-2.94	108.87	113.16
37	Y	607	CHL	CBC-CAC-C3C	-2.94	108.87	113.16
40	g	1623	NEX	C31-C30-C29	-2.93	122.96	127.22
31	B	622	LMG	O1-C7-C8	-2.93	104.01	110.99
27	n	603	CLA	CMB-C2B-C1B	-2.93	123.33	128.31
27	S	604	CLA	O2D-CGD-O1D	-2.93	117.61	123.77
37	y	605	CHL	CBC-CAC-C3C	-2.92	108.89	113.16
27	c	501	CLA	O2D-CGD-O1D	-2.92	117.62	123.77
31	b	622	LMG	O1-C7-C8	-2.92	104.04	110.99
27	c	503	CLA	CMB-C2B-C1B	-2.92	123.35	128.31
27	s	604	CLA	O2D-CGD-O1D	-2.92	117.63	123.77
27	C	501	CLA	O2D-CGD-O1D	-2.92	117.63	123.77
27	N	603	CLA	CMB-C2B-C1B	-2.91	123.36	128.31
40	Y	1623	NEX	C19-C9-C10	-2.91	118.65	122.89
40	y	1623	NEX	C19-C9-C10	-2.91	118.65	122.89
27	b	603	CLA	O2D-CGD-O1D	-2.91	117.64	123.77
27	B	603	CLA	O2D-CGD-O1D	-2.91	117.64	123.77
27	D	402	CLA	CMB-C2B-C1B	-2.91	123.36	128.31
27	d	402	CLA	CMB-C2B-C1B	-2.91	123.36	128.31
38	G	1621	LUT	C10-C11-C12	-2.90	114.15	123.11
38	g	1621	LUT	C10-C11-C12	-2.90	114.15	123.11
37	Y	605	CHL	CBC-CAC-C3C	-2.90	108.93	113.16
27	r	616	CLA	CMB-C2B-C1B	-2.89	123.39	128.31
27	G	603	CLA	CMB-C2B-C1B	-2.89	123.39	128.31
37	g	605	CHL	C4A-C3A-C2A	-2.89	99.54	103.98
37	G	605	CHL	C4A-C3A-C2A	-2.89	99.54	103.98
27	g	602	CLA	O2D-CGD-O1D	-2.88	117.70	123.77
27	Y	614	CLA	O2D-CGD-O1D	-2.88	117.70	123.77
31	B	622	LMG	O6-C1-O1	-2.88	103.09	109.99
39	Y	1622	XAT	C15-C14-C13	-2.88	123.04	127.22
27	R	616	CLA	O2D-CGD-O1D	-2.88	117.72	123.77
27	r	616	CLA	O2D-CGD-O1D	-2.88	117.72	123.77
31	b	622	LMG	O6-C1-O1	-2.87	103.10	109.99
27	g	603	CLA	CMB-C2B-C1B	-2.87	123.43	128.31
38	G	1621	LUT	C31-C30-C29	-2.87	123.05	127.22
38	g	1621	LUT	C31-C30-C29	-2.87	123.05	127.22
29	B	619	BCR	C38-C26-C25	-2.87	121.57	124.62
27	G	602	CLA	O2D-CGD-O1D	-2.86	117.75	123.77
29	a	411	BCR	C23-C24-C25	-2.86	118.94	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	1622	XAT	C15-C14-C13	-2.86	123.07	127.22
40	s	1623	NEX	C35-C34-C33	-2.85	123.07	127.22
37	G	608	CHL	CBC-CAC-C3C	-2.85	108.99	113.16
29	A	411	BCR	C23-C24-C25	-2.85	118.97	127.24
27	C	507	CLA	O2D-CGD-O1D	-2.85	117.78	123.77
27	c	507	CLA	O2D-CGD-O1D	-2.85	117.78	123.77
40	G	1623	NEX	C39-C29-C30	-2.84	118.75	122.89
40	N	1623	NEX	C39-C29-C30	-2.84	118.75	122.89
29	b	619	BCR	C38-C26-C25	-2.84	121.59	124.62
27	y	614	CLA	O2D-CGD-O1D	-2.84	117.79	123.77
27	n	614	CLA	O2D-CGD-O1D	-2.84	117.79	123.77
40	S	1623	NEX	C35-C34-C33	-2.84	123.10	127.22
38	n	1621	LUT	C10-C11-C12	-2.83	114.35	123.11
27	N	614	CLA	O2D-CGD-O1D	-2.83	117.81	123.77
29	c	515	BCR	C20-C21-C22	-2.83	123.10	127.22
29	C	515	BCR	C20-C21-C22	-2.83	123.10	127.22
27	D	403	CLA	O2D-CGD-O1D	-2.83	117.81	123.77
27	d	403	CLA	O2D-CGD-O1D	-2.83	117.81	123.77
29	B	618	BCR	C21-C20-C19	-2.83	114.37	123.11
29	b	618	BCR	C21-C20-C19	-2.83	114.38	123.11
37	g	608	CHL	CBC-CAC-C3C	-2.82	109.04	113.16
27	Y	611	CLA	O2D-CGD-O1D	-2.82	117.84	123.77
27	y	611	CLA	O2D-CGD-O1D	-2.82	117.84	123.77
38	N	1621	LUT	C10-C11-C12	-2.82	114.41	123.11
40	g	1623	NEX	C39-C29-C30	-2.82	118.79	122.89
40	n	1623	NEX	C39-C29-C30	-2.81	118.80	122.89
29	C	517	BCR	C10-C11-C12	-2.81	114.44	123.11
29	c	517	BCR	C10-C11-C12	-2.81	114.44	123.11
28	a	408	PHO	CBD-CHA-C4D	-2.81	105.38	108.54
38	Y	1620	LUT	C31-C30-C29	-2.80	123.15	127.22
39	G	1622	XAT	C15-C35-C34	-2.80	117.19	123.23
27	g	613	CLA	O2D-CGD-O1D	-2.80	117.89	123.77
27	b	605	CLA	O2D-CGD-O1D	-2.79	117.89	123.77
32	C	519	DGD	CDB-CCB-CBB	-2.79	100.05	114.54
32	c	519	DGD	CDB-CCB-CBB	-2.79	100.05	114.54
37	N	607	CHL	OMC-CMC-C2C	-2.79	120.92	124.49
27	B	612	CLA	O2D-CGD-O1D	-2.79	117.90	123.77
38	G	1621	LUT	C11-C10-C9	-2.78	123.18	127.22
38	g	1621	LUT	C11-C10-C9	-2.78	123.18	127.22
27	B	605	CLA	O2D-CGD-O1D	-2.78	117.92	123.77
32	C	520	DGD	O3G-C1D-C2D	-2.78	104.58	108.00
27	B	611	CLA	O2D-CGD-O1D	-2.78	117.92	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	S	1620	LUT	C15-C14-C13	-2.78	123.18	127.22
27	G	613	CLA	O2D-CGD-O1D	-2.78	117.92	123.77
27	b	612	CLA	O2D-CGD-O1D	-2.78	117.93	123.77
39	g	1622	XAT	C15-C35-C34	-2.78	117.25	123.23
27	y	613	CLA	CMB-C2B-C1B	-2.77	123.60	128.31
38	s	1620	LUT	C15-C14-C13	-2.77	123.19	127.22
37	n	606	CHL	OMC-CMC-C2C	-2.77	120.94	124.49
37	n	607	CHL	CBA-CAA-C2A	-2.77	111.80	115.88
28	A	408	PHO	CBD-CHA-C4D	-2.77	105.42	108.54
38	y	1620	LUT	C31-C30-C29	-2.77	123.20	127.22
37	n	607	CHL	OMC-CMC-C2C	-2.77	120.95	124.49
37	y	605	CHL	CBA-CAA-C2A	-2.77	111.80	115.88
27	D	402	CLA	O2D-CGD-O1D	-2.76	117.95	123.77
32	c	520	DGD	O3G-C1D-C2D	-2.76	104.60	108.00
28	A	409	PHO	CMB-C2B-C1B	-2.76	120.65	125.06
29	b	618	BCR	C23-C24-C25	-2.76	119.23	127.24
29	B	620	BCR	C20-C21-C22	-2.75	123.22	127.22
27	Y	613	CLA	CMB-C2B-C1B	-2.75	123.63	128.31
39	N	1622	XAT	C35-C34-C33	-2.75	123.22	127.22
37	N	607	CHL	CBA-CAA-C2A	-2.75	111.82	115.88
29	B	618	BCR	C23-C24-C25	-2.75	119.26	127.24
27	d	402	CLA	O2D-CGD-O1D	-2.74	117.99	123.77
37	Y	605	CHL	CBA-CAA-C2A	-2.74	111.83	115.88
27	b	616	CLA	O2D-CGD-O1D	-2.74	118.00	123.77
27	c	510	CLA	O2D-CGD-O1D	-2.74	118.00	123.77
37	N	606	CHL	OMC-CMC-C2C	-2.74	120.98	124.49
27	C	506	CLA	O2D-CGD-O1D	-2.74	118.00	123.77
31	A	413	LMG	O3-C3-C2	-2.73	104.19	110.36
28	a	409	PHO	CMB-C2B-C1B	-2.73	120.69	125.06
27	c	505	CLA	O2D-CGD-O1D	-2.73	118.02	123.77
27	c	506	CLA	O2D-CGD-O1D	-2.73	118.02	123.77
29	C	514	BCR	C21-C20-C19	-2.73	114.67	123.11
27	b	611	CLA	O2D-CGD-O1D	-2.73	118.02	123.77
27	s	603	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
27	S	603	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
27	B	609	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
31	a	413	LMG	C4-C3-C2	-2.73	105.76	110.79
31	A	413	LMG	C4-C3-C2	-2.73	105.76	110.79
32	C	518	DGD	CDB-CCB-CBB	-2.73	100.37	114.54
27	C	510	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
38	S	1621	LUT	C18-C5-C6	-2.73	121.72	124.62
38	S	1620	LUT	C16-C1-C6	-2.73	106.17	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	s	1620	LUT	C16-C1-C6	-2.73	106.17	110.33
27	s	602	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
27	S	602	CLA	O2D-CGD-O1D	-2.73	118.03	123.77
40	R	623	NEX	C15-C35-C34	-2.72	117.36	123.23
37	G	609	CHL	CBA-CAA-C2A	-2.72	111.86	115.88
32	c	518	DGD	CDB-CCB-CBB	-2.72	100.40	114.54
40	S	1623	NEX	C15-C35-C34	-2.72	117.36	123.23
27	b	609	CLA	O2D-CGD-O1D	-2.72	118.04	123.77
29	c	514	BCR	C7-C8-C9	-2.72	122.10	126.21
40	Y	1623	NEX	C39-C29-C30	-2.72	118.93	122.89
40	s	1623	NEX	C15-C35-C34	-2.72	117.36	123.23
29	c	514	BCR	C21-C20-C19	-2.72	114.71	123.11
39	n	1622	XAT	C35-C34-C33	-2.72	123.27	127.22
27	N	602	CLA	O2D-CGD-O1D	-2.72	118.05	123.77
27	c	513	CLA	O2D-CGD-O1D	-2.72	118.05	123.77
31	a	413	LMG	O3-C3-C2	-2.72	104.23	110.36
27	B	616	CLA	O2D-CGD-O1D	-2.72	118.05	123.77
37	N	606	CHL	CBC-CAC-C3C	-2.72	109.19	113.16
38	g	1620	LUT	C35-C15-C14	-2.72	117.38	123.23
29	b	620	BCR	C20-C21-C22	-2.71	123.28	127.22
27	Y	602	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
27	C	505	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
39	N	1622	XAT	C10-C11-C12	-2.71	114.74	123.11
37	n	606	CHL	CBC-CAC-C3C	-2.71	109.20	113.16
29	C	514	BCR	C7-C8-C9	-2.71	122.12	126.21
38	s	1621	LUT	C18-C5-C6	-2.71	121.74	124.62
27	g	610	CLA	O2D-CGD-O1D	-2.70	118.08	123.77
27	y	602	CLA	O2D-CGD-O1D	-2.70	118.08	123.77
27	G	610	CLA	O2D-CGD-O1D	-2.70	118.08	123.77
27	n	602	CLA	O2D-CGD-O1D	-2.70	118.08	123.77
40	y	1623	NEX	C39-C29-C30	-2.70	118.96	122.89
37	S	606	CHL	OMC-CMC-C2C	-2.70	121.04	124.49
37	s	606	CHL	OMC-CMC-C2C	-2.70	121.04	124.49
40	r	623	NEX	C15-C35-C34	-2.70	117.42	123.23
29	A	411	BCR	C8-C7-C6	-2.69	119.42	127.24
40	G	1623	NEX	C11-C12-C13	-2.69	118.44	126.34
39	n	1622	XAT	C10-C11-C12	-2.69	114.80	123.11
38	N	1620	LUT	C10-C11-C12	-2.69	114.80	123.11
40	g	1623	NEX	C11-C12-C13	-2.69	118.46	126.34
38	G	1620	LUT	C8-C7-C6	-2.69	119.44	127.24
38	G	1620	LUT	C35-C15-C14	-2.69	117.44	123.23
27	C	513	CLA	O2D-CGD-O1D	-2.68	118.12	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	S	612	CLA	O2D-CGD-O1D	-2.68	118.12	123.77
34	d	405	PL9	C36-C37-C38	-2.68	104.57	111.61
29	a	411	BCR	C8-C7-C6	-2.68	119.47	127.24
38	n	1620	LUT	C10-C11-C12	-2.68	114.84	123.11
38	g	1620	LUT	C8-C7-C6	-2.68	119.47	127.24
34	D	405	PL9	C36-C37-C38	-2.67	104.59	111.61
27	G	611	CLA	O2D-CGD-O1D	-2.67	118.14	123.77
37	g	609	CHL	CBA-CAA-C2A	-2.67	111.94	115.88
40	Y	1623	NEX	C31-C30-C29	-2.67	123.34	127.22
27	g	611	CLA	O2D-CGD-O1D	-2.67	118.15	123.77
29	C	514	BCR	C15-C16-C17	-2.67	117.48	123.23
29	c	514	BCR	C15-C16-C17	-2.67	117.48	123.23
27	R	613	CLA	O2D-CGD-O1D	-2.67	118.16	123.77
27	Y	610	CLA	O2D-CGD-O1D	-2.66	118.16	123.77
27	y	610	CLA	O2D-CGD-O1D	-2.66	118.16	123.77
38	r	620	LUT	C35-C34-C33	-2.66	123.35	127.22
32	c	518	DGD	C1E-C2E-C3E	-2.66	104.71	109.98
32	C	518	DGD	C1E-C2E-C3E	-2.66	104.71	109.98
32	h	102	DGD	C1D-C2D-C3D	-2.66	104.71	109.98
27	s	612	CLA	O2D-CGD-O1D	-2.66	118.18	123.77
27	r	610	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
27	S	614	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
27	s	614	CLA	O2D-CGD-O1D	-2.65	118.18	123.77
27	Y	613	CLA	O2D-CGD-O1D	-2.65	118.19	123.77
38	Y	1620	LUT	C35-C15-C14	-2.65	117.52	123.23
38	y	1620	LUT	C35-C15-C14	-2.65	117.52	123.23
37	G	605	CHL	CBC-CAC-C3C	-2.65	109.30	113.16
32	H	102	DGD	C1D-C2D-C3D	-2.65	104.73	109.98
40	y	1623	NEX	C24-C23-C22	-2.64	104.42	110.64
37	y	601	CHL	CAA-C2A-C1A	-2.64	108.89	115.87
27	B	616	CLA	CMB-C2B-C1B	-2.64	123.82	128.31
27	c	509	CLA	C11-C12-C13	-2.64	107.28	115.46
27	C	509	CLA	C11-C12-C13	-2.64	107.28	115.46
27	r	613	CLA	O2D-CGD-O1D	-2.64	118.21	123.77
27	C	507	CLA	CMB-C2B-C1B	-2.64	123.83	128.31
37	Y	601	CHL	CAA-C2A-C1A	-2.64	108.91	115.87
32	C	520	DGD	O2D-C2D-C1D	-2.64	104.16	110.01
40	Y	1623	NEX	C24-C23-C22	-2.64	104.44	110.64
38	g	1620	LUT	C31-C30-C29	-2.64	123.39	127.22
27	s	613	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
40	y	1623	NEX	C31-C30-C29	-2.63	123.39	127.22
37	g	605	CHL	CBC-CAC-C3C	-2.63	109.32	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	610	CLA	O2D-CGD-O1D	-2.63	118.24	123.77
38	g	1621	LUT	C38-C25-C24	-2.62	118.03	123.75
38	R	620	LUT	C35-C34-C33	-2.62	123.41	127.22
32	H	102	DGD	CDB-CCB-CBB	-2.62	100.92	114.54
27	S	613	CLA	O2D-CGD-O1D	-2.62	118.25	123.77
39	Y	1622	XAT	C35-C15-C14	-2.62	117.58	123.23
29	C	514	BCR	C8-C7-C6	-2.62	119.63	127.24
29	c	514	BCR	C8-C7-C6	-2.62	119.64	127.24
27	B	617	CLA	O2D-CGD-O1D	-2.62	118.26	123.77
27	b	617	CLA	O2D-CGD-O1D	-2.62	118.26	123.77
27	c	507	CLA	CMB-C2B-C1B	-2.62	123.86	128.31
32	c	520	DGD	O2D-C2D-C1D	-2.62	104.20	110.01
37	S	608	CHL	OMC-CMC-C2C	-2.62	121.14	124.49
27	R	601	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
32	h	102	DGD	CDB-CCB-CBB	-2.61	100.97	114.54
38	G	1620	LUT	C31-C30-C29	-2.61	123.42	127.22
38	G	1621	LUT	C38-C25-C24	-2.61	118.06	123.75
27	y	613	CLA	O2D-CGD-O1D	-2.61	118.28	123.77
37	G	605	CHL	CBA-CAA-C2A	-2.61	112.03	115.88
38	n	1621	LUT	C38-C25-C24	-2.61	118.07	123.75
38	g	1620	LUT	C16-C1-C6	-2.61	106.35	110.33
27	r	601	CLA	O2D-CGD-O1D	-2.61	118.28	123.77
39	y	1622	XAT	C35-C15-C14	-2.61	117.61	123.23
35	N	2630	LHG	C11-C10-C9	-2.61	101.01	114.54
27	r	602	CLA	O2D-CGD-O1D	-2.60	118.29	123.77
29	a	411	BCR	C16-C15-C14	-2.60	117.63	123.23
35	n	2630	LHG	C11-C10-C9	-2.60	101.04	114.54
37	G	608	CHL	C4A-C3A-C2A	-2.60	99.98	103.98
27	B	604	CLA	O2D-CGD-O1D	-2.60	118.30	123.77
27	R	602	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
38	N	1621	LUT	C38-C25-C24	-2.59	118.10	123.75
27	r	611	CLA	O2D-CGD-O1D	-2.59	118.31	123.77
34	d	405	PL9	C36-C34-C33	-2.59	116.15	120.98
34	D	405	PL9	C36-C34-C33	-2.59	116.15	120.98
31	d	411	LMG	O1-C7-C8	-2.59	104.83	110.99
37	G	601	CHL	OMC-CMC-C2C	-2.59	121.18	124.49
37	g	601	CHL	OMC-CMC-C2C	-2.59	121.18	124.49
27	b	616	CLA	CMB-C2B-C1B	-2.59	123.91	128.31
38	g	1621	LUT	C30-C31-C32	-2.59	115.11	123.11
38	G	1620	LUT	C16-C1-C6	-2.59	106.38	110.33
27	s	611	CLA	O2D-CGD-O1D	-2.59	118.32	123.77
29	A	411	BCR	C16-C15-C14	-2.59	117.65	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	605	CHL	CBA-CAA-C2A	-2.59	112.06	115.88
37	y	601	CHL	OMC-CMC-C2C	-2.59	121.18	124.49
37	g	608	CHL	C4A-C3A-C2A	-2.59	100.00	103.98
38	N	1621	LUT	C16-C1-C6	-2.58	106.38	110.33
37	s	608	CHL	OMC-CMC-C2C	-2.58	121.18	124.49
27	S	611	CLA	O2D-CGD-O1D	-2.58	118.33	123.77
27	R	611	CLA	O2D-CGD-O1D	-2.58	118.34	123.77
38	G	1621	LUT	C30-C31-C32	-2.58	115.14	123.11
37	G	606	CHL	CBC-CAC-C3C	-2.58	109.39	113.16
28	A	409	PHO	CBD-CHA-C4D	-2.58	105.64	108.54
31	D	411	LMG	O1-C7-C8	-2.58	104.86	110.99
31	D	411	LMG	O6-C1-O1	-2.57	103.81	109.99
27	b	604	CLA	O2D-CGD-O1D	-2.57	118.35	123.77
37	y	606	CHL	OMC-CMC-C2C	-2.57	121.20	124.49
29	b	620	BCR	C16-C15-C14	-2.57	117.68	123.23
40	N	1623	NEX	C31-C30-C29	-2.57	123.48	127.22
37	G	609	CHL	OMC-CMC-C2C	-2.57	121.20	124.49
37	g	606	CHL	CBC-CAC-C3C	-2.57	109.41	113.16
29	B	618	BCR	C15-C16-C17	-2.57	117.69	123.23
29	b	618	BCR	C15-C16-C17	-2.57	117.69	123.23
27	R	603	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
37	Y	609	CHL	OMC-CMC-C2C	-2.57	121.20	124.49
27	y	604	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
37	Y	606	CHL	OMC-CMC-C2C	-2.57	121.20	124.49
27	b	611	CLA	CAA-CBA-CGA	-2.57	105.86	113.28
37	g	607	CHL	OMC-CMC-C2C	-2.57	121.21	124.49
32	c	518	DGD	O2D-C2D-C1D	-2.56	104.32	110.01
37	G	607	CHL	OMC-CMC-C2C	-2.56	121.21	124.49
37	g	605	CHL	OMC-CMC-C2C	-2.56	121.21	124.49
32	c	519	DGD	C3G-C2G-C1G	-2.56	106.11	112.08
31	d	411	LMG	O6-C1-O1	-2.56	103.85	109.99
38	n	1621	LUT	C16-C1-C6	-2.56	106.42	110.33
38	R	620	LUT	C10-C11-C12	-2.56	115.20	123.11
38	r	620	LUT	C10-C11-C12	-2.56	115.20	123.11
40	n	1623	NEX	C31-C30-C29	-2.56	123.50	127.22
40	n	1623	NEX	C24-C23-C22	-2.56	104.63	110.64
32	C	518	DGD	O3G-C1D-C2D	-2.56	104.85	108.00
32	C	519	DGD	C3G-C2G-C1G	-2.56	106.12	112.08
27	r	603	CLA	O2D-CGD-O1D	-2.56	118.39	123.77
37	s	607	CHL	C4A-C3A-C2A	-2.56	100.04	103.98
38	y	1621	LUT	C38-C25-C24	-2.56	118.18	123.75
34	d	405	PL9	C22-C23-C24	-2.56	122.11	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	D	405	PL9	C22-C23-C24	-2.56	122.11	127.75
37	Y	601	CHL	OMC-CMC-C2C	-2.56	121.22	124.49
29	B	620	BCR	C16-C15-C14	-2.55	117.72	123.23
27	B	611	CLA	CAA-CBA-CGA	-2.55	105.90	113.28
38	g	1621	LUT	C22-C23-C24	-2.55	108.22	111.19
27	Y	604	CLA	O2D-CGD-O1D	-2.55	118.40	123.77
37	G	605	CHL	OMC-CMC-C2C	-2.55	121.22	124.49
40	N	1623	NEX	C24-C23-C22	-2.55	104.66	110.64
38	Y	1621	LUT	C38-C25-C24	-2.55	118.20	123.75
37	g	609	CHL	OMC-CMC-C2C	-2.55	121.23	124.49
38	S	1620	LUT	C10-C11-C12	-2.55	115.25	123.11
27	b	606	CLA	O2D-CGD-O1D	-2.54	118.41	123.77
28	a	409	PHO	CBD-CHA-C4D	-2.54	105.67	108.54
32	c	518	DGD	O3G-C1D-C2D	-2.54	104.87	108.00
29	c	515	BCR	C4-C5-C6	-2.54	119.94	122.73
29	b	618	BCR	C3-C4-C5	-2.54	109.66	113.87
38	G	1621	LUT	C22-C23-C24	-2.54	108.23	111.19
38	s	1620	LUT	C10-C11-C12	-2.54	115.27	123.11
31	b	622	LMG	C38-C37-C36	-2.54	101.37	114.54
31	B	622	LMG	C38-C37-C36	-2.54	101.37	114.54
37	y	609	CHL	OMC-CMC-C2C	-2.53	121.25	124.49
35	l	101	LHG	C5-O7-C7	-2.53	111.64	117.91
29	C	515	BCR	C33-C5-C6	-2.53	121.92	124.62
38	s	1621	LUT	C31-C30-C29	-2.53	123.54	127.22
38	S	1621	LUT	C31-C30-C29	-2.53	123.54	127.22
32	C	518	DGD	O2D-C2D-C1D	-2.53	104.39	110.01
29	c	515	BCR	C38-C26-C25	-2.53	121.92	124.62
32	C	519	DGD	O2D-C2D-C1D	-2.53	104.39	110.01
32	c	519	DGD	O2D-C2D-C1D	-2.53	104.39	110.01
27	C	512	CLA	O2D-CGD-O1D	-2.53	118.44	123.77
27	c	512	CLA	O2D-CGD-O1D	-2.53	118.44	123.77
35	L	101	LHG	C5-O7-C7	-2.53	111.67	117.91
38	s	1620	LUT	C30-C31-C32	-2.52	115.31	123.11
37	S	607	CHL	C4A-C3A-C2A	-2.52	100.09	103.98
27	B	606	CLA	O2D-CGD-O1D	-2.52	118.46	123.77
29	B	618	BCR	C3-C4-C5	-2.52	109.69	113.87
38	S	1620	LUT	C30-C31-C32	-2.52	115.33	123.11
27	N	612	CLA	O2D-CGD-O1D	-2.52	118.47	123.77
27	n	612	CLA	O2D-CGD-O1D	-2.52	118.47	123.77
27	b	615	CLA	CMB-C2B-C1B	-2.52	124.03	128.31
31	C	521	LMG	O1-C1-C2	-2.51	104.91	108.00
31	c	521	LMG	O1-C1-C2	-2.51	104.91	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	d	409	LHG	C5-O7-C7	-2.51	111.70	117.91
35	D	409	LHG	C5-O7-C7	-2.51	111.70	117.91
29	C	515	BCR	C38-C26-C25	-2.51	121.94	124.62
27	G	604	CLA	O2D-CGD-O1D	-2.51	118.48	123.77
29	C	515	BCR	C4-C5-C6	-2.51	119.97	122.73
40	r	623	NEX	C39-C29-C30	-2.51	119.24	122.89
29	c	515	BCR	C16-C17-C18	-2.51	123.58	127.22
29	C	515	BCR	C16-C17-C18	-2.51	123.58	127.22
31	B	622	LMG	C1-C2-C3	-2.50	105.01	109.98
27	B	615	CLA	CMB-C2B-C1B	-2.50	124.05	128.31
38	N	1621	LUT	C30-C31-C32	-2.50	115.37	123.11
35	g	2630	LHG	C20-C19-C18	-2.50	101.56	114.54
27	N	602	CLA	CMB-C2B-C1B	-2.50	124.06	128.31
27	n	602	CLA	CMB-C2B-C1B	-2.50	124.06	128.31
37	n	607	CHL	C6-C5-C3	-2.50	108.28	112.76
40	g	1623	NEX	C20-C13-C14	-2.50	119.25	122.89
39	y	1622	XAT	C31-C32-C33	-2.50	119.02	126.34
31	b	622	LMG	C1-C2-C3	-2.49	105.04	109.98
35	G	2630	LHG	C20-C19-C18	-2.49	101.59	114.54
29	c	515	BCR	C33-C5-C6	-2.49	121.97	124.62
27	g	604	CLA	O2D-CGD-O1D	-2.49	118.52	123.77
37	N	607	CHL	C6-C5-C3	-2.49	108.29	112.76
27	C	511	CLA	O2D-CGD-O1D	-2.49	118.53	123.77
35	d	409	LHG	C20-C19-C18	-2.49	101.61	114.54
39	Y	1622	XAT	C31-C32-C33	-2.49	119.05	126.34
38	n	1621	LUT	C30-C31-C32	-2.49	115.43	123.11
35	G	2630	LHG	C11-C10-C9	-2.49	101.63	114.54
35	D	410	LHG	C11-C10-C9	-2.49	101.63	114.54
35	d	410	LHG	C11-C10-C9	-2.49	101.63	114.54
37	N	601	CHL	CBC-CAC-C3C	-2.48	109.53	113.16
35	g	2630	LHG	C11-C10-C9	-2.48	101.64	114.54
40	R	623	NEX	C39-C29-C30	-2.48	119.28	122.89
27	a	406	CLA	O2D-CGD-O1D	-2.48	118.54	123.77
31	B	622	LMG	C40-C39-C38	-2.48	101.65	114.54
32	c	520	DGD	C4E-C3E-C2E	-2.48	106.22	110.79
35	D	409	LHG	C20-C19-C18	-2.48	101.67	114.54
37	n	601	CHL	CBC-CAC-C3C	-2.48	109.54	113.16
31	b	622	LMG	C40-C39-C38	-2.48	101.67	114.54
37	s	601	CHL	CAA-C2A-C1A	-2.48	109.33	115.87
27	A	406	CLA	O2D-CGD-O1D	-2.48	118.56	123.77
39	n	1622	XAT	C39-C29-C30	-2.47	119.29	122.89
27	c	511	CLA	O2D-CGD-O1D	-2.47	118.57	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	101	BCR	C23-C24-C25	-2.47	120.08	127.24
39	R	622	XAT	C4-C3-C2	-2.47	104.84	110.64
32	C	520	DGD	C4E-C3E-C2E	-2.47	106.24	110.79
27	Y	612	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
27	y	612	CLA	OBD-CAD-CBD	-2.46	122.22	125.94
35	l	101	LHG	C11-C10-C9	-2.46	101.76	114.54
35	L	101	LHG	C11-C10-C9	-2.46	101.76	114.54
39	N	1622	XAT	C39-C29-C30	-2.46	119.31	122.89
37	y	608	CHL	OMC-CMC-C2C	-2.46	121.34	124.49
27	b	602	CLA	O2D-CGD-O1D	-2.46	118.59	123.77
39	y	1622	XAT	C40-C33-C34	-2.46	119.31	122.89
29	h	101	BCR	C23-C24-C25	-2.46	120.11	127.24
32	C	520	DGD	CDB-CCB-CBB	-2.45	101.79	114.54
40	r	623	NEX	C16-C1-C6	-2.45	108.22	110.47
38	s	1621	LUT	C30-C31-C32	-2.45	115.53	123.11
38	S	1621	LUT	C30-C31-C32	-2.45	115.53	123.11
40	G	1623	NEX	C20-C13-C14	-2.45	119.32	122.89
32	c	520	DGD	CDB-CCB-CBB	-2.45	101.81	114.54
27	C	511	CLA	CAA-CBA-CGA	-2.45	106.19	113.28
29	C	517	BCR	C3-C4-C5	-2.45	109.81	113.87
29	c	517	BCR	C3-C4-C5	-2.45	109.81	113.87
29	A	411	BCR	C28-C27-C26	-2.45	109.81	113.87
35	l	101	LHG	C20-C19-C18	-2.45	101.83	114.54
37	Y	608	CHL	OMC-CMC-C2C	-2.45	121.36	124.49
27	y	603	CLA	OBD-CAD-CBD	-2.45	122.25	125.94
39	r	622	XAT	C4-C3-C2	-2.44	104.89	110.64
31	A	413	LMG	C38-C37-C36	-2.44	101.85	114.54
40	R	623	NEX	C30-C31-C32	-2.44	115.56	123.11
27	R	612	CLA	O2D-CGD-O1D	-2.44	118.63	123.77
27	c	511	CLA	CAA-CBA-CGA	-2.44	106.22	113.28
37	G	607	CHL	CBC-CAC-C3C	-2.44	109.59	113.16
37	S	601	CHL	CAA-C2A-C1A	-2.44	109.42	115.87
29	a	411	BCR	C28-C27-C26	-2.44	109.82	113.87
31	B	622	LMG	O3-C3-C2	-2.44	104.86	110.36
35	L	101	LHG	C20-C19-C18	-2.44	101.87	114.54
39	n	1622	XAT	C30-C31-C32	-2.44	115.58	123.11
29	d	404	BCR	C8-C7-C6	-2.44	120.16	127.24
39	N	1622	XAT	C30-C31-C32	-2.44	115.58	123.11
31	A	413	LMG	C40-C39-C38	-2.44	101.89	114.54
40	R	623	NEX	C16-C1-C6	-2.44	108.23	110.47
40	r	623	NEX	C30-C31-C32	-2.44	115.58	123.11
38	y	1621	LUT	C31-C30-C29	-2.44	123.68	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	S	2630	LHG	C11-C10-C9	-2.43	101.89	114.54
29	H	101	BCR	C39-C30-C25	-2.43	106.61	110.33
31	a	413	LMG	C38-C37-C36	-2.43	101.90	114.54
34	d	405	PL9	C37-C38-C39	-2.43	122.38	127.75
35	s	2630	LHG	C11-C10-C9	-2.43	101.91	114.54
31	b	622	LMG	O3-C3-C2	-2.43	104.88	110.36
27	r	612	CLA	O2D-CGD-O1D	-2.43	118.65	123.77
27	c	512	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
27	C	512	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
27	Y	603	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
39	Y	1622	XAT	C40-C33-C34	-2.43	119.35	122.89
39	r	622	XAT	C31-C30-C29	-2.43	123.69	127.22
37	g	607	CHL	CBC-CAC-C3C	-2.43	109.61	113.16
29	D	404	BCR	C8-C7-C6	-2.43	120.19	127.24
29	h	101	BCR	C21-C20-C19	-2.43	115.61	123.11
37	g	606	CHL	C4A-C3A-C2A	-2.43	100.24	103.98
35	S	2630	LHG	C20-C19-C18	-2.43	101.94	114.54
27	c	504	CLA	O2D-CGD-O1D	-2.43	118.66	123.77
31	a	413	LMG	C40-C39-C38	-2.43	101.94	114.54
27	G	614	CLA	O2D-CGD-O1D	-2.42	118.67	123.77
37	n	606	CHL	CBA-CAA-C2A	-2.42	112.31	115.88
37	N	606	CHL	CBA-CAA-C2A	-2.42	112.31	115.88
29	H	101	BCR	C33-C5-C6	-2.42	122.04	124.62
27	C	509	CLA	O2D-CGD-O1D	-2.42	118.67	123.77
34	D	405	PL9	C37-C38-C39	-2.42	122.41	127.75
32	c	518	DGD	O3E-C3E-C2E	-2.42	104.91	110.36
27	R	609	CLA	O2D-CGD-O1D	-2.42	118.68	123.77
27	b	610	CLA	CAA-CBA-CGA	-2.42	106.29	113.28
27	r	609	CLA	O2D-CGD-O1D	-2.42	118.68	123.77
27	n	604	CLA	O2D-CGD-O1D	-2.42	118.68	123.77
27	n	613	CLA	O2D-CGD-O1D	-2.42	118.68	123.77
27	B	612	CLA	C2C-C1C-NC	-2.41	108.57	110.22
32	C	518	DGD	O3E-C3E-C2E	-2.41	104.92	110.36
35	s	2630	LHG	C20-C19-C18	-2.41	102.01	114.54
37	G	606	CHL	C4A-C3A-C2A	-2.41	100.27	103.98
29	H	101	BCR	C21-C20-C19	-2.41	115.66	123.11
38	R	620	LUT	C16-C1-C6	-2.41	106.65	110.33
35	Y	2630	LHG	C11-C10-C9	-2.41	102.03	114.54
40	y	1623	NEX	C11-C12-C13	-2.41	119.28	126.34
29	C	517	BCR	C8-C7-C6	-2.41	120.25	127.24
35	y	2630	LHG	C11-C10-C9	-2.41	102.04	114.54
29	B	620	BCR	C23-C24-C25	-2.41	120.26	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	H	101	BCR	C8-C7-C6	-2.41	120.26	127.24
29	h	101	BCR	C8-C7-C6	-2.40	120.26	127.24
35	d	408	LHG	C11-C10-C9	-2.40	102.06	114.54
35	D	408	LHG	C11-C10-C9	-2.40	102.06	114.54
27	g	614	CLA	O2D-CGD-O1D	-2.40	118.71	123.77
29	b	620	BCR	C23-C24-C25	-2.40	120.27	127.24
35	y	2630	LHG	C20-C19-C18	-2.40	102.06	114.54
27	c	503	CLA	O2D-CGD-O1D	-2.40	118.71	123.77
27	c	509	CLA	O2D-CGD-O1D	-2.40	118.71	123.77
39	R	622	XAT	C31-C30-C29	-2.40	123.73	127.22
32	C	520	DGD	C3D-C4D-C5D	-2.40	105.95	110.23
27	N	613	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
40	s	1623	NEX	C24-C23-C22	-2.40	105.00	110.64
40	S	1623	NEX	C24-C23-C22	-2.40	105.00	110.64
37	y	601	CHL	O1D-CGD-CBD	-2.40	119.32	124.59
27	B	610	CLA	CAA-CBA-CGA	-2.40	106.34	113.28
27	N	604	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
29	h	101	BCR	C39-C30-C25	-2.40	106.67	110.33
29	c	517	BCR	C8-C7-C6	-2.40	120.28	127.24
27	B	602	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
27	C	504	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
32	c	519	DGD	CBB-CAB-C9B	-2.40	102.09	114.54
37	n	607	CHL	CBC-CAC-C3C	-2.40	109.66	113.16
40	s	1623	NEX	C39-C29-C30	-2.39	119.41	122.89
37	r	607	CHL	O2D-CGD-O1D	-2.39	118.73	123.77
27	B	608	CLA	O2D-CGD-O1D	-2.39	118.73	123.77
27	A	407	CLA	O2D-CGD-O1D	-2.39	118.74	123.77
27	b	608	CLA	O2D-CGD-O1D	-2.39	118.74	123.77
32	C	519	DGD	CBB-CAB-C9B	-2.39	102.12	114.54
35	Y	2630	LHG	C20-C19-C18	-2.39	102.12	114.54
39	r	622	XAT	C30-C31-C32	-2.39	115.72	123.11
38	r	620	LUT	C16-C1-C6	-2.39	106.68	110.33
38	Y	1621	LUT	C31-C30-C29	-2.39	123.75	127.22
38	Y	1620	LUT	C16-C1-C6	-2.38	106.69	110.33
38	y	1620	LUT	C16-C1-C6	-2.38	106.69	110.33
31	c	521	LMG	O2-C2-C1	-2.38	104.72	110.01
40	Y	1623	NEX	C11-C12-C13	-2.38	119.36	126.34
37	Y	601	CHL	O1D-CGD-CBD	-2.38	119.36	124.59
27	a	407	CLA	O2D-CGD-O1D	-2.38	118.76	123.77
34	D	405	PL9	C7-C3-C2	-2.38	119.20	122.66
32	c	520	DGD	C3D-C4D-C5D	-2.38	105.98	110.23
37	R	607	CHL	O2D-CGD-O1D	-2.38	118.76	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	503	CLA	O2D-CGD-O1D	-2.38	118.76	123.77
29	h	101	BCR	C33-C5-C6	-2.38	122.09	124.62
31	C	521	LMG	O2-C2-C1	-2.38	104.73	110.01
31	C	521	LMG	C40-C39-C38	-2.37	102.21	114.54
40	S	1623	NEX	C39-C29-C30	-2.37	119.44	122.89
31	c	521	LMG	C40-C39-C38	-2.37	102.22	114.54
27	D	402	CLA	O2A-CGA-O1A	-2.37	117.29	123.51
39	N	1622	XAT	C24-C23-C22	-2.37	105.07	110.64
37	N	608	CHL	C4A-C3A-C2A	-2.37	100.33	103.98
38	Y	1621	LUT	C16-C1-C6	-2.37	106.71	110.33
38	y	1621	LUT	C16-C1-C6	-2.37	106.71	110.33
35	D	409	LHG	C18-C17-C16	-2.37	102.25	114.54
38	S	1620	LUT	C31-C30-C29	-2.37	123.78	127.22
31	Z	101	LMG	O2-C2-C1	-2.37	104.76	110.01
29	c	516	BCR	C8-C7-C6	-2.37	120.37	127.24
29	C	516	BCR	C8-C7-C6	-2.37	120.37	127.24
35	d	409	LHG	C18-C17-C16	-2.37	102.25	114.54
40	R	623	NEX	C31-C30-C29	-2.36	123.78	127.22
27	S	609	CLA	O2D-CGD-O1D	-2.36	118.79	123.77
39	R	622	XAT	C30-C31-C32	-2.36	115.81	123.11
38	g	1620	LUT	C10-C11-C12	-2.36	115.81	123.11
34	d	405	PL9	C21-C22-C23	-2.36	105.41	111.61
39	n	1622	XAT	C24-C23-C22	-2.36	105.09	110.64
34	d	405	PL9	C7-C3-C2	-2.36	119.23	122.66
37	N	607	CHL	CBC-CAC-C3C	-2.36	109.71	113.16
37	n	608	CHL	C4A-C3A-C2A	-2.36	100.35	103.98
37	y	608	CHL	C4A-C3A-C2A	-2.36	100.35	103.98
40	R	623	NEX	C17-C1-C6	-2.36	108.31	110.47
31	Z	101	LMG	O3-C3-C2	-2.36	105.04	110.36
27	N	603	CLA	O2D-CGD-O1D	-2.36	118.81	123.77
34	D	405	PL9	C21-C22-C23	-2.36	105.42	111.61
31	z	101	LMG	O3-C3-C2	-2.36	105.05	110.36
40	r	623	NEX	C31-C30-C29	-2.35	123.80	127.22
38	G	1620	LUT	C30-C31-C32	-2.35	115.84	123.11
35	D	408	LHG	C27-C26-C25	-2.35	102.35	114.54
38	y	1621	LUT	C15-C35-C34	-2.35	118.17	123.23
31	c	521	LMG	O3-C3-C2	-2.35	105.07	110.36
35	d	408	LHG	C27-C26-C25	-2.35	102.36	114.54
38	s	1620	LUT	C31-C30-C29	-2.34	123.81	127.22
40	r	623	NEX	C17-C1-C6	-2.34	108.32	110.47
35	d	409	LHG	O8-C6-C5	-2.34	102.38	108.70
38	g	1620	LUT	C30-C31-C32	-2.34	115.87	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	s	609	CLA	O2D-CGD-O1D	-2.34	118.84	123.77
27	y	612	CLA	O2D-CGD-O1D	-2.34	118.84	123.77
31	z	101	LMG	O2-C2-C1	-2.34	104.82	110.01
27	c	503	CLA	OBD-CAD-CBD	-2.34	122.41	125.94
35	D	409	LHG	O8-C6-C5	-2.34	102.39	108.70
27	G	603	CLA	O2D-CGD-O1D	-2.34	118.85	123.77
40	N	1623	NEX	C30-C31-C32	-2.34	115.89	123.11
37	Y	608	CHL	C4A-C3A-C2A	-2.33	100.39	103.98
28	a	408	PHO	CBA-CAA-C2A	-2.33	107.94	113.96
27	d	402	CLA	O2A-CGA-O1A	-2.33	117.39	123.51
35	r	2630	LHG	C11-C10-C9	-2.33	102.43	114.54
28	A	408	PHO	CBA-CAA-C2A	-2.33	107.95	113.96
27	b	612	CLA	C2C-C1C-NC	-2.33	108.62	110.22
31	C	521	LMG	O3-C3-C2	-2.33	105.11	110.36
27	n	603	CLA	O2D-CGD-O1D	-2.33	118.87	123.77
35	R	2630	LHG	C11-C10-C9	-2.33	102.45	114.54
35	D	408	LHG	O8-C6-C5	-2.33	102.42	108.70
35	R	2630	LHG	C20-C19-C18	-2.33	102.45	114.54
35	r	2630	LHG	C20-C19-C18	-2.33	102.45	114.54
27	g	603	CLA	O2D-CGD-O1D	-2.32	118.88	123.77
27	C	503	CLA	OBD-CAD-CBD	-2.32	122.43	125.94
38	G	1620	LUT	C10-C11-C12	-2.32	115.93	123.11
31	C	521	LMG	C38-C37-C36	-2.32	102.47	114.54
27	Y	612	CLA	O2D-CGD-O1D	-2.32	118.88	123.77
40	n	1623	NEX	C30-C31-C32	-2.32	115.94	123.11
27	g	612	CLA	O2D-CGD-O1D	-2.32	118.89	123.77
38	Y	1621	LUT	C15-C35-C34	-2.32	118.23	123.23
27	R	616	CLA	O2A-CGA-O1A	-2.32	117.43	123.51
37	y	609	CHL	C3B-CAB-CBB	-2.32	119.70	125.34
37	Y	609	CHL	C3B-CAB-CBB	-2.32	119.70	125.34
31	c	521	LMG	C38-C37-C36	-2.31	102.52	114.54
27	B	614	CLA	O2D-CGD-O1D	-2.31	118.91	123.77
28	a	408	PHO	CMC-C2C-C1C	-2.31	121.38	125.06
36	f	101	HEM	CBA-CAA-C2A	-2.31	108.44	112.49
27	G	612	CLA	O2D-CGD-O1D	-2.30	118.92	123.77
27	r	616	CLA	O2A-CGA-O1A	-2.30	117.47	123.51
32	C	518	DGD	O5D-C6D-C5D	-2.30	105.05	109.14
29	C	514	BCR	C23-C24-C25	-2.30	120.56	127.24
36	F	101	HEM	CBA-CAA-C2A	-2.30	108.45	112.49
35	d	408	LHG	O8-C6-C5	-2.30	102.49	108.70
29	B	619	BCR	C10-C11-C12	-2.30	116.01	123.11
37	S	601	CHL	O1D-CGD-CBD	-2.30	119.54	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	614	CLA	O2D-CGD-O1D	-2.30	118.93	123.77
34	d	405	PL9	C12-C13-C14	-2.30	122.68	127.75
34	D	405	PL9	C12-C13-C14	-2.30	122.68	127.75
29	b	619	BCR	C10-C11-C12	-2.29	116.02	123.11
29	c	514	BCR	C23-C24-C25	-2.29	120.59	127.24
39	Y	1622	XAT	C24-C23-C22	-2.29	105.25	110.64
37	R	607	CHL	O1D-CGD-CBD	-2.29	119.56	124.59
32	c	518	DGD	O5D-C6D-C5D	-2.29	105.06	109.14
38	n	1620	LUT	C16-C1-C6	-2.29	106.84	110.33
29	H	101	BCR	C11-C10-C9	-2.29	123.90	127.22
29	h	101	BCR	C3-C4-C5	-2.28	110.08	113.87
29	H	101	BCR	C3-C4-C5	-2.28	110.08	113.87
38	S	1620	LUT	C8-C7-C6	-2.28	120.61	127.24
35	L	101	LHG	C18-C17-C16	-2.28	102.68	114.54
37	s	601	CHL	O1D-CGD-CBD	-2.28	119.58	124.59
29	b	618	BCR	C8-C7-C6	-2.28	120.62	127.24
27	A	405	CLA	O2D-CGD-O1D	-2.28	118.97	123.77
38	N	1620	LUT	C16-C1-C6	-2.28	106.85	110.33
37	n	605	CHL	O2D-CGD-O1D	-2.28	118.98	123.77
39	y	1622	XAT	C24-C23-C22	-2.28	105.29	110.64
29	b	619	BCR	C27-C26-C25	-2.27	120.23	122.73
27	b	610	CLA	O2A-CGA-O1A	-2.27	117.55	123.51
40	G	1623	NEX	C15-C35-C34	-2.27	118.33	123.23
31	Z	101	LMG	C40-C39-C38	-2.27	102.74	114.54
35	l	101	LHG	C18-C17-C16	-2.27	102.74	114.54
28	A	408	PHO	CMC-C2C-C1C	-2.27	121.43	125.06
31	A	413	LMG	O2-C2-C1	-2.27	104.97	110.01
37	N	606	CHL	O2D-CGD-O1D	-2.27	118.99	123.77
37	r	607	CHL	CBA-CAA-C2A	-2.27	112.53	115.88
37	r	607	CHL	O1D-CGD-CBD	-2.27	119.61	124.59
29	B	618	BCR	C16-C15-C14	-2.27	118.34	123.23
29	b	618	BCR	C16-C15-C14	-2.27	118.34	123.23
38	s	1620	LUT	C8-C7-C6	-2.27	120.66	127.24
29	a	411	BCR	C21-C20-C19	-2.27	116.11	123.11
40	N	1623	NEX	C11-C12-C13	-2.26	119.70	126.34
29	c	514	BCR	C10-C11-C12	-2.26	116.12	123.11
37	n	606	CHL	O2D-CGD-O1D	-2.26	119.00	123.77
29	C	514	BCR	C10-C11-C12	-2.26	116.12	123.11
31	z	101	LMG	C40-C39-C38	-2.26	102.79	114.54
29	A	411	BCR	C21-C20-C19	-2.26	116.12	123.11
40	g	1623	NEX	C15-C35-C34	-2.26	118.36	123.23
31	D	411	LMG	O3-C3-C2	-2.26	105.26	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	610	CLA	O2A-CGA-O1A	-2.26	117.58	123.51
27	y	610	CLA	O2A-CGA-O1A	-2.26	117.58	123.51
27	s	610	CLA	O2D-CGD-O1D	-2.26	119.01	123.77
29	h	101	BCR	C11-C10-C9	-2.26	123.94	127.22
38	n	1620	LUT	C35-C15-C14	-2.26	118.36	123.23
40	R	623	NEX	C24-C23-C22	-2.26	105.33	110.64
27	a	405	CLA	O2D-CGD-O1D	-2.26	119.02	123.77
35	s	2630	LHG	C18-C17-C16	-2.26	102.82	114.54
40	n	1623	NEX	C11-C12-C13	-2.26	119.72	126.34
31	a	413	LMG	O2-C2-C1	-2.26	105.00	110.01
31	d	411	LMG	O3-C3-C2	-2.25	105.28	110.36
35	S	2630	LHG	C18-C17-C16	-2.25	102.85	114.54
29	B	618	BCR	C8-C7-C6	-2.25	120.71	127.24
37	G	605	CHL	O2D-CGD-O1D	-2.25	119.03	123.77
27	B	610	CLA	O2A-CGA-O1A	-2.25	117.61	123.51
40	r	623	NEX	C24-C23-C22	-2.25	105.35	110.64
35	l	101	LHG	C27-C26-C25	-2.25	102.86	114.54
37	G	606	CHL	CAA-C2A-C1A	-2.25	109.93	115.87
37	N	606	CHL	O1D-CGD-CBD	-2.25	119.65	124.59
35	n	2630	LHG	C20-C19-C18	-2.25	102.87	114.54
37	g	605	CHL	O2D-CGD-O1D	-2.25	119.04	123.77
35	L	101	LHG	C27-C26-C25	-2.25	102.88	114.54
38	N	1620	LUT	C35-C15-C14	-2.24	118.39	123.23
35	N	2630	LHG	C27-C26-C25	-2.24	102.89	114.54
35	n	2630	LHG	C27-C26-C25	-2.24	102.89	114.54
31	c	521	LMG	O1-C7-C8	-2.24	105.65	110.99
32	c	518	DGD	O6D-C5D-C6D	-2.24	101.99	106.61
35	d	409	LHG	C27-C26-C25	-2.24	102.90	114.54
35	D	409	LHG	C27-C26-C25	-2.24	102.90	114.54
27	y	603	CLA	O2D-CGD-O1D	-2.24	119.05	123.77
29	C	515	BCR	C23-C24-C25	-2.24	120.74	127.24
37	n	606	CHL	O1D-CGD-CBD	-2.24	119.67	124.59
35	N	2630	LHG	C20-C19-C18	-2.24	102.92	114.54
27	N	614	CLA	O2A-CGA-O1A	-2.24	117.64	123.51
37	N	605	CHL	O2D-CGD-O1D	-2.24	119.06	123.77
38	R	620	LUT	C30-C31-C32	-2.24	116.20	123.11
37	g	606	CHL	CAA-C2A-C1A	-2.24	109.97	115.87
29	a	411	BCR	C10-C11-C12	-2.24	116.20	123.11
38	r	620	LUT	C30-C31-C32	-2.23	116.21	123.11
27	Y	603	CLA	O2D-CGD-O1D	-2.23	119.07	123.77
40	S	1623	NEX	C30-C31-C32	-2.23	116.22	123.11
37	R	607	CHL	CBA-CAA-C2A	-2.23	112.59	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	619	BCR	C23-C24-C25	-2.23	120.77	127.24
31	z	101	LMG	O1-C1-C2	-2.23	105.26	108.00
32	C	518	DGD	O6D-C5D-C6D	-2.23	102.02	106.61
29	c	515	BCR	C23-C24-C25	-2.23	120.78	127.24
27	S	610	CLA	O2D-CGD-O1D	-2.23	119.08	123.77
27	b	613	CLA	CAA-CBA-CGA	-2.23	106.84	113.28
29	B	619	BCR	C23-C24-C25	-2.23	120.78	127.24
29	c	515	BCR	C8-C7-C6	-2.22	120.78	127.24
29	C	515	BCR	C8-C7-C6	-2.22	120.78	127.24
38	S	1621	LUT	C35-C15-C14	-2.22	118.44	123.23
27	n	614	CLA	O2A-CGA-O1A	-2.22	117.68	123.51
31	z	101	LMG	C1-C2-C3	-2.22	105.57	109.98
37	n	601	CHL	CAA-C2A-C1A	-2.22	110.00	115.87
32	H	102	DGD	O3E-C3E-C2E	-2.22	105.35	110.36
40	s	1623	NEX	C30-C31-C32	-2.22	116.25	123.11
29	b	619	BCR	C21-C20-C19	-2.22	116.25	123.11
29	A	411	BCR	C10-C11-C12	-2.22	116.25	123.11
34	d	405	PL9	C46-C47-C48	-2.22	105.79	111.61
27	N	611	CLA	O2A-CGA-O1A	-2.22	117.70	123.51
31	C	521	LMG	O1-C7-C8	-2.22	105.72	110.99
31	A	413	LMG	C9-C8-C7	-2.21	106.92	112.08
37	Y	607	CHL	O2D-CGD-O1D	-2.21	119.11	123.77
37	N	601	CHL	CAA-C2A-C1A	-2.21	110.03	115.87
27	b	605	CLA	O2A-CGA-O1A	-2.21	117.72	123.51
34	D	405	PL9	C46-C47-C48	-2.21	105.81	111.61
27	B	613	CLA	CAA-CBA-CGA	-2.21	106.89	113.28
39	N	1622	XAT	C4-C3-C2	-2.21	105.45	110.64
29	B	619	BCR	C21-C20-C19	-2.21	116.29	123.11
29	B	619	BCR	C27-C26-C25	-2.21	120.31	122.73
37	y	609	CHL	C11-C10-C8	-2.21	108.63	115.46
32	h	102	DGD	O3E-C3E-C2E	-2.21	105.39	110.36
37	N	605	CHL	CBC-CAC-C3C	-2.20	109.94	113.16
35	r	2630	LHG	C27-C26-C25	-2.20	103.09	114.54
27	B	605	CLA	O2A-CGA-O1A	-2.20	117.73	123.51
27	n	611	CLA	O2A-CGA-O1A	-2.20	117.73	123.51
31	Z	101	LMG	C1-C2-C3	-2.20	105.61	109.98
35	R	2630	LHG	C27-C26-C25	-2.20	103.10	114.54
37	g	607	CHL	O2D-CGD-O1D	-2.20	119.13	123.77
37	S	608	CHL	CBA-CAA-C2A	-2.20	112.63	115.88
37	s	608	CHL	CBA-CAA-C2A	-2.20	112.63	115.88
28	a	409	PHO	O2D-CGD-O1D	-2.20	119.14	123.77
37	Y	609	CHL	C11-C10-C8	-2.20	108.66	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	605	CHL	CBC-CAC-C3C	-2.20	109.95	113.16
31	a	413	LMG	C9-C8-C7	-2.20	106.96	112.08
38	N	1620	LUT	C38-C25-C24	-2.20	118.97	123.75
37	G	607	CHL	O2D-CGD-O1D	-2.20	119.15	123.77
27	b	605	CLA	C4B-CHC-C1C	-2.20	124.98	129.34
27	c	503	CLA	C4B-CHC-C1C	-2.19	124.98	129.34
37	y	601	CHL	O2D-CGD-O1D	-2.19	119.15	123.77
40	G	1623	NEX	C24-C23-C22	-2.19	105.49	110.64
40	g	1623	NEX	C24-C23-C22	-2.19	105.49	110.64
37	n	608	CHL	O2D-CGD-O1D	-2.19	119.16	123.77
29	c	516	BCR	C39-C30-C25	-2.19	106.99	110.33
38	Y	1620	LUT	C38-C25-C24	-2.19	118.99	123.75
38	Y	1620	LUT	C8-C7-C6	-2.19	120.89	127.24
38	y	1620	LUT	C8-C7-C6	-2.19	120.89	127.24
37	r	608	CHL	CBA-CAA-C2A	-2.19	112.66	115.88
32	c	518	DGD	CBB-CAB-C9B	-2.19	103.19	114.54
37	y	607	CHL	O2D-CGD-O1D	-2.19	119.17	123.77
32	C	519	DGD	C5B-C4B-C3B	-2.18	103.19	114.54
39	n	1622	XAT	C4-C3-C2	-2.18	105.51	110.64
32	c	519	DGD	C5B-C4B-C3B	-2.18	103.20	114.54
38	s	1621	LUT	C35-C15-C14	-2.18	118.52	123.23
32	C	518	DGD	CBB-CAB-C9B	-2.18	103.21	114.54
38	n	1620	LUT	C38-C25-C24	-2.18	119.00	123.75
27	C	503	CLA	C4B-CHC-C1C	-2.18	125.01	129.34
27	B	605	CLA	C4B-CHC-C1C	-2.18	125.01	129.34
37	Y	601	CHL	O2D-CGD-O1D	-2.18	119.19	123.77
27	A	405	CLA	CAA-CBA-CGA	-2.18	106.99	113.28
38	y	1620	LUT	C38-C25-C24	-2.17	119.01	123.75
37	n	609	CHL	OMC-CMC-C2C	-2.17	121.71	124.49
37	N	609	CHL	OMC-CMC-C2C	-2.17	121.71	124.49
27	b	607	CLA	O2A-CGA-O1A	-2.17	117.82	123.51
35	D	410	LHG	C27-C26-C25	-2.17	103.27	114.54
37	N	608	CHL	O2D-CGD-O1D	-2.17	119.20	123.77
37	g	601	CHL	CAA-C2A-C1A	-2.17	110.14	115.87
27	a	405	CLA	CAA-CBA-CGA	-2.17	107.00	113.28
31	Z	101	LMG	O1-C1-C2	-2.17	105.33	108.00
37	n	601	CHL	O1D-CGD-CBD	-2.17	119.83	124.59
37	N	601	CHL	O1D-CGD-CBD	-2.17	119.83	124.59
35	d	410	LHG	C27-C26-C25	-2.17	103.28	114.54
35	y	2630	LHG	C18-C17-C16	-2.17	103.28	114.54
27	c	509	CLA	CAA-CBA-CGA	-2.17	107.01	113.28
35	Y	2630	LHG	C18-C17-C16	-2.17	103.28	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	509	CLA	CAA-CBA-CGA	-2.17	107.01	113.28
37	G	601	CHL	CAA-C2A-C1A	-2.17	110.14	115.87
31	z	101	LMG	O6-C1-O1	-2.16	104.80	109.99
27	B	607	CLA	O2A-CGA-O1A	-2.16	117.84	123.51
35	y	2630	LHG	C5-O7-C7	-2.16	112.56	117.91
32	C	520	DGD	O6E-C1E-O5D	-2.16	104.80	109.99
35	Y	2630	LHG	C5-O7-C7	-2.16	112.56	117.91
32	c	520	DGD	O6E-C1E-O5D	-2.16	104.80	109.99
27	c	508	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
29	C	516	BCR	C39-C30-C25	-2.16	107.03	110.33
29	b	620	BCR	C10-C11-C12	-2.16	116.44	123.11
28	A	409	PHO	O2D-CGD-O1D	-2.16	119.23	123.77
38	Y	1620	LUT	C15-C35-C34	-2.16	118.58	123.23
38	y	1620	LUT	C15-C35-C34	-2.16	118.58	123.23
38	n	1620	LUT	C31-C30-C29	-2.16	124.08	127.22
31	Z	101	LMG	O6-C1-O1	-2.16	104.82	109.99
37	Y	609	CHL	O2D-CGD-O1D	-2.15	119.23	123.77
39	r	622	XAT	C24-C23-C22	-2.15	105.58	110.64
31	D	411	LMG	O2-C2-C1	-2.15	105.23	110.01
29	D	404	BCR	C28-C27-C26	-2.15	110.30	113.87
37	G	605	CHL	CAA-C2A-C1A	-2.15	110.19	115.87
27	R	601	CLA	O2A-CGA-O1A	-2.15	117.87	123.51
27	B	610	CLA	O2D-CGD-O1D	-2.15	119.24	123.77
31	A	413	LMG	O1-C7-C8	-2.15	105.87	110.99
29	B	620	BCR	C10-C11-C12	-2.15	116.47	123.11
31	a	413	LMG	O1-C7-C8	-2.15	105.88	110.99
32	c	518	DGD	CAB-C9B-C8B	-2.15	103.40	114.54
35	s	2630	LHG	C27-C26-C25	-2.15	103.40	114.54
35	S	2630	LHG	C27-C26-C25	-2.15	103.40	114.54
37	y	607	CHL	O1D-CGD-CBD	-2.14	119.88	124.59
27	C	508	CLA	OBD-CAD-CBD	-2.14	122.70	125.94
27	y	602	CLA	C16-C15-C13	-2.14	108.82	115.46
27	C	503	CLA	O2A-CGA-O1A	-2.14	117.89	123.51
27	r	601	CLA	O2A-CGA-O1A	-2.14	117.90	123.51
32	C	518	DGD	CAB-C9B-C8B	-2.14	103.43	114.54
39	g	1622	XAT	C10-C11-C12	-2.14	116.50	123.11
37	R	608	CHL	CBA-CAA-C2A	-2.14	112.73	115.88
32	c	518	DGD	O5E-C6E-C5E	-2.14	104.16	111.30
32	C	519	DGD	C3D-C4D-C5D	-2.14	106.42	110.23
32	c	519	DGD	C3D-C4D-C5D	-2.14	106.42	110.23
35	g	2630	LHG	C27-C26-C25	-2.14	103.45	114.54
37	Y	607	CHL	O1D-CGD-CBD	-2.14	119.90	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	610	CLA	O2D-CGD-O1D	-2.13	119.28	123.77
39	R	622	XAT	C24-C23-C22	-2.13	105.62	110.64
39	G	1622	XAT	C10-C11-C12	-2.13	116.52	123.11
37	N	607	CHL	O2D-CGD-O1D	-2.13	119.28	123.77
35	g	2630	LHG	C18-C17-C16	-2.13	103.47	114.54
35	G	2630	LHG	C18-C17-C16	-2.13	103.47	114.54
31	d	411	LMG	O2-C2-C1	-2.13	105.28	110.01
35	G	2630	LHG	C27-C26-C25	-2.13	103.47	114.54
37	N	609	CHL	C3B-CAB-CBB	-2.13	120.15	125.34
37	n	607	CHL	O2D-CGD-O1D	-2.13	119.28	123.77
37	g	605	CHL	CAA-C2A-C1A	-2.13	110.24	115.87
38	y	1621	LUT	C22-C23-C24	-2.13	108.71	111.19
32	C	518	DGD	O5E-C6E-C5E	-2.13	104.19	111.30
27	c	506	CLA	OBD-CAD-CBD	-2.13	122.72	125.94
27	C	501	CLA	OBD-CAD-CBD	-2.13	122.73	125.94
27	c	501	CLA	OBD-CAD-CBD	-2.13	122.73	125.94
27	Y	602	CLA	C16-C15-C13	-2.13	108.88	115.46
38	y	1621	LUT	C30-C31-C32	-2.13	116.54	123.11
32	h	102	DGD	O3D-C3D-C4D	-2.12	105.57	110.36
27	B	617	CLA	C4B-CHC-C1C	-2.12	125.12	129.34
27	c	503	CLA	O2A-CGA-O1A	-2.12	117.94	123.51
37	S	606	CHL	O2D-CGD-O1D	-2.12	119.30	123.77
37	n	609	CHL	C3B-CAB-CBB	-2.12	120.17	125.34
38	N	1620	LUT	C31-C30-C29	-2.12	124.14	127.22
29	d	404	BCR	C21-C20-C19	-2.12	116.56	123.11
29	d	404	BCR	C28-C27-C26	-2.12	110.35	113.87
27	b	617	CLA	C4B-CHC-C1C	-2.12	125.13	129.34
37	y	609	CHL	O2D-CGD-O1D	-2.12	119.31	123.77
38	Y	1621	LUT	C22-C23-C24	-2.12	108.72	111.19
27	c	509	CLA	O2A-CGA-O1A	-2.12	117.96	123.51
38	Y	1621	LUT	C30-C31-C32	-2.12	116.57	123.11
27	C	509	CLA	O2A-CGA-O1A	-2.11	117.97	123.51
37	n	605	CHL	CAA-C2A-C1A	-2.11	110.28	115.87
31	Z	101	LMG	C38-C37-C36	-2.11	103.57	114.54
31	z	101	LMG	C38-C37-C36	-2.11	103.58	114.54
29	D	404	BCR	C21-C20-C19	-2.11	116.59	123.11
32	H	102	DGD	O2D-C2D-C1D	-2.11	105.33	110.01
38	R	620	LUT	C38-C25-C24	-2.11	119.15	123.75
31	b	622	LMG	O7-C10-O9	-2.11	117.93	123.67
35	n	2630	LHG	C18-C17-C16	-2.11	103.59	114.54
40	r	623	NEX	C11-C12-C13	-2.11	120.16	126.34
29	C	516	BCR	C10-C11-C12	-2.11	116.60	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	R	623	NEX	C11-C12-C13	-2.11	120.16	126.34
35	N	2630	LHG	C18-C17-C16	-2.11	103.60	114.54
32	h	102	DGD	O2D-C2D-C1D	-2.11	105.33	110.01
27	C	506	CLA	OBD-CAD-CBD	-2.11	122.76	125.94
37	G	601	CHL	O1D-CGD-CBD	-2.10	119.97	124.59
37	g	601	CHL	O1D-CGD-CBD	-2.10	119.97	124.59
29	c	516	BCR	C10-C11-C12	-2.10	116.61	123.11
27	G	613	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
27	g	613	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
27	B	602	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
27	B	604	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
35	N	2630	LHG	O8-C6-C5	-2.10	103.03	108.70
27	b	602	CLA	O2A-CGA-O1A	-2.10	118.01	123.51
27	Y	602	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
38	S	1621	LUT	C7-C8-C9	-2.10	123.04	126.21
31	D	411	LMG	C1-O6-C5	-2.10	109.63	113.74
31	d	411	LMG	C1-O6-C5	-2.10	109.63	113.74
31	B	622	LMG	O7-C10-O9	-2.10	117.97	123.67
38	r	620	LUT	C38-C25-C24	-2.10	119.18	123.75
31	C	521	LMG	C1-C2-C3	-2.10	105.82	109.98
28	a	408	PHO	O2D-CGD-O1D	-2.10	119.36	123.77
27	c	503	CLA	CAA-CBA-CGA	-2.10	107.22	113.28
27	b	604	CLA	O2A-CGA-O1A	-2.10	118.02	123.51
38	n	1620	LUT	C11-C10-C9	-2.09	124.18	127.22
35	n	2630	LHG	O8-C6-C5	-2.09	103.05	108.70
32	c	518	DGD	C5B-C4B-C3B	-2.09	103.67	114.54
29	a	411	BCR	C15-C16-C17	-2.09	118.72	123.23
37	r	606	CHL	C3B-CAB-CBB	-2.09	120.25	125.34
32	H	102	DGD	O5D-C6D-C5D	-2.09	105.42	109.14
31	a	413	LMG	O7-C10-O9	-2.09	117.98	123.67
37	g	606	CHL	O2D-CGD-O1D	-2.09	119.37	123.77
32	C	518	DGD	C5B-C4B-C3B	-2.09	103.69	114.54
32	H	102	DGD	O3D-C3D-C4D	-2.09	105.65	110.36
32	h	102	DGD	O5D-C6D-C5D	-2.09	105.42	109.14
29	d	404	BCR	C15-C14-C13	-2.09	124.18	127.22
29	c	517	BCR	C16-C15-C14	-2.09	118.73	123.23
29	C	517	BCR	C16-C15-C14	-2.09	118.73	123.23
37	y	606	CHL	O1D-CGD-CBD	-2.09	120.01	124.59
37	R	608	CHL	C4A-C3A-C2A	-2.09	100.77	103.98
37	N	605	CHL	CAA-C2A-C1A	-2.09	110.36	115.87
37	G	609	CHL	CBC-CAC-C3C	-2.09	110.11	113.16
29	A	411	BCR	C15-C16-C17	-2.09	118.74	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	606	CHL	O2D-CGD-O1D	-2.08	119.39	123.77
27	R	603	CLA	O2A-CGA-O1A	-2.08	118.05	123.51
27	R	611	CLA	O2A-CGA-O1A	-2.08	118.05	123.51
37	s	606	CHL	O2D-CGD-O1D	-2.08	119.39	123.77
27	r	603	CLA	O2A-CGA-O1A	-2.08	118.05	123.51
37	g	609	CHL	CBC-CAC-C3C	-2.08	110.12	113.16
37	g	601	CHL	O2D-CGD-O1D	-2.08	119.39	123.77
28	A	408	PHO	O2D-CGD-O1D	-2.08	119.39	123.77
37	Y	606	CHL	O1D-CGD-CBD	-2.08	120.02	124.59
31	c	521	LMG	C1-C2-C3	-2.08	105.86	109.98
37	G	601	CHL	O2D-CGD-O1D	-2.08	119.40	123.77
38	S	1621	LUT	C15-C35-C34	-2.08	118.75	123.23
37	R	606	CHL	C3B-CAB-CBB	-2.08	120.29	125.34
27	B	615	CLA	OBD-CAD-CBD	-2.08	122.81	125.94
37	r	608	CHL	C4A-C3A-C2A	-2.07	100.79	103.98
38	s	1621	LUT	C7-C8-C9	-2.07	123.08	126.21
27	C	501	CLA	O2A-CGA-O1A	-2.07	118.08	123.51
27	C	503	CLA	CAA-CBA-CGA	-2.07	107.29	113.28
27	g	604	CLA	C4B-CHC-C1C	-2.07	125.23	129.34
27	G	604	CLA	C4B-CHC-C1C	-2.07	125.23	129.34
27	c	501	CLA	O2A-CGA-O1A	-2.07	118.08	123.51
38	N	1620	LUT	C11-C10-C9	-2.07	124.21	127.22
34	D	405	PL9	O1-C4-C3	-2.07	118.11	120.71
27	C	512	CLA	C4B-CHC-C1C	-2.07	125.23	129.34
38	s	1621	LUT	C15-C35-C34	-2.06	118.78	123.23
35	g	2630	LHG	O8-C23-O10	-2.06	118.10	123.51
31	A	413	LMG	O7-C10-O9	-2.06	118.06	123.67
27	c	512	CLA	C4B-CHC-C1C	-2.06	125.24	129.34
37	r	606	CHL	O2D-CGD-O1D	-2.06	119.43	123.77
37	N	601	CHL	O2D-CGD-O1D	-2.06	119.43	123.77
27	S	610	CLA	O2A-CGA-O1A	-2.06	118.11	123.51
27	b	613	CLA	C11-C12-C13	-2.06	109.09	115.46
37	s	607	CHL	O2D-CGD-O1D	-2.06	119.44	123.77
29	D	404	BCR	C15-C14-C13	-2.06	124.23	127.22
38	G	1621	LUT	C15-C35-C34	-2.06	118.79	123.23
38	g	1621	LUT	C15-C35-C34	-2.06	118.79	123.23
27	n	612	CLA	C4B-CHC-C1C	-2.06	125.25	129.34
27	s	612	CLA	C4B-CHC-C1C	-2.06	125.25	129.34
35	y	2630	LHG	O8-C6-C5	-2.06	103.15	108.70
27	S	612	CLA	C4B-CHC-C1C	-2.06	125.26	129.34
27	s	614	CLA	O2A-CGA-O1A	-2.06	118.12	123.51
27	r	611	CLA	O2A-CGA-O1A	-2.05	118.12	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	G	1621	LUT	C35-C15-C14	-2.05	118.80	123.23
38	g	1621	LUT	C35-C15-C14	-2.05	118.80	123.23
27	b	615	CLA	OBD-CAD-CBD	-2.05	122.84	125.94
27	s	610	CLA	O2A-CGA-O1A	-2.05	118.13	123.51
35	G	2630	LHG	O8-C23-O10	-2.05	118.14	123.51
37	S	607	CHL	O2D-CGD-O1D	-2.05	119.45	123.77
27	N	610	CLA	O2A-CGA-O1A	-2.05	118.14	123.51
27	y	612	CLA	O2A-CGA-O1A	-2.05	118.14	123.51
34	D	405	PL9	O2-C1-C2	-2.05	117.17	121.78
27	Y	612	CLA	O2A-CGA-O1A	-2.05	118.15	123.51
27	n	612	CLA	O2A-CGA-O1A	-2.05	118.15	123.51
37	n	601	CHL	O2D-CGD-O1D	-2.04	119.47	123.77
27	y	602	CLA	OBD-CAD-CBD	-2.04	122.86	125.94
27	S	614	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
27	Y	614	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
27	Y	611	CLA	OBD-CAD-CBD	-2.04	122.86	125.94
27	n	610	CLA	O2A-CGA-O1A	-2.04	118.16	123.51
34	d	405	PL9	C42-C43-C44	-2.04	123.25	127.75
27	B	613	CLA	C11-C12-C13	-2.04	109.14	115.46
35	Y	2630	LHG	O8-C6-C5	-2.04	103.19	108.70
37	R	606	CHL	O2D-CGD-O1D	-2.04	119.47	123.77
27	N	612	CLA	C4B-CHC-C1C	-2.04	125.29	129.34
35	R	2630	LHG	C18-C17-C16	-2.04	103.94	114.54
34	d	405	PL9	O1-C4-C3	-2.04	118.15	120.71
32	c	519	DGD	O6E-C1E-O5D	-2.04	105.10	109.99
29	C	516	BCR	C21-C20-C19	-2.04	116.81	123.11
34	d	405	PL9	O2-C1-C2	-2.04	117.19	121.78
27	N	612	CLA	O2A-CGA-O1A	-2.04	118.17	123.51
37	G	608	CHL	O2D-CGD-O1D	-2.03	119.49	123.77
37	g	608	CHL	O2D-CGD-O1D	-2.03	119.49	123.77
27	S	604	CLA	C4B-CHC-C1C	-2.03	125.30	129.34
27	s	604	CLA	C4B-CHC-C1C	-2.03	125.30	129.34
32	c	519	DGD	C7B-C6B-C5B	-2.03	103.98	114.54
27	y	613	CLA	OBD-CAD-CBD	-2.03	122.87	125.94
34	D	405	PL9	C42-C43-C44	-2.03	123.27	127.75
27	y	611	CLA	OBD-CAD-CBD	-2.03	122.87	125.94
32	C	519	DGD	C7B-C6B-C5B	-2.03	104.00	114.54
35	r	2630	LHG	C18-C17-C16	-2.03	104.00	114.54
29	c	516	BCR	C21-C20-C19	-2.03	116.84	123.11
38	R	620	LUT	C11-C10-C9	-2.03	124.27	127.22
38	r	620	LUT	C11-C10-C9	-2.03	124.27	127.22
29	C	514	BCR	C11-C12-C13	-2.03	120.39	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	1622	XAT	C10-C11-C12	-2.03	116.84	123.11
27	c	513	CLA	O2A-CGA-O1A	-2.03	118.19	123.51
32	C	519	DGD	O6E-C1E-O5D	-2.03	105.13	109.99
38	r	620	LUT	C15-C35-C34	-2.03	118.86	123.23
27	Y	613	CLA	OBD-CAD-CBD	-2.03	122.88	125.94
27	y	614	CLA	O2A-CGA-O1A	-2.02	118.20	123.51
31	a	413	LMG	O6-C1-O1	-2.02	105.14	109.99
32	c	519	DGD	C8B-C7B-C6B	-2.02	104.03	114.54
32	h	102	DGD	C5B-C4B-C3B	-2.02	104.03	114.54
27	g	612	CLA	O2A-CGA-O1A	-2.02	118.21	123.51
32	C	519	DGD	C8B-C7B-C6B	-2.02	104.04	114.54
31	A	413	LMG	O6-C1-O1	-2.02	105.14	109.99
28	a	408	PHO	CHC-C1C-C2C	-2.02	120.83	125.52
32	c	519	DGD	O3E-C3E-C2E	-2.02	105.80	110.36
29	C	514	BCR	C27-C26-C25	-2.02	120.51	122.73
38	R	620	LUT	C15-C35-C34	-2.02	118.88	123.23
32	C	520	DGD	O3D-C3D-C4D	-2.02	105.81	110.36
28	A	408	PHO	CHC-C1C-C2C	-2.02	120.85	125.52
32	H	102	DGD	C5B-C4B-C3B	-2.02	104.08	114.54
27	C	505	CLA	C4B-CHC-C1C	-2.01	125.34	129.34
39	Y	1622	XAT	C10-C11-C12	-2.01	116.88	123.11
28	a	408	PHO	CMB-C2B-C1B	-2.01	121.85	125.06
28	A	408	PHO	CMB-C2B-C1B	-2.01	121.85	125.06
29	c	514	BCR	C11-C12-C13	-2.01	120.45	126.34
29	c	514	BCR	C27-C26-C25	-2.01	120.52	122.73
37	n	609	CHL	O1D-CGD-CBD	-2.01	120.18	124.59
37	N	609	CHL	O1D-CGD-CBD	-2.01	120.18	124.59
27	c	502	CLA	OBD-CAD-CBD	-2.01	122.91	125.94
29	c	515	BCR	C11-C12-C13	-2.01	120.46	126.34
32	C	520	DGD	C5B-C4B-C3B	-2.01	104.12	114.54
40	G	1623	NEX	C19-C9-C10	-2.00	119.97	122.89
27	C	513	CLA	O2A-CGA-O1A	-2.00	118.26	123.51
29	C	515	BCR	C11-C12-C13	-2.00	120.47	126.34
27	C	509	CLA	C11-C10-C8	-2.00	109.26	115.46
32	c	520	DGD	C5B-C4B-C3B	-2.00	104.14	114.54
31	B	622	LMG	O2-C2-C1	-2.00	105.57	110.01
27	G	612	CLA	O2A-CGA-O1A	-2.00	118.26	123.51
31	z	101	LMG	C1-O6-C5	-2.00	109.82	113.74
32	C	519	DGD	O3E-C3E-C2E	-2.00	105.85	110.36
37	y	606	CHL	C4A-C3A-C2A	-2.00	100.90	103.98
37	R	607	CHL	CBC-CAC-C3C	-2.00	110.24	113.16
37	s	606	CHL	CMD-C2D-C3D	2.00	119.70	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	s	603	CLA	CMD-C2D-C3D	2.00	129.00	125.09
38	S	1621	LUT	C40-C33-C32	2.00	121.35	118.08
27	y	613	CLA	O2D-CGD-CBD	2.00	114.11	111.22
40	r	623	NEX	C40-C33-C32	2.00	121.36	118.08
29	A	411	BCR	C37-C22-C23	2.00	121.36	118.08
37	S	606	CHL	CMD-C2D-C3D	2.00	119.71	114.17
30	a	418	SQD	O5-C5-C4	2.01	113.49	109.67
27	R	603	CLA	O2D-CGD-CBD	2.01	114.11	111.22
27	C	507	CLA	CMB-C2B-C3B	2.01	129.02	125.09
27	n	613	CLA	CMD-C2D-C3D	2.01	129.02	125.09
27	b	605	CLA	CBA-CAA-C2A	2.01	119.14	113.96
27	B	605	CLA	CBA-CAA-C2A	2.01	119.14	113.96
27	s	602	CLA	CMD-C2D-C3D	2.01	129.02	125.09
37	g	605	CHL	C4D-C3D-CAD	2.01	109.48	104.88
27	r	601	CLA	O2D-CGD-CBD	2.01	114.12	111.22
30	A	412	SQD	O5-C5-C4	2.01	113.51	109.67
27	R	601	CLA	O2D-CGD-CBD	2.02	114.12	111.22
29	C	515	BCR	C37-C22-C23	2.02	121.38	118.08
37	N	605	CHL	C4D-C3D-CAD	2.02	109.48	104.88
38	s	1621	LUT	C2-C1-C6	2.02	113.62	110.58
27	g	613	CLA	O1D-CGD-CBD	2.02	127.78	124.64
27	C	504	CLA	CMD-C2D-C3D	2.02	129.04	125.09
37	G	605	CHL	C4D-C3D-CAD	2.02	109.50	104.88
27	A	407	CLA	CMD-C2D-C3D	2.02	129.04	125.09
27	c	504	CLA	CMD-C2D-C3D	2.02	129.04	125.09
37	g	607	CHL	C4D-C3D-CAD	2.02	109.50	104.88
40	r	623	NEX	C2-C1-C6	2.02	111.24	109.31
37	g	607	CHL	CHC-C4B-C3B	2.03	123.16	118.13
27	y	614	CLA	O2D-CGD-CBD	2.03	114.14	111.22
30	a	412	SQD	O5-C5-C4	2.03	113.53	109.67
27	a	407	CLA	CMD-C2D-C3D	2.03	129.05	125.09
37	G	607	CHL	C4D-C3D-CAD	2.03	109.51	104.88
40	R	623	NEX	C2-C1-C6	2.03	111.25	109.31
40	y	1623	NEX	C28-C29-C30	2.03	122.22	118.95
27	S	602	CLA	CMD-C2D-C3D	2.03	129.06	125.09
27	B	612	CLA	O1D-CGD-CBD	2.03	127.79	124.64
27	S	604	CLA	O2D-CGD-CBD	2.03	114.14	111.22
37	g	606	CHL	C4D-C3D-CAD	2.03	109.52	104.88
27	b	616	CLA	O1D-CGD-CBD	2.03	127.80	124.64
27	b	613	CLA	C2A-C3A-C4A	2.03	103.92	101.84
38	S	1621	LUT	C2-C1-C6	2.04	113.65	110.58
27	N	613	CLA	CMD-C2D-C3D	2.04	129.07	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	606	CHL	C4D-C3D-CAD	2.04	109.53	104.88
29	c	514	BCR	C33-C5-C4	2.04	117.41	113.47
37	G	607	CHL	CHC-C4B-C3B	2.04	123.19	118.13
37	n	605	CHL	C4D-C3D-CAD	2.04	109.54	104.88
29	C	515	BCR	C2-C1-C6	2.04	113.52	110.48
38	N	1621	LUT	C19-C9-C8	2.04	121.42	118.08
38	y	1620	LUT	C39-C29-C28	2.04	121.42	118.08
38	N	1621	LUT	C39-C29-C28	2.04	121.42	118.08
38	n	1621	LUT	C39-C29-C28	2.04	121.42	118.08
29	C	516	BCR	C35-C13-C12	2.05	121.42	118.08
40	Y	1623	NEX	C28-C29-C30	2.05	122.25	118.95
27	C	508	CLA	CHC-C1C-NC	2.05	127.70	123.92
37	r	606	CHL	C4D-C3D-CAD	2.05	109.55	104.88
29	c	515	BCR	C37-C22-C23	2.05	121.43	118.08
27	n	603	CLA	CMD-C2D-C3D	2.05	129.09	125.09
29	C	514	BCR	C33-C5-C4	2.05	117.43	113.47
27	b	612	CLA	O1D-CGD-CBD	2.05	127.83	124.64
27	B	613	CLA	C2A-C3A-C4A	2.05	103.94	101.84
27	N	603	CLA	CMD-C2D-C3D	2.05	129.10	125.09
37	R	607	CHL	CHB-C1B-C2B	2.06	122.57	116.80
27	Y	614	CLA	O2D-CGD-CBD	2.06	114.18	111.22
37	r	607	CHL	CHB-C1B-C2B	2.06	122.57	116.80
27	A	405	CLA	CMD-C2D-C3D	2.06	129.11	125.09
37	y	605	CHL	CHB-C1B-C2B	2.06	122.58	116.80
29	c	516	BCR	C35-C13-C12	2.06	121.45	118.08
27	n	602	CLA	CMD-C2D-C3D	2.06	129.12	125.09
38	Y	1620	LUT	C19-C9-C8	2.06	121.45	118.08
27	c	508	CLA	CHC-C1C-NC	2.06	127.74	123.92
27	a	405	CLA	CMD-C2D-C3D	2.06	129.12	125.09
30	a	412	SQD	O5-C1-C2	2.06	114.57	110.28
38	Y	1620	LUT	C39-C29-C28	2.06	121.46	118.08
29	H	101	BCR	C29-C30-C25	2.07	113.55	110.48
37	R	606	CHL	C4D-C3D-CAD	2.07	109.60	104.88
27	G	613	CLA	O1D-CGD-CBD	2.07	127.85	124.64
37	Y	605	CHL	CHB-C1B-C2B	2.07	122.60	116.80
38	S	1620	LUT	C20-C13-C12	2.07	121.46	118.08
37	Y	607	CHL	C4D-C3D-CAD	2.07	109.60	104.88
27	n	612	CLA	CMD-C2D-C3D	2.07	129.13	125.09
27	B	603	CLA	O1D-CGD-CBD	2.07	127.85	124.64
37	y	607	CHL	C4D-C3D-CAD	2.07	109.61	104.88
29	b	620	BCR	C37-C22-C23	2.07	121.47	118.08
38	n	1621	LUT	C19-C9-C8	2.07	121.47	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	607	CHL	CHB-C1B-C2B	2.07	122.61	116.80
27	b	616	CLA	O2D-CGD-CBD	2.07	114.20	111.22
39	n	1622	XAT	C19-C9-C8	2.07	121.47	118.08
27	B	616	CLA	O2D-CGD-CBD	2.07	114.20	111.22
37	n	609	CHL	C4D-C3D-CAD	2.07	109.61	104.88
37	N	609	CHL	C4D-C3D-CAD	2.07	109.61	104.88
27	b	616	CLA	CMB-C2B-C3B	2.07	129.14	125.09
37	R	608	CHL	C4D-C3D-CAD	2.07	109.62	104.88
27	r	610	CLA	C2A-C3A-C4A	2.07	103.96	101.84
27	R	610	CLA	C2A-C3A-C4A	2.07	103.96	101.84
37	n	609	CHL	CHB-C1B-C2B	2.07	122.62	116.80
37	N	609	CHL	CHB-C1B-C2B	2.07	122.62	116.80
27	s	604	CLA	O2D-CGD-CBD	2.07	114.21	111.22
38	s	1620	LUT	C20-C13-C12	2.08	121.47	118.08
30	A	412	SQD	C1-O5-C5	2.08	117.82	113.74
29	h	101	BCR	C29-C30-C25	2.08	113.57	110.48
28	A	408	PHO	CBD-CHA-C1A	2.08	130.36	126.70
27	N	612	CLA	CMD-C2D-C3D	2.08	129.16	125.09
38	R	620	LUT	C19-C9-C8	2.08	121.48	118.08
38	r	620	LUT	C19-C9-C8	2.08	121.48	118.08
27	S	613	CLA	O1D-CGD-CBD	2.08	127.87	124.64
27	G	613	CLA	O2D-CGD-CBD	2.08	114.22	111.22
30	a	412	SQD	C1-O5-C5	2.09	117.83	113.74
27	y	610	CLA	O2D-CGD-CBD	2.09	114.23	111.22
37	G	609	CHL	CHC-C4B-C3B	2.09	123.31	118.13
37	r	608	CHL	C4D-C3D-CAD	2.09	109.64	104.88
39	g	1622	XAT	C19-C9-C8	2.09	121.49	118.08
27	n	611	CLA	O1D-CGD-CBD	2.09	127.89	124.64
37	n	607	CHL	CHB-C1B-C2B	2.09	122.66	116.80
27	a	407	CLA	O1D-CGD-CBD	2.09	127.89	124.64
27	N	602	CLA	CMD-C2D-C3D	2.09	129.18	125.09
27	b	615	CLA	CMB-C2B-C3B	2.09	129.18	125.09
29	c	515	BCR	C2-C1-C6	2.09	113.59	110.48
37	g	609	CHL	CHC-C4B-C3B	2.09	123.32	118.13
39	G	1622	XAT	C19-C9-C8	2.09	121.50	118.08
27	b	612	CLA	O2D-CGD-CBD	2.10	114.24	111.22
27	D	403	CLA	O1D-CGD-CBD	2.10	127.90	124.64
27	B	606	CLA	C4A-NA-C1A	2.10	109.04	106.38
27	b	603	CLA	O1D-CGD-CBD	2.10	127.90	124.64
27	Y	610	CLA	O2D-CGD-CBD	2.10	114.24	111.22
27	Y	604	CLA	O2D-CGD-CBD	2.10	114.24	111.22
38	y	1620	LUT	C19-C9-C8	2.10	121.51	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	g	614	CLA	CMD-C2D-C3D	2.10	129.20	125.09
29	B	620	BCR	C37-C22-C23	2.10	121.52	118.08
30	A	412	SQD	O5-C1-C2	2.10	114.65	110.28
27	A	407	CLA	O1D-CGD-CBD	2.10	127.91	124.64
27	s	613	CLA	O1D-CGD-CBD	2.10	127.91	124.64
27	d	403	CLA	O1D-CGD-CBD	2.11	127.91	124.64
38	s	1621	LUT	C39-C29-C28	2.11	121.53	118.08
27	B	616	CLA	CMB-C2B-C3B	2.11	129.21	125.09
27	B	615	CLA	CMB-C2B-C3B	2.11	129.21	125.09
37	g	609	CHL	CED-O2D-CGD	2.11	120.99	115.97
27	G	614	CLA	CMD-C2D-C3D	2.11	129.22	125.09
27	N	611	CLA	O1D-CGD-CBD	2.11	127.92	124.64
28	a	408	PHO	CBD-CHA-C1A	2.11	130.43	126.70
27	g	604	CLA	CMD-C2D-C3D	2.11	129.22	125.09
37	G	601	CHL	CHB-C1B-C2B	2.11	122.73	116.80
28	A	408	PHO	CMC-C2C-C3C	2.11	131.99	125.91
38	g	1621	LUT	C40-C33-C32	2.11	121.54	118.08
27	n	602	CLA	O1D-CGD-CBD	2.12	127.93	124.64
37	n	607	CHL	C4D-C3D-CAD	2.12	109.71	104.88
39	N	1622	XAT	C19-C9-C8	2.12	121.54	118.08
27	G	604	CLA	CMD-C2D-C3D	2.12	129.23	125.09
27	d	403	CLA	O2D-CGD-CBD	2.12	114.27	111.22
27	b	606	CLA	C4A-NA-C1A	2.12	109.07	106.38
27	B	616	CLA	CMD-C2D-C3D	2.12	129.24	125.09
37	y	601	CHL	CHB-C1B-C2B	2.12	122.76	116.80
38	S	1621	LUT	C39-C29-C28	2.12	121.55	118.08
29	B	618	BCR	C29-C30-C25	2.12	113.64	110.48
27	S	614	CLA	O2D-CGD-CBD	2.13	114.28	111.22
27	s	614	CLA	O2D-CGD-CBD	2.13	114.28	111.22
37	G	609	CHL	CED-O2D-CGD	2.13	121.02	115.97
38	G	1621	LUT	C40-C33-C32	2.13	121.56	118.08
39	R	622	XAT	C20-C13-C12	2.13	121.56	118.08
27	D	403	CLA	O2D-CGD-CBD	2.13	114.29	111.22
27	y	604	CLA	O2D-CGD-CBD	2.13	114.29	111.22
38	y	1621	LUT	C39-C29-C28	2.13	121.57	118.08
28	a	408	PHO	CMC-C2C-C3C	2.13	132.04	125.91
37	g	601	CHL	CHB-C1B-C2B	2.13	122.79	116.80
27	n	614	CLA	CMD-C2D-C3D	2.13	129.26	125.09
27	y	603	CLA	O1D-CGD-CBD	2.13	127.96	124.64
27	C	513	CLA	O1D-CGD-CBD	2.13	127.96	124.64
37	R	606	CHL	CHC-C4B-C3B	2.13	123.43	118.13
29	b	618	BCR	C29-C30-C25	2.13	113.65	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	B	621	SQD	C44-O6-C1	2.13	118.27	113.81
29	h	101	BCR	C38-C26-C27	2.14	117.60	113.47
37	Y	601	CHL	CHB-C1B-C2B	2.14	122.79	116.80
27	B	612	CLA	O2D-CGD-CBD	2.14	114.30	111.22
37	N	607	CHL	C4D-C3D-CAD	2.14	109.76	104.88
27	g	604	CLA	O1D-CGD-CBD	2.14	127.97	124.64
27	b	607	CLA	O1D-CGD-CBD	2.14	127.97	124.64
29	H	101	BCR	C38-C26-C27	2.14	117.61	113.47
27	N	602	CLA	O1D-CGD-CBD	2.14	127.97	124.64
30	b	621	SQD	C44-O6-C1	2.15	118.30	113.81
27	N	614	CLA	CMD-C2D-C3D	2.15	129.28	125.09
37	r	606	CHL	CHC-C4B-C3B	2.15	123.46	118.13
37	n	606	CHL	C4D-C3D-CAD	2.15	109.78	104.88
27	G	604	CLA	O1D-CGD-CBD	2.15	127.98	124.64
27	r	610	CLA	O1D-CGD-CBD	2.15	127.98	124.64
27	R	610	CLA	O1D-CGD-CBD	2.15	127.98	124.64
27	B	607	CLA	O1D-CGD-CBD	2.15	127.98	124.64
38	Y	1621	LUT	C2-C3-C4	2.15	113.61	110.29
38	y	1621	LUT	C2-C3-C4	2.15	113.61	110.29
27	g	610	CLA	O2D-CGD-CBD	2.15	114.32	111.22
27	b	616	CLA	CMD-C2D-C3D	2.15	129.30	125.09
27	c	513	CLA	O1D-CGD-CBD	2.16	127.99	124.64
27	S	610	CLA	CMD-C2D-C3D	2.16	129.31	125.09
38	S	1620	LUT	C39-C29-C28	2.16	121.61	118.08
39	r	622	XAT	C20-C13-C12	2.16	121.61	118.08
27	R	609	CLA	CMD-C2D-C3D	2.16	129.31	125.09
27	B	615	CLA	O2D-CGD-CBD	2.16	114.33	111.22
27	Y	603	CLA	O1D-CGD-CBD	2.16	127.99	124.64
27	B	603	CLA	C2A-C1A-CHA	2.16	127.28	123.80
37	N	606	CHL	C4D-C3D-CAD	2.16	109.81	104.88
27	n	610	CLA	CMD-C2D-C3D	2.16	129.31	125.09
27	r	609	CLA	CMD-C2D-C3D	2.16	129.31	125.09
27	r	604	CLA	CMD-C2D-C3D	2.16	129.31	125.09
27	G	610	CLA	O2D-CGD-CBD	2.16	114.33	111.22
27	g	613	CLA	O2D-CGD-CBD	2.16	114.34	111.22
27	N	610	CLA	CMD-C2D-C3D	2.16	129.32	125.09
38	s	1620	LUT	C39-C29-C28	2.16	121.62	118.08
27	B	615	CLA	CMD-C2D-C3D	2.17	129.32	125.09
39	y	1622	XAT	O4-C5-C18	2.17	117.54	114.99
39	Y	1622	XAT	O4-C5-C18	2.17	117.54	114.99
27	s	610	CLA	CMD-C2D-C3D	2.17	129.33	125.09
27	b	607	CLA	CMD-C2D-C3D	2.17	129.33	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	s	1621	LUT	C19-C9-C8	2.17	121.63	118.08
38	s	1621	LUT	C18-C5-C4	2.17	118.22	114.25
38	G	1620	LUT	C20-C13-C12	2.17	121.63	118.08
38	G	1620	LUT	C18-C5-C4	2.17	118.22	114.25
37	s	606	CHL	C4D-C3D-CAD	2.17	109.84	104.88
27	B	607	CLA	CMD-C2D-C3D	2.17	129.34	125.09
37	S	606	CHL	C4D-C3D-CAD	2.17	109.85	104.88
29	C	514	BCR	C37-C22-C23	2.18	121.64	118.08
27	b	615	CLA	CMD-C2D-C3D	2.18	129.35	125.09
37	N	608	CHL	CMD-C2D-C3D	2.18	120.20	114.17
37	n	608	CHL	CMD-C2D-C3D	2.18	120.20	114.17
38	Y	1621	LUT	C39-C29-C28	2.18	121.65	118.08
27	b	603	CLA	C2A-C1A-CHA	2.18	127.31	123.80
37	Y	606	CHL	C4D-C3D-CAD	2.18	109.87	104.88
38	S	1621	LUT	C19-C9-C8	2.18	121.65	118.08
27	N	604	CLA	CMD-C2D-C3D	2.18	129.36	125.09
37	g	601	CHL	C4D-C3D-CAD	2.19	109.88	104.88
27	n	604	CLA	CMD-C2D-C3D	2.19	129.37	125.09
27	b	614	CLA	C4A-NA-C1A	2.19	109.16	106.38
27	B	614	CLA	C4A-NA-C1A	2.19	109.16	106.38
27	c	508	CLA	O1D-CGD-CBD	2.19	128.05	124.64
38	g	1620	LUT	C18-C5-C4	2.19	118.26	114.25
37	g	608	CHL	CHB-C1B-C2B	2.20	122.96	116.80
27	b	615	CLA	O2D-CGD-CBD	2.20	114.39	111.22
27	C	508	CLA	O1D-CGD-CBD	2.20	128.05	124.64
27	C	503	CLA	O1D-CGD-CBD	2.20	128.06	124.64
37	g	608	CHL	C4D-C3D-CAD	2.20	109.90	104.88
38	g	1620	LUT	C20-C13-C12	2.20	121.68	118.08
27	R	604	CLA	CMD-C2D-C3D	2.20	129.39	125.09
37	G	608	CHL	CHB-C1B-C2B	2.20	122.98	116.80
37	G	608	CHL	C4D-C3D-CAD	2.20	109.91	104.88
37	G	601	CHL	C4D-C3D-CAD	2.20	109.91	104.88
37	y	606	CHL	C4D-C3D-CAD	2.20	109.91	104.88
37	Y	605	CHL	C4D-C3D-CAD	2.21	109.92	104.88
27	y	614	CLA	O1D-CGD-CBD	2.21	128.07	124.64
31	A	413	LMG	O6-C1-C2	2.21	114.87	110.28
38	S	1621	LUT	C18-C5-C4	2.21	118.28	114.25
38	n	1620	LUT	C39-C29-C28	2.21	121.69	118.08
29	c	514	BCR	C37-C22-C23	2.21	121.69	118.08
27	c	506	CLA	O1D-CGD-CBD	2.21	128.08	124.64
27	C	506	CLA	O1D-CGD-CBD	2.21	128.08	124.64
38	n	1620	LUT	C18-C5-C4	2.22	118.30	114.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	608	CHL	C4D-C3D-CAD	2.22	109.94	104.88
27	G	613	CLA	CMD-C2D-C3D	2.22	129.43	125.09
31	a	413	LMG	O6-C1-C2	2.22	114.89	110.28
37	G	601	CHL	CMD-C2D-C3D	2.22	120.31	114.17
27	S	604	CLA	CMD-C2D-C3D	2.22	129.43	125.09
27	c	501	CLA	CMD-C2D-C3D	2.22	129.43	125.09
27	A	410	CLA	CMD-C2D-C3D	2.22	129.43	125.09
27	a	410	CLA	CMD-C2D-C3D	2.22	129.43	125.09
27	c	509	CLA	CMD-C2D-C3D	2.22	129.44	125.09
29	C	514	BCR	C34-C9-C8	2.22	121.72	118.08
27	y	613	CLA	CMD-C2D-C3D	2.22	129.44	125.09
39	R	622	XAT	C19-C9-C8	2.23	121.72	118.08
27	b	615	CLA	O1D-CGD-CBD	2.23	128.10	124.64
27	C	510	CLA	CMD-C2D-C3D	2.23	129.44	125.09
37	y	605	CHL	C4D-C3D-CAD	2.23	109.97	104.88
38	N	1620	LUT	C39-C29-C28	2.23	121.72	118.08
27	c	503	CLA	O1D-CGD-CBD	2.23	128.10	124.64
27	B	604	CLA	C4A-NA-C1A	2.23	109.21	106.38
27	C	509	CLA	CMD-C2D-C3D	2.23	129.45	125.09
39	r	622	XAT	C19-C9-C8	2.23	121.73	118.08
27	c	510	CLA	O1D-CGD-CBD	2.23	128.11	124.64
27	g	602	CLA	C2A-C3A-C4A	2.23	104.12	101.84
27	Y	614	CLA	O1D-CGD-CBD	2.23	128.11	124.64
29	c	514	BCR	C34-C9-C8	2.23	121.73	118.08
27	g	613	CLA	CMD-C2D-C3D	2.23	129.46	125.09
38	N	1620	LUT	C18-C5-C4	2.24	118.33	114.25
37	G	608	CHL	CMD-C2D-C3D	2.24	120.35	114.17
27	s	604	CLA	CMD-C2D-C3D	2.24	129.47	125.09
27	C	501	CLA	CMD-C2D-C3D	2.24	129.47	125.09
37	N	608	CHL	C4D-C3D-CAD	2.24	110.00	104.88
37	g	601	CHL	CMD-C2D-C3D	2.24	120.37	114.17
27	b	604	CLA	C4A-NA-C1A	2.24	109.22	106.38
27	B	615	CLA	O1D-CGD-CBD	2.24	128.12	124.64
27	B	603	CLA	C4A-NA-C1A	2.24	109.22	106.38
36	f	101	HEM	CMC-C2C-C3C	2.24	129.48	125.09
36	F	101	HEM	CMC-C2C-C3C	2.24	129.48	125.09
27	G	602	CLA	C2A-C3A-C4A	2.25	104.14	101.84
27	b	603	CLA	C4A-NA-C1A	2.25	109.23	106.38
37	Y	609	CHL	CHB-C1B-C2B	2.25	123.11	116.80
27	n	603	CLA	O1D-CGD-CBD	2.25	128.13	124.64
27	C	510	CLA	O1D-CGD-CBD	2.25	128.13	124.64
27	y	604	CLA	CMD-C2D-C3D	2.25	129.48	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	601	CHL	CMD-C2D-C3D	2.25	120.39	114.17
27	S	611	CLA	CMD-C2D-C3D	2.25	129.49	125.09
27	s	611	CLA	CMD-C2D-C3D	2.25	129.49	125.09
27	c	510	CLA	CMD-C2D-C3D	2.25	129.49	125.09
27	b	603	CLA	O2D-CGD-CBD	2.25	114.46	111.22
37	y	609	CHL	CHB-C1B-C2B	2.25	123.12	116.80
37	g	608	CHL	CMD-C2D-C3D	2.25	120.40	114.17
37	n	605	CHL	CHB-C1B-C2B	2.25	123.12	116.80
37	N	605	CHL	CHB-C1B-C2B	2.25	123.12	116.80
37	n	601	CHL	CMD-C2D-C3D	2.25	120.40	114.17
37	y	608	CHL	C4D-C3D-CAD	2.25	110.03	104.88
27	Y	613	CLA	CMD-C2D-C3D	2.25	129.50	125.09
27	s	612	CLA	O1D-CGD-CBD	2.26	128.15	124.64
27	C	503	CLA	C4A-NA-C1A	2.26	109.24	106.38
27	S	612	CLA	O1D-CGD-CBD	2.26	128.15	124.64
27	y	602	CLA	CMD-C2D-C3D	2.26	129.51	125.09
27	s	604	CLA	O1D-CGD-CBD	2.26	128.16	124.64
37	s	606	CHL	CHB-C1B-C2B	2.27	123.16	116.80
27	N	603	CLA	O1D-CGD-CBD	2.27	128.16	124.64
27	n	611	CLA	CMD-C2D-C3D	2.27	129.53	125.09
39	r	622	XAT	C40-C33-C32	2.27	121.80	118.08
27	C	511	CLA	O2D-CGD-CBD	2.27	114.50	111.22
37	s	601	CHL	CHC-C4B-C3B	2.28	123.78	118.13
27	c	502	CLA	O1D-CGD-CBD	2.28	128.18	124.64
38	g	1620	LUT	C2-C1-C6	2.28	114.01	110.58
27	B	603	CLA	O2D-CGD-CBD	2.28	114.51	111.22
30	A	412	SQD	O48-C23-C24	2.28	118.87	111.85
37	S	608	CHL	CHB-C4A-C3A	2.28	123.29	117.08
27	c	511	CLA	O2D-CGD-CBD	2.28	114.51	111.22
37	r	607	CHL	CHC-C4B-C3B	2.28	123.80	118.13
30	a	412	SQD	O48-C23-C24	2.28	118.88	111.85
27	Y	604	CLA	CMD-C2D-C3D	2.28	129.56	125.09
37	s	608	CHL	CHB-C4A-C3A	2.28	123.30	117.08
37	S	606	CHL	CHB-C1B-C2B	2.28	123.21	116.80
37	R	607	CHL	CHC-C4B-C3B	2.29	123.80	118.13
37	Y	608	CHL	C4D-C3D-CAD	2.29	110.10	104.88
27	g	603	CLA	O1D-CGD-CBD	2.29	128.20	124.64
27	C	502	CLA	O1D-CGD-CBD	2.29	128.20	124.64
27	N	611	CLA	CMD-C2D-C3D	2.29	129.56	125.09
27	G	603	CLA	O1D-CGD-CBD	2.29	128.20	124.64
37	Y	607	CHL	CHC-C4B-C3B	2.29	123.82	118.13
37	y	608	CHL	CHC-C4B-C3B	2.29	123.82	118.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	R	622	XAT	C40-C33-C32	2.29	121.83	118.08
37	y	607	CHL	CHC-C4B-C3B	2.29	123.82	118.13
29	b	619	BCR	C33-C5-C4	2.30	117.91	113.47
27	c	502	CLA	CMD-C2D-C3D	2.30	129.58	125.09
27	g	612	CLA	CMD-C2D-C3D	2.30	129.58	125.09
29	B	619	BCR	C33-C5-C4	2.30	117.92	113.47
37	G	601	CHL	CHC-C4B-C3B	2.30	123.84	118.13
37	S	601	CHL	CHC-C4B-C3B	2.30	123.84	118.13
27	c	503	CLA	C4A-NA-C1A	2.30	109.30	106.38
38	G	1620	LUT	C2-C1-C6	2.30	114.05	110.58
27	G	612	CLA	CMD-C2D-C3D	2.30	129.59	125.09
35	G	2630	LHG	O8-C23-C24	2.31	118.95	111.85
27	C	502	CLA	CMD-C2D-C3D	2.31	129.61	125.09
27	C	507	CLA	O1D-CGD-CBD	2.32	128.24	124.64
37	g	601	CHL	CHC-C4B-C3B	2.32	123.88	118.13
27	D	403	CLA	CMD-C2D-C3D	2.32	129.62	125.09
27	S	604	CLA	O1D-CGD-CBD	2.32	128.24	124.64
27	c	505	CLA	CMD-C2D-C3D	2.32	129.62	125.09
37	Y	608	CHL	CHC-C4B-C3B	2.32	123.89	118.13
35	g	2630	LHG	O8-C23-C24	2.32	118.99	111.85
35	D	409	LHG	O8-C23-C24	2.32	119.00	111.85
27	C	505	CLA	CMD-C2D-C3D	2.32	129.63	125.09
27	d	403	CLA	CMD-C2D-C3D	2.32	129.63	125.09
27	Y	602	CLA	CMD-C2D-C3D	2.32	129.63	125.09
29	H	101	BCR	C35-C13-C12	2.33	121.89	118.08
27	B	606	CLA	CMB-C2B-C3B	2.33	129.64	125.09
29	h	101	BCR	C35-C13-C12	2.33	121.89	118.08
27	g	603	CLA	CMB-C2B-C3B	2.33	129.65	125.09
36	F	101	HEM	CMB-C2B-C3B	2.33	129.65	125.09
27	G	602	CLA	O1D-CGD-CBD	2.33	128.26	124.64
27	b	606	CLA	CMB-C2B-C3B	2.33	129.65	125.09
27	r	616	CLA	CMB-C2B-C3B	2.33	129.65	125.09
35	d	409	LHG	O8-C23-C24	2.33	119.03	111.85
27	y	612	CLA	C4A-NA-C1A	2.33	109.34	106.38
27	G	611	CLA	CMD-C2D-C3D	2.33	129.66	125.09
36	f	101	HEM	CMB-C2B-C3B	2.34	129.66	125.09
27	g	602	CLA	O1D-CGD-CBD	2.34	128.27	124.64
27	R	601	CLA	CMD-C2D-C3D	2.34	129.66	125.09
27	y	603	CLA	CMD-C2D-C3D	2.34	129.66	125.09
27	c	507	CLA	O1D-CGD-CBD	2.34	128.28	124.64
27	C	506	CLA	CMD-C2D-C3D	2.34	129.66	125.09
27	C	508	CLA	O2D-CGD-CBD	2.34	114.60	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	603	CLA	CMB-C2B-C3B	2.35	129.68	125.09
27	g	611	CLA	CMD-C2D-C3D	2.35	129.69	125.09
27	B	606	CLA	O1D-CGD-CBD	2.35	128.30	124.64
27	b	605	CLA	CMD-C2D-C3D	2.36	129.69	125.09
27	c	506	CLA	CMD-C2D-C3D	2.36	129.69	125.09
27	B	605	CLA	CMD-C2D-C3D	2.36	129.69	125.09
27	c	508	CLA	CMD-C2D-C3D	2.36	129.70	125.09
27	y	611	CLA	CMD-C2D-C3D	2.36	129.70	125.09
37	N	608	CHL	CHC-C4B-C3B	2.36	123.98	118.13
27	Y	603	CLA	CMD-C2D-C3D	2.36	129.70	125.09
27	N	604	CLA	O1D-CGD-CBD	2.36	128.31	124.64
27	b	606	CLA	O1D-CGD-CBD	2.36	128.31	124.64
27	R	616	CLA	CMB-C2B-C3B	2.36	129.71	125.09
27	C	508	CLA	CMD-C2D-C3D	2.36	129.71	125.09
27	Y	612	CLA	C4A-NA-C1A	2.36	109.38	106.38
27	r	601	CLA	CMD-C2D-C3D	2.37	129.72	125.09
27	r	613	CLA	O2D-CGD-CBD	2.37	114.64	111.22
27	C	503	CLA	CMD-C2D-C3D	2.38	129.74	125.09
38	G	1621	LUT	C19-C9-C8	2.38	121.97	118.08
27	c	508	CLA	O2D-CGD-CBD	2.38	114.65	111.22
27	G	613	CLA	C4A-NA-C1A	2.38	109.39	106.38
27	Y	611	CLA	CMD-C2D-C3D	2.38	129.74	125.09
27	c	503	CLA	CMD-C2D-C3D	2.38	129.74	125.09
27	g	613	CLA	C4A-NA-C1A	2.38	109.40	106.38
27	c	512	CLA	O1D-CGD-CBD	2.38	128.34	124.64
37	n	608	CHL	CHC-C4B-C3B	2.38	124.04	118.13
27	B	603	CLA	CMD-C2D-C3D	2.38	129.75	125.09
27	C	505	CLA	O1D-CGD-CBD	2.38	128.34	124.64
27	Y	613	CLA	CMB-C2B-C3B	2.38	129.75	125.09
27	c	509	CLA	O1D-CGD-CBD	2.39	128.35	124.64
27	S	603	CLA	C4A-NA-C1A	2.39	109.41	106.38
27	Y	603	CLA	C4A-NA-C1A	2.39	109.41	106.38
27	s	603	CLA	C4A-NA-C1A	2.39	109.41	106.38
27	n	604	CLA	O1D-CGD-CBD	2.39	128.36	124.64
29	c	515	BCR	C33-C5-C4	2.39	118.10	113.47
31	a	413	LMG	C1-O6-C5	2.39	118.44	113.74
31	A	413	LMG	C1-O6-C5	2.39	118.44	113.74
37	g	608	CHL	CHC-C4B-C3B	2.39	124.07	118.13
27	Y	603	CLA	CMB-C2B-C3B	2.39	129.77	125.09
27	D	402	CLA	CMB-C2B-C3B	2.40	129.77	125.09
29	C	515	BCR	C33-C5-C4	2.40	118.10	113.47
27	N	603	CLA	CMB-C2B-C3B	2.40	129.78	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	603	CLA	CMD-C2D-C3D	2.40	129.78	125.09
27	G	604	CLA	CMB-C2B-C3B	2.40	129.78	125.09
38	g	1621	LUT	C19-C9-C8	2.40	122.00	118.08
27	C	501	CLA	C4A-NA-C1A	2.40	109.42	106.38
27	c	501	CLA	C4A-NA-C1A	2.40	109.42	106.38
27	b	603	CLA	CMD-C2D-C3D	2.40	129.78	125.09
27	R	613	CLA	O2D-CGD-CBD	2.40	114.68	111.22
27	y	613	CLA	CMB-C2B-C3B	2.40	129.78	125.09
27	S	602	CLA	C2A-C3A-C4A	2.40	104.30	101.84
30	a	418	SQD	C1-C2-C3	2.40	114.74	109.98
27	Y	613	CLA	C4A-NA-C1A	2.40	109.42	106.38
27	c	505	CLA	O1D-CGD-CBD	2.40	128.37	124.64
27	C	509	CLA	O1D-CGD-CBD	2.40	128.37	124.64
27	y	603	CLA	CMB-C2B-C3B	2.40	129.79	125.09
29	B	619	BCR	C38-C26-C27	2.40	118.12	113.47
37	y	608	CHL	CMD-C2D-C3D	2.40	120.82	114.17
27	d	402	CLA	CMB-C2B-C3B	2.41	129.79	125.09
27	C	506	CLA	C4A-NA-C1A	2.41	109.43	106.38
37	G	608	CHL	CHC-C4B-C3B	2.41	124.11	118.13
27	n	603	CLA	CMB-C2B-C3B	2.41	129.80	125.09
27	r	603	CLA	CMD-C2D-C3D	2.41	129.80	125.09
27	C	512	CLA	O1D-CGD-CBD	2.41	128.38	124.64
28	a	408	PHO	C3D-C4D-CHA	2.41	113.00	107.14
27	B	604	CLA	CMD-C2D-C3D	2.41	129.80	125.09
28	A	408	PHO	C3D-C4D-CHA	2.41	113.00	107.14
28	a	409	PHO	C3D-C4D-CHA	2.41	113.01	107.14
30	A	418	SQD	C1-C2-C3	2.41	114.77	109.98
27	r	609	CLA	CMB-C2B-C3B	2.41	129.81	125.09
27	g	604	CLA	CMB-C2B-C3B	2.41	129.81	125.09
27	y	603	CLA	C4A-NA-C1A	2.42	109.44	106.38
37	g	609	CHL	CMD-C2D-C3D	2.42	120.85	114.17
27	g	603	CLA	CMD-C2D-C3D	2.42	129.82	125.09
27	G	603	CLA	CMD-C2D-C3D	2.42	129.82	125.09
27	b	604	CLA	CMD-C2D-C3D	2.42	129.82	125.09
37	Y	608	CHL	CMD-C2D-C3D	2.42	120.87	114.17
37	G	609	CHL	CMD-C2D-C3D	2.42	120.87	114.17
27	S	609	CLA	C4A-NA-C1A	2.42	109.45	106.38
27	R	609	CLA	CMB-C2B-C3B	2.42	129.83	125.09
27	R	612	CLA	CMB-C2B-C3B	2.42	129.83	125.09
37	Y	605	CHL	CMD-C2D-C3D	2.42	120.87	114.17
37	G	607	CHL	O2A-CGA-CBA	2.42	119.31	111.85
37	y	605	CHL	CMD-C2D-C3D	2.42	120.88	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	409	PHO	C3D-C4D-CHA	2.43	113.04	107.14
37	n	609	CHL	O2A-CGA-CBA	2.43	119.32	111.85
27	a	406	CLA	O2D-CGD-CBD	2.43	114.72	111.22
37	R	608	CHL	O2A-CGA-CBA	2.43	119.32	111.85
27	B	607	CLA	C4A-NA-C1A	2.43	109.46	106.38
29	b	619	BCR	C38-C26-C27	2.43	118.17	113.47
37	r	608	CHL	O2A-CGA-CBA	2.43	119.33	111.85
27	b	607	CLA	C4A-NA-C1A	2.43	109.46	106.38
27	s	609	CLA	C4A-NA-C1A	2.43	109.46	106.38
37	n	605	CHL	CHC-C4B-C3B	2.43	124.17	118.13
27	C	501	CLA	O2D-CGD-CBD	2.43	114.73	111.22
27	b	609	CLA	CMD-C2D-C3D	2.43	129.85	125.09
27	A	406	CLA	O2D-CGD-CBD	2.43	114.73	111.22
37	G	606	CHL	CMD-C2D-C3D	2.44	120.90	114.17
37	g	607	CHL	O2A-CGA-CBA	2.44	119.35	111.85
27	B	617	CLA	O2D-CGD-CBD	2.44	114.73	111.22
27	b	617	CLA	O2D-CGD-CBD	2.44	114.73	111.22
37	N	609	CHL	O2A-CGA-CBA	2.44	119.35	111.85
27	s	602	CLA	C2A-C3A-C4A	2.44	104.34	101.84
27	y	610	CLA	CMD-C2D-C3D	2.44	129.86	125.09
37	y	606	CHL	CHC-C4B-C3B	2.44	124.18	118.13
37	Y	606	CHL	CHC-C4B-C3B	2.44	124.19	118.13
37	g	609	CHL	CHB-C1B-C2B	2.44	123.65	116.80
37	g	606	CHL	CMD-C2D-C3D	2.44	120.92	114.17
27	y	613	CLA	C4A-NA-C1A	2.44	109.48	106.38
27	c	501	CLA	O2D-CGD-CBD	2.44	114.74	111.22
27	B	609	CLA	CMD-C2D-C3D	2.44	129.86	125.09
27	Y	610	CLA	CMD-C2D-C3D	2.44	129.87	125.09
29	c	516	BCR	C38-C26-C27	2.45	118.20	113.47
38	n	1620	LUT	C19-C9-C8	2.45	122.08	118.08
37	N	605	CHL	CHC-C4B-C3B	2.45	124.20	118.13
27	C	510	CLA	C4A-NA-C1A	2.45	109.48	106.38
37	S	607	CHL	CMD-C2D-C3D	2.45	120.94	114.17
27	S	612	CLA	CMD-C2D-C3D	2.45	129.88	125.09
37	N	605	CHL	CMD-C2D-C3D	2.45	120.95	114.17
29	C	517	BCR	C36-C18-C19	2.45	122.09	118.08
35	L	101	LHG	O8-C23-C24	2.45	119.40	111.85
27	r	616	CLA	C4A-NA-C1A	2.45	109.49	106.38
27	c	510	CLA	C4A-NA-C1A	2.45	109.49	106.38
27	c	506	CLA	C4A-NA-C1A	2.46	109.49	106.38
27	C	501	CLA	CMB-C2B-C3B	2.46	129.89	125.09
27	R	611	CLA	CMB-C2B-C3B	2.46	129.90	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	r	611	CLA	CMB-C2B-C3B	2.46	129.90	125.09
37	n	605	CHL	CMD-C2D-C3D	2.46	120.97	114.17
27	N	611	CLA	CMB-C2B-C3B	2.46	129.90	125.09
27	c	501	CLA	CMB-C2B-C3B	2.46	129.90	125.09
27	S	611	CLA	C4A-NA-C1A	2.46	109.50	106.38
37	G	609	CHL	CHB-C1B-C2B	2.46	123.71	116.80
27	B	608	CLA	C4A-NA-C1A	2.46	109.50	106.38
38	N	1620	LUT	C19-C9-C8	2.46	122.11	118.08
27	r	612	CLA	CMB-C2B-C3B	2.46	129.91	125.09
27	s	611	CLA	C4A-NA-C1A	2.47	109.51	106.38
27	d	402	CLA	O2D-CGD-CBD	2.47	114.78	111.22
27	b	608	CLA	C4A-NA-C1A	2.47	109.51	106.38
35	n	2630	LHG	O8-C23-C24	2.47	119.44	111.85
27	G	612	CLA	CMB-C2B-C3B	2.47	129.92	125.09
27	Y	602	CLA	CMB-C2B-C3B	2.47	129.92	125.09
35	l	101	LHG	O8-C23-C24	2.47	119.45	111.85
27	s	612	CLA	CMD-C2D-C3D	2.47	129.93	125.09
27	R	603	CLA	C4A-NA-C1A	2.47	109.52	106.38
37	s	607	CHL	CMD-C2D-C3D	2.47	121.01	114.17
29	c	517	BCR	C36-C18-C19	2.47	122.13	118.08
27	n	614	CLA	O2D-CGD-CBD	2.47	114.79	111.22
29	C	516	BCR	C38-C26-C27	2.47	118.26	113.47
27	R	601	CLA	C4A-NA-C1A	2.48	109.52	106.38
27	C	502	CLA	C4A-NA-C1A	2.48	109.52	106.38
37	n	609	CHL	CMD-C2D-C3D	2.48	121.02	114.17
37	N	609	CHL	CMD-C2D-C3D	2.48	121.02	114.17
27	b	613	CLA	O1D-CGD-CBD	2.48	128.49	124.64
27	r	601	CLA	CAC-C3C-C4C	2.48	128.48	124.82
27	b	605	CLA	CMB-C2B-C3B	2.48	129.94	125.09
27	B	605	CLA	CMB-C2B-C3B	2.48	129.94	125.09
27	N	614	CLA	O2D-CGD-CBD	2.48	114.80	111.22
27	b	614	CLA	CMD-C2D-C3D	2.48	129.94	125.09
27	B	614	CLA	CMD-C2D-C3D	2.48	129.94	125.09
27	S	613	CLA	C4A-NA-C1A	2.48	109.53	106.38
27	s	613	CLA	C4A-NA-C1A	2.48	109.53	106.38
27	S	603	CLA	O1D-CGD-CBD	2.48	128.50	124.64
27	s	603	CLA	O1D-CGD-CBD	2.49	128.50	124.64
35	N	2630	LHG	O8-C23-C24	2.49	119.50	111.85
27	b	616	CLA	C4A-NA-C1A	2.49	109.53	106.38
27	g	612	CLA	CMB-C2B-C3B	2.49	129.95	125.09
27	Y	602	CLA	O1D-CGD-CBD	2.49	128.51	124.64
37	S	601	CHL	CMD-C2D-C3D	2.49	121.05	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	606	CHL	CMD-C2D-C3D	2.49	121.06	114.17
27	r	601	CLA	C4A-NA-C1A	2.49	109.54	106.38
27	B	610	CLA	O1D-CGD-CBD	2.49	128.51	124.64
37	r	608	CHL	CHC-C4B-C3B	2.49	124.31	118.13
27	r	612	CLA	C4A-NA-C1A	2.49	109.54	106.38
27	b	605	CLA	C2A-C3A-C4A	2.49	104.39	101.84
27	B	605	CLA	C2A-C3A-C4A	2.49	104.39	101.84
27	b	610	CLA	C4A-NA-C1A	2.50	109.54	106.38
27	D	402	CLA	O2D-CGD-CBD	2.50	114.82	111.22
27	R	612	CLA	CMD-C2D-C3D	2.50	129.97	125.09
37	N	606	CHL	CMD-C2D-C3D	2.50	121.08	114.17
27	R	603	CLA	CMB-C2B-C3B	2.50	129.97	125.09
27	y	602	CLA	CMB-C2B-C3B	2.50	129.97	125.09
27	y	602	CLA	O1D-CGD-CBD	2.50	128.52	124.64
27	R	616	CLA	C4A-NA-C1A	2.50	109.55	106.38
37	g	605	CHL	CMD-C2D-C3D	2.50	121.08	114.17
27	g	604	CLA	C4A-NA-C1A	2.50	109.55	106.38
27	G	604	CLA	C4A-NA-C1A	2.50	109.55	106.38
27	c	502	CLA	C4A-NA-C1A	2.50	109.56	106.38
27	r	603	CLA	CMB-C2B-C3B	2.51	129.99	125.09
27	B	610	CLA	C4A-NA-C1A	2.51	109.56	106.38
27	n	611	CLA	CMB-C2B-C3B	2.51	129.99	125.09
37	y	606	CHL	CMD-C2D-C3D	2.51	121.11	114.17
37	G	605	CHL	CMD-C2D-C3D	2.51	121.11	114.17
37	s	601	CHL	CMD-C2D-C3D	2.51	121.11	114.17
37	R	606	CHL	O2A-CGA-CBA	2.51	119.58	111.85
27	B	602	CLA	CMB-C2B-C3B	2.51	130.00	125.09
27	b	602	CLA	CMB-C2B-C3B	2.51	130.00	125.09
27	G	611	CLA	O2D-CGD-CBD	2.51	114.84	111.22
27	S	612	CLA	C4A-NA-C1A	2.51	109.57	106.38
37	N	607	CHL	CHC-C4B-C3B	2.52	124.37	118.13
37	n	607	CHL	CHC-C4B-C3B	2.52	124.37	118.13
27	B	605	CLA	O1D-CGD-CBD	2.52	128.55	124.64
27	n	610	CLA	C4A-NA-C1A	2.52	109.57	106.38
37	Y	606	CHL	CMD-C2D-C3D	2.52	121.13	114.17
30	b	621	SQD	C1-O5-C5	2.52	118.68	113.74
27	c	507	CLA	C4A-NA-C1A	2.52	109.57	106.38
27	R	611	CLA	O1D-CGD-CBD	2.52	128.56	124.64
27	B	613	CLA	O1D-CGD-CBD	2.52	128.56	124.64
27	b	610	CLA	O1D-CGD-CBD	2.52	128.56	124.64
37	r	606	CHL	O2A-CGA-CBA	2.52	119.61	111.85
27	D	403	CLA	C4A-NA-C1A	2.52	109.58	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	403	CLA	C4A-NA-C1A	2.52	109.58	106.38
27	R	612	CLA	C4A-NA-C1A	2.52	109.58	106.38
27	B	608	CLA	O1D-CGD-CBD	2.52	128.56	124.64
37	R	608	CHL	CHC-C4B-C3B	2.52	124.39	118.13
38	Y	1620	LUT	C20-C13-C12	2.52	122.21	118.08
30	B	621	SQD	C1-O5-C5	2.52	118.70	113.74
27	B	616	CLA	C4A-NA-C1A	2.53	109.58	106.38
27	n	612	CLA	CMB-C2B-C3B	2.53	130.03	125.09
30	A	418	SQD	C4-C3-C2	2.53	115.44	110.79
27	s	612	CLA	C4A-NA-C1A	2.53	109.59	106.38
30	A	418	SQD	O48-C23-C24	2.53	119.64	111.85
29	b	618	BCR	C38-C26-C27	2.53	118.37	113.47
27	g	611	CLA	O2D-CGD-CBD	2.53	114.87	111.22
27	c	507	CLA	CMD-C2D-C3D	2.53	130.04	125.09
27	r	611	CLA	O1D-CGD-CBD	2.53	128.58	124.64
27	b	605	CLA	O1D-CGD-CBD	2.53	128.58	124.64
27	B	610	CLA	CMD-C2D-C3D	2.53	130.05	125.09
27	r	603	CLA	C4A-NA-C1A	2.54	109.59	106.38
27	N	612	CLA	CMB-C2B-C3B	2.54	130.05	125.09
27	g	602	CLA	C4A-NA-C1A	2.54	109.60	106.38
27	b	608	CLA	O1D-CGD-CBD	2.54	128.59	124.64
27	C	507	CLA	C4A-NA-C1A	2.54	109.60	106.38
29	B	618	BCR	C33-C5-C4	2.54	118.38	113.47
27	R	601	CLA	CAC-C3C-C4C	2.54	128.57	124.82
27	r	612	CLA	CMD-C2D-C3D	2.54	130.06	125.09
27	R	602	CLA	CMB-C2B-C3B	2.54	130.06	125.09
27	b	609	CLA	O2D-CGD-CBD	2.54	114.89	111.22
30	a	418	SQD	O48-C23-C24	2.54	119.68	111.85
38	y	1620	LUT	C20-C13-C12	2.54	122.24	118.08
27	c	512	CLA	CMD-C2D-C3D	2.54	130.06	125.09
28	a	409	PHO	CBD-CHA-C1A	2.55	131.19	126.70
37	N	607	CHL	C4-C3-C5	2.55	119.25	115.37
37	n	607	CHL	C4-C3-C5	2.55	119.25	115.37
27	G	602	CLA	C4A-NA-C1A	2.55	109.61	106.38
37	N	607	CHL	O2A-CGA-CBA	2.55	119.68	111.85
30	a	418	SQD	C4-C3-C2	2.55	115.47	110.79
27	B	609	CLA	O2D-CGD-CBD	2.55	114.89	111.22
37	R	608	CHL	CMD-C2D-C3D	2.55	121.22	114.17
37	n	607	CHL	O2A-CGA-CBA	2.55	119.70	111.85
27	s	614	CLA	C4A-NA-C1A	2.55	109.61	106.38
37	Y	605	CHL	O2A-CGA-CBA	2.55	119.71	111.85
27	b	610	CLA	CMD-C2D-C3D	2.56	130.09	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	S	614	CLA	C4A-NA-C1A	2.56	109.62	106.38
29	B	618	BCR	C38-C26-C27	2.56	118.42	113.47
38	n	1621	LUT	C2-C1-C6	2.56	114.43	110.58
27	b	607	CLA	O2D-CGD-CBD	2.56	114.91	111.22
38	r	620	LUT	C18-C5-C4	2.56	118.92	114.25
37	N	606	CHL	O2A-CGA-CBA	2.56	119.73	111.85
37	R	608	CHL	CHB-C1B-C2B	2.56	123.99	116.80
29	b	618	BCR	C33-C5-C4	2.56	118.42	113.47
38	R	620	LUT	C18-C5-C4	2.56	118.93	114.25
37	n	606	CHL	O2A-CGA-CBA	2.56	119.73	111.85
27	R	602	CLA	O1D-CGD-CBD	2.56	128.62	124.64
37	r	608	CHL	CHB-C1B-C2B	2.56	124.00	116.80
28	A	409	PHO	CBD-CHA-C1A	2.57	131.23	126.70
27	b	609	CLA	C4A-NA-C1A	2.57	109.64	106.38
27	r	602	CLA	CMB-C2B-C3B	2.57	130.11	125.09
27	b	612	CLA	C4A-NA-C1A	2.57	109.64	106.38
27	B	612	CLA	C4A-NA-C1A	2.57	109.64	106.38
27	N	610	CLA	C4A-NA-C1A	2.57	109.64	106.38
27	c	505	CLA	C4A-NA-C1A	2.57	109.64	106.38
37	r	608	CHL	CMD-C2D-C3D	2.57	121.27	114.17
27	R	611	CLA	C4A-NA-C1A	2.57	109.64	106.38
27	r	611	CLA	C4A-NA-C1A	2.57	109.64	106.38
39	n	1622	XAT	C40-C33-C32	2.57	122.28	118.08
27	b	615	CLA	C4A-NA-C1A	2.57	109.64	106.38
37	y	605	CHL	O2A-CGA-CBA	2.57	119.76	111.85
27	S	609	CLA	CMB-C2B-C3B	2.57	130.12	125.09
27	B	615	CLA	C4A-NA-C1A	2.57	109.64	106.38
27	B	602	CLA	C4A-NA-C1A	2.57	109.64	106.38
38	N	1621	LUT	C2-C1-C6	2.57	114.45	110.58
27	B	607	CLA	O2D-CGD-CBD	2.57	114.93	111.22
27	s	614	CLA	CMB-C2B-C3B	2.57	130.12	125.09
27	C	507	CLA	CMD-C2D-C3D	2.58	130.13	125.09
27	b	602	CLA	C4A-NA-C1A	2.58	109.65	106.38
27	B	611	CLA	CMD-C2D-C3D	2.58	130.13	125.09
30	A	418	SQD	O8-S-C6	2.58	110.35	104.99
30	a	418	SQD	O8-S-C6	2.58	110.35	104.99
27	C	512	CLA	CMD-C2D-C3D	2.58	130.13	125.09
27	s	609	CLA	CMB-C2B-C3B	2.58	130.13	125.09
30	B	621	SQD	O6-C1-C2	2.58	111.17	108.00
27	B	609	CLA	C4A-NA-C1A	2.58	109.65	106.38
38	R	620	LUT	C2-C1-C6	2.58	114.47	110.58
38	r	620	LUT	C2-C1-C6	2.59	114.48	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	611	CLA	CMD-C2D-C3D	2.59	130.16	125.09
27	C	505	CLA	C4A-NA-C1A	2.59	109.67	106.38
27	r	610	CLA	CMB-C2B-C3B	2.60	130.16	125.09
37	Y	601	CHL	CHC-C4B-C3B	2.60	124.57	118.13
37	y	601	CHL	CHC-C4B-C3B	2.60	124.57	118.13
37	Y	609	CHL	CMD-C2D-C3D	2.60	121.36	114.17
37	y	609	CHL	CMD-C2D-C3D	2.60	121.36	114.17
27	b	617	CLA	C4A-NA-C1A	2.60	109.68	106.38
37	Y	601	CHL	CMD-C2D-C3D	2.60	121.36	114.17
27	r	602	CLA	O1D-CGD-CBD	2.60	128.68	124.64
37	N	601	CHL	CHB-C1B-C2B	2.60	124.10	116.80
27	S	614	CLA	CMB-C2B-C3B	2.60	130.18	125.09
27	N	610	CLA	CMB-C2B-C3B	2.60	130.18	125.09
37	n	601	CHL	CHB-C1B-C2B	2.60	124.10	116.80
37	R	606	CHL	CMD-C2D-C3D	2.60	121.37	114.17
27	R	616	CLA	O2D-CGD-CBD	2.60	114.97	111.22
27	r	616	CLA	O2D-CGD-CBD	2.60	114.97	111.22
27	G	612	CLA	C4A-NA-C1A	2.60	109.68	106.38
27	Y	614	CLA	C4A-NA-C1A	2.61	109.68	106.38
27	G	611	CLA	CMB-C2B-C3B	2.61	130.18	125.09
39	N	1622	XAT	C40-C33-C32	2.61	122.34	118.08
37	r	606	CHL	CMD-C2D-C3D	2.61	121.38	114.17
27	Y	611	CLA	C4A-NA-C1A	2.61	109.69	106.38
27	a	407	CLA	C4A-NA-C1A	2.61	109.69	106.38
27	y	611	CLA	C4A-NA-C1A	2.61	109.69	106.38
37	S	601	CHL	O2A-CGA-CBA	2.61	119.89	111.85
27	s	610	CLA	C4A-NA-C1A	2.61	109.69	106.38
29	A	411	BCR	C33-C5-C4	2.62	118.53	113.47
27	C	503	CLA	CMB-C2B-C3B	2.62	130.21	125.09
37	s	601	CHL	O2A-CGA-CBA	2.62	119.91	111.85
27	b	611	CLA	CMB-C2B-C3B	2.62	130.21	125.09
27	n	610	CLA	CMB-C2B-C3B	2.62	130.21	125.09
27	s	602	CLA	O1D-CGD-CBD	2.62	128.71	124.64
27	g	611	CLA	CMB-C2B-C3B	2.62	130.21	125.09
27	R	610	CLA	CMB-C2B-C3B	2.62	130.21	125.09
27	G	613	CLA	CMB-C2B-C3B	2.62	130.21	125.09
27	S	602	CLA	O1D-CGD-CBD	2.62	128.71	124.64
27	B	617	CLA	C4A-NA-C1A	2.62	109.71	106.38
30	b	621	SQD	O6-C1-C2	2.62	111.23	108.00
27	S	610	CLA	C4A-NA-C1A	2.62	109.71	106.38
27	g	613	CLA	CMB-C2B-C3B	2.62	130.22	125.09
30	b	621	SQD	O48-C23-C24	2.63	119.93	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	611	CLA	CMB-C2B-C3B	2.63	130.23	125.09
37	N	606	CHL	CHC-C4B-C3B	2.63	124.66	118.13
27	c	503	CLA	CMB-C2B-C3B	2.63	130.23	125.09
27	G	603	CLA	C4A-NA-C1A	2.63	109.72	106.38
27	b	611	CLA	O1D-CGD-CBD	2.63	128.73	124.64
27	g	612	CLA	C4A-NA-C1A	2.63	109.72	106.38
29	a	411	BCR	C33-C5-C4	2.63	118.57	113.47
37	y	601	CHL	CMD-C2D-C3D	2.64	121.46	114.17
27	b	607	CLA	CMB-C2B-C3B	2.64	130.25	125.09
37	y	607	CHL	O2A-CGA-CBA	2.64	119.97	111.85
27	s	602	CLA	CMB-C2B-C3B	2.64	130.25	125.09
27	S	602	CLA	CMB-C2B-C3B	2.64	130.25	125.09
27	B	607	CLA	CMB-C2B-C3B	2.64	130.25	125.09
27	Y	614	CLA	CMB-C2B-C3B	2.64	130.25	125.09
37	n	606	CHL	CHC-C4B-C3B	2.64	124.69	118.13
27	B	611	CLA	C4A-NA-C1A	2.64	109.73	106.38
27	b	611	CLA	C4A-NA-C1A	2.64	109.73	106.38
38	Y	1621	LUT	C38-C25-C26	2.64	118.02	116.04
30	B	621	SQD	O48-C23-C24	2.64	119.99	111.85
37	g	606	CHL	O2A-CGA-CBA	2.64	119.99	111.85
38	y	1621	LUT	C38-C25-C26	2.64	118.02	116.04
27	g	603	CLA	C4A-NA-C1A	2.64	109.73	106.38
27	G	610	CLA	C4A-NA-C1A	2.65	109.74	106.38
27	G	602	CLA	CMD-C2D-C3D	2.65	130.27	125.09
27	A	407	CLA	C4A-NA-C1A	2.65	109.74	106.38
37	G	606	CHL	O2A-CGA-CBA	2.65	120.01	111.85
27	g	610	CLA	C4A-NA-C1A	2.65	109.75	106.38
27	G	614	CLA	CMB-C2B-C3B	2.66	130.29	125.09
27	N	613	CLA	C4A-NA-C1A	2.66	109.76	106.38
27	B	611	CLA	O1D-CGD-CBD	2.66	128.78	124.64
27	y	614	CLA	CMB-C2B-C3B	2.66	130.30	125.09
37	Y	607	CHL	O2A-CGA-CBA	2.67	120.05	111.85
27	y	610	CLA	C4A-NA-C1A	2.67	109.76	106.38
37	R	607	CHL	CMD-C2D-C3D	2.67	121.56	114.17
37	r	607	CHL	CMD-C2D-C3D	2.67	121.56	114.17
38	y	1621	LUT	C18-C5-C4	2.67	119.13	114.25
38	N	1620	LUT	C2-C1-C6	2.67	114.60	110.58
27	n	613	CLA	C4A-NA-C1A	2.67	109.77	106.38
37	g	605	CHL	CHB-C1B-C2B	2.67	124.30	116.80
27	y	612	CLA	CMD-C2D-C3D	2.67	130.32	125.09
39	G	1622	XAT	O4-C5-C18	2.68	118.14	114.99
35	r	2630	LHG	O8-C23-C24	2.68	120.09	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	G	605	CHL	CHB-C1B-C2B	2.68	124.32	116.80
27	y	614	CLA	C4A-NA-C1A	2.68	109.78	106.38
35	R	2630	LHG	O8-C23-C24	2.68	120.10	111.85
29	c	516	BCR	C33-C5-C4	2.68	118.66	113.47
27	g	614	CLA	CMB-C2B-C3B	2.68	130.34	125.09
38	G	1621	LUT	C18-C5-C4	2.68	119.15	114.25
38	g	1621	LUT	C18-C5-C4	2.68	119.15	114.25
37	g	606	CHL	CHC-C4B-C3B	2.68	124.79	118.13
27	Y	612	CLA	CMD-C2D-C3D	2.69	130.34	125.09
37	G	606	CHL	CHC-C4B-C3B	2.69	124.80	118.13
39	g	1622	XAT	O4-C5-C18	2.69	118.16	114.99
38	n	1620	LUT	C2-C1-C6	2.69	114.63	110.58
29	C	516	BCR	C33-C5-C4	2.69	118.67	113.47
37	S	608	CHL	CMD-C2D-C3D	2.69	121.61	114.17
38	Y	1621	LUT	C18-C5-C4	2.69	119.17	114.25
27	s	612	CLA	CMB-C2B-C3B	2.69	130.35	125.09
37	y	609	CHL	O2A-CGA-CBA	2.69	120.14	111.85
27	g	602	CLA	CMD-C2D-C3D	2.70	130.36	125.09
27	N	611	CLA	C4A-NA-C1A	2.70	109.80	106.38
27	Y	610	CLA	C4A-NA-C1A	2.70	109.80	106.38
37	s	608	CHL	CMD-C2D-C3D	2.70	121.63	114.17
27	R	613	CLA	CMB-C2B-C3B	2.70	130.37	125.09
27	Y	602	CLA	C4A-NA-C1A	2.70	109.81	106.38
27	n	602	CLA	C4A-NA-C1A	2.70	109.81	106.38
27	s	602	CLA	C4A-NA-C1A	2.70	109.81	106.38
27	S	604	CLA	CMB-C2B-C3B	2.71	130.38	125.09
27	n	612	CLA	C4A-NA-C1A	2.71	109.81	106.38
30	A	412	SQD	O8-S-C6	2.71	110.61	104.99
37	Y	609	CHL	O2A-CGA-CBA	2.71	120.18	111.85
37	Y	605	CHL	O2D-CGD-CBD	2.71	118.63	111.23
37	Y	601	CHL	O2A-CGA-CBA	2.71	120.19	111.85
37	y	601	CHL	O2A-CGA-CBA	2.71	120.19	111.85
27	n	611	CLA	C4A-NA-C1A	2.71	109.82	106.38
27	n	610	CLA	O2D-CGD-CBD	2.71	115.13	111.22
27	S	611	CLA	CMB-C2B-C3B	2.71	130.39	125.09
27	S	613	CLA	CMD-C2D-C3D	2.71	130.40	125.09
27	r	613	CLA	CMB-C2B-C3B	2.71	130.40	125.09
27	N	603	CLA	C4A-NA-C1A	2.71	109.82	106.38
27	n	614	CLA	C4A-NA-C1A	2.72	109.83	106.38
37	s	606	CHL	O2A-CGA-CBA	2.72	120.22	111.85
37	y	605	CHL	O2D-CGD-CBD	2.72	118.66	111.23
37	N	605	CHL	O2A-CGA-CBA	2.72	120.22	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	g	614	CLA	C4A-NA-C1A	2.72	109.83	106.38
27	C	509	CLA	C4A-NA-C1A	2.72	109.83	106.38
27	S	612	CLA	CMB-C2B-C3B	2.72	130.41	125.09
37	n	605	CHL	O2A-CGA-CBA	2.72	120.23	111.85
27	G	614	CLA	C4A-NA-C1A	2.72	109.83	106.38
27	R	604	CLA	C4A-NA-C1A	2.72	109.83	106.38
27	r	604	CLA	C4A-NA-C1A	2.72	109.83	106.38
27	a	406	CLA	C4A-NA-C1A	2.73	109.84	106.38
30	a	412	SQD	O8-S-C6	2.73	110.65	104.99
27	G	611	CLA	C4A-NA-C1A	2.73	109.84	106.38
37	n	607	CHL	CMD-C2D-C3D	2.73	121.71	114.17
27	s	611	CLA	CMB-C2B-C3B	2.73	130.42	125.09
27	R	602	CLA	C4A-NA-C1A	2.73	109.84	106.38
27	R	609	CLA	C4A-NA-C1A	2.73	109.84	106.38
27	c	509	CLA	C4A-NA-C1A	2.73	109.84	106.38
27	r	602	CLA	C4A-NA-C1A	2.73	109.84	106.38
37	S	606	CHL	O2A-CGA-CBA	2.73	120.26	111.85
37	Y	607	CHL	CMD-C2D-C3D	2.74	121.74	114.17
27	N	612	CLA	C4A-NA-C1A	2.74	109.85	106.38
37	N	607	CHL	CMD-C2D-C3D	2.74	121.74	114.17
27	s	604	CLA	CMB-C2B-C3B	2.74	130.44	125.09
27	N	614	CLA	C4A-NA-C1A	2.74	109.85	106.38
37	y	607	CHL	CMD-C2D-C3D	2.74	121.74	114.17
37	G	605	CHL	CHC-C4B-C3B	2.74	124.93	118.13
27	R	613	CLA	C4A-NA-C1A	2.74	109.86	106.38
27	A	405	CLA	C4A-NA-C1A	2.74	109.86	106.38
35	Y	2630	LHG	O8-C23-C24	2.74	120.29	111.85
38	s	1620	LUT	C2-C1-C6	2.74	114.71	110.58
35	y	2630	LHG	O8-C23-C24	2.74	120.30	111.85
27	N	610	CLA	O2D-CGD-CBD	2.75	115.18	111.22
27	C	513	CLA	C4A-NA-C1A	2.75	109.86	106.38
27	N	613	CLA	CMB-C2B-C3B	2.75	130.46	125.09
27	n	613	CLA	CMB-C2B-C3B	2.75	130.46	125.09
27	s	613	CLA	CMD-C2D-C3D	2.75	130.47	125.09
27	y	602	CLA	C4A-NA-C1A	2.75	109.87	106.38
27	S	602	CLA	C4A-NA-C1A	2.75	109.87	106.38
27	n	603	CLA	C4A-NA-C1A	2.75	109.87	106.38
37	g	605	CHL	CHC-C4B-C3B	2.75	124.96	118.13
27	N	602	CLA	C4A-NA-C1A	2.76	109.88	106.38
38	S	1620	LUT	C2-C1-C6	2.76	114.74	110.58
27	Y	611	CLA	CMB-C2B-C3B	2.76	130.49	125.09
27	y	611	CLA	CMB-C2B-C3B	2.76	130.49	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	n	601	CHL	O2A-CGA-CBA	2.76	120.35	111.85
27	C	512	CLA	C4A-NA-C1A	2.76	109.88	106.38
27	g	611	CLA	C4A-NA-C1A	2.77	109.89	106.38
27	c	504	CLA	C4A-NA-C1A	2.77	109.89	106.38
27	r	609	CLA	C4A-NA-C1A	2.77	109.89	106.38
27	N	604	CLA	C4A-NA-C1A	2.77	109.89	106.38
27	r	613	CLA	C4A-NA-C1A	2.77	109.89	106.38
38	n	1621	LUT	C18-C5-C4	2.77	119.32	114.25
27	c	512	CLA	C4A-NA-C1A	2.77	109.90	106.38
27	B	604	CLA	CMB-C2B-C3B	2.78	130.53	125.09
27	b	604	CLA	CMB-C2B-C3B	2.78	130.53	125.09
37	N	601	CHL	O2A-CGA-CBA	2.78	120.41	111.85
30	A	412	SQD	C44-O6-C1	2.78	119.63	113.81
27	c	513	CLA	C4A-NA-C1A	2.79	109.91	106.38
37	g	609	CHL	O2A-CGA-CBA	2.79	120.44	111.85
37	s	606	CHL	O2D-CGD-CBD	2.79	118.86	111.23
38	N	1621	LUT	C18-C5-C4	2.79	119.35	114.25
37	S	606	CHL	O2D-CGD-CBD	2.79	118.86	111.23
27	C	508	CLA	C4A-NA-C1A	2.79	109.92	106.38
27	N	604	CLA	CMB-C2B-C3B	2.80	130.56	125.09
27	a	405	CLA	C4A-NA-C1A	2.80	109.93	106.38
27	C	504	CLA	C4A-NA-C1A	2.80	109.93	106.38
27	y	604	CLA	C4A-NA-C1A	2.80	109.93	106.38
27	Y	604	CLA	C4A-NA-C1A	2.80	109.93	106.38
27	n	604	CLA	CMB-C2B-C3B	2.80	130.56	125.09
37	G	608	CHL	O2D-CGD-CBD	2.80	118.88	111.23
37	g	608	CHL	O2D-CGD-CBD	2.80	118.88	111.23
30	a	412	SQD	C44-O6-C1	2.80	119.67	113.81
37	G	609	CHL	O2A-CGA-CBA	2.80	120.47	111.85
27	n	604	CLA	C4A-NA-C1A	2.80	109.93	106.38
30	B	621	SQD	O5-C5-C4	2.81	115.02	109.67
30	b	621	SQD	O5-C5-C4	2.81	115.02	109.67
27	b	603	CLA	CMB-C2B-C3B	2.81	130.58	125.09
27	Y	612	CLA	CMB-C2B-C3B	2.81	130.59	125.09
27	y	612	CLA	CMB-C2B-C3B	2.81	130.59	125.09
27	N	614	CLA	CMB-C2B-C3B	2.81	130.59	125.09
27	n	614	CLA	CMB-C2B-C3B	2.81	130.59	125.09
27	b	613	CLA	C4A-NA-C1A	2.81	109.95	106.38
27	A	406	CLA	C4A-NA-C1A	2.81	109.95	106.38
27	B	613	CLA	C4A-NA-C1A	2.82	109.95	106.38
27	y	604	CLA	CMB-C2B-C3B	2.82	130.60	125.09
27	c	508	CLA	CMB-C2B-C3B	2.82	130.61	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	612	CLA	CMD-C2D-C3D	2.83	130.62	125.09
27	Y	604	CLA	CMB-C2B-C3B	2.83	130.62	125.09
29	c	517	BCR	C33-C5-C4	2.83	118.94	113.47
29	C	517	BCR	C33-C5-C4	2.83	118.94	113.47
27	B	603	CLA	CMB-C2B-C3B	2.83	130.62	125.09
27	c	511	CLA	C4A-NA-C1A	2.84	109.98	106.38
27	c	508	CLA	C4A-NA-C1A	2.84	109.98	106.38
37	G	607	CHL	CMD-C2D-C3D	2.84	122.03	114.17
37	g	607	CHL	CMD-C2D-C3D	2.84	122.03	114.17
27	r	604	CLA	CMB-C2B-C3B	2.84	130.65	125.09
37	N	608	CHL	O2A-CGA-CBA	2.85	120.61	111.85
27	c	504	CLA	CMB-C2B-C3B	2.85	130.65	125.09
27	B	612	CLA	CMD-C2D-C3D	2.85	130.65	125.09
37	G	608	CHL	O2A-CGA-CBA	2.85	120.61	111.85
27	C	508	CLA	CMB-C2B-C3B	2.85	130.66	125.09
37	g	605	CHL	O2A-CGA-CBA	2.85	120.62	111.85
37	G	605	CHL	O2A-CGA-CBA	2.85	120.62	111.85
37	g	608	CHL	O2A-CGA-CBA	2.85	120.62	111.85
35	D	410	LHG	O8-C23-C24	2.85	120.63	111.85
35	d	410	LHG	O8-C23-C24	2.85	120.63	111.85
27	B	610	CLA	CMB-C2B-C3B	2.85	130.67	125.09
27	r	610	CLA	C4A-NA-C1A	2.86	110.00	106.38
27	R	610	CLA	C4A-NA-C1A	2.86	110.00	106.38
37	N	601	CHL	CHC-C4B-C3B	2.86	125.22	118.13
37	y	608	CHL	O2D-CGD-CBD	2.86	119.03	111.23
37	Y	608	CHL	O2D-CGD-CBD	2.86	119.03	111.23
37	s	607	CHL	O2A-CGA-CBA	2.86	120.65	111.85
37	S	607	CHL	O2A-CGA-CBA	2.86	120.65	111.85
27	b	610	CLA	CMB-C2B-C3B	2.86	130.68	125.09
27	R	604	CLA	CMB-C2B-C3B	2.86	130.68	125.09
27	C	504	CLA	CMB-C2B-C3B	2.86	130.68	125.09
37	n	601	CHL	CHC-C4B-C3B	2.86	125.23	118.13
27	A	410	CLA	C4A-NA-C1A	2.86	110.01	106.38
37	n	608	CHL	O2A-CGA-CBA	2.86	120.66	111.85
37	G	601	CHL	O2A-CGA-CBA	2.86	120.66	111.85
38	G	1621	LUT	C38-C25-C26	2.86	118.18	116.04
35	d	408	LHG	O8-C23-C24	2.87	120.67	111.85
35	D	408	LHG	O8-C23-C24	2.87	120.69	111.85
27	c	513	CLA	CMD-C2D-C3D	2.87	130.71	125.09
27	d	402	CLA	CMD-C2D-C3D	2.88	130.71	125.09
37	g	601	CHL	O2A-CGA-CBA	2.88	120.71	111.85
27	a	410	CLA	C4A-NA-C1A	2.88	110.03	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	513	CLA	CMD-C2D-C3D	2.88	130.73	125.09
27	D	402	CLA	CMD-C2D-C3D	2.89	130.73	125.09
27	b	614	CLA	CMB-C2B-C3B	2.89	130.74	125.09
27	r	602	CLA	CMD-C2D-C3D	2.90	130.75	125.09
27	R	602	CLA	CMD-C2D-C3D	2.90	130.76	125.09
37	Y	608	CHL	O2A-CGA-CBA	2.90	120.78	111.85
27	C	511	CLA	C4A-NA-C1A	2.90	110.06	106.38
38	g	1621	LUT	C38-C25-C26	2.90	118.21	116.04
38	S	1620	LUT	C18-C5-C4	2.90	119.55	114.25
38	s	1620	LUT	C18-C5-C4	2.90	119.55	114.25
37	Y	606	CHL	O2A-CGA-CBA	2.91	120.79	111.85
37	y	608	CHL	O2A-CGA-CBA	2.91	120.80	111.85
37	y	606	CHL	O2A-CGA-CBA	2.91	120.81	111.85
27	s	604	CLA	C4A-NA-C1A	2.91	110.07	106.38
27	D	402	CLA	C4A-NA-C1A	2.91	110.08	106.38
27	B	614	CLA	CMB-C2B-C3B	2.92	130.80	125.09
29	D	404	BCR	C33-C5-C4	2.92	119.12	113.47
27	G	602	CLA	CMB-C2B-C3B	2.92	130.81	125.09
27	g	602	CLA	CMB-C2B-C3B	2.92	130.81	125.09
27	d	402	CLA	C4A-NA-C1A	2.93	110.10	106.38
38	g	1621	LUT	C2-C1-C6	2.94	115.00	110.58
27	N	611	CLA	O2D-CGD-CBD	2.94	115.46	111.22
27	S	604	CLA	C4A-NA-C1A	2.94	110.11	106.38
27	S	613	CLA	CMB-C2B-C3B	2.95	130.85	125.09
27	s	613	CLA	CMB-C2B-C3B	2.95	130.85	125.09
37	N	601	CHL	C2D-C3D-C4D	2.95	107.55	103.46
29	d	404	BCR	C33-C5-C4	2.95	119.18	113.47
27	A	410	CLA	O2D-CGD-CBD	2.95	115.48	111.22
30	a	418	SQD	C44-O6-C1	2.96	119.99	113.81
37	R	607	CHL	C2D-C3D-C4D	2.96	107.56	103.46
37	r	607	CHL	C2D-C3D-C4D	2.96	107.56	103.46
37	r	608	CHL	O2D-CGD-CBD	2.96	119.31	111.23
27	b	613	CLA	CMD-C2D-C3D	2.96	130.87	125.09
37	n	601	CHL	C2D-C3D-C4D	2.96	107.57	103.46
27	y	611	CLA	O2D-CGD-CBD	2.96	115.50	111.22
37	y	601	CHL	C4-C3-C5	2.96	119.89	115.37
27	Y	611	CLA	O2D-CGD-CBD	2.97	115.50	111.22
38	G	1621	LUT	C2-C1-C6	2.97	115.05	110.58
27	B	613	CLA	CMD-C2D-C3D	2.97	130.89	125.09
37	S	608	CHL	O2D-CGD-CBD	2.97	119.34	111.23
37	Y	601	CHL	C4-C3-C5	2.97	119.90	115.37
27	R	601	CLA	CMB-C2B-C3B	2.97	130.90	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	r	601	CLA	CMB-C2B-C3B	2.97	130.91	125.09
37	R	607	CHL	O2A-CGA-CBA	2.97	121.00	111.85
27	n	611	CLA	O2D-CGD-CBD	2.98	115.51	111.22
30	A	418	SQD	C44-O6-C1	2.98	120.03	113.81
40	G	1623	NEX	O24-C25-C38	2.98	118.50	114.99
37	s	608	CHL	O2A-CGA-CBA	2.98	121.03	111.85
37	R	608	CHL	O2D-CGD-CBD	2.98	119.39	111.23
37	s	608	CHL	O2D-CGD-CBD	2.99	119.39	111.23
37	g	609	CHL	O2D-CGD-CBD	2.99	119.40	111.23
37	G	609	CHL	O2D-CGD-CBD	2.99	119.40	111.23
37	S	601	CHL	C2D-C3D-C4D	2.99	107.61	103.46
27	a	410	CLA	O2D-CGD-CBD	2.99	115.53	111.22
37	s	606	CHL	CHC-C4B-C3B	2.99	125.56	118.13
37	r	607	CHL	O2A-CGA-CBA	2.99	121.06	111.85
37	S	608	CHL	O2A-CGA-CBA	2.99	121.06	111.85
35	s	2630	LHG	O8-C23-C24	3.00	121.08	111.85
35	S	2630	LHG	O8-C23-C24	3.00	121.09	111.85
27	b	612	CLA	CMB-C2B-C3B	3.02	130.99	125.09
37	S	606	CHL	CHC-C4B-C3B	3.02	125.62	118.13
27	B	612	CLA	CMB-C2B-C3B	3.02	131.00	125.09
27	s	603	CLA	CMB-C2B-C3B	3.02	131.00	125.09
27	a	410	CLA	CMB-C2B-C3B	3.03	131.02	125.09
37	s	601	CHL	C2D-C3D-C4D	3.04	107.67	103.46
37	s	607	CHL	CHC-C4B-C3B	3.04	125.67	118.13
37	S	607	CHL	CHC-C4B-C3B	3.04	125.67	118.13
27	c	512	CLA	CMB-C2B-C3B	3.04	131.03	125.09
27	C	512	CLA	CMB-C2B-C3B	3.05	131.04	125.09
40	g	1623	NEX	O24-C25-C38	3.05	118.58	114.99
27	S	603	CLA	CMB-C2B-C3B	3.05	131.05	125.09
27	g	610	CLA	CMB-C2B-C3B	3.05	131.06	125.09
27	B	609	CLA	CMB-C2B-C3B	3.05	131.06	125.09
27	A	410	CLA	CMB-C2B-C3B	3.05	131.06	125.09
27	b	605	CLA	C4A-NA-C1A	3.06	110.26	106.38
27	B	605	CLA	C4A-NA-C1A	3.06	110.26	106.38
37	R	606	CHL	O2D-CGD-CBD	3.06	119.59	111.23
37	G	606	CHL	C2D-C3D-C4D	3.06	107.71	103.46
37	r	606	CHL	O2D-CGD-CBD	3.07	119.62	111.23
31	a	413	LMG	O6-C5-C4	3.07	115.53	109.67
27	b	609	CLA	CMB-C2B-C3B	3.08	131.10	125.09
28	A	408	PHO	O1D-CGD-CBD	3.08	129.43	124.64
27	G	610	CLA	CMB-C2B-C3B	3.09	131.12	125.09
37	y	606	CHL	C2D-C3D-C4D	3.09	107.74	103.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	413	LMG	O6-C5-C4	3.09	115.56	109.67
28	a	408	PHO	O1D-CGD-CBD	3.09	129.45	124.64
27	r	604	CLA	O2D-CGD-CBD	3.09	115.68	111.22
37	g	606	CHL	C2D-C3D-C4D	3.09	107.75	103.46
27	B	617	CLA	CMB-C2B-C3B	3.10	131.15	125.09
27	b	617	CLA	CMB-C2B-C3B	3.10	131.15	125.09
37	y	607	CHL	C2D-C3D-C4D	3.11	107.78	103.46
37	g	601	CHL	C4-C3-C5	3.12	120.12	115.37
37	G	601	CHL	C2D-C3D-C4D	3.12	107.78	103.46
37	G	606	CHL	O2D-CGD-CBD	3.12	119.75	111.23
37	Y	607	CHL	C2D-C3D-C4D	3.12	107.79	103.46
37	g	606	CHL	O2D-CGD-CBD	3.12	119.76	111.23
27	R	604	CLA	O2D-CGD-CBD	3.12	115.72	111.22
37	G	607	CHL	C2D-C3D-C4D	3.13	107.80	103.46
37	g	607	CHL	C2D-C3D-C4D	3.13	107.81	103.46
37	Y	606	CHL	C2D-C3D-C4D	3.14	107.81	103.46
37	G	601	CHL	C4-C3-C5	3.14	120.16	115.37
27	c	502	CLA	CMB-C2B-C3B	3.14	131.24	125.09
37	r	606	CHL	C2D-C3D-C4D	3.15	107.83	103.46
37	y	609	CHL	C4-C3-C5	3.15	120.17	115.37
37	s	607	CHL	CHB-C1B-C2B	3.15	125.65	116.80
37	R	606	CHL	C2D-C3D-C4D	3.16	107.84	103.46
27	C	502	CLA	CMB-C2B-C3B	3.16	131.26	125.09
37	S	607	CHL	CHB-C1B-C2B	3.17	125.69	116.80
37	s	606	CHL	C2D-C3D-C4D	3.17	107.86	103.46
37	Y	609	CHL	C4-C3-C5	3.17	120.20	115.37
37	g	601	CHL	C2D-C3D-C4D	3.17	107.86	103.46
37	S	606	CHL	C2D-C3D-C4D	3.18	107.87	103.46
27	b	608	CLA	CMB-C2B-C3B	3.18	131.31	125.09
37	y	605	CHL	C2D-C3D-C4D	3.19	107.88	103.46
27	c	509	CLA	CMB-C2B-C3B	3.19	131.33	125.09
27	C	509	CLA	CMB-C2B-C3B	3.19	131.34	125.09
37	Y	605	CHL	C2D-C3D-C4D	3.21	107.91	103.46
37	n	609	CHL	C2D-C3D-C4D	3.21	107.92	103.46
37	N	609	CHL	C2D-C3D-C4D	3.21	107.92	103.46
37	g	605	CHL	C2D-C3D-C4D	3.21	107.92	103.46
37	n	609	CHL	O2D-CGD-CBD	3.21	120.01	111.23
37	N	609	CHL	O2D-CGD-CBD	3.21	120.01	111.23
27	a	406	CLA	CMB-C2B-C3B	3.22	131.39	125.09
37	n	608	CHL	O2D-CGD-CBD	3.23	120.06	111.23
27	B	608	CLA	CMB-C2B-C3B	3.23	131.41	125.09
27	c	511	CLA	CMB-C2B-C3B	3.24	131.42	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	608	CHL	O2D-CGD-CBD	3.24	120.08	111.23
37	N	605	CHL	C2D-C3D-C4D	3.24	107.96	103.46
27	A	405	CLA	CMB-C2B-C3B	3.24	131.43	125.09
37	S	607	CHL	C2D-C3D-C4D	3.24	107.96	103.46
27	a	405	CLA	CMB-C2B-C3B	3.24	131.43	125.09
27	y	610	CLA	CMB-C2B-C3B	3.24	131.43	125.09
27	c	510	CLA	CMB-C2B-C3B	3.25	131.44	125.09
27	A	406	CLA	CMB-C2B-C3B	3.25	131.44	125.09
27	C	510	CLA	CMB-C2B-C3B	3.25	131.44	125.09
37	y	609	CHL	O2D-CGD-CBD	3.25	120.11	111.23
37	S	608	CHL	C2D-C3D-C4D	3.26	107.98	103.46
27	C	506	CLA	CMB-C2B-C3B	3.26	131.46	125.09
37	S	608	CHL	CHB-C1B-C2B	3.26	125.95	116.80
37	n	605	CHL	C2D-C3D-C4D	3.26	107.98	103.46
27	C	511	CLA	CMB-C2B-C3B	3.26	131.47	125.09
27	B	613	CLA	CMB-C2B-C3B	3.26	131.47	125.09
37	s	608	CHL	CHB-C1B-C2B	3.26	125.96	116.80
37	G	605	CHL	C2D-C3D-C4D	3.27	108.00	103.46
37	s	607	CHL	C2D-C3D-C4D	3.27	108.00	103.46
27	A	407	CLA	CMB-C2B-C3B	3.27	131.48	125.09
37	Y	609	CHL	O2D-CGD-CBD	3.27	120.17	111.23
38	n	1621	LUT	C38-C25-C26	3.27	118.49	116.04
37	s	608	CHL	C2D-C3D-C4D	3.27	108.00	103.46
37	y	606	CHL	O2D-CGD-CBD	3.27	120.18	111.23
37	Y	606	CHL	O2D-CGD-CBD	3.27	120.18	111.23
37	N	607	CHL	C2D-C3D-C4D	3.27	108.00	103.46
27	Y	610	CLA	CMB-C2B-C3B	3.28	131.50	125.09
37	N	607	CHL	O2D-CGD-CBD	3.28	120.20	111.23
37	n	607	CHL	O2D-CGD-CBD	3.29	120.22	111.23
27	a	407	CLA	CMB-C2B-C3B	3.29	131.52	125.09
27	c	506	CLA	CMB-C2B-C3B	3.29	131.52	125.09
37	n	607	CHL	C2D-C3D-C4D	3.29	108.03	103.46
37	Y	601	CHL	C2D-C3D-C4D	3.29	108.03	103.46
37	g	607	CHL	O2D-CGD-CBD	3.30	120.25	111.23
37	S	608	CHL	CHC-C4B-C3B	3.30	126.32	118.13
37	s	608	CHL	CHC-C4B-C3B	3.31	126.34	118.13
37	G	607	CHL	O2D-CGD-CBD	3.31	120.27	111.23
28	A	409	PHO	O1D-CGD-CBD	3.31	129.79	124.64
27	b	613	CLA	CMB-C2B-C3B	3.32	131.57	125.09
38	N	1621	LUT	C38-C25-C26	3.32	118.52	116.04
39	g	1622	XAT	O24-C25-C38	3.32	118.91	114.99
37	s	607	CHL	O2D-CGD-CBD	3.33	120.32	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	N	606	CHL	C2D-C3D-C4D	3.33	108.08	103.46
37	y	601	CHL	C2D-C3D-C4D	3.33	108.09	103.46
37	S	607	CHL	O2D-CGD-CBD	3.33	120.34	111.23
39	G	1622	XAT	O24-C25-C38	3.34	118.92	114.99
37	n	606	CHL	C2D-C3D-C4D	3.34	108.09	103.46
30	b	621	SQD	O47-C7-C8	3.34	118.57	111.53
27	C	513	CLA	CMB-C2B-C3B	3.34	131.62	125.09
27	c	513	CLA	CMB-C2B-C3B	3.35	131.63	125.09
37	y	609	CHL	C2D-C3D-C4D	3.35	108.11	103.46
30	B	621	SQD	O47-C7-C8	3.36	118.61	111.53
37	Y	609	CHL	C2D-C3D-C4D	3.36	108.12	103.46
28	a	409	PHO	O1D-CGD-CBD	3.37	129.88	124.64
37	y	608	CHL	C2D-C3D-C4D	3.37	108.14	103.46
27	S	610	CLA	CMB-C2B-C3B	3.38	131.70	125.09
37	Y	608	CHL	C2D-C3D-C4D	3.39	108.16	103.46
39	n	1622	XAT	O4-C5-C18	3.40	119.00	114.99
37	s	601	CHL	O2D-CGD-CBD	3.41	120.54	111.23
37	g	605	CHL	O2D-CGD-CBD	3.42	120.56	111.23
37	S	601	CHL	O2D-CGD-CBD	3.42	120.58	111.23
27	s	610	CLA	CMB-C2B-C3B	3.42	131.78	125.09
37	G	605	CHL	O2D-CGD-CBD	3.43	120.59	111.23
37	G	601	CHL	O2D-CGD-CBD	3.44	120.62	111.23
37	g	601	CHL	O2D-CGD-CBD	3.44	120.63	111.23
37	N	605	CHL	O2D-CGD-CBD	3.45	120.67	111.23
39	N	1622	XAT	O4-C5-C18	3.46	119.06	114.99
37	n	605	CHL	O2D-CGD-CBD	3.46	120.69	111.23
37	n	601	CHL	O2D-CGD-CBD	3.47	120.70	111.23
37	N	601	CHL	O2D-CGD-CBD	3.48	120.74	111.23
27	D	403	CLA	CMB-C2B-C3B	3.50	131.92	125.09
27	d	403	CLA	CMB-C2B-C3B	3.53	132.00	125.09
37	g	609	CHL	C2D-C3D-C4D	3.53	108.36	103.46
37	y	607	CHL	O2D-CGD-CBD	3.56	120.95	111.23
37	G	609	CHL	C2D-C3D-C4D	3.57	108.41	103.46
37	Y	607	CHL	O2D-CGD-CBD	3.57	120.98	111.23
37	G	608	CHL	C2D-C3D-C4D	3.57	108.42	103.46
38	r	620	LUT	C38-C25-C26	3.59	118.72	116.04
29	b	620	BCR	C33-C5-C4	3.60	120.43	113.47
29	B	620	BCR	C33-C5-C4	3.60	120.43	113.47
38	R	620	LUT	C38-C25-C26	3.62	118.75	116.04
37	g	608	CHL	C2D-C3D-C4D	3.63	108.50	103.46
34	d	405	PL9	C40-C39-C41	3.66	120.94	115.37
30	A	412	SQD	O47-C7-C8	3.66	119.25	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	412	SQD	O47-C7-C8	3.66	119.25	111.53
37	N	608	CHL	C2D-C3D-C4D	3.68	108.57	103.46
37	n	606	CHL	O2D-CGD-CBD	3.69	121.32	111.23
37	n	608	CHL	C2D-C3D-C4D	3.70	108.60	103.46
34	D	405	PL9	C40-C39-C41	3.70	121.01	115.37
37	N	606	CHL	O2D-CGD-CBD	3.71	121.35	111.23
27	C	505	CLA	CMB-C2B-C3B	3.71	132.34	125.09
27	c	505	CLA	CMB-C2B-C3B	3.71	132.34	125.09
37	Y	601	CHL	O2D-CGD-CBD	3.74	121.44	111.23
37	y	601	CHL	O2D-CGD-CBD	3.76	121.52	111.23
37	r	607	CHL	O2D-CGD-CBD	3.82	121.66	111.23
37	R	607	CHL	O2D-CGD-CBD	3.82	121.68	111.23
30	a	418	SQD	O47-C7-C8	3.84	119.62	111.53
30	A	418	SQD	O47-C7-C8	3.85	119.65	111.53
37	R	608	CHL	C2D-C3D-C4D	3.88	108.85	103.46
35	n	2630	LHG	O4-P-O5	3.89	132.78	112.56
35	N	2630	LHG	O4-P-O5	3.89	132.78	112.56
37	g	607	CHL	CHD-C1D-C2D	3.89	127.72	116.80
37	G	607	CHL	CHD-C1D-C2D	3.90	127.74	116.80
37	y	608	CHL	CHD-C1D-C2D	3.90	127.76	116.80
37	Y	608	CHL	CHD-C1D-C2D	3.90	127.76	116.80
37	r	608	CHL	C2D-C3D-C4D	3.92	108.90	103.46
37	n	607	CHL	CHD-C1D-C2D	3.92	127.81	116.80
30	A	418	SQD	O9-S-C6	3.92	109.69	106.92
35	D	410	LHG	O4-P-O5	3.94	133.07	112.56
35	d	410	LHG	O4-P-O5	3.94	133.07	112.56
37	N	607	CHL	CHD-C1D-C2D	3.95	127.88	116.80
30	a	418	SQD	O9-S-C6	3.95	109.70	106.92
35	L	101	LHG	O4-P-O5	3.95	133.14	112.56
37	Y	607	CHL	CHD-C1D-C2D	3.96	127.91	116.80
37	y	607	CHL	CHD-C1D-C2D	3.96	127.91	116.80
35	l	101	LHG	O4-P-O5	3.96	133.18	112.56
35	d	409	LHG	O4-P-O5	3.97	133.23	112.56
35	D	409	LHG	O4-P-O5	3.98	133.25	112.56
35	r	2630	LHG	O4-P-O5	3.98	133.27	112.56
35	R	2630	LHG	O4-P-O5	3.98	133.28	112.56
35	G	2630	LHG	O4-P-O5	3.99	133.32	112.56
37	Y	606	CHL	CHD-C1D-C2D	3.99	128.00	116.80
35	Y	2630	LHG	O4-P-O5	4.00	133.35	112.56
35	y	2630	LHG	O4-P-O5	4.00	133.36	112.56
39	R	622	XAT	O24-C25-C38	4.00	119.70	114.99
35	g	2630	LHG	O4-P-O5	4.00	133.37	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	y	606	CHL	CHD-C1D-C2D	4.00	128.03	116.80
35	D	408	LHG	O4-P-O5	4.00	133.39	112.56
35	d	408	LHG	O4-P-O5	4.02	133.45	112.56
37	y	605	CHL	CHD-C1D-C2D	4.02	128.08	116.80
37	Y	605	CHL	CHD-C1D-C2D	4.02	128.08	116.80
39	r	622	XAT	O24-C25-C38	4.06	119.78	114.99
37	n	608	CHL	CHD-C1D-C2D	4.07	128.21	116.80
37	N	608	CHL	CHD-C1D-C2D	4.07	128.22	116.80
35	s	2630	LHG	O4-P-O5	4.07	133.76	112.56
35	S	2630	LHG	O4-P-O5	4.08	133.79	112.56
37	R	607	CHL	CHD-C1D-C2D	4.09	128.27	116.80
37	r	607	CHL	CHD-C1D-C2D	4.09	128.27	116.80
37	R	606	CHL	CHD-C1D-C2D	4.09	128.28	116.80
37	r	606	CHL	CHD-C1D-C2D	4.11	128.34	116.80
37	n	606	CHL	CHD-C1D-C2D	4.13	128.38	116.80
37	N	606	CHL	CHD-C1D-C2D	4.13	128.38	116.80
37	S	601	CHL	CHD-C1D-C2D	4.17	128.51	116.80
37	s	601	CHL	CHD-C1D-C2D	4.17	128.52	116.80
37	r	608	CHL	CHD-C1D-C2D	4.19	128.57	116.80
37	R	608	CHL	CHD-C1D-C2D	4.20	128.59	116.80
37	n	609	CHL	CHD-C1D-C2D	4.21	128.62	116.80
37	G	601	CHL	CHD-C1D-C2D	4.21	128.62	116.80
37	N	609	CHL	CHD-C1D-C2D	4.22	128.65	116.80
37	g	601	CHL	CHD-C1D-C2D	4.22	128.65	116.80
37	Y	609	CHL	CHD-C1D-C2D	4.22	128.66	116.80
37	y	609	CHL	CHD-C1D-C2D	4.24	128.70	116.80
37	g	608	CHL	CHD-C1D-C2D	4.29	128.84	116.80
37	G	608	CHL	CHD-C1D-C2D	4.29	128.85	116.80
37	Y	601	CHL	CHD-C1D-C2D	4.30	128.87	116.80
37	G	606	CHL	CHD-C1D-C2D	4.30	128.87	116.80
37	y	601	CHL	CHD-C1D-C2D	4.31	128.89	116.80
37	n	605	CHL	CHD-C1D-C2D	4.32	128.94	116.80
37	g	606	CHL	CHD-C1D-C2D	4.32	128.94	116.80
37	N	605	CHL	CHD-C1D-C2D	4.34	128.97	116.80
37	G	605	CHL	CHD-C1D-C2D	4.38	129.10	116.80
37	g	605	CHL	CHD-C1D-C2D	4.40	129.16	116.80
40	r	623	NEX	O24-C25-C38	4.45	120.23	114.99
40	R	623	NEX	O24-C25-C38	4.46	120.25	114.99
37	N	601	CHL	CHD-C1D-C2D	4.52	129.49	116.80
37	n	601	CHL	CHD-C1D-C2D	4.53	129.51	116.80
37	g	609	CHL	CHD-C1D-C2D	4.55	129.57	116.80
37	G	609	CHL	CHD-C1D-C2D	4.55	129.58	116.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	y	1622	XAT	O24-C25-C38	4.63	120.44	114.99
39	Y	1622	XAT	O24-C25-C38	4.63	120.44	114.99
40	N	1623	NEX	O24-C25-C38	4.63	120.44	114.99
37	S	607	CHL	CHD-C1D-C2D	4.65	129.86	116.80
37	s	607	CHL	CHD-C1D-C2D	4.66	129.88	116.80
40	n	1623	NEX	O24-C25-C38	4.67	120.49	114.99
37	S	608	CHL	CHD-C1D-C2D	4.69	129.96	116.80
37	s	608	CHL	CHD-C1D-C2D	4.70	129.98	116.80
37	S	606	CHL	CHD-C1D-C2D	4.70	130.00	116.80
37	s	606	CHL	CHD-C1D-C2D	4.71	130.01	116.80
39	r	622	XAT	O4-C5-C18	4.72	120.55	114.99
39	R	622	XAT	O4-C5-C18	4.72	120.55	114.99
38	y	1620	LUT	C38-C25-C26	4.75	119.59	116.04
40	Y	1623	NEX	O24-C25-C38	4.77	120.61	114.99
40	y	1623	NEX	O24-C25-C38	4.77	120.61	114.99
38	Y	1620	LUT	C38-C25-C26	4.80	119.63	116.04
40	S	1623	NEX	O24-C25-C38	4.94	120.80	114.99
39	n	1622	XAT	O24-C25-C38	4.96	120.83	114.99
38	s	1621	LUT	C38-C25-C26	4.96	119.75	116.04
39	N	1622	XAT	O24-C25-C38	4.97	120.84	114.99
38	S	1621	LUT	C38-C25-C26	4.97	119.76	116.04
40	s	1623	NEX	O24-C25-C38	4.97	120.84	114.99
38	G	1620	LUT	C38-C25-C26	5.18	119.92	116.04
38	g	1620	LUT	C38-C25-C26	5.21	119.94	116.04
38	s	1620	LUT	C38-C25-C26	5.72	120.32	116.04
38	S	1620	LUT	C38-C25-C26	5.73	120.33	116.04
38	n	1620	LUT	C38-C25-C26	6.01	120.53	116.04
30	A	412	SQD	O9-S-C6	6.07	111.19	106.92
30	a	412	SQD	O9-S-C6	6.08	111.20	106.92
38	N	1620	LUT	C38-C25-C26	6.12	120.62	116.04
30	A	412	SQD	O7-S-C6	6.21	111.30	106.92
30	a	412	SQD	O7-S-C6	6.22	111.30	106.92
37	s	607	CHL	C3D-C4D-ND	6.32	114.91	103.52
37	r	608	CHL	C3D-C4D-ND	6.33	114.93	103.52
37	R	608	CHL	C3D-C4D-ND	6.35	114.95	103.52
37	S	607	CHL	C3D-C4D-ND	6.35	114.96	103.52
37	G	608	CHL	C3D-C4D-ND	6.43	115.11	103.52
37	g	608	CHL	C3D-C4D-ND	6.44	115.12	103.52
37	s	608	CHL	C3D-C4D-ND	6.50	115.22	103.52
37	S	608	CHL	C3D-C4D-ND	6.51	115.25	103.52
37	n	607	CHL	C3D-C4D-ND	6.51	115.25	103.52
37	N	607	CHL	C3D-C4D-ND	6.51	115.25	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Y	607	CHL	C3D-C4D-ND	6.57	115.35	103.52
37	y	607	CHL	C3D-C4D-ND	6.57	115.36	103.52
37	G	605	CHL	C3D-C4D-ND	6.58	115.38	103.52
37	G	609	CHL	C3D-C4D-ND	6.59	115.39	103.52
37	g	609	CHL	C3D-C4D-ND	6.60	115.41	103.52
37	g	605	CHL	C3D-C4D-ND	6.61	115.43	103.52
37	S	606	CHL	C3D-C4D-ND	6.62	115.44	103.52
37	s	606	CHL	C3D-C4D-ND	6.62	115.44	103.52
37	n	608	CHL	C3D-C4D-ND	6.62	115.44	103.52
30	b	621	SQD	O7-S-C6	6.63	111.59	106.92
37	N	608	CHL	C3D-C4D-ND	6.63	115.47	103.52
30	B	621	SQD	O7-S-C6	6.64	111.60	106.92
37	y	608	CHL	C3D-C4D-ND	6.67	115.54	103.52
37	y	601	CHL	C3D-C4D-ND	6.67	115.54	103.52
37	Y	609	CHL	C3D-C4D-ND	6.68	115.55	103.52
37	Y	608	CHL	C3D-C4D-ND	6.68	115.56	103.52
37	y	609	CHL	C3D-C4D-ND	6.69	115.58	103.52
37	Y	601	CHL	C3D-C4D-ND	6.71	115.61	103.52
37	n	609	CHL	C3D-C4D-ND	6.77	115.71	103.52
37	N	609	CHL	C3D-C4D-ND	6.77	115.71	103.52
37	N	605	CHL	C3D-C4D-ND	6.78	115.73	103.52
37	r	606	CHL	C3D-C4D-ND	6.79	115.75	103.52
37	n	605	CHL	C3D-C4D-ND	6.79	115.75	103.52
37	g	607	CHL	C3D-C4D-ND	6.80	115.76	103.52
37	G	607	CHL	C3D-C4D-ND	6.81	115.78	103.52
37	R	606	CHL	C3D-C4D-ND	6.81	115.80	103.52
37	n	606	CHL	C3D-C4D-ND	6.82	115.80	103.52
37	N	606	CHL	C3D-C4D-ND	6.83	115.82	103.52
37	n	601	CHL	C3D-C4D-ND	6.83	115.83	103.52
37	N	601	CHL	C3D-C4D-ND	6.84	115.85	103.52
37	g	601	CHL	C3D-C4D-ND	6.85	115.86	103.52
37	Y	606	CHL	C3D-C4D-ND	6.85	115.86	103.52
37	Y	605	CHL	C3D-C4D-ND	6.86	115.87	103.52
37	R	607	CHL	C3D-C4D-ND	6.87	115.90	103.52
37	r	607	CHL	C3D-C4D-ND	6.87	115.90	103.52
37	G	601	CHL	C3D-C4D-ND	6.88	115.91	103.52
37	y	606	CHL	C3D-C4D-ND	6.88	115.92	103.52
37	y	605	CHL	C3D-C4D-ND	6.90	115.94	103.52
37	s	601	CHL	C3D-C4D-ND	6.90	115.95	103.52
37	g	606	CHL	C3D-C4D-ND	6.90	115.96	103.52
37	S	601	CHL	C3D-C4D-ND	6.93	116.00	103.52
37	G	606	CHL	C3D-C4D-ND	6.95	116.04	103.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	418	SQD	O7-S-C6	7.05	111.89	106.92
30	a	418	SQD	O7-S-C6	7.08	111.91	106.92
30	b	621	SQD	O9-S-C6	8.81	113.12	106.92
30	B	621	SQD	O9-S-C6	8.85	113.16	106.92

All (466) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	y	603	CLA	NC
27	y	603	CLA	ND
27	y	603	CLA	NA
27	N	611	CLA	NC
27	N	611	CLA	ND
27	N	611	CLA	NA
27	r	610	CLA	NC
27	r	610	CLA	ND
27	r	610	CLA	NA
27	N	614	CLA	NC
27	N	614	CLA	ND
27	N	614	CLA	NA
27	s	603	CLA	NC
27	s	603	CLA	NA
27	c	503	CLA	NC
27	c	503	CLA	ND
27	c	503	CLA	NA
27	S	614	CLA	NC
27	S	614	CLA	ND
27	S	614	CLA	NA
27	A	410	CLA	NC
27	A	410	CLA	ND
27	A	410	CLA	NA
27	A	407	CLA	NC
27	A	407	CLA	ND
27	A	407	CLA	NA
27	b	605	CLA	NC
27	b	605	CLA	ND
27	b	605	CLA	NA
27	r	609	CLA	NC
27	r	609	CLA	NA
27	r	609	CLA	ND
27	C	511	CLA	NC
27	C	511	CLA	ND

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Mol	Chain	Res	Type	Atom
27	C	511	CLA	NA
27	g	611	CLA	NC
27	g	611	CLA	ND
27	g	611	CLA	NA
27	D	402	CLA	NC
27	D	402	CLA	ND
27	D	402	CLA	NA
27	B	617	CLA	NC
27	B	617	CLA	ND
27	B	617	CLA	NA
27	b	613	CLA	NC
27	b	613	CLA	ND
27	b	613	CLA	NA
27	C	501	CLA	NC
27	C	501	CLA	NA
27	C	501	CLA	ND
27	B	615	CLA	NC
27	B	615	CLA	ND
27	B	615	CLA	NA
27	N	612	CLA	NC
27	N	612	CLA	ND
27	N	612	CLA	NA
27	g	603	CLA	NC
27	g	603	CLA	ND
27	g	603	CLA	NA
27	S	609	CLA	NC
27	S	609	CLA	ND
27	S	609	CLA	NA
27	G	610	CLA	NC
27	G	610	CLA	ND
27	G	610	CLA	NA
27	b	606	CLA	NC
27	b	606	CLA	ND
27	b	606	CLA	NA
27	B	613	CLA	NC
27	B	613	CLA	ND
27	B	613	CLA	NA
27	Y	613	CLA	NC
27	Y	613	CLA	ND
27	Y	613	CLA	NA
27	c	512	CLA	NC
27	c	512	CLA	ND

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Mol	Chain	Res	Type	Atom
27	c	512	CLA	NA
27	G	602	CLA	NC
27	G	602	CLA	ND
27	G	602	CLA	NA
27	B	602	CLA	NC
27	B	602	CLA	ND
27	B	602	CLA	NA
27	Y	602	CLA	NC
27	Y	602	CLA	ND
27	Y	602	CLA	NA
27	A	405	CLA	NC
27	A	405	CLA	ND
27	A	405	CLA	NA
27	S	613	CLA	NC
27	S	613	CLA	ND
27	S	613	CLA	NA
27	b	612	CLA	NC
27	b	612	CLA	ND
27	b	612	CLA	NA
27	C	505	CLA	NC
27	C	505	CLA	ND
27	C	505	CLA	NA
27	G	613	CLA	NC
27	G	613	CLA	ND
27	G	613	CLA	NA
27	B	611	CLA	NC
27	B	611	CLA	ND
27	B	611	CLA	NA
27	n	603	CLA	NC
27	n	603	CLA	ND
27	n	603	CLA	NA
27	R	616	CLA	NC
27	R	616	CLA	ND
27	R	616	CLA	NA
27	R	604	CLA	NC
27	R	604	CLA	ND
27	R	604	CLA	NA
27	S	604	CLA	NC
27	S	604	CLA	ND
27	S	604	CLA	NA
27	a	405	CLA	NC
27	a	405	CLA	ND

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Mol	Chain	Res	Type	Atom
27	a	405	CLA	NA
27	B	616	CLA	NC
27	B	616	CLA	ND
27	B	616	CLA	NA
27	c	504	CLA	NC
27	c	504	CLA	ND
27	c	504	CLA	NA
27	B	612	CLA	NC
27	B	612	CLA	ND
27	B	612	CLA	NA
27	n	612	CLA	NC
27	n	612	CLA	ND
27	n	612	CLA	NA
27	N	602	CLA	NC
27	N	602	CLA	ND
27	N	602	CLA	NA
27	s	609	CLA	NC
27	s	609	CLA	ND
27	s	609	CLA	NA
27	r	601	CLA	NC
27	r	601	CLA	ND
27	r	601	CLA	NA
27	g	610	CLA	NC
27	g	610	CLA	ND
27	g	610	CLA	NA
27	s	612	CLA	NC
27	s	612	CLA	ND
27	s	612	CLA	NA
27	Y	611	CLA	NC
27	Y	611	CLA	ND
27	Y	611	CLA	NA
27	S	603	CLA	NC
27	S	603	CLA	NA
27	s	602	CLA	NC
27	s	602	CLA	ND
27	s	602	CLA	NA
27	y	613	CLA	NC
27	y	613	CLA	ND
27	y	613	CLA	NA
27	R	611	CLA	NC
27	R	611	CLA	ND
27	R	611	CLA	NA

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Mol	Chain	Res	Type	Atom
27	b	604	CLA	NC
27	b	604	CLA	NA
27	b	604	CLA	ND
27	Y	614	CLA	NC
27	Y	614	CLA	ND
27	Y	614	CLA	NA
27	C	512	CLA	NC
27	C	512	CLA	ND
27	C	512	CLA	NA
27	b	614	CLA	NC
27	b	614	CLA	ND
27	b	614	CLA	NA
27	a	407	CLA	NC
27	a	407	CLA	ND
27	a	407	CLA	NA
27	R	609	CLA	NC
27	R	609	CLA	NA
27	R	609	CLA	ND
27	b	603	CLA	NC
27	b	603	CLA	ND
27	b	603	CLA	NA
27	G	614	CLA	NC
27	G	614	CLA	ND
27	G	614	CLA	NA
27	c	509	CLA	NC
27	c	509	CLA	ND
27	c	509	CLA	NA
27	Y	612	CLA	NC
27	Y	612	CLA	ND
27	Y	612	CLA	NA
27	B	609	CLA	NC
27	B	609	CLA	ND
27	B	609	CLA	NA
27	R	603	CLA	NC
27	R	603	CLA	ND
27	R	603	CLA	NA
27	c	513	CLA	NC
27	c	513	CLA	ND
27	c	513	CLA	NA
27	S	611	CLA	NC
27	S	611	CLA	ND
27	S	611	CLA	NA

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Mol	Chain	Res	Type	Atom
27	g	613	CLA	NC
27	g	613	CLA	ND
27	g	613	CLA	NA
27	Y	610	CLA	NC
27	Y	610	CLA	NA
27	Y	610	CLA	ND
27	B	614	CLA	NC
27	B	614	CLA	ND
27	B	614	CLA	NA
27	b	611	CLA	NC
27	b	611	CLA	ND
27	b	611	CLA	NA
27	r	616	CLA	NC
27	r	616	CLA	ND
27	r	616	CLA	NA
27	B	603	CLA	NC
27	B	603	CLA	ND
27	B	603	CLA	NA
27	B	606	CLA	NC
27	B	606	CLA	ND
27	B	606	CLA	NA
27	n	614	CLA	NC
27	n	614	CLA	ND
27	n	614	CLA	NA
27	C	503	CLA	NC
27	C	503	CLA	ND
27	C	503	CLA	NA
27	R	610	CLA	NC
27	R	610	CLA	ND
27	R	610	CLA	NA
27	r	611	CLA	NC
27	r	611	CLA	ND
27	r	611	CLA	NA
27	r	612	CLA	NC
27	r	612	CLA	ND
27	r	612	CLA	NA
27	R	613	CLA	NC
27	R	613	CLA	ND
27	R	613	CLA	NA
27	c	506	CLA	NC
27	c	506	CLA	ND
27	c	506	CLA	NA

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Mol	Chain	Res	Type	Atom
27	N	610	CLA	NC
27	N	610	CLA	NA
27	N	610	CLA	ND
27	C	508	CLA	NC
27	C	508	CLA	ND
27	C	508	CLA	NA
27	C	507	CLA	NC
27	C	507	CLA	ND
27	C	507	CLA	NA
27	g	612	CLA	NC
27	g	612	CLA	ND
27	g	612	CLA	NA
27	y	614	CLA	NC
27	y	614	CLA	ND
27	y	614	CLA	NA
27	c	505	CLA	NC
27	c	505	CLA	ND
27	c	505	CLA	NA
27	b	615	CLA	NC
27	b	615	CLA	ND
27	b	615	CLA	NA
27	Y	603	CLA	NC
27	Y	603	CLA	ND
27	Y	603	CLA	NA
27	A	406	CLA	NC
27	A	406	CLA	ND
27	A	406	CLA	NA
27	g	614	CLA	NC
27	g	614	CLA	ND
27	g	614	CLA	NA
27	n	604	CLA	NC
27	n	604	CLA	ND
27	n	604	CLA	NA
27	D	403	CLA	NC
27	D	403	CLA	ND
27	D	403	CLA	NA
27	y	612	CLA	NC
27	y	612	CLA	ND
27	y	612	CLA	NA
27	y	604	CLA	NC
27	y	604	CLA	ND
27	y	604	CLA	NA

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Mol	Chain	Res	Type	Atom
27	C	513	CLA	NC
27	C	513	CLA	ND
27	C	513	CLA	NA
27	s	611	CLA	NC
27	s	611	CLA	ND
27	s	611	CLA	NA
27	a	410	CLA	NC
27	a	410	CLA	ND
27	a	410	CLA	NA
27	B	605	CLA	NC
27	B	605	CLA	ND
27	B	605	CLA	NA
27	c	502	CLA	NC
27	c	502	CLA	ND
27	c	502	CLA	NA
27	g	602	CLA	NC
27	g	602	CLA	ND
27	g	602	CLA	NA
27	c	511	CLA	NC
27	c	511	CLA	ND
27	c	511	CLA	NA
27	G	611	CLA	NC
27	G	611	CLA	ND
27	G	611	CLA	NA
27	N	604	CLA	NC
27	N	604	CLA	ND
27	N	604	CLA	NA
27	d	403	CLA	NC
27	d	403	CLA	ND
27	d	403	CLA	NA
27	C	510	CLA	NC
27	C	510	CLA	ND
27	C	510	CLA	NA
27	g	604	CLA	NC
27	g	604	CLA	ND
27	g	604	CLA	NA
27	B	604	CLA	NC
27	B	604	CLA	NA
27	B	604	CLA	ND
27	c	501	CLA	NC
27	c	501	CLA	NA
27	c	501	CLA	ND

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Mol	Chain	Res	Type	Atom
27	S	610	CLA	NC
27	S	610	CLA	NA
27	S	610	CLA	ND
27	G	603	CLA	NC
27	G	603	CLA	ND
27	G	603	CLA	NA
27	n	611	CLA	NC
27	n	611	CLA	ND
27	n	611	CLA	NA
27	r	604	CLA	NC
27	r	604	CLA	ND
27	r	604	CLA	NA
27	s	604	CLA	NC
27	s	604	CLA	ND
27	s	604	CLA	NA
27	B	608	CLA	NC
27	B	608	CLA	ND
27	B	608	CLA	NA
27	N	613	CLA	NC
27	N	613	CLA	ND
27	N	613	CLA	NA
27	b	616	CLA	NC
27	b	616	CLA	ND
27	b	616	CLA	NA
27	n	602	CLA	NC
27	n	602	CLA	ND
27	n	602	CLA	NA
27	B	610	CLA	NC
27	B	610	CLA	ND
27	B	610	CLA	NA
27	b	617	CLA	NC
27	b	617	CLA	ND
27	b	617	CLA	NA
27	R	601	CLA	NC
27	R	601	CLA	ND
27	R	601	CLA	NA
27	y	611	CLA	NC
27	y	611	CLA	ND
27	y	611	CLA	NA
27	C	502	CLA	NC
27	C	502	CLA	ND
27	C	502	CLA	NA

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Mol	Chain	Res	Type	Atom
27	N	603	CLA	NC
27	N	603	CLA	ND
27	N	603	CLA	NA
27	c	508	CLA	NC
27	c	508	CLA	ND
27	c	508	CLA	NA
27	C	509	CLA	NC
27	C	509	CLA	ND
27	C	509	CLA	NA
27	c	507	CLA	NC
27	c	507	CLA	ND
27	c	507	CLA	NA
27	G	612	CLA	NC
27	G	612	CLA	ND
27	G	612	CLA	NA
27	r	602	CLA	NC
27	r	602	CLA	NA
27	r	602	CLA	ND
27	b	609	CLA	NC
27	b	609	CLA	ND
27	b	609	CLA	NA
27	r	603	CLA	NC
27	r	603	CLA	ND
27	r	603	CLA	NA
27	s	610	CLA	NC
27	s	610	CLA	NA
27	s	610	CLA	ND
27	y	610	CLA	NC
27	y	610	CLA	NA
27	y	610	CLA	ND
27	a	406	CLA	NC
27	a	406	CLA	ND
27	a	406	CLA	NA
27	b	602	CLA	NC
27	b	602	CLA	ND
27	b	602	CLA	NA
27	r	613	CLA	NC
27	r	613	CLA	ND
27	r	613	CLA	NA
27	S	612	CLA	NC
27	S	612	CLA	ND
27	S	612	CLA	NA

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Mol	Chain	Res	Type	Atom
27	d	402	CLA	NC
27	d	402	CLA	ND
27	d	402	CLA	NA
27	R	612	CLA	NC
27	R	612	CLA	ND
27	R	612	CLA	NA
27	b	608	CLA	NC
27	b	608	CLA	ND
27	b	608	CLA	NA
27	b	607	CLA	NC
27	b	607	CLA	ND
27	b	607	CLA	NA
27	y	602	CLA	NC
27	y	602	CLA	ND
27	y	602	CLA	NA
27	S	602	CLA	NC
27	S	602	CLA	ND
27	S	602	CLA	NA
27	s	613	CLA	NC
27	s	613	CLA	ND
27	s	613	CLA	NA
27	n	613	CLA	NC
27	n	613	CLA	ND
27	n	613	CLA	NA
27	R	602	CLA	NC
27	R	602	CLA	NA
27	R	602	CLA	ND
27	b	610	CLA	NC
27	b	610	CLA	ND
27	b	610	CLA	NA
27	C	506	CLA	NC
27	C	506	CLA	ND
27	C	506	CLA	NA
27	n	610	CLA	NC
27	n	610	CLA	NA
27	n	610	CLA	ND
27	B	607	CLA	NC
27	B	607	CLA	ND
27	B	607	CLA	NA
27	c	510	CLA	NC
27	c	510	CLA	ND
27	c	510	CLA	NA

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Mol	Chain	Res	Type	Atom
27	s	614	CLA	NC
27	s	614	CLA	ND
27	s	614	CLA	NA
27	G	604	CLA	NC
27	G	604	CLA	ND
27	G	604	CLA	NA
27	C	504	CLA	NC
27	C	504	CLA	ND
27	C	504	CLA	NA
27	Y	604	CLA	NC
27	Y	604	CLA	ND
27	Y	604	CLA	NA

There are no torsion outliers.

There are no ring outliers.

155 monomers are involved in 855 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	401	OEX	2	0
27	A	405	CLA	11	0
27	A	406	CLA	8	0
27	A	407	CLA	7	0
28	A	408	PHO	5	0
28	A	409	PHO	5	0
27	A	410	CLA	8	0
29	A	411	BCR	6	0
30	A	412	SQD	3	0
31	A	413	LMG	8	0
30	A	418	SQD	3	0
27	B	602	CLA	7	0
27	B	603	CLA	11	0
27	B	604	CLA	10	0
27	B	605	CLA	9	0
27	B	606	CLA	7	0
27	B	607	CLA	7	0
27	B	608	CLA	6	0
27	B	609	CLA	9	0
27	B	610	CLA	12	0
27	B	611	CLA	3	0
27	B	612	CLA	5	0
27	B	613	CLA	13	0
27	B	614	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	615	CLA	6	0
27	B	616	CLA	7	0
27	B	617	CLA	4	0
29	B	618	BCR	10	0
29	B	619	BCR	8	0
29	B	620	BCR	2	0
30	B	621	SQD	3	0
31	B	622	LMG	10	0
27	C	501	CLA	3	0
27	C	502	CLA	9	0
27	C	503	CLA	8	0
27	C	504	CLA	6	0
27	C	505	CLA	8	0
27	C	506	CLA	8	0
27	C	507	CLA	5	0
27	C	508	CLA	5	0
27	C	509	CLA	5	0
27	C	510	CLA	9	0
27	C	511	CLA	10	0
27	C	512	CLA	3	0
27	C	513	CLA	5	0
29	C	514	BCR	7	0
29	C	515	BCR	6	0
29	C	516	BCR	10	0
29	C	517	BCR	8	0
32	C	518	DGD	5	0
32	C	519	DGD	6	0
32	C	520	DGD	20	0
31	C	521	LMG	5	0
33	D	401	BCT	5	0
27	D	402	CLA	9	0
27	D	403	CLA	7	0
29	D	404	BCR	5	0
34	D	405	PL9	9	0
35	D	408	LHG	5	0
35	D	409	LHG	4	0
35	D	410	LHG	5	0
31	D	411	LMG	3	0
36	F	101	HEM	5	0
38	G	1620	LUT	9	0
38	G	1621	LUT	7	0
39	G	1622	XAT	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	G	1623	NEX	3	0
35	G	2630	LHG	14	0
37	G	601	CHL	14	0
27	G	602	CLA	8	0
27	G	603	CLA	2	0
27	G	604	CLA	3	0
37	G	605	CHL	6	0
37	G	606	CHL	3	0
37	G	607	CHL	5	0
37	G	608	CHL	6	0
37	G	609	CHL	5	0
27	G	610	CLA	14	0
27	G	611	CLA	9	0
27	G	612	CLA	1	0
27	G	613	CLA	4	0
27	G	614	CLA	3	0
29	H	101	BCR	7	0
32	H	102	DGD	10	0
35	L	101	LHG	7	0
38	N	1620	LUT	10	0
38	N	1621	LUT	8	0
39	N	1622	XAT	8	0
40	N	1623	NEX	3	0
35	N	2630	LHG	7	0
37	N	601	CHL	9	0
27	N	602	CLA	10	0
27	N	603	CLA	1	0
37	N	605	CHL	6	0
37	N	606	CHL	4	0
37	N	607	CHL	10	0
37	N	608	CHL	5	0
37	N	609	CHL	7	0
27	N	610	CLA	12	0
27	N	611	CLA	3	0
27	N	612	CLA	3	0
27	N	613	CLA	3	0
27	N	614	CLA	3	0
35	R	2630	LHG	3	0
27	R	601	CLA	5	0
27	R	602	CLA	14	0
27	R	604	CLA	5	0
37	R	606	CHL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	R	607	CHL	4	0
37	R	608	CHL	11	0
27	R	609	CLA	5	0
27	R	610	CLA	11	0
27	R	611	CLA	4	0
27	R	612	CLA	1	0
27	R	613	CLA	9	0
27	R	616	CLA	6	0
38	R	620	LUT	13	0
39	R	622	XAT	8	0
40	R	623	NEX	6	0
38	S	1620	LUT	8	0
38	S	1621	LUT	11	0
40	S	1623	NEX	5	0
35	S	2630	LHG	3	0
37	S	601	CHL	2	0
27	S	602	CLA	5	0
27	S	603	CLA	3	0
27	S	604	CLA	7	0
37	S	606	CHL	4	0
37	S	607	CHL	3	0
37	S	608	CHL	4	0
27	S	609	CLA	4	0
27	S	610	CLA	13	0
27	S	611	CLA	2	0
27	S	612	CLA	3	0
27	S	613	CLA	4	0
27	S	614	CLA	4	0
38	Y	1620	LUT	8	0
38	Y	1621	LUT	9	0
39	Y	1622	XAT	10	0
40	Y	1623	NEX	5	0
35	Y	2630	LHG	8	0
37	Y	601	CHL	9	0
27	Y	602	CLA	10	0
27	Y	603	CLA	5	0
27	Y	604	CLA	4	0
37	Y	605	CHL	5	0
37	Y	607	CHL	6	0
37	Y	608	CHL	3	0
37	Y	609	CHL	8	0
27	Y	610	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	Y	611	CLA	7	0
27	Y	612	CLA	5	0
27	Y	613	CLA	7	0
27	Y	614	CLA	2	0
31	Z	101	LMG	6	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.