



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 13, 2017 – 08:32 AM EDT

PDB ID : 5XNL
EMDB ID: : EMD-6741
Title : Structure of stacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : unknown
Resolution : 2.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

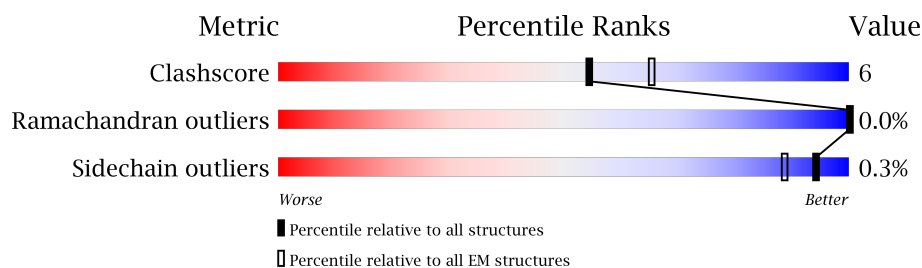
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.









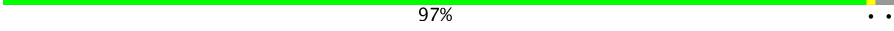

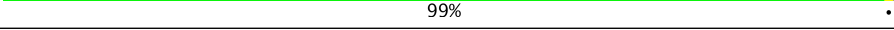

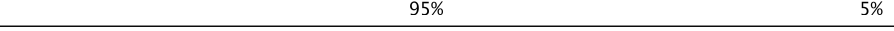
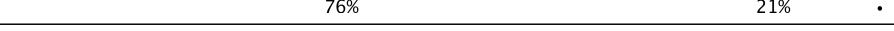
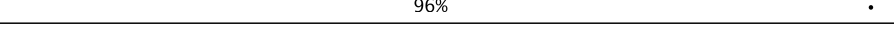






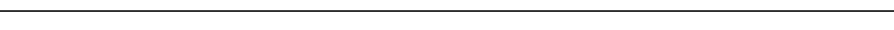

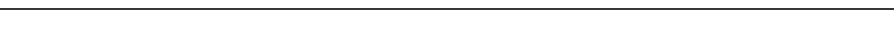
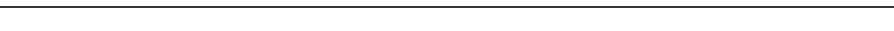


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1	232	
1	2	232	
1	5	232	
1	6	232	
1	G	232	
1	N	232	
1	Y	232	
1	g	232	
1	n	232	


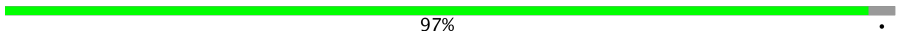

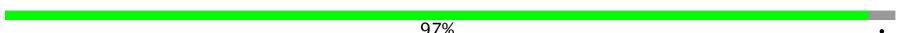

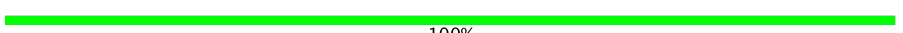












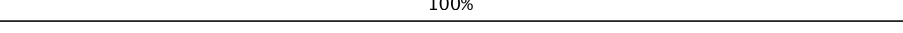
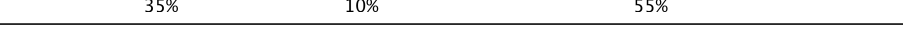


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Mol	Chain	Length	Quality of chain
1	y	232	 94% 6%
2	3	243	 77% 14% 9%
2	7	243	 77% 14% 9%
3	4	210	 80% 13% 6%
3	8	210	 79% 15% 6%
4	A	344	 71% 26% .
4	a	344	 97% . .
5	B	507	 80% 18% ..
5	b	507	 99% ..
6	C	473	 74% 21% 5%
6	c	473	 95% 5%
7	D	353	 76% 21% .
7	d	353	 96% .
8	E	83	 81% 10% 10%
8	e	83	 89% . 10%
9	F	39	 72% 5% 23%
9	f	39	 77% 23%
10	H	73	 67% 14% . 18%
10	h	73	 81% . 18%
11	I	36	 81% 14% 6%
11	i	36	 94% 6%
12	J	40	 75% 13% 13%
12	j	40	 85% . 13%
13	K	61	 49% 11% 39%
13	k	61	 61% 39%

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Mol	Chain	Length	Quality of chain
14	L	38	 66% 32% .
14	l	38	 97% .
15	M	34	 82% 15% .
15	m	34	 97% .
16	O	248	 78% 22%
16	o	248	 100%
17	P	186	 82% 18%
17	p	186	 100%
18	Q	148	 73% 14% 13%
18	q	148	 87% 13%
19	R	246	 76% 19% 5%
19	r	246	 95% 5%
20	S	244	 71% 18% 11%
20	s	244	 89% 11%
21	T	35	 74% 17% 9%
21	t	35	 91% 9%
22	W	54	 89% 11%
22	w	54	 100%
23	X	86	 35% 10% 55%
23	x	86	 45% 55%
24	Z	62	 84% 16%
24	z	62	 100%

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
26	CLA	1	602	X	-	-	-
26	CLA	1	603	X	-	-	-
26	CLA	1	604	X	-	-	-
26	CLA	1	610	X	-	-	-
26	CLA	1	611	X	-	-	-
26	CLA	1	612	X	-	-	-
26	CLA	1	613	X	-	-	-
26	CLA	1	614	X	-	-	-
26	CLA	2	602	X	-	-	-
26	CLA	2	603	X	-	-	-
26	CLA	2	604	X	-	-	-
26	CLA	2	610	X	-	-	-
26	CLA	2	611	X	-	-	-
26	CLA	2	612	X	-	-	-
26	CLA	2	613	X	-	-	-
26	CLA	2	614	X	-	-	-
26	CLA	3	602	X	-	-	-
26	CLA	3	603	X	-	-	-
26	CLA	3	604	X	-	-	-
26	CLA	3	610	X	-	-	-
26	CLA	3	611	X	-	-	-
26	CLA	3	612	X	-	-	-
26	CLA	3	613	X	-	-	-
26	CLA	3	614	X	-	-	-
26	CLA	4	602	X	-	-	-
26	CLA	4	603	X	-	-	-
26	CLA	4	604	X	-	-	-
26	CLA	4	610	X	-	-	-
26	CLA	4	611	X	-	-	-
26	CLA	4	612	X	-	-	-
26	CLA	5	602	X	-	-	-
26	CLA	5	603	X	-	-	-
26	CLA	5	604	X	-	-	-
26	CLA	5	610	X	-	-	-
26	CLA	5	611	X	-	-	-
26	CLA	5	612	X	-	-	-
26	CLA	5	613	X	-	-	-
26	CLA	5	614	X	-	-	-
26	CLA	6	602	X	-	-	-
26	CLA	6	603	X	-	-	-
26	CLA	6	604	X	-	-	-
26	CLA	6	610	X	-	-	-
26	CLA	6	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	6	612	X	-	-	-
26	CLA	6	613	X	-	-	-
26	CLA	6	614	X	-	-	-
26	CLA	7	602	X	-	-	-
26	CLA	7	603	X	-	-	-
26	CLA	7	604	X	-	-	-
26	CLA	7	610	X	-	-	-
26	CLA	7	611	X	-	-	-
26	CLA	7	612	X	-	-	-
26	CLA	7	613	X	-	-	-
26	CLA	7	614	X	-	-	-
26	CLA	8	602	X	-	-	-
26	CLA	8	603	X	-	-	-
26	CLA	8	604	X	-	-	-
26	CLA	8	610	X	-	-	-
26	CLA	8	611	X	-	-	-
26	CLA	8	612	X	-	-	-
26	CLA	A	405	X	-	-	-
26	CLA	A	406	X	-	-	-
26	CLA	A	407	X	-	-	-
26	CLA	A	410	X	-	-	-
26	CLA	B	602	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	608	X	-	-	-
26	CLA	B	609	X	-	-	-
26	CLA	B	610	X	-	-	-
26	CLA	B	611	X	-	-	-
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	614	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	B	617	X	-	-	-
26	CLA	C	501	X	-	-	-
26	CLA	C	502	X	-	-	-
26	CLA	C	503	X	-	-	-
26	CLA	C	504	X	-	-	-
26	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	508	X	-	-	-
26	CLA	C	509	X	-	-	-
26	CLA	C	510	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	C	513	X	-	-	-
26	CLA	D	402	X	-	-	-
26	CLA	D	403	X	-	-	-
26	CLA	G	602	X	-	-	-
26	CLA	G	603	X	-	-	-
26	CLA	G	604	X	-	-	-
26	CLA	G	610	X	-	-	-
26	CLA	G	611	X	-	-	-
26	CLA	G	612	X	-	-	-
26	CLA	G	613	X	-	-	-
26	CLA	G	614	X	-	-	-
26	CLA	N	602	X	-	-	-
26	CLA	N	603	X	-	-	-
26	CLA	N	604	X	-	-	-
26	CLA	N	610	X	-	-	-
26	CLA	N	611	X	-	-	-
26	CLA	N	612	X	-	-	-
26	CLA	N	613	X	-	-	-
26	CLA	N	614	X	-	-	-
26	CLA	R	601	X	-	-	-
26	CLA	R	602	X	-	-	-
26	CLA	R	603	X	-	-	-
26	CLA	R	604	X	-	-	-
26	CLA	R	609	X	-	-	-
26	CLA	R	610	X	-	-	-
26	CLA	R	611	X	-	-	-
26	CLA	R	612	X	-	-	-
26	CLA	R	613	X	-	-	-
26	CLA	R	616	X	-	-	-
26	CLA	S	602	X	-	-	-
26	CLA	S	603	X	-	-	-
26	CLA	S	604	X	-	-	-
26	CLA	S	609	X	-	-	-
26	CLA	S	610	X	-	-	-
26	CLA	S	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	S	612	X	-	-	-
26	CLA	S	613	X	-	-	-
26	CLA	S	614	X	-	-	-
26	CLA	Y	602	X	-	-	-
26	CLA	Y	603	X	-	-	-
26	CLA	Y	604	X	-	-	-
26	CLA	Y	610	X	-	-	-
26	CLA	Y	611	X	-	-	-
26	CLA	Y	612	X	-	-	-
26	CLA	Y	613	X	-	-	-
26	CLA	Y	614	X	-	-	-
26	CLA	a	405	X	-	-	-
26	CLA	a	406	X	-	-	-
26	CLA	a	407	X	-	-	-
26	CLA	a	410	X	-	-	-
26	CLA	b	602	X	-	-	-
26	CLA	b	603	X	-	-	-
26	CLA	b	604	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-
26	CLA	b	608	X	-	-	-
26	CLA	b	609	X	-	-	-
26	CLA	b	610	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	615	X	-	-	-
26	CLA	b	616	X	-	-	-
26	CLA	b	617	X	-	-	-
26	CLA	c	501	X	-	-	-
26	CLA	c	502	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-
26	CLA	c	507	X	-	-	-
26	CLA	c	508	X	-	-	-
26	CLA	c	509	X	-	-	-
26	CLA	c	510	X	-	-	-
26	CLA	c	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	c	512	X	-	-	-
26	CLA	c	513	X	-	-	-
26	CLA	d	402	X	-	-	-
26	CLA	d	403	X	-	-	-
26	CLA	g	602	X	-	-	-
26	CLA	g	603	X	-	-	-
26	CLA	g	604	X	-	-	-
26	CLA	g	610	X	-	-	-
26	CLA	g	611	X	-	-	-
26	CLA	g	612	X	-	-	-
26	CLA	g	613	X	-	-	-
26	CLA	g	614	X	-	-	-
26	CLA	n	602	X	-	-	-
26	CLA	n	603	X	-	-	-
26	CLA	n	604	X	-	-	-
26	CLA	n	610	X	-	-	-
26	CLA	n	611	X	-	-	-
26	CLA	n	612	X	-	-	-
26	CLA	n	613	X	-	-	-
26	CLA	n	614	X	-	-	-
26	CLA	r	601	X	-	-	-
26	CLA	r	602	X	-	-	-
26	CLA	r	603	X	-	-	-
26	CLA	r	604	X	-	-	-
26	CLA	r	609	X	-	-	-
26	CLA	r	610	X	-	-	-
26	CLA	r	611	X	-	-	-
26	CLA	r	612	X	-	-	-
26	CLA	r	613	X	-	-	-
26	CLA	r	616	X	-	-	-
26	CLA	s	602	X	-	-	-
26	CLA	s	603	X	-	-	-
26	CLA	s	604	X	-	-	-
26	CLA	s	609	X	-	-	-
26	CLA	s	610	X	-	-	-
26	CLA	s	611	X	-	-	-
26	CLA	s	612	X	-	-	-
26	CLA	s	613	X	-	-	-
26	CLA	s	614	X	-	-	-
26	CLA	y	602	X	-	-	-
26	CLA	y	603	X	-	-	-
26	CLA	y	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	y	610	X	-	-	-
26	CLA	y	611	X	-	-	-
26	CLA	y	612	X	-	-	-
26	CLA	y	613	X	-	-	-
26	CLA	y	614	X	-	-	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 98986 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 Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	5	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	6	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		
2	7	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		
4	a	334	Total	C	N	O	S	0	0
			2616	1708	431	464	13		

- Molecule 5 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		
5	b	503	Total	C	N	O	S	0	0
			3948	2581	669	686	12		

- Molecule 6 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		
6	c	450	Total	C	N	O	S	0	0
			3497	2300	583	604	10		

- Molecule 7 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		
7	d	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		

- Molecule 8 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	75	Total	C	N	O	0	0
			612	400	100	112		
8	e	75	Total	C	N	O	0	0
			612	400	100	112		

- Molecule 9 is a protein called Cytochrome b559 subunit beta, PsbF.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
9	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
10	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

- Molecule 11 is a protein called Photosystem II reaction center protein I, PsbI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
11	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total	C	N	O	0	0
			256	174	39	43		
12	j	35	Total	C	N	O	0	0
			256	174	39	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	37	Total	C	N	O	S	0	0
			306	215	44	46	1		
13	k	37	Total	C	N	O	S	0	0
			306	215	44	46	1		

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

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

- Molecule 15 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
15	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

- Molecule 16 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		
16	o	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

- Molecule 17 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		
17	p	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		

- Molecule 18 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	129	Total	C	N	O	0	0
			1034	661	177	196		
18	q	129	Total	C	N	O	0	0
			1034	661	177	196		

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	234	Total	C	N	O	S	0	0
			1835	1194	297	341	3		

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		
20	s	218	Total	C	N	O	S	0	0
			1689	1107	273	305	4		

- Molecule 21 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	32	Total	C	N	O	S	0	0
			261	182	37	41	1		
21	t	32	Total	C	N	O	S	0	0
			261	182	37	41	1		

- Molecule 22 is a protein called Photosystem II reaction center protein W.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	54	Total	C	N	O	S	0	0
			419	275	61	82	1		
22	w	54	Total	C	N	O	S	0	0
			419	275	61	82	1		

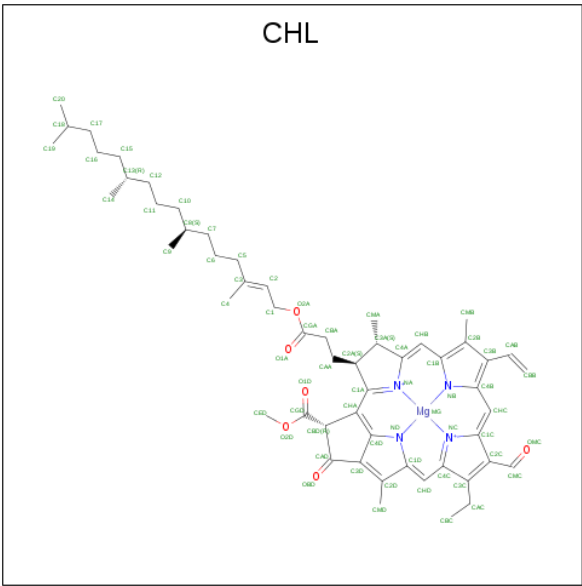
- Molecule 23 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	39	Total	C	N	O	0	0
			276	180	46	50		
23	x	39	Total	C	N	O	0	0
			276	180	46	50		

- Molecule 24 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		
24	z	62	Total	C	N	O	S	0	0
			464	312	69	82	1		

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
25	1	1	309	243	6	24	36	0
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
25	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
25	1	1	309	243	6	24	36	0
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
25	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
25	2	1	306	240	6	24	36	0
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
25	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
25	2	1	306	240	6	24	36	0
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
25	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
			Total	C	Mg	N	O	
			316	250	6	24	36	
			Total	C	Mg	N	O	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
25	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
25	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
25	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
25	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
25	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
25	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
25	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
25	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
25	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
25	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
25	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
25	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
25	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
25	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
25	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
25	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
25	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0

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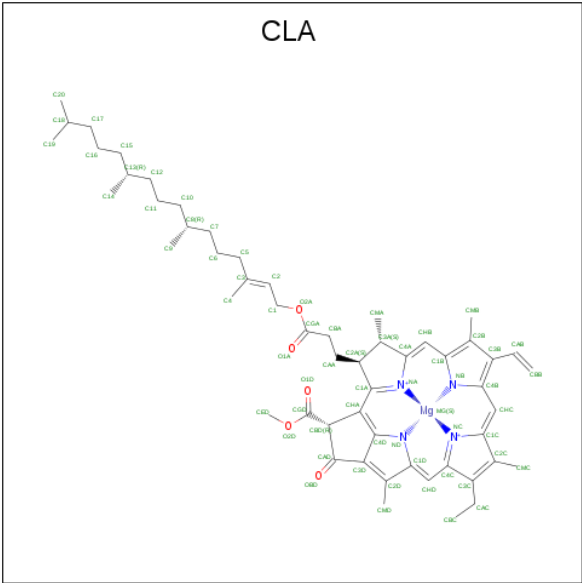
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	

- Molecule 26 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
26	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	

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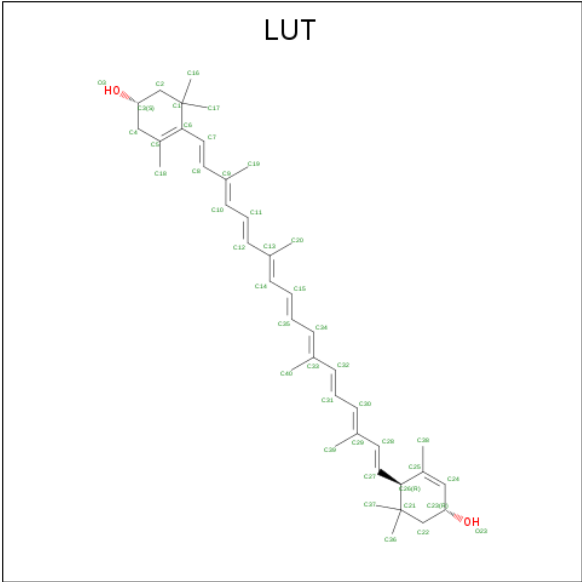
Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	n	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	
26	r	1	Total	C	Mg	N	O	0
			543	443	10	40	50	

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Mol	Chain	Residues	Atoms					AltConf
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	s	1	Total	C	Mg	N	O	0
			465	375	9	36	45	
26	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
26	y	1	Total	C	Mg	N	O	0
			473	393	8	32	40	

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



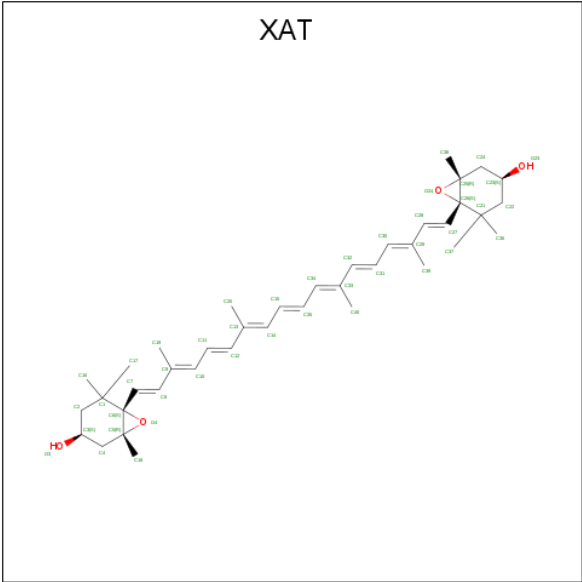
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			84	80	4	
27	1	1	Total	C	O	0
			84	80	4	
27	2	1	Total	C	O	0
			84	80	4	
27	2	1	Total	C	O	0
			84	80	4	
27	3	1	Total	C	O	0
			84	80	4	
27	3	1	Total	C	O	0
			84	80	4	
27	4	1	Total	C	O	0
			42	40	2	
27	G	1	Total	C	O	0
			84	80	4	
27	G	1	Total	C	O	0
			84	80	4	
27	N	1	Total	C	O	0
			84	80	4	
27	N	1	Total	C	O	0
			84	80	4	
27	R	1	Total	C	O	0
			42	40	2	
27	S	1	Total	C	O	0
			84	80	4	
27	S	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
27	Y	1	Total	C	O	0
			84	80	4	
27	Y	1	Total	C	O	0
			84	80	4	
27	5	1	Total	C	O	0
			84	80	4	
27	5	1	Total	C	O	0
			84	80	4	
27	6	1	Total	C	O	0
			84	80	4	
27	6	1	Total	C	O	0
			84	80	4	
27	7	1	Total	C	O	0
			84	80	4	
27	7	1	Total	C	O	0
			84	80	4	
27	8	1	Total	C	O	0
			42	40	2	
27	g	1	Total	C	O	0
			84	80	4	
27	g	1	Total	C	O	0
			84	80	4	
27	n	1	Total	C	O	0
			84	80	4	
27	n	1	Total	C	O	0
			84	80	4	
27	r	1	Total	C	O	0
			42	40	2	
27	s	1	Total	C	O	0
			84	80	4	
27	s	1	Total	C	O	0
			84	80	4	
27	y	1	Total	C	O	0
			84	80	4	
27	y	1	Total	C	O	0
			84	80	4	

- Molecule 28 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).



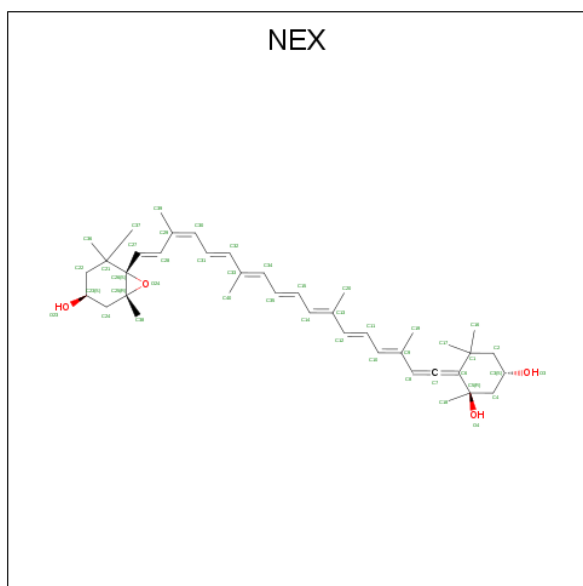
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	4	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	R	1	Total	C	O	0
			44	40	4	
28	Y	1	Total	C	O	0
			44	40	4	
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	7	1	Total	C	O	0
			44	40	4	
28	8	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	

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

- Molecule 29 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



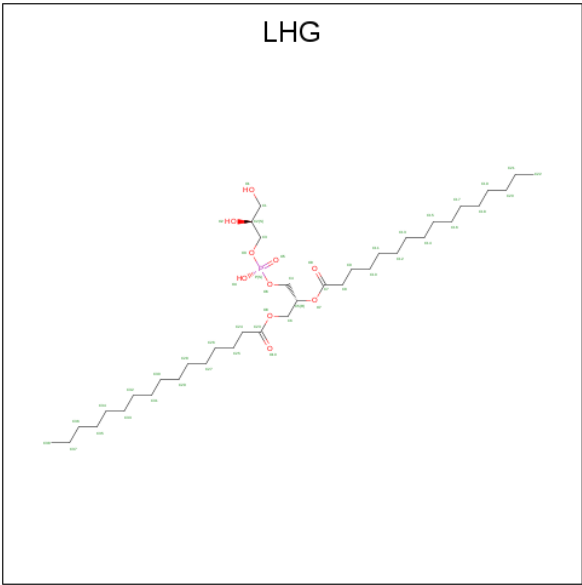
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			44	40	4	
29	2	1	Total	C	O	0
			44	40	4	
29	3	1	Total	C	O	0
			44	40	4	
29	G	1	Total	C	O	0
			44	40	4	
29	N	1	Total	C	O	0
			44	40	4	
29	R	1	Total	C	O	0
			44	40	4	
29	S	1	Total	C	O	0
			44	40	4	
29	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
29	5	1	Total	C	O	0
			44	40	4	
29	6	1	Total	C	O	0
			44	40	4	
29	7	1	Total	C	O	0
			44	40	4	
29	g	1	Total	C	O	0
			44	40	4	
29	n	1	Total	C	O	0
			44	40	4	
29	r	1	Total	C	O	0
			44	40	4	
29	s	1	Total	C	O	0
			44	40	4	
29	y	1	Total	C	O	0
			44	40	4	

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



Mol	Chain	Residues	Atoms				AltConf
30	1	1	Total	C	O	P	0
			41	30	10	1	
30	2	1	Total	C	O	P	0
			37	26	10	1	
30	3	1	Total	C	O	P	0
			47	36	10	1	

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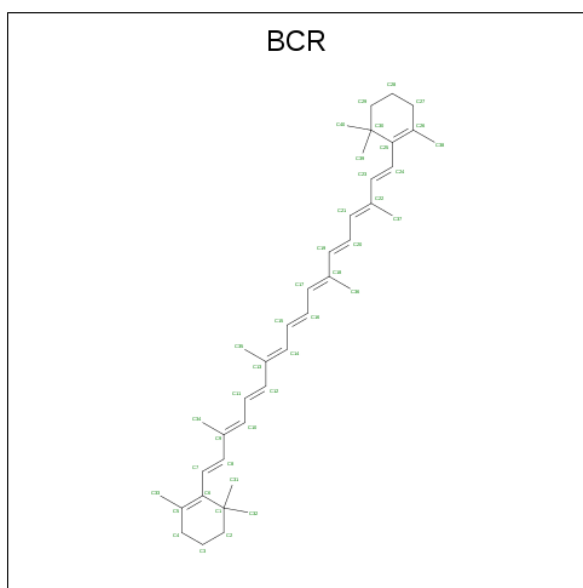
Mol	Chain	Residues	Atoms				AltConf
30	4	1	Total	C	O	P	0
			21	10	10	1	
30	B	1	Total	C	O	P	0
			96	74	20	2	
30	B	1	Total	C	O	P	0
			96	74	20	2	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			42	31	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	5	1	Total	C	O	P	0
			41	30	10	1	
30	6	1	Total	C	O	P	0
			37	26	10	1	
30	7	1	Total	C	O	P	0
			47	36	10	1	
30	8	1	Total	C	O	P	0
			21	10	10	1	
30	b	1	Total	C	O	P	0
			96	74	20	2	
30	b	1	Total	C	O	P	0
			96	74	20	2	

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Mol	Chain	Residues	Atoms				AltConf
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	g	1	Total	C	O	P	0
			49	38	10	1	
30	l	1	Total	C	O	P	0
			49	38	10	1	
30	n	1	Total	C	O	P	0
			49	38	10	1	
30	r	1	Total	C	O	P	0
			42	31	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



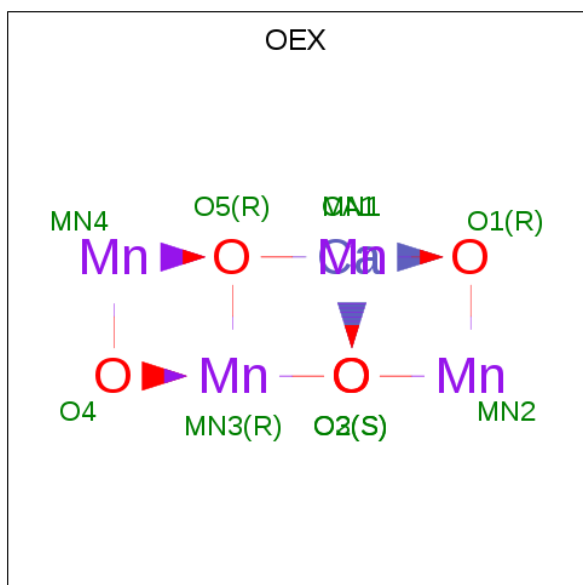
Mol	Chain	Residues	Atoms	AltConf
31	4	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 120 120	0
31	B	1	Total C 120 120	0
31	B	1	Total C 120 120	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	8	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	d	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
31	h	1	Total	C	0
			40	40	
31	t	1	Total	C	0
			40	40	

- Molecule 32 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 33 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

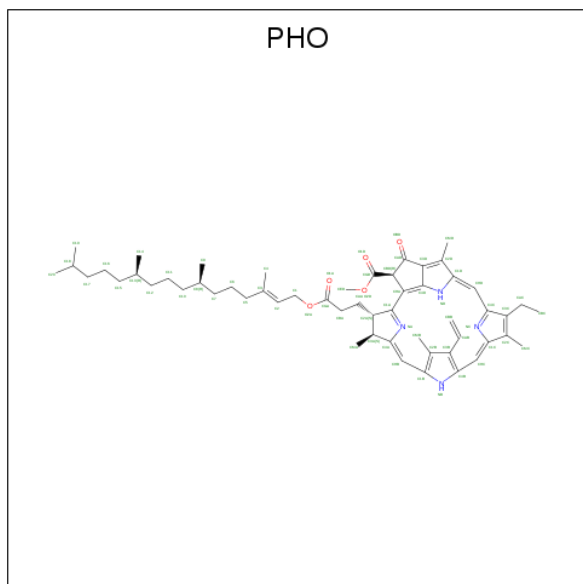
Mol	Chain	Residues	Atoms		AltConf
34	A	2	Total	Cl	0
			2	2	

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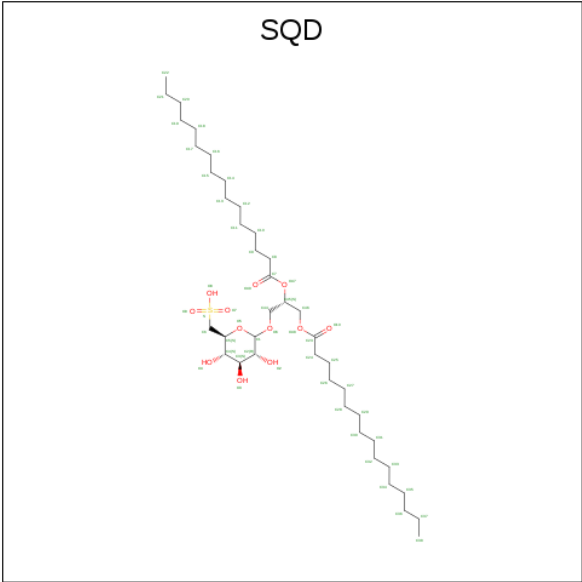
Mol	Chain	Residues	Atoms		AltConf
34	a	2	Total	Cl	0
			2	2	

- Molecule 35 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



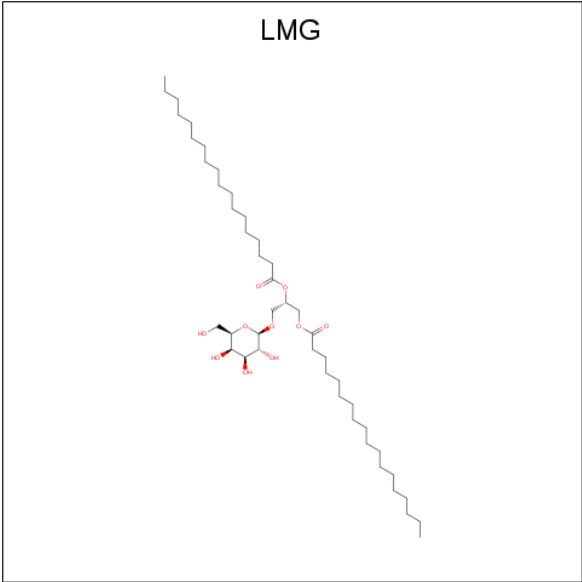
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			128	110	8	10	
35	A	1	Total	C	N	O	0
			128	110	8	10	
35	a	1	Total	C	N	O	0
			128	110	8	10	
35	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



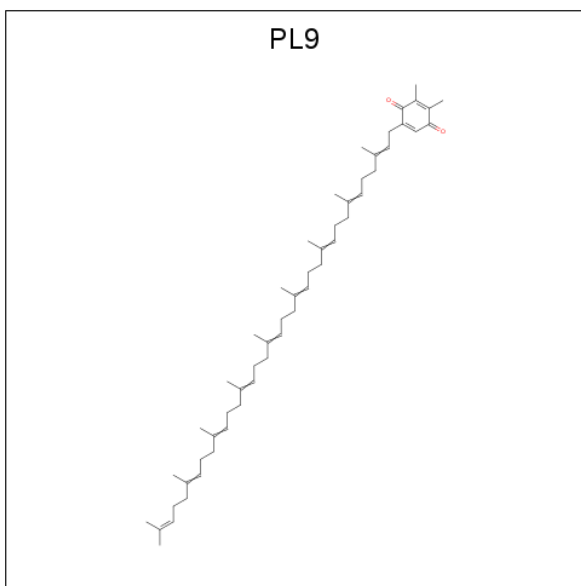
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	S	0
			104	78	24	2	
36	A	1	Total	C	O	S	0
			104	78	24	2	
36	B	1	Total	C	O	S	0
			96	70	24	2	
36	B	1	Total	C	O	S	0
			96	70	24	2	
36	a	1	Total	C	O	S	0
			104	78	24	2	
36	a	1	Total	C	O	S	0
			104	78	24	2	
36	b	1	Total	C	O	S	0
			96	70	24	2	
36	b	1	Total	C	O	S	0
			96	70	24	2	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



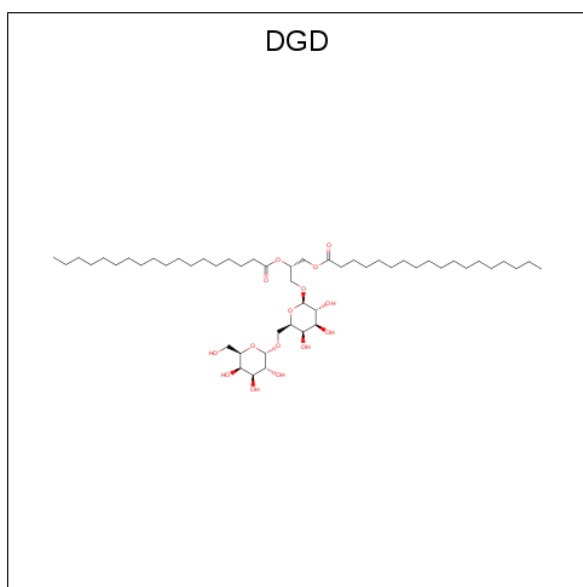
Mol	Chain	Residues	Atoms			AltConf
37	A	1	Total	C	O	0
			88	68	20	
37	A	1	Total	C	O	0
			88	68	20	
37	B	1	Total	C	O	0
			106	86	20	
37	B	1	Total	C	O	0
			106	86	20	
37	C	1	Total	C	O	0
			51	41	10	
37	D	1	Total	C	O	0
			46	36	10	
37	Z	1	Total	C	O	0
			51	41	10	
37	a	1	Total	C	O	0
			88	68	20	
37	a	1	Total	C	O	0
			88	68	20	
37	b	1	Total	C	O	0
			106	86	20	
37	b	1	Total	C	O	0
			106	86	20	
37	c	1	Total	C	O	0
			51	41	10	
37	d	1	Total	C	O	0
			46	36	10	
37	z	1	Total	C	O	0
			51	41	10	

- Molecule 38 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: $C_{53}H_{80}O_2$).



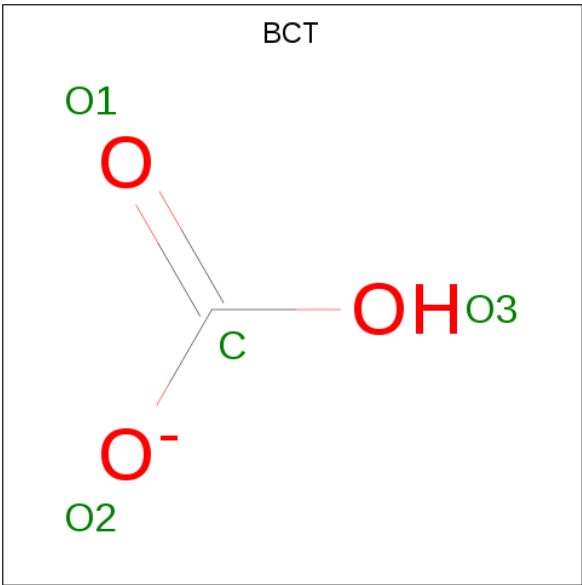
Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			13	11	2	
38	D	1	Total	C	O	0
			55	53	2	
38	a	1	Total	C	O	0
			13	11	2	
38	d	1	Total	C	O	0
			55	53	2	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



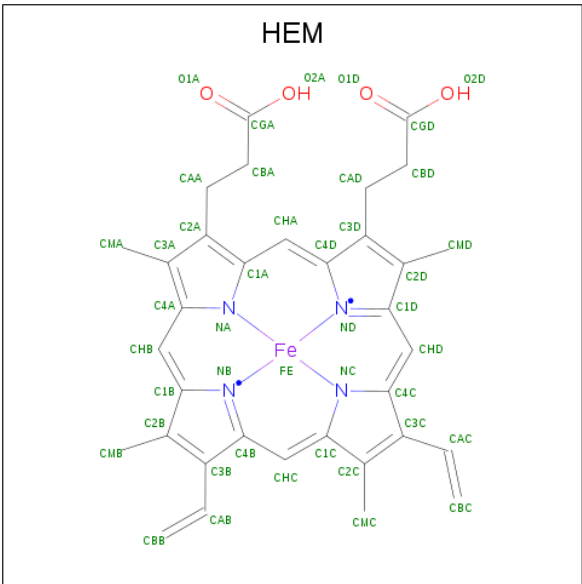
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			59	44	15	
39	C	1	Total	C	O	0
			177	132	45	
39	C	1	Total	C	O	0
			177	132	45	
39	C	1	Total	C	O	0
			177	132	45	
39	H	1	Total	C	O	0
			62	47	15	
39	b	1	Total	C	O	0
			59	44	15	
39	c	1	Total	C	O	0
			177	132	45	
39	c	1	Total	C	O	0
			177	132	45	
39	c	1	Total	C	O	0
			177	132	45	
39	h	1	Total	C	O	0
			62	47	15	

- Molecule 40 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	96	Total	O	0
			96	96	
42	B	89	Total	O	0
			89	89	
42	C	68	Total	O	0
			68	68	
42	D	58	Total	O	0
			58	58	
42	E	10	Total	O	0
			10	10	
42	F	2	Total	O	0
			2	2	
42	G	15	Total	O	0
			15	15	
42	H	16	Total	O	0
			16	16	
42	J	3	Total	O	0
			3	3	
42	K	2	Total	O	0
			2	2	
42	L	10	Total	O	0
			10	10	
42	M	4	Total	O	0
			4	4	
42	N	20	Total	O	0
			20	20	
42	O	31	Total	O	0
			31	31	
42	P	16	Total	O	0
			16	16	
42	R	30	Total	O	0
			30	30	
42	S	14	Total	O	0
			14	14	
42	T	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
42	W	4	Total 4	O 4	0
42	X	5	Total 5	O 5	0
42	Y	39	Total 39	O 39	0
42	Z	4	Total 4	O 4	0
42	a	96	Total 96	O 96	0
42	b	89	Total 89	O 89	0
42	c	68	Total 68	O 68	0
42	d	58	Total 58	O 58	0
42	e	10	Total 10	O 10	0
42	f	2	Total 2	O 2	0
42	g	15	Total 15	O 15	0
42	h	16	Total 16	O 16	0
42	j	3	Total 3	O 3	0
42	k	2	Total 2	O 2	0
42	l	10	Total 10	O 10	0
42	m	4	Total 4	O 4	0
42	n	20	Total 20	O 20	0
42	o	31	Total 31	O 31	0
42	p	16	Total 16	O 16	0
42	r	30	Total 30	O 30	0
42	s	14	Total 14	O 14	0

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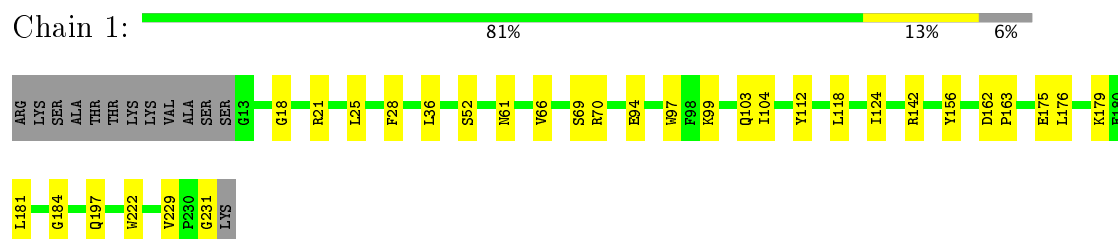
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
42	t	2	Total 2	O 2	0
42	w	4	Total 4	O 4	0
42	x	5	Total 5	O 5	0
42	y	39	Total 39	O 39	0
42	z	4	Total 4	O 4	0

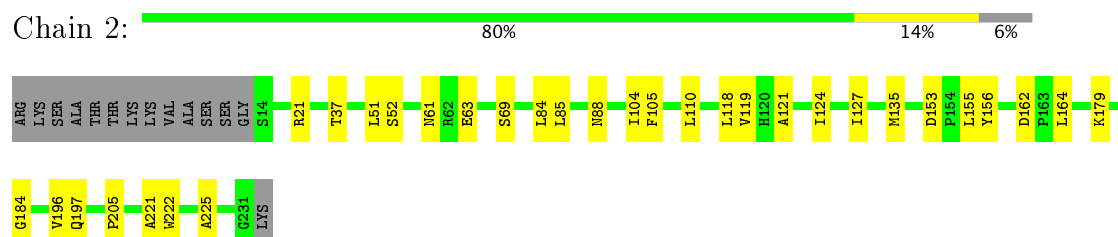
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

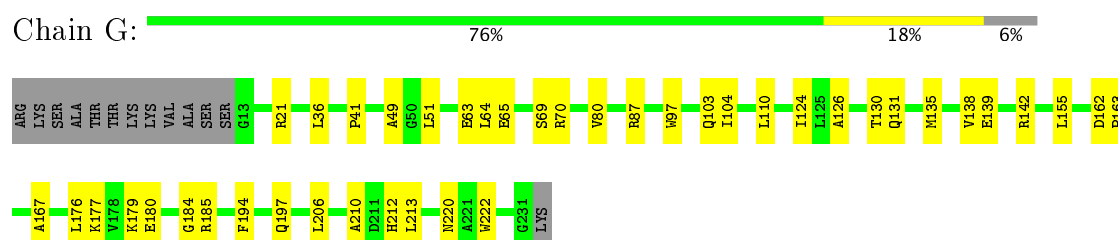
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



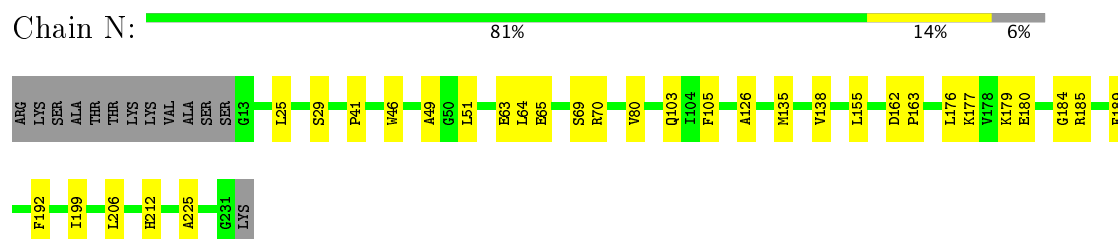
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



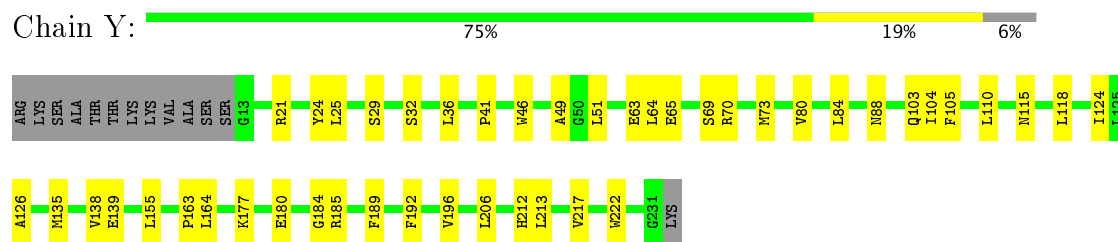
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



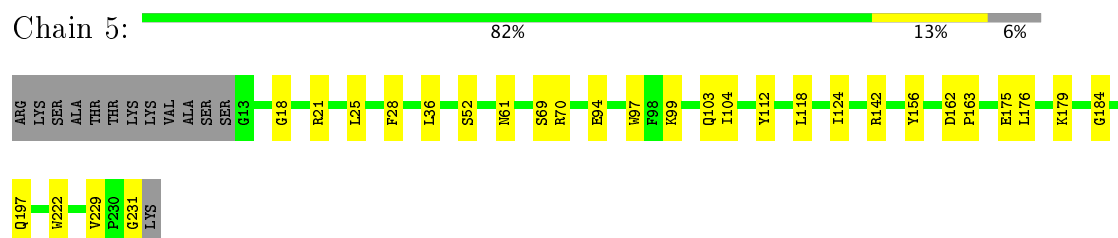
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



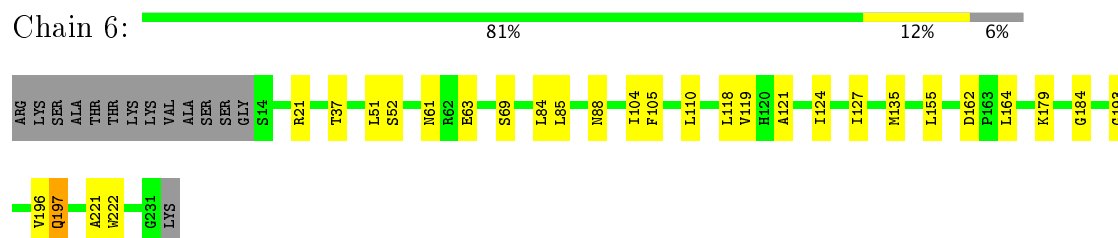
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



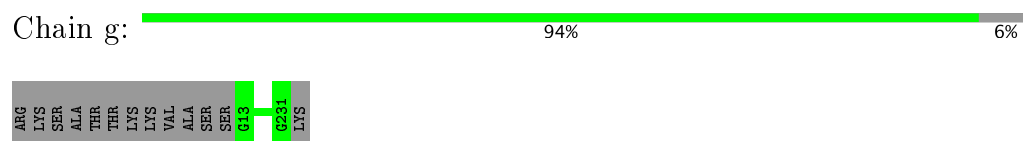
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



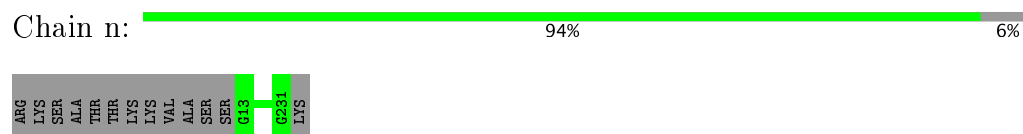
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



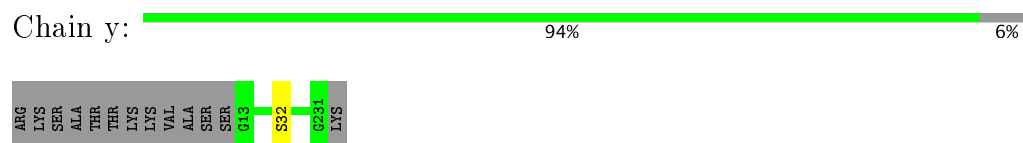
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic




- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

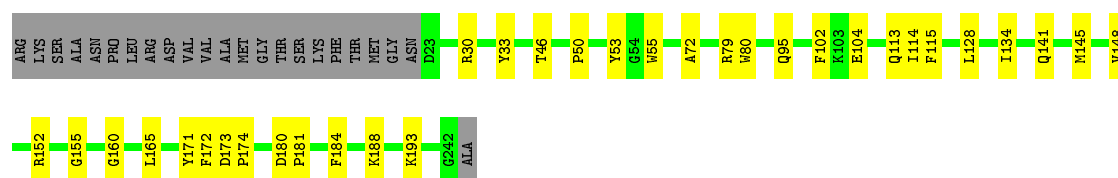


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic




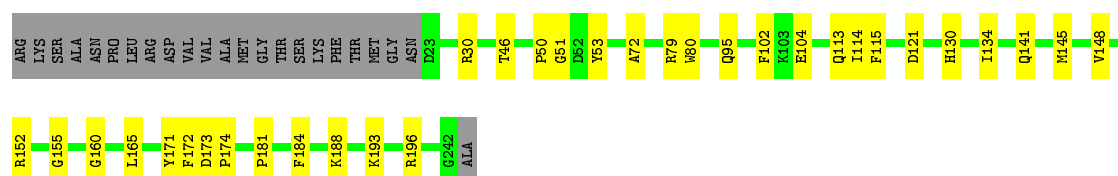
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 




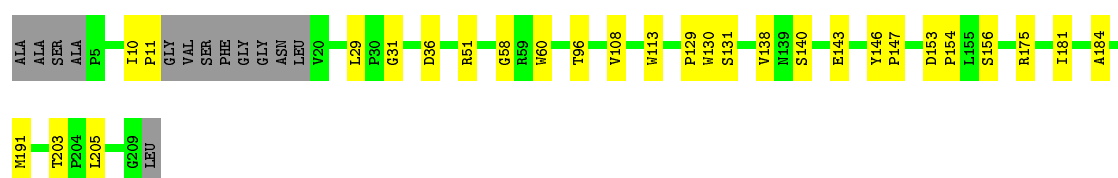
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 




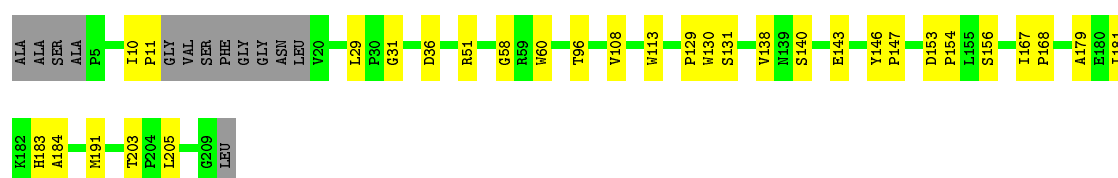
- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

Chain 4: 



- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

Chain 8: 



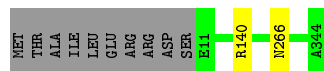
- Molecule 4: Photosystem II protein D1

Chain A: 




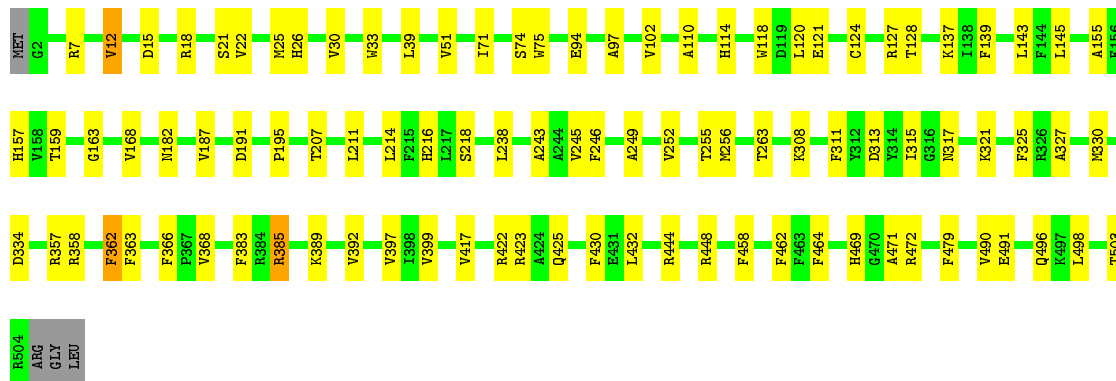
- Molecule 4: Photosystem II protein D1

Chain a:  97%



- Molecule 5: Photosystem II CP47 reaction center protein

Chain B:  80%



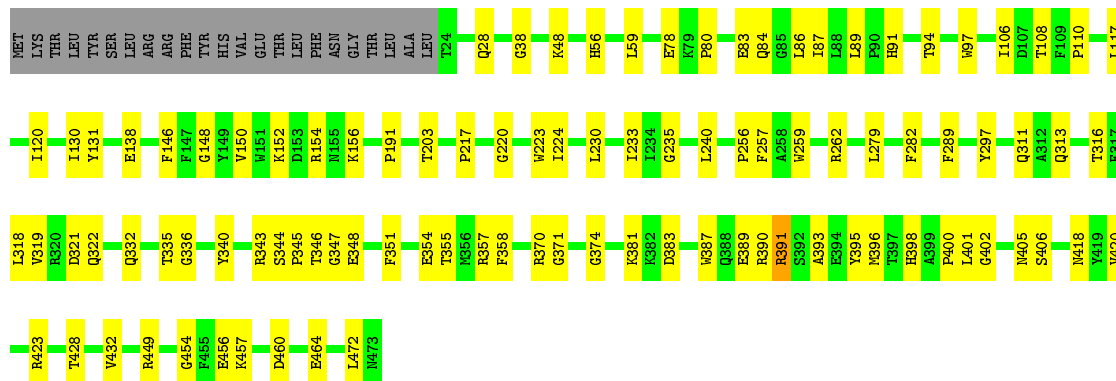
- Molecule 5: Photosystem II CP47 reaction center protein

Chain b:  99%



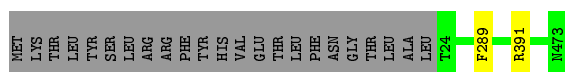
- Molecule 6: Photosystem II CP43 reaction center protein

Chain C:  74%



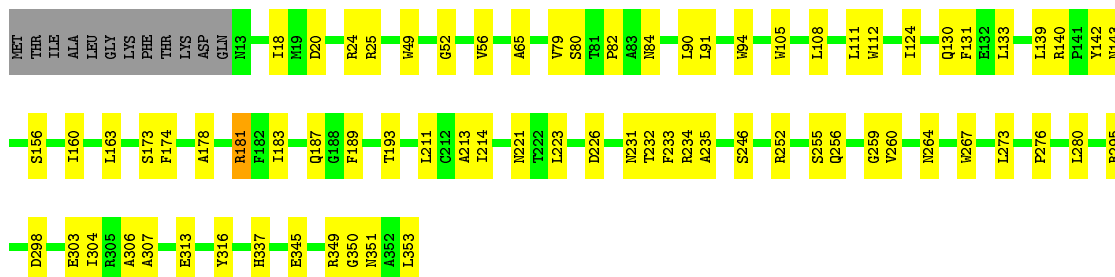
- Molecule 6: Photosystem II CP43 reaction center protein

Chain c:  95%



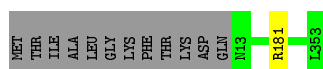
- Molecule 7: Photosystem II D2 protein

Chain D: 76% 21% .



- Molecule 7: Photosystem II D2 protein

Chain d: 96% .



- Molecule 8: Cytochrome b559 subunit alpha

Chain E: 81% 10% 10%



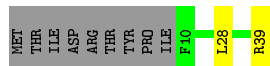
- Molecule 8: Cytochrome b559 subunit alpha

Chain e: 89% 10%



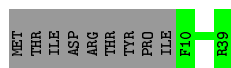
- Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain F: 72% 5% 23%



- Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain f: 77% 23%




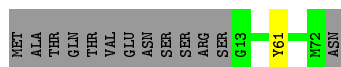
- Molecule 10: Photosystem II reaction center protein H

Chain H: 




- Molecule 10: Photosystem II reaction center protein H

Chain h: 



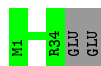
- Molecule 11: Photosystem II reaction center protein I, PsbI

Chain I: 



- Molecule 11: Photosystem II reaction center protein I, PsbI

Chain i: 




- Molecule 12: Photosystem II reaction center protein J

Chain J: 



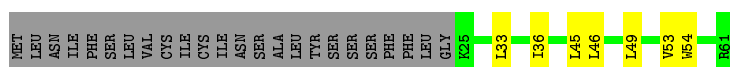
- Molecule 12: Photosystem II reaction center protein J

Chain j: 



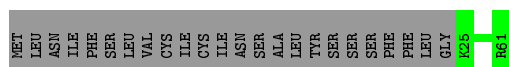
- Molecule 13: Photosystem II reaction center protein K

Chain K: 



- Molecule 13: Photosystem II reaction center protein K

Chain k: 



- Molecule 14: Photosystem II reaction center protein L

Chain L: 66% 32%



- Molecule 14: Photosystem II reaction center protein L

Chain l: 97%



- Molecule 15: Photosystem II reaction center protein M

Chain M: 82% 15%



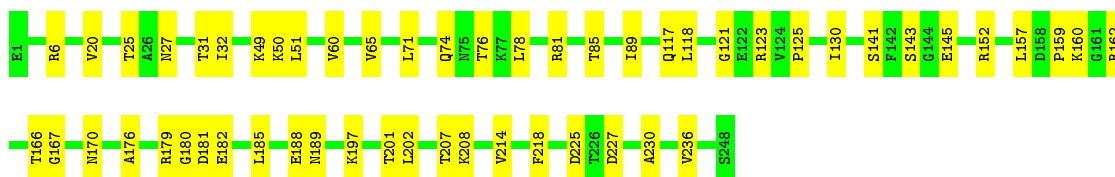
- Molecule 15: Photosystem II reaction center protein M

Chain m: 97%



- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O: 78% 22%



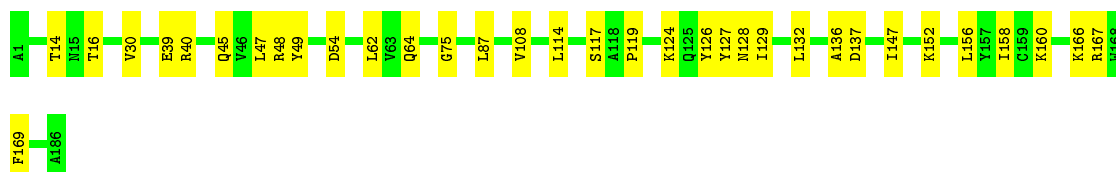
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 100%

There are no outlier residues recorded for this chain.

- Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

Chain P: 82% 18%



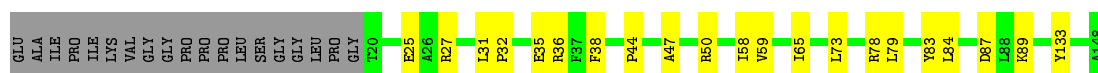
- Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

Chain p: 100%

There are no outlier residues recorded for this chain.

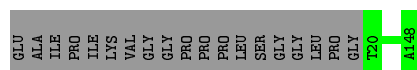
- Molecule 18: Oxygen-evolving enhancer protein 3

Chain Q: 73%



- Molecule 18: Oxygen-evolving enhancer protein 3

Chain q: 87%



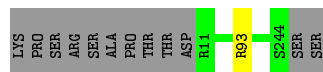
- Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain R: 76%



- Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain r: 95%



- Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

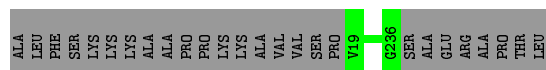
Chain S: 71%





- Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain s: 89% 11%



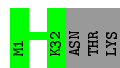
- Molecule 21: Photosystem II reaction center protein T

Chain T: 74% 17% 9%



- Molecule 21: Photosystem II reaction center protein T

Chain t: 91% 9%



- Molecule 22: Photosystem II reaction center protein W

Chain W: 89% 11%



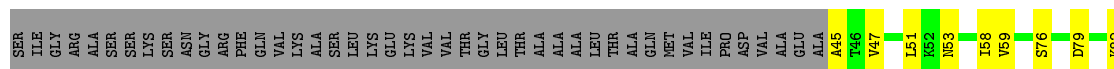
- Molecule 22: Photosystem II reaction center protein W

Chain w: 100%

There are no outlier residues recorded for this chain.

- Molecule 23: Photosystem II reaction center protein X

Chain X: 35% 10% 55%

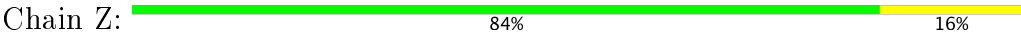


- Molecule 23: Photosystem II reaction center protein X

Chain x: 45% 55%



- Molecule 24: Photosystem II reaction center protein Z



- Molecule 24: Photosystem II reaction center protein Z



There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	136521	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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	1	0.36	0/1720	0.50	0/2342
1	2	0.32	0/1716	0.51	1/2337 (0.0%)
1	5	0.37	0/1720	0.50	0/2342
1	6	0.33	0/1716	0.51	1/2337 (0.0%)
1	G	0.39	0/1720	0.52	0/2342
1	N	0.44	0/1720	0.56	0/2342
1	Y	0.43	0/1720	0.55	0/2342
1	g	0.39	0/1720	0.52	0/2342
1	n	0.45	0/1720	0.56	0/2342
1	y	0.43	0/1720	0.55	0/2342
10	H	0.50	0/461	0.56	0/626
10	h	0.50	0/461	0.56	0/626
11	I	0.52	0/286	0.68	0/386
11	i	0.52	0/286	0.68	0/386
12	J	0.58	1/262 (0.4%)	0.70	0/354
12	j	0.58	1/262 (0.4%)	0.70	0/354
13	K	0.48	0/318	0.63	0/434
13	k	0.48	0/318	0.63	0/434
14	L	0.57	0/319	0.59	0/434
14	l	0.57	0/319	0.59	0/434
15	M	0.44	0/260	0.66	0/355
15	m	0.44	0/260	0.66	0/355
16	O	0.43	0/1906	0.60	0/2575
16	o	0.43	0/1906	0.60	0/2575
17	P	0.54	0/1464	0.63	0/1978
17	p	0.54	0/1464	0.63	0/1978
18	Q	0.29	0/1051	0.59	0/1414
18	q	0.29	0/1051	0.59	0/1414
19	R	0.50	0/1886	0.59	0/2569
19	r	0.50	0/1886	0.59	0/2569
2	3	0.37	0/1759	0.53	0/2396

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	7	0.37	0/1759	0.53	0/2396
20	S	0.43	0/1736	0.65	0/2359
20	s	0.43	0/1736	0.65	0/2359
21	T	0.46	0/269	0.51	0/365
21	t	0.46	0/269	0.51	0/365
22	W	0.55	0/429	0.63	0/581
22	w	0.55	0/429	0.63	0/581
23	X	0.33	0/279	0.48	0/380
23	x	0.33	0/279	0.48	0/380
24	Z	0.42	0/474	0.55	0/648
24	z	0.42	0/474	0.55	0/648
3	4	0.34	0/1586	0.55	0/2158
3	8	0.34	0/1586	0.55	0/2158
4	A	0.54	0/2697	0.62	1/3677 (0.0%)
4	a	0.54	0/2697	0.62	1/3677 (0.0%)
5	B	0.54	0/4081	0.60	0/5556
5	b	0.54	0/4081	0.61	0/5556
6	C	0.58	0/3614	0.63	0/4922
6	c	0.58	0/3614	0.63	0/4922
7	D	0.47	0/2804	0.61	0/3823
7	d	0.48	0/2804	0.61	0/3823
8	E	0.47	0/630	0.52	0/857
8	e	0.48	0/630	0.52	0/857
9	F	0.60	0/248	0.64	0/335
9	f	0.60	0/248	0.64	0/335
All	All	0.47	2/74830 (0.0%)	0.59	4/101774 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	j	11	TRP	CB-CG	-5.25	1.40	1.50
12	J	11	TRP	CB-CG	-5.24	1.40	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	197	GLN	CA-CB-CG	5.70	125.94	113.40
1	2	197	GLN	CA-CB-CG	5.69	125.92	113.40
4	A	140	ARG	NE-CZ-NH1	-5.28	117.66	120.30
4	a	140	ARG	NE-CZ-NH1	-5.28	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	23	0
1	2	1664	0	1593	24	0
1	5	1668	0	1596	21	0
1	6	1664	0	1593	22	0
1	G	1668	0	1596	35	0
1	N	1668	0	1596	26	0
1	Y	1668	0	1596	36	0
1	g	1668	0	1596	0	0
1	n	1668	0	1596	0	0
1	y	1668	0	1596	0	0
2	3	1707	0	1659	23	0
2	7	1707	0	1659	23	0
3	4	1534	0	1486	21	0
3	8	1534	0	1486	22	0
4	A	2616	0	2522	101	0
4	a	2616	0	2522	0	0
5	B	3948	0	3818	85	0
5	b	3948	0	3818	0	0
6	C	3497	0	3422	92	0
6	c	3497	0	3422	0	0
7	D	2712	0	2604	78	0
7	d	2712	0	2604	0	0
8	E	612	0	595	5	0
8	e	612	0	595	0	0
9	F	241	0	246	2	0
9	f	241	0	246	0	0
10	H	452	0	473	17	0
10	h	452	0	473	0	0
11	I	278	0	291	7	0
11	i	278	0	291	0	0
12	J	256	0	269	4	0
12	j	256	0	269	0	0
13	K	306	0	313	7	0
13	k	306	0	313	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L	311	0	299	13	0
14	l	311	0	299	0	0
15	M	256	0	284	5	0
15	m	256	0	284	0	0
16	O	1870	0	1851	36	0
16	o	1870	0	1851	0	0
17	P	1434	0	1392	23	0
17	p	1434	0	1392	0	0
18	Q	1034	0	1075	22	0
18	q	1034	0	1075	0	0
19	R	1835	0	1801	46	0
19	r	1835	0	1801	0	0
20	S	1689	0	1670	39	0
20	s	1689	0	1670	0	0
21	T	261	0	280	9	0
21	t	261	0	280	0	0
22	W	419	0	402	5	0
22	w	419	0	402	0	0
23	X	276	0	301	8	0
23	x	276	0	301	0	0
24	Z	464	0	493	9	0
24	z	464	0	493	0	0
25	1	309	0	244	11	0
25	2	306	0	238	5	0
25	3	316	0	254	17	0
25	4	229	0	152	7	0
25	5	309	0	244	11	0
25	6	306	0	238	6	0
25	7	316	0	254	18	0
25	8	229	0	152	7	0
25	G	355	0	335	26	0
25	N	362	0	350	13	0
25	R	225	0	201	13	0
25	S	196	0	144	5	0
25	Y	362	0	350	15	0
25	g	355	0	335	0	0
25	n	362	0	350	0	0
25	r	225	0	201	0	0
25	s	196	0	144	0	0
25	y	362	0	350	0	0
26	1	412	0	348	10	0
26	2	391	0	314	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	3	426	0	373	12	0
26	4	270	0	198	4	0
26	5	412	0	348	9	0
26	6	391	0	314	9	0
26	7	426	0	373	10	0
26	8	270	0	198	3	0
26	A	240	0	242	20	0
26	B	1040	0	1152	66	0
26	C	845	0	936	47	0
26	D	130	0	144	10	0
26	G	477	0	477	25	0
26	N	473	0	468	28	0
26	R	543	0	490	36	0
26	S	465	0	393	22	0
26	Y	473	0	468	27	0
26	a	240	0	242	0	0
26	b	1040	0	1152	0	0
26	c	845	0	936	0	0
26	d	130	0	144	0	0
26	g	477	0	477	0	0
26	n	473	0	468	0	0
26	r	543	0	490	0	0
26	s	465	0	393	0	0
26	y	473	0	468	0	0
27	1	84	0	112	9	0
27	2	84	0	112	8	0
27	3	84	0	112	7	0
27	4	42	0	56	2	0
27	5	84	0	112	8	0
27	6	84	0	112	6	0
27	7	84	0	112	5	0
27	8	42	0	56	3	0
27	G	84	0	112	14	0
27	N	84	0	112	11	0
27	R	42	0	56	5	0
27	S	84	0	112	7	0
27	Y	84	0	112	10	0
27	g	84	0	112	0	0
27	n	84	0	112	0	0
27	r	42	0	56	0	0
27	s	84	0	112	0	0
27	y	84	0	112	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	1	44	0	56	4	0
28	2	44	0	56	6	0
28	3	44	0	56	3	0
28	4	44	0	56	2	0
28	5	44	0	56	3	0
28	6	44	0	56	4	0
28	7	44	0	56	3	0
28	8	44	0	56	3	0
28	G	44	0	56	6	0
28	N	44	0	56	7	0
28	R	44	0	56	5	0
28	Y	44	0	56	7	0
28	g	44	0	56	0	0
28	n	44	0	56	0	0
28	r	44	0	56	0	0
28	y	44	0	56	0	0
29	1	44	0	56	2	0
29	2	44	0	56	1	0
29	3	44	0	56	3	0
29	5	44	0	56	2	0
29	6	44	0	56	0	0
29	7	44	0	56	3	0
29	G	44	0	56	5	0
29	N	44	0	56	2	0
29	R	44	0	56	6	0
29	S	44	0	56	3	0
29	Y	44	0	56	3	0
29	g	44	0	56	0	0
29	n	44	0	56	0	0
29	r	44	0	56	0	0
29	s	44	0	56	0	0
29	y	44	0	56	0	0
30	1	41	0	55	2	0
30	2	37	0	44	1	0
30	3	47	0	67	2	0
30	4	21	0	12	1	0
30	5	41	0	55	2	0
30	6	37	0	44	1	0
30	7	47	0	67	1	0
30	8	21	0	12	1	0
30	B	96	0	141	6	0
30	C	147	0	222	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	D	138	0	195	18	0
30	G	49	0	74	5	0
30	L	49	0	74	3	0
30	N	49	0	74	4	0
30	R	42	0	57	5	0
30	S	49	0	74	5	0
30	Y	49	0	74	4	0
30	b	96	0	141	0	0
30	c	147	0	222	0	0
30	d	138	0	195	0	0
30	g	49	0	74	0	0
30	l	49	0	74	0	0
30	n	49	0	74	0	0
30	r	42	0	57	0	0
30	s	49	0	74	0	0
30	y	49	0	74	0	0
31	4	40	0	56	7	0
31	8	40	0	56	8	0
31	A	40	0	56	6	0
31	B	120	0	168	16	0
31	C	160	0	224	24	0
31	D	40	0	56	3	0
31	H	40	0	56	7	0
31	T	40	0	56	10	0
31	a	40	0	56	0	0
31	b	120	0	168	0	0
31	c	160	0	224	0	0
31	d	40	0	56	0	0
31	h	40	0	56	0	0
31	t	40	0	56	0	0
32	A	10	0	0	0	0
32	a	10	0	0	0	0
33	A	1	0	0	0	0
33	a	1	0	0	0	0
34	A	2	0	0	0	0
34	a	2	0	0	0	0
35	A	128	0	148	11	0
35	a	128	0	148	0	0
36	A	104	0	144	13	0
36	B	96	0	126	8	0
36	a	104	0	144	0	0
36	b	96	0	126	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A	88	0	116	2	0
37	B	106	0	158	8	0
37	C	51	0	72	1	0
37	D	46	0	62	2	0
37	Z	51	0	72	6	0
37	a	88	0	116	0	0
37	b	106	0	158	0	0
37	c	51	0	72	0	0
37	d	46	0	62	0	0
37	z	51	0	72	0	0
38	A	13	0	7	1	0
38	D	55	0	80	2	0
38	a	13	0	7	0	0
38	d	55	0	80	0	0
39	B	59	0	76	5	0
39	C	177	0	227	6	0
39	H	62	0	82	4	0
39	b	59	0	76	0	0
39	c	177	0	227	0	0
39	h	62	0	82	0	0
40	D	4	0	0	0	0
40	d	4	0	0	0	0
41	F	43	0	30	0	0
41	f	43	0	30	0	0
42	A	96	0	0	0	0
42	B	89	0	0	0	0
42	C	68	0	0	0	0
42	D	58	0	0	0	0
42	E	10	0	0	0	0
42	F	2	0	0	0	0
42	G	15	0	0	1	0
42	H	16	0	0	0	0
42	J	3	0	0	0	0
42	K	2	0	0	0	0
42	L	10	0	0	0	0
42	M	4	0	0	0	0
42	N	20	0	0	0	0
42	O	31	0	0	0	0
42	P	16	0	0	0	0
42	R	30	0	0	0	0
42	S	14	0	0	1	0
42	T	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	W	4	0	0	0	0
42	X	5	0	0	0	0
42	Y	39	0	0	0	0
42	Z	4	0	0	0	0
42	a	96	0	0	0	0
42	b	89	0	0	0	0
42	c	68	0	0	0	0
42	d	58	0	0	0	0
42	e	10	0	0	0	0
42	f	2	0	0	0	0
42	g	15	0	0	0	0
42	h	16	0	0	0	0
42	j	3	0	0	0	0
42	k	2	0	0	0	0
42	l	10	0	0	0	0
42	m	4	0	0	0	0
42	n	20	0	0	0	0
42	o	31	0	0	0	0
42	p	16	0	0	0	0
42	r	30	0	0	0	0
42	s	14	0	0	0	0
42	t	2	0	0	0	0
42	w	4	0	0	0	0
42	x	5	0	0	0	0
42	y	39	0	0	0	0
42	z	4	0	0	0	0
All	All	98986	0	97642	1210	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 6.

All (1210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:611:CLA:HAB	3:8:130:TRP:CD1	175.49	0.87
3:4:130:TRP:CD1	26:R:611:CLA:HAB	2.08	0.87
31:4:623:BCR:HC42	26:R:601:CLA:HBB1	1.62	0.82
26:R:601:CLA:HBB1	31:8:623:BCR:HC42	166.40	0.79
6:C:383:ASP:HB3	18:Q:79:LEU:HD21	1.65	0.78
3:4:130:TRP:HD1	26:R:611:CLA:HAB	1.48	0.78
26:R:611:CLA:HAB	3:8:130:TRP:HD1	174.94	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:7:602:CLA:HAB	27:7:1621:LUT:H32	1.67	0.75
20:S:139:VAL:HG22	25:S:607:CHL:HBC1	1.69	0.75
19:R:93:ARG:NH1	19:R:96:GLU:OE2	2.20	0.75
4:A:257:ARG:CD	5:B:498:LEU:HD21	2.18	0.74
26:3:602:CLA:HAB	27:3:1621:LUT:H32	1.67	0.74
5:B:12:VAL:HG12	26:B:613:CLA:HMC2	1.71	0.73
5:B:385:ARG:NH1	16:O:167:GLY:O	2.22	0.73
31:C:517:BCR:H332	24:Z:12:LEU:HD23	1.71	0.73
26:N:610:CLA:H71	26:N:612:CLA:H101	1.71	0.73
4:A:257:ARG:HD3	5:B:498:LEU:HD21	1.70	0.72
5:B:121:GLU:HG3	10:H:16:ARG:HD3	1.71	0.72
26:5:602:CLA:HAB	27:5:1621:LUT:H32	1.72	0.72
26:B:603:CLA:H12	10:H:61:TYR:CD2	2.26	0.71
30:C:2630:LHG:H152	30:S:2630:LHG:H111	1.72	0.70
30:D:409:LHG:H291	21:T:17:ILE:HG23	1.72	0.70
4:A:243:GLU:N	4:A:243:GLU:OE2	2.24	0.70
26:1:602:CLA:HAB	27:1:1621:LUT:H32	1.72	0.70
26:G:610:CLA:H52	27:G:1620:LUT:H28	1.74	0.70
36:A:418:SQD:C26	31:T:101:BCR:H333	2.22	0.69
35:A:409:PHO:HBC3	7:D:280:LEU:HD22	1.75	0.69
36:B:623:SQD:H281	15:M:21:PHE:HB2	1.75	0.69
36:B:621:SQD:H352	31:T:101:BCR:H362	28.49	0.68
7:D:260:VAL:HG21	30:D:409:LHG:H281	1.76	0.68
30:D:409:LHG:H322	21:T:21:ILE:HD11	1.76	0.68
6:C:472:LEU:HD21	7:D:256:GLN:HE21	1.58	0.68
4:A:221:SER:HA	7:D:140:ARG:HB2	1.75	0.67
20:S:202:GLY:O	20:S:206:GLN:HB3	1.93	0.67
6:C:393:ALA:HB1	18:Q:27:ARG:HG3	1.77	0.67
5:B:75:TRP:HB3	39:B:626:DGD:HD5	1.76	0.67
26:7:611:CLA:H3A	3:8:131:SER:HA	1.77	0.67
19:R:30:GLY:H	19:R:93:ARG:NH2	1.93	0.66
5:B:15:ASP:OD2	14:L:5:ASN:ND2	2.28	0.66
20:S:100:LYS:NZ	20:S:216:GLU:OE1	2.28	0.66
5:B:311:PHE:O	5:B:317:ASN:ND2	2.29	0.66
26:B:604:CLA:HAB	26:B:606:CLA:H152	1.78	0.66
7:D:193:THR:HG23	26:D:402:CLA:HBC2	1.78	0.66
26:3:611:CLA:H3A	3:4:131:SER:HA	1.77	0.66
4:A:40:THR:HG23	26:A:410:CLA:HBB1	1.78	0.66
28:N:1622:XAT:H363	30:N:2630:LHG:HC41	1.77	0.65
7:D:173:SER:HB2	7:D:178:ALA:HB1	1.79	0.65
19:R:163:ASN:HD22	26:R:616:CLA:HBC3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:A:418:SQD:H181	30:D:409:LHG:H382	1.78	0.65
7:D:124:ILE:HD11	39:H:102:DGD:HAH2	1.79	0.65
1:N:135:MET:HA	1:N:138:VAL:HG22	1.79	0.65
6:C:297:TYR:O	6:C:423:ARG:NH2	2.30	0.65
21:T:15:GLY:HA2	31:T:101:BCR:H12C	1.79	0.65
26:G:613:CLA:H162	26:G:614:CLA:H2	1.79	0.64
4:A:217:SER:HA	7:D:273:LEU:HD12	1.79	0.64
4:A:82:ILE:HB	4:A:174:LEU:HB2	1.79	0.64
19:R:214:VAL:HG12	26:R:613:CLA:HMD3	1.79	0.64
1:G:139:GLU:HG3	25:G:609:CHL:C4B	2.28	0.64
31:C:517:BCR:H312	13:K:33:LEU:HD13	1.80	0.64
1:Y:135:MET:HA	1:Y:138:VAL:HG22	1.80	0.64
8:E:57:THR:O	8:E:61:GLN:NE2	2.31	0.64
6:C:86:LEU:HD13	6:C:89:LEU:HD12	1.80	0.63
17:P:117:SER:HB2	17:P:128:ASN:HB2	1.80	0.63
25:G:606:CHL:HMB1	25:G:609:CHL:HAC1	1.80	0.63
4:A:143:ILE:HG13	7:D:221:ASN:HD22	1.63	0.63
26:3:603:CLA:HMA2	26:3:603:CLA:H2	1.81	0.63
1:6:85:LEU:HD23	1:6:88:ASN:HD22	1.64	0.63
30:B:2631:LHG:H242	30:B:2631:LHG:HC91	1.81	0.63
5:B:187:VAL:HG23	26:B:602:CLA:HMD3	1.81	0.63
30:C:2630:LHG:H101	26:S:611:CLA:HAB	1.81	0.63
14:L:15:ARG:NH2	21:T:25:GLU:OE1	2.32	0.62
12:J:40:LEU:HD11	17:P:14:THR:HG22	1.81	0.62
4:A:243:GLU:CD	4:A:243:GLU:H	2.03	0.62
19:R:21:PRO:HD2	19:R:24:LEU:HD13	1.80	0.62
26:7:603:CLA:HMA2	26:7:603:CLA:H2	1.81	0.62
1:G:70:ARG:NE	1:G:180:GLU:OE2	2.33	0.62
1:G:142:ARG:NH2	25:G:609:CHL:O1D	2.32	0.62
1:1:163:PRO:HD2	27:1:1620:LUT:H23	1.81	0.61
16:O:117:GLN:HE21	16:O:121:GLY:HA2	1.65	0.61
16:O:51:LEU:HB3	16:O:89:ILE:HB	1.82	0.61
25:7:606:CHL:HBB2	25:7:607:CHL:HBB1	1.82	0.61
38:D:405:PL9:H111	30:D:409:LHG:HC92	1.81	0.61
1:Y:115:ASN:HB3	1:Y:118:LEU:HD12	1.82	0.61
26:A:407:CLA:HAB	26:D:402:CLA:H72	1.82	0.61
1:2:85:LEU:HD23	1:2:88:ASN:HD22	1.64	0.61
6:C:240:LEU:HD21	26:C:501:CLA:CHC	2.31	0.61
20:S:147:GLY:HA2	26:S:609:CLA:HAB	1.83	0.61
2:3:171:TYR:O	2:3:172:PHE:HB2	2.00	0.61
25:3:606:CHL:HBB2	25:3:607:CHL:HBB1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:159:LEU:HD22	26:C:505:CLA:H202	1.83	0.61
19:R:97:LEU:HB3	19:R:172:LEU:HD11	1.82	0.61
2:7:171:TYR:O	2:7:172:PHE:HB2	2.00	0.61
6:C:130:ILE:HD11	31:C:517:BCR:H21C	1.83	0.61
31:B:620:BCR:H271	21:T:22:PHE:HB3	46.51	0.60
1:5:163:PRO:HD2	27:5:1620:LUT:H23	1.81	0.60
26:7:603:CLA:HMD1	25:7:609:CHL:HBA2	1.83	0.60
19:R:100:GLY:HA3	19:R:202:ALA:HB1	1.84	0.60
25:R:606:CHL:HBA2	29:R:623:NEX:H403	1.83	0.60
26:A:410:CLA:HAA2	37:A:413:LMG:H112	1.82	0.60
4:A:65:GLU:OE2	4:A:334:ARG:NH2	2.35	0.60
4:A:63:ILE:HB	6:C:335:THR:HG21	1.84	0.60
8:E:69:ARG:NH2	10:H:62:ASN:O	2.34	0.60
4:A:136:ARG:NH1	11:I:27:ASP:OD1	2.33	0.60
1:Y:164:LEU:HD12	27:Y:1620:LUT:H222	1.84	0.60
26:2:603:CLA:HMD1	25:2:609:CHL:HBA2	1.83	0.60
26:8:610:CLA:HAB	27:8:620:LUT:H32	1.84	0.60
26:C:511:CLA:HBA1	31:C:517:BCR:H271	1.84	0.60
20:S:200:MET:HG2	27:S:1621:LUT:H14	1.83	0.60
4:A:27:ARG:NH2	7:D:259:GLY:O	2.33	0.59
1:N:51:LEU:HD13	26:N:602:CLA:H42	1.84	0.59
16:O:81:ARG:NH1	22:W:9:GLU:OE2	2.30	0.59
26:3:603:CLA:HMD1	25:3:609:CHL:HBA2	1.83	0.59
1:G:103:GLN:NE2	26:G:604:CLA:O1D	2.36	0.59
5:B:191:ASP:HB2	10:H:70:ILE:HG12	1.84	0.59
26:C:503:CLA:H172	26:C:510:CLA:HBB2	1.85	0.59
31:C:516:BCR:H373	13:K:49:LEU:HD13	1.84	0.59
26:Y:603:CLA:HMD3	25:Y:607:CHL:H193	1.84	0.59
20:S:170:PHE:O	27:S:1620:LUT:H24	2.03	0.59
26:6:603:CLA:HMD1	25:6:609:CHL:HBA2	1.83	0.59
6:C:313:GLN:HG3	6:C:396:MET:HE3	1.86	0.59
25:1:607:CHL:HAA2	28:3:1622:XAT:H41	1.84	0.58
5:B:145:LEU:HB3	26:B:605:CLA:H162	1.84	0.58
18:Q:50:ARG:NH1	18:Q:87:ASP:OD1	2.36	0.58
35:A:409:PHO:H3A	26:D:402:CLA:H142	1.84	0.58
4:A:42:LEU:HD23	36:A:418:SQD:H212	1.85	0.58
31:B:618:BCR:H322	37:B:622:LMG:H111	1.85	0.58
4:A:335:ASN:HA	7:D:351:ASN:HD22	1.69	0.58
5:B:334:ASP:HB3	16:O:176:ALA:HB1	1.86	0.58
26:B:608:CLA:H2	37:B:622:LMG:H151	1.85	0.58
26:6:611:CLA:HBA2	26:6:612:CLA:HMD1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:391:ARG:NH1	6:C:395:TYR:OH	2.36	0.58
6:C:78:GLU:HB2	18:Q:32:PRO:HB3	1.86	0.58
25:G:606:CHL:CBA	29:G:1623:NEX:H403	2.34	0.58
26:4:610:CLA:HAB	27:4:620:LUT:H32	1.84	0.58
26:5:603:CLA:HMD1	25:5:609:CHL:HBA2	1.86	0.58
20:S:166:PRO:HB3	25:S:608:CHL:HBC2	1.85	0.58
7:D:187:GLN:HB2	26:D:402:CLA:HBC1	1.86	0.58
17:P:62:LEU:HD11	17:P:158:ILE:HD12	1.86	0.58
4:A:131:TRP:CH2	6:C:449:ARG:HD2	2.39	0.57
1:N:70:ARG:NE	1:N:180:GLU:OE2	2.37	0.57
5:B:127:ARG:HG3	5:B:128:THR:HG23	1.86	0.57
26:G:602:CLA:H92	26:G:603:CLA:HMA1	1.86	0.57
26:2:611:CLA:HBA2	26:2:612:CLA:HMD1	1.86	0.57
5:B:496:GLN:HB2	5:B:503:THR:HB	1.86	0.57
6:C:148:GLY:O	6:C:156:LYS:NZ	2.37	0.57
6:C:332:GLN:HE21	6:C:336:GLY:HA2	1.70	0.57
1:2:51:LEU:HD13	26:2:602:CLA:H42	1.86	0.57
25:5:607:CHL:HAA2	28:7:1622:XAT:H41	1.84	0.57
4:A:341:LEU:H	6:C:313:GLN:HE22	1.53	0.57
6:C:343:ARG:NH1	6:C:347:GLY:O	2.38	0.57
4:A:131:TRP:CZ2	6:C:449:ARG:HD2	2.40	0.57
8:E:14:ILE:O	8:E:20:TRP:NE1	2.38	0.57
26:R:613:CLA:H111	30:R:2630:LHG:H292	1.86	0.57
1:6:51:LEU:HD13	26:6:602:CLA:H42	1.86	0.57
1:N:192:PHE:CD2	26:N:602:CLA:H171	2.40	0.57
4:A:140:ARG:NH1	7:D:232:THR:HG21	2.20	0.57
19:R:96:GLU:HB2	26:R:602:CLA:C1B	2.35	0.57
26:8:612:CLA:H2A	26:8:612:CLA:HED2	1.87	0.57
5:B:30:VAL:HG11	26:B:613:CLA:H112	1.87	0.57
26:B:603:CLA:H12	10:H:61:TYR:HD2	1.69	0.57
6:C:387:TRP:HB2	18:Q:38:PHE:HD2	1.70	0.57
1:2:21:ARG:NH1	1:2:37:THR:O	2.38	0.56
4:A:140:ARG:HB2	7:D:221:ASN:HA	1.87	0.56
4:A:340:PRO:HB2	17:P:166:LYS:HB3	1.86	0.56
26:B:615:CLA:H8	31:B:618:BCR:H362	1.88	0.56
26:N:610:CLA:H92	27:N:1620:LUT:H371	1.87	0.56
20:S:125:ASN:ND2	20:S:130:ASN:OD1	2.38	0.56
26:1:603:CLA:HMD1	25:1:609:CHL:HBA2	1.86	0.56
4:A:234:ASN:HB3	7:D:264:ASN:HD21	1.70	0.56
6:C:83:GLU:OE2	6:C:398:HIS:NE2	2.38	0.56
26:4:612:CLA:HED2	26:4:612:CLA:H2A	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:GLU:HA	1:G:155:LEU:HD21	1.86	0.56
26:N:603:CLA:HMD1	25:N:609:CHL:HBA2	1.87	0.56
4:A:147:TYR:OH	35:A:408:PHO:O1A	2.22	0.56
5:B:334:ASP:N	5:B:334:ASP:OD1	2.39	0.56
1:G:126:ALA:HB3	25:G:605:CHL:HMC	1.88	0.56
17:P:39:GLU:O	17:P:40:ARG:NH1	2.35	0.56
26:B:605:CLA:H203	30:B:2631:LHG:H342	1.87	0.56
1:6:222:TRP:HB3	2:7:115:PHE:HZ	1.71	0.56
7:D:183:ILE:HA	26:D:402:CLA:HMD2	1.88	0.56
25:Y:601:CHL:HMA3	30:Y:2630:LHG:H121	1.88	0.56
25:2:606:CHL:HMB1	25:2:609:CHL:HAC1	1.88	0.56
26:3:611:CLA:HBA1	26:3:612:CLA:HMD1	1.88	0.56
1:6:21:ARG:NH1	1:6:37:THR:O	2.38	0.56
3:8:138:VAL:HG22	3:8:140:SER:H	1.71	0.56
1:5:99:LYS:HA	25:5:607:CHL:HED3	1.87	0.56
4:A:64:ARG:O	16:O:152:ARG:NH1	2.33	0.56
26:C:501:CLA:HBB1	26:C:507:CLA:H41	1.88	0.56
7:D:307:ALA:O	16:O:188:GLU:HG3	2.06	0.56
26:G:603:CLA:H12	1:N:51:LEU:HD11	1.88	0.56
1:G:64:LEU:HD11	1:N:49:ALA:HA	1.88	0.55
1:1:99:LYS:HA	25:1:607:CHL:HED3	1.87	0.55
1:2:222:TRP:HB3	2:3:115:PHE:HZ	1.71	0.55
35:A:409:PHO:OBD	7:D:130:GLN:NE2	2.39	0.55
25:6:606:CHL:HMB1	25:6:609:CHL:HAC1	1.88	0.55
26:C:509:CLA:H192	26:C:512:CLA:HMD2	1.88	0.55
16:O:74:GLN:HE21	16:O:118:LEU:HD22	1.70	0.55
6:C:48:LYS:HE2	6:C:138:GLU:HG2	1.88	0.55
26:C:502:CLA:HBB2	26:C:510:CLA:H151	1.88	0.55
31:C:516:BCR:H311	24:Z:20:LEU:HD11	1.89	0.55
16:O:32:ILE:HG23	16:O:208:LYS:HE2	1.88	0.55
3:4:138:VAL:HG22	3:4:140:SER:H	1.71	0.55
1:5:21:ARG:NH2	1:5:36:LEU:O	2.40	0.55
20:S:146:VAL:HG11	26:S:609:CLA:HMC3	1.88	0.55
1:6:110:LEU:HD21	26:6:604:CLA:HAA2	1.88	0.55
1:G:163:PRO:HD2	27:G:1620:LUT:H23	1.89	0.55
19:R:135:TYR:CD2	25:Y:605:CHL:H11	144.85	0.55
1:5:103:GLN:HE22	26:5:604:CLA:HED3	1.72	0.55
4:A:305:SER:HA	12:J:39:SER:HB3	1.89	0.55
26:A:406:CLA:H72	35:A:408:PHO:HMB3	1.89	0.55
6:C:454:GLY:O	11:I:34:ARG:NH2	2.40	0.55
26:R:612:CLA:H2A	26:R:612:CLA:H2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:110:LEU:HD21	26:2:604:CLA:HAA2	1.88	0.55
1:5:104:ILE:HG21	1:5:124:ILE:HD13	1.88	0.55
26:7:611:CLA:HBA1	26:7:612:CLA:HMD1	1.88	0.55
19:R:30:GLY:H	19:R:93:ARG:HH22	1.55	0.55
2:7:114:ILE:HG21	2:7:134:ILE:HD13	1.90	0.54
1:G:51:LEU:HD11	26:Y:603:CLA:H12	1.90	0.54
1:1:103:GLN:HE22	26:1:604:CLA:HED3	1.72	0.54
1:5:197:GLN:HE22	27:5:1620:LUT:H42	1.71	0.54
2:7:79:ARG:NH1	25:7:608:CHL:OBD	2.40	0.54
1:N:64:LEU:HD11	1:Y:49:ALA:HA	1.89	0.54
5:B:124:CYS:O	10:H:24:LYS:NZ	2.40	0.54
20:S:210:THR:HG22	20:S:233:VAL:HG11	1.89	0.54
1:1:104:ILE:HG21	1:1:124:ILE:HD13	1.88	0.54
1:N:63:GLU:HA	1:N:155:LEU:HD21	1.88	0.54
2:3:114:ILE:HG21	2:3:134:ILE:HD13	1.89	0.54
4:A:24:THR:O	7:D:252:ARG:NH2	2.39	0.54
6:C:318:LEU:HD12	6:C:340:TYR:HB3	1.90	0.54
20:S:60:ASP:OD1	27:S:1621:LUT:O23	2.26	0.54
1:Y:163:PRO:HD2	27:Y:1620:LUT:H23	1.90	0.54
30:B:2630:LHG:H341	37:B:2633:LMG:H202	1.89	0.54
5:B:256:MET:HA	5:B:263:THR:HG21	1.90	0.54
3:4:129:PRO:HD3	26:R:601:CLA:HBB2	1.90	0.54
20:S:50:THR:O	20:S:50:THR:HG22	2.08	0.54
1:1:197:GLN:HE22	27:1:1620:LUT:H42	1.71	0.54
2:7:173:ASP:OD1	27:7:1620:LUT:O23	2.26	0.54
4:A:85:THR:HA	4:A:109:GLY:HA3	1.90	0.54
31:C:516:BCR:HC21	24:Z:13:ILE:HG23	1.89	0.54
4:A:267:ASN:ND2	7:D:233:PHE:O	2.40	0.54
1:1:21:ARG:NH2	1:1:36:LEU:O	2.40	0.54
1:6:164:LEU:HD12	27:6:1620:LUT:H222	1.90	0.54
1:G:49:ALA:HA	1:Y:64:LEU:HD11	1.90	0.54
19:R:135:TYR:HD2	25:Y:605:CHL:H11	145.18	0.54
20:S:212:GLU:OE2	20:S:220:LYS:NZ	2.41	0.54
1:Y:80:VAL:HG13	1:Y:206:LEU:HD11	1.90	0.54
3:8:58:GLY:HA3	3:8:184:ALA:HB1	1.90	0.53
30:C:523:LHG:H112	30:C:523:LHG:H241	1.89	0.53
3:4:191:MET:HG2	28:4:622:XAT:H12	1.90	0.53
3:4:58:GLY:HA3	3:4:184:ALA:HB1	1.90	0.53
26:7:603:CLA:HED2	25:7:609:CHL:H93	1.91	0.53
7:D:303:GLU:OE1	16:O:160:LYS:HE2	2.08	0.53
1:Y:217:VAL:O	1:Y:217:VAL:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:212:HIS:CG	26:N:613:CLA:HAA2	2.44	0.53
20:S:172:PRO:HD2	27:S:1620:LUT:H23	1.89	0.53
31:C:517:BCR:H333	24:Z:9:VAL:HG13	1.91	0.53
3:8:191:MET:HG2	28:8:622:XAT:H12	1.90	0.53
5:B:121:GLU:HG3	10:H:16:ARG:CD	2.39	0.53
7:D:313:GLU:HB2	16:O:159:PRO:HG3	1.90	0.53
16:O:207:THR:HG22	16:O:214:VAL:HG22	1.91	0.53
19:R:227:TRP:HB2	27:R:620:LUT:H21	1.90	0.53
4:A:45:THR:HG23	26:A:406:CLA:H201	1.91	0.53
1:N:65:GLU:OE2	1:N:185:ARG:NE	2.41	0.53
26:C:513:CLA:H71	30:C:2630:LHG:H122	1.91	0.53
4:A:129:ARG:NH2	7:D:256:GLN:O	2.42	0.53
25:G:606:CHL:HBA1	29:G:1623:NEX:H403	1.90	0.53
16:O:65:VAL:HA	16:O:71:LEU:HD21	1.91	0.53
1:Y:51:LEU:HD13	26:Y:602:CLA:H42	1.91	0.53
24:Z:23:VAL:HB	24:Z:24:PRO:HD3	1.91	0.53
2:3:173:ASP:OD1	27:3:1620:LUT:O23	2.26	0.53
5:B:472:ARG:HD3	5:B:479:PHE:CE1	2.44	0.53
16:O:143:SER:HA	16:O:201:THR:HA	1.91	0.53
1:Y:104:ILE:HG21	1:Y:124:ILE:HD13	1.91	0.53
4:A:183:MET:HA	26:A:405:CLA:HMD2	1.92	0.53
5:B:30:VAL:HG12	26:B:606:CLA:HHD	1.91	0.53
1:2:164:LEU:HD12	27:2:1620:LUT:H222	1.90	0.52
2:7:141:GLN:HE22	25:7:607:CHL:HMC	1.74	0.52
26:R:601:CLA:HBB2	3:8:129:PRO:HD3	170.23	0.52
4:A:198:HIS:HA	4:A:286:THR:HG22	1.91	0.52
6:C:402:GLY:HA3	6:C:420:VAL:HG22	1.92	0.52
1:G:176:LEU:HD23	1:G:179:LYS:HD2	1.91	0.52
1:G:69:SER:HB3	1:G:184:GLY:HA3	1.91	0.52
1:N:225:ALA:HA	28:N:1622:XAT:H42	1.91	0.52
17:P:87:LEU:O	17:P:160:LYS:NZ	2.41	0.52
26:R:602:CLA:H72	28:R:622:XAT:H28	1.90	0.52
4:A:43:THR:HG23	31:A:411:BCR:H362	1.91	0.52
14:L:20:TRP:HA	14:L:20:TRP:CE3	2.45	0.52
16:O:180:GLY:O	16:O:189:ASN:ND2	2.42	0.52
16:O:227:ASP:HB3	16:O:230:ALA:HB3	1.91	0.52
18:Q:50:ARG:HD2	18:Q:83:TYR:CD1	2.44	0.52
35:A:408:PHO:H51	36:A:418:SQD:H201	1.91	0.52
7:D:108:LEU:HD23	8:E:66:ILE:HD13	1.92	0.52
6:C:282:PHE:HE1	26:C:501:CLA:H111	1.74	0.52
30:D:409:LHG:HC11	14:L:14:ASN:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:602:CLA:H101	27:Y:1621:LUT:H371	1.91	0.52
4:A:288:LEU:HD22	6:C:432:VAL:HG22	1.91	0.52
5:B:255:THR:HG21	26:B:603:CLA:HED1	1.92	0.52
18:Q:58:ILE:HD11	18:Q:84:LEU:HD11	1.92	0.52
20:S:99:ASN:ND2	20:S:103:ALA:O	2.43	0.52
4:A:47:VAL:HG21	4:A:114:LEU:HD22	1.92	0.52
3:4:29:LEU:HD11	3:4:51:ARG:HD3	1.92	0.52
19:R:59:LYS:HE2	19:R:61:LEU:HD21	1.92	0.52
1:Y:63:GLU:HA	1:Y:155:LEU:HD21	1.92	0.52
26:3:603:CLA:HED2	25:3:609:CHL:H93	1.91	0.52
4:A:215:HIS:HB2	38:A:414:PL9:HC8	1.92	0.52
5:B:157:HIS:HE1	26:B:607:CLA:NA	2.07	0.52
7:D:79:VAL:HB	7:D:174:PHE:HB2	1.92	0.52
20:S:113:LYS:HA	25:S:607:CHL:HED3	1.91	0.52
25:8:606:CHL:HAA1	31:8:623:BCR:H19C	1.92	0.52
1:G:139:GLU:HG3	25:G:609:CHL:NB	2.25	0.52
25:1:601:CHL:HMA3	30:1:2630:LHG:H121	1.92	0.52
2:3:104:GLU:O	2:3:113:GLN:NE2	2.43	0.52
25:4:606:CHL:HAA1	31:4:623:BCR:H19C	1.92	0.52
25:G:601:CHL:HHC	25:G:601:CHL:HBB1	1.92	0.52
26:G:611:CLA:HMB3	30:G:2630:LHG:HC12	1.91	0.52
1:G:197:GLN:HG3	26:G:613:CLA:C1D	2.39	0.52
26:C:511:CLA:C4D	13:K:54:TRP:HH2	2.24	0.52
4:A:317:TRP:HZ3	7:D:181:ARG:HD2	1.75	0.51
1:N:80:VAL:HG13	1:N:206:LEU:HD11	1.91	0.51
6:C:131:TYR:OH	20:S:38:GLY:HA3	2.11	0.51
2:3:141:GLN:HE22	25:3:607:CHL:HMC	1.74	0.51
2:7:30:ARG:NH1	2:7:46:THR:O	2.43	0.51
4:A:27:ARG:NH1	7:D:255:SER:O	2.37	0.51
25:G:606:CHL:HBB2	25:G:607:CHL:HBB1	1.92	0.51
2:7:104:GLU:O	2:7:113:GLN:NE2	2.43	0.51
25:5:607:CHL:HBB1	25:7:601:CHL:H141	1.92	0.51
28:6:1622:XAT:H41	25:7:607:CHL:HAA2	1.93	0.51
4:A:84:PRO:HA	4:A:112:TYR:CG	2.45	0.51
6:C:396:MET:SD	18:Q:27:ARG:NH2	2.81	0.51
6:C:28:GLN:NE2	7:D:234:ARG:NE	2.59	0.51
10:H:33:VAL:HG21	19:R:48:PHE:HE1	1.74	0.51
16:O:60:VAL:HG22	16:O:236:VAL:HG22	1.92	0.51
17:P:108:VAL:HB	17:P:136:ALA:HB2	1.92	0.51
20:S:189:GLU:HG3	26:S:610:CLA:C4B	2.41	0.51
2:3:30:ARG:NH1	2:3:46:THR:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:162:ASP:OD1	27:5:1620:LUT:O23	2.28	0.51
1:6:104:ILE:HG21	1:6:124:ILE:HD13	1.92	0.51
3:8:29:LEU:HD11	3:8:51:ARG:HD3	1.92	0.51
5:B:168:VAL:HG13	5:B:195:PRO:HG2	1.93	0.51
6:C:94:THR:HG22	26:C:501:CLA:HED1	1.93	0.51
7:D:211:LEU:HA	7:D:214:ILE:HG22	1.92	0.51
21:T:17:ILE:HG22	31:T:101:BCR:H313	1.93	0.51
25:1:607:CHL:HBB1	25:3:601:CHL:H141	1.92	0.51
5:B:423:ARG:NH1	5:B:430:PHE:O	2.44	0.51
5:B:71:ILE:HD13	26:B:607:CLA:HED3	1.92	0.51
6:C:108:THR:O	6:C:108:THR:HG22	2.11	0.51
7:D:306:ALA:HB3	16:O:160:LYS:HE3	1.93	0.51
1:2:162:ASP:OD1	27:2:1620:LUT:O23	2.29	0.51
28:2:1622:XAT:H41	25:3:607:CHL:HAA2	1.93	0.51
4:A:170:ASP:OD2	6:C:357:ARG:NH1	2.40	0.51
5:B:315:ILE:HG12	5:B:321:LYS:HG3	1.92	0.51
26:C:510:CLA:H122	26:C:510:CLA:HMA3	1.93	0.51
7:D:25:ARG:NH1	23:X:79:ASP:O	2.43	0.51
1:2:104:ILE:HG21	1:2:124:ILE:HD13	1.92	0.51
26:4:611:CLA:HBA2	26:4:612:CLA:HMD1	1.92	0.51
25:5:601:CHL:HMA3	30:5:2630:LHG:H121	1.92	0.51
1:6:69:SER:HB3	1:6:184:GLY:HA3	1.93	0.51
25:7:606:CHL:HBA2	29:7:1623:NEX:H403	1.93	0.51
30:C:2630:LHG:H223	26:S:614:CLA:H2	1.93	0.51
7:D:18:ILE:HG22	23:X:76:SER:HB3	1.93	0.51
26:N:602:CLA:H203	27:N:1621:LUT:H391	1.93	0.51
1:2:69:SER:HB3	1:2:184:GLY:HA3	1.93	0.51
2:3:79:ARG:NH1	25:3:608:CHL:OBD	2.40	0.51
2:3:95:GLN:HE22	2:3:102:PHE:H	1.59	0.51
1:5:69:SER:HB3	1:5:184:GLY:HA3	1.93	0.51
2:7:95:GLN:HE22	2:7:102:PHE:H	1.59	0.51
5:B:157:HIS:HA	5:B:163:GLY:HA3	1.93	0.51
5:B:399:VAL:HG12	5:B:417:VAL:HG22	1.93	0.51
17:P:119:PRO:HG2	17:P:126:TYR:HB2	1.93	0.51
6:C:345:PRO:HB3	16:O:81:ARG:HD3	1.94	0.50
1:G:162:ASP:OD1	27:G:1620:LUT:O23	2.28	0.50
6:C:370:ARG:HH11	6:C:370:ARG:HG3	1.77	0.50
6:C:28:GLN:NE2	7:D:231:ASN:HD22	2.09	0.50
20:S:154:ILE:HD11	26:S:609:CLA:HMA1	1.93	0.50
1:Y:65:GLU:OE2	1:Y:185:ARG:NE	2.43	0.50
1:1:69:SER:HB3	1:1:184:GLY:HA3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:85:LEU:HA	1:2:88:ASN:HB2	1.94	0.50
4:A:114:LEU:O	4:A:118:HIS:ND1	2.33	0.50
4:A:116:VAL:HG13	4:A:158:PHE:HB3	1.93	0.50
26:B:611:CLA:H141	26:B:613:CLA:HBD	1.93	0.50
26:B:614:CLA:H172	31:B:619:BCR:H312	1.94	0.50
26:B:615:CLA:H43	36:B:621:SQD:H122	1.94	0.50
1:G:135:MET:HA	1:G:138:VAL:HG22	1.93	0.50
20:S:202:GLY:O	20:S:206:GLN:CB	2.59	0.50
25:Y:601:CHL:HHC	25:Y:601:CHL:HBB1	1.93	0.50
6:C:117:LEU:HD22	37:Z:101:LMG:H391	1.94	0.50
1:1:162:ASP:OD1	27:1:1620:LUT:O23	2.28	0.50
25:3:606:CHL:HBA2	29:3:1623:NEX:H403	1.93	0.50
6:C:262:ARG:NH1	30:C:522:LHG:O5	2.34	0.50
1:Y:212:HIS:CG	26:Y:613:CLA:HAA2	2.47	0.50
4:A:316:THR:HG22	7:D:65:ALA:HB3	1.93	0.50
5:B:366:PHE:HD2	5:B:425:GLN:HE21	1.58	0.50
5:B:330:MET:HA	5:B:444:ARG:HB2	1.94	0.50
6:C:460:ASP:HB2	11:I:34:ARG:NH1	2.26	0.50
1:1:176:LEU:HD23	1:1:179:LYS:HD2	1.93	0.50
1:5:176:LEU:HD23	1:5:179:LYS:HD2	1.93	0.50
26:8:611:CLA:HBA2	26:8:612:CLA:HMD1	1.92	0.50
4:A:96:ILE:HG12	4:A:105:TRP:CE2	2.47	0.50
5:B:256:MET:O	5:B:448:ARG:NH1	2.42	0.50
7:D:142:TYR:HB3	7:D:273:LEU:HD11	1.93	0.50
1:Y:41:PRO:HG3	1:Y:177:LYS:HB3	1.94	0.50
1:6:162:ASP:OD1	27:6:1620:LUT:O23	2.29	0.50
4:A:22:THR:HB	4:A:136:ARG:HE	1.77	0.50
26:B:604:CLA:H2	26:B:606:CLA:H91	1.94	0.50
26:1:602:CLA:H92	26:1:603:CLA:HMA1	1.94	0.50
1:5:18:GLY:O	1:5:21:ARG:NH1	2.41	0.50
6:C:150:VAL:HG12	6:C:152:LYS:H	1.77	0.50
1:N:176:LEU:HD23	1:N:179:LYS:HD2	1.94	0.50
25:N:608:CHL:HBB1	25:N:608:CHL:HHC	1.93	0.50
20:S:39:LEU:HD22	24:Z:41:PHE:HE1	1.77	0.50
4:A:254:TYR:CD1	7:D:133:LEU:HD22	2.47	0.49
26:D:403:CLA:H13	23:X:58:ILE:HG22	1.94	0.49
17:P:45:GLN:HA	17:P:62:LEU:HA	1.94	0.49
22:W:17:LEU:HA	22:W:22:LEU:HD23	1.94	0.49
28:2:1622:XAT:H393	30:2:2630:LHG:HC92	1.94	0.49
26:5:602:CLA:H92	26:5:603:CLA:HMA1	1.93	0.49
26:A:405:CLA:H122	35:A:408:PHO:H3A	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:91:LEU:HD11	4:A:163:ILE:HA	1.94	0.49
5:B:26:HIS:HB2	26:B:613:CLA:HMB2	1.95	0.49
14:L:30:VAL:O	14:L:34:ASN:ND2	2.45	0.49
25:N:601:CHL:HHC	25:N:601:CHL:HBB1	1.94	0.49
19:R:161:GLN:HG3	25:R:608:CHL:HBB1	1.93	0.49
1:6:85:LEU:HA	1:6:88:ASN:HB2	1.94	0.49
36:B:621:SQD:H262	36:B:623:SQD:H102	1.94	0.49
4:A:77:ILE:HD11	21:T:6:TYR:HB3	1.95	0.49
28:Y:1622:XAT:H363	30:Y:2630:LHG:HC41	1.94	0.49
25:8:606:CHL:HAA1	31:8:623:BCR:H21C	1.94	0.49
5:B:249:ALA:HA	5:B:252:VAL:HG22	1.94	0.49
6:C:406:SER:HA	6:C:420:VAL:HG23	1.94	0.49
20:S:100:LYS:NZ	42:S:1101:HOH:O	2.45	0.49
26:G:613:CLA:H91	30:G:2630:LHG:H321	1.95	0.49
26:N:610:CLA:H52	27:N:1620:LUT:H28	1.94	0.49
2:3:50:PRO:HG3	2:3:188:LYS:HD3	1.95	0.49
4:A:330:VAL:O	7:D:350:GLY:N	2.46	0.49
7:D:52:GLY:HA3	7:D:79:VAL:HG22	1.94	0.49
1:G:80:VAL:HG13	1:G:206:LEU:HD11	1.95	0.49
10:H:49:LEU:HB3	31:H:101:BCR:H14C	1.94	0.49
1:N:69:SER:HB3	1:N:184:GLY:HA3	1.93	0.49
26:Y:602:CLA:H92	26:Y:603:CLA:HMA1	1.95	0.49
5:B:327:ALA:HB1	37:B:622:LMG:HC8	1.94	0.49
1:G:220:ASN:HB2	26:G:614:CLA:HED1	1.95	0.49
25:4:606:CHL:HAA1	31:4:623:BCR:H21C	1.94	0.49
25:G:601:CHL:HMA3	30:G:2630:LHG:H121	1.95	0.49
7:D:267:TRP:HH2	30:L:101:LHG:H102	1.78	0.49
26:R:613:CLA:HBB	25:R:614:CHL:HHD	1.95	0.49
30:C:522:LHG:H181	22:W:31:GLY:HA3	1.94	0.49
25:Y:608:CHL:H11	27:Y:1620:LUT:H383	1.94	0.49
1:Y:69:SER:HB3	1:Y:184:GLY:HA3	1.94	0.49
1:5:52:SER:OG	1:5:61:ASN:ND2	2.45	0.49
26:B:617:CLA:H91	31:B:620:BCR:H14C	1.95	0.49
7:D:156:SER:HA	7:D:160:ILE:HB	1.95	0.49
26:N:603:CLA:H12	1:Y:51:LEU:HD11	1.95	0.49
1:1:52:SER:OG	1:1:61:ASN:ND2	2.45	0.49
25:1:606:CHL:HMB1	25:1:609:CHL:HAC1	1.95	0.49
2:3:53:TYR:OH	2:3:193:LYS:NZ	2.41	0.49
28:6:1622:XAT:H393	30:6:2630:LHG:HC92	1.94	0.49
5:B:207:THR:HG21	37:B:2633:LMG:H351	1.94	0.49
6:C:217:PRO:HA	6:C:223:TRP:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:80:PRO:O	6:C:84:GLN:HG3	2.13	0.49
1:G:194:PHE:HE1	27:G:1620:LUT:H41	1.78	0.49
25:G:609:CHL:H43	25:N:601:CHL:H12	1.95	0.49
5:B:120:LEU:HD23	10:H:15:ARG:HB3	1.95	0.49
1:N:41:PRO:HG3	1:N:177:LYS:HB3	1.94	0.49
16:O:145:GLU:HB3	16:O:197:LYS:HE2	1.95	0.49
25:Y:608:CHL:HBB1	25:Y:608:CHL:HHC	1.95	0.49
3:8:154:PRO:HD2	27:8:620:LUT:H23	1.94	0.48
6:C:370:ARG:HG3	6:C:370:ARG:NH1	2.28	0.48
26:C:508:CLA:HBC2	30:D:410:LHG:H341	1.94	0.48
20:S:235:ALA:HB2	24:Z:59:SER:HB3	1.95	0.48
2:7:50:PRO:HG3	2:7:188:LYS:HD3	1.95	0.48
5:B:313:ASP:OD2	5:B:358:ARG:NH2	2.32	0.48
26:C:510:CLA:H2	26:C:510:CLA:HMA2	1.95	0.48
7:D:20:ASP:OD2	7:D:24:ARG:NH1	2.39	0.48
31:D:404:BCR:H383	37:D:411:LMG:H182	1.94	0.48
15:M:5:ILE:HG23	15:M:5:ILE:HG23	0.00	0.48
19:R:194:LEU:HB3	26:R:610:CLA:H3A	1.95	0.48
1:1:18:GLY:O	1:1:21:ARG:NH1	2.41	0.48
4:A:92:HIS:CE1	6:C:220:GLY:HA3	2.49	0.48
19:R:182:LEU:HD12	27:R:620:LUT:H222	1.95	0.48
31:4:623:BCR:HC22	30:R:2630:LHG:HC92	1.95	0.48
1:5:156:TYR:HB3	26:5:610:CLA:HED2	1.94	0.48
26:B:607:CLA:HBC1	30:B:2630:LHG:H101	1.96	0.48
1:G:87:ARG:HH12	1:G:210:ALA:CB	2.27	0.48
1:1:156:TYR:HB3	26:1:610:CLA:HED2	1.94	0.48
4:A:44:ALA:HB2	4:A:118:HIS:HB2	1.95	0.48
5:B:71:ILE:HD11	26:B:607:CLA:H2A	1.95	0.48
26:C:504:CLA:H42	39:C:519:DGD:HB32	1.96	0.48
6:C:28:GLN:NE2	7:D:234:ARG:HE	2.12	0.48
7:D:349:ARG:NH1	7:D:353:LEU:O	2.40	0.48
7:D:90:LEU:HG	10:H:62:ASN:HD22	1.78	0.48
7:D:90:LEU:HG	10:H:62:ASN:ND2	2.28	0.48
1:1:97:TRP:O	27:1:1621:LUT:O3	2.32	0.48
1:G:65:GLU:OE2	1:G:185:ARG:NE	2.47	0.48
1:Y:110:LEU:HD22	25:Y:606:CHL:HMD2	1.96	0.48
3:4:203:THR:HG22	3:4:205:LEU:H	1.79	0.48
3:4:154:PRO:HD2	27:4:620:LUT:H23	1.94	0.48
4:A:341:LEU:H	6:C:313:GLN:NE2	2.12	0.48
26:A:410:CLA:H11	11:I:9:TYR:CZ	2.48	0.48
5:B:392:VAL:HG13	5:B:397:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C:515:BCR:HC42	11:I:23:PHE:HB2	1.96	0.48
7:D:226:ASP:HB2	7:D:235:ALA:HB1	1.96	0.48
16:O:6:ARG:HG2	16:O:31:THR:HB	1.96	0.48
25:Y:607:CHL:H142	25:Y:609:CHL:H101	1.96	0.48
1:2:179:LYS:HD3	26:2:612:CLA:HAA2	1.96	0.48
25:5:606:CHL:HMB1	25:5:609:CHL:HAC1	1.95	0.48
3:8:113:TRP:HB2	25:8:609:CHL:HMA1	1.96	0.48
26:C:503:CLA:H151	26:C:510:CLA:HBB2	1.96	0.48
7:D:142:TYR:OH	30:D:408:LHG:O4	2.20	0.48
1:6:121:ALA:HB1	1:6:127:ILE:HD11	1.95	0.48
4:A:234:ASN:HB3	7:D:264:ASN:ND2	2.29	0.48
7:D:298:ASP:HA	7:D:316:TYR:OH	2.14	0.48
25:G:607:CHL:HAA2	28:N:1622:XAT:H41	1.96	0.48
26:S:603:CLA:H2A	26:S:603:CLA:HED2	1.96	0.48
1:Y:110:LEU:O	1:Y:110:LEU:HD23	2.14	0.48
28:Y:1622:XAT:H12	30:Y:2630:LHG:H212	1.96	0.48
1:Y:126:ALA:HB3	25:Y:605:CHL:HMC	1.96	0.48
1:1:112:TYR:HD2	1:1:118:LEU:HD13	1.79	0.48
1:2:52:SER:OG	1:2:61:ASN:ND2	2.47	0.48
5:B:114:HIS:HE1	26:B:617:CLA:ND	2.11	0.48
5:B:321:LYS:NZ	5:B:363:PHE:O	2.47	0.48
26:C:506:CLA:H41	26:C:506:CLA:H62	1.68	0.48
30:R:2630:LHG:HC92	31:8:623:BCR:HC22	160.01	0.48
25:1:607:CHL:H8	25:1:607:CHL:HMB2	1.96	0.47
1:6:179:LYS:HD3	26:6:612:CLA:HAA2	1.96	0.47
2:7:72:ALA:HA	2:7:165:LEU:HD11	1.96	0.47
4:A:228:THR:HA	19:R:58:ALA:HA	1.96	0.47
1:N:105:PHE:HZ	1:Y:222:TRP:HB3	1.79	0.47
20:S:53:VAL:HG21	20:S:71:PHE:HE2	1.79	0.47
1:1:94:GLU:N	1:1:103:GLN:OE1	2.45	0.47
26:1:613:CLA:H2	26:1:613:CLA:H61	1.67	0.47
25:5:607:CHL:HMB2	25:5:607:CHL:H8	1.96	0.47
4:A:231:GLU:O	5:B:7:ARG:NH1	2.47	0.47
6:C:230:LEU:HD23	6:C:233:ILE:HD12	1.96	0.47
6:C:91:HIS:NE2	26:C:502:CLA:O1D	2.44	0.47
25:G:601:CHL:H152	25:Y:607:CHL:HBB1	1.97	0.47
26:B:602:CLA:H12	26:B:602:CLA:H52	1.72	0.47
17:P:169:PHE:HB2	18:Q:27:ARG:HB3	1.96	0.47
6:C:106:ILE:HG21	18:Q:89:LYS:HE2	1.96	0.47
1:5:97:TRP:O	27:5:1621:LUT:O3	2.32	0.47
5:B:490:VAL:HG23	5:B:491:GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:179:ARG:O	16:O:182:GLU:HG2	2.14	0.47
20:S:154:ILE:CG1	26:S:609:CLA:HMA1	2.44	0.47
1:2:118:LEU:HD23	25:2:605:CHL:HED2	1.96	0.47
3:4:113:TRP:HB2	25:4:609:CHL:HMA1	1.96	0.47
4:A:286:THR:HB	26:A:405:CLA:O1D	2.14	0.47
4:A:39:PRO:HG3	31:A:411:BCR:HC8	1.97	0.47
6:C:311:GLN:OE1	6:C:355:THR:OG1	2.28	0.47
4:A:279:PRO:HG2	7:D:213:ALA:HB2	1.97	0.47
1:N:103:GLN:HE22	26:N:604:CLA:HED2	1.80	0.47
28:N:1622:XAT:H15	28:N:1622:XAT:H201	1.64	0.47
25:Y:607:CHL:H2	25:Y:607:CHL:H62	1.57	0.47
1:2:121:ALA:HB1	1:2:127:ILE:HD11	1.95	0.47
1:6:52:SER:OG	1:6:61:ASN:ND2	2.47	0.47
5:B:33:TRP:CD1	31:T:101:BCR:H381	36.17	0.47
26:C:505:CLA:H43	31:C:515:BCR:H331	1.96	0.47
28:G:1622:XAT:H391	28:G:1622:XAT:H31	1.71	0.47
18:Q:31:LEU:HB2	18:Q:36:ARG:HD3	1.97	0.47
19:R:204:LEU:HD13	26:R:611:CLA:HBC1	1.97	0.47
30:C:2630:LHG:H222	30:S:2630:LHG:H331	1.96	0.47
26:A:405:CLA:H162	26:A:406:CLA:H102	1.97	0.47
5:B:471:ALA:HB2	7:D:131:PHE:HE1	1.80	0.47
4:A:221:SER:HB2	7:D:140:ARG:O	2.15	0.47
1:G:41:PRO:HG3	1:G:177:LYS:HB3	1.97	0.47
6:C:460:ASP:HB2	11:I:34:ARG:HH12	1.80	0.47
29:S:1623:NEX:H201	29:S:1623:NEX:H15	1.79	0.47
30:B:2631:LHG:H161	30:B:2631:LHG:H341	1.97	0.47
26:C:503:CLA:HAB	26:C:512:CLA:H41	1.95	0.47
1:G:194:PHE:HE1	27:G:1620:LUT:C5	2.28	0.47
1:G:110:LEU:HD21	26:G:604:CLA:HAA1	1.96	0.47
19:R:185:ALA:HB1	19:R:191:LYS:HG3	1.97	0.47
28:Y:1622:XAT:H201	28:Y:1622:XAT:H15	1.76	0.47
3:8:203:THR:HG22	3:8:205:LEU:H	1.79	0.47
31:8:623:BCR:H341	31:8:623:BCR:H11C	1.69	0.47
6:C:279:LEU:HD11	26:C:507:CLA:HBA1	1.97	0.47
5:B:245:VAL:HG21	26:B:613:CLA:HED3	1.96	0.47
5:B:238:LEU:HB2	26:B:613:CLA:HMD3	1.96	0.47
26:B:612:CLA:H8	26:B:614:CLA:H51	1.96	0.47
31:B:618:BCR:H351	31:B:618:BCR:H15C	1.75	0.47
6:C:387:TRP:HD1	18:Q:83:TYR:CZ	2.33	0.47
31:C:517:BCR:H371	31:C:517:BCR:H24C	1.72	0.47
28:G:1622:XAT:O23	30:G:2630:LHG:O1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:613:CLA:H2	26:G:613:CLA:H61	1.64	0.47
1:1:229:VAL:HG22	1:1:231:GLY:H	1.80	0.47
28:6:1622:XAT:H15	28:6:1622:XAT:H201	1.79	0.47
7:D:260:VAL:HG12	30:D:409:LHG:HC82	1.97	0.47
27:G:1621:LUT:H201	27:G:1621:LUT:H15	1.79	0.47
1:Y:21:ARG:NH2	1:Y:36:LEU:O	2.48	0.47
1:1:222:TRP:HB3	1:2:105:PHE:HZ	1.80	0.46
28:2:1622:XAT:H391	28:2:1622:XAT:H31	1.75	0.46
1:5:112:TYR:HD2	1:5:118:LEU:HD13	1.79	0.46
4:A:250:ALA:HB1	7:D:139:LEU:HD21	1.97	0.46
36:B:623:SQD:H62	14:L:8:GLU:HB3	1.97	0.46
18:Q:50:ARG:HH11	18:Q:87:ASP:HB2	1.80	0.46
19:R:29:VAL:H	19:R:93:ARG:HH21	1.62	0.46
19:R:180:ASP:OD1	27:R:620:LUT:O23	2.32	0.46
1:Y:41:PRO:HG3	1:Y:177:LYS:HD3	1.98	0.46
36:A:418:SQD:H382	5:B:102:VAL:HG11	64.77	0.46
5:B:368:VAL:HG21	5:B:422:ARG:HG2	1.97	0.46
31:B:619:BCR:H391	39:B:626:DGD:HBF1	1.97	0.46
6:C:456:GLU:OE2	6:C:457:LYS:NZ	2.48	0.46
4:A:160:ILE:HD11	39:C:518:DGD:HBT2	1.97	0.46
28:G:1622:XAT:H201	28:G:1622:XAT:H15	1.71	0.46
31:C:516:BCR:H363	13:K:46:LEU:HD22	1.98	0.46
25:N:607:CHL:H2	25:N:607:CHL:H62	1.56	0.46
19:R:133:SER:O	19:R:140:LEU:N	2.35	0.46
19:R:151:GLU:OE1	25:R:607:CHL:HMC	2.16	0.46
28:1:1622:XAT:H31	28:1:1622:XAT:H391	1.72	0.46
1:2:84:LEU:O	1:2:88:ASN:N	2.48	0.46
35:A:408:PHO:H62	35:A:408:PHO:H92	1.77	0.46
5:B:51:VAL:HG13	5:B:308:LYS:HB2	1.98	0.46
31:B:618:BCR:H383	36:B:621:SQD:H101	1.97	0.46
17:P:54:ASP:HB2	17:P:167:ARG:HE	1.80	0.46
5:B:211:LEU:HD22	26:R:603:CLA:H111	1.98	0.46
19:R:101:ARG:NH2	25:R:608:CHL:OBD	2.37	0.46
3:4:31:GLY:HA3	3:4:181:ILE:HG21	1.98	0.46
1:5:94:GLU:N	1:5:103:GLN:OE1	2.45	0.46
6:C:257:PHE:HA	30:C:523:LHG:HC11	1.98	0.46
28:G:1622:XAT:H371	30:G:2630:LHG:H362	1.98	0.46
2:3:72:ALA:HA	2:3:165:LEU:HD11	1.96	0.46
26:5:613:CLA:H2	26:5:613:CLA:H61	1.67	0.46
1:5:222:TRP:HB3	1:6:105:PHE:HZ	1.80	0.46
2:7:181:PRO:HA	2:7:184:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:214:MET:HE2	4:A:255:PHE:CE1	2.52	0.46
26:D:403:CLA:H152	23:X:59:VAL:HA	1.97	0.46
4:A:77:ILE:HB	14:L:34:ASN:HD21	1.80	0.46
1:N:199:ILE:HG13	25:N:607:CHL:H42	1.98	0.46
26:S:614:CLA:HBC1	30:S:2630:LHG:H372	1.97	0.46
20:S:95:PRO:HG3	26:S:604:CLA:C1D	2.46	0.46
28:Y:1622:XAT:H12	30:Y:2630:LHG:H191	1.98	0.46
1:Y:213:LEU:HD21	26:Y:614:CLA:HMC3	1.98	0.46
4:A:42:LEU:HD23	36:A:418:SQD:C21	2.46	0.46
4:A:63:ILE:HG21	4:A:336:ALA:HA	1.97	0.46
5:B:389:LYS:N	7:D:345:GLU:OE2	2.46	0.46
31:D:404:BCR:H351	31:D:404:BCR:H15C	1.84	0.46
26:C:506:CLA:H71	11:I:20:ILE:HD13	1.98	0.46
19:R:174:PRO:HD3	25:R:608:CHL:HMD2	1.98	0.46
29:S:1623:NEX:H11	29:S:1623:NEX:H191	1.75	0.46
1:6:118:LEU:HD23	25:6:605:CHL:HED2	1.96	0.46
5:B:114:HIS:HE1	26:B:617:CLA:C1D	2.29	0.46
26:B:616:CLA:H121	26:B:617:CLA:HMA3	1.98	0.46
6:C:371:GLY:N	6:C:374:GLY:O	2.49	0.46
31:C:517:BCR:H15C	31:C:517:BCR:H351	1.81	0.46
25:N:606:CHL:HMB1	25:N:609:CHL:HAC1	1.98	0.46
19:R:102:TRP:CD1	26:R:609:CLA:HMD3	2.51	0.46
6:C:316:THR:HG21	18:Q:27:ARG:NH2	2.30	0.46
31:C:516:BCR:H21C	12:J:15:THR:HG23	1.98	0.46
17:P:137:ASP:N	17:P:137:ASP:OD1	2.49	0.46
19:R:181:PRO:HD2	27:R:620:LUT:H23	1.98	0.46
2:3:155:GLY:HA2	25:3:608:CHL:HAC1	1.98	0.46
36:B:621:SQD:H321	36:B:621:SQD:H351	1.68	0.46
6:C:191:PRO:HA	18:Q:78:ARG:HG2	1.98	0.46
6:C:223:TRP:CG	6:C:224:ILE:N	2.83	0.46
37:C:521:LMG:H361	13:K:45:LEU:HD11	1.98	0.46
30:C:522:LHG:HC91	30:C:522:LHG:H242	1.98	0.46
26:N:610:CLA:H41	26:N:610:CLA:H62	1.71	0.46
27:1:1620:LUT:H35	27:1:1620:LUT:H401	1.84	0.45
28:1:1622:XAT:H201	28:1:1622:XAT:H15	1.73	0.45
25:4:601:CHL:H3A	25:4:601:CHL:HBA1	1.66	0.45
4:A:166:GLY:HA3	6:C:358:PHE:HE1	1.81	0.45
26:B:607:CLA:HMC2	30:B:2631:LHG:H322	1.98	0.45
6:C:344:SER:OG	6:C:348:GLU:OE1	2.32	0.45
6:C:400:PRO:O	6:C:401:LEU:HD12	2.16	0.45
26:C:512:CLA:H202	26:C:513:CLA:H111	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:39:ARG:NH2	17:P:16:THR:OG1	2.45	0.45
26:R:601:CLA:HBA1	26:R:601:CLA:H3A	1.44	0.45
29:R:623:NEX:H11	29:R:623:NEX:H191	1.73	0.45
3:4:36:ASP:OD1	28:4:622:XAT:O23	2.34	0.45
26:C:510:CLA:H61	26:C:510:CLA:H2	1.77	0.45
7:D:56:VAL:HG21	7:D:111:LEU:HD12	1.99	0.45
1:G:213:LEU:HD21	26:G:614:CLA:HMC3	1.98	0.45
26:G:602:CLA:H101	27:G:1621:LUT:H371	1.98	0.45
1:N:41:PRO:HG3	1:N:177:LYS:HD3	1.98	0.45
20:S:79:LEU:HD13	20:S:164:LEU:HD23	1.98	0.45
36:A:418:SQD:H262	31:T:101:BCR:H333	1.96	0.45
23:X:47:VAL:HA	23:X:51:LEU:HD23	1.98	0.45
1:Y:103:GLN:HE22	26:Y:604:CLA:HED2	1.81	0.45
26:Y:603:CLA:HBB1	26:Y:603:CLA:HHC	1.98	0.45
3:4:96:THR:HG21	19:R:235:LEU:HA	1.99	0.45
26:R:616:CLA:HBA2	26:R:616:CLA:H3A	1.65	0.45
1:5:229:VAL:HG22	1:5:231:GLY:H	1.80	0.45
25:G:601:CHL:H102	28:G:1622:XAT:H14	1.98	0.45
25:G:607:CHL:HBB2	25:G:609:CHL:HBC1	1.99	0.45
20:S:55:GLY:HA3	20:S:194:ARG:HH12	1.82	0.45
22:W:47:ASP:OD1	22:W:47:ASP:N	2.49	0.45
1:Y:70:ARG:NE	1:Y:180:GLU:OE2	2.49	0.45
1:Y:24:TYR:CG	1:Y:46:TRP:HB2	2.51	0.45
25:4:601:CHL:HBC1	30:4:2630:LHG:HC2	1.99	0.45
26:B:602:CLA:HBB2	31:H:101:BCR:H351	1.98	0.45
26:C:512:CLA:HMB3	31:C:514:BCR:H391	1.98	0.45
5:B:383:PHE:N	7:D:345:GLU:O	2.50	0.45
14:L:5:ASN:HB3	14:L:8:GLU:HG3	1.98	0.45
25:N:601:CHL:HMA3	30:N:2630:LHG:H121	1.99	0.45
19:R:127:VAL:HA	19:R:130:VAL:HG22	1.98	0.45
6:C:110:PRO:HG3	37:Z:101:LMG:H121	1.97	0.45
27:3:1621:LUT:H201	27:3:1621:LUT:H15	1.80	0.45
4:A:193:LEU:HD21	26:A:405:CLA:HMC3	1.99	0.45
26:B:605:CLA:H161	26:B:605:CLA:H141	1.80	0.45
26:C:513:CLA:HMC2	31:C:514:BCR:H372	1.99	0.45
5:B:362:PHE:HB3	7:D:189:PHE:CD2	2.52	0.45
29:N:1623:NEX:H401	29:N:1623:NEX:H35	1.86	0.45
26:N:603:CLA:H91	25:N:609:CHL:H112	1.98	0.45
16:O:162:ARG:NH1	16:O:189:ASN:OD1	2.44	0.45
16:O:202:LEU:HD23	16:O:218:PHE:HB3	1.98	0.45
19:R:187:ASP:HA	19:R:188:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:238:THR:HG22	19:R:239:ILE:H	1.81	0.45
1:Y:192:PHE:CD2	26:Y:602:CLA:H171	2.52	0.45
27:1:1621:LUT:H35	27:1:1621:LUT:H401	1.87	0.45
2:3:80:TRP:CE2	25:3:608:CHL:HED2	2.52	0.45
3:4:153:ASP:HB3	3:4:156:SER:HA	1.99	0.45
3:8:31:GLY:HA3	3:8:181:ILE:HG21	1.98	0.45
25:8:601:CHL:HBC1	30:8:2630:LHG:HC2	1.99	0.45
5:B:366:PHE:O	5:B:425:GLN:NE2	2.45	0.45
6:C:322:GLN:NE2	6:C:381:LYS:HA	2.32	0.45
26:C:508:CLA:H142	26:C:510:CLA:H102	1.98	0.45
31:C:515:BCR:H15C	31:C:515:BCR:H351	1.81	0.45
26:G:611:CLA:H61	26:G:611:CLA:H41	1.85	0.45
1:G:97:TRP:O	27:G:1621:LUT:O3	2.35	0.45
1:N:162:ASP:OD1	27:N:1620:LUT:O23	2.35	0.45
17:P:129:ILE:HG23	17:P:147:ILE:HB	1.99	0.45
26:Y:613:CLA:H2	26:Y:613:CLA:H61	1.66	0.45
27:3:1620:LUT:H15	27:3:1620:LUT:H201	1.84	0.45
6:C:38:GLY:HA3	26:C:511:CLA:HMD3	1.99	0.45
25:G:606:CHL:HBB2	25:G:607:CHL:CBB	2.47	0.45
31:H:101:BCR:H371	31:H:101:BCR:H24C	1.74	0.45
26:N:610:CLA:H92	26:N:610:CLA:H61	1.83	0.45
17:P:75:GLY:O	17:P:127:TYR:OH	2.31	0.45
5:B:214:LEU:HB3	26:R:603:CLA:HED1	1.98	0.45
26:C:503:CLA:HMA1	37:Z:101:LMG:H191	1.99	0.45
3:8:36:ASP:OD1	28:8:622:XAT:O23	2.34	0.45
26:C:512:CLA:C1B	31:C:514:BCR:H401	2.46	0.45
19:R:124:ALA:HB1	26:R:604:CLA:HED1	1.99	0.45
19:R:155:ILE:HG13	25:R:606:CHL:HMB3	1.99	0.45
28:R:622:XAT:H35	28:R:622:XAT:H401	1.77	0.45
26:Y:603:CLA:HMA2	26:Y:603:CLA:H2	1.99	0.45
28:7:1622:XAT:H201	28:7:1622:XAT:H15	1.77	0.45
25:G:608:CHL:HBB1	25:G:608:CHL:HHC	1.99	0.45
7:D:163:LEU:HD13	39:H:102:DGD:HB92	1.99	0.45
27:Y:1621:LUT:H15	27:Y:1621:LUT:H201	1.81	0.45
2:3:181:PRO:HA	2:3:184:PHE:HB3	1.98	0.44
28:7:1622:XAT:H391	28:7:1622:XAT:H31	1.72	0.44
4:A:228:THR:OG1	4:A:230:ASN:OD1	2.28	0.44
26:A:410:CLA:H72	26:A:410:CLA:H112	1.74	0.44
7:D:52:GLY:HA2	7:D:56:VAL:HB	1.99	0.44
1:N:192:PHE:CE2	26:N:602:CLA:H171	2.52	0.44
26:R:612:CLA:HBB1	26:R:612:CLA:HHC	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:101:BCR:H351	31:T:101:BCR:H15C	1.83	0.44
25:1:607:CHL:H142	25:1:609:CHL:H101	1.99	0.44
28:2:1622:XAT:H191	28:2:1622:XAT:H11	1.83	0.44
1:2:221:ALA:N	26:2:613:CLA:O1A	2.49	0.44
26:3:603:CLA:H91	25:3:609:CHL:H121	1.99	0.44
2:3:160:GLY:HA3	25:3:608:CHL:HBC3	1.99	0.44
1:5:142:ARG:NH2	25:5:609:CHL:O1D	2.45	0.44
4:A:267:ASN:HD22	36:A:412:SQD:H3	1.83	0.44
5:B:155:ALA:O	5:B:159:THR:OG1	2.36	0.44
5:B:458:PHE:HB3	26:B:605:CLA:HBC2	1.99	0.44
6:C:97:TRP:HH2	26:C:502:CLA:H151	1.82	0.44
16:O:170:ASN:ND2	16:O:181:ASP:OD1	2.51	0.44
19:R:229:THR:HG22	19:R:237:THR:HG21	1.99	0.44
26:R:603:CLA:H2A	26:R:603:CLA:HED2	2.00	0.44
26:S:613:CLA:H61	26:S:613:CLA:H2	1.74	0.44
1:6:51:LEU:HD12	27:6:1621:LUT:H221	2.00	0.44
1:6:84:LEU:O	1:6:88:ASN:N	2.48	0.44
2:7:155:GLY:HA2	25:7:608:CHL:HAC1	1.98	0.44
29:7:1623:NEX:H35	29:7:1623:NEX:H401	1.90	0.44
26:B:605:CLA:H93	26:B:606:CLA:HAB	2.00	0.44
26:B:611:CLA:H102	26:B:616:CLA:HAA1	1.98	0.44
5:B:462:PHE:CE2	26:B:614:CLA:HMB3	2.52	0.44
6:C:319:VAL:HG11	6:C:389:GLU:HG2	1.99	0.44
26:B:602:CLA:HAC1	31:H:101:BCR:H383	1.99	0.44
16:O:89:ILE:HD13	16:O:130:ILE:HD11	2.00	0.44
16:O:27:ASN:O	16:O:85:THR:OG1	2.33	0.44
1:Y:25:LEU:HB2	1:Y:29:SER:HA	1.99	0.44
26:1:602:CLA:HBA1	27:1:1621:LUT:H382	1.99	0.44
1:2:51:LEU:HD12	27:2:1621:LUT:H221	2.00	0.44
2:7:80:TRP:CE2	25:7:608:CHL:HED2	2.52	0.44
4:A:304:GLN:HG2	4:A:313:VAL:HG11	2.00	0.44
35:A:408:PHO:H42	30:D:409:LHG:H342	2.00	0.44
26:B:605:CLA:HAB	26:B:605:CLA:HHC	1.83	0.44
6:C:154:ARG:HB3	6:C:256:PRO:HG2	1.98	0.44
27:G:1621:LUT:H372	26:Y:603:CLA:HED3	2.00	0.44
19:R:21:PRO:CD	19:R:24:LEU:HD13	2.47	0.44
20:S:85:ALA:O	20:S:89:ALA:N	2.46	0.44
1:Y:84:LEU:O	1:Y:88:ASN:ND2	2.51	0.44
28:1:1622:XAT:H12	30:1:2630:LHG:H182	1.99	0.44
1:1:25:LEU:HB3	1:1:28:PHE:HB2	1.99	0.44
2:7:174:PRO:HD2	27:7:1620:LUT:H23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:1620:LUT:H35	27:7:1620:LUT:H401	1.87	0.44
25:7:606:CHL:HMC	25:7:607:CHL:C4C	2.47	0.44
4:A:254:TYR:HE2	7:D:143:ASN:HD22	1.65	0.44
26:A:405:CLA:H193	26:A:405:CLA:H161	1.77	0.44
1:N:126:ALA:HB3	25:N:605:CHL:HMC	2.00	0.44
25:N:607:CHL:H111	25:N:607:CHL:H143	1.71	0.44
29:R:623:NEX:H15	29:R:623:NEX:H201	1.80	0.44
29:Y:1623:NEX:H191	29:Y:1623:NEX:H11	1.84	0.44
26:Y:602:CLA:H161	26:Y:602:CLA:H193	1.78	0.44
26:Y:612:CLA:H142	26:Y:612:CLA:H111	1.86	0.44
1:2:196:VAL:HG12	26:2:613:CLA:HMD3	2.00	0.44
2:3:174:PRO:HD2	27:3:1620:LUT:H23	1.99	0.44
27:3:1620:LUT:H35	27:3:1620:LUT:H401	1.87	0.44
28:5:1622:XAT:H12	30:5:2630:LHG:H182	1.99	0.44
2:7:53:TYR:OH	2:7:193:LYS:NZ	2.41	0.44
5:B:334:ASP:HB2	5:B:432:LEU:HD13	1.99	0.44
5:B:464:PHE:HD2	26:B:612:CLA:HAC2	1.82	0.44
26:B:614:CLA:H41	26:B:614:CLA:H61	1.68	0.44
26:C:502:CLA:H13	26:C:502:CLA:H171	1.81	0.44
25:R:606:CHL:HMB1	26:R:609:CLA:HBC2	2.00	0.44
1:1:142:ARG:NH2	25:1:609:CHL:O1D	2.45	0.44
25:3:606:CHL:HMC	25:3:607:CHL:C4C	2.48	0.44
26:5:602:CLA:HBA1	27:5:1621:LUT:H382	1.99	0.44
4:A:22:THR:HG22	4:A:136:ARG:HH11	1.83	0.44
31:B:620:BCR:H11C	31:B:620:BCR:H341	1.81	0.44
26:C:502:CLA:HAB	26:C:502:CLA:HHC	1.81	0.44
28:N:1622:XAT:H191	28:N:1622:XAT:H11	1.91	0.44
1:N:189:PHE:HD1	26:N:602:CLA:H201	1.82	0.44
18:Q:50:ARG:HH11	18:Q:87:ASP:CB	2.31	0.44
26:R:611:CLA:H3A	26:R:611:CLA:HBA2	1.57	0.44
29:Y:1623:NEX:H35	29:Y:1623:NEX:H401	1.83	0.44
26:1:613:CLA:H2	26:1:614:CLA:HMD1	1.99	0.44
1:6:196:VAL:HG12	26:6:613:CLA:HMD3	2.00	0.44
2:7:160:GLY:HA3	25:7:608:CHL:HBC3	1.99	0.44
19:R:235:LEU:HA	3:8:96:THR:HG21	169.28	0.44
4:A:93:PHE:HZ	26:A:410:CLA:HAA1	1.83	0.44
26:B:606:CLA:H143	26:B:611:CLA:HMA2	2.00	0.44
26:B:613:CLA:H171	26:B:614:CLA:HBB2	2.00	0.44
4:A:46:SER:HB3	39:B:626:DGD:HBN2	59.96	0.44
5:B:362:PHE:HB3	7:D:189:PHE:HD2	1.83	0.44
26:D:403:CLA:H61	26:D:403:CLA:H102	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:49:TRP:HA	7:D:79:VAL:HG21	2.00	0.44
7:D:84:ASN:HD22	7:D:337:HIS:CD2	2.36	0.44
30:S:2630:LHG:H282	30:S:2630:LHG:HC91	1.99	0.44
26:Y:602:CLA:H172	26:Y:602:CLA:H13	1.64	0.44
1:Y:73:MET:SD	26:Y:610:CLA:HAB	2.58	0.44
28:3:1622:XAT:H31	28:3:1622:XAT:H391	1.72	0.44
5:B:182:ASN:HA	37:B:2633:LMG:HC62	2.00	0.44
26:B:613:CLA:H61	26:B:613:CLA:H102	1.81	0.44
1:G:104:ILE:HG21	1:G:124:ILE:HD13	1.99	0.44
27:G:1621:LUT:H401	27:G:1621:LUT:H35	1.82	0.44
26:B:603:CLA:H12	10:H:61:TYR:CE2	2.53	0.44
26:R:613:CLA:H92	30:R:2630:LHG:H171	2.00	0.44
25:Y:601:CHL:H91	25:Y:601:CHL:H112	1.80	0.44
25:6:609:CHL:H61	25:6:609:CHL:H93	1.89	0.43
1:6:221:ALA:N	26:6:613:CLA:O1A	2.49	0.43
18:Q:65:ILE:HG12	18:Q:73:LEU:HD22	1.99	0.43
25:S:606:CHL:HMC	25:S:607:CHL:C1C	2.48	0.43
28:Y:1622:XAT:H11	28:Y:1622:XAT:H191	1.83	0.43
1:5:70:ARG:NH1	25:5:608:CHL:OBD	2.42	0.43
25:6:607:CHL:H91	25:6:607:CHL:H112	1.80	0.43
26:A:405:CLA:H102	35:A:408:PHO:HAA1	2.00	0.43
6:C:117:LEU:HD12	37:Z:101:LMG:H202	2.00	0.43
6:C:59:LEU:HD13	26:C:510:CLA:HMD2	2.00	0.43
26:G:613:CLA:HBB1	27:G:1620:LUT:H192	2.00	0.43
39:H:102:DGD:HB62	39:H:102:DGD:HB91	1.67	0.43
19:R:81:GLN:HE21	26:R:616:CLA:HED3	1.83	0.43
20:S:222:LEU:HD11	26:S:614:CLA:HMC3	1.99	0.43
25:1:609:CHL:H112	25:1:609:CHL:H91	1.83	0.43
1:6:63:GLU:HA	1:6:155:LEU:HD11	2.00	0.43
37:B:622:LMG:HC91	15:M:6:LEU:HD22	2.01	0.43
6:C:120:ILE:HG23	24:Z:47:TRP:CH2	2.53	0.43
30:D:409:LHG:H141	30:D:409:LHG:H292	2.00	0.43
1:Y:110:LEU:HD23	1:Y:110:LEU:C	2.39	0.43
2:3:152:ARG:NH2	25:3:609:CHL:O1D	2.52	0.43
1:5:25:LEU:HB3	1:5:28:PHE:HB2	1.99	0.43
27:7:1621:LUT:H15	27:7:1621:LUT:H201	1.80	0.43
3:8:153:ASP:HB3	3:8:156:SER:HA	1.99	0.43
28:8:622:XAT:H15	28:8:622:XAT:H201	1.87	0.43
26:B:615:CLA:H92	26:B:615:CLA:H61	1.86	0.43
26:C:501:CLA:H41	26:C:501:CLA:H61	1.90	0.43
7:D:304:ILE:HD13	15:M:2:GLU:OE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:603:CLA:C3D	25:N:609:CHL:H2	2.49	0.43
26:N:603:CLA:H61	26:N:603:CLA:H92	1.76	0.43
17:P:114:LEU:HD11	17:P:132:LEU:HB2	2.01	0.43
17:P:30:VAL:HG11	17:P:49:TYR:CD2	2.53	0.43
26:7:603:CLA:H91	25:7:609:CHL:H121	2.00	0.43
26:A:406:CLA:H162	26:A:406:CLA:H202	1.85	0.43
5:B:139:PHE:CZ	5:B:143:LEU:HD22	2.54	0.43
26:B:603:CLA:H61	26:B:603:CLA:H93	1.78	0.43
7:D:91:LEU:O	7:D:105:TRP:NE1	2.31	0.43
28:G:1622:XAT:H11	28:G:1622:XAT:H191	1.93	0.43
1:G:167:ALA:HB2	26:G:610:CLA:HAA1	2.01	0.43
26:G:603:CLA:HBB1	26:G:603:CLA:HHC	2.00	0.43
16:O:78:LEU:HB3	22:W:3:ASP:OD2	2.19	0.43
28:R:622:XAT:H201	28:R:622:XAT:H15	1.87	0.43
27:S:1621:LUT:H35	27:S:1621:LUT:H401	1.83	0.43
25:5:607:CHL:H142	25:5:609:CHL:H101	1.99	0.43
2:7:145:MET:HA	2:7:148:VAL:HG22	2.01	0.43
5:B:469:HIS:CE1	26:B:612:CLA:NA	2.86	0.43
6:C:56:HIS:HB2	26:C:509:CLA:HMB2	2.00	0.43
1:G:130:THR:HB	42:G:664:HOH:O	2.19	0.43
29:3:1623:NEX:H201	29:3:1623:NEX:H15	1.71	0.43
28:5:1622:XAT:H191	28:5:1622:XAT:H11	1.79	0.43
1:6:135:MET:HG3	25:6:606:CHL:HMB3	2.00	0.43
26:7:602:CLA:H111	26:7:602:CLA:H93	1.91	0.43
5:B:145:LEU:HD22	26:B:605:CLA:H18	2.00	0.43
6:C:28:GLN:HE22	7:D:231:ASN:HD22	1.65	0.43
6:C:418:ASN:HD21	39:C:519:DGD:HD4	1.84	0.43
1:G:131:GLN:OE1	25:G:607:CHL:HMC	2.19	0.43
29:G:1623:NEX:H191	29:G:1623:NEX:H11	1.78	0.43
27:N:1621:LUT:H15	27:N:1621:LUT:H201	1.84	0.43
16:O:125:PRO:HG2	16:O:225:ASP:HB3	2.00	0.43
26:5:613:CLA:H2	26:5:614:CLA:HMD1	1.99	0.43
4:A:214:MET:HE2	4:A:255:PHE:CD1	2.54	0.43
4:A:337:HIS:CE1	7:D:353:LEU:HD11	2.54	0.43
26:B:614:CLA:H102	26:B:614:CLA:H62	1.81	0.43
6:C:217:PRO:HG3	39:C:518:DGD:HA71	2.01	0.43
7:D:82:PRO:HD3	7:D:112:TRP:HB3	2.01	0.43
26:N:602:CLA:H13	26:N:602:CLA:H172	1.83	0.43
26:Y:603:CLA:H61	26:Y:603:CLA:H2	1.75	0.43
1:2:135:MET:HG3	25:2:606:CHL:HMB3	2.00	0.43
26:3:613:CLA:H61	26:3:613:CLA:H2	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:411:BCR:H11C	31:A:411:BCR:H341	1.88	0.43
31:B:619:BCR:H20C	31:B:619:BCR:H361	1.87	0.43
37:A:413:LMG:H352	6:C:217:PRO:HB3	2.01	0.43
28:N:1622:XAT:H391	28:N:1622:XAT:H31	1.81	0.43
26:N:613:CLA:H2	26:N:613:CLA:H61	1.61	0.43
16:O:185:LEU:HA	16:O:188:GLU:OE2	2.19	0.43
19:R:234:PRO:HB2	19:R:235:LEU:HD12	2.00	0.43
27:S:1620:LUT:H401	27:S:1620:LUT:H35	1.79	0.43
36:A:418:SQD:H261	31:T:101:BCR:H333	2.00	0.43
26:1:603:CLA:H8	26:3:602:CLA:H91	2.01	0.43
1:2:63:GLU:HA	1:2:155:LEU:HD11	2.00	0.43
2:7:152:ARG:NH2	25:7:609:CHL:O1D	2.52	0.43
4:A:301:ASN:OD1	4:A:303:ASN:ND2	2.52	0.43
4:A:308:ASP:HB2	8:E:52:PRO:O	2.19	0.43
31:A:411:BCR:H15C	31:A:411:BCR:H351	1.86	0.43
6:C:28:GLN:HE21	7:D:234:ARG:HE	1.67	0.43
26:C:501:CLA:HMD2	26:C:502:CLA:H101	2.00	0.43
25:R:606:CHL:H112	25:R:606:CHL:H92	1.93	0.43
26:G:603:CLA:H42	26:Y:603:CLA:H41	2.01	0.43
25:7:609:CHL:H112	25:7:609:CHL:H91	1.83	0.42
3:8:143:GLU:H	3:8:146:TYR:HB2	1.84	0.42
36:A:418:SQD:H461	36:A:418:SQD:H92	2.01	0.42
4:A:56:PRO:HB2	16:O:123:ARG:NH2	2.34	0.42
26:B:612:CLA:H2	26:B:612:CLA:H61	1.69	0.42
26:B:613:CLA:H13	26:B:614:CLA:HBB2	2.01	0.42
31:B:619:BCR:HC42	37:B:622:LMG:H341	2.01	0.42
16:O:157:LEU:HD21	16:O:166:THR:HG23	2.01	0.42
19:R:135:TYR:HD1	26:R:604:CLA:HBA1	1.84	0.42
26:Y:602:CLA:CAB	27:Y:1621:LUT:H32	2.49	0.42
4:A:131:TRP:CZ3	26:C:505:CLA:HAA2	2.54	0.42
5:B:110:ALA:HB2	31:B:620:BCR:H17C	2.01	0.42
4:A:269:ARG:NH2	7:D:235:ALA:HB3	2.33	0.42
1:N:46:TRP:CE3	27:N:1621:LUT:H383	2.54	0.42
19:R:174:PRO:HB3	25:R:608:CHL:HBC2	2.00	0.42
25:R:614:CHL:HAB	26:7:614:CLA:CBB	178.95	0.42
20:S:185:LEU:HD23	20:S:188:LYS:HD2	2.01	0.42
31:T:101:BCR:H11C	31:T:101:BCR:H341	1.75	0.42
29:1:1623:NEX:H15	29:1:1623:NEX:H201	1.84	0.42
27:5:1621:LUT:H35	27:5:1621:LUT:H401	1.87	0.42
5:B:18:ARG:HG3	5:B:118:TRP:HB3	2.02	0.42
30:D:409:LHG:H181	21:T:17:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:607:CHL:HBB1	27:G:1621:LUT:H161	2.01	0.42
5:B:325:PHE:CG	14:L:35:TYR:HB3	2.55	0.42
26:3:614:CLA:CBB	25:R:614:CHL:HAB	2.49	0.42
26:R:602:CLA:H101	28:R:622:XAT:H371	2.02	0.42
29:R:623:NEX:H401	29:R:623:NEX:H35	1.87	0.42
30:S:2630:LHG:H172	30:S:2630:LHG:H201	1.85	0.42
28:Y:1622:XAT:H31	28:Y:1622:XAT:H391	1.73	0.42
25:2:607:CHL:H112	25:2:607:CHL:H91	1.80	0.42
31:4:623:BCR:H11C	31:4:623:BCR:H341	1.69	0.42
29:5:1623:NEX:H191	29:5:1623:NEX:H11	1.88	0.42
26:5:603:CLA:H8	26:7:602:CLA:H91	2.01	0.42
25:8:601:CHL:H3A	25:8:601:CHL:HBA1	1.66	0.42
4:A:38:ILE:HA	36:A:418:SQD:H171	2.02	0.42
26:B:603:CLA:H41	26:B:603:CLA:H62	1.84	0.42
31:B:619:BCR:H351	31:B:619:BCR:H15C	1.78	0.42
4:A:166:GLY:HA3	6:C:358:PHE:CE1	2.54	0.42
31:C:514:BCR:H351	31:C:514:BCR:H15C	1.79	0.42
6:C:84:GLN:HB2	6:C:86:LEU:HG	2.02	0.42
31:H:101:BCR:H341	31:H:101:BCR:H11C	1.82	0.42
31:H:101:BCR:H292	23:X:45:ALA:HB1	2.00	0.42
26:N:611:CLA:H61	26:N:611:CLA:H92	1.80	0.42
26:R:609:CLA:HHC	26:R:609:CLA:HBB1	2.00	0.42
26:Y:611:CLA:HHC	26:Y:611:CLA:HBB1	2.01	0.42
27:1:1621:LUT:H201	27:1:1621:LUT:H15	1.79	0.42
28:3:1622:XAT:H11	28:3:1622:XAT:H191	1.88	0.42
26:A:405:CLA:H171	26:A:406:CLA:H111	2.01	0.42
26:B:609:CLA:H192	10:H:58:LEU:CD2	2.50	0.42
26:B:616:CLA:H61	26:B:616:CLA:H2	1.78	0.42
16:O:49:LYS:HE2	16:O:50:LYS:HZ3	1.88	0.42
28:2:1622:XAT:H15	28:2:1622:XAT:H201	1.79	0.42
27:3:1621:LUT:H35	27:3:1621:LUT:H401	1.90	0.42
3:4:143:GLU:H	3:4:146:TYR:HB2	1.84	0.42
2:7:121:ASP:OD1	2:7:130:HIS:ND1	2.36	0.42
5:B:496:GLN:HE22	23:X:82:LYS:HG3	1.84	0.42
31:B:620:BCR:H351	31:B:620:BCR:H15C	1.82	0.42
4:A:341:LEU:N	6:C:313:GLN:HE22	2.17	0.42
13:K:33:LEU:HD22	13:K:36:ILE:HD11	2.01	0.42
26:N:613:CLA:H91	30:N:2630:LHG:H321	2.01	0.42
3:4:60:TRP:CE2	25:4:608:CHL:HED2	2.55	0.42
31:4:623:BCR:H15C	31:4:623:BCR:H351	1.72	0.42
2:7:51:GLY:O	2:7:196:ARG:NH2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:60:TRP:CE2	25:8:608:CHL:HED2	2.55	0.42
4:A:202:VAL:HA	4:A:205:VAL:HG22	2.01	0.42
26:B:604:CLA:H62	26:B:604:CLA:H41	1.80	0.42
16:O:20:VAL:HG13	16:O:25:THR:HB	2.01	0.42
26:R:613:CLA:H91	26:R:613:CLA:H112	1.82	0.42
27:Y:1621:LUT:H401	27:Y:1621:LUT:H35	1.80	0.42
3:8:147:PRO:HB3	25:8:608:CHL:HBC2	2.01	0.42
3:8:108:VAL:HG21	31:8:623:BCR:H16C	2.02	0.42
26:B:608:CLA:H62	26:B:608:CLA:H93	1.83	0.42
5:B:74:SER:OG	5:B:94:GLU:OE2	2.37	0.42
7:D:94:TRP:HB2	23:X:53:ASN:HB3	2.01	0.42
18:Q:44:PRO:HA	18:Q:47:ALA:HB3	2.01	0.42
20:S:150:GLU:OE1	20:S:153:ARG:NH2	2.42	0.42
26:S:610:CLA:H43	26:S:612:CLA:HBA1	2.02	0.42
26:S:613:CLA:HMB3	27:S:1620:LUT:H162	2.02	0.42
36:A:418:SQD:C22	31:T:101:BCR:H323	2.50	0.42
25:Y:606:CHL:HMB1	25:Y:609:CHL:HAC1	2.02	0.42
29:5:1623:NEX:H15	29:5:1623:NEX:H201	1.85	0.42
31:8:623:BCR:H351	31:8:623:BCR:H15C	1.72	0.42
4:A:202:VAL:HG13	26:A:405:CLA:HMB3	2.02	0.42
26:C:513:CLA:H102	31:C:514:BCR:H23C	2.02	0.42
1:G:21:ARG:NH2	1:G:36:LEU:O	2.53	0.42
26:G:611:CLA:H91	26:G:611:CLA:H112	1.86	0.42
26:S:604:CLA:C1C	29:S:1623:NEX:H222	2.50	0.42
3:4:10:ILE:HG23	3:4:11:PRO:HD3	2.02	0.42
26:6:614:CLA:HBA1	26:6:614:CLA:H3A	1.86	0.42
5:B:218:SER:HA	19:R:86:VAL:HG21	2.02	0.42
6:C:321:ASP:OD2	6:C:340:TYR:OH	2.31	0.42
26:C:504:CLA:H143	26:C:504:CLA:H112	1.84	0.42
4:A:159:LEU:CD2	26:C:505:CLA:H202	2.49	0.42
26:C:508:CLA:H122	26:C:508:CLA:H161	1.87	0.42
26:C:510:CLA:H193	26:C:510:CLA:H162	1.76	0.42
26:C:513:CLA:H11	31:C:514:BCR:H381	2.01	0.42
29:N:1623:NEX:H201	29:N:1623:NEX:H15	1.76	0.42
25:7:606:CHL:HMB1	25:7:609:CHL:HAC1	2.02	0.41
3:8:167:ILE:HA	3:8:168:PRO:HD3	1.90	0.41
27:8:620:LUT:H15	27:8:620:LUT:H201	1.86	0.41
26:D:402:CLA:H112	26:D:402:CLA:H142	1.83	0.41
26:B:609:CLA:H192	10:H:58:LEU:HD23	2.02	0.41
26:N:602:CLA:HBA1	27:N:1621:LUT:H382	2.03	0.41
18:Q:32:PRO:HD2	18:Q:35:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:R:21:PRO:HB2	19:R:24:LEU:CD1	2.50	0.41
26:R:613:CLA:C1C	26:R:613:CLA:H51	2.50	0.41
20:S:154:ILE:HD11	26:S:609:CLA:CMA	2.50	0.41
1:1:175:GLU:HG2	1:1:179:LYS:HE3	2.01	0.41
27:2:1621:LUT:H201	27:2:1621:LUT:H15	1.80	0.41
29:2:1623:NEX:H201	29:2:1623:NEX:H15	1.83	0.41
1:5:175:GLU:HG2	1:5:179:LYS:HE3	2.01	0.41
30:D:409:LHG:H182	14:L:23:LEU:HD11	2.02	0.41
25:G:608:CHL:H202	26:G:610:CLA:H161	2.02	0.41
17:P:45:GLN:NE2	17:P:48:ARG:HB2	2.36	0.41
2:3:145:MET:HA	2:3:148:VAL:HG22	2.01	0.41
25:3:606:CHL:HMB1	25:3:609:CHL:HAC1	2.02	0.41
29:7:1623:NEX:H11	29:7:1623:NEX:H191	1.75	0.41
5:B:243:ALA:HA	5:B:246:PHE:CE2	2.56	0.41
6:C:390:ARG:HH12	18:Q:25:GLU:HB2	1.86	0.41
31:C:517:BCR:H361	31:C:517:BCR:H20C	1.89	0.41
4:A:213:ALA:HB2	7:D:276:PRO:HG2	2.02	0.41
25:G:607:CHL:H143	25:G:607:CHL:H111	1.72	0.41
1:G:212:HIS:CG	26:G:613:CLA:HAA2	2.55	0.41
1:N:25:LEU:HB2	1:N:29:SER:HA	2.02	0.41
28:Y:1622:XAT:H401	28:Y:1622:XAT:H35	1.86	0.41
2:3:193:LYS:HZ1	30:3:2630:LHG:P	2.43	0.41
4:A:143:ILE:HG13	7:D:221:ASN:ND2	2.34	0.41
4:A:286:THR:HG21	26:A:405:CLA:HMA3	2.03	0.41
26:B:603:CLA:H111	26:B:603:CLA:H91	1.82	0.41
6:C:259:TRP:HH2	26:C:507:CLA:H201	1.85	0.41
30:D:409:LHG:C18	21:T:17:ILE:HD11	2.50	0.41
10:H:30:TYR:CE1	19:R:50:LEU:HG	2.55	0.41
26:N:602:CLA:H101	27:N:1621:LUT:H371	2.02	0.41
26:N:610:CLA:H101	26:N:612:CLA:H142	2.01	0.41
30:R:2630:LHG:H281	30:R:2630:LHG:H102	2.02	0.41
1:Y:196:VAL:HG12	26:Y:613:CLA:HMD3	2.02	0.41
26:2:602:CLA:HBA1	27:2:1621:LUT:H382	2.02	0.41
3:4:175:ARG:NH1	26:4:612:CLA:O1A	2.46	0.41
4:A:257:ARG:HD2	5:B:498:LEU:HD21	2.01	0.41
5:B:75:TRP:CE2	39:B:626:DGD:HG32	2.55	0.41
6:C:318:LEU:HD13	6:C:351:PHE:HE1	1.85	0.41
6:C:97:TRP:NE1	37:Z:101:LMG:H151	2.36	0.41
25:G:607:CHL:H203	25:G:607:CHL:H161	1.91	0.41
14:L:25:ILE:HA	14:L:25:ILE:HD13	1.91	0.41
26:N:610:CLA:H161	26:N:610:CLA:H141	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:610:CLA:HBB1	26:N:612:CLA:H3A	2.03	0.41
26:G:602:CLA:H91	26:Y:603:CLA:H8	2.03	0.41
30:C:522:LHG:H192	26:Y:612:CLA:H101	2.03	0.41
29:1:1623:NEX:H191	29:1:1623:NEX:H11	1.88	0.41
26:B:612:CLA:H62	26:B:612:CLA:H92	1.87	0.41
36:B:623:SQD:H101	15:M:23:LEU:HD22	14.82	0.41
26:C:506:CLA:H162	26:C:506:CLA:H143	1.94	0.41
31:H:101:BCR:H15C	31:H:101:BCR:H351	1.86	0.41
26:B:603:CLA:H171	39:H:102:DGD:HAW1	2.02	0.41
20:S:55:GLY:O	20:S:194:ARG:NH2	2.54	0.41
1:G:222:TRP:HB3	1:Y:105:PHE:HZ	1.85	0.41
1:1:70:ARG:NH1	25:1:608:CHL:OBD	2.42	0.41
28:6:1622:XAT:H11	28:6:1622:XAT:H191	1.83	0.41
4:A:344:ALA:HB3	6:C:354:GLU:HB3	2.03	0.41
31:A:411:BCR:H24C	31:A:411:BCR:H371	1.88	0.41
36:A:412:SQD:H131	30:D:410:LHG:H142	2.03	0.41
5:B:137:LYS:HZ1	10:H:29:GLU:CD	2.23	0.41
5:B:357:ARG:NH1	5:B:358:ARG:O	2.54	0.41
26:B:607:CLA:H142	26:B:607:CLA:H111	1.93	0.41
26:D:402:CLA:H143	26:D:402:CLA:H161	1.91	0.41
31:D:404:BCR:H382	37:D:411:LMG:H341	2.02	0.41
26:G:610:CLA:H41	26:G:610:CLA:H62	1.91	0.41
19:R:147:LEU:HA	19:R:147:LEU:HD23	1.87	0.41
27:R:620:LUT:H15	27:R:620:LUT:H201	1.90	0.41
25:R:606:CHL:H8	29:R:623:NEX:H35	2.03	0.41
1:Y:139:GLU:HG3	25:Y:609:CHL:C4B	2.51	0.41
29:Y:1623:NEX:H201	29:Y:1623:NEX:H15	1.78	0.41
1:Y:217:VAL:CG1	1:Y:217:VAL:O	2.68	0.41
26:Y:613:CLA:H193	26:Y:613:CLA:H161	1.89	0.41
27:2:1620:LUT:H35	27:2:1620:LUT:H401	1.82	0.41
3:4:147:PRO:HB3	25:4:608:CHL:HBC2	2.01	0.41
3:8:10:ILE:HG23	3:8:11:PRO:HD3	2.02	0.41
26:B:611:CLA:H162	26:B:611:CLA:H143	1.96	0.41
9:F:28:LEU:HD22	12:J:24:LEU:HD21	2.03	0.41
1:G:194:PHE:CE1	27:G:1620:LUT:H41	2.55	0.41
14:L:27:VAL:HG11	30:L:101:LHG:H201	2.02	0.41
17:P:124:LYS:HE3	17:P:152:LYS:HD2	2.03	0.41
18:Q:59:VAL:O	18:Q:133:TYR:OH	2.38	0.41
1:2:205:PRO:O	27:2:1620:LUT:O3	2.30	0.41
35:A:408:PHO:H12	35:A:408:PHO:HBA2	1.92	0.41
4:A:48:PHE:CD1	4:A:82:ILE:HD12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:75:TRP:CZ2	39:B:626:DGD:HG11	2.56	0.41
30:D:410:LHG:O1	30:D:410:LHG:O3	2.34	0.41
25:G:607:CHL:H62	25:G:607:CHL:H2	1.70	0.41
27:N:1621:LUT:H35	27:N:1621:LUT:H401	1.88	0.41
30:N:2630:LHG:H312	30:N:2630:LHG:H341	1.81	0.41
20:S:86:MET:HE3	26:S:610:CLA:HMC3	2.09	0.41
27:Y:1620:LUT:H401	27:Y:1620:LUT:H35	1.94	0.41
24:Z:19:LEU:HA	24:Z:19:LEU:HD23	1.94	0.41
25:5:607:CHL:H2	25:5:607:CHL:H62	1.88	0.41
4:A:269:ARG:NE	7:D:223:LEU:HD22	2.36	0.41
5:B:25:MET:HG2	31:B:618:BCR:H23C	2.03	0.41
31:B:619:BCR:H24C	31:B:619:BCR:H371	1.86	0.41
29:G:1623:NEX:H15	29:G:1623:NEX:H201	1.80	0.41
17:P:47:LEU:HD13	17:P:49:TYR:HD1	1.86	0.41
17:P:64:GLN:O	17:P:156:LEU:N	2.41	0.41
17:P:87:LEU:HD11	17:P:158:ILE:HG21	2.02	0.41
37:Z:101:LMG:H291	37:Z:101:LMG:HC91	1.64	0.41
1:2:225:ALA:HB1	28:2:1622:XAT:H183	2.02	0.41
2:3:180:ASP:HA	2:3:181:PRO:HD3	1.93	0.41
4:A:106:LEU:HD11	31:A:411:BCR:H292	2.03	0.41
6:C:203:THR:O	6:C:235:GLY:HA3	2.21	0.41
6:C:405:ASN:HB3	39:C:520:DGD:HG2	2.02	0.41
6:C:464:GLU:OE2	7:D:246:SER:OG	2.37	0.41
25:G:601:CHL:H62	25:G:601:CHL:H41	1.88	0.41
16:O:76:THR:HG22	16:O:118:LEU:HD23	2.03	0.41
26:R:602:CLA:CAB	28:R:622:XAT:H32	2.51	0.41
20:S:154:ILE:HG13	26:S:609:CLA:HMA1	2.03	0.41
26:Y:603:CLA:H3A	26:Y:603:CLA:HBA1	1.80	0.41
1:Y:189:PHE:CE2	26:Y:613:CLA:HAB	2.57	0.41
1:1:181:LEU:HA	1:1:181:LEU:HD23	1.95	0.40
28:5:1622:XAT:H201	28:5:1622:XAT:H15	1.73	0.40
26:6:602:CLA:HBA1	27:6:1621:LUT:H382	2.02	0.40
2:7:193:LYS:NZ	30:7:2630:LHG:O5	2.52	0.40
2:7:152:ARG:HH21	25:7:609:CHL:HMA3	1.86	0.40
31:8:623:BCR:H361	31:8:623:BCR:H20C	1.86	0.40
4:A:140:ARG:HH11	4:A:140:ARG:HD2	1.68	0.40
26:B:602:CLA:H112	26:B:602:CLA:H142	1.90	0.40
26:B:610:CLA:HAB	26:B:610:CLA:HHC	1.85	0.40
26:B:613:CLA:H162	26:B:613:CLA:H122	1.93	0.40
26:C:507:CLA:H142	31:C:515:BCR:H362	2.02	0.40
7:D:80:SER:HA	7:D:173:SER:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:G:1620:LUT:H401	27:G:1620:LUT:H35	1.87	0.40
27:Y:1620:LUT:H201	27:Y:1620:LUT:H15	1.92	0.40
28:1:1622:XAT:H401	28:1:1622:XAT:H35	1.89	0.40
1:1:66:VAL:HG22	1:1:181:LEU:HD21	2.04	0.40
29:3:1623:NEX:H191	29:3:1623:NEX:H11	1.75	0.40
2:3:33:TYR:CG	2:3:55:TRP:HB2	2.56	0.40
26:3:603:CLA:HBC1	25:3:609:CHL:HBC2	2.04	0.40
3:4:108:VAL:HG21	31:4:623:BCR:H16C	2.02	0.40
4:A:140:ARG:HH22	30:D:410:LHG:HC41	1.87	0.40
5:B:216:HIS:HE1	26:B:610:CLA:C1A	2.35	0.40
39:C:519:DGD:HBN1	39:C:519:DGD:HBW1	1.85	0.40
29:G:1623:NEX:H401	29:G:1623:NEX:H35	1.88	0.40
27:N:1620:LUT:H201	27:N:1620:LUT:H15	1.93	0.40
17:P:169:PHE:CB	18:Q:27:ARG:HD3	2.52	0.40
26:S:604:CLA:HBA2	26:S:604:CLA:H3A	1.95	0.40
25:7:601:CHL:H92	25:7:601:CHL:H62	1.86	0.40
3:8:179:ALA:O	3:8:183:HIS:ND1	2.38	0.40
4:A:292:THR:HG22	6:C:428:THR:HB	2.03	0.40
7:D:189:PHE:O	7:D:295:ARG:NE	2.55	0.40
26:A:405:CLA:C19	30:D:409:LHG:H332	2.52	0.40
1:G:51:LEU:HD13	26:G:602:CLA:H42	2.04	0.40
25:G:605:CHL:H3A	25:G:605:CHL:HBA2	1.86	0.40
26:G:610:CLA:H172	26:G:610:CLA:H13	1.86	0.40
31:C:516:BCR:H19C	13:K:53:VAL:HG21	2.04	0.40
14:L:24:LEU:HB2	30:L:101:LHG:H162	2.03	0.40
26:R:604:CLA:C1C	29:R:623:NEX:H222	2.52	0.40
20:S:154:ILE:HD11	26:S:609:CLA:H3A	2.04	0.40
20:S:146:VAL:CG1	26:S:609:CLA:HMC3	2.51	0.40
27:Y:1620:LUT:H391	27:Y:1620:LUT:H31	1.96	0.40
27:2:1620:LUT:H191	27:2:1620:LUT:H11	1.94	0.40
27:5:1621:LUT:H201	27:5:1621:LUT:H15	1.79	0.40
1:6:193:GLY:O	1:6:197:GLN:HG2	2.22	0.40
4:A:104:GLU:OE2	4:A:108:ASN:ND2	2.55	0.40
5:B:12:VAL:HG11	5:B:22:VAL:HG21	2.04	0.40
5:B:39:LEU:HG	5:B:97:ALA:HB1	2.04	0.40
6:C:346:THR:OG1	6:C:348:GLU:OE1	2.37	0.40
1:N:163:PRO:HD2	27:N:1620:LUT:H23	2.03	0.40
26:N:613:CLA:H121	28:N:1622:XAT:H34	2.03	0.40
16:O:141:SER:OG	16:O:201:THR:OG1	2.39	0.40
19:R:93:ARG:HA	19:R:93:ARG:HD3	1.97	0.40
26:S:610:CLA:H62	26:S:610:CLA:H41	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:602:CLA:H93	26:1:602:CLA:H111	1.91	0.40
1:2:153:ASP:OD2	1:2:156:TYR:N	2.53	0.40
2:3:128:LEU:HD23	25:3:605:CHL:HED2	2.03	0.40
26:3:611:CLA:C1B	30:3:2630:LHG:HC31	2.52	0.40
27:6:1620:LUT:H35	27:6:1620:LUT:H401	1.82	0.40
27:6:1621:LUT:H35	27:6:1621:LUT:H401	1.85	0.40
4:A:49:ILE:HG23	38:D:405:PL9:H501	2.04	0.40
5:B:18:ARG:O	5:B:21:SER:HB3	2.22	0.40
6:C:146:PHE:HB3	30:C:2630:LHG:HC12	2.03	0.40
6:C:87:ILE:O	6:C:91:HIS:ND1	2.55	0.40
25:G:601:CHL:H91	25:G:601:CHL:H112	1.74	0.40
26:N:603:CLA:HAC2	25:N:607:CHL:H18	2.04	0.40
20:S:104:ASN:HB3	20:S:128:GLY:HA2	2.03	0.40
25:S:607:CHL:H91	25:S:607:CHL:H112	1.92	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	1	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	2	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	32	60
1	5	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	6	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	32	60
1	G	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	N	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	Y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	g	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	n	217/232 (94%)	214 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
2	3	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
2	7	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
3	8	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
4	A	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
4	a	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
5	B	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
5	b	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
6	c	448/473 (95%)	442 (99%)	6 (1%)	0	100	100
7	D	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
7	d	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
8	E	73/83 (88%)	73 (100%)	0	0	100	100
8	e	73/83 (88%)	73 (100%)	0	0	100	100
9	F	28/39 (72%)	28 (100%)	0	0	100	100
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	58 (100%)	0	0	100	100
10	h	58/73 (80%)	58 (100%)	0	0	100	100
11	I	32/36 (89%)	32 (100%)	0	0	100	100
11	i	32/36 (89%)	32 (100%)	0	0	100	100
12	J	33/40 (82%)	33 (100%)	0	0	100	100
12	j	33/40 (82%)	33 (100%)	0	0	100	100
13	K	35/61 (57%)	35 (100%)	0	0	100	100
13	k	35/61 (57%)	35 (100%)	0	0	100	100
14	L	35/38 (92%)	35 (100%)	0	0	100	100
14	l	35/38 (92%)	35 (100%)	0	0	100	100
15	M	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
15	m	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
16	O	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
16	o	246/248 (99%)	240 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	P	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
17	p	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
18	Q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
18	q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
19	R	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
19	r	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
20	S	216/244 (88%)	209 (97%)	7 (3%)	0	100	100
20	s	216/244 (88%)	208 (96%)	8 (4%)	0	100	100
21	T	30/35 (86%)	30 (100%)	0	0	100	100
21	t	30/35 (86%)	30 (100%)	0	0	100	100
22	W	52/54 (96%)	52 (100%)	0	0	100	100
22	w	52/54 (96%)	52 (100%)	0	0	100	100
23	X	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
23	x	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
24	Z	60/62 (97%)	60 (100%)	0	0	100	100
24	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	9248/10006 (92%)	9056 (98%)	190 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	119	VAL
1	6	119	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5	171/182 (94%)	171 (100%)	0	100	100
1	6	171/182 (94%)	171 (100%)	0	100	100
1	G	171/182 (94%)	171 (100%)	0	100	100
1	N	171/182 (94%)	171 (100%)	0	100	100
1	Y	171/182 (94%)	170 (99%)	1 (1%)	89	97
1	g	171/182 (94%)	171 (100%)	0	100	100
1	n	171/182 (94%)	171 (100%)	0	100	100
1	y	171/182 (94%)	170 (99%)	1 (1%)	89	97
2	3	175/193 (91%)	175 (100%)	0	100	100
2	7	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
3	8	154/162 (95%)	154 (100%)	0	100	100
4	A	270/279 (97%)	269 (100%)	1 (0%)	93	98
4	a	270/279 (97%)	269 (100%)	1 (0%)	93	98
5	B	400/403 (99%)	397 (99%)	3 (1%)	85	95
5	b	400/403 (99%)	397 (99%)	3 (1%)	85	95
6	C	352/373 (94%)	350 (99%)	2 (1%)	89	97
6	c	352/373 (94%)	350 (99%)	2 (1%)	89	97
7	D	275/285 (96%)	274 (100%)	1 (0%)	93	98
7	d	275/285 (96%)	274 (100%)	1 (0%)	93	98
8	E	67/73 (92%)	66 (98%)	1 (2%)	70	90
8	e	67/73 (92%)	66 (98%)	1 (2%)	70	90
9	F	25/34 (74%)	25 (100%)	0	100	100
9	f	25/34 (74%)	25 (100%)	0	100	100
10	H	49/61 (80%)	48 (98%)	1 (2%)	60	86
10	h	49/61 (80%)	48 (98%)	1 (2%)	60	86
11	I	31/33 (94%)	31 (100%)	0	100	100
11	i	31/33 (94%)	31 (100%)	0	100	100
12	J	26/30 (87%)	26 (100%)	0	100	100
12	j	26/30 (87%)	26 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	k	32/54 (59%)	32 (100%)	0	100	100
14	L	35/36 (97%)	35 (100%)	0	100	100
14	l	35/36 (97%)	35 (100%)	0	100	100
15	M	29/30 (97%)	29 (100%)	0	100	100
15	m	29/30 (97%)	29 (100%)	0	100	100
16	O	204/204 (100%)	204 (100%)	0	100	100
16	o	204/204 (100%)	204 (100%)	0	100	100
17	P	150/150 (100%)	150 (100%)	0	100	100
17	p	150/150 (100%)	150 (100%)	0	100	100
18	Q	112/125 (90%)	112 (100%)	0	100	100
18	q	112/125 (90%)	112 (100%)	0	100	100
19	R	191/202 (95%)	190 (100%)	1 (0%)	91	97
19	r	191/202 (95%)	190 (100%)	1 (0%)	91	97
20	S	170/190 (90%)	170 (100%)	0	100	100
20	s	170/190 (90%)	170 (100%)	0	100	100
21	T	29/32 (91%)	29 (100%)	0	100	100
21	t	29/32 (91%)	29 (100%)	0	100	100
22	W	44/44 (100%)	44 (100%)	0	100	100
22	w	44/44 (100%)	44 (100%)	0	100	100
23	X	32/67 (48%)	32 (100%)	0	100	100
23	x	32/67 (48%)	32 (100%)	0	100	100
24	Z	54/54 (100%)	54 (100%)	0	100	100
24	z	54/54 (100%)	54 (100%)	0	100	100
All	All	7522/8048 (94%)	7500 (100%)	22 (0%)	94	98

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	266	ASN
5	B	12	VAL
5	B	362	PHE
5	B	385	ARG
6	C	289	PHE
6	C	391	ARG

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Mol	Chain	Res	Type
7	D	181	ARG
8	E	18	ARG
10	H	61	TYR
19	R	93	ARG
1	Y	32	SER
4	a	266	ASN
5	b	12	VAL
5	b	362	PHE
5	b	385	ARG
6	c	289	PHE
6	c	391	ARG
7	d	181	ARG
8	e	18	ARG
10	h	61	TYR
19	r	93	ARG
1	y	32	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	2	61	ASN
1	2	88	ASN
2	3	95	GLN
2	3	113	GLN
2	3	219	ASN
4	A	234	ASN
4	A	266	ASN
4	A	303	ASN
5	B	216	HIS
5	B	332	ASN
5	B	343	HIS
5	B	496	GLN
6	C	28	GLN
6	C	313	GLN
6	C	332	GLN
7	D	84	ASN
7	D	143	ASN
7	D	221	ASN
7	D	351	ASN
9	F	38	GLN
16	O	74	GLN

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Mol	Chain	Res	Type
17	P	112	ASN
18	Q	75	ASN
18	Q	99	GLN
19	R	47	GLN
19	R	56	ASN
19	R	236	HIS
1	Y	88	ASN
1	5	61	ASN
1	6	61	ASN
1	6	88	ASN
2	7	95	GLN
2	7	113	GLN
2	7	219	ASN
4	a	234	ASN
4	a	266	ASN
4	a	303	ASN
5	b	216	HIS
5	b	332	ASN
5	b	343	HIS
5	b	496	GLN
6	c	28	GLN
6	c	313	GLN
6	c	332	GLN
7	d	84	ASN
7	d	143	ASN
7	d	221	ASN
7	d	351	ASN
9	f	38	GLN
16	o	74	GLN
17	p	112	ASN
18	q	75	ASN
18	q	99	GLN
19	r	47	GLN
19	r	56	ASN
19	r	236	HIS
1	y	88	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 490 ligands modelled in this entry, 6 are monoatomic - leaving 484 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$
27	LUT	1	1620	-	41,43,43	0.78	0	50,60,60	1.82	15 (30%)
27	LUT	1	1621	-	41,43,43	0.90	2 (4%)	50,60,60	1.81	15 (30%)
28	XAT	1	1622	-	39,47,47	0.88	0	54,74,74	2.79	21 (38%)
29	NEX	1	1623	-	38,46,46	0.97	1 (2%)	49,70,70	2.43	13 (26%)
30	LHG	1	2630	26	40,40,48	0.70	1 (2%)	41,46,54	1.37	6 (14%)
25	CHL	1	601	1	41,54,74	4.97	24 (58%)	24,90,114	3.48	14 (58%)
26	CLA	1	602	1	52,69,73	1.18	7 (13%)	60,108,113	1.31	8 (13%)
26	CLA	1	603	1	46,63,73	1.19	7 (15%)	53,101,113	1.54	10 (18%)
26	CLA	1	604	-	41,58,73	1.32	7 (17%)	47,95,113	1.57	9 (19%)
25	CHL	1	605	1	41,54,74	4.91	24 (58%)	24,90,114	3.50	16 (66%)
25	CHL	1	606	-	41,54,74	5.03	24 (58%)	24,90,114	3.55	15 (62%)
25	CHL	1	607	-	61,71,74	4.15	26 (42%)	46,110,114	2.58	17 (36%)
25	CHL	1	608	-	41,54,74	4.93	24 (58%)	24,90,114	3.33	14 (58%)
25	CHL	1	609	1	60,70,74	4.23	28 (46%)	46,109,114	2.70	18 (39%)
26	CLA	1	610	1	47,64,73	1.24	7 (14%)	54,102,113	1.33	8 (14%)
26	CLA	1	611	30	33,53,73	1.37	5 (15%)	37,89,113	1.42	7 (18%)
26	CLA	1	612	1	33,53,73	1.41	6 (18%)	37,89,113	1.56	9 (24%)
26	CLA	1	613	1	46,63,73	1.20	6 (13%)	53,101,113	1.31	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	1	614	1	33,53,73	1.38	5 (15%)	37,89,113	1.46	5 (13%)
27	LUT	2	1620	-	41,43,43	0.80	0	50,60,60	1.86	15 (30%)
27	LUT	2	1621	-	41,43,43	0.83	1 (2%)	50,60,60	1.68	15 (30%)
28	XAT	2	1622	-	39,47,47	0.89	0	54,74,74	2.86	20 (37%)
29	NEX	2	1623	-	38,46,46	0.91	1 (2%)	49,70,70	2.43	15 (30%)
30	LHG	2	2630	26	36,36,48	0.73	0	37,42,54	1.30	4 (10%)
25	CHL	2	601	1	41,54,74	5.00	25 (60%)	24,90,114	3.73	15 (62%)
26	CLA	2	602	1	52,69,73	1.14	5 (9%)	60,108,113	1.34	6 (10%)
26	CLA	2	603	1	46,63,73	1.21	5 (10%)	53,101,113	1.54	11 (20%)
26	CLA	2	604	-	33,53,73	1.41	5 (15%)	37,89,113	1.53	6 (16%)
25	CHL	2	605	1	41,54,74	4.81	24 (58%)	24,90,114	3.51	16 (66%)
25	CHL	2	606	-	41,54,74	4.96	24 (58%)	24,90,114	3.45	15 (62%)
25	CHL	2	607	-	59,69,74	4.10	24 (40%)	45,108,114	2.61	17 (37%)
25	CHL	2	608	-	41,54,74	4.89	25 (60%)	24,90,114	3.42	14 (58%)
25	CHL	2	609	1	59,69,74	4.16	27 (45%)	45,108,114	2.74	20 (44%)
26	CLA	2	610	1	41,58,73	1.24	6 (14%)	47,95,113	1.40	8 (17%)
26	CLA	2	611	30	33,53,73	1.33	5 (15%)	37,89,113	1.48	8 (21%)
26	CLA	2	612	1	33,53,73	1.35	5 (15%)	37,89,113	1.64	8 (21%)
26	CLA	2	613	1	33,53,73	1.36	6 (18%)	37,89,113	1.43	5 (13%)
26	CLA	2	614	1	33,53,73	1.33	4 (12%)	37,89,113	1.42	5 (13%)
27	LUT	3	1620	-	41,43,43	0.83	0	50,60,60	1.88	13 (26%)
27	LUT	3	1621	-	41,43,43	0.84	1 (2%)	50,60,60	1.67	12 (24%)
28	XAT	3	1622	-	39,47,47	1.00	2 (5%)	54,74,74	2.85	24 (44%)
29	NEX	3	1623	-	38,46,46	0.85	0	49,70,70	2.43	17 (34%)
30	LHG	3	2630	26	46,46,48	0.69	1 (2%)	47,52,54	1.27	5 (10%)
25	CHL	3	601	2	62,72,74	4.18	26 (41%)	48,111,114	2.65	13 (27%)
26	CLA	3	602	2	51,68,73	1.16	7 (13%)	59,107,113	1.36	8 (13%)
26	CLA	3	603	2	46,63,73	1.20	8 (17%)	53,101,113	1.54	12 (22%)
26	CLA	3	604	-	33,53,73	1.37	7 (21%)	37,89,113	1.56	6 (16%)
25	CHL	3	605	2	41,54,74	4.83	22 (53%)	24,90,114	3.54	17 (70%)
25	CHL	3	606	-	41,54,74	4.96	24 (58%)	24,90,114	3.57	17 (70%)
25	CHL	3	607	-	51,61,74	4.50	26 (50%)	35,98,114	3.01	16 (45%)
25	CHL	3	608	-	41,54,74	5.01	26 (63%)	24,90,114	3.39	13 (54%)
25	CHL	3	609	2	59,69,74	4.22	25 (42%)	45,108,114	2.71	18 (40%)
26	CLA	3	610	2	51,68,73	1.17	7 (13%)	59,107,113	1.30	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	3	611	30	46,63,73	1.34	6 (13%)	53,101,113	1.45	12 (22%)
26	CLA	3	612	2	33,53,73	1.40	7 (21%)	37,89,113	1.80	9 (24%)
26	CLA	3	613	2	49,66,73	1.17	7 (14%)	56,104,113	1.36	7 (12%)
26	CLA	3	614	2	39,56,73	1.31	6 (15%)	45,92,113	1.28	7 (15%)
30	LHG	4	2630	26	20,20,48	0.89	0	21,26,54	1.34	2 (9%)
25	CHL	4	601	3	36,53,74	5.04	20 (55%)	19,89,114	3.78	12 (63%)
26	CLA	4	602	3	33,53,73	1.35	7 (21%)	37,89,113	1.63	7 (18%)
26	CLA	4	603	3	33,53,73	1.36	6 (18%)	37,89,113	1.59	8 (21%)
26	CLA	4	604	-	33,53,73	1.38	5 (15%)	37,89,113	1.43	6 (16%)
25	CHL	4	606	-	41,54,74	4.96	23 (56%)	24,90,114	3.53	16 (66%)
25	CHL	4	607	-	41,54,74	4.89	24 (58%)	24,90,114	3.42	14 (58%)
25	CHL	4	608	-	41,54,74	4.98	25 (60%)	24,90,114	3.37	14 (58%)
25	CHL	4	609	3	41,54,74	4.99	25 (60%)	24,90,114	3.39	15 (62%)
26	CLA	4	610	3	33,53,73	1.41	7 (21%)	37,89,113	1.36	5 (13%)
26	CLA	4	611	30	33,53,73	1.35	5 (15%)	37,89,113	1.48	6 (16%)
26	CLA	4	612	3	33,53,73	1.35	5 (15%)	37,89,113	1.58	7 (18%)
27	LUT	4	620	-	41,43,43	0.79	0	50,60,60	2.02	17 (34%)
28	XAT	4	622	-	39,47,47	0.90	0	54,74,74	2.62	20 (37%)
31	BCR	4	623	-	41,41,41	0.73	0	56,56,56	2.30	16 (28%)
27	LUT	5	1620	-	41,43,43	0.79	0	50,60,60	1.81	15 (30%)
27	LUT	5	1621	-	41,43,43	0.89	2 (4%)	50,60,60	1.81	15 (30%)
28	XAT	5	1622	-	39,47,47	0.88	0	54,74,74	2.79	21 (38%)
29	NEX	5	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.42	13 (26%)
30	LHG	5	2630	26	40,40,48	0.70	1 (2%)	41,46,54	1.36	6 (14%)
25	CHL	5	601	1	41,54,74	4.97	24 (58%)	24,90,114	3.48	14 (58%)
26	CLA	5	602	1	52,69,73	1.18	7 (13%)	60,108,113	1.32	8 (13%)
26	CLA	5	603	1	46,63,73	1.19	5 (10%)	53,101,113	1.55	10 (18%)
26	CLA	5	604	-	41,58,73	1.32	7 (17%)	47,95,113	1.56	9 (19%)
25	CHL	5	605	1	41,54,74	4.91	24 (58%)	24,90,114	3.50	16 (66%)
25	CHL	5	606	-	41,54,74	5.03	24 (58%)	24,90,114	3.55	15 (62%)
25	CHL	5	607	-	61,71,74	4.15	27 (44%)	46,110,114	2.58	17 (36%)
25	CHL	5	608	-	41,54,74	4.93	24 (58%)	24,90,114	3.33	14 (58%)
25	CHL	5	609	1	60,70,74	4.23	27 (45%)	46,109,114	2.71	18 (39%)
26	CLA	5	610	1	47,64,73	1.25	7 (14%)	54,102,113	1.33	8 (14%)
26	CLA	5	611	30	33,53,73	1.37	5 (15%)	37,89,113	1.43	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	5	612	1	33,53,73	1.42	6 (18%)	37,89,113	1.56	9 (24%)
26	CLA	5	613	1	46,63,73	1.20	6 (13%)	53,101,113	1.32	6 (11%)
26	CLA	5	614	1	33,53,73	1.38	5 (15%)	37,89,113	1.46	5 (13%)
27	LUT	6	1620	-	41,43,43	0.80	0	50,60,60	1.85	15 (30%)
27	LUT	6	1621	-	41,43,43	0.83	1 (2%)	50,60,60	1.68	15 (30%)
28	XAT	6	1622	-	39,47,47	0.89	0	54,74,74	2.85	20 (37%)
29	NEX	6	1623	-	38,46,46	0.91	1 (2%)	49,70,70	2.43	15 (30%)
30	LHG	6	2630	26	36,36,48	0.73	0	37,42,54	1.30	4 (10%)
25	CHL	6	601	1	41,54,74	5.01	25 (60%)	24,90,114	3.74	15 (62%)
26	CLA	6	602	1	52,69,73	1.14	5 (9%)	60,108,113	1.34	6 (10%)
26	CLA	6	603	1	46,63,73	1.21	5 (10%)	53,101,113	1.54	11 (20%)
26	CLA	6	604	-	33,53,73	1.40	5 (15%)	37,89,113	1.53	6 (16%)
25	CHL	6	605	1	41,54,74	4.81	24 (58%)	24,90,114	3.50	16 (66%)
25	CHL	6	606	-	41,54,74	4.97	24 (58%)	24,90,114	3.45	15 (62%)
25	CHL	6	607	-	59,69,74	4.10	24 (40%)	45,108,114	2.61	17 (37%)
25	CHL	6	608	-	41,54,74	4.89	25 (60%)	24,90,114	3.41	14 (58%)
25	CHL	6	609	1	59,69,74	4.17	26 (44%)	45,108,114	2.74	20 (44%)
26	CLA	6	610	1	41,58,73	1.24	6 (14%)	47,95,113	1.39	8 (17%)
26	CLA	6	611	30	33,53,73	1.33	5 (15%)	37,89,113	1.48	8 (21%)
26	CLA	6	612	1	33,53,73	1.35	5 (15%)	37,89,113	1.64	8 (21%)
26	CLA	6	613	1	33,53,73	1.36	6 (18%)	37,89,113	1.43	5 (13%)
26	CLA	6	614	1	33,53,73	1.34	4 (12%)	37,89,113	1.42	5 (13%)
27	LUT	7	1620	-	41,43,43	0.83	0	50,60,60	1.87	13 (26%)
27	LUT	7	1621	-	41,43,43	0.85	1 (2%)	50,60,60	1.67	12 (24%)
28	XAT	7	1622	-	39,47,47	1.01	2 (5%)	54,74,74	2.85	22 (40%)
29	NEX	7	1623	-	38,46,46	0.85	0	49,70,70	2.42	17 (34%)
30	LHG	7	2630	26	46,46,48	0.69	1 (2%)	47,52,54	1.27	5 (10%)
25	CHL	7	601	2	62,72,74	4.18	26 (41%)	48,111,114	2.64	13 (27%)
26	CLA	7	602	2	51,68,73	1.17	7 (13%)	59,107,113	1.37	8 (13%)
26	CLA	7	603	2	46,63,73	1.20	8 (17%)	53,101,113	1.55	12 (22%)
26	CLA	7	604	-	33,53,73	1.37	7 (21%)	37,89,113	1.56	6 (16%)
25	CHL	7	605	2	41,54,74	4.83	22 (53%)	24,90,114	3.54	17 (70%)
25	CHL	7	606	-	41,54,74	4.97	24 (58%)	24,90,114	3.57	17 (70%)
25	CHL	7	607	-	51,61,74	4.50	25 (49%)	35,98,114	3.01	16 (45%)
25	CHL	7	608	-	41,54,74	5.00	26 (63%)	24,90,114	3.39	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	7	609	2	59,69,74	4.22	25 (42%)	45,108,114	2.71	18 (40%)
26	CLA	7	610	2	51,68,73	1.17	7 (13%)	59,107,113	1.31	8 (13%)
26	CLA	7	611	30	46,63,73	1.34	7 (15%)	53,101,113	1.44	12 (22%)
26	CLA	7	612	2	33,53,73	1.40	7 (21%)	37,89,113	1.80	9 (24%)
26	CLA	7	613	2	49,66,73	1.17	7 (14%)	56,104,113	1.36	8 (14%)
26	CLA	7	614	2	39,56,73	1.31	6 (15%)	45,92,113	1.27	7 (15%)
30	LHG	8	2630	26	20,20,48	0.89	0	21,26,54	1.34	2 (9%)
25	CHL	8	601	3	36,53,74	5.04	20 (55%)	19,89,114	3.78	12 (63%)
26	CLA	8	602	3	33,53,73	1.35	7 (21%)	37,89,113	1.63	8 (21%)
26	CLA	8	603	3	33,53,73	1.36	6 (18%)	37,89,113	1.59	8 (21%)
26	CLA	8	604	-	33,53,73	1.38	5 (15%)	37,89,113	1.43	6 (16%)
25	CHL	8	606	-	41,54,74	4.96	23 (56%)	24,90,114	3.52	16 (66%)
25	CHL	8	607	-	41,54,74	4.89	24 (58%)	24,90,114	3.43	14 (58%)
25	CHL	8	608	-	41,54,74	4.98	25 (60%)	24,90,114	3.37	14 (58%)
25	CHL	8	609	3	41,54,74	4.99	25 (60%)	24,90,114	3.40	15 (62%)
26	CLA	8	610	3	33,53,73	1.41	7 (21%)	37,89,113	1.36	5 (13%)
26	CLA	8	611	30	33,53,73	1.35	5 (15%)	37,89,113	1.49	6 (16%)
26	CLA	8	612	3	33,53,73	1.35	5 (15%)	37,89,113	1.57	7 (18%)
27	LUT	8	620	-	41,43,43	0.79	0	50,60,60	2.02	18 (36%)
28	XAT	8	622	-	39,47,47	0.91	0	54,74,74	2.62	20 (37%)
31	BCR	8	623	-	41,41,41	0.73	0	56,56,56	2.31	17 (30%)
32	OEX	A	401	4,6	0,15,15	0.00	-	0,32,32	0.00	-
26	CLA	A	405	4	56,73,73	1.30	6 (10%)	65,113,113	1.55	12 (18%)
26	CLA	A	406	42	56,73,73	1.10	6 (10%)	65,113,113	1.63	13 (20%)
26	CLA	A	407	42	41,58,73	1.31	6 (14%)	47,95,113	1.58	9 (19%)
35	PHO	A	408	-	67,69,69	1.26	8 (11%)	87,99,99	1.33	15 (17%)
35	PHO	A	409	-	67,69,69	1.24	6 (8%)	87,99,99	1.28	10 (11%)
26	CLA	A	410	4	51,68,73	1.18	7 (13%)	59,107,113	1.57	10 (16%)
31	BCR	A	411	-	41,41,41	0.77	0	56,56,56	1.78	12 (21%)
36	SQD	A	412	-	49,50,54	0.96	6 (12%)	59,61,65	1.89	11 (18%)
37	LMG	A	413	-	48,48,55	0.79	0	56,56,63	1.32	6 (10%)
38	PL9	A	414	-	13,13,55	0.87	0	17,17,69	1.57	4 (23%)
37	LMG	A	415	-	40,40,55	0.86	0	48,48,63	1.30	5 (10%)
36	SQD	A	418	-	53,54,54	0.92	5 (9%)	63,65,65	1.89	13 (20%)
30	LHG	B	2630	-	46,46,48	0.64	1 (2%)	47,52,54	1.30	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	B	2631	-	48,48,48	0.67	2 (4%)	49,54,54	1.24	6 (12%)
37	LMG	B	2633	-	55,55,55	0.79	3 (5%)	63,63,63	1.34	6 (9%)
26	CLA	B	602	42	56,73,73	1.16	7 (12%)	65,113,113	1.24	7 (10%)
26	CLA	B	603	5	56,73,73	1.13	5 (8%)	65,113,113	1.44	9 (13%)
26	CLA	B	604	5	56,73,73	1.20	7 (12%)	65,113,113	1.45	8 (12%)
26	CLA	B	605	5	56,73,73	1.34	6 (10%)	65,113,113	1.86	19 (29%)
26	CLA	B	606	5	56,73,73	1.23	8 (14%)	65,113,113	1.52	9 (13%)
26	CLA	B	607	5	56,73,73	1.13	6 (10%)	65,113,113	1.55	12 (18%)
26	CLA	B	608	42	56,73,73	1.21	6 (10%)	65,113,113	1.46	10 (15%)
26	CLA	B	609	5	56,73,73	1.04	5 (8%)	65,113,113	1.65	12 (18%)
26	CLA	B	610	5	56,73,73	1.12	6 (10%)	65,113,113	1.51	10 (15%)
26	CLA	B	611	42	56,73,73	1.14	7 (12%)	65,113,113	1.55	12 (18%)
26	CLA	B	612	5	56,73,73	1.17	6 (10%)	65,113,113	1.59	11 (16%)
26	CLA	B	613	5	56,73,73	1.23	7 (12%)	65,113,113	1.77	10 (15%)
26	CLA	B	614	5	56,73,73	1.16	6 (10%)	65,113,113	1.33	8 (12%)
26	CLA	B	615	5	56,73,73	1.14	7 (12%)	65,113,113	1.33	9 (13%)
26	CLA	B	616	5	56,73,73	1.16	8 (14%)	65,113,113	1.37	13 (20%)
26	CLA	B	617	5	56,73,73	1.15	5 (8%)	65,113,113	1.59	14 (21%)
31	BCR	B	618	-	41,41,41	0.82	1 (2%)	56,56,56	1.84	13 (23%)
31	BCR	B	619	-	41,41,41	0.78	0	56,56,56	1.80	17 (30%)
31	BCR	B	620	-	41,41,41	0.78	1 (2%)	56,56,56	1.98	15 (26%)
36	SQD	B	621	-	53,54,54	0.94	4 (7%)	63,65,65	1.90	14 (22%)
37	LMG	B	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.31	6 (10%)
36	SQD	B	623	-	41,42,54	1.10	5 (12%)	51,53,65	2.08	11 (21%)
39	DGD	B	626	-	60,60,67	1.04	3 (5%)	74,74,81	1.41	13 (17%)
30	LHG	C	2630	-	48,48,48	0.64	1 (2%)	49,54,54	1.34	7 (14%)
26	CLA	C	501	6	56,73,73	1.13	7 (12%)	65,113,113	1.33	9 (13%)
26	CLA	C	502	6	56,73,73	1.11	5 (8%)	65,113,113	1.52	11 (16%)
26	CLA	C	503	6	56,73,73	1.13	6 (10%)	65,113,113	1.35	11 (16%)
26	CLA	C	504	42	56,73,73	1.07	7 (12%)	65,113,113	1.62	8 (12%)
26	CLA	C	505	6	56,73,73	1.19	6 (10%)	65,113,113	1.50	12 (18%)
26	CLA	C	506	6	56,73,73	1.14	6 (10%)	65,113,113	1.52	11 (16%)
26	CLA	C	507	42	56,73,73	1.18	8 (14%)	65,113,113	1.52	11 (16%)
26	CLA	C	508	6	56,73,73	1.15	7 (12%)	65,113,113	1.85	12 (18%)
26	CLA	C	509	6	56,73,73	1.19	8 (14%)	65,113,113	1.62	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	C	510	6	56,73,73	1.11	4 (7%)	65,113,113	1.51	9 (13%)
26	CLA	C	511	6	56,73,73	1.12	6 (10%)	65,113,113	1.39	9 (13%)
26	CLA	C	512	6	56,73,73	1.09	7 (12%)	65,113,113	1.49	10 (15%)
26	CLA	C	513	6	56,73,73	1.06	5 (8%)	65,113,113	1.57	14 (21%)
31	BCR	C	514	-	41,41,41	0.88	1 (2%)	56,56,56	1.73	12 (21%)
31	BCR	C	515	-	41,41,41	0.91	2 (4%)	56,56,56	2.01	17 (30%)
31	BCR	C	516	-	41,41,41	0.72	0	56,56,56	1.98	17 (30%)
31	BCR	C	517	-	41,41,41	0.88	1 (2%)	56,56,56	2.08	11 (19%)
39	DGD	C	518	-	56,56,67	1.18	7 (12%)	70,70,81	1.60	15 (21%)
39	DGD	C	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.50	14 (18%)
39	DGD	C	520	-	61,61,67	1.18	9 (14%)	75,75,81	1.50	15 (20%)
37	LMG	C	521	-	51,51,55	0.80	2 (3%)	59,59,63	1.40	6 (10%)
30	LHG	C	522	-	48,48,48	0.67	1 (2%)	49,54,54	1.29	8 (16%)
30	LHG	C	523	-	48,48,48	0.65	0	49,54,54	1.22	5 (10%)
40	BCT	D	401	33	0,3,3	0.00	-	0,3,3	0.00	-
26	CLA	D	402	7	56,73,73	1.30	8 (14%)	65,113,113	1.57	11 (16%)
26	CLA	D	403	7	56,73,73	1.06	4 (7%)	65,113,113	1.65	12 (18%)
31	BCR	D	404	-	41,41,41	0.73	0	56,56,56	1.83	13 (23%)
38	PL9	D	405	-	55,55,55	1.78	10 (18%)	69,69,69	1.51	11 (15%)
30	LHG	D	408	-	45,45,48	0.75	1 (2%)	46,51,54	1.30	5 (10%)
30	LHG	D	409	-	48,48,48	0.73	1 (2%)	49,54,54	1.33	7 (14%)
30	LHG	D	410	-	42,42,48	0.66	1 (2%)	43,48,54	1.24	4 (9%)
37	LMG	D	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.50	5 (9%)
41	HEM	F	101	9,8	28,50,50	1.81	4 (14%)	17,82,82	1.71	4 (23%)
27	LUT	G	1620	-	41,43,43	0.76	0	50,60,60	1.67	12 (24%)
27	LUT	G	1621	-	41,43,43	0.89	1 (2%)	50,60,60	1.99	17 (34%)
28	XAT	G	1622	-	39,47,47	0.95	1 (2%)	54,74,74	2.91	22 (40%)
29	NEX	G	1623	-	38,46,46	0.98	2 (5%)	49,70,70	2.43	14 (28%)
30	LHG	G	2630	26	48,48,48	0.64	1 (2%)	49,54,54	1.30	6 (12%)
25	CHL	G	601	1	64,74,74	4.13	26 (40%)	51,114,114	2.66	17 (33%)
26	CLA	G	602	1	56,73,73	1.10	5 (8%)	65,113,113	1.57	12 (18%)
26	CLA	G	603	1	56,73,73	1.14	7 (12%)	65,113,113	1.56	15 (23%)
26	CLA	G	604	42	41,58,73	1.35	5 (12%)	47,95,113	1.73	10 (21%)
25	CHL	G	605	1	41,54,74	4.78	23 (56%)	24,90,114	3.52	13 (54%)
25	CHL	G	606	42	48,58,74	4.60	25 (52%)	32,94,114	3.16	18 (56%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	G	607	42	64,74,74	4.10	26 (40%)	51,114,114	2.43	16 (31%)
25	CHL	G	608	42	64,74,74	4.04	26 (40%)	51,114,114	2.49	15 (29%)
25	CHL	G	609	1	59,69,74	4.23	25 (42%)	45,108,114	2.92	17 (37%)
26	CLA	G	610	1	55,72,73	1.08	5 (9%)	63,111,113	1.42	9 (14%)
26	CLA	G	611	30	51,68,73	1.19	5 (9%)	59,107,113	1.51	8 (13%)
26	CLA	G	612	1	51,68,73	1.10	5 (9%)	59,107,113	1.40	9 (15%)
26	CLA	G	613	1	56,73,73	1.10	5 (8%)	65,113,113	1.24	8 (12%)
26	CLA	G	614	1	39,56,73	1.28	4 (10%)	45,92,113	1.42	6 (13%)
31	BCR	H	101	-	41,41,41	0.76	0	56,56,56	1.89	10 (17%)
39	DGD	H	102	-	63,63,67	1.09	7 (11%)	77,77,81	1.43	10 (12%)
30	LHG	L	101	-	48,48,48	0.88	1 (2%)	49,54,54	1.32	6 (12%)
27	LUT	N	1620	-	41,43,43	0.79	0	50,60,60	1.71	13 (26%)
27	LUT	N	1621	-	41,43,43	0.89	2 (4%)	50,60,60	1.90	15 (30%)
28	XAT	N	1622	-	39,47,47	0.90	0	54,74,74	3.01	23 (42%)
29	NEX	N	1623	-	38,46,46	0.88	1 (2%)	49,70,70	2.39	15 (30%)
30	LHG	N	2630	26	48,48,48	0.65	1 (2%)	49,54,54	1.31	6 (12%)
25	CHL	N	601	1	64,74,74	4.05	26 (40%)	51,114,114	2.66	16 (31%)
26	CLA	N	602	1	56,73,73	1.10	5 (8%)	65,113,113	1.56	11 (16%)
26	CLA	N	603	1	56,73,73	1.19	8 (14%)	65,113,113	1.51	14 (21%)
26	CLA	N	604	42	41,58,73	1.37	6 (14%)	47,95,113	1.80	10 (21%)
25	CHL	N	605	1	46,56,74	4.75	24 (52%)	30,92,114	3.28	15 (50%)
25	CHL	N	606	42	48,58,74	4.58	26 (54%)	32,94,114	3.11	15 (46%)
25	CHL	N	607	42	64,74,74	4.10	25 (39%)	51,114,114	2.32	11 (21%)
25	CHL	N	608	42	64,74,74	4.05	25 (39%)	51,114,114	2.58	18 (35%)
25	CHL	N	609	1	64,74,74	4.17	26 (40%)	51,114,114	2.61	15 (29%)
26	CLA	N	610	1	56,73,73	1.07	6 (10%)	65,113,113	1.46	13 (20%)
26	CLA	N	611	30	51,68,73	1.17	5 (9%)	59,107,113	1.29	8 (13%)
26	CLA	N	612	1	51,68,73	1.11	6 (11%)	59,107,113	1.43	10 (16%)
26	CLA	N	613	1	51,68,73	1.13	5 (9%)	59,107,113	1.44	8 (13%)
26	CLA	N	614	1	39,56,73	1.19	4 (10%)	45,92,113	1.64	7 (15%)
30	LHG	R	2630	26	41,41,48	0.69	1 (2%)	42,47,54	1.30	7 (16%)
26	CLA	R	601	19	40,57,73	1.23	4 (10%)	46,93,113	1.92	12 (26%)
26	CLA	R	602	19	51,68,73	1.12	4 (7%)	59,107,113	1.54	10 (16%)
26	CLA	R	603	19	51,68,73	1.12	4 (7%)	59,107,113	1.70	14 (23%)
26	CLA	R	604	42	39,56,73	1.28	4 (10%)	45,92,113	1.76	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	R	606	42	64,74,74	4.04	25 (39%)	51,114,114	2.54	18 (35%)
25	CHL	R	607	42	54,64,74	4.46	26 (48%)	39,102,114	2.88	18 (46%)
25	CHL	R	608	42	59,69,74	4.38	27 (45%)	45,108,114	2.63	15 (33%)
26	CLA	R	609	19	49,66,73	1.14	5 (10%)	56,104,113	1.45	9 (16%)
26	CLA	R	610	19	56,73,73	1.13	6 (10%)	65,113,113	1.44	11 (16%)
26	CLA	R	611	30	40,57,73	1.28	4 (10%)	46,93,113	1.75	12 (26%)
26	CLA	R	612	19	40,57,73	1.25	5 (12%)	46,93,113	1.45	9 (19%)
26	CLA	R	613	19	51,68,73	1.17	6 (11%)	59,107,113	1.17	6 (10%)
25	CHL	R	614	19	40,50,74	5.00	25 (62%)	25,85,114	3.38	15 (60%)
26	CLA	R	616	19	33,53,73	1.43	5 (15%)	37,89,113	1.39	6 (16%)
27	LUT	R	620	-	41,43,43	0.86	2 (4%)	50,60,60	1.85	15 (30%)
28	XAT	R	622	-	39,47,47	0.94	0	54,74,74	2.77	21 (38%)
29	NEX	R	623	-	38,46,46	1.03	3 (7%)	49,70,70	2.54	18 (36%)
27	LUT	S	1620	-	41,43,43	0.79	0	50,60,60	1.74	9 (18%)
27	LUT	S	1621	-	41,43,43	0.84	1 (2%)	50,60,60	1.89	17 (34%)
29	NEX	S	1623	-	38,46,46	0.89	1 (2%)	49,70,70	2.27	15 (30%)
30	LHG	S	2630	26	48,48,48	0.72	1 (2%)	49,54,54	1.28	7 (14%)
25	CHL	S	601	20	41,54,74	5.18	24 (58%)	24,90,114	3.35	13 (54%)
26	CLA	S	602	20	52,69,73	1.15	5 (9%)	60,108,113	1.52	10 (16%)
26	CLA	S	603	20	33,53,73	1.37	6 (18%)	37,89,113	1.85	10 (27%)
26	CLA	S	604	42	41,58,73	1.28	4 (9%)	47,95,113	1.79	9 (19%)
25	CHL	S	606	42	41,54,74	4.78	23 (56%)	24,90,114	3.50	15 (62%)
25	CHL	S	607	42	56,66,74	4.24	25 (44%)	40,104,114	2.80	15 (37%)
25	CHL	S	608	-	41,54,74	4.96	23 (56%)	24,90,114	3.38	12 (50%)
26	CLA	S	609	20	33,53,73	1.36	5 (15%)	37,89,113	1.43	6 (16%)
26	CLA	S	610	20	46,63,73	1.16	6 (13%)	53,101,113	1.60	9 (16%)
26	CLA	S	611	30	47,64,73	1.22	6 (12%)	54,102,113	1.37	8 (14%)
26	CLA	S	612	20	40,57,73	1.20	5 (12%)	46,93,113	1.70	8 (17%)
26	CLA	S	613	20	46,63,73	1.15	5 (10%)	53,101,113	1.49	7 (13%)
26	CLA	S	614	20	40,57,73	1.19	4 (10%)	46,93,113	1.73	7 (15%)
31	BCR	T	101	-	41,41,41	0.74	0	56,56,56	2.55	19 (33%)
27	LUT	Y	1620	-	41,43,43	0.86	2 (4%)	50,60,60	1.77	13 (26%)
27	LUT	Y	1621	-	41,43,43	0.87	1 (2%)	50,60,60	1.69	13 (26%)
28	XAT	Y	1622	-	39,47,47	1.06	2 (5%)	54,74,74	3.00	20 (37%)
29	NEX	Y	1623	-	38,46,46	0.92	1 (2%)	49,70,70	2.59	17 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	Y	2630	26	48,48,48	0.78	2 (4%)	49,54,54	1.25	6 (12%)
25	CHL	Y	601	1	64,74,74	4.19	26 (40%)	51,114,114	2.66	16 (31%)
26	CLA	Y	602	1	56,73,73	1.14	5 (8%)	65,113,113	1.50	12 (18%)
26	CLA	Y	603	1	56,73,73	1.17	7 (12%)	65,113,113	1.49	14 (21%)
26	CLA	Y	604	42	41,58,73	1.36	6 (14%)	47,95,113	1.76	11 (23%)
25	CHL	Y	605	1	46,56,74	4.71	26 (56%)	30,92,114	3.13	14 (46%)
25	CHL	Y	606	42	48,58,74	4.81	28 (58%)	32,94,114	3.06	16 (50%)
25	CHL	Y	607	42	64,74,74	4.22	27 (42%)	51,114,114	2.45	16 (31%)
25	CHL	Y	608	42	64,74,74	4.13	25 (39%)	51,114,114	2.61	18 (35%)
25	CHL	Y	609	1	64,74,74	4.15	27 (42%)	51,114,114	2.74	16 (31%)
26	CLA	Y	610	1	51,68,73	1.20	7 (13%)	59,107,113	1.34	8 (13%)
26	CLA	Y	611	30	51,68,73	1.17	6 (11%)	59,107,113	1.42	11 (18%)
26	CLA	Y	612	1	51,68,73	1.20	6 (11%)	59,107,113	1.44	10 (16%)
26	CLA	Y	613	1	56,73,73	1.12	6 (10%)	65,113,113	1.34	10 (15%)
26	CLA	Y	614	1	39,56,73	1.28	6 (15%)	45,92,113	1.53	9 (20%)
37	LMG	Z	101	-	51,51,55	0.85	1 (1%)	59,59,63	1.35	6 (10%)
32	OEX	a	401	4,6	0,15,15	0.00	-	0,32,32	0.00	-
26	CLA	a	405	4	56,73,73	1.30	6 (10%)	65,113,113	1.55	12 (18%)
26	CLA	a	406	42	56,73,73	1.10	6 (10%)	65,113,113	1.63	13 (20%)
26	CLA	a	407	42	41,58,73	1.30	7 (17%)	47,95,113	1.58	9 (19%)
35	PHO	a	408	-	67,69,69	1.25	8 (11%)	87,99,99	1.32	15 (17%)
35	PHO	a	409	-	67,69,69	1.24	6 (8%)	87,99,99	1.28	10 (11%)
26	CLA	a	410	4	51,68,73	1.18	7 (13%)	59,107,113	1.57	10 (16%)
31	BCR	a	411	-	41,41,41	0.77	0	56,56,56	1.78	12 (21%)
36	SQD	a	412	-	49,50,54	0.96	6 (12%)	59,61,65	1.90	12 (20%)
37	LMG	a	413	-	48,48,55	0.80	0	56,56,63	1.32	6 (10%)
38	PL9	a	414	-	13,13,55	0.87	0	17,17,69	1.57	4 (23%)
37	LMG	a	415	-	40,40,55	0.86	0	48,48,63	1.31	5 (10%)
36	SQD	a	418	-	53,54,54	0.92	5 (9%)	63,65,65	1.90	13 (20%)
30	LHG	b	2630	-	46,46,48	0.64	1 (2%)	47,52,54	1.30	6 (12%)
30	LHG	b	2631	-	48,48,48	0.66	2 (4%)	49,54,54	1.24	6 (12%)
37	LMG	b	2633	-	55,55,55	0.79	3 (5%)	63,63,63	1.34	6 (9%)
26	CLA	b	602	42	56,73,73	1.15	7 (12%)	65,113,113	1.24	7 (10%)
26	CLA	b	603	5	56,73,73	1.12	5 (8%)	65,113,113	1.44	8 (12%)
26	CLA	b	604	5	56,73,73	1.19	7 (12%)	65,113,113	1.44	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	b	605	5	56,73,73	1.34	6 (10%)	65,113,113	1.86	19 (29%)
26	CLA	b	606	5	56,73,73	1.23	7 (12%)	65,113,113	1.52	9 (13%)
26	CLA	b	607	5	56,73,73	1.13	6 (10%)	65,113,113	1.55	13 (20%)
26	CLA	b	608	42	56,73,73	1.21	6 (10%)	65,113,113	1.46	10 (15%)
26	CLA	b	609	5	56,73,73	1.04	4 (7%)	65,113,113	1.65	12 (18%)
26	CLA	b	610	5	56,73,73	1.12	6 (10%)	65,113,113	1.51	10 (15%)
26	CLA	b	611	42	56,73,73	1.14	7 (12%)	65,113,113	1.56	12 (18%)
26	CLA	b	612	5	56,73,73	1.17	6 (10%)	65,113,113	1.59	11 (16%)
26	CLA	b	613	5	56,73,73	1.23	7 (12%)	65,113,113	1.78	10 (15%)
26	CLA	b	614	5	56,73,73	1.17	6 (10%)	65,113,113	1.33	8 (12%)
26	CLA	b	615	5	56,73,73	1.13	7 (12%)	65,113,113	1.33	9 (13%)
26	CLA	b	616	5	56,73,73	1.16	8 (14%)	65,113,113	1.37	13 (20%)
26	CLA	b	617	5	56,73,73	1.15	5 (8%)	65,113,113	1.59	14 (21%)
31	BCR	b	618	-	41,41,41	0.83	1 (2%)	56,56,56	1.84	13 (23%)
31	BCR	b	619	-	41,41,41	0.78	0	56,56,56	1.80	16 (28%)
31	BCR	b	620	-	41,41,41	0.78	1 (2%)	56,56,56	1.98	15 (26%)
36	SQD	b	621	-	53,54,54	0.94	4 (7%)	63,65,65	1.90	14 (22%)
37	LMG	b	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.31	6 (10%)
36	SQD	b	623	-	41,42,54	1.10	5 (12%)	51,53,65	2.08	11 (21%)
39	DGD	b	626	-	60,60,67	1.04	3 (5%)	74,74,81	1.41	13 (17%)
30	LHG	c	2630	-	48,48,48	0.64	1 (2%)	49,54,54	1.34	7 (14%)
26	CLA	c	501	6	56,73,73	1.13	7 (12%)	65,113,113	1.32	9 (13%)
26	CLA	c	502	6	56,73,73	1.11	4 (7%)	65,113,113	1.51	11 (16%)
26	CLA	c	503	6	56,73,73	1.12	6 (10%)	65,113,113	1.35	11 (16%)
26	CLA	c	504	42	56,73,73	1.07	5 (8%)	65,113,113	1.62	9 (13%)
26	CLA	c	505	6	56,73,73	1.19	6 (10%)	65,113,113	1.50	12 (18%)
26	CLA	c	506	6	56,73,73	1.14	5 (8%)	65,113,113	1.52	10 (15%)
26	CLA	c	507	42	56,73,73	1.18	8 (14%)	65,113,113	1.52	11 (16%)
26	CLA	c	508	6	56,73,73	1.14	7 (12%)	65,113,113	1.84	12 (18%)
26	CLA	c	509	6	56,73,73	1.19	8 (14%)	65,113,113	1.62	11 (16%)
26	CLA	c	510	6	56,73,73	1.11	4 (7%)	65,113,113	1.50	9 (13%)
26	CLA	c	511	6	56,73,73	1.12	6 (10%)	65,113,113	1.39	9 (13%)
26	CLA	c	512	6	56,73,73	1.09	7 (12%)	65,113,113	1.49	9 (13%)
26	CLA	c	513	6	56,73,73	1.06	5 (8%)	65,113,113	1.57	14 (21%)
31	BCR	c	514	-	41,41,41	0.88	2 (4%)	56,56,56	1.73	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	c	515	-	41,41,41	0.91	2 (4%)	56,56,56	2.01	17 (30%)
31	BCR	c	516	-	41,41,41	0.72	0	56,56,56	1.98	17 (30%)
31	BCR	c	517	-	41,41,41	0.87	1 (2%)	56,56,56	2.09	11 (19%)
39	DGD	c	518	-	56,56,67	1.18	7 (12%)	70,70,81	1.60	15 (21%)
39	DGD	c	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.50	13 (16%)
39	DGD	c	520	-	61,61,67	1.18	9 (14%)	75,75,81	1.50	15 (20%)
37	LMG	c	521	-	51,51,55	0.80	2 (3%)	59,59,63	1.40	6 (10%)
30	LHG	c	522	-	48,48,48	0.68	1 (2%)	49,54,54	1.29	8 (16%)
30	LHG	c	523	-	48,48,48	0.65	0	49,54,54	1.21	5 (10%)
40	BCT	d	401	33	0,3,3	0.00	-	0,3,3	0.00	-
26	CLA	d	402	7	56,73,73	1.29	8 (14%)	65,113,113	1.57	12 (18%)
26	CLA	d	403	7	56,73,73	1.06	4 (7%)	65,113,113	1.65	12 (18%)
31	BCR	d	404	-	41,41,41	0.73	0	56,56,56	1.83	13 (23%)
38	PL9	d	405	-	55,55,55	1.78	11 (20%)	69,69,69	1.51	10 (14%)
30	LHG	d	408	-	45,45,48	0.75	1 (2%)	46,51,54	1.30	5 (10%)
30	LHG	d	409	-	48,48,48	0.73	1 (2%)	49,54,54	1.33	7 (14%)
30	LHG	d	410	-	42,42,48	0.67	1 (2%)	43,48,54	1.24	4 (9%)
37	LMG	d	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.50	5 (9%)
41	HEM	f	101	9,8	28,50,50	1.80	4 (14%)	17,82,82	1.71	4 (23%)
27	LUT	g	1620	-	41,43,43	0.76	0	50,60,60	1.66	12 (24%)
27	LUT	g	1621	-	41,43,43	0.90	1 (2%)	50,60,60	1.99	17 (34%)
28	XAT	g	1622	-	39,47,47	0.95	1 (2%)	54,74,74	2.92	22 (40%)
29	NEX	g	1623	-	38,46,46	0.98	2 (5%)	49,70,70	2.43	14 (28%)
30	LHG	g	2630	26	48,48,48	0.65	1 (2%)	49,54,54	1.30	6 (12%)
25	CHL	g	601	1	64,74,74	4.13	26 (40%)	51,114,114	2.66	17 (33%)
26	CLA	g	602	1	56,73,73	1.10	5 (8%)	65,113,113	1.57	12 (18%)
26	CLA	g	603	1	56,73,73	1.14	7 (12%)	65,113,113	1.57	15 (23%)
26	CLA	g	604	42	41,58,73	1.36	5 (12%)	47,95,113	1.73	10 (21%)
25	CHL	g	605	1	41,54,74	4.78	23 (56%)	24,90,114	3.52	13 (54%)
25	CHL	g	606	42	48,58,74	4.60	25 (52%)	32,94,114	3.16	18 (56%)
25	CHL	g	607	42	64,74,74	4.10	26 (40%)	51,114,114	2.43	16 (31%)
25	CHL	g	608	42	64,74,74	4.04	26 (40%)	51,114,114	2.50	15 (29%)
25	CHL	g	609	1	59,69,74	4.23	26 (44%)	45,108,114	2.92	17 (37%)
26	CLA	g	610	1	55,72,73	1.08	5 (9%)	63,111,113	1.42	9 (14%)
26	CLA	g	611	30	51,68,73	1.19	5 (9%)	59,107,113	1.51	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	g	612	1	51,68,73	1.11	5 (9%)	59,107,113	1.40	9 (15%)
26	CLA	g	613	1	56,73,73	1.10	5 (8%)	65,113,113	1.24	8 (12%)
26	CLA	g	614	1	39,56,73	1.27	4 (10%)	45,92,113	1.42	6 (13%)
31	BCR	h	101	-	41,41,41	0.76	0	56,56,56	1.88	10 (17%)
39	DGD	h	102	-	63,63,67	1.10	7 (11%)	77,77,81	1.43	10 (12%)
30	LHG	l	101	-	48,48,48	0.88	1 (2%)	49,54,54	1.32	6 (12%)
27	LUT	n	1620	-	41,43,43	0.79	0	50,60,60	1.71	13 (26%)
27	LUT	n	1621	-	41,43,43	0.89	2 (4%)	50,60,60	1.90	15 (30%)
28	XAT	n	1622	-	39,47,47	0.90	0	54,74,74	3.01	23 (42%)
29	NEX	n	1623	-	38,46,46	0.88	1 (2%)	49,70,70	2.39	16 (32%)
30	LHG	n	2630	26	48,48,48	0.65	1 (2%)	49,54,54	1.31	6 (12%)
25	CHL	n	601	1	64,74,74	4.05	26 (40%)	51,114,114	2.66	16 (31%)
26	CLA	n	602	1	56,73,73	1.10	5 (8%)	65,113,113	1.56	11 (16%)
26	CLA	n	603	1	56,73,73	1.19	8 (14%)	65,113,113	1.52	14 (21%)
26	CLA	n	604	42	41,58,73	1.37	6 (14%)	47,95,113	1.80	9 (19%)
25	CHL	n	605	1	46,56,74	4.75	24 (52%)	30,92,114	3.28	15 (50%)
25	CHL	n	606	42	48,58,74	4.58	26 (54%)	32,94,114	3.10	15 (46%)
25	CHL	n	607	42	64,74,74	4.10	25 (39%)	51,114,114	2.32	12 (23%)
25	CHL	n	608	42	64,74,74	4.05	25 (39%)	51,114,114	2.58	18 (35%)
25	CHL	n	609	1	64,74,74	4.17	26 (40%)	51,114,114	2.61	15 (29%)
26	CLA	n	610	1	56,73,73	1.06	6 (10%)	65,113,113	1.46	12 (18%)
26	CLA	n	611	30	51,68,73	1.17	5 (9%)	59,107,113	1.29	8 (13%)
26	CLA	n	612	1	51,68,73	1.11	6 (11%)	59,107,113	1.44	10 (16%)
26	CLA	n	613	1	51,68,73	1.13	5 (9%)	59,107,113	1.44	8 (13%)
26	CLA	n	614	1	39,56,73	1.19	4 (10%)	45,92,113	1.64	8 (17%)
30	LHG	r	2630	26	41,41,48	0.69	1 (2%)	42,47,54	1.30	7 (16%)
26	CLA	r	601	19	40,57,73	1.23	4 (10%)	46,93,113	1.92	12 (26%)
26	CLA	r	602	19	51,68,73	1.13	4 (7%)	59,107,113	1.54	10 (16%)
26	CLA	r	603	19	51,68,73	1.12	4 (7%)	59,107,113	1.70	14 (23%)
26	CLA	r	604	42	39,56,73	1.28	4 (10%)	45,92,113	1.76	10 (22%)
25	CHL	r	606	42	64,74,74	4.04	25 (39%)	51,114,114	2.54	18 (35%)
25	CHL	r	607	42	54,64,74	4.46	26 (48%)	39,102,114	2.88	18 (46%)
25	CHL	r	608	42	59,69,74	4.37	27 (45%)	45,108,114	2.63	15 (33%)
26	CLA	r	609	19	49,66,73	1.15	5 (10%)	56,104,113	1.45	9 (16%)
26	CLA	r	610	19	56,73,73	1.14	7 (12%)	65,113,113	1.44	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	r	611	30	40,57,73	1.28	5 (12%)	46,93,113	1.75	12 (26%)
26	CLA	r	612	19	40,57,73	1.25	5 (12%)	46,93,113	1.46	9 (19%)
26	CLA	r	613	19	51,68,73	1.17	6 (11%)	59,107,113	1.17	7 (11%)
25	CHL	r	614	19	40,50,74	5.00	24 (60%)	25,85,114	3.38	15 (60%)
26	CLA	r	616	19	33,53,73	1.43	5 (15%)	37,89,113	1.39	6 (16%)
27	LUT	r	620	-	41,43,43	0.87	2 (4%)	50,60,60	1.85	15 (30%)
28	XAT	r	622	-	39,47,47	0.94	0	54,74,74	2.78	21 (38%)
29	NEX	r	623	-	38,46,46	1.02	3 (7%)	49,70,70	2.54	18 (36%)
27	LUT	s	1620	-	41,43,43	0.78	0	50,60,60	1.74	9 (18%)
27	LUT	s	1621	-	41,43,43	0.84	1 (2%)	50,60,60	1.89	17 (34%)
29	NEX	s	1623	-	38,46,46	0.88	1 (2%)	49,70,70	2.27	15 (30%)
30	LHG	s	2630	26	48,48,48	0.72	1 (2%)	49,54,54	1.28	7 (14%)
25	CHL	s	601	20	41,54,74	5.18	24 (58%)	24,90,114	3.35	14 (58%)
26	CLA	s	602	20	52,69,73	1.15	5 (9%)	60,108,113	1.52	9 (15%)
26	CLA	s	603	20	33,53,73	1.37	6 (18%)	37,89,113	1.85	10 (27%)
26	CLA	s	604	42	41,58,73	1.28	4 (9%)	47,95,113	1.79	10 (21%)
25	CHL	s	606	42	41,54,74	4.77	23 (56%)	24,90,114	3.50	15 (62%)
25	CHL	s	607	42	56,66,74	4.23	24 (42%)	40,104,114	2.80	15 (37%)
25	CHL	s	608	-	41,54,74	4.96	23 (56%)	24,90,114	3.38	12 (50%)
26	CLA	s	609	20	33,53,73	1.36	5 (15%)	37,89,113	1.43	6 (16%)
26	CLA	s	610	20	46,63,73	1.17	6 (13%)	53,101,113	1.60	9 (16%)
26	CLA	s	611	30	47,64,73	1.22	6 (12%)	54,102,113	1.37	8 (14%)
26	CLA	s	612	20	40,57,73	1.20	5 (12%)	46,93,113	1.70	8 (17%)
26	CLA	s	613	20	46,63,73	1.15	5 (10%)	53,101,113	1.49	7 (13%)
26	CLA	s	614	20	40,57,73	1.19	4 (10%)	46,93,113	1.73	7 (15%)
31	BCR	t	101	-	41,41,41	0.74	0	56,56,56	2.54	18 (32%)
27	LUT	y	1620	-	41,43,43	0.87	2 (4%)	50,60,60	1.77	13 (26%)
27	LUT	y	1621	-	41,43,43	0.88	1 (2%)	50,60,60	1.69	13 (26%)
28	XAT	y	1622	-	39,47,47	1.06	2 (5%)	54,74,74	3.00	20 (37%)
29	NEX	y	1623	-	38,46,46	0.92	1 (2%)	49,70,70	2.59	17 (34%)
30	LHG	y	2630	26	48,48,48	0.78	2 (4%)	49,54,54	1.25	6 (12%)
25	CHL	y	601	1	64,74,74	4.19	26 (40%)	51,114,114	2.66	16 (31%)
26	CLA	y	602	1	56,73,73	1.14	5 (8%)	65,113,113	1.49	12 (18%)
26	CLA	y	603	1	56,73,73	1.16	7 (12%)	65,113,113	1.49	14 (21%)
26	CLA	y	604	42	41,58,73	1.36	6 (14%)	47,95,113	1.76	11 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	y	605	1	46,56,74	4.71	25 (54%)	30,92,114	3.13	14 (46%)
25	CHL	y	606	42	48,58,74	4.82	29 (60%)	32,94,114	3.07	16 (50%)
25	CHL	y	607	42	64,74,74	4.21	27 (42%)	51,114,114	2.45	15 (29%)
25	CHL	y	608	42	64,74,74	4.13	25 (39%)	51,114,114	2.61	18 (35%)
25	CHL	y	609	1	64,74,74	4.14	27 (42%)	51,114,114	2.74	15 (29%)
26	CLA	y	610	1	51,68,73	1.20	7 (13%)	59,107,113	1.34	8 (13%)
26	CLA	y	611	30	51,68,73	1.17	6 (11%)	59,107,113	1.42	11 (18%)
26	CLA	y	612	1	51,68,73	1.20	6 (11%)	59,107,113	1.44	10 (16%)
26	CLA	y	613	1	56,73,73	1.12	6 (10%)	65,113,113	1.34	10 (15%)
26	CLA	y	614	1	39,56,73	1.28	7 (17%)	45,92,113	1.53	9 (20%)
37	LMG	z	101	-	51,51,55	0.85	1 (1%)	59,59,63	1.35	6 (10%)

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
27	LUT	1	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	1	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	1	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	1	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	1	2630	26	-	0/45/45/53	0/0/0/0
25	CHL	1	601	1	-	0/15/153/177	0/0/9/9
26	CLA	1	602	1	3/3/19/25	0/33/131/135	0/0/9/9
26	CLA	1	603	1	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	1	604	-	2/2/17/25	0/19/117/135	0/0/9/9
25	CHL	1	605	1	-	0/15/153/177	0/0/9/9
25	CHL	1	606	-	-	0/15/153/177	0/0/9/9
25	CHL	1	607	-	-	0/38/174/177	0/0/9/9
25	CHL	1	608	-	-	0/15/153/177	0/0/9/9
25	CHL	1	609	1	-	0/37/173/177	0/0/9/9
26	CLA	1	610	1	3/3/18/25	0/27/125/135	0/0/9/9
26	CLA	1	611	30	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	1	612	1	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	1	613	1	2/2/18/25	0/25/123/135	0/0/9/9
26	CLA	1	614	1	3/3/16/25	0/11/111/135	0/0/9/9
27	LUT	2	1620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LUT	2	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	2	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	2	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	2	2630	26	-	0/41/41/53	0/0/0/0
25	CHL	2	601	1	-	0/15/153/177	0/0/9/9
26	CLA	2	602	1	3/3/19/25	0/33/131/135	0/0/9/9
26	CLA	2	603	1	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	2	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	2	605	1	-	0/15/153/177	0/0/9/9
25	CHL	2	606	-	-	0/15/153/177	0/0/9/9
25	CHL	2	607	-	-	0/35/171/177	0/0/9/9
25	CHL	2	608	-	-	0/15/153/177	0/0/9/9
25	CHL	2	609	1	-	0/35/171/177	0/0/9/9
26	CLA	2	610	1	3/3/17/25	0/19/117/135	0/0/9/9
26	CLA	2	611	30	2/2/16/25	0/11/111/135	0/0/9/9
26	CLA	2	612	1	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	2	613	1	2/2/16/25	0/11/111/135	0/0/9/9
26	CLA	2	614	1	3/3/16/25	0/11/111/135	0/0/9/9
27	LUT	3	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	3	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	3	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	3	2630	26	-	0/51/51/53	0/0/0/0
25	CHL	3	601	2	-	0/39/175/177	0/0/9/9
26	CLA	3	602	2	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	3	603	2	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	3	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	3	605	2	-	0/15/153/177	0/0/9/9
25	CHL	3	606	-	-	0/15/153/177	0/0/9/9
25	CHL	3	607	-	-	0/26/162/177	0/0/9/9
25	CHL	3	608	-	-	0/15/153/177	0/0/9/9
25	CHL	3	609	2	-	0/35/171/177	0/0/9/9
26	CLA	3	610	2	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	3	611	30	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	3	612	2	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	3	613	2	3/3/18/25	0/29/127/135	0/0/9/9
26	CLA	3	614	2	3/3/16/25	0/17/115/135	0/0/9/9
30	LHG	4	2630	26	-	0/23/23/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	4	601	3	-	0/9/151/177	0/0/9/9
26	CLA	4	602	3	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	4	603	3	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	4	604	-	2/2/16/25	0/11/111/135	0/0/9/9
25	CHL	4	606	-	-	0/15/153/177	0/0/9/9
25	CHL	4	607	-	-	0/15/153/177	0/0/9/9
25	CHL	4	608	-	-	0/15/153/177	0/0/9/9
25	CHL	4	609	3	-	0/15/153/177	0/0/9/9
26	CLA	4	610	3	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	4	611	30	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	4	612	3	3/3/16/25	0/11/111/135	0/0/9/9
27	LUT	4	620	-	-	0/29/67/67	0/2/2/2
28	XAT	4	622	-	-	0/31/93/93	0/2/4/4
31	BCR	4	623	-	-	0/29/63/63	0/2/2/2
27	LUT	5	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	5	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	5	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	5	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	5	2630	26	-	0/45/45/53	0/0/0/0
25	CHL	5	601	1	-	0/15/153/177	0/0/9/9
26	CLA	5	602	1	3/3/19/25	0/33/131/135	0/0/9/9
26	CLA	5	603	1	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	5	604	-	2/2/17/25	0/19/117/135	0/0/9/9
25	CHL	5	605	1	-	0/15/153/177	0/0/9/9
25	CHL	5	606	-	-	0/15/153/177	0/0/9/9
25	CHL	5	607	-	-	0/38/174/177	0/0/9/9
25	CHL	5	608	-	-	0/15/153/177	0/0/9/9
25	CHL	5	609	1	-	0/37/173/177	0/0/9/9
26	CLA	5	610	1	3/3/18/25	0/27/125/135	0/0/9/9
26	CLA	5	611	30	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	5	612	1	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	5	613	1	2/2/18/25	0/25/123/135	0/0/9/9
26	CLA	5	614	1	3/3/16/25	0/11/111/135	0/0/9/9
27	LUT	6	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	6	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	6	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	6	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	6	2630	26	-	0/41/41/53	0/0/0/0
25	CHL	6	601	1	-	0/15/153/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	6	602	1	3/3/19/25	0/33/131/135	0/0/9/9
26	CLA	6	603	1	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	6	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	6	605	1	-	0/15/153/177	0/0/9/9
25	CHL	6	606	-	-	0/15/153/177	0/0/9/9
25	CHL	6	607	-	-	0/35/171/177	0/0/9/9
25	CHL	6	608	-	-	0/15/153/177	0/0/9/9
25	CHL	6	609	1	-	0/35/171/177	0/0/9/9
26	CLA	6	610	1	3/3/17/25	0/19/117/135	0/0/9/9
26	CLA	6	611	30	2/2/16/25	0/11/111/135	0/0/9/9
26	CLA	6	612	1	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	6	613	1	2/2/16/25	0/11/111/135	0/0/9/9
26	CLA	6	614	1	3/3/16/25	0/11/111/135	0/0/9/9
27	LUT	7	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	7	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	7	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	7	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	7	2630	26	-	0/51/51/53	0/0/0/0
25	CHL	7	601	2	-	0/39/175/177	0/0/9/9
26	CLA	7	602	2	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	7	603	2	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	7	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	7	605	2	-	0/15/153/177	0/0/9/9
25	CHL	7	606	-	-	0/15/153/177	0/0/9/9
25	CHL	7	607	-	-	0/26/162/177	0/0/9/9
25	CHL	7	608	-	-	0/15/153/177	0/0/9/9
25	CHL	7	609	2	-	0/35/171/177	0/0/9/9
26	CLA	7	610	2	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	7	611	30	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	7	612	2	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	7	613	2	3/3/18/25	0/29/127/135	0/0/9/9
26	CLA	7	614	2	3/3/16/25	0/17/115/135	0/0/9/9
30	LHG	8	2630	26	-	0/23/23/53	0/0/0/0
25	CHL	8	601	3	-	0/9/151/177	0/0/9/9
26	CLA	8	602	3	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	8	603	3	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	8	604	-	2/2/16/25	0/11/111/135	0/0/9/9
25	CHL	8	606	-	-	0/15/153/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	8	607	-	-	0/15/153/177	0/0/9/9
25	CHL	8	608	-	-	0/15/153/177	0/0/9/9
25	CHL	8	609	3	-	0/15/153/177	0/0/9/9
26	CLA	8	610	3	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	8	611	30	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	8	612	3	3/3/16/25	0/11/111/135	0/0/9/9
27	LUT	8	620	-	-	0/29/67/67	0/2/2/2
28	XAT	8	622	-	-	0/31/93/93	0/2/4/4
31	BCR	8	623	-	-	0/29/63/63	0/2/2/2
32	OEX	A	401	4,6	-	0/0/68/68	0/0/6/6
26	CLA	A	405	4	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	A	406	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	A	407	42	2/2/17/25	0/19/117/135	0/0/9/9
35	PHO	A	408	-	-	0/53/103/103	0/1/6/6
35	PHO	A	409	-	-	0/53/103/103	0/1/6/6
26	CLA	A	410	4	3/3/19/25	0/31/129/135	0/0/9/9
31	BCR	A	411	-	-	0/29/63/63	0/2/2/2
36	SQD	A	412	-	-	1/45/65/69	0/1/1/1
37	LMG	A	413	-	-	0/43/63/70	0/1/1/1
38	PL9	A	414	-	-	0/5/18/73	0/1/1/1
37	LMG	A	415	-	-	0/35/55/70	0/1/1/1
36	SQD	A	418	-	-	0/49/69/69	0/1/1/1
30	LHG	B	2630	-	-	0/51/51/53	0/0/0/0
30	LHG	B	2631	-	-	0/53/53/53	0/0/0/0
37	LMG	B	2633	-	-	0/50/70/70	0/1/1/1
26	CLA	B	602	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	603	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	604	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	605	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	606	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	607	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	608	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	609	5	2/2/20/25	0/37/135/135	0/0/9/9
26	CLA	B	610	5	2/2/20/25	0/37/135/135	0/0/9/9
26	CLA	B	611	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	612	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	613	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	614	5	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	B	615	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	616	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	B	617	5	3/3/20/25	0/37/135/135	0/0/9/9
31	BCR	B	618	-	-	0/29/63/63	0/2/2/2
31	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	BCR	B	620	-	-	0/29/63/63	0/2/2/2
36	SQD	B	621	-	-	0/49/69/69	0/1/1/1
37	LMG	B	622	-	-	0/46/66/70	0/1/1/1
36	SQD	B	623	-	-	0/37/57/69	0/1/1/1
39	DGD	B	626	-	-	0/48/88/95	0/2/2/2
30	LHG	C	2630	-	-	0/53/53/53	0/0/0/0
26	CLA	C	501	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	502	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	503	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	504	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	505	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	506	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	507	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	508	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	509	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	510	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	511	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	512	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	C	513	6	2/2/20/25	0/37/135/135	0/0/9/9
31	BCR	C	514	-	-	0/29/63/63	0/2/2/2
31	BCR	C	515	-	-	0/29/63/63	0/2/2/2
31	BCR	C	516	-	-	0/29/63/63	0/2/2/2
31	BCR	C	517	-	-	0/29/63/63	0/2/2/2
39	DGD	C	518	-	-	0/44/84/95	0/2/2/2
39	DGD	C	519	-	-	0/51/91/95	0/2/2/2
39	DGD	C	520	-	-	0/49/89/95	0/2/2/2
37	LMG	C	521	-	-	0/46/66/70	0/1/1/1
30	LHG	C	522	-	-	0/53/53/53	0/0/0/0
30	LHG	C	523	-	-	0/53/53/53	0/0/0/0
40	BCT	D	401	33	-	0/0/0/0	0/0/0/0
26	CLA	D	402	7	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	D	403	7	2/2/20/25	0/37/135/135	0/0/9/9
31	BCR	D	404	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PL9	D	405	-	-	0/53/73/73	0/1/1/1
30	LHG	D	408	-	-	0/50/50/53	0/0/0/0
30	LHG	D	409	-	-	0/53/53/53	0/0/0/0
30	LHG	D	410	-	-	0/47/47/53	0/0/0/0
37	LMG	D	411	-	-	0/41/61/70	0/1/1/1
41	HEM	F	101	9,8	-	0/6/54/54	0/0/8/8
27	LUT	G	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	G	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	G	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	G	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	G	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	G	601	1	-	0/41/177/177	0/0/9/9
26	CLA	G	602	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	G	603	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	G	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	G	605	1	-	0/15/153/177	0/0/9/9
25	CHL	G	606	42	-	0/22/158/177	0/0/9/9
25	CHL	G	607	42	-	0/41/177/177	0/0/9/9
25	CHL	G	608	42	-	0/41/177/177	0/0/9/9
25	CHL	G	609	1	-	0/35/171/177	0/0/9/9
26	CLA	G	610	1	3/3/19/25	0/36/134/135	0/0/9/9
26	CLA	G	611	30	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	G	612	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	G	613	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	G	614	1	3/3/16/25	0/17/115/135	0/0/9/9
31	BCR	H	101	-	-	0/29/63/63	0/2/2/2
39	DGD	H	102	-	-	0/51/91/95	0/2/2/2
30	LHG	L	101	-	-	0/53/53/53	0/0/0/0
27	LUT	N	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	N	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	N	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	N	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	N	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	N	601	1	-	0/41/177/177	0/0/9/9
26	CLA	N	602	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	N	603	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	N	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	N	605	1	-	0/20/156/177	0/0/9/9
25	CHL	N	606	42	-	0/22/158/177	0/0/9/9
25	CHL	N	607	42	-	0/41/177/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	N	608	42	-	0/41/177/177	0/0/9/9
25	CHL	N	609	1	-	0/41/177/177	0/0/9/9
26	CLA	N	610	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	N	611	30	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	N	612	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	N	613	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	N	614	1	3/3/16/25	0/17/115/135	0/0/9/9
30	LHG	R	2630	26	-	0/46/46/53	0/0/0/0
26	CLA	R	601	19	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	R	602	19	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	R	603	19	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	R	604	42	3/3/16/25	0/17/115/135	0/0/9/9
25	CHL	R	606	42	-	0/41/177/177	0/0/9/9
25	CHL	R	607	42	-	0/29/165/177	0/0/9/9
25	CHL	R	608	42	-	0/35/171/177	0/0/9/9
26	CLA	R	609	19	3/3/18/25	0/29/127/135	0/0/9/9
26	CLA	R	610	19	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	R	611	30	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	R	612	19	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	R	613	19	3/3/19/25	0/31/129/135	0/0/9/9
25	CHL	R	614	19	-	0/12/148/177	0/0/9/9
26	CLA	R	616	19	2/2/16/25	0/11/111/135	0/0/9/9
27	LUT	R	620	-	-	0/29/67/67	0/2/2/2
28	XAT	R	622	-	-	0/31/93/93	0/2/4/4
29	NEX	R	623	-	-	0/27/83/83	0/2/3/3
27	LUT	S	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
29	NEX	S	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	S	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	S	601	20	-	0/15/153/177	0/0/9/9
26	CLA	S	602	20	3/3/19/25	0/33/131/135	0/0/9/9
26	CLA	S	603	20	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	S	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	S	606	42	-	0/15/153/177	0/0/9/9
25	CHL	S	607	42	-	0/32/168/177	0/0/9/9
25	CHL	S	608	-	-	0/15/153/177	0/0/9/9
26	CLA	S	609	20	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	S	610	20	3/3/18/25	0/25/123/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	S	611	30	3/3/18/25	0/27/125/135	0/0/9/9
26	CLA	S	612	20	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	S	613	20	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	S	614	20	3/3/16/25	0/18/116/135	0/0/9/9
31	BCR	T	101	-	-	0/29/63/63	0/2/2/2
27	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	Y	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	Y	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	Y	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	Y	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	Y	601	1	-	0/41/177/177	0/0/9/9
26	CLA	Y	602	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	Y	603	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	Y	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	Y	605	1	-	0/20/156/177	0/0/9/9
25	CHL	Y	606	42	-	0/22/158/177	0/0/9/9
25	CHL	Y	607	42	-	0/41/177/177	0/0/9/9
25	CHL	Y	608	42	-	0/41/177/177	0/0/9/9
25	CHL	Y	609	1	-	0/41/177/177	0/0/9/9
26	CLA	Y	610	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	Y	611	30	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	Y	612	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	Y	613	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	Y	614	1	3/3/16/25	0/17/115/135	0/0/9/9
37	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
32	OEX	a	401	4,6	-	0/0/68/68	0/0/6/6
26	CLA	a	405	4	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	a	406	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	a	407	42	2/2/17/25	0/19/117/135	0/0/9/9
35	PHO	a	408	-	-	0/53/103/103	0/1/6/6
35	PHO	a	409	-	-	0/53/103/103	0/1/6/6
26	CLA	a	410	4	3/3/19/25	0/31/129/135	0/0/9/9
31	BCR	a	411	-	-	0/29/63/63	0/2/2/2
36	SQD	a	412	-	-	1/45/65/69	0/1/1/1
37	LMG	a	413	-	-	0/43/63/70	0/1/1/1
38	PL9	a	414	-	-	0/5/18/73	0/1/1/1
37	LMG	a	415	-	-	0/35/55/70	0/1/1/1
36	SQD	a	418	-	-	0/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	b	2630	-	-	0/51/51/53	0/0/0/0
30	LHG	b	2631	-	-	0/53/53/53	0/0/0/0
37	LMG	b	2633	-	-	0/50/70/70	0/1/1/1
26	CLA	b	602	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	603	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	604	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	605	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	606	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	607	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	608	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	609	5	2/2/20/25	0/37/135/135	0/0/9/9
26	CLA	b	610	5	2/2/20/25	0/37/135/135	0/0/9/9
26	CLA	b	611	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	612	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	613	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	614	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	615	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	616	5	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	b	617	5	3/3/20/25	0/37/135/135	0/0/9/9
31	BCR	b	618	-	-	0/29/63/63	0/2/2/2
31	BCR	b	619	-	-	0/29/63/63	0/2/2/2
31	BCR	b	620	-	-	0/29/63/63	0/2/2/2
36	SQD	b	621	-	-	0/49/69/69	0/1/1/1
37	LMG	b	622	-	-	0/46/66/70	0/1/1/1
36	SQD	b	623	-	-	0/37/57/69	0/1/1/1
39	DGD	b	626	-	-	0/48/88/95	0/2/2/2
30	LHG	c	2630	-	-	0/53/53/53	0/0/0/0
26	CLA	c	501	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	502	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	503	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	504	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	505	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	506	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	507	42	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	508	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	509	6	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	c	510	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	511	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	512	6	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	c	513	6	2/2/20/25	0/37/135/135	0/0/9/9
31	BCR	c	514	-	-	0/29/63/63	0/2/2/2
31	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	BCR	c	516	-	-	0/29/63/63	0/2/2/2
31	BCR	c	517	-	-	0/29/63/63	0/2/2/2
39	DGD	c	518	-	-	0/44/84/95	0/2/2/2
39	DGD	c	519	-	-	0/51/91/95	0/2/2/2
39	DGD	c	520	-	-	0/49/89/95	0/2/2/2
37	LMG	c	521	-	-	0/46/66/70	0/1/1/1
30	LHG	c	522	-	-	0/53/53/53	0/0/0/0
30	LHG	c	523	-	-	0/53/53/53	0/0/0/0
40	BCT	d	401	33	-	0/0/0/0	0/0/0/0
26	CLA	d	402	7	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	d	403	7	2/2/20/25	0/37/135/135	0/0/9/9
31	BCR	d	404	-	-	0/29/63/63	0/2/2/2
38	PL9	d	405	-	-	0/53/73/73	0/1/1/1
30	LHG	d	408	-	-	0/50/50/53	0/0/0/0
30	LHG	d	409	-	-	0/53/53/53	0/0/0/0
30	LHG	d	410	-	-	0/47/47/53	0/0/0/0
37	LMG	d	411	-	-	0/41/61/70	0/1/1/1
41	HEM	f	101	9,8	-	0/6/54/54	0/0/8/8
27	LUT	g	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	g	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	g	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	g	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	g	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	g	601	1	-	0/41/177/177	0/0/9/9
26	CLA	g	602	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	g	603	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	g	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	g	605	1	-	0/15/153/177	0/0/9/9
25	CHL	g	606	42	-	0/22/158/177	0/0/9/9
25	CHL	g	607	42	-	0/41/177/177	0/0/9/9
25	CHL	g	608	42	-	0/41/177/177	0/0/9/9
25	CHL	g	609	1	-	0/35/171/177	0/0/9/9
26	CLA	g	610	1	3/3/19/25	0/36/134/135	0/0/9/9
26	CLA	g	611	30	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	g	612	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	g	613	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	g	614	1	3/3/16/25	0/17/115/135	0/0/9/9
31	BCR	h	101	-	-	0/29/63/63	0/2/2/2
39	DGD	h	102	-	-	0/51/91/95	0/2/2/2
30	LHG	l	101	-	-	0/53/53/53	0/0/0/0
27	LUT	n	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	n	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	n	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	n	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	n	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	n	601	1	-	0/41/177/177	0/0/9/9
26	CLA	n	602	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	n	603	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	n	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	n	605	1	-	0/20/156/177	0/0/9/9
25	CHL	n	606	42	-	0/22/158/177	0/0/9/9
25	CHL	n	607	42	-	0/41/177/177	0/0/9/9
25	CHL	n	608	42	-	0/41/177/177	0/0/9/9
25	CHL	n	609	1	-	0/41/177/177	0/0/9/9
26	CLA	n	610	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	n	611	30	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	n	612	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	n	613	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	n	614	1	3/3/16/25	0/17/115/135	0/0/9/9
30	LHG	r	2630	26	-	0/46/46/53	0/0/0/0
26	CLA	r	601	19	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	r	602	19	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	r	603	19	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	r	604	42	3/3/16/25	0/17/115/135	0/0/9/9
25	CHL	r	606	42	-	0/41/177/177	0/0/9/9
25	CHL	r	607	42	-	0/29/165/177	0/0/9/9
25	CHL	r	608	42	-	0/35/171/177	0/0/9/9
26	CLA	r	609	19	3/3/18/25	0/29/127/135	0/0/9/9
26	CLA	r	610	19	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	r	611	30	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	r	612	19	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	r	613	19	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	r	614	19	-	0/12/148/177	0/0/9/9
26	CLA	r	616	19	2/2/16/25	0/11/111/135	0/0/9/9
27	LUT	r	620	-	-	0/29/67/67	0/2/2/2
28	XAT	r	622	-	-	0/31/93/93	0/2/4/4
29	NEX	r	623	-	-	0/27/83/83	0/2/3/3
27	LUT	s	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	s	1621	-	-	0/29/67/67	0/2/2/2
29	NEX	s	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	s	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	s	601	20	-	0/15/153/177	0/0/9/9
26	CLA	s	602	20	3/3/19/25	0/33/131/135	0/0/9/9
26	CLA	s	603	20	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	s	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	s	606	42	-	0/15/153/177	0/0/9/9
25	CHL	s	607	42	-	0/32/168/177	0/0/9/9
25	CHL	s	608	-	-	0/15/153/177	0/0/9/9
26	CLA	s	609	20	3/3/16/25	0/11/111/135	0/0/9/9
26	CLA	s	610	20	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	s	611	30	3/3/18/25	0/27/125/135	0/0/9/9
26	CLA	s	612	20	3/3/16/25	0/18/116/135	0/0/9/9
26	CLA	s	613	20	3/3/18/25	0/25/123/135	0/0/9/9
26	CLA	s	614	20	3/3/16/25	0/18/116/135	0/0/9/9
31	BCR	t	101	-	-	0/29/63/63	0/2/2/2
27	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
27	LUT	y	1621	-	-	0/29/67/67	0/2/2/2
28	XAT	y	1622	-	-	0/31/93/93	0/2/4/4
29	NEX	y	1623	-	-	0/27/83/83	0/2/3/3
30	LHG	y	2630	26	-	0/53/53/53	0/0/0/0
25	CHL	y	601	1	-	0/41/177/177	0/0/9/9
26	CLA	y	602	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	y	603	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	y	604	42	3/3/17/25	0/19/117/135	0/0/9/9
25	CHL	y	605	1	-	0/20/156/177	0/0/9/9
25	CHL	y	606	42	-	0/22/158/177	0/0/9/9
25	CHL	y	607	42	-	0/41/177/177	0/0/9/9
25	CHL	y	608	42	-	0/41/177/177	0/0/9/9
25	CHL	y	609	1	-	0/41/177/177	0/0/9/9
26	CLA	y	610	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	y	611	30	3/3/19/25	0/31/129/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	y	612	1	3/3/19/25	0/31/129/135	0/0/9/9
26	CLA	y	613	1	3/3/20/25	0/37/135/135	0/0/9/9
26	CLA	y	614	1	3/3/16/25	0/17/115/135	0/0/9/9
37	LMG	z	101	-	-	0/46/66/70	0/1/1/1

All (3986) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	608	CHL	C3D-C4D	-20.66	1.31	1.54
25	r	608	CHL	C3D-C4D	-20.63	1.31	1.54
25	Y	601	CHL	C3D-C4D	-20.62	1.31	1.54
25	y	601	CHL	C3D-C4D	-20.62	1.31	1.54
25	y	608	CHL	C3D-C4D	-20.57	1.31	1.54
25	Y	608	CHL	C3D-C4D	-20.56	1.31	1.54
25	3	601	CHL	C3D-C4D	-20.16	1.31	1.54
25	7	601	CHL	C3D-C4D	-20.16	1.31	1.54
25	S	601	CHL	C3D-C4D	-20.13	1.31	1.54
25	s	601	CHL	C3D-C4D	-20.13	1.31	1.54
25	G	601	CHL	C3D-C4D	-20.07	1.31	1.54
25	g	601	CHL	C3D-C4D	-20.07	1.31	1.54
25	y	606	CHL	C3D-C4D	-20.05	1.31	1.54
25	g	608	CHL	C3D-C4D	-20.02	1.32	1.54
25	n	601	CHL	C3D-C4D	-20.00	1.32	1.54
25	G	608	CHL	C3D-C4D	-19.99	1.32	1.54
25	Y	606	CHL	C3D-C4D	-19.98	1.32	1.54
25	N	601	CHL	C3D-C4D	-19.95	1.32	1.54
25	1	601	CHL	C3D-C4D	-19.91	1.32	1.54
25	N	608	CHL	C3D-C4D	-19.88	1.32	1.54
25	n	608	CHL	C3D-C4D	-19.88	1.32	1.54
25	5	601	CHL	C3D-C4D	-19.86	1.32	1.54
25	6	601	CHL	C3D-C4D	-19.85	1.32	1.54
25	2	601	CHL	C3D-C4D	-19.81	1.32	1.54
25	R	606	CHL	C3D-C4D	-19.65	1.32	1.54
25	r	606	CHL	C3D-C4D	-19.65	1.32	1.54
25	7	606	CHL	C3D-C4D	-19.63	1.32	1.54
25	Y	609	CHL	C3D-C4D	-19.62	1.32	1.54
25	y	609	CHL	C3D-C4D	-19.62	1.32	1.54
25	Y	607	CHL	C3D-C4D	-19.59	1.32	1.54
25	S	608	CHL	C3D-C4D	-19.57	1.32	1.54
25	3	608	CHL	C3D-C4D	-19.57	1.32	1.54
25	3	606	CHL	C3D-C4D	-19.54	1.32	1.54
25	8	609	CHL	C3D-C4D	-19.54	1.32	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	608	CHL	C3D-C4D	-19.53	1.32	1.54
25	1	608	CHL	C3D-C4D	-19.53	1.32	1.54
25	y	607	CHL	C3D-C4D	-19.53	1.32	1.54
25	7	608	CHL	C3D-C4D	-19.52	1.32	1.54
25	s	608	CHL	C3D-C4D	-19.51	1.32	1.54
25	n	609	CHL	C3D-C4D	-19.50	1.32	1.54
25	N	609	CHL	C3D-C4D	-19.50	1.32	1.54
25	r	607	CHL	C3D-C4D	-19.47	1.32	1.54
25	R	607	CHL	C3D-C4D	-19.47	1.32	1.54
25	1	606	CHL	C3D-C4D	-19.46	1.32	1.54
25	4	609	CHL	C3D-C4D	-19.46	1.32	1.54
25	5	606	CHL	C3D-C4D	-19.44	1.32	1.54
25	Y	605	CHL	C3D-C4D	-19.44	1.32	1.54
25	5	609	CHL	C3D-C4D	-19.43	1.32	1.54
25	1	609	CHL	C3D-C4D	-19.43	1.32	1.54
25	4	608	CHL	C3D-C4D	-19.42	1.32	1.54
25	y	605	CHL	C3D-C4D	-19.42	1.32	1.54
25	G	607	CHL	C3D-C4D	-19.40	1.32	1.54
25	8	608	CHL	C3D-C4D	-19.39	1.32	1.54
25	3	609	CHL	C3D-C4D	-19.37	1.32	1.54
25	7	609	CHL	C3D-C4D	-19.37	1.32	1.54
25	4	606	CHL	C3D-C4D	-19.37	1.32	1.54
25	8	606	CHL	C3D-C4D	-19.36	1.32	1.54
25	g	607	CHL	C3D-C4D	-19.35	1.32	1.54
25	7	607	CHL	C3D-C4D	-19.35	1.32	1.54
25	2	608	CHL	C3D-C4D	-19.32	1.32	1.54
25	6	608	CHL	C3D-C4D	-19.29	1.32	1.54
25	3	607	CHL	C3D-C4D	-19.29	1.32	1.54
25	1	605	CHL	C3D-C4D	-19.29	1.32	1.54
25	5	605	CHL	C3D-C4D	-19.29	1.32	1.54
25	6	609	CHL	C3D-C4D	-19.27	1.32	1.54
25	6	606	CHL	C3D-C4D	-19.25	1.32	1.54
25	n	605	CHL	C3D-C4D	-19.25	1.32	1.54
25	N	605	CHL	C3D-C4D	-19.24	1.32	1.54
25	N	606	CHL	C3D-C4D	-19.23	1.32	1.54
25	n	606	CHL	C3D-C4D	-19.23	1.32	1.54
25	2	609	CHL	C3D-C4D	-19.19	1.32	1.54
25	2	606	CHL	C3D-C4D	-19.18	1.32	1.54
25	G	606	CHL	C3D-C4D	-19.16	1.32	1.54
25	g	606	CHL	C3D-C4D	-19.15	1.32	1.54
25	8	607	CHL	C3D-C4D	-19.13	1.33	1.54
25	N	607	CHL	C3D-C4D	-19.11	1.33	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	607	CHL	C3D-C4D	-19.11	1.33	1.54
25	4	607	CHL	C3D-C4D	-19.10	1.33	1.54
25	g	605	CHL	C3D-C4D	-18.99	1.33	1.54
25	5	607	CHL	C3D-C4D	-18.99	1.33	1.54
25	G	605	CHL	C3D-C4D	-18.96	1.33	1.54
25	1	607	CHL	C3D-C4D	-18.95	1.33	1.54
25	r	614	CHL	C3D-C4D	-18.92	1.33	1.54
25	R	614	CHL	C3D-C4D	-18.92	1.33	1.54
25	G	609	CHL	C3D-C4D	-18.86	1.33	1.54
25	g	609	CHL	C3D-C4D	-18.86	1.33	1.54
25	7	605	CHL	C3D-C4D	-18.83	1.33	1.54
25	8	601	CHL	C3D-C4D	-18.83	1.33	1.54
25	3	605	CHL	C3D-C4D	-18.83	1.33	1.54
25	6	607	CHL	C3D-C4D	-18.81	1.33	1.54
25	4	601	CHL	C3D-C4D	-18.78	1.33	1.54
25	s	606	CHL	C3D-C4D	-18.78	1.33	1.54
25	S	606	CHL	C3D-C4D	-18.78	1.33	1.54
25	2	607	CHL	C3D-C4D	-18.74	1.33	1.54
25	S	607	CHL	C3D-C4D	-18.62	1.33	1.54
25	6	605	CHL	C3D-C4D	-18.60	1.33	1.54
25	2	605	CHL	C3D-C4D	-18.60	1.33	1.54
25	s	607	CHL	C3D-C4D	-18.56	1.33	1.54
25	s	601	CHL	CHB-C4A	-8.86	1.31	1.52
25	S	601	CHL	CHB-C4A	-8.85	1.31	1.52
25	n	609	CHL	CHB-C4A	-8.72	1.31	1.52
25	N	609	CHL	CHB-C4A	-8.72	1.31	1.52
25	g	607	CHL	CHB-C4A	-8.68	1.31	1.52
25	G	607	CHL	CHB-C4A	-8.66	1.31	1.52
25	Y	609	CHL	CHB-C4A	-8.63	1.32	1.52
25	3	601	CHL	CHB-C4A	-8.62	1.32	1.52
25	7	601	CHL	CHB-C4A	-8.61	1.32	1.52
25	y	609	CHL	CHB-C4A	-8.60	1.32	1.52
25	Y	601	CHL	CHB-C4A	-8.60	1.32	1.52
25	y	601	CHL	CHB-C4A	-8.60	1.32	1.52
25	G	601	CHL	CHB-C4A	-8.58	1.32	1.52
25	g	601	CHL	CHB-C4A	-8.57	1.32	1.52
25	Y	607	CHL	CHB-C4A	-8.53	1.32	1.52
25	y	607	CHL	CHB-C4A	-8.52	1.32	1.52
25	G	609	CHL	CHB-C4A	-8.52	1.32	1.52
25	g	609	CHL	CHB-C4A	-8.50	1.32	1.52
25	N	608	CHL	CHB-C4A	-8.42	1.32	1.52
25	n	608	CHL	CHB-C4A	-8.42	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	609	CHL	CHB-C4A	-8.41	1.32	1.52
25	2	601	CHL	CHB-C4A	-8.40	1.32	1.52
25	6	601	CHL	CHB-C4A	-8.40	1.32	1.52
25	4	609	CHL	CHB-C4A	-8.40	1.32	1.52
25	N	601	CHL	CHB-C4A	-8.39	1.32	1.52
25	n	601	CHL	CHB-C4A	-8.39	1.32	1.52
25	5	607	CHL	CHB-C4A	-8.38	1.32	1.52
25	R	607	CHL	CHB-C4A	-8.37	1.32	1.52
25	r	607	CHL	CHB-C4A	-8.36	1.32	1.52
25	1	607	CHL	CHB-C4A	-8.36	1.32	1.52
25	N	607	CHL	CHB-C4A	-8.35	1.32	1.52
25	n	607	CHL	CHB-C4A	-8.34	1.32	1.52
25	S	607	CHL	CHB-C4A	-8.32	1.32	1.52
25	y	608	CHL	CHB-C4A	-8.31	1.32	1.52
25	G	606	CHL	CHB-C4A	-8.31	1.32	1.52
25	Y	608	CHL	CHB-C4A	-8.31	1.32	1.52
25	r	608	CHL	CHB-C4A	-8.30	1.32	1.52
25	R	608	CHL	CHB-C4A	-8.30	1.32	1.52
25	s	607	CHL	CHB-C4A	-8.29	1.32	1.52
25	g	606	CHL	CHB-C4A	-8.29	1.32	1.52
25	N	605	CHL	CHB-C4A	-8.28	1.32	1.52
25	7	607	CHL	CHB-C4A	-8.28	1.32	1.52
25	3	607	CHL	CHB-C4A	-8.27	1.32	1.52
25	8	606	CHL	CHB-C4A	-8.27	1.32	1.52
25	Y	606	CHL	CHB-C4A	-8.26	1.32	1.52
25	r	606	CHL	CHB-C4A	-8.26	1.32	1.52
25	7	606	CHL	CHB-C4A	-8.26	1.32	1.52
25	3	606	CHL	CHB-C4A	-8.26	1.32	1.52
25	4	606	CHL	CHB-C4A	-8.26	1.32	1.52
25	1	606	CHL	CHB-C4A	-8.25	1.32	1.52
25	n	605	CHL	CHB-C4A	-8.25	1.32	1.52
25	7	609	CHL	CHB-C4A	-8.25	1.32	1.52
25	3	609	CHL	CHB-C4A	-8.25	1.32	1.52
25	R	606	CHL	CHB-C4A	-8.24	1.33	1.52
25	y	606	CHL	CHB-C4A	-8.24	1.33	1.52
25	5	606	CHL	CHB-C4A	-8.23	1.33	1.52
25	3	608	CHL	CHB-C4A	-8.22	1.33	1.52
25	n	609	CHL	C3B-C2B	-8.22	1.45	1.55
25	7	608	CHL	CHB-C4A	-8.22	1.33	1.52
25	G	608	CHL	CHB-C4A	-8.21	1.33	1.52
25	g	608	CHL	CHB-C4A	-8.21	1.33	1.52
25	g	605	CHL	CHB-C4A	-8.21	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	605	CHL	CHB-C4A	-8.21	1.33	1.52
25	6	606	CHL	CHB-C4A	-8.20	1.33	1.52
25	2	606	CHL	CHB-C4A	-8.20	1.33	1.52
25	5	601	CHL	CHB-C4A	-8.20	1.33	1.52
25	5	605	CHL	CHB-C4A	-8.20	1.33	1.52
25	N	609	CHL	C3B-C2B	-8.19	1.45	1.55
25	1	601	CHL	CHB-C4A	-8.19	1.33	1.52
25	6	607	CHL	CHB-C4A	-8.18	1.33	1.52
25	1	605	CHL	CHB-C4A	-8.18	1.33	1.52
25	2	607	CHL	CHB-C4A	-8.18	1.33	1.52
25	5	609	CHL	CHB-C4A	-8.17	1.33	1.52
25	1	609	CHL	CHB-C4A	-8.17	1.33	1.52
25	n	609	CHL	C1B-NB	-8.16	1.32	1.50
25	N	609	CHL	C1B-NB	-8.16	1.32	1.50
25	Y	601	CHL	C3B-C2B	-8.12	1.45	1.55
25	y	601	CHL	C3B-C2B	-8.12	1.45	1.55
25	n	606	CHL	CHB-C4A	-8.09	1.33	1.52
25	N	606	CHL	CHB-C4A	-8.08	1.33	1.52
25	8	601	CHL	CHB-C4A	-8.08	1.33	1.52
25	2	605	CHL	CHB-C4A	-8.07	1.33	1.52
25	5	608	CHL	CHB-C4A	-8.06	1.33	1.52
25	1	608	CHL	CHB-C4A	-8.06	1.33	1.52
25	4	601	CHL	CHB-C4A	-8.06	1.33	1.52
25	r	614	CHL	CHB-C4A	-8.05	1.33	1.52
25	R	614	CHL	CHB-C4A	-8.05	1.33	1.52
25	6	605	CHL	CHB-C4A	-8.05	1.33	1.52
25	y	607	CHL	C3B-C2B	-8.04	1.45	1.55
25	Y	607	CHL	C3B-C2B	-8.04	1.45	1.55
25	6	608	CHL	CHB-C4A	-8.01	1.33	1.52
25	2	608	CHL	CHB-C4A	-8.01	1.33	1.52
25	3	605	CHL	CHB-C4A	-8.00	1.33	1.52
25	7	605	CHL	CHB-C4A	-8.00	1.33	1.52
25	R	608	CHL	C3B-C2B	-7.99	1.45	1.55
25	r	608	CHL	C3B-C2B	-7.99	1.45	1.55
25	S	608	CHL	CHB-C4A	-7.99	1.33	1.52
25	4	608	CHL	CHB-C4A	-7.98	1.33	1.52
25	Y	605	CHL	CHB-C4A	-7.98	1.33	1.52
25	8	608	CHL	CHB-C4A	-7.98	1.33	1.52
25	2	609	CHL	CHB-C4A	-7.97	1.33	1.52
25	s	608	CHL	CHB-C4A	-7.97	1.33	1.52
25	y	605	CHL	CHB-C4A	-7.96	1.33	1.52
25	6	609	CHL	CHB-C4A	-7.95	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	609	CHL	C1B-NB	-7.94	1.33	1.50
25	Y	609	CHL	C1B-NB	-7.94	1.33	1.50
25	G	607	CHL	C3B-C2B	-7.94	1.45	1.55
25	g	607	CHL	C3B-C2B	-7.94	1.45	1.55
25	g	609	CHL	C1B-NB	-7.93	1.33	1.50
25	5	607	CHL	C3B-C2B	-7.92	1.45	1.55
25	l	607	CHL	C3B-C2B	-7.92	1.45	1.55
25	G	609	CHL	C1B-NB	-7.92	1.33	1.50
25	S	606	CHL	CHB-C4A	-7.91	1.33	1.52
25	s	606	CHL	CHB-C4A	-7.91	1.33	1.52
25	8	607	CHL	CHB-C4A	-7.90	1.33	1.52
25	y	607	CHL	C4B-NB	-7.88	1.33	1.50
25	y	606	CHL	C1B-NB	-7.88	1.33	1.50
25	Y	606	CHL	C1B-NB	-7.88	1.33	1.50
25	4	607	CHL	CHB-C4A	-7.87	1.33	1.52
25	Y	607	CHL	C4B-NB	-7.86	1.33	1.50
25	Y	601	CHL	C1B-NB	-7.83	1.33	1.50
25	y	601	CHL	C1B-NB	-7.83	1.33	1.50
25	S	601	CHL	C3B-C2B	-7.79	1.45	1.55
25	s	601	CHL	C3B-C2B	-7.79	1.45	1.55
25	R	608	CHL	C1B-NB	-7.79	1.33	1.50
25	N	607	CHL	C1B-NB	-7.79	1.33	1.50
25	r	608	CHL	C1B-NB	-7.79	1.33	1.50
25	n	607	CHL	C1B-NB	-7.79	1.33	1.50
25	Y	607	CHL	C1B-NB	-7.77	1.33	1.50
25	y	609	CHL	C3B-C2B	-7.77	1.45	1.55
25	Y	609	CHL	C3B-C2B	-7.77	1.45	1.55
25	G	601	CHL	C1B-NB	-7.76	1.33	1.50
25	g	601	CHL	C1B-NB	-7.76	1.33	1.50
25	y	607	CHL	C1B-NB	-7.76	1.33	1.50
25	5	606	CHL	C3B-C2B	-7.75	1.45	1.55
25	7	607	CHL	C1B-NB	-7.73	1.33	1.50
25	3	607	CHL	C1B-NB	-7.72	1.33	1.50
25	S	607	CHL	C3B-C2B	-7.72	1.45	1.55
25	s	607	CHL	C3B-C2B	-7.72	1.45	1.55
25	l	606	CHL	C1B-NB	-7.72	1.33	1.50
25	5	606	CHL	C1B-NB	-7.72	1.33	1.50
25	l	606	CHL	C3B-C2B	-7.71	1.45	1.55
25	y	608	CHL	C3B-C2B	-7.71	1.46	1.55
25	N	608	CHL	C3B-C2B	-7.71	1.46	1.55
25	n	608	CHL	C3B-C2B	-7.70	1.46	1.55
25	R	607	CHL	C3B-C2B	-7.69	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	606	CHL	C3B-C2B	-7.69	1.46	1.55
25	r	606	CHL	C3B-C2B	-7.69	1.46	1.55
25	g	601	CHL	C3B-C2B	-7.67	1.46	1.55
25	Y	608	CHL	C3B-C2B	-7.67	1.46	1.55
25	5	609	CHL	C1B-NB	-7.66	1.33	1.50
25	1	609	CHL	C1B-NB	-7.66	1.33	1.50
25	r	607	CHL	C3B-C2B	-7.65	1.46	1.55
25	G	601	CHL	C3B-C2B	-7.65	1.46	1.55
25	3	609	CHL	C1B-NB	-7.64	1.33	1.50
25	7	609	CHL	C1B-NB	-7.64	1.33	1.50
25	S	607	CHL	C1B-NB	-7.63	1.33	1.50
25	r	607	CHL	C1B-NB	-7.63	1.33	1.50
25	R	607	CHL	C1B-NB	-7.63	1.33	1.50
25	s	607	CHL	C1B-NB	-7.63	1.33	1.50
25	G	609	CHL	C3B-C2B	-7.63	1.46	1.55
25	g	609	CHL	C3B-C2B	-7.61	1.46	1.55
25	G	607	CHL	C4B-NB	-7.61	1.34	1.50
25	g	607	CHL	C4B-NB	-7.61	1.34	1.50
25	3	601	CHL	C1B-NB	-7.61	1.34	1.50
25	7	601	CHL	C1B-NB	-7.60	1.34	1.50
25	r	607	CHL	C4B-NB	-7.58	1.34	1.50
25	3	601	CHL	C3B-C2B	-7.58	1.46	1.55
25	7	609	CHL	C3B-C2B	-7.58	1.46	1.55
25	g	608	CHL	C3B-C2B	-7.58	1.46	1.55
25	7	601	CHL	C3B-C2B	-7.57	1.46	1.55
25	3	606	CHL	C1B-NB	-7.57	1.34	1.50
25	7	606	CHL	C1B-NB	-7.57	1.34	1.50
25	R	607	CHL	C4B-NB	-7.56	1.34	1.50
25	2	601	CHL	C1B-NB	-7.56	1.34	1.50
25	N	601	CHL	C1B-NB	-7.56	1.34	1.50
25	n	601	CHL	C1B-NB	-7.55	1.34	1.50
25	2	609	CHL	C1B-NB	-7.55	1.34	1.50
25	S	608	CHL	C4B-NB	-7.55	1.34	1.50
25	S	601	CHL	C1B-NB	-7.54	1.34	1.50
25	s	601	CHL	C1B-NB	-7.54	1.34	1.50
25	N	605	CHL	C1B-NB	-7.54	1.34	1.50
25	n	605	CHL	C1B-NB	-7.54	1.34	1.50
25	1	609	CHL	C3B-C2B	-7.54	1.46	1.55
25	3	609	CHL	C3B-C2B	-7.54	1.46	1.55
25	3	607	CHL	C4B-NB	-7.54	1.34	1.50
25	G	608	CHL	C3B-C2B	-7.54	1.46	1.55
25	6	601	CHL	C1B-NB	-7.53	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	608	CHL	C4B-NB	-7.53	1.34	1.50
25	7	607	CHL	C4B-NB	-7.53	1.34	1.50
25	N	601	CHL	C3B-C2B	-7.52	1.46	1.55
25	5	609	CHL	C3B-C2B	-7.52	1.46	1.55
25	6	609	CHL	C1B-NB	-7.52	1.34	1.50
25	N	605	CHL	C3B-C2B	-7.51	1.46	1.55
25	N	607	CHL	C4B-NB	-7.51	1.34	1.50
25	Y	608	CHL	C4B-NB	-7.50	1.34	1.50
25	1	609	CHL	C4B-NB	-7.50	1.34	1.50
25	n	607	CHL	C4B-NB	-7.50	1.34	1.50
25	r	606	CHL	C1B-NB	-7.50	1.34	1.50
25	R	606	CHL	C1B-NB	-7.49	1.34	1.50
25	5	609	CHL	C4B-NB	-7.49	1.34	1.50
25	y	608	CHL	C4B-NB	-7.48	1.34	1.50
25	8	606	CHL	C1B-NB	-7.47	1.34	1.50
25	4	606	CHL	C1B-NB	-7.47	1.34	1.50
25	n	601	CHL	C3B-C2B	-7.47	1.46	1.55
25	n	605	CHL	C3B-C2B	-7.46	1.46	1.55
25	Y	608	CHL	C1B-NB	-7.46	1.34	1.50
25	7	609	CHL	C4B-NB	-7.46	1.34	1.50
25	N	608	CHL	C1B-NB	-7.46	1.34	1.50
25	y	608	CHL	C1B-NB	-7.45	1.34	1.50
25	g	608	CHL	C1B-NB	-7.45	1.34	1.50
25	G	608	CHL	C1B-NB	-7.45	1.34	1.50
25	G	607	CHL	C1B-NB	-7.44	1.34	1.50
25	g	607	CHL	C1B-NB	-7.44	1.34	1.50
25	2	606	CHL	C1B-NB	-7.44	1.34	1.50
25	3	609	CHL	C4B-NB	-7.43	1.34	1.50
25	4	609	CHL	C1B-NB	-7.43	1.34	1.50
25	8	608	CHL	C3B-C2B	-7.43	1.46	1.55
25	r	608	CHL	C4B-NB	-7.41	1.34	1.50
25	n	608	CHL	C1B-NB	-7.41	1.34	1.50
25	6	607	CHL	C1B-NB	-7.41	1.34	1.50
25	2	607	CHL	C1B-NB	-7.40	1.34	1.50
25	8	609	CHL	C1B-NB	-7.40	1.34	1.50
25	4	607	CHL	C1B-NB	-7.40	1.34	1.50
25	8	607	CHL	C1B-NB	-7.40	1.34	1.50
25	6	606	CHL	C1B-NB	-7.40	1.34	1.50
25	8	609	CHL	C3B-C2B	-7.40	1.46	1.55
25	4	608	CHL	C3B-C2B	-7.39	1.46	1.55
25	5	607	CHL	C1B-NB	-7.38	1.34	1.50
25	1	607	CHL	C1B-NB	-7.38	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	609	CHL	C4B-NB	-7.38	1.34	1.50
25	4	609	CHL	C3B-C2B	-7.38	1.46	1.55
25	4	609	CHL	C4B-NB	-7.38	1.34	1.50
25	R	614	CHL	C4B-NB	-7.38	1.34	1.50
25	r	614	CHL	C4B-NB	-7.38	1.34	1.50
25	5	607	CHL	C4B-NB	-7.37	1.34	1.50
25	1	607	CHL	C4B-NB	-7.37	1.34	1.50
25	1	608	CHL	C1B-NB	-7.37	1.34	1.50
25	R	608	CHL	C4B-NB	-7.37	1.34	1.50
25	6	606	CHL	C3B-C2B	-7.36	1.46	1.55
25	5	608	CHL	C1B-NB	-7.35	1.34	1.50
25	6	601	CHL	C4B-NB	-7.35	1.34	1.50
25	3	608	CHL	C4B-NB	-7.35	1.34	1.50
25	2	606	CHL	C3B-C2B	-7.35	1.46	1.55
25	r	614	CHL	C3B-C2B	-7.34	1.46	1.55
25	R	614	CHL	C3B-C2B	-7.34	1.46	1.55
25	Y	606	CHL	C4B-NB	-7.34	1.34	1.50
25	y	606	CHL	C4B-NB	-7.34	1.34	1.50
25	n	606	CHL	C4B-NB	-7.34	1.34	1.50
25	G	606	CHL	C1B-NB	-7.34	1.34	1.50
25	g	606	CHL	C1B-NB	-7.34	1.34	1.50
25	5	608	CHL	C3B-C2B	-7.34	1.46	1.55
25	1	608	CHL	C3B-C2B	-7.34	1.46	1.55
25	N	606	CHL	C1B-NB	-7.34	1.34	1.50
25	n	606	CHL	C1B-NB	-7.33	1.34	1.50
25	7	606	CHL	C3B-C2B	-7.33	1.46	1.55
25	3	606	CHL	C3B-C2B	-7.33	1.46	1.55
25	8	601	CHL	C4B-NB	-7.33	1.34	1.50
25	2	601	CHL	C4B-NB	-7.33	1.34	1.50
25	N	606	CHL	C4B-NB	-7.33	1.34	1.50
25	4	601	CHL	C4B-NB	-7.32	1.34	1.50
25	G	609	CHL	C4B-NB	-7.32	1.34	1.50
25	g	609	CHL	C4B-NB	-7.32	1.34	1.50
25	7	608	CHL	C4B-NB	-7.32	1.34	1.50
25	6	605	CHL	C1B-NB	-7.31	1.34	1.50
25	7	608	CHL	C1B-NB	-7.31	1.34	1.50
25	N	608	CHL	C4B-NB	-7.31	1.34	1.50
25	3	608	CHL	C1B-NB	-7.31	1.34	1.50
25	6	609	CHL	C4B-NB	-7.31	1.34	1.50
25	S	608	CHL	C1B-NB	-7.31	1.34	1.50
25	s	608	CHL	C1B-NB	-7.31	1.34	1.50
25	5	601	CHL	C1B-NB	-7.30	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	601	CHL	C1B-NB	-7.30	1.34	1.50
25	y	605	CHL	C3B-C2B	-7.29	1.46	1.55
25	6	607	CHL	C4B-NB	-7.29	1.34	1.50
25	S	601	CHL	C4B-NB	-7.29	1.34	1.50
25	2	607	CHL	C4B-NB	-7.29	1.34	1.50
25	2	609	CHL	C4B-NB	-7.29	1.34	1.50
25	1	601	CHL	C4B-NB	-7.29	1.34	1.50
25	5	601	CHL	C4B-NB	-7.28	1.34	1.50
25	8	606	CHL	C3B-C2B	-7.28	1.46	1.55
25	n	608	CHL	C4B-NB	-7.28	1.34	1.50
25	2	605	CHL	C1B-NB	-7.28	1.34	1.50
25	s	601	CHL	C4B-NB	-7.28	1.34	1.50
25	6	601	CHL	C3B-C2B	-7.28	1.46	1.55
25	Y	605	CHL	C3B-C2B	-7.28	1.46	1.55
25	y	605	CHL	C1B-NB	-7.27	1.34	1.50
25	2	609	CHL	C3B-C2B	-7.27	1.46	1.55
25	4	606	CHL	C3B-C2B	-7.27	1.46	1.55
25	S	606	CHL	C3B-C2B	-7.27	1.46	1.55
25	6	609	CHL	C3B-C2B	-7.27	1.46	1.55
25	S	607	CHL	C4B-NB	-7.27	1.34	1.50
25	s	607	CHL	C4B-NB	-7.27	1.34	1.50
25	y	601	CHL	C4B-NB	-7.27	1.34	1.50
25	6	606	CHL	C4B-NB	-7.27	1.34	1.50
25	2	606	CHL	C4B-NB	-7.27	1.34	1.50
25	6	605	CHL	C4B-NB	-7.26	1.34	1.50
25	S	606	CHL	C1B-NB	-7.26	1.34	1.50
25	s	606	CHL	C1B-NB	-7.26	1.34	1.50
25	n	607	CHL	C3B-C2B	-7.26	1.46	1.55
25	2	605	CHL	C4B-NB	-7.25	1.34	1.50
25	4	608	CHL	C4B-NB	-7.25	1.34	1.50
25	n	605	CHL	C4B-NB	-7.25	1.34	1.50
25	1	606	CHL	C4B-NB	-7.25	1.34	1.50
25	4	607	CHL	C4B-NB	-7.25	1.34	1.50
25	5	606	CHL	C4B-NB	-7.25	1.34	1.50
25	Y	601	CHL	C4B-NB	-7.24	1.34	1.50
25	Y	605	CHL	C1B-NB	-7.24	1.34	1.50
25	4	601	CHL	C1B-NB	-7.24	1.34	1.50
25	N	605	CHL	C4B-NB	-7.24	1.34	1.50
25	2	601	CHL	C3B-C2B	-7.23	1.46	1.55
25	8	601	CHL	C1B-NB	-7.23	1.34	1.50
25	s	606	CHL	C3B-C2B	-7.22	1.46	1.55
25	8	607	CHL	C4B-NB	-7.22	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	607	CHL	C3B-C2B	-7.21	1.46	1.55
25	G	606	CHL	C4B-NB	-7.21	1.34	1.50
25	g	606	CHL	C4B-NB	-7.21	1.34	1.50
25	8	608	CHL	C4B-NB	-7.21	1.34	1.50
25	7	601	CHL	C4B-NB	-7.21	1.34	1.50
25	3	601	CHL	C4B-NB	-7.21	1.34	1.50
25	7	605	CHL	C1B-NB	-7.21	1.34	1.50
25	4	607	CHL	C3B-C2B	-7.20	1.46	1.55
25	8	607	CHL	C3B-C2B	-7.20	1.46	1.55
25	2	607	CHL	C3B-C2B	-7.20	1.46	1.55
25	6	607	CHL	C3B-C2B	-7.20	1.46	1.55
25	7	606	CHL	C4B-NB	-7.20	1.34	1.50
25	3	605	CHL	C4B-NB	-7.19	1.34	1.50
25	3	606	CHL	C4B-NB	-7.19	1.34	1.50
25	1	605	CHL	C1B-NB	-7.18	1.34	1.50
25	5	605	CHL	C1B-NB	-7.18	1.34	1.50
25	3	605	CHL	C1B-NB	-7.18	1.34	1.50
25	r	614	CHL	C1B-NB	-7.18	1.34	1.50
25	R	614	CHL	C1B-NB	-7.18	1.34	1.50
25	7	605	CHL	C4B-NB	-7.17	1.34	1.50
25	n	609	CHL	C4B-NB	-7.16	1.34	1.50
25	g	605	CHL	C3B-C2B	-7.16	1.46	1.55
25	G	605	CHL	C3B-C2B	-7.16	1.46	1.55
25	G	601	CHL	C4B-NB	-7.16	1.34	1.50
25	1	605	CHL	C4B-NB	-7.15	1.34	1.50
25	Y	606	CHL	C3B-C2B	-7.15	1.46	1.55
25	7	607	CHL	C3B-C2B	-7.15	1.46	1.55
25	4	606	CHL	C4B-NB	-7.14	1.35	1.50
25	5	605	CHL	C4B-NB	-7.14	1.35	1.50
25	N	609	CHL	C4B-NB	-7.14	1.35	1.50
25	g	601	CHL	C4B-NB	-7.14	1.35	1.50
25	2	608	CHL	C4B-NB	-7.13	1.35	1.50
25	8	606	CHL	C4B-NB	-7.13	1.35	1.50
25	y	606	CHL	C3B-C2B	-7.13	1.46	1.55
25	Y	609	CHL	C4B-NB	-7.12	1.35	1.50
25	6	608	CHL	C1B-NB	-7.12	1.35	1.50
25	2	608	CHL	C1B-NB	-7.12	1.35	1.50
25	6	608	CHL	C4B-NB	-7.11	1.35	1.50
25	3	607	CHL	C3B-C2B	-7.11	1.46	1.55
25	Y	606	CHL	C1D-ND	-7.10	1.35	1.50
25	y	606	CHL	C1D-ND	-7.10	1.35	1.50
25	y	605	CHL	C4B-NB	-7.10	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	605	CHL	C4B-NB	-7.10	1.35	1.50
25	n	601	CHL	C4B-NB	-7.09	1.35	1.50
25	y	609	CHL	C4B-NB	-7.09	1.35	1.50
25	4	608	CHL	C1B-NB	-7.09	1.35	1.50
25	5	608	CHL	C4B-NB	-7.09	1.35	1.50
25	1	608	CHL	C4B-NB	-7.09	1.35	1.50
25	r	606	CHL	C4B-NB	-7.09	1.35	1.50
25	N	601	CHL	C4B-NB	-7.08	1.35	1.50
25	7	608	CHL	C3B-C2B	-7.08	1.46	1.55
25	8	608	CHL	C1B-NB	-7.07	1.35	1.50
25	G	606	CHL	C3B-C2B	-7.07	1.46	1.55
25	g	606	CHL	C3B-C2B	-7.07	1.46	1.55
25	R	606	CHL	C4B-NB	-7.06	1.35	1.50
25	3	608	CHL	C3B-C2B	-7.05	1.46	1.55
25	5	605	CHL	C3B-C2B	-7.04	1.46	1.55
25	1	605	CHL	C3B-C2B	-7.02	1.46	1.55
25	G	605	CHL	C1B-NB	-6.99	1.35	1.50
25	g	605	CHL	C1B-NB	-6.98	1.35	1.50
25	G	608	CHL	C4B-NB	-6.97	1.35	1.50
25	g	608	CHL	C4B-NB	-6.96	1.35	1.50
25	y	607	CHL	C1D-ND	-6.94	1.35	1.50
25	Y	607	CHL	C1D-ND	-6.94	1.35	1.50
25	1	601	CHL	C3B-C2B	-6.92	1.46	1.55
25	5	601	CHL	C3B-C2B	-6.91	1.46	1.55
25	y	609	CHL	C1D-ND	-6.90	1.35	1.50
25	Y	609	CHL	C1D-ND	-6.90	1.35	1.50
25	6	608	CHL	C3B-C2B	-6.90	1.47	1.55
25	r	608	CHL	C4D-ND	-6.88	1.35	1.50
25	2	608	CHL	C3B-C2B	-6.88	1.47	1.55
25	1	606	CHL	C1D-ND	-6.88	1.35	1.50
25	y	605	CHL	C1D-ND	-6.88	1.35	1.50
25	5	606	CHL	C1D-ND	-6.88	1.35	1.50
25	g	605	CHL	C4B-NB	-6.86	1.35	1.50
25	G	605	CHL	C4B-NB	-6.86	1.35	1.50
25	n	605	CHL	C1D-ND	-6.86	1.35	1.50
25	5	609	CHL	C1D-ND	-6.85	1.35	1.50
25	1	609	CHL	C1D-ND	-6.85	1.35	1.50
25	Y	605	CHL	C1D-ND	-6.84	1.35	1.50
25	R	608	CHL	C4D-ND	-6.84	1.35	1.50
25	N	605	CHL	C1D-ND	-6.83	1.35	1.50
38	D	405	PL9	C7-C3	-6.82	1.44	1.51
25	2	609	CHL	C1D-ND	-6.82	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	605	CHL	C3B-C2B	-6.80	1.47	1.55
25	7	605	CHL	C3B-C2B	-6.80	1.47	1.55
25	6	609	CHL	C1D-ND	-6.80	1.35	1.50
38	d	405	PL9	C7-C3	-6.79	1.44	1.51
25	S	606	CHL	C1D-ND	-6.79	1.35	1.50
25	3	601	CHL	C1D-ND	-6.79	1.35	1.50
25	s	606	CHL	C1D-ND	-6.79	1.35	1.50
25	8	609	CHL	C1D-ND	-6.79	1.35	1.50
25	4	609	CHL	C1D-ND	-6.78	1.35	1.50
25	G	607	CHL	C1D-ND	-6.77	1.35	1.50
25	R	608	CHL	C1D-ND	-6.77	1.35	1.50
25	r	608	CHL	C1D-ND	-6.77	1.35	1.50
25	g	607	CHL	C1D-ND	-6.77	1.35	1.50
25	n	606	CHL	C3B-C2B	-6.77	1.47	1.55
25	7	601	CHL	C1D-ND	-6.76	1.35	1.50
25	3	609	CHL	C1D-ND	-6.75	1.35	1.50
25	7	609	CHL	C1D-ND	-6.75	1.35	1.50
25	N	606	CHL	C3B-C2B	-6.75	1.47	1.55
25	7	608	CHL	C1D-ND	-6.75	1.35	1.50
25	S	608	CHL	C1D-ND	-6.75	1.35	1.50
25	s	608	CHL	C1D-ND	-6.75	1.35	1.50
25	s	608	CHL	C3B-C2B	-6.74	1.47	1.55
25	8	607	CHL	C1D-ND	-6.74	1.35	1.50
25	N	607	CHL	C1D-ND	-6.73	1.35	1.50
25	3	608	CHL	C1D-ND	-6.73	1.35	1.50
25	3	607	CHL	C1D-ND	-6.71	1.35	1.50
25	7	607	CHL	C1D-ND	-6.71	1.35	1.50
25	4	607	CHL	C1D-ND	-6.71	1.35	1.50
25	S	608	CHL	C3B-C2B	-6.71	1.47	1.55
25	4	606	CHL	C1D-ND	-6.70	1.35	1.50
25	8	606	CHL	C1D-ND	-6.70	1.35	1.50
25	n	607	CHL	C1D-ND	-6.70	1.35	1.50
25	1	601	CHL	C1D-ND	-6.69	1.35	1.50
25	y	608	CHL	C1D-ND	-6.69	1.35	1.50
25	Y	608	CHL	C1D-ND	-6.69	1.35	1.50
25	R	607	CHL	C1D-ND	-6.69	1.35	1.50
25	3	606	CHL	C1D-ND	-6.68	1.35	1.50
25	7	606	CHL	C1D-ND	-6.68	1.35	1.50
25	5	601	CHL	C1D-ND	-6.68	1.35	1.50
25	6	606	CHL	C1D-ND	-6.68	1.35	1.50
25	N	606	CHL	C1D-ND	-6.68	1.36	1.50
25	n	608	CHL	C4D-ND	-6.68	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	606	CHL	C1D-ND	-6.68	1.36	1.50
25	2	606	CHL	C1D-ND	-6.68	1.36	1.50
25	4	608	CHL	C1D-ND	-6.67	1.36	1.50
25	3	605	CHL	C1D-ND	-6.66	1.36	1.50
25	r	607	CHL	C1D-ND	-6.66	1.36	1.50
25	2	607	CHL	C1D-ND	-6.66	1.36	1.50
25	Y	606	CHL	C4D-ND	-6.66	1.36	1.50
25	y	606	CHL	C4D-ND	-6.66	1.36	1.50
25	S	601	CHL	C1D-ND	-6.66	1.36	1.50
25	s	601	CHL	C1D-ND	-6.66	1.36	1.50
25	2	605	CHL	C3B-C2B	-6.66	1.47	1.55
25	N	609	CHL	C1D-ND	-6.65	1.36	1.50
25	n	609	CHL	C1D-ND	-6.65	1.36	1.50
25	N	608	CHL	C4D-ND	-6.65	1.36	1.50
25	7	605	CHL	C1D-ND	-6.65	1.36	1.50
25	G	601	CHL	C1D-ND	-6.64	1.36	1.50
25	g	601	CHL	C1D-ND	-6.64	1.36	1.50
25	8	608	CHL	C1D-ND	-6.64	1.36	1.50
25	8	601	CHL	C1D-ND	-6.63	1.36	1.50
25	4	601	CHL	C1D-ND	-6.63	1.36	1.50
25	6	605	CHL	C3B-C2B	-6.62	1.47	1.55
25	6	607	CHL	C1D-ND	-6.62	1.36	1.50
25	5	605	CHL	C1D-ND	-6.62	1.36	1.50
25	N	608	CHL	C1D-ND	-6.62	1.36	1.50
25	1	605	CHL	C1D-ND	-6.62	1.36	1.50
25	G	606	CHL	C1D-ND	-6.60	1.36	1.50
25	g	606	CHL	C1D-ND	-6.60	1.36	1.50
25	5	608	CHL	C1D-ND	-6.59	1.36	1.50
25	1	608	CHL	C1D-ND	-6.58	1.36	1.50
25	n	601	CHL	C1D-ND	-6.58	1.36	1.50
25	n	608	CHL	C1D-ND	-6.57	1.36	1.50
25	6	608	CHL	C1D-ND	-6.57	1.36	1.50
25	N	601	CHL	C1D-ND	-6.56	1.36	1.50
25	y	608	CHL	C4D-ND	-6.56	1.36	1.50
25	Y	608	CHL	C4D-ND	-6.56	1.36	1.50
25	S	607	CHL	C1D-ND	-6.55	1.36	1.50
25	y	607	CHL	C4D-ND	-6.55	1.36	1.50
25	Y	607	CHL	C4D-ND	-6.55	1.36	1.50
25	r	614	CHL	C1D-ND	-6.54	1.36	1.50
25	R	614	CHL	C1D-ND	-6.54	1.36	1.50
25	s	607	CHL	C1D-ND	-6.54	1.36	1.50
25	S	606	CHL	C4B-NB	-6.54	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	606	CHL	C4B-NB	-6.53	1.36	1.50
25	2	608	CHL	C1D-ND	-6.53	1.36	1.50
25	2	601	CHL	C1D-ND	-6.53	1.36	1.50
25	5	607	CHL	C1D-ND	-6.52	1.36	1.50
25	1	607	CHL	C1D-ND	-6.52	1.36	1.50
25	6	601	CHL	C1D-ND	-6.52	1.36	1.50
25	Y	601	CHL	C1D-ND	-6.51	1.36	1.50
25	y	601	CHL	C1D-ND	-6.51	1.36	1.50
25	G	609	CHL	C1D-ND	-6.50	1.36	1.50
25	g	609	CHL	C1D-ND	-6.50	1.36	1.50
25	7	608	CHL	C4D-ND	-6.49	1.36	1.50
25	1	609	CHL	C4D-ND	-6.48	1.36	1.50
25	3	608	CHL	C4D-ND	-6.47	1.36	1.50
25	r	607	CHL	C4D-ND	-6.46	1.36	1.50
25	G	605	CHL	C1D-ND	-6.46	1.36	1.50
25	5	609	CHL	C4D-ND	-6.46	1.36	1.50
25	n	607	CHL	C4D-ND	-6.45	1.36	1.50
25	g	605	CHL	C1D-ND	-6.45	1.36	1.50
25	N	607	CHL	C4D-ND	-6.45	1.36	1.50
25	R	607	CHL	C4D-ND	-6.44	1.36	1.50
25	r	606	CHL	C1D-ND	-6.44	1.36	1.50
25	R	606	CHL	C1D-ND	-6.43	1.36	1.50
25	g	608	CHL	C1D-ND	-6.43	1.36	1.50
25	G	608	CHL	C1D-ND	-6.43	1.36	1.50
25	6	605	CHL	C1D-ND	-6.41	1.36	1.50
25	2	605	CHL	C1D-ND	-6.41	1.36	1.50
25	S	608	CHL	C4D-ND	-6.38	1.36	1.50
25	s	608	CHL	C4D-ND	-6.38	1.36	1.50
25	G	601	CHL	C4D-ND	-6.38	1.36	1.50
25	n	609	CHL	C4D-ND	-6.37	1.36	1.50
25	N	609	CHL	C4D-ND	-6.37	1.36	1.50
25	Y	609	CHL	C4D-ND	-6.36	1.36	1.50
25	5	608	CHL	C4D-ND	-6.36	1.36	1.50
25	1	608	CHL	C4D-ND	-6.36	1.36	1.50
25	g	601	CHL	C4D-ND	-6.36	1.36	1.50
25	4	608	CHL	C4D-ND	-6.36	1.36	1.50
25	8	608	CHL	C4D-ND	-6.36	1.36	1.50
25	y	609	CHL	C4D-ND	-6.34	1.36	1.50
25	G	608	CHL	C4D-ND	-6.34	1.36	1.50
25	Y	601	CHL	C4D-ND	-6.33	1.36	1.50
25	y	601	CHL	C4D-ND	-6.32	1.36	1.50
25	N	601	CHL	C4D-ND	-6.32	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	605	CHL	C4D-ND	-6.30	1.36	1.50
25	Y	605	CHL	C4D-ND	-6.30	1.36	1.50
25	g	608	CHL	C4D-ND	-6.30	1.36	1.50
25	7	601	CHL	C4D-ND	-6.30	1.36	1.50
25	r	614	CHL	C4D-ND	-6.28	1.36	1.50
25	3	601	CHL	C4D-ND	-6.28	1.36	1.50
25	n	601	CHL	C4D-ND	-6.27	1.36	1.50
25	R	614	CHL	C4D-ND	-6.27	1.36	1.50
25	7	609	CHL	C4D-ND	-6.27	1.36	1.50
25	g	607	CHL	C4D-ND	-6.26	1.36	1.50
25	3	606	CHL	C4D-ND	-6.26	1.36	1.50
25	5	605	CHL	C4D-ND	-6.26	1.36	1.50
25	6	608	CHL	C4D-ND	-6.26	1.36	1.50
25	7	607	CHL	C4D-ND	-6.25	1.36	1.50
25	3	607	CHL	C4D-ND	-6.25	1.36	1.50
25	7	606	CHL	C4D-ND	-6.25	1.36	1.50
25	2	608	CHL	C4D-ND	-6.25	1.36	1.50
25	G	609	CHL	C4D-ND	-6.24	1.36	1.50
25	3	609	CHL	C4D-ND	-6.24	1.36	1.50
25	g	609	CHL	C4D-ND	-6.23	1.36	1.50
25	G	607	CHL	C4D-ND	-6.22	1.36	1.50
25	4	609	CHL	C4D-ND	-6.22	1.36	1.50
25	1	605	CHL	C4D-ND	-6.22	1.36	1.50
25	4	601	CHL	C3B-C2B	-6.18	1.47	1.55
25	N	607	CHL	C3B-C4B	-6.18	1.47	1.54
25	n	607	CHL	C3B-C4B	-6.18	1.47	1.54
25	8	609	CHL	C4D-ND	-6.18	1.37	1.50
25	6	609	CHL	C4D-ND	-6.17	1.37	1.50
25	4	601	CHL	C4D-ND	-6.16	1.37	1.50
25	4	606	CHL	C4D-ND	-6.15	1.37	1.50
25	8	606	CHL	C4D-ND	-6.15	1.37	1.50
25	y	607	CHL	C3B-C4B	-6.15	1.47	1.54
25	5	601	CHL	C4D-ND	-6.15	1.37	1.50
25	1	601	CHL	C4D-ND	-6.15	1.37	1.50
25	2	609	CHL	C4D-ND	-6.14	1.37	1.50
25	5	609	CHL	C3B-C4B	-6.14	1.47	1.54
25	1	609	CHL	C3B-C4B	-6.14	1.47	1.54
25	8	601	CHL	C3B-C2B	-6.13	1.47	1.55
25	8	601	CHL	C4D-ND	-6.12	1.37	1.50
25	R	606	CHL	C4D-ND	-6.12	1.37	1.50
25	5	607	CHL	C4D-ND	-6.11	1.37	1.50
25	1	607	CHL	C4D-ND	-6.11	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	606	CHL	C4D-ND	-6.11	1.37	1.50
25	2	606	CHL	C4D-ND	-6.10	1.37	1.50
25	6	606	CHL	C4D-ND	-6.10	1.37	1.50
25	S	607	CHL	C4D-ND	-6.10	1.37	1.50
25	s	607	CHL	C4D-ND	-6.10	1.37	1.50
25	Y	607	CHL	C3B-C4B	-6.09	1.47	1.54
25	S	601	CHL	C4D-ND	-6.09	1.37	1.50
25	6	601	CHL	C4D-ND	-6.09	1.37	1.50
25	s	601	CHL	C4D-ND	-6.07	1.37	1.50
25	2	601	CHL	C4D-ND	-6.07	1.37	1.50
25	S	606	CHL	C4D-ND	-6.06	1.37	1.50
25	s	606	CHL	C4D-ND	-6.06	1.37	1.50
25	4	607	CHL	C4D-ND	-6.04	1.37	1.50
25	5	606	CHL	C4D-ND	-6.02	1.37	1.50
25	3	605	CHL	C4D-ND	-6.02	1.37	1.50
25	7	605	CHL	C4D-ND	-6.02	1.37	1.50
25	6	605	CHL	C4D-ND	-6.00	1.37	1.50
25	2	605	CHL	C4D-ND	-6.00	1.37	1.50
25	8	607	CHL	C4D-ND	-6.00	1.37	1.50
25	2	607	CHL	C4D-ND	-5.99	1.37	1.50
25	n	606	CHL	C4D-ND	-5.99	1.37	1.50
25	1	606	CHL	C4D-ND	-5.98	1.37	1.50
25	N	606	CHL	C4D-ND	-5.98	1.37	1.50
25	6	607	CHL	C4D-ND	-5.98	1.37	1.50
25	n	605	CHL	C4D-ND	-5.96	1.37	1.50
25	N	605	CHL	C4D-ND	-5.95	1.37	1.50
25	R	614	CHL	C3B-C4B	-5.89	1.47	1.54
25	G	606	CHL	C4D-ND	-5.87	1.37	1.50
25	g	606	CHL	C4D-ND	-5.87	1.37	1.50
25	y	606	CHL	C3B-C4B	-5.87	1.47	1.54
25	r	614	CHL	C3B-C4B	-5.85	1.47	1.54
25	Y	606	CHL	C3B-C4B	-5.83	1.47	1.54
25	4	608	CHL	C3B-C4B	-5.79	1.47	1.54
25	8	608	CHL	C3B-C4B	-5.79	1.47	1.54
25	Y	606	CHL	CHD-C1D	-5.77	1.44	1.53
25	Y	607	CHL	C4A-C3A	-5.74	1.47	1.53
25	y	606	CHL	CHD-C1D	-5.74	1.44	1.53
25	R	608	CHL	C3B-C4B	-5.72	1.47	1.54
25	y	607	CHL	C4A-C3A	-5.68	1.47	1.53
25	G	605	CHL	C4D-ND	-5.67	1.38	1.50
25	5	606	CHL	C3B-C4B	-5.67	1.47	1.54
25	r	608	CHL	C3B-C4B	-5.66	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	605	CHL	C4D-ND	-5.66	1.38	1.50
25	7	608	CHL	C3B-C4B	-5.66	1.47	1.54
25	1	606	CHL	C3B-C4B	-5.64	1.48	1.54
25	3	608	CHL	C3B-C4B	-5.63	1.48	1.54
25	N	606	CHL	C3B-C4B	-5.59	1.48	1.54
25	6	609	CHL	C3B-C4B	-5.56	1.48	1.54
25	2	609	CHL	C3B-C4B	-5.54	1.48	1.54
25	n	606	CHL	C3B-C4B	-5.52	1.48	1.54
25	4	609	CHL	C3B-C4B	-5.51	1.48	1.54
25	8	609	CHL	C3B-C4B	-5.51	1.48	1.54
25	Y	609	CHL	C3B-C4B	-5.51	1.48	1.54
25	y	609	CHL	C3B-C4B	-5.49	1.48	1.54
25	8	607	CHL	C3B-C4B	-5.49	1.48	1.54
25	1	607	CHL	C3B-C4B	-5.47	1.48	1.54
25	5	607	CHL	C3B-C4B	-5.44	1.48	1.54
25	4	607	CHL	C3B-C4B	-5.43	1.48	1.54
25	n	607	CHL	C4A-C3A	-5.40	1.47	1.53
25	3	609	CHL	C3B-C4B	-5.39	1.48	1.54
25	7	609	CHL	C3B-C4B	-5.39	1.48	1.54
25	g	609	CHL	C3B-C4B	-5.35	1.48	1.54
25	4	608	CHL	CHD-C1D	-5.34	1.45	1.53
25	8	608	CHL	CHD-C1D	-5.34	1.45	1.53
25	N	607	CHL	C4A-C3A	-5.34	1.47	1.53
25	y	605	CHL	CHD-C1D	-5.34	1.45	1.53
25	Y	605	CHL	CHD-C1D	-5.34	1.45	1.53
25	6	607	CHL	C3B-C4B	-5.33	1.48	1.54
25	G	606	CHL	C3B-C4B	-5.33	1.48	1.54
25	Y	607	CHL	CHD-C1D	-5.32	1.45	1.53
25	S	607	CHL	C3B-C4B	-5.32	1.48	1.54
25	G	609	CHL	CHC-C4B	-5.32	1.45	1.53
25	n	607	CHL	CHD-C1D	-5.31	1.45	1.53
25	y	607	CHL	CHD-C1D	-5.31	1.45	1.53
25	g	606	CHL	C3B-C4B	-5.31	1.48	1.54
25	2	607	CHL	C3B-C4B	-5.30	1.48	1.54
25	N	609	CHL	C4A-C3A	-5.30	1.47	1.53
25	1	605	CHL	C3B-C4B	-5.30	1.48	1.54
25	5	605	CHL	C3B-C4B	-5.29	1.48	1.54
25	g	609	CHL	CHC-C4B	-5.28	1.45	1.53
25	G	609	CHL	C3B-C4B	-5.28	1.48	1.54
25	y	601	CHL	C4A-C3A	-5.28	1.47	1.53
25	N	607	CHL	CHB-C1B	-5.28	1.45	1.53
25	n	607	CHL	CHB-C1B	-5.28	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	607	CHL	CHD-C1D	-5.27	1.45	1.53
25	G	601	CHL	C4A-C3A	-5.27	1.47	1.53
25	s	607	CHL	C3B-C4B	-5.25	1.48	1.54
25	n	609	CHL	CHB-C1B	-5.24	1.45	1.53
25	n	609	CHL	C4A-C3A	-5.23	1.47	1.53
25	7	608	CHL	CHD-C1D	-5.23	1.45	1.53
25	3	608	CHL	CHD-C1D	-5.23	1.45	1.53
25	g	601	CHL	C4A-C3A	-5.22	1.47	1.53
25	N	609	CHL	C3B-C4B	-5.22	1.48	1.54
25	Y	601	CHL	C4A-C3A	-5.22	1.47	1.53
25	N	609	CHL	CHB-C1B	-5.21	1.45	1.53
25	s	601	CHL	CHB-C1B	-5.21	1.45	1.53
25	n	609	CHL	C3B-C4B	-5.20	1.48	1.54
25	Y	601	CHL	CHB-C1B	-5.19	1.45	1.53
25	5	607	CHL	C4A-C3A	-5.19	1.47	1.53
25	1	607	CHL	C4A-C3A	-5.19	1.47	1.53
25	3	605	CHL	C3B-C4B	-5.19	1.48	1.54
25	y	607	CHL	CHB-C1B	-5.19	1.45	1.53
25	Y	607	CHL	CHB-C1B	-5.19	1.45	1.53
25	S	601	CHL	CHB-C1B	-5.16	1.45	1.53
25	y	609	CHL	CHC-C4B	-5.16	1.45	1.53
25	Y	609	CHL	CHC-C4B	-5.16	1.45	1.53
25	7	605	CHL	C3B-C4B	-5.16	1.48	1.54
25	y	601	CHL	CHB-C1B	-5.15	1.45	1.53
25	G	607	CHL	C4A-C3A	-5.15	1.47	1.53
25	g	607	CHL	C4A-C3A	-5.15	1.47	1.53
25	5	608	CHL	CHD-C1D	-5.13	1.45	1.53
25	2	605	CHL	C3B-C4B	-5.10	1.48	1.54
25	r	607	CHL	CHD-C1D	-5.10	1.45	1.53
25	G	609	CHL	CHB-C1B	-5.09	1.45	1.53
25	g	609	CHL	CHB-C1B	-5.08	1.45	1.53
25	1	608	CHL	CHD-C1D	-5.08	1.45	1.53
25	s	607	CHL	C4A-C3A	-5.06	1.47	1.53
25	N	609	CHL	CHC-C4B	-5.06	1.45	1.53
25	6	606	CHL	C3B-C4B	-5.06	1.48	1.54
25	2	606	CHL	C3B-C4B	-5.06	1.48	1.54
25	R	607	CHL	CHD-C1D	-5.06	1.45	1.53
25	Y	609	CHL	CHB-C1B	-5.05	1.45	1.53
25	6	605	CHL	C3B-C4B	-5.05	1.48	1.54
25	7	606	CHL	C3B-C4B	-5.05	1.48	1.54
25	y	608	CHL	CHD-C1D	-5.04	1.45	1.53
25	n	609	CHL	CHC-C4B	-5.04	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	609	CHL	CHB-C1B	-5.03	1.45	1.53
25	G	607	CHL	CHB-C1B	-5.02	1.45	1.53
25	S	607	CHL	C4A-C3A	-5.01	1.47	1.53
25	Y	608	CHL	CHD-C1D	-5.00	1.45	1.53
25	3	606	CHL	C3B-C4B	-5.00	1.48	1.54
25	g	608	CHL	CHD-C1D	-5.00	1.45	1.53
25	g	607	CHL	CHB-C1B	-4.99	1.45	1.53
25	G	608	CHL	CHD-C1D	-4.98	1.45	1.53
25	8	601	CHL	C3B-C4B	-4.96	1.48	1.54
25	4	601	CHL	C3B-C4B	-4.96	1.48	1.54
25	G	601	CHL	CHD-C1D	-4.95	1.45	1.53
25	N	608	CHL	CHD-C1D	-4.95	1.45	1.53
25	g	601	CHL	CHD-C1D	-4.95	1.45	1.53
25	n	608	CHL	CHD-C1D	-4.93	1.45	1.53
25	y	601	CHL	CHC-C4B	-4.92	1.45	1.53
25	Y	601	CHL	CHC-C4B	-4.92	1.45	1.53
25	S	608	CHL	CHD-C1D	-4.90	1.45	1.53
25	R	608	CHL	CHD-C1D	-4.89	1.45	1.53
25	r	608	CHL	CHD-C1D	-4.89	1.45	1.53
25	N	605	CHL	C3B-C4B	-4.89	1.48	1.54
25	N	605	CHL	C4A-C3A	-4.87	1.48	1.53
25	R	607	CHL	CHB-C1B	-4.87	1.45	1.53
25	s	608	CHL	CHD-C1D	-4.86	1.45	1.53
25	5	607	CHL	CHB-C1B	-4.86	1.45	1.53
25	1	607	CHL	CHB-C1B	-4.86	1.45	1.53
25	n	605	CHL	C3B-C4B	-4.85	1.48	1.54
25	n	605	CHL	C4A-C3A	-4.85	1.48	1.53
25	5	601	CHL	C3B-C4B	-4.84	1.48	1.54
25	1	601	CHL	C3B-C4B	-4.84	1.48	1.54
25	S	607	CHL	CHC-C4B	-4.84	1.45	1.53
25	s	607	CHL	CHC-C4B	-4.84	1.45	1.53
25	S	601	CHL	C4A-C3A	-4.84	1.48	1.53
25	N	605	CHL	CHD-C1D	-4.82	1.45	1.53
25	r	607	CHL	CHB-C1B	-4.82	1.45	1.53
25	n	605	CHL	CHD-C1D	-4.82	1.45	1.53
25	S	607	CHL	CHD-C1D	-4.81	1.45	1.53
25	s	607	CHL	CHD-C1D	-4.81	1.45	1.53
25	7	607	CHL	C3B-C4B	-4.81	1.48	1.54
25	3	607	CHL	C3B-C4B	-4.81	1.48	1.54
25	s	601	CHL	C4A-C3A	-4.81	1.48	1.53
25	7	601	CHL	CHB-C1B	-4.81	1.45	1.53
25	3	601	CHL	CHB-C1B	-4.81	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	608	CHL	CHD-C1D	-4.80	1.45	1.53
25	2	608	CHL	C3B-C4B	-4.80	1.48	1.54
25	6	608	CHL	C3B-C4B	-4.80	1.48	1.54
25	s	608	CHL	C3B-C4B	-4.79	1.48	1.54
25	6	608	CHL	CHD-C1D	-4.78	1.46	1.53
25	3	607	CHL	C4A-C3A	-4.78	1.48	1.53
25	G	601	CHL	CHB-C1B	-4.77	1.46	1.53
25	s	606	CHL	CHD-C1D	-4.77	1.46	1.53
25	S	606	CHL	CHD-C1D	-4.76	1.46	1.53
25	7	607	CHL	C4A-C3A	-4.75	1.48	1.53
25	1	609	CHL	CHC-C4B	-4.75	1.46	1.53
25	N	601	CHL	CHD-C1D	-4.75	1.46	1.53
25	n	601	CHL	CHD-C1D	-4.75	1.46	1.53
25	S	601	CHL	C3B-C4B	-4.74	1.49	1.54
25	s	601	CHL	C3B-C4B	-4.74	1.49	1.54
25	g	601	CHL	CHB-C1B	-4.74	1.46	1.53
25	G	607	CHL	C3B-C4B	-4.74	1.49	1.54
25	n	601	CHL	CHB-C1B	-4.74	1.46	1.53
25	r	607	CHL	C4A-C3A	-4.74	1.48	1.53
25	R	607	CHL	C4A-C3A	-4.74	1.48	1.53
25	5	609	CHL	CHC-C4B	-4.73	1.46	1.53
25	Y	607	CHL	CHC-C4B	-4.73	1.46	1.53
25	7	601	CHL	CHD-C1D	-4.73	1.46	1.53
25	3	601	CHL	CHD-C1D	-4.73	1.46	1.53
25	r	607	CHL	C3B-C4B	-4.73	1.49	1.54
25	R	607	CHL	C3B-C4B	-4.73	1.49	1.54
25	S	608	CHL	C3B-C4B	-4.72	1.49	1.54
25	y	607	CHL	CHC-C4B	-4.72	1.46	1.53
25	G	607	CHL	CHD-C1D	-4.71	1.46	1.53
25	g	607	CHL	CHD-C1D	-4.71	1.46	1.53
25	4	606	CHL	C3B-C4B	-4.71	1.49	1.54
25	N	601	CHL	CHB-C1B	-4.71	1.46	1.53
25	n	607	CHL	CHC-C4B	-4.71	1.46	1.53
25	g	607	CHL	C3B-C4B	-4.70	1.49	1.54
25	N	607	CHL	CHC-C4B	-4.69	1.46	1.53
25	6	601	CHL	CHB-C1B	-4.67	1.46	1.53
25	Y	606	CHL	CHC-C4B	-4.67	1.46	1.53
25	8	606	CHL	C3B-C4B	-4.66	1.49	1.54
25	R	614	CHL	CHD-C1D	-4.65	1.46	1.53
25	S	607	CHL	CHB-C1B	-4.63	1.46	1.53
25	s	607	CHL	CHB-C1B	-4.63	1.46	1.53
25	2	601	CHL	CHB-C1B	-4.63	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	606	CHL	CHC-C4B	-4.63	1.46	1.53
25	7	601	CHL	C4A-C3A	-4.63	1.48	1.53
25	3	601	CHL	C4A-C3A	-4.63	1.48	1.53
25	5	607	CHL	CHD-C1D	-4.62	1.46	1.53
25	1	607	CHL	CHD-C1D	-4.62	1.46	1.53
25	r	614	CHL	CHD-C1D	-4.61	1.46	1.53
25	Y	605	CHL	C3B-C4B	-4.60	1.49	1.54
25	Y	601	CHL	C3B-C4B	-4.59	1.49	1.54
25	r	614	CHL	CHC-C4B	-4.59	1.46	1.53
25	y	601	CHL	C3B-C4B	-4.57	1.49	1.54
25	R	607	CHL	CHC-C4B	-4.56	1.46	1.53
25	y	605	CHL	C3B-C4B	-4.56	1.49	1.54
25	6	605	CHL	CHD-C1D	-4.55	1.46	1.53
25	2	605	CHL	CHD-C1D	-4.55	1.46	1.53
25	Y	609	CHL	CHD-C1D	-4.55	1.46	1.53
25	3	606	CHL	CHD-C1D	-4.55	1.46	1.53
25	G	609	CHL	C4A-C3A	-4.55	1.48	1.53
25	r	607	CHL	CHC-C4B	-4.54	1.46	1.53
25	3	605	CHL	CHD-C1D	-4.54	1.46	1.53
25	7	605	CHL	CHD-C1D	-4.54	1.46	1.53
25	1	606	CHL	CHD-C1D	-4.54	1.46	1.53
25	g	609	CHL	C4A-C3A	-4.54	1.48	1.53
25	2	609	CHL	CHD-C1D	-4.54	1.46	1.53
25	6	609	CHL	CHD-C1D	-4.54	1.46	1.53
25	R	614	CHL	CHC-C4B	-4.54	1.46	1.53
25	y	609	CHL	CHD-C1D	-4.53	1.46	1.53
25	N	606	CHL	CHD-C1D	-4.53	1.46	1.53
25	n	606	CHL	CHD-C1D	-4.53	1.46	1.53
25	7	606	CHL	CHD-C1D	-4.53	1.46	1.53
25	n	608	CHL	CHB-C1B	-4.53	1.46	1.53
25	5	607	CHL	CHC-C4B	-4.52	1.46	1.53
25	1	607	CHL	CHC-C4B	-4.52	1.46	1.53
25	Y	608	CHL	C3B-C4B	-4.52	1.49	1.54
25	1	608	CHL	C3B-C4B	-4.51	1.49	1.54
25	n	605	CHL	CHB-C1B	-4.51	1.46	1.53
25	N	605	CHL	CHB-C1B	-4.50	1.46	1.53
25	5	606	CHL	CHD-C1D	-4.50	1.46	1.53
25	y	608	CHL	CHC-C4B	-4.48	1.46	1.53
25	y	608	CHL	C3B-C4B	-4.48	1.49	1.54
25	6	607	CHL	CHD-C1D	-4.48	1.46	1.53
25	Y	608	CHL	CHC-C4B	-4.48	1.46	1.53
25	N	608	CHL	CHB-C1B	-4.47	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	605	CHL	CHD-C1D	-4.47	1.46	1.53
25	6	607	CHL	CHB-C1B	-4.47	1.46	1.53
25	G	605	CHL	CHD-C1D	-4.47	1.46	1.53
25	1	605	CHL	CHD-C1D	-4.47	1.46	1.53
25	5	605	CHL	CHD-C1D	-4.47	1.46	1.53
25	5	608	CHL	C3B-C4B	-4.46	1.49	1.54
25	5	609	CHL	CHD-C1D	-4.46	1.46	1.53
25	2	607	CHL	CHB-C1B	-4.45	1.46	1.53
25	Y	601	CHL	CHD-C1D	-4.45	1.46	1.53
25	y	601	CHL	CHD-C1D	-4.45	1.46	1.53
25	S	601	CHL	CHC-C4B	-4.44	1.46	1.53
25	y	608	CHL	CHB-C1B	-4.44	1.46	1.53
25	Y	608	CHL	CHB-C1B	-4.44	1.46	1.53
25	6	601	CHL	C3B-C4B	-4.44	1.49	1.54
25	N	601	CHL	C4A-C3A	-4.44	1.48	1.53
25	n	601	CHL	C4A-C3A	-4.44	1.48	1.53
25	4	606	CHL	CHD-C1D	-4.44	1.46	1.53
25	6	601	CHL	CHD-C1D	-4.43	1.46	1.53
25	Y	609	CHL	C4A-C3A	-4.43	1.48	1.53
25	3	609	CHL	CHC-C4B	-4.43	1.46	1.53
25	g	601	CHL	C3B-C4B	-4.43	1.49	1.54
25	6	609	CHL	CHC-C4B	-4.43	1.46	1.53
25	5	609	CHL	C4A-C3A	-4.43	1.48	1.53
25	G	601	CHL	C3B-C4B	-4.43	1.49	1.54
25	2	601	CHL	C3B-C4B	-4.42	1.49	1.54
25	2	607	CHL	CHD-C1D	-4.42	1.46	1.53
25	2	609	CHL	CHC-C4B	-4.42	1.46	1.53
25	2	601	CHL	CHD-C1D	-4.42	1.46	1.53
25	N	609	CHL	CHD-C1D	-4.42	1.46	1.53
25	7	609	CHL	CHC-C4B	-4.41	1.46	1.53
25	R	606	CHL	C3B-C4B	-4.41	1.49	1.54
25	R	608	CHL	CHB-C1B	-4.41	1.46	1.53
25	r	608	CHL	CHB-C1B	-4.41	1.46	1.53
25	g	601	CHL	CHC-C4B	-4.41	1.46	1.53
25	s	601	CHL	CHC-C4B	-4.41	1.46	1.53
25	2	606	CHL	CHD-C1D	-4.41	1.46	1.53
25	6	606	CHL	CHD-C1D	-4.40	1.46	1.53
25	8	606	CHL	CHD-C1D	-4.40	1.46	1.53
25	1	609	CHL	CHD-C1D	-4.40	1.46	1.53
25	8	601	CHL	C4A-C3A	-4.40	1.48	1.53
25	G	606	CHL	CHB-C1B	-4.38	1.46	1.53
25	g	609	CHL	CHD-C1D	-4.38	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	606	CHL	CHB-C1B	-4.38	1.46	1.53
25	y	609	CHL	C4A-C3A	-4.38	1.48	1.53
25	G	609	CHL	CHD-C1D	-4.37	1.46	1.53
25	R	606	CHL	CHD-C1D	-4.37	1.46	1.53
25	G	601	CHL	CHC-C4B	-4.37	1.46	1.53
25	2	607	CHL	CHC-C4B	-4.37	1.46	1.53
25	6	607	CHL	CHC-C4B	-4.37	1.46	1.53
25	4	601	CHL	C4A-C3A	-4.37	1.48	1.53
25	n	609	CHL	CHD-C1D	-4.36	1.46	1.53
25	1	609	CHL	C4A-C3A	-4.36	1.48	1.53
25	y	606	CHL	CHD-C4C	-4.36	1.45	1.53
25	r	606	CHL	C3B-C4B	-4.35	1.49	1.54
25	7	606	CHL	CHB-C1B	-4.34	1.46	1.53
25	r	606	CHL	CHD-C1D	-4.34	1.46	1.53
25	Y	606	CHL	CHD-C4C	-4.34	1.45	1.53
25	g	606	CHL	CHD-C1D	-4.34	1.46	1.53
25	y	608	CHL	C4A-C3A	-4.34	1.48	1.53
25	S	608	CHL	CHC-C4B	-4.33	1.46	1.53
25	R	606	CHL	CHB-C1B	-4.33	1.46	1.53
25	G	608	CHL	CHB-C1B	-4.33	1.46	1.53
25	r	606	CHL	CHB-C1B	-4.33	1.46	1.53
25	5	606	CHL	CHC-C4B	-4.33	1.46	1.53
25	Y	606	CHL	CHB-C1B	-4.32	1.46	1.53
25	n	605	CHL	CHC-C4B	-4.32	1.46	1.53
25	1	606	CHL	CHC-C4B	-4.32	1.46	1.53
25	3	606	CHL	CHB-C1B	-4.32	1.46	1.53
25	8	606	CHL	C4A-C3A	-4.31	1.48	1.53
25	5	609	CHL	CHB-C1B	-4.31	1.46	1.53
25	g	608	CHL	CHB-C1B	-4.31	1.46	1.53
25	1	609	CHL	CHB-C1B	-4.31	1.46	1.53
25	G	606	CHL	CHD-C1D	-4.31	1.46	1.53
26	Y	604	CLA	CMB-C2B	-4.31	1.42	1.51
26	y	604	CLA	CMB-C2B	-4.31	1.42	1.51
25	s	608	CHL	CHC-C4B	-4.30	1.46	1.53
25	6	601	CHL	CHC-C4B	-4.30	1.46	1.53
25	2	607	CHL	C4A-C3A	-4.30	1.48	1.53
25	1	605	CHL	CHB-C1B	-4.30	1.46	1.53
25	N	605	CHL	CHC-C4B	-4.30	1.46	1.53
25	y	606	CHL	CHB-C1B	-4.30	1.46	1.53
25	4	607	CHL	CHC-C4B	-4.29	1.46	1.53
25	8	607	CHL	CHC-C4B	-4.29	1.46	1.53
25	R	608	CHL	CHC-C4B	-4.29	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	608	CHL	CHC-C4B	-4.29	1.46	1.53
25	4	609	CHL	CHC-C4B	-4.29	1.46	1.53
25	5	606	CHL	CHB-C1B	-4.29	1.46	1.53
25	Y	608	CHL	C4A-C3A	-4.29	1.48	1.53
25	5	605	CHL	CHB-C1B	-4.28	1.46	1.53
25	7	607	CHL	CHB-C1B	-4.27	1.46	1.53
25	3	607	CHL	CHB-C1B	-4.27	1.46	1.53
26	B	605	CLA	CMD-C2D	-4.27	1.42	1.51
25	7	608	CHL	CHC-C4B	-4.27	1.46	1.53
25	3	608	CHL	CHC-C4B	-4.27	1.46	1.53
25	4	606	CHL	C4A-C3A	-4.27	1.48	1.53
25	6	606	CHL	CHB-C1B	-4.27	1.46	1.53
25	5	601	CHL	CHB-C1B	-4.27	1.46	1.53
25	G	608	CHL	CHC-C4B	-4.27	1.46	1.53
25	2	606	CHL	CHB-C1B	-4.27	1.46	1.53
25	6	607	CHL	C4A-C3A	-4.27	1.48	1.53
25	2	601	CHL	CHC-C4B	-4.26	1.46	1.53
26	b	605	CLA	CMD-C2D	-4.25	1.42	1.51
25	R	608	CHL	C3D-C2D	-4.25	1.44	1.55
25	1	606	CHL	CHB-C1B	-4.25	1.46	1.53
25	g	608	CHL	CHC-C4B	-4.25	1.46	1.53
25	R	606	CHL	C4A-C3A	-4.24	1.48	1.53
25	1	601	CHL	CHB-C1B	-4.24	1.46	1.53
25	r	608	CHL	C3D-C2D	-4.24	1.44	1.55
25	7	601	CHL	C3B-C4B	-4.24	1.49	1.54
25	8	609	CHL	CHC-C4B	-4.24	1.46	1.53
25	4	609	CHL	CHB-C1B	-4.24	1.46	1.53
25	8	609	CHL	CHB-C1B	-4.24	1.46	1.53
25	3	608	CHL	CHB-C1B	-4.23	1.46	1.53
25	3	601	CHL	C3B-C4B	-4.22	1.49	1.54
25	8	609	CHL	C4A-C3A	-4.22	1.48	1.53
25	4	609	CHL	C4A-C3A	-4.21	1.48	1.53
26	N	604	CLA	CMB-C2B	-4.20	1.43	1.51
25	s	608	CHL	C4A-C3A	-4.20	1.48	1.53
25	g	608	CHL	C3B-C4B	-4.20	1.49	1.54
25	7	601	CHL	C3D-C2D	-4.20	1.44	1.55
25	y	605	CHL	CHB-C1B	-4.20	1.46	1.53
25	Y	605	CHL	CHB-C1B	-4.20	1.46	1.53
25	4	607	CHL	CHD-C1D	-4.20	1.46	1.53
25	n	601	CHL	C3B-C4B	-4.20	1.49	1.54
25	r	606	CHL	C4A-C3A	-4.20	1.48	1.53
25	Y	601	CHL	CHC-C1C	-4.19	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	609	CHL	CHB-C1B	-4.19	1.46	1.53
25	S	608	CHL	C4A-C3A	-4.19	1.48	1.53
25	6	606	CHL	CHC-C4B	-4.19	1.46	1.53
25	7	608	CHL	CHB-C1B	-4.19	1.46	1.53
25	7	606	CHL	C4A-C3A	-4.19	1.48	1.53
25	y	601	CHL	CHC-C1C	-4.19	1.45	1.53
25	3	601	CHL	C3D-C2D	-4.18	1.44	1.55
25	y	606	CHL	CHC-C1C	-4.17	1.45	1.53
25	N	601	CHL	C3B-C4B	-4.17	1.49	1.54
25	4	606	CHL	CHB-C1B	-4.17	1.47	1.53
25	7	609	CHL	CHB-C1B	-4.17	1.47	1.53
25	8	606	CHL	CHB-C1B	-4.17	1.47	1.53
25	7	607	CHL	CHC-C4B	-4.16	1.47	1.53
25	5	605	CHL	CHC-C4B	-4.16	1.47	1.53
26	n	604	CLA	CMB-C2B	-4.16	1.43	1.51
25	3	607	CHL	CHC-C4B	-4.16	1.47	1.53
25	2	606	CHL	CHC-C4B	-4.15	1.47	1.53
25	8	607	CHL	CHD-C1D	-4.15	1.47	1.53
25	G	605	CHL	CHB-C1B	-4.15	1.47	1.53
25	1	605	CHL	CHC-C4B	-4.15	1.47	1.53
25	5	606	CHL	C4A-C3A	-4.15	1.48	1.53
25	g	605	CHL	CHB-C1B	-4.15	1.47	1.53
25	n	608	CHL	CHC-C4B	-4.15	1.47	1.53
25	3	606	CHL	C4A-C3A	-4.15	1.48	1.53
25	8	606	CHL	CHC-C4B	-4.14	1.47	1.53
25	N	608	CHL	CHC-C4B	-4.14	1.47	1.53
25	4	606	CHL	CHC-C4B	-4.14	1.47	1.53
25	N	606	CHL	CHC-C4B	-4.14	1.47	1.53
25	5	601	CHL	CHC-C4B	-4.13	1.47	1.53
25	1	601	CHL	CHC-C4B	-4.13	1.47	1.53
25	3	606	CHL	CHC-C4B	-4.13	1.47	1.53
26	G	604	CLA	CMB-C2B	-4.13	1.43	1.51
26	g	604	CLA	CMB-C2B	-4.13	1.43	1.51
25	Y	606	CHL	C4A-C3A	-4.13	1.48	1.53
25	G	608	CHL	C3B-C4B	-4.13	1.49	1.54
25	7	606	CHL	CHC-C4B	-4.13	1.47	1.53
25	Y	606	CHL	CHC-C1C	-4.13	1.45	1.53
25	y	606	CHL	C4A-C3A	-4.13	1.48	1.53
25	G	601	CHL	C3D-C2D	-4.12	1.44	1.55
25	g	601	CHL	C3D-C2D	-4.12	1.44	1.55
25	n	606	CHL	CHC-C4B	-4.11	1.47	1.53
25	R	606	CHL	CHC-C4B	-4.11	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	606	CHL	CHC-C4B	-4.11	1.47	1.53
25	G	609	CHL	CHC-C1C	-4.11	1.45	1.53
26	b	613	CLA	CMD-C2D	-4.11	1.42	1.51
25	g	605	CHL	C4A-C3A	-4.11	1.48	1.53
26	B	613	CLA	CMD-C2D	-4.11	1.42	1.51
25	l	606	CHL	C4A-C3A	-4.10	1.48	1.53
25	s	601	CHL	CHD-C1D	-4.09	1.47	1.53
25	N	601	CHL	CHC-C4B	-4.09	1.47	1.53
25	n	601	CHL	CHC-C4B	-4.09	1.47	1.53
25	7	605	CHL	CHB-C1B	-4.09	1.47	1.53
25	Y	606	CHL	C3D-C2D	-4.08	1.44	1.55
25	r	614	CHL	CHB-C1B	-4.08	1.47	1.53
25	g	609	CHL	CHC-C1C	-4.08	1.45	1.53
25	3	605	CHL	CHB-C1B	-4.07	1.47	1.53
25	R	614	CHL	CHB-C1B	-4.07	1.47	1.53
25	3	609	CHL	C4A-C3A	-4.07	1.48	1.53
25	y	606	CHL	C3D-C2D	-4.07	1.44	1.55
25	S	601	CHL	CHD-C1D	-4.06	1.47	1.53
25	N	607	CHL	CHD-C4C	-4.06	1.45	1.53
25	G	605	CHL	C4A-C3A	-4.06	1.48	1.53
25	6	601	CHL	C4A-C3A	-4.05	1.48	1.53
25	l	608	CHL	CHC-C4B	-4.05	1.47	1.53
25	n	607	CHL	CHD-C4C	-4.05	1.46	1.53
25	7	609	CHL	C4A-C3A	-4.05	1.48	1.53
25	G	607	CHL	CHC-C4B	-4.05	1.47	1.53
25	g	607	CHL	CHC-C4B	-4.05	1.47	1.53
25	8	608	CHL	C4A-C3A	-4.05	1.48	1.53
25	R	614	CHL	C4A-C3A	-4.05	1.48	1.53
25	5	608	CHL	CHC-C4B	-4.05	1.47	1.53
25	y	607	CHL	CHD-C4C	-4.04	1.46	1.53
25	Y	607	CHL	CHD-C4C	-4.04	1.46	1.53
25	r	608	CHL	CHD-C4C	-4.04	1.46	1.53
25	N	608	CHL	C4A-C3A	-4.04	1.48	1.53
25	4	609	CHL	CHD-C1D	-4.03	1.47	1.53
25	N	608	CHL	C3B-C4B	-4.03	1.49	1.54
25	Y	601	CHL	C3D-C2D	-4.03	1.44	1.55
25	R	608	CHL	CHD-C4C	-4.03	1.46	1.53
25	G	606	CHL	CHC-C4B	-4.03	1.47	1.53
25	g	606	CHL	CHC-C4B	-4.03	1.47	1.53
25	y	601	CHL	C3D-C2D	-4.03	1.44	1.55
25	5	608	CHL	CHB-C1B	-4.02	1.47	1.53
25	l	608	CHL	CHB-C1B	-4.02	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	606	CHL	CHB-C1B	-4.02	1.47	1.53
25	5	605	CHL	C4A-C3A	-4.02	1.49	1.53
25	1	605	CHL	C4A-C3A	-4.01	1.49	1.53
25	3	605	CHL	C4A-C3A	-4.01	1.49	1.53
25	7	605	CHL	C4A-C3A	-4.01	1.49	1.53
25	4	608	CHL	C4A-C3A	-4.01	1.49	1.53
25	n	608	CHL	C4A-C3A	-4.01	1.49	1.53
25	6	605	CHL	CHB-C1B	-4.01	1.47	1.53
25	2	605	CHL	CHB-C1B	-4.01	1.47	1.53
25	Y	607	CHL	CHC-C1C	-4.01	1.46	1.53
25	7	601	CHL	C1A-CHA	-4.00	1.47	1.53
25	3	601	CHL	C1A-CHA	-4.00	1.47	1.53
25	4	608	CHL	CHC-C4B	-4.00	1.47	1.53
25	r	614	CHL	C4A-C3A	-4.00	1.49	1.53
25	n	608	CHL	C3D-C2D	-4.00	1.44	1.55
25	N	606	CHL	CHB-C1B	-3.99	1.47	1.53
25	y	607	CHL	CHC-C1C	-3.99	1.46	1.53
25	8	609	CHL	CHD-C1D	-3.99	1.47	1.53
25	g	608	CHL	C3D-C2D	-3.99	1.44	1.55
25	2	601	CHL	C4A-C3A	-3.99	1.49	1.53
25	N	608	CHL	C3D-C2D	-3.98	1.44	1.55
25	n	608	CHL	C3B-C4B	-3.98	1.49	1.54
25	8	608	CHL	CHC-C4B	-3.98	1.47	1.53
25	4	608	CHL	CHB-C1B	-3.97	1.47	1.53
25	8	608	CHL	CHB-C1B	-3.97	1.47	1.53
25	N	609	CHL	CHC-C1C	-3.97	1.46	1.53
25	6	608	CHL	CHC-C4B	-3.97	1.47	1.53
25	G	608	CHL	C3D-C2D	-3.96	1.44	1.55
25	2	608	CHL	CHB-C1B	-3.96	1.47	1.53
25	6	608	CHL	CHB-C1B	-3.96	1.47	1.53
25	7	607	CHL	CHD-C1D	-3.96	1.47	1.53
25	3	601	CHL	CHC-C4B	-3.96	1.47	1.53
30	l	101	LHG	O7-C5	-3.96	1.36	1.46
25	g	605	CHL	C3B-C4B	-3.96	1.49	1.54
38	D	405	PL9	C3-C4	-3.96	1.42	1.49
38	d	405	PL9	C3-C4	-3.96	1.42	1.49
25	n	609	CHL	CHC-C1C	-3.95	1.46	1.53
25	2	608	CHL	CHC-C4B	-3.95	1.47	1.53
25	n	601	CHL	C3D-C2D	-3.95	1.44	1.55
41	F	101	HEM	C3C-C2C	-3.95	1.35	1.40
25	S	608	CHL	CHB-C1B	-3.94	1.47	1.53
25	s	608	CHL	C3D-C2D	-3.94	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	601	CHL	CHB-C1B	-3.94	1.47	1.53
25	4	601	CHL	CHB-C1B	-3.94	1.47	1.53
25	G	605	CHL	C3B-C4B	-3.94	1.49	1.54
25	N	601	CHL	C3D-C2D	-3.93	1.44	1.55
25	1	608	CHL	C3D-C2D	-3.93	1.44	1.55
30	L	101	LHG	O7-C5	-3.93	1.36	1.46
25	s	608	CHL	CHB-C1B	-3.93	1.47	1.53
25	7	601	CHL	CHC-C4B	-3.93	1.47	1.53
25	6	606	CHL	C4A-C3A	-3.92	1.49	1.53
25	2	606	CHL	C4A-C3A	-3.92	1.49	1.53
25	y	605	CHL	C4A-C3A	-3.92	1.49	1.53
25	Y	605	CHL	C4A-C3A	-3.92	1.49	1.53
25	7	608	CHL	C4A-C3A	-3.92	1.49	1.53
25	3	608	CHL	C4A-C3A	-3.92	1.49	1.53
25	5	608	CHL	C3D-C2D	-3.92	1.44	1.55
25	3	607	CHL	CHD-C1D	-3.92	1.47	1.53
25	2	601	CHL	C3D-C2D	-3.92	1.44	1.55
25	6	601	CHL	C3D-C2D	-3.92	1.44	1.55
25	4	601	CHL	CHD-C1D	-3.91	1.47	1.53
25	S	608	CHL	C3D-C2D	-3.90	1.44	1.55
25	Y	605	CHL	CHD-C4C	-3.90	1.46	1.53
41	f	101	HEM	C3C-C2C	-3.90	1.35	1.40
25	6	605	CHL	CHC-C4B	-3.90	1.47	1.53
25	5	609	CHL	CHC-C1C	-3.89	1.46	1.53
25	3	609	CHL	CHD-C1D	-3.89	1.47	1.53
26	A	405	CLA	CMC-C2C	-3.89	1.42	1.50
26	a	405	CLA	CMC-C2C	-3.89	1.42	1.50
25	y	605	CHL	CHD-C4C	-3.88	1.46	1.53
25	y	608	CHL	C3D-C2D	-3.88	1.44	1.55
25	Y	608	CHL	C3D-C2D	-3.88	1.44	1.55
25	y	609	CHL	CHC-C1C	-3.88	1.46	1.53
25	Y	609	CHL	CHC-C1C	-3.88	1.46	1.53
25	S	601	CHL	C1A-CHA	-3.88	1.47	1.53
25	s	601	CHL	C1A-CHA	-3.88	1.47	1.53
25	1	609	CHL	CHC-C1C	-3.88	1.46	1.53
25	y	605	CHL	CHC-C4B	-3.88	1.47	1.53
25	Y	605	CHL	CHC-C4B	-3.88	1.47	1.53
26	d	402	CLA	CMD-C2D	-3.87	1.43	1.51
25	7	609	CHL	CHD-C1D	-3.87	1.47	1.53
25	8	601	CHL	CHC-C4B	-3.87	1.47	1.53
25	4	601	CHL	CHC-C4B	-3.87	1.47	1.53
25	y	607	CHL	C3D-C2D	-3.87	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	605	CHL	CHC-C4B	-3.87	1.47	1.53
25	Y	607	CHL	C3D-C2D	-3.87	1.45	1.55
25	8	601	CHL	CHD-C1D	-3.87	1.47	1.53
25	5	601	CHL	CHD-C1D	-3.87	1.47	1.53
26	D	402	CLA	CMD-C2D	-3.86	1.43	1.51
25	5	601	CHL	C1A-CHA	-3.85	1.47	1.53
25	1	601	CHL	C1A-CHA	-3.85	1.47	1.53
25	3	605	CHL	CHC-C4B	-3.85	1.47	1.53
25	7	605	CHL	CHC-C4B	-3.85	1.47	1.53
25	5	601	CHL	C4A-C3A	-3.85	1.49	1.53
25	1	601	CHL	C4A-C3A	-3.85	1.49	1.53
25	1	601	CHL	CHD-C1D	-3.83	1.47	1.53
26	C	505	CLA	CMD-C2D	-3.83	1.43	1.51
26	b	604	CLA	CMB-C2B	-3.83	1.43	1.51
26	B	604	CLA	CMB-C2B	-3.83	1.43	1.51
26	c	505	CLA	CMD-C2D	-3.82	1.43	1.51
25	4	607	CHL	C4A-C3A	-3.81	1.49	1.53
38	d	405	PL9	C6-C1	-3.81	1.41	1.48
26	c	508	CLA	CMB-C2B	-3.80	1.43	1.51
25	6	605	CHL	C4A-C3A	-3.79	1.49	1.53
26	c	506	CLA	CMB-C2B	-3.79	1.44	1.51
25	2	601	CHL	C1A-CHA	-3.79	1.47	1.53
25	6	601	CHL	C1A-CHA	-3.79	1.47	1.53
25	7	608	CHL	C3D-C2D	-3.79	1.45	1.55
26	C	508	CLA	CMB-C2B	-3.79	1.44	1.51
25	S	601	CHL	C3D-C2D	-3.78	1.45	1.55
25	s	601	CHL	C3D-C2D	-3.78	1.45	1.55
25	2	608	CHL	C3D-C2D	-3.78	1.45	1.55
25	6	608	CHL	C3D-C2D	-3.78	1.45	1.55
25	3	608	CHL	C3D-C2D	-3.78	1.45	1.55
26	C	506	CLA	CMB-C2B	-3.77	1.44	1.51
38	D	405	PL9	C6-C1	-3.77	1.41	1.48
25	R	607	CHL	C3D-C2D	-3.77	1.45	1.55
25	4	607	CHL	CHB-C1B	-3.77	1.47	1.53
25	g	601	CHL	CHC-C1C	-3.77	1.46	1.53
25	G	601	CHL	CHC-C1C	-3.76	1.46	1.53
25	8	607	CHL	C4A-C3A	-3.76	1.49	1.53
25	r	607	CHL	C3D-C2D	-3.76	1.45	1.55
25	s	607	CHL	CHC-C1C	-3.76	1.46	1.53
25	S	607	CHL	CHC-C1C	-3.75	1.46	1.53
26	B	605	CLA	CMB-C2B	-3.75	1.44	1.51
26	b	605	CLA	CMB-C2B	-3.75	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	608	CHL	C3D-C2D	-3.74	1.45	1.55
25	8	608	CHL	C3D-C2D	-3.74	1.45	1.55
25	N	601	CHL	CHC-C1C	-3.74	1.46	1.53
25	5	601	CHL	C3D-C2D	-3.74	1.45	1.55
25	S	606	CHL	CHB-C1B	-3.74	1.47	1.53
25	s	606	CHL	CHB-C1B	-3.74	1.47	1.53
25	1	601	CHL	C3D-C2D	-3.74	1.45	1.55
25	s	606	CHL	C3B-C4B	-3.73	1.50	1.54
25	2	605	CHL	C4A-C3A	-3.73	1.49	1.53
25	n	601	CHL	CHC-C1C	-3.72	1.46	1.53
25	S	606	CHL	C3B-C4B	-3.72	1.50	1.54
25	8	607	CHL	CHB-C1B	-3.72	1.47	1.53
38	D	405	PL9	C7-C8	-3.71	1.45	1.50
25	n	607	CHL	C3D-C2D	-3.70	1.45	1.55
25	5	607	CHL	C3D-C2D	-3.70	1.45	1.55
25	1	607	CHL	C3D-C2D	-3.70	1.45	1.55
25	2	609	CHL	CHB-C1B	-3.69	1.47	1.53
25	G	606	CHL	C4A-C3A	-3.69	1.49	1.53
25	5	608	CHL	C4A-C3A	-3.69	1.49	1.53
25	g	606	CHL	C4A-C3A	-3.69	1.49	1.53
25	1	608	CHL	C4A-C3A	-3.69	1.49	1.53
25	6	606	CHL	CHC-C1C	-3.69	1.46	1.53
25	2	606	CHL	CHC-C1C	-3.69	1.46	1.53
25	7	606	CHL	C3D-C2D	-3.68	1.45	1.55
25	3	606	CHL	C3D-C2D	-3.68	1.45	1.55
25	6	609	CHL	CHB-C1B	-3.68	1.47	1.53
25	N	607	CHL	C3D-C2D	-3.68	1.45	1.55
26	G	611	CLA	CMB-C2B	-3.68	1.44	1.51
25	G	608	CHL	C4A-C3A	-3.68	1.49	1.53
25	5	609	CHL	C3D-C2D	-3.68	1.45	1.55
25	1	609	CHL	C3D-C2D	-3.68	1.45	1.55
25	2	609	CHL	C4A-C3A	-3.67	1.49	1.53
25	6	609	CHL	C4A-C3A	-3.67	1.49	1.53
25	r	606	CHL	C3D-C2D	-3.66	1.45	1.55
38	d	405	PL9	C7-C8	-3.66	1.45	1.50
25	S	601	CHL	C1A-C2A	-3.65	1.49	1.53
25	G	607	CHL	C3D-C2D	-3.65	1.45	1.55
25	g	607	CHL	C3D-C2D	-3.65	1.45	1.55
25	R	606	CHL	C3D-C2D	-3.65	1.45	1.55
26	g	611	CLA	CMB-C2B	-3.65	1.44	1.51
25	3	609	CHL	C1A-CHA	-3.64	1.48	1.53
25	7	609	CHL	C1A-CHA	-3.64	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	606	CHL	CHC-C1C	-3.64	1.46	1.53
25	g	609	CHL	C3D-C2D	-3.64	1.45	1.55
25	1	606	CHL	C3D-C2D	-3.64	1.45	1.55
25	5	606	CHL	C3D-C2D	-3.64	1.45	1.55
25	G	601	CHL	C1A-CHA	-3.64	1.48	1.53
25	g	601	CHL	C1A-CHA	-3.64	1.48	1.53
25	G	609	CHL	C3D-C2D	-3.63	1.45	1.55
25	N	605	CHL	CHD-C4C	-3.63	1.46	1.53
25	s	601	CHL	C1A-C2A	-3.62	1.49	1.53
26	B	608	CLA	CMB-C2B	-3.62	1.44	1.51
25	Y	601	CHL	C1A-C2A	-3.62	1.49	1.53
25	y	601	CHL	C1A-C2A	-3.62	1.49	1.53
25	3	606	CHL	CHC-C1C	-3.62	1.46	1.53
25	S	608	CHL	CHD-C4C	-3.62	1.46	1.53
25	s	608	CHL	CHD-C4C	-3.62	1.46	1.53
25	y	601	CHL	C1A-CHA	-3.62	1.48	1.53
25	1	608	CHL	CHD-C4C	-3.61	1.46	1.53
25	g	608	CHL	C4A-C3A	-3.61	1.49	1.53
26	b	608	CLA	CMB-C2B	-3.61	1.44	1.51
25	2	606	CHL	C3D-C2D	-3.60	1.45	1.55
25	R	608	CHL	CBD-CAD	-3.60	1.47	1.53
25	6	606	CHL	C3D-C2D	-3.60	1.45	1.55
25	R	607	CHL	CHD-C4C	-3.59	1.46	1.53
25	N	606	CHL	C4A-C3A	-3.59	1.49	1.53
25	n	606	CHL	C4A-C3A	-3.59	1.49	1.53
25	n	605	CHL	CHD-C4C	-3.59	1.46	1.53
25	4	608	CHL	CHD-C4C	-3.59	1.46	1.53
25	5	608	CHL	CHD-C4C	-3.59	1.46	1.53
25	G	601	CHL	C1A-C2A	-3.58	1.49	1.53
25	g	601	CHL	C1A-C2A	-3.58	1.49	1.53
25	r	607	CHL	CHD-C4C	-3.58	1.46	1.53
25	S	607	CHL	C3D-C2D	-3.58	1.45	1.55
25	s	607	CHL	C3D-C2D	-3.58	1.45	1.55
25	N	605	CHL	C3D-C2D	-3.58	1.45	1.55
25	r	608	CHL	CBD-CAD	-3.58	1.47	1.53
25	6	608	CHL	C4A-C3A	-3.58	1.49	1.53
25	Y	601	CHL	C1A-CHA	-3.57	1.48	1.53
41	F	101	HEM	C3B-C2B	-3.57	1.35	1.40
25	y	608	CHL	CHD-C4C	-3.57	1.46	1.53
25	Y	608	CHL	CHD-C4C	-3.56	1.46	1.53
41	f	101	HEM	C3B-C2B	-3.56	1.35	1.40
25	G	606	CHL	C3D-C2D	-3.56	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	606	CHL	C3D-C2D	-3.56	1.45	1.55
25	n	605	CHL	C3D-C2D	-3.56	1.45	1.55
25	8	608	CHL	CHD-C4C	-3.55	1.46	1.53
25	7	609	CHL	CHC-C1C	-3.54	1.46	1.53
25	6	601	CHL	C1A-C2A	-3.54	1.49	1.53
25	2	608	CHL	C4A-C3A	-3.54	1.49	1.53
25	1	608	CHL	CHC-C1C	-3.54	1.46	1.53
26	B	612	CLA	CMC-C2C	-3.53	1.43	1.50
26	b	612	CLA	CMC-C2C	-3.53	1.43	1.50
25	N	606	CHL	C3D-C2D	-3.53	1.45	1.55
25	R	614	CHL	C3D-C2D	-3.52	1.45	1.55
25	2	607	CHL	C3D-C2D	-3.52	1.45	1.55
25	6	607	CHL	C3D-C2D	-3.52	1.45	1.55
25	r	614	CHL	C3D-C2D	-3.52	1.45	1.55
25	n	606	CHL	C3D-C2D	-3.51	1.45	1.55
25	8	606	CHL	CHC-C1C	-3.51	1.46	1.53
25	y	605	CHL	C3D-C2D	-3.51	1.45	1.55
25	5	608	CHL	CHC-C1C	-3.51	1.46	1.53
25	3	609	CHL	CHC-C1C	-3.51	1.46	1.53
39	c	520	DGD	O5D-C6D	-3.51	1.37	1.43
25	y	609	CHL	C3D-C2D	-3.50	1.45	1.55
25	Y	609	CHL	C3D-C2D	-3.50	1.45	1.55
25	1	605	CHL	C3D-C2D	-3.50	1.45	1.55
25	5	605	CHL	C3D-C2D	-3.50	1.45	1.55
26	5	604	CLA	CMB-C2B	-3.50	1.44	1.51
25	2	601	CHL	C1A-C2A	-3.50	1.49	1.53
25	2	609	CHL	C3D-C2D	-3.50	1.46	1.55
25	N	601	CHL	C1A-CHA	-3.50	1.48	1.53
25	n	601	CHL	C1A-CHA	-3.50	1.48	1.53
25	Y	605	CHL	C3D-C2D	-3.50	1.46	1.55
25	S	606	CHL	C3D-C2D	-3.49	1.46	1.55
25	s	606	CHL	C3D-C2D	-3.49	1.46	1.55
26	1	604	CLA	CMB-C2B	-3.49	1.44	1.51
25	N	608	CHL	CHD-C4C	-3.49	1.46	1.53
25	r	608	CHL	C4A-C3A	-3.49	1.49	1.53
25	n	608	CHL	CHD-C4C	-3.48	1.46	1.53
25	3	601	CHL	C1A-C2A	-3.48	1.49	1.53
25	8	607	CHL	C3D-C2D	-3.48	1.46	1.55
39	C	520	DGD	O5D-C6D	-3.48	1.37	1.43
26	B	612	CLA	CMB-C2B	-3.47	1.44	1.51
26	b	612	CLA	CMB-C2B	-3.47	1.44	1.51
26	D	402	CLA	CMB-C2B	-3.47	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	402	CLA	CMB-C2B	-3.47	1.44	1.51
25	2	601	CHL	CHC-C1C	-3.47	1.47	1.53
25	n	609	CHL	C3D-C2D	-3.47	1.46	1.55
25	6	609	CHL	C3D-C2D	-3.47	1.46	1.55
25	4	606	CHL	CHC-C1C	-3.47	1.47	1.53
25	4	606	CHL	C3D-C2D	-3.46	1.46	1.55
25	4	607	CHL	C3D-C2D	-3.46	1.46	1.55
25	7	601	CHL	C1A-C2A	-3.46	1.49	1.53
25	N	609	CHL	C3D-C2D	-3.46	1.46	1.55
26	a	405	CLA	CMD-C2D	-3.45	1.44	1.51
26	n	603	CLA	C3B-C2B	-3.45	1.35	1.40
25	N	609	CHL	C2B-C1B	-3.45	1.46	1.53
25	7	606	CHL	C1A-CHA	-3.45	1.48	1.53
26	N	603	CLA	C3B-C2B	-3.44	1.35	1.40
25	8	606	CHL	C3D-C2D	-3.44	1.46	1.55
25	Y	608	CHL	C1A-CHA	-3.44	1.48	1.53
25	4	609	CHL	C1A-CHA	-3.44	1.48	1.53
26	Y	603	CLA	C3B-C2B	-3.44	1.35	1.40
25	N	607	CHL	CHC-C1C	-3.44	1.47	1.53
25	n	607	CHL	CHC-C1C	-3.44	1.47	1.53
25	2	609	CHL	CHC-C1C	-3.44	1.47	1.53
25	R	608	CHL	C4A-C3A	-3.44	1.49	1.53
26	A	405	CLA	CMD-C2D	-3.43	1.44	1.51
25	8	609	CHL	C1A-CHA	-3.43	1.48	1.53
26	7	611	CLA	CMB-C2B	-3.43	1.44	1.51
26	3	611	CLA	CMB-C2B	-3.43	1.44	1.51
25	S	606	CHL	CHC-C4B	-3.43	1.48	1.53
25	s	606	CHL	CHC-C4B	-3.43	1.48	1.53
39	b	626	DGD	O2G-C2G	-3.43	1.37	1.46
39	B	626	DGD	O2G-C2G	-3.43	1.37	1.46
25	6	601	CHL	CHC-C1C	-3.43	1.47	1.53
25	n	609	CHL	C2B-C1B	-3.43	1.46	1.53
25	4	609	CHL	C3D-C2D	-3.42	1.46	1.55
25	8	609	CHL	C3D-C2D	-3.42	1.46	1.55
25	r	607	CHL	CHC-C1C	-3.42	1.47	1.53
25	y	608	CHL	C1A-CHA	-3.42	1.48	1.53
25	3	606	CHL	C1A-CHA	-3.42	1.48	1.53
25	3	608	CHL	CHD-C4C	-3.42	1.47	1.53
25	R	607	CHL	CHC-C1C	-3.41	1.47	1.53
25	8	606	CHL	C1A-CHA	-3.41	1.48	1.53
25	7	608	CHL	CHD-C4C	-3.41	1.47	1.53
25	3	609	CHL	C3D-C2D	-3.41	1.46	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	609	CHL	C3D-C2D	-3.41	1.46	1.55
25	1	601	CHL	C1A-C2A	-3.41	1.49	1.53
25	6	609	CHL	CHC-C1C	-3.41	1.47	1.53
25	4	608	CHL	C1A-CHA	-3.40	1.48	1.53
25	8	608	CHL	C1A-CHA	-3.40	1.48	1.53
25	S	606	CHL	CHD-C4C	-3.40	1.47	1.53
26	y	603	CLA	C3B-C2B	-3.39	1.35	1.40
25	3	605	CHL	C3D-C2D	-3.39	1.46	1.55
25	N	606	CHL	CHC-C1C	-3.39	1.47	1.53
25	n	606	CHL	CHC-C1C	-3.39	1.47	1.53
26	B	617	CLA	CMC-C2C	-3.38	1.43	1.50
26	b	617	CLA	CMC-C2C	-3.38	1.43	1.50
25	N	605	CHL	CHC-C1C	-3.38	1.47	1.53
25	6	608	CHL	CHD-C4C	-3.38	1.47	1.53
25	n	605	CHL	CHC-C1C	-3.38	1.47	1.53
26	7	611	CLA	C3B-C2B	-3.37	1.35	1.40
26	3	611	CLA	C3B-C2B	-3.37	1.35	1.40
25	5	601	CHL	C1A-C2A	-3.37	1.49	1.53
25	7	605	CHL	C3D-C2D	-3.37	1.46	1.55
25	2	608	CHL	CHD-C4C	-3.37	1.47	1.53
25	s	606	CHL	CHD-C4C	-3.37	1.47	1.53
25	g	605	CHL	CHC-C4B	-3.37	1.48	1.53
25	4	606	CHL	C1A-CHA	-3.36	1.48	1.53
25	6	605	CHL	C3D-C2D	-3.36	1.46	1.55
25	2	605	CHL	C3D-C2D	-3.36	1.46	1.55
25	7	607	CHL	C3D-C2D	-3.35	1.46	1.55
25	3	607	CHL	C3D-C2D	-3.35	1.46	1.55
25	1	605	CHL	C1A-CHA	-3.34	1.48	1.53
25	5	605	CHL	C1A-CHA	-3.34	1.48	1.53
25	1	606	CHL	CHC-C1C	-3.34	1.47	1.53
25	5	606	CHL	CHC-C1C	-3.34	1.47	1.53
25	y	601	CHL	CBD-CAD	-3.34	1.48	1.53
25	R	606	CHL	CHD-C4C	-3.34	1.47	1.53
25	r	606	CHL	CHD-C4C	-3.34	1.47	1.53
25	6	608	CHL	CHC-C1C	-3.33	1.47	1.53
25	3	606	CHL	CHD-C4C	-3.33	1.47	1.53
25	g	605	CHL	C3D-C2D	-3.33	1.46	1.55
25	G	605	CHL	C3D-C2D	-3.33	1.46	1.55
25	G	605	CHL	CHC-C4B	-3.33	1.48	1.53
25	R	608	CHL	CHC-C1C	-3.32	1.47	1.53
25	r	608	CHL	CHC-C1C	-3.32	1.47	1.53
25	8	607	CHL	CHC-C1C	-3.32	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	601	CHL	CHC-C1C	-3.32	1.47	1.53
25	4	607	CHL	CHC-C1C	-3.32	1.47	1.53
25	r	608	CHL	C3D-CAD	-3.32	1.45	1.51
25	N	606	CHL	CHD-C4C	-3.32	1.47	1.53
25	R	606	CHL	C1A-CHA	-3.31	1.48	1.53
25	Y	601	CHL	CBD-CAD	-3.31	1.48	1.53
25	S	601	CHL	CHC-C1C	-3.31	1.47	1.53
25	7	606	CHL	CHD-C4C	-3.31	1.47	1.53
25	S	607	CHL	CHD-C4C	-3.31	1.47	1.53
25	g	606	CHL	CHC-C1C	-3.31	1.47	1.53
25	y	609	CHL	C2B-C1B	-3.31	1.46	1.53
25	5	607	CHL	CHC-C1C	-3.30	1.47	1.53
25	1	607	CHL	CHC-C1C	-3.30	1.47	1.53
30	d	409	LHG	O7-C5	-3.30	1.38	1.46
26	c	509	CLA	CMD-C2D	-3.30	1.44	1.51
26	C	509	CLA	CMD-C2D	-3.30	1.44	1.51
26	b	615	CLA	CMD-C2D	-3.30	1.44	1.51
26	B	615	CLA	CMD-C2D	-3.30	1.44	1.51
30	D	409	LHG	O7-C5	-3.29	1.38	1.46
25	n	606	CHL	CHD-C4C	-3.29	1.47	1.53
25	2	608	CHL	CHC-C1C	-3.29	1.47	1.53
25	Y	609	CHL	C2B-C1B	-3.29	1.46	1.53
25	r	606	CHL	C1A-CHA	-3.28	1.48	1.53
25	g	608	CHL	CHD-C4C	-3.28	1.47	1.53
25	G	606	CHL	CHC-C1C	-3.28	1.47	1.53
25	1	606	CHL	CHD-C4C	-3.28	1.47	1.53
25	5	606	CHL	CHD-C4C	-3.28	1.47	1.53
25	R	608	CHL	C3D-CAD	-3.27	1.45	1.51
25	G	606	CHL	C1A-C2A	-3.27	1.49	1.53
25	g	606	CHL	C1A-C2A	-3.27	1.49	1.53
25	G	608	CHL	CHD-C4C	-3.27	1.47	1.53
25	1	605	CHL	CHD-C4C	-3.27	1.47	1.53
25	S	606	CHL	C4A-C3A	-3.27	1.49	1.53
25	s	606	CHL	C4A-C3A	-3.27	1.49	1.53
25	1	605	CHL	CHC-C1C	-3.27	1.47	1.53
25	7	605	CHL	CHC-C1C	-3.26	1.47	1.53
25	R	614	CHL	CHC-C1C	-3.26	1.47	1.53
25	5	605	CHL	CHC-C1C	-3.26	1.47	1.53
25	7	608	CHL	CHC-C1C	-3.26	1.47	1.53
25	5	605	CHL	CHD-C4C	-3.26	1.47	1.53
25	s	607	CHL	CHD-C4C	-3.25	1.47	1.53
25	3	605	CHL	CHC-C1C	-3.25	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	614	CHL	CHC-C1C	-3.24	1.47	1.53
25	8	601	CHL	C3D-C2D	-3.24	1.46	1.55
26	B	604	CLA	CMD-C2D	-3.23	1.44	1.51
25	6	607	CHL	CHC-C1C	-3.23	1.47	1.53
25	y	608	CHL	CHC-C1C	-3.23	1.47	1.53
35	a	408	PHO	C1C-NC	-3.23	1.31	1.38
35	A	408	PHO	C1C-NC	-3.23	1.31	1.38
26	b	604	CLA	CMD-C2D	-3.23	1.44	1.51
25	r	606	CHL	C1A-C2A	-3.23	1.49	1.53
25	r	614	CHL	CHD-C4C	-3.23	1.47	1.53
25	y	609	CHL	CHD-C4C	-3.22	1.47	1.53
25	N	608	CHL	CHC-C1C	-3.22	1.47	1.53
25	n	608	CHL	CHC-C1C	-3.22	1.47	1.53
25	Y	608	CHL	CHC-C1C	-3.21	1.47	1.53
25	3	608	CHL	CHC-C1C	-3.21	1.47	1.53
25	g	607	CHL	CHD-C4C	-3.21	1.47	1.53
26	N	603	CLA	CMD-C2D	-3.21	1.44	1.51
25	4	601	CHL	C3D-C2D	-3.21	1.46	1.55
26	n	603	CLA	CMD-C2D	-3.21	1.44	1.51
25	Y	609	CHL	CHD-C4C	-3.20	1.47	1.53
25	n	609	CHL	CHD-C4C	-3.20	1.47	1.53
25	N	609	CHL	CHD-C4C	-3.20	1.47	1.53
25	g	607	CHL	C3B-CAB	-3.20	1.47	1.50
25	g	605	CHL	CHD-C4C	-3.20	1.47	1.53
25	G	605	CHL	CHD-C4C	-3.20	1.47	1.53
25	R	606	CHL	C1A-C2A	-3.20	1.49	1.53
25	G	607	CHL	CHD-C4C	-3.20	1.47	1.53
25	N	601	CHL	C1A-C2A	-3.20	1.49	1.53
25	y	608	CHL	C1A-C2A	-3.20	1.49	1.53
25	Y	608	CHL	C1A-C2A	-3.20	1.49	1.53
26	C	502	CLA	CMB-C2B	-3.20	1.45	1.51
26	c	502	CLA	CMB-C2B	-3.20	1.45	1.51
30	d	408	LHG	O7-C5	-3.20	1.38	1.46
25	S	606	CHL	C1A-CHA	-3.20	1.48	1.53
25	G	607	CHL	C3B-CAB	-3.20	1.47	1.50
25	S	608	CHL	CHC-C1C	-3.19	1.47	1.53
25	R	614	CHL	CHD-C4C	-3.19	1.47	1.53
25	s	608	CHL	CHC-C1C	-3.19	1.47	1.53
25	y	605	CHL	CHC-C1C	-3.19	1.47	1.53
25	2	607	CHL	CHC-C1C	-3.19	1.47	1.53
25	y	609	CHL	C1A-CHA	-3.19	1.48	1.53
25	Y	609	CHL	C1A-CHA	-3.19	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	611	CLA	CMD-C2D	-3.19	1.44	1.51
26	Y	611	CLA	CMD-C2D	-3.19	1.44	1.51
25	n	609	CHL	C1A-CHA	-3.19	1.48	1.53
25	N	609	CHL	C1A-CHA	-3.19	1.48	1.53
25	n	601	CHL	C1A-C2A	-3.18	1.49	1.53
25	1	601	CHL	CHC-C1C	-3.18	1.47	1.53
26	5	610	CLA	C3B-C2B	-3.18	1.36	1.40
38	D	405	PL9	C52-C5	-3.18	1.43	1.50
38	d	405	PL9	C52-C5	-3.18	1.43	1.50
25	s	606	CHL	C1A-CHA	-3.18	1.48	1.53
26	c	509	CLA	CMB-C2B	-3.17	1.45	1.51
26	C	509	CLA	CMB-C2B	-3.17	1.45	1.51
30	D	408	LHG	O7-C5	-3.17	1.38	1.46
25	g	608	CHL	CHC-C1C	-3.17	1.47	1.53
25	G	608	CHL	CHC-C1C	-3.17	1.47	1.53
25	6	605	CHL	CHD-C4C	-3.17	1.47	1.53
29	1	1623	NEX	C7-C8	-3.17	1.26	1.32
25	5	601	CHL	CHC-C1C	-3.17	1.47	1.53
35	A	409	PHO	C1C-NC	-3.17	1.31	1.38
25	7	608	CHL	C1A-CHA	-3.17	1.48	1.53
25	3	608	CHL	C1A-CHA	-3.17	1.48	1.53
26	C	510	CLA	CMD-C2D	-3.17	1.44	1.51
26	1	610	CLA	C3B-C2B	-3.16	1.36	1.40
25	R	606	CHL	CHC-C1C	-3.16	1.47	1.53
26	5	612	CLA	C3B-C2B	-3.16	1.36	1.40
26	G	603	CLA	C3B-C2B	-3.16	1.36	1.40
26	g	603	CLA	C3B-C2B	-3.16	1.36	1.40
25	1	606	CHL	C1A-CHA	-3.16	1.48	1.53
26	c	510	CLA	CMD-C2D	-3.16	1.44	1.51
25	y	607	CHL	C3B-CAB	-3.16	1.47	1.50
26	r	610	CLA	C3B-C2B	-3.16	1.36	1.40
35	a	409	PHO	C1C-NC	-3.15	1.31	1.38
26	B	616	CLA	C3B-C2B	-3.15	1.36	1.40
25	2	605	CHL	CHD-C4C	-3.15	1.47	1.53
26	R	610	CLA	C3B-C2B	-3.15	1.36	1.40
25	r	606	CHL	CHC-C1C	-3.15	1.47	1.53
25	2	606	CHL	CHD-C4C	-3.15	1.47	1.53
25	Y	607	CHL	C3B-CAB	-3.14	1.47	1.50
25	Y	605	CHL	CHC-C1C	-3.14	1.47	1.53
25	4	609	CHL	CHC-C1C	-3.14	1.47	1.53
25	8	609	CHL	CHC-C1C	-3.14	1.47	1.53
25	G	601	CHL	CBD-CAD	-3.14	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	601	CHL	CBD-CAD	-3.14	1.48	1.53
25	2	608	CHL	C1A-CHA	-3.13	1.48	1.53
29	5	1623	NEX	C7-C8	-3.13	1.26	1.32
25	2	605	CHL	CHC-C1C	-3.13	1.47	1.53
26	b	616	CLA	C3B-C2B	-3.13	1.36	1.40
25	6	606	CHL	CHD-C4C	-3.13	1.47	1.53
25	5	606	CHL	C1A-CHA	-3.13	1.48	1.53
25	g	605	CHL	C1A-C2A	-3.12	1.50	1.53
25	G	605	CHL	C1A-C2A	-3.12	1.50	1.53
26	1	612	CLA	C3B-C2B	-3.12	1.36	1.40
25	6	605	CHL	CHC-C1C	-3.12	1.47	1.53
29	R	623	NEX	C7-C8	-3.12	1.26	1.32
29	r	623	NEX	C7-C8	-3.12	1.26	1.32
25	3	607	CHL	CHC-C1C	-3.11	1.47	1.53
39	c	518	DGD	O1G-C1G	-3.11	1.38	1.45
25	Y	606	CHL	C2B-C1B	-3.11	1.47	1.53
25	y	606	CHL	C2B-C1B	-3.11	1.47	1.53
26	b	607	CLA	CMD-C2D	-3.11	1.44	1.51
26	B	607	CLA	CMD-C2D	-3.11	1.44	1.51
25	5	607	CHL	C3B-CAB	-3.11	1.47	1.50
25	1	607	CHL	CHD-C4C	-3.11	1.47	1.53
25	5	609	CHL	C1A-CHA	-3.11	1.48	1.53
25	1	609	CHL	C1A-CHA	-3.11	1.48	1.53
26	b	609	CLA	CMD-C2D	-3.11	1.45	1.51
26	B	609	CLA	CMD-C2D	-3.11	1.45	1.51
25	5	607	CHL	CHD-C4C	-3.11	1.47	1.53
25	3	605	CHL	CHD-C4C	-3.10	1.47	1.53
25	7	605	CHL	CHD-C4C	-3.10	1.47	1.53
25	7	607	CHL	CHC-C1C	-3.10	1.47	1.53
26	s	604	CLA	CMB-C2B	-3.10	1.45	1.51
26	B	613	CLA	CMB-C2B	-3.10	1.45	1.51
26	S	604	CLA	CMB-C2B	-3.10	1.45	1.51
26	b	613	CLA	CMB-C2B	-3.10	1.45	1.51
25	s	601	CHL	C2B-C1B	-3.10	1.47	1.53
39	C	518	DGD	O1G-C1G	-3.10	1.38	1.45
38	D	405	PL9	C53-C6	-3.09	1.44	1.50
38	d	405	PL9	C53-C6	-3.09	1.44	1.50
25	G	609	CHL	C2B-C1B	-3.09	1.47	1.53
25	g	609	CHL	C2B-C1B	-3.09	1.47	1.53
25	7	601	CHL	CHC-C1C	-3.09	1.47	1.53
25	3	601	CHL	CHC-C1C	-3.09	1.47	1.53
25	6	608	CHL	C1A-CHA	-3.09	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	601	CHL	C2B-C1B	-3.09	1.47	1.53
25	1	607	CHL	C3B-CAB	-3.09	1.47	1.50
25	4	607	CHL	C1A-CHA	-3.08	1.49	1.53
26	r	616	CLA	CMB-C2B	-3.08	1.45	1.51
26	B	614	CLA	CMB-C2B	-3.07	1.45	1.51
25	G	607	CHL	C1A-CHA	-3.07	1.49	1.53
25	g	607	CHL	C1A-CHA	-3.07	1.49	1.53
25	2	609	CHL	CHD-C4C	-3.07	1.47	1.53
25	S	606	CHL	CHC-C1C	-3.07	1.47	1.53
25	N	608	CHL	C1A-CHA	-3.06	1.49	1.53
25	n	608	CHL	C1A-CHA	-3.06	1.49	1.53
25	G	609	CHL	CHD-C4C	-3.06	1.47	1.53
25	g	609	CHL	CHD-C4C	-3.06	1.47	1.53
29	y	1623	NEX	C7-C8	-3.06	1.26	1.32
25	8	607	CHL	C1A-CHA	-3.06	1.49	1.53
25	R	608	CHL	C2B-C1B	-3.06	1.47	1.53
25	6	606	CHL	C1A-CHA	-3.06	1.49	1.53
25	s	606	CHL	CHC-C1C	-3.05	1.47	1.53
25	r	608	CHL	C2B-C1B	-3.05	1.47	1.53
26	1	604	CLA	C3B-C2B	-3.04	1.36	1.40
26	5	604	CLA	C3B-C2B	-3.04	1.36	1.40
25	g	605	CHL	C1A-CHA	-3.04	1.49	1.53
25	S	606	CHL	C2A-C3A	-3.04	1.49	1.55
26	b	606	CLA	CMB-C2B	-3.04	1.45	1.51
26	B	606	CLA	CMB-C2B	-3.04	1.45	1.51
25	Y	606	CHL	C1A-CHA	-3.04	1.49	1.53
25	Y	608	CHL	CBD-CAD	-3.04	1.48	1.53
26	b	606	CLA	CMD-C2D	-3.04	1.45	1.51
26	B	606	CLA	CMD-C2D	-3.04	1.45	1.51
25	S	608	CHL	C1A-CHA	-3.04	1.49	1.53
26	y	610	CLA	C3B-C2B	-3.03	1.36	1.40
26	b	614	CLA	CMB-C2B	-3.03	1.45	1.51
26	R	616	CLA	CMB-C2B	-3.03	1.45	1.51
26	Y	610	CLA	C3B-C2B	-3.03	1.36	1.40
25	G	605	CHL	C1A-CHA	-3.03	1.49	1.53
25	s	606	CHL	C2A-C3A	-3.02	1.49	1.55
26	C	501	CLA	C3B-C2B	-3.02	1.36	1.40
26	c	501	CLA	C3B-C2B	-3.02	1.36	1.40
29	6	1623	NEX	C7-C8	-3.02	1.26	1.32
25	6	609	CHL	CHD-C4C	-3.02	1.47	1.53
29	Y	1623	NEX	C7-C8	-3.02	1.26	1.32
39	c	519	DGD	O1G-C1G	-3.02	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	519	DGD	O1G-C1G	-3.02	1.38	1.45
25	s	608	CHL	C1A-CHA	-3.01	1.49	1.53
25	g	607	CHL	C2B-C1B	-3.01	1.47	1.53
26	Y	613	CLA	CMD-C2D	-3.01	1.45	1.51
26	y	613	CLA	CMD-C2D	-3.01	1.45	1.51
25	y	606	CHL	C1A-CHA	-3.01	1.49	1.53
25	2	607	CHL	CHD-C4C	-3.01	1.47	1.53
25	6	607	CHL	CHD-C4C	-3.01	1.47	1.53
26	c	512	CLA	CMD-C2D	-3.01	1.45	1.51
37	D	411	LMG	O8-C9	-3.01	1.38	1.45
25	G	606	CHL	CHD-C4C	-3.01	1.47	1.53
25	8	608	CHL	CHC-C1C	-3.01	1.47	1.53
29	2	1623	NEX	C7-C8	-3.01	1.27	1.32
25	G	607	CHL	C2B-C1B	-3.00	1.47	1.53
25	g	606	CHL	C1A-CHA	-3.00	1.49	1.53
26	B	607	CLA	CMC-C2C	-3.00	1.44	1.50
25	4	608	CHL	CHC-C1C	-3.00	1.47	1.53
26	Y	610	CLA	CMD-C2D	-3.00	1.45	1.51
26	y	610	CLA	CMD-C2D	-3.00	1.45	1.51
25	4	606	CHL	C1A-C2A	-3.00	1.50	1.53
25	2	606	CHL	C1A-CHA	-3.00	1.49	1.53
25	g	606	CHL	CHD-C4C	-3.00	1.47	1.53
25	y	608	CHL	CBD-CAD	-3.00	1.48	1.53
26	6	604	CLA	CMB-C2B	-3.00	1.45	1.51
25	G	608	CHL	C1A-CHA	-3.00	1.49	1.53
25	N	601	CHL	CHD-C4C	-2.99	1.47	1.53
25	n	601	CHL	CHD-C4C	-2.99	1.47	1.53
26	b	607	CLA	CMC-C2C	-2.99	1.44	1.50
25	Y	606	CHL	C3D-CAD	-2.99	1.45	1.51
25	y	606	CHL	C3D-CAD	-2.99	1.45	1.51
25	1	609	CHL	CHD-C4C	-2.99	1.47	1.53
26	2	604	CLA	CMB-C2B	-2.98	1.45	1.51
39	C	520	DGD	O1G-C1G	-2.98	1.38	1.45
39	c	520	DGD	O1G-C1G	-2.98	1.38	1.45
25	Y	608	CHL	C2B-C1B	-2.98	1.47	1.53
26	b	608	CLA	CMD-C2D	-2.98	1.45	1.51
26	C	512	CLA	CMD-C2D	-2.97	1.45	1.51
25	G	606	CHL	C1A-CHA	-2.97	1.49	1.53
37	d	411	LMG	O8-C9	-2.97	1.38	1.45
26	y	612	CLA	CMD-C2D	-2.97	1.45	1.51
26	Y	612	CLA	CMD-C2D	-2.97	1.45	1.51
26	C	512	CLA	CMB-C2B	-2.97	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	512	CLA	CMB-C2B	-2.97	1.45	1.51
26	y	603	CLA	CMB-C2B	-2.96	1.45	1.51
25	y	608	CHL	C2B-C1B	-2.96	1.47	1.53
26	C	504	CLA	CMB-C2B	-2.96	1.45	1.51
25	5	609	CHL	CHD-C4C	-2.96	1.47	1.53
26	Y	603	CLA	CMB-C2B	-2.96	1.45	1.51
25	g	608	CHL	C1A-CHA	-2.96	1.49	1.53
26	b	606	CLA	CMC-C2C	-2.96	1.44	1.50
26	B	606	CLA	CMC-C2C	-2.96	1.44	1.50
26	B	604	CLA	C3B-C2B	-2.95	1.36	1.40
25	G	608	CHL	CBD-CAD	-2.95	1.48	1.53
25	N	606	CHL	C1A-CHA	-2.95	1.49	1.53
25	y	609	CHL	CBD-CAD	-2.95	1.48	1.53
25	Y	609	CHL	CBD-CAD	-2.95	1.48	1.53
26	b	603	CLA	CMB-C2B	-2.95	1.45	1.51
26	B	603	CLA	CMB-C2B	-2.95	1.45	1.51
26	c	507	CLA	CMB-C2B	-2.95	1.45	1.51
25	Y	607	CHL	C2B-C1B	-2.95	1.47	1.53
25	g	608	CHL	CBD-CAD	-2.95	1.48	1.53
25	n	606	CHL	C1A-CHA	-2.94	1.49	1.53
25	N	601	CHL	CBD-CAD	-2.94	1.48	1.53
25	n	601	CHL	CBD-CAD	-2.94	1.48	1.53
26	s	610	CLA	CMB-C2B	-2.94	1.45	1.51
26	B	608	CLA	CMD-C2D	-2.94	1.45	1.51
25	8	606	CHL	C1A-C2A	-2.94	1.50	1.53
25	R	607	CHL	C1A-CHA	-2.94	1.49	1.53
25	g	601	CHL	CHD-C4C	-2.93	1.47	1.53
25	R	614	CHL	C1A-C2A	-2.93	1.50	1.53
25	4	608	CHL	C3B-CAB	-2.93	1.47	1.50
25	4	608	CHL	CBD-CAD	-2.93	1.48	1.53
25	r	607	CHL	C1A-CHA	-2.93	1.49	1.53
26	S	610	CLA	CMB-C2B	-2.93	1.45	1.51
25	n	609	CHL	C2A-C3A	-2.93	1.49	1.55
25	N	609	CHL	C2A-C3A	-2.93	1.49	1.55
25	8	601	CHL	CHC-C1C	-2.93	1.47	1.53
25	y	607	CHL	C2B-C1B	-2.93	1.47	1.53
26	Y	612	CLA	C3B-C2B	-2.92	1.36	1.40
25	8	606	CHL	CHD-C4C	-2.92	1.47	1.53
26	c	504	CLA	CMB-C2B	-2.92	1.45	1.51
25	4	601	CHL	CHC-C1C	-2.92	1.47	1.53
25	4	606	CHL	CHD-C4C	-2.92	1.47	1.53
25	G	601	CHL	CHD-C4C	-2.91	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	614	CLA	CMD-C2D	-2.91	1.45	1.51
26	Y	614	CLA	CMD-C2D	-2.91	1.45	1.51
26	n	603	CLA	CMB-C2B	-2.91	1.45	1.51
26	b	604	CLA	C3B-C2B	-2.91	1.36	1.40
29	n	1623	NEX	C7-C8	-2.91	1.27	1.32
26	8	604	CLA	CMB-C2B	-2.91	1.45	1.51
26	4	604	CLA	CMB-C2B	-2.91	1.45	1.51
26	C	507	CLA	CMB-C2B	-2.91	1.45	1.51
25	8	608	CHL	C3B-CAB	-2.91	1.47	1.50
26	c	511	CLA	CMD-C2D	-2.90	1.45	1.51
26	C	511	CLA	CMD-C2D	-2.90	1.45	1.51
26	5	610	CLA	CMB-C2B	-2.90	1.45	1.51
26	1	610	CLA	CMB-C2B	-2.90	1.45	1.51
26	y	612	CLA	C3B-C2B	-2.90	1.36	1.40
26	3	610	CLA	CMB-C2B	-2.90	1.45	1.51
26	7	610	CLA	CMB-C2B	-2.90	1.45	1.51
25	r	614	CHL	C1A-C2A	-2.90	1.50	1.53
26	c	501	CLA	CMD-C2D	-2.90	1.45	1.51
26	y	611	CLA	C3B-C2B	-2.90	1.36	1.40
26	B	615	CLA	CMB-C2B	-2.90	1.45	1.51
25	8	608	CHL	CBD-CAD	-2.89	1.48	1.53
26	3	604	CLA	CMB-C2B	-2.89	1.45	1.51
26	Y	611	CLA	C3B-C2B	-2.89	1.36	1.40
25	R	606	CHL	CBD-CAD	-2.89	1.48	1.53
26	b	615	CLA	CMB-C2B	-2.89	1.45	1.51
26	c	505	CLA	CMB-C2B	-2.89	1.45	1.51
26	C	505	CLA	CMB-C2B	-2.89	1.45	1.51
29	N	1623	NEX	C7-C8	-2.89	1.27	1.32
26	C	501	CLA	CMD-C2D	-2.89	1.45	1.51
25	7	608	CHL	C3D-CAD	-2.89	1.46	1.51
25	3	608	CHL	C3D-CAD	-2.89	1.46	1.51
26	N	603	CLA	CMB-C2B	-2.89	1.45	1.51
39	c	520	DGD	O2G-C2G	-2.89	1.39	1.46
26	7	604	CLA	CMB-C2B	-2.89	1.45	1.51
25	5	608	CHL	C1A-CHA	-2.89	1.49	1.53
25	y	605	CHL	C1A-CHA	-2.89	1.49	1.53
26	n	604	CLA	C3B-C2B	-2.88	1.36	1.40
26	b	614	CLA	CMD-C2D	-2.88	1.45	1.51
26	A	405	CLA	CMB-C2B	-2.88	1.45	1.51
26	s	602	CLA	CMD-C2D	-2.88	1.45	1.51
26	7	611	CLA	CMD-C2D	-2.88	1.45	1.51
26	3	611	CLA	CMD-C2D	-2.88	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	405	CLA	CMB-C2B	-2.88	1.45	1.51
26	A	410	CLA	CMB-C2B	-2.88	1.45	1.51
25	1	605	CHL	C1A-C2A	-2.88	1.50	1.53
25	n	607	CHL	C2B-C1B	-2.87	1.47	1.53
26	3	610	CLA	C3B-C2B	-2.87	1.36	1.40
26	7	610	CLA	C3B-C2B	-2.87	1.36	1.40
26	A	410	CLA	CMD-C2D	-2.87	1.45	1.51
26	Y	603	CLA	CMD-C2D	-2.87	1.45	1.51
26	b	608	CLA	C3B-C2B	-2.87	1.36	1.40
25	r	614	CHL	C1A-CHA	-2.87	1.49	1.53
25	R	614	CHL	C1A-CHA	-2.87	1.49	1.53
26	B	614	CLA	CMD-C2D	-2.87	1.45	1.51
26	a	410	CLA	CMB-C2B	-2.87	1.45	1.51
26	S	602	CLA	CMD-C2D	-2.86	1.45	1.51
25	N	607	CHL	C2B-C1B	-2.86	1.47	1.53
39	C	520	DGD	O2G-C2G	-2.86	1.39	1.46
26	r	604	CLA	CMB-C2B	-2.86	1.45	1.51
26	R	604	CLA	CMB-C2B	-2.86	1.45	1.51
26	G	611	CLA	CMD-C2D	-2.86	1.45	1.51
26	y	603	CLA	CMD-C2D	-2.86	1.45	1.51
26	6	613	CLA	CMD-C2D	-2.86	1.45	1.51
26	2	613	CLA	CMD-C2D	-2.86	1.45	1.51
25	1	606	CHL	C1A-C2A	-2.86	1.50	1.53
26	3	612	CLA	CMD-C2D	-2.85	1.45	1.51
26	7	612	CLA	CMD-C2D	-2.85	1.45	1.51
25	3	609	CHL	C1A-C2A	-2.85	1.50	1.53
25	7	609	CHL	C1A-C2A	-2.85	1.50	1.53
26	S	603	CLA	CMD-C2D	-2.85	1.45	1.51
25	7	601	CHL	CBD-CAD	-2.85	1.48	1.53
25	3	601	CHL	CBD-CAD	-2.85	1.48	1.53
26	a	410	CLA	CMD-C2D	-2.85	1.45	1.51
26	b	616	CLA	CMB-C2B	-2.85	1.45	1.51
26	R	610	CLA	CMB-C2B	-2.85	1.45	1.51
26	r	610	CLA	CMB-C2B	-2.85	1.45	1.51
26	B	616	CLA	CMB-C2B	-2.85	1.45	1.51
26	Y	610	CLA	CMB-C2B	-2.85	1.45	1.51
26	y	610	CLA	CMB-C2B	-2.85	1.45	1.51
25	5	606	CHL	C1A-C2A	-2.85	1.50	1.53
26	s	603	CLA	CMD-C2D	-2.85	1.45	1.51
26	B	602	CLA	CMB-C2B	-2.85	1.45	1.51
26	N	602	CLA	CMD-C2D	-2.85	1.45	1.51
26	1	610	CLA	C3B-CAB	-2.85	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	608	CHL	C1A-CHA	-2.84	1.49	1.53
26	7	612	CLA	C3B-C2B	-2.84	1.36	1.40
26	B	608	CLA	C3B-C2B	-2.84	1.36	1.40
26	N	604	CLA	C3B-C2B	-2.84	1.36	1.40
25	2	609	CHL	C1A-CHA	-2.84	1.49	1.53
26	b	602	CLA	CMB-C2B	-2.83	1.45	1.51
25	5	607	CHL	C1A-CHA	-2.83	1.49	1.53
25	1	607	CHL	C1A-CHA	-2.83	1.49	1.53
26	g	611	CLA	CMD-C2D	-2.83	1.45	1.51
26	B	602	CLA	C3B-C2B	-2.83	1.36	1.40
26	b	602	CLA	C3B-C2B	-2.83	1.36	1.40
26	n	602	CLA	CMD-C2D	-2.83	1.45	1.51
25	1	606	CHL	C2B-C1B	-2.83	1.47	1.53
25	S	601	CHL	CHD-C4C	-2.83	1.48	1.53
25	s	601	CHL	CHD-C4C	-2.83	1.48	1.53
39	h	102	DGD	O5D-C6D	-2.83	1.38	1.43
39	H	102	DGD	O5D-C6D	-2.83	1.38	1.43
26	B	610	CLA	CMD-C2D	-2.83	1.45	1.51
25	Y	605	CHL	C1A-CHA	-2.83	1.49	1.53
26	6	603	CLA	CMB-C2B	-2.83	1.45	1.51
26	5	610	CLA	C3B-CAB	-2.83	1.42	1.47
25	6	609	CHL	C1A-CHA	-2.83	1.49	1.53
25	6	605	CHL	C1A-CHA	-2.82	1.49	1.53
26	R	613	CLA	CMB-C2B	-2.82	1.45	1.51
26	r	613	CLA	CMB-C2B	-2.82	1.45	1.51
25	r	606	CHL	CBD-CAD	-2.82	1.48	1.53
25	7	609	CHL	C2B-C1B	-2.82	1.47	1.53
26	b	603	CLA	CMD-C2D	-2.82	1.45	1.51
26	B	603	CLA	CMD-C2D	-2.82	1.45	1.51
25	5	606	CHL	C2B-C1B	-2.82	1.47	1.53
26	g	603	CLA	CMD-C2D	-2.82	1.45	1.51
25	R	607	CHL	C1A-C2A	-2.82	1.50	1.53
26	2	603	CLA	CMB-C2B	-2.82	1.45	1.51
26	B	610	CLA	CMB-C2B	-2.82	1.45	1.51
26	c	503	CLA	CMD-C2D	-2.82	1.45	1.51
25	5	605	CHL	C1A-C2A	-2.82	1.50	1.53
26	r	613	CLA	CMD-C2D	-2.82	1.45	1.51
26	a	407	CLA	CMB-C2B	-2.82	1.45	1.51
26	C	503	CLA	CMD-C2D	-2.82	1.45	1.51
26	G	603	CLA	CMD-C2D	-2.81	1.45	1.51
25	8	609	CHL	CHD-C4C	-2.81	1.48	1.53
25	5	607	CHL	C1A-C2A	-2.81	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	607	CHL	C1A-C2A	-2.81	1.50	1.53
26	B	609	CLA	CMB-C2B	-2.81	1.45	1.51
25	r	607	CHL	C1A-C2A	-2.81	1.50	1.53
25	3	609	CHL	C2B-C1B	-2.81	1.47	1.53
26	5	613	CLA	CMD-C2D	-2.81	1.45	1.51
25	G	608	CHL	C3D-CAD	-2.80	1.46	1.51
25	3	606	CHL	C2B-C1B	-2.80	1.47	1.53
25	2	605	CHL	C1A-CHA	-2.80	1.49	1.53
25	r	607	CHL	C2B-C1B	-2.80	1.47	1.53
26	3	612	CLA	C3B-C2B	-2.79	1.36	1.40
26	2	602	CLA	CMD-C2D	-2.79	1.45	1.51
26	6	602	CLA	CMD-C2D	-2.79	1.45	1.51
25	7	601	CHL	CHD-C4C	-2.79	1.48	1.53
25	3	601	CHL	CHD-C4C	-2.79	1.48	1.53
25	S	601	CHL	C3B-CAB	-2.79	1.47	1.50
26	b	610	CLA	CMD-C2D	-2.79	1.45	1.51
26	N	604	CLA	CMD-C2D	-2.79	1.45	1.51
25	s	601	CHL	C3B-CAB	-2.79	1.47	1.50
25	4	609	CHL	CHD-C4C	-2.79	1.48	1.53
26	A	407	CLA	CMB-C2B	-2.79	1.46	1.51
26	b	610	CLA	CMB-C2B	-2.78	1.46	1.51
26	B	611	CLA	CMB-C2B	-2.78	1.46	1.51
26	y	611	CLA	CMB-C2B	-2.78	1.46	1.51
26	2	603	CLA	CMD-C2D	-2.78	1.45	1.51
39	h	102	DGD	O3G-C3G	-2.78	1.38	1.43
39	H	102	DGD	O3G-C3G	-2.78	1.38	1.43
26	c	507	CLA	CMC-C2C	-2.78	1.44	1.50
30	c	522	LHG	O7-C5	-2.78	1.39	1.46
30	C	522	LHG	O7-C5	-2.78	1.39	1.46
26	3	613	CLA	C3B-C2B	-2.78	1.36	1.40
26	7	613	CLA	C3B-C2B	-2.78	1.36	1.40
26	R	613	CLA	CMD-C2D	-2.77	1.45	1.51
26	B	602	CLA	CMD-C2D	-2.77	1.45	1.51
26	y	602	CLA	CMD-C2D	-2.77	1.45	1.51
26	Y	602	CLA	CMD-C2D	-2.77	1.45	1.51
26	1	613	CLA	CMD-C2D	-2.77	1.45	1.51
26	C	503	CLA	CMB-C2B	-2.77	1.46	1.51
26	c	503	CLA	CMB-C2B	-2.77	1.46	1.51
26	b	609	CLA	CMB-C2B	-2.77	1.46	1.51
26	s	602	CLA	CMB-C2B	-2.77	1.46	1.51
26	n	604	CLA	CMD-C2D	-2.77	1.45	1.51
37	D	411	LMG	O1-C7	-2.77	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	d	411	LMG	O1-C7	-2.77	1.38	1.43
25	g	608	CHL	C3D-CAD	-2.77	1.46	1.51
26	g	613	CLA	CMD-C2D	-2.77	1.45	1.51
26	G	613	CLA	CMD-C2D	-2.77	1.45	1.51
25	Y	601	CHL	C3D-CAD	-2.76	1.46	1.51
25	y	601	CHL	C3D-CAD	-2.76	1.46	1.51
26	b	611	CLA	CMB-C2B	-2.76	1.46	1.51
25	R	607	CHL	C2B-C1B	-2.76	1.47	1.53
26	3	614	CLA	CMD-C2D	-2.76	1.45	1.51
39	C	518	DGD	O3E-C3E	-2.76	1.36	1.43
26	G	604	CLA	CMD-C2D	-2.76	1.45	1.51
26	C	507	CLA	CMC-C2C	-2.76	1.44	1.50
26	b	607	CLA	CMB-C2B	-2.76	1.46	1.51
26	Y	611	CLA	CMB-C2B	-2.76	1.46	1.51
26	B	607	CLA	CMB-C2B	-2.76	1.46	1.51
39	c	518	DGD	O2G-C2G	-2.76	1.39	1.46
26	3	612	CLA	CMB-C2B	-2.76	1.46	1.51
25	7	606	CHL	C2B-C1B	-2.76	1.47	1.53
25	Y	606	CHL	CBD-CAD	-2.75	1.48	1.53
25	y	606	CHL	CBD-CAD	-2.75	1.48	1.53
26	S	602	CLA	CMB-C2B	-2.75	1.46	1.51
39	c	518	DGD	O3E-C3E	-2.75	1.36	1.43
27	N	1621	LUT	C22-C21	-2.75	1.51	1.54
25	4	609	CHL	C1A-C2A	-2.75	1.50	1.53
25	8	609	CHL	C1A-C2A	-2.75	1.50	1.53
26	7	612	CLA	CMB-C2B	-2.75	1.46	1.51
26	3	603	CLA	C3B-C2B	-2.75	1.36	1.40
25	G	606	CHL	C2B-C1B	-2.75	1.47	1.53
26	b	602	CLA	CMD-C2D	-2.75	1.45	1.51
26	b	616	CLA	CMD-C2D	-2.74	1.45	1.51
25	3	609	CHL	CHD-C4C	-2.74	1.48	1.53
25	7	609	CHL	CHD-C4C	-2.74	1.48	1.53
26	r	603	CLA	CMB-C2B	-2.74	1.46	1.51
26	6	603	CLA	CMD-C2D	-2.74	1.45	1.51
26	B	616	CLA	CMD-C2D	-2.74	1.45	1.51
25	5	608	CHL	C3D-CAD	-2.74	1.46	1.51
25	1	608	CHL	C3D-CAD	-2.74	1.46	1.51
26	b	605	CLA	CMA-C3A	-2.73	1.47	1.53
26	7	603	CLA	C3B-C2B	-2.73	1.36	1.40
25	g	606	CHL	C2B-C1B	-2.73	1.47	1.53
26	a	406	CLA	CMB-C2B	-2.73	1.46	1.51
25	y	607	CHL	C3D-CAD	-2.73	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	504	CLA	CMD-C2D	-2.73	1.45	1.51
25	8	607	CHL	CHD-C4C	-2.73	1.48	1.53
25	g	605	CHL	CHC-C1C	-2.73	1.48	1.53
26	3	614	CLA	C3B-C2B	-2.73	1.36	1.40
26	R	603	CLA	CMB-C2B	-2.73	1.46	1.51
26	7	614	CLA	CMD-C2D	-2.73	1.45	1.51
39	C	518	DGD	O2G-C2G	-2.73	1.39	1.46
26	s	612	CLA	CMD-C2D	-2.73	1.45	1.51
26	S	612	CLA	CMD-C2D	-2.73	1.45	1.51
26	g	604	CLA	CMD-C2D	-2.73	1.45	1.51
26	y	602	CLA	CMB-C2B	-2.72	1.46	1.51
26	Y	602	CLA	CMB-C2B	-2.72	1.46	1.51
26	4	603	CLA	CMB-C2B	-2.72	1.46	1.51
25	y	606	CHL	C1A-C2A	-2.72	1.50	1.53
26	7	613	CLA	CMB-C2B	-2.72	1.46	1.51
26	B	605	CLA	CMA-C3A	-2.72	1.47	1.53
26	R	603	CLA	CMD-C2D	-2.72	1.45	1.51
26	5	604	CLA	CMD-C2D	-2.72	1.45	1.51
26	7	614	CLA	C3B-C2B	-2.72	1.36	1.40
25	Y	607	CHL	C3D-CAD	-2.72	1.46	1.51
25	G	605	CHL	CHC-C1C	-2.72	1.48	1.53
30	S	2630	LHG	O7-C5	-2.72	1.39	1.46
30	s	2630	LHG	O7-C5	-2.72	1.39	1.46
25	3	606	CHL	C1A-C2A	-2.72	1.50	1.53
25	5	609	CHL	CBD-CAD	-2.72	1.49	1.53
26	C	504	CLA	CMD-C2D	-2.71	1.45	1.51
26	A	406	CLA	CMB-C2B	-2.71	1.46	1.51
26	G	602	CLA	CMB-C2B	-2.71	1.46	1.51
25	6	601	CHL	CHD-C4C	-2.71	1.48	1.53
26	r	603	CLA	CMD-C2D	-2.71	1.45	1.51
25	5	606	CHL	CBD-CAD	-2.71	1.49	1.53
26	3	613	CLA	CMB-C2B	-2.71	1.46	1.51
26	b	608	CLA	CMC-C2C	-2.71	1.44	1.50
26	b	611	CLA	CMD-C2D	-2.71	1.45	1.51
25	G	607	CHL	C2A-C3A	-2.71	1.49	1.55
25	g	607	CHL	C2A-C3A	-2.71	1.49	1.55
25	1	606	CHL	CBD-CAD	-2.71	1.49	1.53
25	7	607	CHL	CHD-C4C	-2.71	1.48	1.53
25	7	601	CHL	C2B-C1B	-2.71	1.47	1.53
25	3	601	CHL	C2B-C1B	-2.71	1.47	1.53
26	B	608	CLA	CMC-C2C	-2.71	1.44	1.50
27	g	1621	LUT	C22-C21	-2.71	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	602	CLA	CMB-C2B	-2.71	1.46	1.51
25	r	606	CHL	C2B-C1B	-2.71	1.47	1.53
25	7	606	CHL	C1A-C2A	-2.71	1.50	1.53
25	g	601	CHL	C3D-CAD	-2.71	1.46	1.51
26	1	604	CLA	CMD-C2D	-2.71	1.45	1.51
26	B	611	CLA	CMD-C2D	-2.71	1.45	1.51
26	6	610	CLA	CMB-C2B	-2.70	1.46	1.51
26	2	610	CLA	CMB-C2B	-2.70	1.46	1.51
25	2	601	CHL	CHD-C4C	-2.70	1.48	1.53
25	Y	607	CHL	CBD-CAD	-2.70	1.49	1.53
26	Y	614	CLA	CMB-C2B	-2.70	1.46	1.51
25	4	607	CHL	CHD-C4C	-2.70	1.48	1.53
25	Y	606	CHL	C1A-C2A	-2.70	1.50	1.53
26	g	604	CLA	C3B-C2B	-2.70	1.36	1.40
25	3	607	CHL	CHD-C4C	-2.70	1.48	1.53
26	5	602	CLA	C3B-C2B	-2.69	1.36	1.40
26	g	610	CLA	CMB-C2B	-2.69	1.46	1.51
26	c	502	CLA	CMD-C2D	-2.69	1.45	1.51
35	a	409	PHO	CMD-C2D	-2.69	1.44	1.50
35	A	409	PHO	CMD-C2D	-2.69	1.44	1.50
26	G	604	CLA	C3B-C2B	-2.69	1.36	1.40
25	y	607	CHL	CBD-CAD	-2.69	1.49	1.53
25	2	606	CHL	C1A-C2A	-2.69	1.50	1.53
26	g	602	CLA	CMC-C2C	-2.69	1.45	1.50
26	G	602	CLA	CMC-C2C	-2.69	1.45	1.50
26	D	402	CLA	CMC-C2C	-2.68	1.45	1.50
26	d	402	CLA	CMC-C2C	-2.68	1.45	1.50
26	8	603	CLA	CMB-C2B	-2.68	1.46	1.51
26	Y	604	CLA	CMD-C2D	-2.68	1.45	1.51
26	y	604	CLA	CMD-C2D	-2.68	1.45	1.51
25	G	601	CHL	C3D-CAD	-2.68	1.46	1.51
26	S	604	CLA	CMD-C2D	-2.68	1.45	1.51
26	C	502	CLA	CMD-C2D	-2.68	1.45	1.51
26	R	610	CLA	CMD-C2D	-2.68	1.45	1.51
26	r	610	CLA	CMD-C2D	-2.68	1.45	1.51
27	n	1621	LUT	C22-C21	-2.68	1.51	1.54
26	8	610	CLA	CMB-C2B	-2.68	1.46	1.51
26	y	614	CLA	CMB-C2B	-2.68	1.46	1.51
25	4	608	CHL	C1A-C2A	-2.68	1.50	1.53
25	8	608	CHL	C1A-C2A	-2.68	1.50	1.53
25	R	606	CHL	C2B-C1B	-2.68	1.47	1.53
25	y	607	CHL	C2A-C3A	-2.68	1.49	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	605	CHL	C1A-C2A	-2.68	1.50	1.53
26	4	610	CLA	CMB-C2B	-2.68	1.46	1.51
26	C	508	CLA	CMC-C2C	-2.67	1.45	1.50
26	s	614	CLA	CMD-C2D	-2.67	1.45	1.51
25	1	609	CHL	CBD-CAD	-2.67	1.49	1.53
27	G	1621	LUT	C22-C21	-2.67	1.51	1.54
26	c	508	CLA	CMC-C2C	-2.67	1.45	1.50
25	y	609	CHL	C2A-C3A	-2.67	1.49	1.55
25	Y	609	CHL	C2A-C3A	-2.67	1.49	1.55
26	g	602	CLA	CMD-C2D	-2.67	1.45	1.51
26	G	602	CLA	CMD-C2D	-2.67	1.45	1.51
26	s	604	CLA	CMD-C2D	-2.67	1.45	1.51
26	3	602	CLA	CMB-C2B	-2.67	1.46	1.51
26	7	602	CLA	CMB-C2B	-2.67	1.46	1.51
26	S	614	CLA	CMD-C2D	-2.67	1.45	1.51
26	3	614	CLA	CMB-C2B	-2.67	1.46	1.51
26	7	614	CLA	CMB-C2B	-2.67	1.46	1.51
26	4	610	CLA	CMD-C2D	-2.67	1.45	1.51
25	5	608	CHL	C2A-C3A	-2.66	1.49	1.55
25	1	608	CHL	C2A-C3A	-2.66	1.49	1.55
25	1	607	CHL	C2A-C3A	-2.66	1.49	1.55
26	8	610	CLA	CMD-C2D	-2.66	1.45	1.51
25	G	601	CHL	C2B-C1B	-2.66	1.48	1.53
25	g	601	CHL	C2B-C1B	-2.66	1.48	1.53
26	N	610	CLA	CMB-C2B	-2.66	1.46	1.51
26	Y	613	CLA	CMB-C2B	-2.66	1.46	1.51
26	y	613	CLA	CMB-C2B	-2.66	1.46	1.51
26	n	610	CLA	CMB-C2B	-2.66	1.46	1.51
26	g	611	CLA	C3B-C2B	-2.66	1.36	1.40
25	Y	607	CHL	C2A-C3A	-2.66	1.49	1.55
25	5	607	CHL	C2A-C3A	-2.66	1.49	1.55
26	A	406	CLA	CMD-C2D	-2.66	1.45	1.51
26	a	406	CLA	CMD-C2D	-2.66	1.45	1.51
25	R	606	CHL	C2A-C3A	-2.66	1.49	1.55
25	r	606	CHL	C2A-C3A	-2.66	1.49	1.55
26	1	602	CLA	C3B-C2B	-2.66	1.36	1.40
26	3	603	CLA	CMB-C2B	-2.66	1.46	1.51
26	7	603	CLA	CMB-C2B	-2.66	1.46	1.51
25	2	609	CHL	CBD-CAD	-2.66	1.49	1.53
26	S	613	CLA	CMB-C2B	-2.66	1.46	1.51
26	s	613	CLA	CMB-C2B	-2.66	1.46	1.51
26	4	610	CLA	C3B-C2B	-2.66	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	606	CHL	C1A-C2A	-2.66	1.50	1.53
26	r	604	CLA	CMD-C2D	-2.66	1.45	1.51
26	R	604	CLA	CMD-C2D	-2.66	1.45	1.51
26	y	612	CLA	CMB-C2B	-2.66	1.46	1.51
26	Y	612	CLA	CMB-C2B	-2.66	1.46	1.51
25	N	608	CHL	C2B-C1B	-2.65	1.48	1.53
25	n	608	CHL	C2B-C1B	-2.65	1.48	1.53
26	c	511	CLA	CMB-C2B	-2.65	1.46	1.51
26	5	613	CLA	CMB-C2B	-2.65	1.46	1.51
26	G	610	CLA	CMB-C2B	-2.65	1.46	1.51
26	7	602	CLA	C3B-C2B	-2.65	1.36	1.40
27	Y	1621	LUT	C22-C21	-2.65	1.51	1.54
26	2	602	CLA	CMB-C2B	-2.65	1.46	1.51
26	N	613	CLA	CMD-C2D	-2.65	1.45	1.51
26	n	613	CLA	CMD-C2D	-2.65	1.45	1.51
25	G	607	CHL	CHC-C1C	-2.65	1.48	1.53
26	C	511	CLA	CMB-C2B	-2.65	1.46	1.51
26	C	501	CLA	CMB-C2B	-2.65	1.46	1.51
25	N	605	CHL	C1A-C2A	-2.65	1.50	1.53
26	8	604	CLA	C3B-C2B	-2.65	1.36	1.40
39	h	102	DGD	O4D-C4D	-2.64	1.36	1.43
39	H	102	DGD	O4D-C4D	-2.64	1.36	1.43
25	5	607	CHL	CBD-CAD	-2.64	1.49	1.53
25	1	607	CHL	CBD-CAD	-2.64	1.49	1.53
25	Y	601	CHL	C2B-C1B	-2.64	1.48	1.53
26	3	603	CLA	CMD-C2D	-2.64	1.46	1.51
26	n	614	CLA	CMD-C2D	-2.64	1.46	1.51
30	Y	2630	LHG	O7-C5	-2.64	1.39	1.46
30	y	2630	LHG	O7-C5	-2.64	1.39	1.46
25	Y	606	CHL	C2D-C1D	-2.64	1.48	1.53
25	y	606	CHL	C2D-C1D	-2.64	1.48	1.53
27	y	1621	LUT	C22-C21	-2.64	1.51	1.54
26	7	603	CLA	CMD-C2D	-2.63	1.46	1.51
26	5	603	CLA	CMB-C2B	-2.63	1.46	1.51
26	1	603	CLA	CMB-C2B	-2.63	1.46	1.51
26	6	602	CLA	CMB-C2B	-2.63	1.46	1.51
29	g	1623	NEX	O4-C5	-2.63	1.38	1.43
29	G	1623	NEX	O4-C5	-2.63	1.38	1.43
25	y	601	CHL	C2B-C1B	-2.63	1.48	1.53
26	5	612	CLA	CMD-C2D	-2.63	1.46	1.51
26	1	612	CLA	CMD-C2D	-2.63	1.46	1.51
26	6	604	CLA	CMD-C2D	-2.63	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	602	CLA	C3B-C2B	-2.63	1.36	1.40
26	5	612	CLA	CMB-C2B	-2.63	1.46	1.51
26	1	612	CLA	CMB-C2B	-2.63	1.46	1.51
26	c	507	CLA	CMD-C2D	-2.63	1.46	1.51
25	8	601	CHL	CHD-C4C	-2.63	1.48	1.53
25	6	608	CHL	C1A-C2A	-2.63	1.50	1.53
26	8	610	CLA	C3B-C2B	-2.63	1.36	1.40
26	G	611	CLA	C3B-C2B	-2.63	1.36	1.40
25	G	606	CHL	C3B-CAB	-2.63	1.48	1.50
25	g	606	CHL	C3B-CAB	-2.63	1.48	1.50
26	1	602	CLA	CMD-C2D	-2.63	1.46	1.51
26	2	604	CLA	CMD-C2D	-2.63	1.46	1.51
26	5	602	CLA	CMD-C2D	-2.63	1.46	1.51
25	n	608	CHL	CBD-CAD	-2.62	1.49	1.53
25	g	607	CHL	CHC-C1C	-2.62	1.48	1.53
26	d	403	CLA	CMB-C2B	-2.62	1.46	1.51
26	7	610	CLA	CMD-C2D	-2.62	1.46	1.51
25	6	609	CHL	CBD-CAD	-2.62	1.49	1.53
26	S	613	CLA	CMD-C2D	-2.62	1.46	1.51
25	1	606	CHL	C2A-C3A	-2.62	1.49	1.55
26	b	617	CLA	CMD-C2D	-2.62	1.46	1.51
25	N	608	CHL	C3D-CAD	-2.62	1.46	1.51
25	n	608	CHL	C3D-CAD	-2.62	1.46	1.51
26	1	613	CLA	CMB-C2B	-2.62	1.46	1.51
25	7	606	CHL	C2A-C3A	-2.62	1.49	1.55
25	N	605	CHL	C1A-CHA	-2.62	1.49	1.53
25	n	605	CHL	C1A-CHA	-2.62	1.49	1.53
39	h	102	DGD	O1G-C1G	-2.62	1.39	1.45
26	G	614	CLA	CMD-C2D	-2.61	1.46	1.51
26	2	614	CLA	CMD-C2D	-2.61	1.46	1.51
25	S	606	CHL	C1A-C2A	-2.61	1.50	1.53
25	s	606	CHL	C1A-C2A	-2.61	1.50	1.53
26	n	602	CLA	CMB-C2B	-2.61	1.46	1.51
26	N	602	CLA	CMB-C2B	-2.61	1.46	1.51
26	g	614	CLA	CMD-C2D	-2.61	1.46	1.51
25	G	607	CHL	CBD-CAD	-2.61	1.49	1.53
25	2	601	CHL	C2A-C3A	-2.61	1.49	1.55
26	D	403	CLA	CMD-C2D	-2.61	1.46	1.51
25	s	601	CHL	CBD-CAD	-2.61	1.49	1.53
26	y	602	CLA	CMC-C2C	-2.61	1.45	1.50
26	Y	602	CLA	CMC-C2C	-2.61	1.45	1.50
26	R	616	CLA	CMD-C2D	-2.61	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	616	CLA	CMD-C2D	-2.61	1.46	1.51
26	N	614	CLA	CMD-C2D	-2.61	1.46	1.51
25	4	601	CHL	CHD-C4C	-2.61	1.48	1.53
29	S	1623	NEX	C7-C8	-2.61	1.27	1.32
29	s	1623	NEX	C7-C8	-2.61	1.27	1.32
25	8	608	CHL	C3D-CAD	-2.61	1.46	1.51
26	s	613	CLA	CMD-C2D	-2.61	1.46	1.51
25	6	606	CHL	C2B-C1B	-2.61	1.48	1.53
25	7	608	CHL	CBD-CAD	-2.61	1.49	1.53
26	B	612	CLA	CMD-C2D	-2.61	1.46	1.51
26	b	612	CLA	CMD-C2D	-2.61	1.46	1.51
26	6	613	CLA	CMB-C2B	-2.61	1.46	1.51
26	2	613	CLA	CMB-C2B	-2.61	1.46	1.51
26	3	613	CLA	CMD-C2D	-2.60	1.46	1.51
26	7	613	CLA	CMD-C2D	-2.60	1.46	1.51
26	c	501	CLA	CMB-C2B	-2.60	1.46	1.51
25	y	608	CHL	C3D-CAD	-2.60	1.46	1.51
25	Y	608	CHL	C3D-CAD	-2.60	1.46	1.51
26	5	611	CLA	CMB-C2B	-2.60	1.46	1.51
26	1	611	CLA	CMB-C2B	-2.60	1.46	1.51
25	Y	601	CHL	CHD-C4C	-2.60	1.48	1.53
25	y	601	CHL	CHD-C4C	-2.60	1.48	1.53
26	5	614	CLA	CMB-C2B	-2.60	1.46	1.51
26	1	614	CLA	CMB-C2B	-2.60	1.46	1.51
25	N	608	CHL	CBD-CAD	-2.60	1.49	1.53
26	5	603	CLA	CMD-C2D	-2.60	1.46	1.51
25	3	606	CHL	CBD-CAD	-2.60	1.49	1.53
26	B	617	CLA	CMD-C2D	-2.60	1.46	1.51
25	6	601	CHL	C2A-C3A	-2.60	1.49	1.55
25	7	606	CHL	CBD-CAD	-2.60	1.49	1.53
25	g	607	CHL	CBD-CAD	-2.60	1.49	1.53
26	5	614	CLA	CMD-C2D	-2.60	1.46	1.51
26	C	507	CLA	CMD-C2D	-2.59	1.46	1.51
25	2	608	CHL	C1A-C2A	-2.59	1.50	1.53
25	8	607	CHL	C1A-C2A	-2.59	1.50	1.53
26	D	403	CLA	CMB-C2B	-2.59	1.46	1.51
26	A	407	CLA	CMD-C2D	-2.59	1.46	1.51
26	R	611	CLA	C3B-C2B	-2.59	1.36	1.40
26	r	611	CLA	C3B-C2B	-2.59	1.36	1.40
26	3	610	CLA	CMD-C2D	-2.59	1.46	1.51
25	3	606	CHL	C2A-C3A	-2.59	1.49	1.55
26	N	611	CLA	CMB-C2B	-2.59	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	611	CLA	CMB-C2B	-2.59	1.46	1.51
25	7	601	CHL	C2A-C3A	-2.59	1.49	1.55
25	3	601	CHL	C2A-C3A	-2.59	1.49	1.55
26	R	602	CLA	CMB-C2B	-2.59	1.46	1.51
26	r	602	CLA	CMB-C2B	-2.59	1.46	1.51
26	6	614	CLA	CMD-C2D	-2.59	1.46	1.51
26	6	614	CLA	CMB-C2B	-2.59	1.46	1.51
25	7	605	CHL	C1A-CHA	-2.59	1.49	1.53
26	s	611	CLA	CMB-C2B	-2.59	1.46	1.51
26	S	611	CLA	CMB-C2B	-2.59	1.46	1.51
25	3	601	CHL	C3D-CAD	-2.59	1.46	1.51
25	6	608	CHL	C2A-C3A	-2.59	1.49	1.55
39	H	102	DGD	O1G-C1G	-2.59	1.39	1.45
25	7	607	CHL	C1A-CHA	-2.58	1.49	1.53
26	c	513	CLA	CMD-C2D	-2.58	1.46	1.51
25	g	608	CHL	C1A-C2A	-2.58	1.50	1.53
25	1	605	CHL	C2A-C3A	-2.58	1.49	1.55
25	5	605	CHL	C2A-C3A	-2.58	1.49	1.55
25	3	607	CHL	C1A-CHA	-2.58	1.49	1.53
25	3	608	CHL	CBD-CAD	-2.58	1.49	1.53
26	r	609	CLA	CMD-C2D	-2.58	1.46	1.51
26	B	611	CLA	CMC-C2C	-2.58	1.45	1.50
26	6	612	CLA	CMB-C2B	-2.58	1.46	1.51
25	5	606	CHL	C2A-C3A	-2.58	1.49	1.55
26	1	610	CLA	CMD-C2D	-2.58	1.46	1.51
26	6	610	CLA	C3B-C2B	-2.58	1.36	1.40
26	2	610	CLA	C3B-C2B	-2.58	1.36	1.40
26	N	611	CLA	CMD-C2D	-2.58	1.46	1.51
26	n	611	CLA	CMD-C2D	-2.58	1.46	1.51
26	5	610	CLA	CMD-C2D	-2.58	1.46	1.51
25	2	606	CHL	C2B-C1B	-2.58	1.48	1.53
26	4	604	CLA	C3B-C2B	-2.57	1.37	1.40
26	c	508	CLA	CMD-C2D	-2.57	1.46	1.51
26	1	614	CLA	CMD-C2D	-2.57	1.46	1.51
26	g	603	CLA	CMB-C2B	-2.57	1.46	1.51
26	4	612	CLA	CMB-C2B	-2.57	1.46	1.51
26	G	603	CLA	CMB-C2B	-2.57	1.46	1.51
26	d	403	CLA	CMD-C2D	-2.57	1.46	1.51
25	4	608	CHL	C3D-CAD	-2.57	1.46	1.51
26	g	613	CLA	CMB-C2B	-2.57	1.46	1.51
26	G	613	CLA	CMB-C2B	-2.57	1.46	1.51
26	a	407	CLA	CMD-C2D	-2.57	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	601	CHL	CBD-CAD	-2.57	1.49	1.53
25	G	609	CHL	C1A-CHA	-2.57	1.49	1.53
25	g	609	CHL	C1A-CHA	-2.57	1.49	1.53
26	2	612	CLA	CMB-C2B	-2.57	1.46	1.51
26	R	611	CLA	CMB-C2B	-2.57	1.46	1.51
25	3	605	CHL	C1A-CHA	-2.57	1.49	1.53
25	2	607	CHL	C3B-CAB	-2.57	1.48	1.50
25	N	601	CHL	C2B-C1B	-2.56	1.48	1.53
25	n	601	CHL	C2B-C1B	-2.56	1.48	1.53
26	C	508	CLA	CMD-C2D	-2.56	1.46	1.51
26	1	602	CLA	CMB-C2B	-2.56	1.46	1.51
26	5	602	CLA	CMB-C2B	-2.56	1.46	1.51
25	2	608	CHL	C2A-C3A	-2.56	1.50	1.55
26	S	611	CLA	CMD-C2D	-2.56	1.46	1.51
26	y	610	CLA	CMC-C2C	-2.56	1.45	1.50
26	s	611	CLA	CMD-C2D	-2.56	1.46	1.51
25	6	607	CHL	C3B-CAB	-2.56	1.48	1.50
26	1	603	CLA	CMD-C2D	-2.56	1.46	1.51
25	1	609	CHL	C2A-C3A	-2.56	1.50	1.55
26	2	614	CLA	CMB-C2B	-2.56	1.46	1.51
25	y	605	CHL	C2B-C1B	-2.56	1.48	1.53
25	Y	605	CHL	C2B-C1B	-2.56	1.48	1.53
25	2	607	CHL	CBD-CAD	-2.56	1.49	1.53
25	6	607	CHL	CBD-CAD	-2.56	1.49	1.53
26	N	612	CLA	CMD-C2D	-2.56	1.46	1.51
26	n	612	CLA	CMD-C2D	-2.56	1.46	1.51
26	c	507	CLA	C3B-C2B	-2.55	1.37	1.40
25	4	607	CHL	C1A-C2A	-2.55	1.50	1.53
26	R	612	CLA	CMD-C2D	-2.55	1.46	1.51
26	r	612	CLA	CMD-C2D	-2.55	1.46	1.51
26	Y	610	CLA	CMC-C2C	-2.55	1.45	1.50
26	b	611	CLA	CMC-C2C	-2.55	1.45	1.50
25	7	601	CHL	C3D-CAD	-2.55	1.46	1.51
26	B	607	CLA	C3B-C2B	-2.54	1.37	1.40
25	5	609	CHL	C2A-C3A	-2.54	1.50	1.55
26	3	602	CLA	CMC-C2C	-2.54	1.45	1.50
26	7	602	CLA	CMC-C2C	-2.54	1.45	1.50
27	y	1620	LUT	C30-C29	-2.54	1.32	1.35
25	4	609	CHL	C2B-C1B	-2.54	1.48	1.53
25	G	608	CHL	C1A-C2A	-2.54	1.50	1.53
26	6	612	CLA	C3B-C2B	-2.54	1.37	1.40
26	b	607	CLA	C3B-C2B	-2.54	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	609	CLA	CMD-C2D	-2.54	1.46	1.51
26	4	602	CLA	CMB-C2B	-2.54	1.46	1.51
26	N	610	CLA	CMD-C2D	-2.54	1.46	1.51
26	n	610	CLA	CMD-C2D	-2.54	1.46	1.51
26	2	604	CLA	C3B-C2B	-2.54	1.37	1.40
26	6	604	CLA	C3B-C2B	-2.54	1.37	1.40
25	N	607	CHL	C3D-CAD	-2.54	1.46	1.51
25	2	608	CHL	C3D-CAD	-2.54	1.46	1.51
26	C	513	CLA	CMD-C2D	-2.54	1.46	1.51
25	6	608	CHL	C3D-CAD	-2.54	1.46	1.51
26	8	612	CLA	CMB-C2B	-2.54	1.46	1.51
26	2	612	CLA	C3B-C2B	-2.53	1.37	1.40
26	r	611	CLA	CMB-C2B	-2.53	1.46	1.51
26	1	602	CLA	C3B-CAB	-2.53	1.42	1.47
26	6	603	CLA	C3B-C2B	-2.53	1.37	1.40
26	8	602	CLA	CMB-C2B	-2.53	1.46	1.51
26	a	410	CLA	C3B-C2B	-2.52	1.37	1.40
25	g	608	CHL	C2B-C1B	-2.52	1.48	1.53
25	8	609	CHL	C2B-C1B	-2.52	1.48	1.53
26	2	603	CLA	C3B-C2B	-2.52	1.37	1.40
26	S	609	CLA	CMB-C2B	-2.52	1.46	1.51
26	C	507	CLA	C3B-C2B	-2.52	1.37	1.40
26	8	603	CLA	CMD-C2D	-2.52	1.46	1.51
26	6	611	CLA	CMB-C2B	-2.52	1.46	1.51
26	r	609	CLA	C3B-C2B	-2.52	1.37	1.40
26	R	609	CLA	C3B-C2B	-2.52	1.37	1.40
25	G	608	CHL	C2B-C1B	-2.52	1.48	1.53
25	n	607	CHL	C3D-CAD	-2.51	1.46	1.51
26	R	602	CLA	CMD-C2D	-2.51	1.46	1.51
26	r	602	CLA	CMD-C2D	-2.51	1.46	1.51
25	y	607	CHL	C2D-C1D	-2.51	1.48	1.53
26	1	611	CLA	CMD-C2D	-2.51	1.46	1.51
26	5	611	CLA	CMD-C2D	-2.51	1.46	1.51
25	N	608	CHL	C2A-C3A	-2.51	1.50	1.55
25	n	608	CHL	C2A-C3A	-2.51	1.50	1.55
26	4	603	CLA	CMD-C2D	-2.51	1.46	1.51
26	S	603	CLA	CMB-C2B	-2.51	1.46	1.51
39	C	520	DGD	O3G-C3G	-2.50	1.39	1.43
39	c	520	DGD	O3G-C3G	-2.50	1.39	1.43
39	c	519	DGD	O5D-C6D	-2.50	1.39	1.43
39	C	519	DGD	O5D-C6D	-2.50	1.39	1.43
25	r	608	CHL	C2A-C3A	-2.50	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	611	CLA	CMB-C2B	-2.50	1.46	1.51
26	8	611	CLA	CMB-C2B	-2.50	1.46	1.51
26	R	612	CLA	CMB-C2B	-2.50	1.46	1.51
26	2	611	CLA	CMB-C2B	-2.50	1.46	1.51
26	A	410	CLA	C3B-C2B	-2.50	1.37	1.40
26	R	609	CLA	CMB-C2B	-2.50	1.46	1.51
26	c	506	CLA	CMD-C2D	-2.50	1.46	1.51
25	r	608	CHL	C1A-CHA	-2.50	1.49	1.53
25	G	609	CHL	CBD-CAD	-2.49	1.49	1.53
26	N	612	CLA	CMB-C2B	-2.49	1.46	1.51
26	n	612	CLA	CMB-C2B	-2.49	1.46	1.51
25	6	606	CHL	C2A-C3A	-2.49	1.50	1.55
26	4	602	CLA	CMD-C2D	-2.49	1.46	1.51
26	8	602	CLA	CMD-C2D	-2.49	1.46	1.51
26	3	602	CLA	CMD-C2D	-2.49	1.46	1.51
26	7	602	CLA	CMD-C2D	-2.49	1.46	1.51
26	5	602	CLA	C3B-CAB	-2.49	1.42	1.47
25	n	609	CHL	CBD-CAD	-2.49	1.49	1.53
25	N	606	CHL	CBD-CAD	-2.49	1.49	1.53
25	n	606	CHL	CBD-CAD	-2.49	1.49	1.53
26	6	612	CLA	CMD-C2D	-2.49	1.46	1.51
26	r	612	CLA	CMB-C2B	-2.49	1.46	1.51
26	s	609	CLA	CMB-C2B	-2.49	1.46	1.51
25	s	601	CHL	C2A-C3A	-2.49	1.50	1.55
26	g	612	CLA	CMB-C2B	-2.49	1.46	1.51
26	G	612	CLA	CMB-C2B	-2.49	1.46	1.51
25	g	605	CHL	C2B-C1B	-2.49	1.48	1.53
25	G	605	CHL	C2B-C1B	-2.49	1.48	1.53
25	R	608	CHL	C2A-C3A	-2.48	1.50	1.55
25	r	607	CHL	CBD-CAD	-2.48	1.49	1.53
25	R	608	CHL	C1A-CHA	-2.48	1.49	1.53
26	s	603	CLA	CMB-C2B	-2.48	1.46	1.51
26	C	506	CLA	CMD-C2D	-2.48	1.46	1.51
26	b	608	CLA	C4B-CHC	-2.48	1.33	1.40
26	2	612	CLA	CMD-C2D	-2.48	1.46	1.51
26	B	602	CLA	CMC-C2C	-2.48	1.45	1.50
26	b	602	CLA	CMC-C2C	-2.48	1.45	1.50
26	B	608	CLA	C4B-CHC	-2.48	1.33	1.40
35	a	408	PHO	CMB-C2B	-2.48	1.45	1.50
26	r	610	CLA	CMC-C2C	-2.48	1.45	1.50
25	r	614	CHL	C3B-CAB	-2.48	1.48	1.50
25	N	609	CHL	CBD-CAD	-2.48	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	609	CLA	CMB-C2B	-2.48	1.46	1.51
27	Y	1620	LUT	C30-C29	-2.47	1.32	1.35
26	R	611	CLA	CMD-C2D	-2.47	1.46	1.51
26	r	611	CLA	CMD-C2D	-2.47	1.46	1.51
27	6	1621	LUT	C22-C21	-2.47	1.51	1.54
25	G	609	CHL	C2A-C3A	-2.47	1.50	1.55
25	g	609	CHL	C2A-C3A	-2.47	1.50	1.55
25	Y	608	CHL	C2A-C3A	-2.47	1.50	1.55
25	4	608	CHL	C2A-C3A	-2.47	1.50	1.55
25	n	605	CHL	C3B-CAB	-2.47	1.48	1.50
35	A	409	PHO	CMC-C2C	-2.47	1.45	1.50
25	R	614	CHL	C3B-CAB	-2.47	1.48	1.50
26	8	604	CLA	CMD-C2D	-2.47	1.46	1.51
26	b	606	CLA	C3B-C2B	-2.46	1.37	1.40
26	B	606	CLA	C3B-C2B	-2.46	1.37	1.40
25	g	609	CHL	CBD-CAD	-2.46	1.49	1.53
25	S	601	CHL	C2A-C3A	-2.46	1.50	1.55
26	R	610	CLA	CMC-C2C	-2.46	1.45	1.50
25	Y	607	CHL	C2D-C1D	-2.46	1.48	1.53
25	R	607	CHL	CBD-CAD	-2.46	1.49	1.53
26	g	610	CLA	CMD-C2D	-2.46	1.46	1.51
26	b	611	CLA	C3B-C2B	-2.46	1.37	1.40
27	2	1621	LUT	C22-C21	-2.46	1.51	1.54
25	8	608	CHL	C2A-C3A	-2.46	1.50	1.55
26	G	613	CLA	C3B-C2B	-2.46	1.37	1.40
25	2	606	CHL	C2A-C3A	-2.46	1.50	1.55
25	N	607	CHL	CBD-CAD	-2.46	1.49	1.53
25	n	607	CHL	CBD-CAD	-2.46	1.49	1.53
25	y	607	CHL	C1A-C2A	-2.46	1.50	1.53
26	B	615	CLA	CMC-C2C	-2.46	1.45	1.50
26	6	611	CLA	CMD-C2D	-2.45	1.46	1.51
26	2	611	CLA	CMD-C2D	-2.45	1.46	1.51
35	A	408	PHO	CMB-C2B	-2.45	1.45	1.50
25	4	606	CHL	C2A-C3A	-2.45	1.50	1.55
25	3	608	CHL	C1A-C2A	-2.45	1.50	1.53
25	g	607	CHL	C1A-C2A	-2.45	1.50	1.53
26	4	612	CLA	CMD-C2D	-2.45	1.46	1.51
26	8	612	CLA	CMD-C2D	-2.45	1.46	1.51
25	y	608	CHL	C2A-C3A	-2.45	1.50	1.55
26	3	604	CLA	C3B-C2B	-2.45	1.37	1.40
25	5	601	CHL	CHD-C4C	-2.45	1.48	1.53
25	1	601	CHL	CHD-C4C	-2.45	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	601	CHL	C3D-CAD	-2.45	1.46	1.51
25	G	606	CHL	C2A-C3A	-2.45	1.50	1.55
26	N	614	CLA	CMB-C2B	-2.45	1.46	1.51
25	8	609	CHL	C3B-CAB	-2.44	1.48	1.50
35	a	409	PHO	CMC-C2C	-2.44	1.45	1.50
39	C	518	DGD	O5D-C6D	-2.44	1.39	1.43
25	n	609	CHL	CMB-C2B	-2.44	1.48	1.53
25	N	609	CHL	CMB-C2B	-2.44	1.48	1.53
26	b	617	CLA	CMB-C2B	-2.44	1.46	1.51
26	b	613	CLA	CMC-C2C	-2.44	1.45	1.50
28	y	1622	XAT	C10-C9	-2.44	1.32	1.35
28	Y	1622	XAT	C10-C9	-2.44	1.32	1.35
25	7	608	CHL	C1A-C2A	-2.44	1.50	1.53
26	4	604	CLA	CMD-C2D	-2.44	1.46	1.51
26	G	610	CLA	CMD-C2D	-2.44	1.46	1.51
39	h	102	DGD	O2G-C2G	-2.44	1.40	1.46
26	C	513	CLA	CMB-C2B	-2.43	1.46	1.51
25	N	601	CHL	C3D-CAD	-2.43	1.46	1.51
25	8	606	CHL	C2A-C3A	-2.43	1.50	1.55
26	7	604	CLA	C3B-C2B	-2.43	1.37	1.40
25	5	609	CHL	C2B-C1B	-2.43	1.48	1.53
25	1	609	CHL	C2B-C1B	-2.43	1.48	1.53
26	n	614	CLA	CMB-C2B	-2.43	1.46	1.51
26	g	612	CLA	CMD-C2D	-2.43	1.46	1.51
26	G	612	CLA	CMD-C2D	-2.43	1.46	1.51
30	1	2630	LHG	O7-C5	-2.43	1.40	1.46
39	c	518	DGD	O5D-C6D	-2.43	1.39	1.43
25	g	605	CHL	C2A-C3A	-2.43	1.50	1.55
25	g	606	CHL	C2A-C3A	-2.43	1.50	1.55
26	B	615	CLA	C3B-C2B	-2.42	1.37	1.40
26	c	513	CLA	CMB-C2B	-2.42	1.46	1.51
25	G	605	CHL	C2A-C3A	-2.42	1.50	1.55
25	G	607	CHL	C1A-C2A	-2.42	1.50	1.53
38	d	405	PL9	C11-C9	-2.42	1.46	1.51
25	6	601	CHL	C3D-CAD	-2.42	1.46	1.51
39	c	519	DGD	O2G-C2G	-2.42	1.40	1.46
25	Y	605	CHL	CBD-CAD	-2.42	1.49	1.53
30	5	2630	LHG	O7-C5	-2.42	1.40	1.46
39	C	519	DGD	O2G-C2G	-2.42	1.40	1.46
39	H	102	DGD	O2G-C2G	-2.42	1.40	1.46
26	s	610	CLA	CMD-C2D	-2.42	1.46	1.51
26	B	613	CLA	CMC-C2C	-2.42	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	601	CHL	C2A-C3A	-2.42	1.50	1.55
25	5	608	CHL	C2B-C1B	-2.42	1.48	1.53
25	1	608	CHL	C2B-C1B	-2.42	1.48	1.53
25	N	605	CHL	C3B-CAB	-2.42	1.48	1.50
26	4	611	CLA	CMD-C2D	-2.42	1.46	1.51
25	4	609	CHL	C3B-CAB	-2.42	1.48	1.50
26	N	613	CLA	CMB-C2B	-2.42	1.46	1.51
26	n	613	CLA	CMB-C2B	-2.42	1.46	1.51
25	y	609	CHL	C1A-C2A	-2.41	1.50	1.53
25	Y	609	CHL	C1A-C2A	-2.41	1.50	1.53
26	g	614	CLA	CMB-C2B	-2.41	1.46	1.51
26	b	615	CLA	CMC-C2C	-2.41	1.45	1.50
26	3	604	CLA	CMD-C2D	-2.41	1.46	1.51
26	7	604	CLA	CMD-C2D	-2.41	1.46	1.51
31	c	515	BCR	C21-C22	-2.41	1.32	1.35
26	b	615	CLA	C3B-C2B	-2.41	1.37	1.40
26	8	611	CLA	CMD-C2D	-2.41	1.46	1.51
26	B	602	CLA	C3B-CAB	-2.41	1.43	1.47
26	b	602	CLA	C3B-CAB	-2.41	1.43	1.47
25	n	601	CHL	C3D-CAD	-2.41	1.46	1.51
26	n	602	CLA	CMC-C2C	-2.40	1.45	1.50
26	N	602	CLA	CMC-C2C	-2.40	1.45	1.50
26	C	510	CLA	CMB-C2B	-2.40	1.46	1.51
26	c	510	CLA	CMB-C2B	-2.40	1.46	1.51
39	C	519	DGD	O6D-C5D	-2.40	1.38	1.44
26	D	402	CLA	C3B-C2B	-2.40	1.37	1.40
25	s	606	CHL	C2B-C1B	-2.40	1.48	1.53
25	2	606	CHL	CBD-CAD	-2.40	1.49	1.53
26	g	613	CLA	C3B-C2B	-2.40	1.37	1.40
25	6	606	CHL	CBD-CAD	-2.40	1.49	1.53
26	s	610	CLA	C3B-C2B	-2.40	1.37	1.40
26	S	610	CLA	C3B-C2B	-2.40	1.37	1.40
26	B	613	CLA	CMA-C3A	-2.40	1.47	1.53
26	B	617	CLA	CMB-C2B	-2.40	1.46	1.51
26	C	513	CLA	CMC-C2C	-2.40	1.45	1.50
26	S	610	CLA	CMD-C2D	-2.40	1.46	1.51
26	6	610	CLA	CMD-C2D	-2.40	1.46	1.51
31	b	618	BCR	C21-C22	-2.40	1.32	1.35
31	C	515	BCR	C21-C22	-2.40	1.32	1.35
25	2	608	CHL	C2B-C1B	-2.40	1.48	1.53
25	S	606	CHL	C2B-C1B	-2.40	1.48	1.53
25	3	608	CHL	C2A-C3A	-2.40	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	601	CHL	C2A-C3A	-2.40	1.50	1.55
25	8	606	CHL	C2B-C1B	-2.39	1.48	1.53
26	c	513	CLA	CMC-C2C	-2.39	1.45	1.50
26	d	402	CLA	C3B-C2B	-2.39	1.37	1.40
26	y	604	CLA	C3B-C2B	-2.39	1.37	1.40
39	c	519	DGD	O6D-C5D	-2.39	1.38	1.44
25	6	608	CHL	C2B-C1B	-2.39	1.48	1.53
25	N	607	CHL	C3B-CAB	-2.39	1.48	1.50
26	2	610	CLA	CMD-C2D	-2.39	1.46	1.51
26	B	611	CLA	C3B-C2B	-2.39	1.37	1.40
25	y	605	CHL	CBD-CAD	-2.39	1.49	1.53
25	5	605	CHL	CBD-CAD	-2.39	1.49	1.53
31	B	618	BCR	C21-C22	-2.39	1.32	1.35
29	r	623	NEX	C30-C29	-2.39	1.32	1.35
38	D	405	PL9	C11-C9	-2.39	1.46	1.51
25	N	606	CHL	C2B-C1B	-2.39	1.48	1.53
25	n	606	CHL	C2B-C1B	-2.39	1.48	1.53
39	b	626	DGD	O3G-C3G	-2.38	1.39	1.43
26	r	612	CLA	C3B-C2B	-2.38	1.37	1.40
26	R	612	CLA	C3B-C2B	-2.38	1.37	1.40
25	4	609	CHL	C2A-C3A	-2.38	1.50	1.55
25	2	601	CHL	C2B-C1B	-2.38	1.48	1.53
25	6	601	CHL	C2B-C1B	-2.38	1.48	1.53
26	b	613	CLA	CMA-C3A	-2.38	1.47	1.53
26	s	614	CLA	CMB-C2B	-2.38	1.46	1.51
26	S	614	CLA	CMB-C2B	-2.38	1.46	1.51
25	n	607	CHL	C2A-C3A	-2.38	1.50	1.55
26	2	602	CLA	CMC-C2C	-2.38	1.45	1.50
25	Y	607	CHL	C1A-C2A	-2.38	1.50	1.53
25	6	607	CHL	C1A-CHA	-2.38	1.50	1.53
26	5	603	CLA	C3B-C2B	-2.38	1.37	1.40
25	n	607	CHL	C3B-CAB	-2.38	1.48	1.50
29	R	623	NEX	C30-C29	-2.37	1.32	1.35
25	7	608	CHL	C2A-C3A	-2.37	1.50	1.55
28	y	1622	XAT	C34-C33	-2.37	1.32	1.35
26	6	602	CLA	CMC-C2C	-2.37	1.45	1.50
28	Y	1622	XAT	C34-C33	-2.37	1.32	1.35
25	8	609	CHL	C2A-C3A	-2.37	1.50	1.55
25	4	606	CHL	C2B-C1B	-2.37	1.48	1.53
26	1	602	CLA	CMC-C2C	-2.37	1.45	1.50
26	5	602	CLA	CMC-C2C	-2.37	1.45	1.50
26	G	614	CLA	CMB-C2B	-2.37	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	607	CHL	C2A-C3A	-2.37	1.50	1.55
25	1	605	CHL	CBD-CAD	-2.37	1.49	1.53
25	2	607	CHL	C1A-CHA	-2.36	1.50	1.53
26	3	610	CLA	C3B-CAB	-2.36	1.43	1.47
37	B	622	LMG	O7-C8	-2.36	1.40	1.46
25	7	607	CHL	C2B-C1B	-2.36	1.48	1.53
35	a	408	PHO	CHC-C4B	-2.36	1.34	1.40
26	s	602	CLA	CMC-C2C	-2.36	1.45	1.50
25	R	607	CHL	C2A-C3A	-2.36	1.50	1.55
26	S	602	CLA	CMC-C2C	-2.36	1.45	1.50
26	y	614	CLA	C3B-C2B	-2.36	1.37	1.40
37	b	622	LMG	O7-C8	-2.36	1.40	1.46
25	5	609	CHL	C3B-CAB	-2.36	1.48	1.50
25	4	606	CHL	CBD-CAD	-2.36	1.49	1.53
26	3	612	CLA	CMC-C2C	-2.35	1.45	1.50
25	8	606	CHL	CBD-CAD	-2.35	1.49	1.53
25	s	607	CHL	C2B-C1B	-2.35	1.48	1.53
25	N	606	CHL	C1A-C2A	-2.35	1.50	1.53
35	A	408	PHO	CHC-C4B	-2.35	1.34	1.40
26	6	611	CLA	C3B-C2B	-2.35	1.37	1.40
26	Y	604	CLA	C3B-C2B	-2.35	1.37	1.40
26	2	611	CLA	C3B-C2B	-2.35	1.37	1.40
36	a	412	SQD	O2-C2	-2.35	1.37	1.43
25	2	608	CHL	CBD-CAD	-2.35	1.49	1.53
25	6	608	CHL	CBD-CAD	-2.35	1.49	1.53
39	B	626	DGD	O3G-C3G	-2.35	1.39	1.43
26	A	407	CLA	C3B-C2B	-2.35	1.37	1.40
26	b	605	CLA	C3B-C2B	-2.35	1.37	1.40
25	r	607	CHL	C2A-C3A	-2.35	1.50	1.55
25	1	608	CHL	C1A-C2A	-2.35	1.50	1.53
25	S	607	CHL	C2B-C1B	-2.35	1.48	1.53
26	7	612	CLA	CMC-C2C	-2.34	1.45	1.50
25	S	608	CHL	C3D-CAD	-2.34	1.47	1.51
25	s	608	CHL	C3D-CAD	-2.34	1.47	1.51
36	A	412	SQD	O2-C2	-2.34	1.37	1.43
25	G	608	CHL	C2A-C3A	-2.34	1.50	1.55
25	3	607	CHL	C2B-C1B	-2.34	1.48	1.53
30	3	2630	LHG	O7-C5	-2.34	1.40	1.46
25	8	601	CHL	C1A-CHA	-2.34	1.50	1.53
25	2	605	CHL	CBD-CAD	-2.34	1.49	1.53
26	S	609	CLA	CMD-C2D	-2.34	1.46	1.51
26	7	610	CLA	C3B-CAB	-2.34	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	610	CLA	C3B-CAB	-2.33	1.43	1.47
26	S	610	CLA	C3B-CAB	-2.33	1.43	1.47
30	G	2630	LHG	O7-C5	-2.33	1.40	1.46
30	g	2630	LHG	O7-C5	-2.33	1.40	1.46
25	3	606	CHL	C3D-CAD	-2.33	1.47	1.51
25	7	606	CHL	C3D-CAD	-2.33	1.47	1.51
25	g	608	CHL	C2A-C3A	-2.33	1.50	1.55
26	1	603	CLA	C3B-C2B	-2.33	1.37	1.40
26	b	605	CLA	CMC-C2C	-2.33	1.45	1.50
25	n	607	CHL	C2D-C1D	-2.33	1.48	1.53
25	1	606	CHL	C3B-CAB	-2.33	1.48	1.50
25	5	608	CHL	C1A-C2A	-2.33	1.50	1.53
25	n	608	CHL	C1A-C2A	-2.33	1.50	1.53
25	8	608	CHL	C2B-C1B	-2.33	1.48	1.53
26	R	601	CLA	CMB-C2B	-2.33	1.46	1.51
25	N	607	CHL	C2D-C1D	-2.33	1.48	1.53
25	4	609	CHL	CBD-CAD	-2.32	1.49	1.53
25	2	601	CHL	CBD-CAD	-2.32	1.49	1.53
25	6	601	CHL	CBD-CAD	-2.32	1.49	1.53
26	r	601	CLA	CMB-C2B	-2.32	1.46	1.51
26	s	609	CLA	CMD-C2D	-2.32	1.46	1.51
26	c	512	CLA	C3B-C2B	-2.32	1.37	1.40
25	4	608	CHL	C2B-C1B	-2.32	1.48	1.53
26	A	410	CLA	C3B-CAB	-2.32	1.43	1.47
26	a	410	CLA	C3B-CAB	-2.32	1.43	1.47
26	8	612	CLA	C3B-C2B	-2.32	1.37	1.40
26	r	601	CLA	CMD-C2D	-2.32	1.46	1.51
26	R	601	CLA	CMD-C2D	-2.32	1.46	1.51
25	N	608	CHL	C1A-C2A	-2.32	1.50	1.53
25	7	605	CHL	C2A-C3A	-2.31	1.50	1.55
30	b	2630	LHG	O7-C5	-2.31	1.40	1.46
30	B	2630	LHG	O7-C5	-2.31	1.40	1.46
25	r	607	CHL	C3D-CAD	-2.31	1.47	1.51
26	4	612	CLA	C3B-C2B	-2.31	1.37	1.40
25	n	606	CHL	C1A-C2A	-2.31	1.50	1.53
26	B	605	CLA	CMC-C2C	-2.31	1.45	1.50
26	C	508	CLA	C4B-CHC	-2.31	1.34	1.40
26	c	508	CLA	C4B-CHC	-2.31	1.34	1.40
31	C	517	BCR	C21-C22	-2.31	1.32	1.35
25	3	605	CHL	C2A-C3A	-2.31	1.50	1.55
26	Y	613	CLA	C3B-C2B	-2.31	1.37	1.40
26	y	613	CLA	C3B-C2B	-2.31	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	611	CLA	C3B-C2B	-2.31	1.37	1.40
25	4	601	CHL	C1A-CHA	-2.31	1.50	1.53
25	r	614	CHL	C3D-CAD	-2.31	1.47	1.51
25	R	614	CHL	C3D-CAD	-2.31	1.47	1.51
25	6	605	CHL	CBD-CAD	-2.30	1.49	1.53
30	7	2630	LHG	O7-C5	-2.30	1.40	1.46
35	a	408	PHO	CMC-C2C	-2.30	1.45	1.50
35	A	408	PHO	CMC-C2C	-2.30	1.45	1.50
25	7	609	CHL	CBD-CAD	-2.30	1.49	1.53
26	Y	614	CLA	C3B-C2B	-2.30	1.37	1.40
25	1	609	CHL	C3B-CAB	-2.30	1.48	1.50
25	2	605	CHL	C2A-C3A	-2.30	1.50	1.55
25	N	601	CHL	C2A-C3A	-2.30	1.50	1.55
25	Y	607	CHL	C1A-CHA	-2.30	1.50	1.53
26	B	610	CLA	CMC-C2C	-2.30	1.45	1.50
26	b	610	CLA	CMC-C2C	-2.30	1.45	1.50
26	a	407	CLA	C3B-C2B	-2.30	1.37	1.40
26	n	603	CLA	CMC-C2C	-2.30	1.45	1.50
26	C	512	CLA	C3B-C2B	-2.30	1.37	1.40
25	1	609	CHL	C3D-CAD	-2.29	1.47	1.51
25	Y	605	CHL	C2A-C3A	-2.29	1.50	1.55
25	5	601	CHL	CBD-CAD	-2.29	1.49	1.53
25	1	601	CHL	CBD-CAD	-2.29	1.49	1.53
36	b	623	SQD	O2-C2	-2.29	1.37	1.43
25	3	609	CHL	CBD-CAD	-2.29	1.49	1.53
25	8	609	CHL	CBD-CAD	-2.29	1.49	1.53
26	B	605	CLA	C3B-C2B	-2.29	1.37	1.40
25	y	605	CHL	C2A-C3A	-2.29	1.50	1.55
30	B	2631	LHG	O7-C5	-2.29	1.40	1.46
26	b	604	CLA	CMC-C2C	-2.29	1.45	1.50
26	N	603	CLA	CMC-C2C	-2.29	1.45	1.50
25	5	609	CHL	C3D-CAD	-2.29	1.47	1.51
25	R	607	CHL	C3D-CAD	-2.29	1.47	1.51
31	c	517	BCR	C21-C22	-2.28	1.32	1.35
26	B	604	CLA	CMC-C2C	-2.28	1.45	1.50
25	y	607	CHL	C1A-CHA	-2.28	1.50	1.53
30	n	2630	LHG	O7-C5	-2.28	1.40	1.46
25	7	609	CHL	C2A-C3A	-2.28	1.50	1.55
26	b	616	CLA	CMC-C2C	-2.28	1.45	1.50
26	B	616	CLA	CMC-C2C	-2.28	1.45	1.50
25	6	605	CHL	C2A-C3A	-2.28	1.50	1.55
35	A	408	PHO	CMD-C2D	-2.28	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	506	CLA	CMC-C2C	-2.28	1.45	1.50
25	1	607	CHL	C2B-C1B	-2.28	1.48	1.53
25	3	609	CHL	C2A-C3A	-2.27	1.50	1.55
30	C	2630	LHG	O7-C5	-2.27	1.40	1.46
26	5	614	CLA	C3B-C2B	-2.27	1.37	1.40
26	1	614	CLA	C3B-C2B	-2.27	1.37	1.40
30	N	2630	LHG	O7-C5	-2.27	1.40	1.46
26	c	506	CLA	CMC-C2C	-2.27	1.45	1.50
25	n	601	CHL	C2A-C3A	-2.27	1.50	1.55
25	5	607	CHL	C2B-C1B	-2.27	1.48	1.53
36	B	623	SQD	O2-C2	-2.27	1.37	1.43
26	c	507	CLA	CAC-C3C	-2.27	1.45	1.51
25	6	605	CHL	C1A-C2A	-2.27	1.51	1.53
25	2	605	CHL	C1A-C2A	-2.27	1.51	1.53
26	1	611	CLA	C3B-C2B	-2.27	1.37	1.40
26	S	609	CLA	C3B-C2B	-2.27	1.37	1.40
26	s	609	CLA	C3B-C2B	-2.27	1.37	1.40
25	N	609	CHL	C1A-C2A	-2.27	1.51	1.53
26	1	613	CLA	C3B-C2B	-2.26	1.37	1.40
25	N	606	CHL	C3B-CAB	-2.26	1.48	1.50
25	n	606	CHL	C3B-CAB	-2.26	1.48	1.50
30	R	2630	LHG	O7-C5	-2.26	1.40	1.46
26	c	509	CLA	CMA-C3A	-2.26	1.48	1.53
26	C	509	CLA	CMA-C3A	-2.26	1.48	1.53
26	R	616	CLA	C3B-C2B	-2.26	1.37	1.40
25	G	601	CHL	C2A-C3A	-2.26	1.50	1.55
25	g	601	CHL	C2A-C3A	-2.26	1.50	1.55
25	2	607	CHL	C2B-C1B	-2.26	1.48	1.53
25	G	609	CHL	C3D-CAD	-2.26	1.47	1.51
26	s	603	CLA	C3B-C2B	-2.26	1.37	1.40
26	y	611	CLA	CMC-C2C	-2.26	1.45	1.50
26	Y	611	CLA	CMC-C2C	-2.26	1.45	1.50
25	3	605	CHL	CBD-CAD	-2.26	1.49	1.53
30	r	2630	LHG	O7-C5	-2.26	1.40	1.46
26	R	613	CLA	C3B-C2B	-2.26	1.37	1.40
26	r	613	CLA	C3B-C2B	-2.26	1.37	1.40
25	N	605	CHL	C2B-C1B	-2.26	1.48	1.53
25	n	605	CHL	C2B-C1B	-2.26	1.48	1.53
36	B	623	SQD	O4-C4	-2.26	1.37	1.43
30	b	2631	LHG	O7-C5	-2.26	1.40	1.46
30	c	2630	LHG	O7-C5	-2.26	1.40	1.46
25	3	608	CHL	C2B-C1B	-2.25	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	601	CHL	C2B-C1B	-2.25	1.48	1.53
25	1	601	CHL	C2B-C1B	-2.25	1.48	1.53
26	8	603	CLA	C3B-C2B	-2.25	1.37	1.40
26	4	603	CLA	C3B-C2B	-2.25	1.37	1.40
25	y	609	CHL	CMB-C2B	-2.25	1.48	1.53
25	Y	609	CHL	CMB-C2B	-2.25	1.48	1.53
25	g	609	CHL	C3D-CAD	-2.25	1.47	1.51
39	C	520	DGD	O2E-C2E	-2.25	1.37	1.43
39	c	520	DGD	O2E-C2E	-2.25	1.37	1.43
25	7	608	CHL	C2B-C1B	-2.25	1.48	1.53
25	5	606	CHL	C3B-CAB	-2.24	1.48	1.50
27	7	1621	LUT	C22-C21	-2.24	1.52	1.54
35	a	408	PHO	CMD-C2D	-2.24	1.45	1.50
26	C	502	CLA	C4B-CHC	-2.24	1.34	1.40
26	C	507	CLA	CAC-C3C	-2.24	1.45	1.51
36	b	623	SQD	O4-C4	-2.24	1.37	1.43
25	6	607	CHL	C2B-C1B	-2.24	1.48	1.53
39	c	520	DGD	O4D-C4D	-2.24	1.37	1.43
39	C	520	DGD	O4D-C4D	-2.24	1.37	1.43
26	7	610	CLA	CMC-C2C	-2.24	1.45	1.50
26	Y	610	CLA	C3B-CAB	-2.24	1.43	1.47
26	y	610	CLA	C3B-CAB	-2.24	1.43	1.47
39	C	520	DGD	O3D-C3D	-2.24	1.37	1.43
39	c	520	DGD	O3D-C3D	-2.24	1.37	1.43
27	1	1621	LUT	C22-C21	-2.23	1.52	1.54
25	4	607	CHL	C2B-C1B	-2.23	1.48	1.53
26	6	613	CLA	C3B-C2B	-2.23	1.37	1.40
25	n	609	CHL	C1A-C2A	-2.23	1.51	1.53
35	A	408	PHO	CAA-C2A	-2.23	1.49	1.54
26	S	612	CLA	CMB-C2B	-2.23	1.47	1.51
26	r	616	CLA	C3B-C2B	-2.23	1.37	1.40
26	B	606	CLA	C3B-CAB	-2.23	1.43	1.47
25	5	605	CHL	C2B-C1B	-2.23	1.48	1.53
26	3	602	CLA	C3B-CAB	-2.23	1.43	1.47
26	7	602	CLA	C3B-CAB	-2.23	1.43	1.47
25	Y	601	CHL	C2A-C3A	-2.22	1.50	1.55
27	3	1621	LUT	C22-C21	-2.22	1.52	1.54
25	1	608	CHL	CBD-CAD	-2.22	1.49	1.53
25	y	605	CHL	C3B-CAB	-2.22	1.48	1.50
25	Y	605	CHL	C3B-CAB	-2.22	1.48	1.50
25	N	605	CHL	C2A-C3A	-2.22	1.50	1.55
25	n	605	CHL	C2A-C3A	-2.22	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	408	PHO	CAA-C2A	-2.22	1.49	1.54
26	c	502	CLA	C4B-CHC	-2.22	1.34	1.40
26	A	406	CLA	CAC-C3C	-2.22	1.45	1.51
25	8	607	CHL	C2B-C1B	-2.22	1.48	1.53
26	b	606	CLA	C3B-CAB	-2.22	1.43	1.47
36	A	418	SQD	O2-C2	-2.21	1.37	1.43
25	1	605	CHL	C2B-C1B	-2.21	1.48	1.53
26	s	612	CLA	CMB-C2B	-2.21	1.47	1.51
26	C	505	CLA	CMC-C2C	-2.21	1.46	1.50
26	N	611	CLA	C3B-C2B	-2.21	1.37	1.40
26	n	611	CLA	C3B-C2B	-2.21	1.37	1.40
39	C	519	DGD	O4E-C4E	-2.21	1.37	1.43
39	c	519	DGD	O4E-C4E	-2.21	1.37	1.43
25	y	601	CHL	C2A-C3A	-2.21	1.50	1.55
25	7	605	CHL	CBD-CAD	-2.21	1.49	1.53
26	B	614	CLA	CMC-C2C	-2.21	1.46	1.50
25	8	607	CHL	C3B-CAB	-2.21	1.48	1.50
27	5	1621	LUT	C22-C21	-2.20	1.52	1.54
26	c	505	CLA	CMC-C2C	-2.20	1.46	1.50
25	Y	606	CHL	C2A-C3A	-2.20	1.50	1.55
25	y	606	CHL	C2A-C3A	-2.20	1.50	1.55
25	4	607	CHL	C3B-CAB	-2.20	1.48	1.50
25	6	607	CHL	C2A-C3A	-2.20	1.50	1.55
39	b	626	DGD	O1G-C1G	-2.20	1.40	1.45
39	B	626	DGD	O1G-C1G	-2.20	1.40	1.45
26	a	406	CLA	CAC-C3C	-2.20	1.45	1.51
25	s	607	CHL	C3B-CAB	-2.20	1.48	1.50
26	B	613	CLA	C3B-CAB	-2.20	1.43	1.47
31	C	514	BCR	C21-C22	-2.20	1.32	1.35
25	5	608	CHL	CBD-CAD	-2.20	1.49	1.53
36	a	412	SQD	O4-C4	-2.19	1.37	1.43
36	A	412	SQD	O4-C4	-2.19	1.37	1.43
26	G	603	CLA	CAC-C3C	-2.19	1.45	1.51
26	3	610	CLA	CMC-C2C	-2.19	1.46	1.50
26	g	603	CLA	CAC-C3C	-2.19	1.45	1.51
25	r	608	CHL	C3B-CAB	-2.19	1.48	1.50
26	c	505	CLA	C3B-C2B	-2.19	1.37	1.40
26	5	613	CLA	C3B-C2B	-2.19	1.37	1.40
25	6	609	CHL	C2A-C3A	-2.19	1.50	1.55
25	2	609	CHL	C3B-CAB	-2.19	1.48	1.50
26	B	611	CLA	C3B-CAB	-2.19	1.43	1.47
39	h	102	DGD	O2D-C2D	-2.18	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	H	102	DGD	O2D-C2D	-2.18	1.37	1.43
25	2	609	CHL	C2A-C3A	-2.18	1.50	1.55
26	C	508	CLA	C3B-C2B	-2.18	1.37	1.40
26	2	613	CLA	C3B-C2B	-2.18	1.37	1.40
26	3	613	CLA	CMC-C2C	-2.18	1.46	1.50
26	C	505	CLA	C3B-C2B	-2.18	1.37	1.40
25	r	606	CHL	C3D-CAD	-2.18	1.47	1.51
26	b	615	CLA	C3B-CAB	-2.18	1.43	1.47
36	a	418	SQD	O2-C2	-2.18	1.37	1.43
26	8	610	CLA	C3B-CAB	-2.18	1.43	1.47
26	4	610	CLA	C3B-CAB	-2.18	1.43	1.47
39	h	102	DGD	O2E-C2E	-2.18	1.37	1.43
39	H	102	DGD	O2E-C2E	-2.18	1.37	1.43
26	B	603	CLA	CMC-C2C	-2.18	1.46	1.50
36	A	418	SQD	O3-C3	-2.18	1.37	1.43
36	a	418	SQD	O3-C3	-2.18	1.37	1.43
26	S	603	CLA	C3B-C2B	-2.17	1.37	1.40
26	7	613	CLA	CMC-C2C	-2.17	1.46	1.50
25	7	607	CHL	C2A-C3A	-2.17	1.50	1.55
25	3	607	CHL	C2A-C3A	-2.17	1.50	1.55
26	b	614	CLA	CMC-C2C	-2.17	1.46	1.50
25	6	605	CHL	C2B-C1B	-2.17	1.48	1.53
25	2	605	CHL	C2B-C1B	-2.17	1.48	1.53
37	C	521	LMG	O1-C7	-2.17	1.39	1.43
25	r	607	CHL	C3B-CAB	-2.17	1.48	1.50
26	b	611	CLA	C3B-CAB	-2.17	1.43	1.47
26	b	613	CLA	C3B-CAB	-2.17	1.43	1.47
27	r	620	LUT	C22-C21	-2.17	1.52	1.54
25	s	607	CHL	CBD-CAD	-2.17	1.49	1.53
25	S	607	CHL	C3B-CAB	-2.17	1.48	1.50
26	8	610	CLA	CMC-C2C	-2.17	1.46	1.50
26	4	610	CLA	CMC-C2C	-2.17	1.46	1.50
26	B	615	CLA	C3B-CAB	-2.17	1.43	1.47
26	N	604	CLA	CMC-C2C	-2.17	1.46	1.50
26	c	509	CLA	C3B-CAB	-2.17	1.43	1.47
28	7	1622	XAT	C34-C33	-2.17	1.32	1.35
28	3	1622	XAT	C34-C33	-2.17	1.32	1.35
25	R	608	CHL	C2D-C1D	-2.16	1.48	1.53
27	r	620	LUT	C30-C29	-2.16	1.32	1.35
27	R	620	LUT	C30-C29	-2.16	1.32	1.35
26	c	508	CLA	C3B-C2B	-2.16	1.37	1.40
26	C	507	CLA	C3B-CAB	-2.16	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	606	CHL	C3B-CAB	-2.16	1.48	1.50
25	S	607	CHL	C1A-CHA	-2.16	1.50	1.53
25	s	607	CHL	C1A-CHA	-2.16	1.50	1.53
25	1	607	CHL	C3D-CAD	-2.16	1.47	1.51
26	s	612	CLA	CMC-C2C	-2.16	1.46	1.50
26	S	612	CLA	CMC-C2C	-2.16	1.46	1.50
25	r	608	CHL	C2D-C1D	-2.16	1.48	1.53
31	c	514	BCR	C21-C22	-2.16	1.32	1.35
31	C	515	BCR	C10-C9	-2.15	1.32	1.35
26	c	505	CLA	C4B-CHC	-2.15	1.34	1.40
25	2	607	CHL	C2A-C3A	-2.15	1.50	1.55
30	y	2630	LHG	O8-C6	-2.15	1.40	1.45
26	y	603	CLA	CMC-C2C	-2.15	1.46	1.50
26	n	604	CLA	CMC-C2C	-2.15	1.46	1.50
26	Y	603	CLA	CMC-C2C	-2.15	1.46	1.50
26	c	503	CLA	C3B-C2B	-2.15	1.37	1.40
38	D	405	PL9	C16-C14	-2.15	1.46	1.51
38	d	405	PL9	C16-C14	-2.15	1.46	1.51
26	s	611	CLA	CMC-C2C	-2.15	1.46	1.50
26	Y	612	CLA	CMC-C2C	-2.15	1.46	1.50
26	A	410	CLA	CMC-C2C	-2.15	1.46	1.50
26	a	410	CLA	CMC-C2C	-2.15	1.46	1.50
26	C	503	CLA	C3B-C2B	-2.15	1.37	1.40
25	R	606	CHL	C3D-CAD	-2.15	1.47	1.51
25	6	609	CHL	C2B-C1B	-2.15	1.49	1.53
25	4	607	CHL	CBD-CAD	-2.15	1.49	1.53
25	8	607	CHL	CBD-CAD	-2.15	1.49	1.53
26	8	611	CLA	C3B-C2B	-2.15	1.37	1.40
26	C	505	CLA	C4B-CHC	-2.15	1.34	1.40
25	S	608	CHL	C1A-C2A	-2.15	1.51	1.53
25	s	608	CHL	C1A-C2A	-2.15	1.51	1.53
25	R	607	CHL	C3B-CAB	-2.15	1.48	1.50
26	y	612	CLA	CMC-C2C	-2.14	1.46	1.50
26	c	507	CLA	C3B-CAB	-2.14	1.43	1.47
26	C	509	CLA	C3B-CAB	-2.14	1.43	1.47
27	S	1621	LUT	C30-C29	-2.14	1.32	1.35
26	b	603	CLA	CMC-C2C	-2.14	1.46	1.50
26	7	611	CLA	C4B-CHC	-2.14	1.34	1.40
26	c	511	CLA	CMC-C2C	-2.14	1.46	1.50
26	C	511	CLA	CMC-C2C	-2.14	1.46	1.50
26	s	611	CLA	C3B-CAB	-2.14	1.43	1.47
25	2	606	CHL	C3B-CAB	-2.14	1.48	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	609	CHL	C3D-CAD	-2.14	1.47	1.51
36	B	621	SQD	O2-C2	-2.14	1.38	1.43
26	S	611	CLA	CMC-C2C	-2.14	1.46	1.50
31	c	515	BCR	C10-C9	-2.13	1.33	1.35
27	s	1621	LUT	C30-C29	-2.13	1.33	1.35
26	G	612	CLA	C3B-C2B	-2.13	1.37	1.40
30	Y	2630	LHG	O8-C6	-2.13	1.40	1.45
25	2	609	CHL	C2B-C1B	-2.13	1.49	1.53
37	c	521	LMG	O1-C7	-2.13	1.40	1.43
26	4	602	CLA	C3B-C2B	-2.13	1.37	1.40
26	8	602	CLA	C3B-C2B	-2.13	1.37	1.40
25	6	609	CHL	C3B-CAB	-2.13	1.48	1.50
36	b	621	SQD	O2-C2	-2.13	1.38	1.43
25	7	607	CHL	CBD-CAD	-2.13	1.49	1.53
25	3	607	CHL	CBD-CAD	-2.13	1.49	1.53
38	D	405	PL9	C31-C29	-2.13	1.46	1.51
38	d	405	PL9	C31-C29	-2.13	1.46	1.51
27	R	620	LUT	C22-C21	-2.13	1.52	1.54
27	1	1621	LUT	C1-C6	-2.12	1.50	1.53
25	3	605	CHL	C1A-C2A	-2.12	1.51	1.53
25	7	605	CHL	C1A-C2A	-2.12	1.51	1.53
25	S	608	CHL	C2B-C1B	-2.12	1.49	1.53
39	C	520	DGD	O3E-C3E	-2.12	1.38	1.43
25	S	607	CHL	CBD-CAD	-2.12	1.49	1.53
26	c	503	CLA	CMC-C2C	-2.12	1.46	1.50
26	a	406	CLA	C4B-CHC	-2.12	1.34	1.40
25	N	606	CHL	C2A-C3A	-2.12	1.50	1.55
26	1	610	CLA	CMC-C2C	-2.12	1.46	1.50
39	c	520	DGD	O3E-C3E	-2.12	1.38	1.43
26	N	613	CLA	CMC-C2C	-2.12	1.46	1.50
26	C	503	CLA	CMC-C2C	-2.12	1.46	1.50
26	A	407	CLA	C3B-CAB	-2.11	1.43	1.47
26	4	611	CLA	C3B-C2B	-2.11	1.37	1.40
26	C	504	CLA	CMC-C2C	-2.11	1.46	1.50
26	n	613	CLA	CMC-C2C	-2.11	1.46	1.50
25	R	608	CHL	C3B-CAB	-2.11	1.48	1.50
26	D	402	CLA	CMA-C3A	-2.11	1.48	1.53
26	d	402	CLA	CMA-C3A	-2.11	1.48	1.53
26	n	603	CLA	CAC-C3C	-2.11	1.45	1.51
26	N	603	CLA	CAC-C3C	-2.11	1.45	1.51
26	B	616	CLA	C4B-CHC	-2.11	1.34	1.40
26	c	506	CLA	C3B-C2B	-2.11	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	506	CLA	C3B-C2B	-2.11	1.37	1.40
26	a	407	CLA	C3B-CAB	-2.11	1.43	1.47
25	5	607	CHL	C3D-CAD	-2.11	1.47	1.51
25	s	608	CHL	C2B-C1B	-2.11	1.49	1.53
26	G	610	CLA	C3B-C2B	-2.11	1.37	1.40
26	5	610	CLA	CMC-C2C	-2.11	1.46	1.50
25	3	608	CHL	C3B-CAB	-2.11	1.48	1.50
26	c	504	CLA	CMC-C2C	-2.11	1.46	1.50
26	S	611	CLA	C3B-CAB	-2.11	1.43	1.47
26	y	604	CLA	CMC-C2C	-2.11	1.46	1.50
26	S	603	CLA	C3B-CAB	-2.11	1.43	1.47
25	N	609	CHL	C3D-CAD	-2.11	1.47	1.51
39	c	518	DGD	O3G-C3G	-2.10	1.40	1.43
26	b	616	CLA	C4B-CHC	-2.10	1.34	1.40
26	3	611	CLA	C4B-CHC	-2.10	1.34	1.40
30	D	410	LHG	O7-C5	-2.10	1.41	1.46
26	C	501	CLA	CMC-C2C	-2.10	1.46	1.50
26	y	614	CLA	C3B-CAB	-2.10	1.43	1.47
25	S	607	CHL	C3D-CAD	-2.10	1.47	1.51
37	b	2633	LMG	O2-C2	-2.10	1.38	1.43
36	B	621	SQD	O3-C3	-2.10	1.38	1.43
26	b	604	CLA	C3B-CAB	-2.10	1.43	1.47
26	Y	614	CLA	C3B-CAB	-2.10	1.43	1.47
36	A	418	SQD	O4-C4	-2.10	1.38	1.43
36	a	418	SQD	O4-C4	-2.10	1.38	1.43
26	c	504	CLA	CAC-C3C	-2.10	1.45	1.51
25	5	609	CHL	C1A-C2A	-2.10	1.51	1.53
25	1	601	CHL	C3D-CAD	-2.09	1.47	1.51
26	b	614	CLA	C3B-C2B	-2.09	1.37	1.40
25	N	606	CHL	C3D-CAD	-2.09	1.47	1.51
25	n	606	CHL	C3D-CAD	-2.09	1.47	1.51
26	3	603	CLA	C3B-CAB	-2.09	1.43	1.47
26	7	603	CLA	C3B-CAB	-2.09	1.43	1.47
36	B	623	SQD	O3-C3	-2.09	1.38	1.43
36	b	623	SQD	O3-C3	-2.09	1.38	1.43
26	s	603	CLA	C3B-CAB	-2.09	1.43	1.47
26	A	406	CLA	C4B-CHC	-2.09	1.34	1.40
25	1	609	CHL	C1A-C2A	-2.09	1.51	1.53
30	d	410	LHG	O7-C5	-2.09	1.41	1.46
25	n	606	CHL	C2A-C3A	-2.09	1.50	1.55
26	Y	613	CLA	CMC-C2C	-2.08	1.46	1.50
26	Y	604	CLA	CMC-C2C	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	402	CLA	C3B-CAB	-2.08	1.43	1.47
25	y	605	CHL	C3D-CAD	-2.08	1.47	1.51
25	Y	605	CHL	C3D-CAD	-2.08	1.47	1.51
27	5	1621	LUT	C1-C6	-2.08	1.50	1.53
26	y	613	CLA	CMC-C2C	-2.08	1.46	1.50
26	4	602	CLA	CMC-C2C	-2.08	1.46	1.50
25	1	609	CHL	CBD-CGD	-2.08	1.48	1.52
26	g	612	CLA	C3B-C2B	-2.08	1.37	1.40
25	5	601	CHL	C3D-CAD	-2.08	1.47	1.51
36	a	412	SQD	O3-C3	-2.08	1.38	1.43
36	A	412	SQD	O3-C3	-2.08	1.38	1.43
26	C	512	CLA	C3B-CAB	-2.08	1.43	1.47
26	c	512	CLA	C3B-CAB	-2.08	1.43	1.47
26	c	501	CLA	CMC-C2C	-2.08	1.46	1.50
25	s	606	CHL	CBD-CAD	-2.08	1.49	1.53
26	C	512	CLA	CMC-C2C	-2.08	1.46	1.50
26	c	512	CLA	CMC-C2C	-2.08	1.46	1.50
26	c	507	CLA	C4B-CHC	-2.08	1.34	1.40
39	C	518	DGD	O3G-C3G	-2.08	1.40	1.43
25	6	609	CHL	C1A-C2A	-2.08	1.51	1.53
25	Y	609	CHL	C3D-CAD	-2.07	1.47	1.51
25	s	607	CHL	C3D-CAD	-2.07	1.47	1.51
26	4	602	CLA	C3B-CAB	-2.07	1.43	1.47
25	G	607	CHL	C3D-CAD	-2.07	1.47	1.51
26	S	613	CLA	CMC-C2C	-2.07	1.46	1.50
26	C	504	CLA	CAC-C3C	-2.07	1.45	1.51
26	C	507	CLA	C4B-CHC	-2.07	1.34	1.40
25	r	614	CHL	C2B-C1B	-2.07	1.49	1.53
25	R	614	CHL	C2B-C1B	-2.07	1.49	1.53
25	S	606	CHL	CBD-CAD	-2.07	1.50	1.53
26	C	501	CLA	C3B-CAB	-2.07	1.43	1.47
26	c	501	CLA	C3B-CAB	-2.07	1.43	1.47
26	8	602	CLA	CMC-C2C	-2.07	1.46	1.50
36	b	621	SQD	O3-C3	-2.07	1.38	1.43
26	s	613	CLA	CMC-C2C	-2.07	1.46	1.50
26	d	402	CLA	C3B-CAB	-2.06	1.43	1.47
26	n	612	CLA	C3B-C2B	-2.06	1.37	1.40
26	G	603	CLA	CMC-C2C	-2.06	1.46	1.50
26	g	603	CLA	CMC-C2C	-2.06	1.46	1.50
25	7	607	CHL	C3D-CAD	-2.06	1.47	1.51
26	N	603	CLA	C3B-CAB	-2.06	1.43	1.47
25	y	606	CHL	CMD-C2D	-2.06	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	2633	LMG	O2-C2	-2.06	1.38	1.43
26	8	603	CLA	CMC-C2C	-2.06	1.46	1.50
26	N	610	CLA	CMC-C2C	-2.06	1.46	1.50
25	8	607	CHL	C2A-C3A	-2.06	1.51	1.55
26	1	613	CLA	CMC-C2C	-2.06	1.46	1.50
29	r	623	NEX	O24-C25	-2.05	1.43	1.46
26	8	602	CLA	C3B-CAB	-2.05	1.43	1.47
26	c	511	CLA	CMA-C3A	-2.05	1.48	1.53
25	5	609	CHL	CBD-CGD	-2.05	1.48	1.52
26	y	603	CLA	CAC-C3C	-2.05	1.45	1.51
26	5	613	CLA	CMC-C2C	-2.05	1.46	1.50
26	N	612	CLA	CMC-C2C	-2.05	1.46	1.50
26	N	610	CLA	C3B-CAB	-2.05	1.43	1.47
26	6	610	CLA	C3B-CAB	-2.05	1.43	1.47
26	3	613	CLA	C3B-CAB	-2.05	1.43	1.47
25	y	609	CHL	C3D-CAD	-2.05	1.47	1.51
39	C	518	DGD	O4D-C4D	-2.05	1.38	1.43
39	c	518	DGD	O4D-C4D	-2.05	1.38	1.43
25	Y	605	CHL	C1A-C2A	-2.05	1.51	1.53
25	s	608	CHL	CBD-CAD	-2.05	1.50	1.53
38	D	405	PL9	C46-C44	-2.05	1.46	1.51
38	d	405	PL9	C46-C44	-2.05	1.46	1.51
26	7	613	CLA	C3B-CAB	-2.05	1.43	1.47
26	B	604	CLA	C3B-CAB	-2.05	1.43	1.47
26	6	613	CLA	CMC-C2C	-2.05	1.46	1.50
27	y	1620	LUT	C22-C21	-2.05	1.52	1.54
37	D	411	LMG	O7-C8	-2.05	1.41	1.46
37	d	411	LMG	O7-C8	-2.05	1.41	1.46
26	3	611	CLA	C3B-CAB	-2.05	1.43	1.47
26	3	604	CLA	C3B-CAB	-2.05	1.43	1.47
26	7	604	CLA	C3B-CAB	-2.05	1.43	1.47
26	7	604	CLA	CMC-C2C	-2.05	1.46	1.50
29	R	623	NEX	O24-C25	-2.05	1.43	1.46
25	S	608	CHL	CBD-CAD	-2.04	1.50	1.53
36	A	412	SQD	O47-C45	-2.04	1.41	1.46
26	3	604	CLA	CMC-C2C	-2.04	1.46	1.50
25	4	607	CHL	C2A-C3A	-2.04	1.51	1.55
26	2	613	CLA	CMC-C2C	-2.04	1.46	1.50
26	n	610	CLA	CMC-C2C	-2.04	1.46	1.50
25	g	607	CHL	C3D-CAD	-2.04	1.47	1.51
26	Y	603	CLA	CAC-C3C	-2.04	1.45	1.51
27	n	1621	LUT	C10-C9	-2.04	1.33	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	1621	LUT	C10-C9	-2.04	1.33	1.35
26	g	610	CLA	C3B-C2B	-2.04	1.37	1.40
29	g	1623	NEX	C7-C8	-2.04	1.28	1.32
26	a	405	CLA	C1C-NC	-2.04	1.34	1.37
25	4	601	CHL	C2B-C1B	-2.04	1.49	1.53
26	3	603	CLA	CAC-C3C	-2.04	1.45	1.51
26	n	610	CLA	C3B-CAB	-2.04	1.43	1.47
26	2	610	CLA	C3B-CAB	-2.04	1.43	1.47
26	7	603	CLA	C4B-CHC	-2.04	1.34	1.40
25	Y	606	CHL	CMD-C2D	-2.04	1.48	1.53
26	3	614	CLA	CMC-C2C	-2.03	1.46	1.50
25	5	607	CHL	CBD-CGD	-2.03	1.48	1.52
26	c	509	CLA	C3B-C2B	-2.03	1.37	1.40
26	7	614	CLA	CMC-C2C	-2.03	1.46	1.50
25	Y	606	CHL	CMB-C2B	-2.03	1.48	1.53
26	1	604	CLA	CMC-C2C	-2.03	1.46	1.50
26	5	604	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	614	CLA	C3B-C2B	-2.03	1.37	1.40
26	4	603	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	610	CLA	C4B-CHC	-2.03	1.34	1.40
26	b	610	CLA	C4B-CHC	-2.03	1.34	1.40
25	y	606	CHL	CMB-C2B	-2.03	1.49	1.53
26	n	612	CLA	CMC-C2C	-2.03	1.46	1.50
26	3	603	CLA	C4B-CHC	-2.03	1.34	1.40
39	C	520	DGD	O4E-C4E	-2.03	1.38	1.43
26	r	613	CLA	C3B-CAB	-2.03	1.43	1.47
25	3	607	CHL	C3B-CAB	-2.03	1.48	1.50
25	3	607	CHL	C3D-CAD	-2.03	1.47	1.51
28	G	1622	XAT	C10-C9	-2.03	1.33	1.35
28	g	1622	XAT	C10-C9	-2.03	1.33	1.35
25	R	614	CHL	CBD-CAD	-2.03	1.50	1.53
26	r	610	CLA	C3B-CAB	-2.03	1.43	1.47
26	7	603	CLA	CAC-C3C	-2.03	1.45	1.51
26	B	606	CLA	CMA-C3A	-2.03	1.48	1.53
25	2	609	CHL	C1A-C2A	-2.02	1.51	1.53
26	c	509	CLA	CMC-C2C	-2.02	1.46	1.50
26	C	509	CLA	CMC-C2C	-2.02	1.46	1.50
25	7	607	CHL	C3B-CAB	-2.02	1.48	1.50
26	b	616	CLA	C3B-CAB	-2.02	1.43	1.47
26	B	616	CLA	C3B-CAB	-2.02	1.43	1.47
39	C	518	DGD	O2D-C2D	-2.02	1.38	1.43
26	C	511	CLA	CMA-C3A	-2.02	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	a	412	SQD	O47-C45	-2.02	1.41	1.46
26	n	603	CLA	C3B-CAB	-2.02	1.43	1.47
26	C	509	CLA	C3B-C2B	-2.02	1.37	1.40
26	3	612	CLA	C3B-CAB	-2.02	1.43	1.47
26	7	612	CLA	C3B-CAB	-2.02	1.43	1.47
26	1	604	CLA	C3B-CAB	-2.02	1.43	1.47
25	1	605	CHL	C3D-CAD	-2.02	1.47	1.51
29	G	1623	NEX	C7-C8	-2.02	1.28	1.32
26	B	612	CLA	C4B-CHC	-2.02	1.34	1.40
26	1	603	CLA	CMC-C2C	-2.02	1.46	1.50
26	r	611	CLA	C3B-CAB	-2.02	1.43	1.47
25	S	607	CHL	C2A-C3A	-2.02	1.51	1.55
38	d	405	PL9	C36-C34	-2.02	1.46	1.51
26	C	504	CLA	C4B-CHC	-2.02	1.34	1.40
39	c	518	DGD	O2D-C2D	-2.02	1.38	1.43
26	y	614	CLA	CMC-C2C	-2.02	1.46	1.50
26	R	613	CLA	C3B-CAB	-2.02	1.43	1.47
26	B	609	CLA	CMC-C2C	-2.01	1.46	1.50
25	7	608	CHL	C3B-CAB	-2.01	1.48	1.50
26	N	612	CLA	C3B-C2B	-2.01	1.37	1.40
25	2	609	CHL	CBD-CGD	-2.01	1.48	1.52
31	c	514	BCR	C10-C9	-2.01	1.33	1.35
26	b	607	CLA	C4B-CHC	-2.01	1.34	1.40
26	B	607	CLA	C4B-CHC	-2.01	1.34	1.40
27	Y	1620	LUT	C22-C21	-2.01	1.52	1.54
25	3	607	CHL	C1A-C2A	-2.01	1.51	1.53
26	C	502	CLA	CAC-C3C	-2.01	1.45	1.51
26	7	611	CLA	C3B-CAB	-2.01	1.43	1.47
25	5	605	CHL	C3D-CAD	-2.01	1.47	1.51
25	8	601	CHL	C2B-C1B	-2.01	1.49	1.53
39	c	520	DGD	O4E-C4E	-2.01	1.38	1.43
26	5	604	CLA	C3B-CAB	-2.01	1.43	1.47
26	a	407	CLA	CAC-C3C	-2.01	1.45	1.51
26	b	612	CLA	C4B-CHC	-2.01	1.34	1.40
26	1	603	CLA	CAC-C3C	-2.00	1.45	1.51
26	1	612	CLA	CMC-C2C	-2.00	1.46	1.50
26	5	612	CLA	C3B-CAB	-2.00	1.43	1.47
25	y	606	CHL	C3B-CAB	-2.00	1.48	1.50
31	b	620	BCR	C1-C6	-2.00	1.51	1.53
31	B	620	BCR	C1-C6	-2.00	1.51	1.53
25	g	609	CHL	CMB-C2B	-2.00	1.49	1.53
26	A	405	CLA	C1C-NC	-2.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	7	1622	XAT	O4-C5	-2.00	1.43	1.46
28	3	1622	XAT	O4-C5	-2.00	1.43	1.46
26	7	611	CLA	CHC-C1C	2.00	1.41	1.35
26	C	504	CLA	CHC-C1C	2.00	1.41	1.35
26	C	506	CLA	CHC-C1C	2.01	1.41	1.35
25	1	609	CHL	CMC-C2C	2.01	1.48	1.45
25	g	605	CHL	CMC-C2C	2.01	1.48	1.45
25	R	608	CHL	CMC-C2C	2.01	1.48	1.45
25	r	608	CHL	CMC-C2C	2.01	1.48	1.45
25	G	605	CHL	CMC-C2C	2.02	1.48	1.45
26	C	508	CLA	CHC-C1C	2.02	1.41	1.35
26	c	508	CLA	CHC-C1C	2.02	1.41	1.35
25	3	601	CHL	CMC-C2C	2.03	1.48	1.45
26	A	406	CLA	CHC-C1C	2.03	1.41	1.35
25	4	609	CHL	CMC-C2C	2.04	1.48	1.45
25	8	609	CHL	CMC-C2C	2.04	1.48	1.45
25	n	601	CHL	CMC-C2C	2.04	1.48	1.45
25	G	606	CHL	CMC-C2C	2.05	1.48	1.45
25	g	606	CHL	CMC-C2C	2.05	1.48	1.45
26	a	406	CLA	CHC-C1C	2.05	1.41	1.35
26	7	603	CLA	CHC-C1C	2.05	1.41	1.35
25	7	601	CHL	CMC-C2C	2.05	1.48	1.45
25	g	601	CHL	CMC-C2C	2.06	1.48	1.45
25	N	601	CHL	CMC-C2C	2.06	1.48	1.45
26	3	603	CLA	CHC-C1C	2.06	1.41	1.35
37	c	521	LMG	C4-C5	2.06	1.57	1.53
37	C	521	LMG	C4-C5	2.07	1.57	1.53
26	b	610	CLA	CHC-C1C	2.08	1.41	1.35
35	a	409	PHO	C1A-NA	2.09	1.41	1.37
35	A	409	PHO	C1A-NA	2.09	1.41	1.37
25	g	608	CHL	CMC-C2C	2.09	1.48	1.45
25	G	608	CHL	CMC-C2C	2.09	1.48	1.45
25	2	601	CHL	CMC-C2C	2.09	1.48	1.45
25	6	601	CHL	CMC-C2C	2.09	1.48	1.45
26	b	616	CLA	CHC-C1C	2.10	1.41	1.35
25	G	601	CHL	CMC-C2C	2.10	1.48	1.45
26	B	610	CLA	CHC-C1C	2.11	1.41	1.35
26	7	612	CLA	CHC-C1C	2.11	1.41	1.35
26	Y	604	CLA	CHC-C1C	2.11	1.41	1.35
26	y	604	CLA	CHC-C1C	2.11	1.41	1.35
26	B	616	CLA	CHC-C1C	2.11	1.41	1.35
37	B	2633	LMG	C3-C2	2.13	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	2633	LMG	C3-C2	2.13	1.57	1.52
25	R	614	CHL	CMC-C2C	2.14	1.49	1.45
25	r	614	CHL	CMC-C2C	2.14	1.49	1.45
26	3	612	CLA	CHC-C1C	2.14	1.41	1.35
30	B	2631	LHG	P-O6	2.14	1.68	1.59
25	2	605	CHL	CMC-C2C	2.14	1.49	1.45
30	b	2631	LHG	P-O6	2.14	1.68	1.59
25	6	605	CHL	CMC-C2C	2.15	1.49	1.45
26	5	603	CLA	CHC-C1C	2.15	1.41	1.35
26	1	603	CLA	CHC-C1C	2.15	1.41	1.35
25	8	601	CHL	CMC-C2C	2.15	1.49	1.45
26	a	407	CLA	CHC-C1C	2.15	1.41	1.35
25	4	601	CHL	CMC-C2C	2.16	1.49	1.45
26	A	407	CLA	CHC-C1C	2.17	1.41	1.35
26	r	616	CLA	CHC-C1C	2.17	1.41	1.35
26	b	611	CLA	CHC-C1C	2.17	1.41	1.35
26	B	612	CLA	CHC-C1C	2.17	1.41	1.35
26	b	612	CLA	CHC-C1C	2.17	1.41	1.35
26	b	614	CLA	CHC-C1C	2.18	1.41	1.35
26	B	614	CLA	CHC-C1C	2.18	1.41	1.35
26	S	610	CLA	CHB-C4A	2.18	1.36	1.33
26	R	616	CLA	CHC-C1C	2.19	1.41	1.35
26	B	611	CLA	CHC-C1C	2.19	1.41	1.35
26	s	603	CLA	CHC-C1C	2.20	1.41	1.35
26	S	603	CLA	CHC-C1C	2.20	1.41	1.35
25	2	608	CHL	CMC-C2C	2.21	1.49	1.45
25	6	608	CHL	CMC-C2C	2.21	1.49	1.45
25	2	609	CHL	CMC-C2C	2.21	1.49	1.45
25	6	609	CHL	CMC-C2C	2.21	1.49	1.45
26	B	604	CLA	CHC-C1C	2.21	1.41	1.35
25	r	608	CHL	OBD-CAD	2.21	1.25	1.21
25	Y	609	CHL	CMC-C2C	2.22	1.49	1.45
26	2	612	CLA	CHC-C1C	2.22	1.41	1.35
26	b	604	CLA	CHC-C1C	2.22	1.41	1.35
26	7	614	CLA	CHC-C1C	2.23	1.41	1.35
26	A	405	CLA	CHC-C1C	2.23	1.41	1.35
26	a	405	CLA	CHC-C1C	2.23	1.41	1.35
25	R	608	CHL	OBD-CAD	2.23	1.25	1.21
26	R	603	CLA	CHC-C1C	2.23	1.41	1.35
26	7	613	CLA	CHC-C1C	2.23	1.41	1.35
26	r	603	CLA	CHC-C1C	2.23	1.41	1.35
26	6	612	CLA	CHC-C1C	2.24	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	2633	LMG	C7-C8	2.24	1.57	1.50
26	c	513	CLA	CHC-C1C	2.24	1.41	1.35
26	s	610	CLA	CHB-C4A	2.24	1.36	1.33
26	Y	613	CLA	CHC-C1C	2.25	1.41	1.35
26	y	613	CLA	CHC-C1C	2.25	1.41	1.35
26	b	606	CLA	CHC-C1C	2.25	1.41	1.35
26	B	606	CLA	CHC-C1C	2.25	1.41	1.35
26	C	513	CLA	CHC-C1C	2.25	1.41	1.35
37	B	2633	LMG	C7-C8	2.25	1.57	1.50
26	N	613	CLA	CHC-C1C	2.25	1.41	1.35
26	n	613	CLA	CHC-C1C	2.25	1.41	1.35
26	3	613	CLA	CHC-C1C	2.25	1.41	1.35
26	3	614	CLA	CHC-C1C	2.25	1.41	1.35
25	3	609	CHL	CMC-C2C	2.25	1.49	1.45
25	7	609	CHL	CMC-C2C	2.25	1.49	1.45
26	s	611	CLA	CHC-C1C	2.25	1.41	1.35
26	8	604	CLA	CHC-C1C	2.25	1.41	1.35
26	4	604	CLA	CHC-C1C	2.25	1.41	1.35
26	N	610	CLA	CHC-C1C	2.25	1.41	1.35
26	n	610	CLA	CHC-C1C	2.25	1.41	1.35
26	Y	610	CLA	CHB-C4A	2.26	1.36	1.33
26	y	610	CLA	CHB-C4A	2.26	1.36	1.33
25	y	609	CHL	CMC-C2C	2.26	1.49	1.45
26	5	612	CLA	CHC-C1C	2.26	1.41	1.35
26	1	612	CLA	CHC-C1C	2.26	1.41	1.35
26	1	613	CLA	CHC-C1C	2.26	1.41	1.35
26	S	611	CLA	CHC-C1C	2.27	1.41	1.35
26	A	410	CLA	CHC-C1C	2.27	1.41	1.35
26	c	512	CLA	CHC-C1C	2.27	1.41	1.35
26	5	613	CLA	CHC-C1C	2.28	1.41	1.35
26	C	512	CLA	CHB-C4A	2.28	1.36	1.33
26	c	512	CLA	CHB-C4A	2.28	1.36	1.33
26	G	604	CLA	CHC-C1C	2.29	1.41	1.35
25	7	608	CHL	CMC-C2C	2.29	1.49	1.45
26	b	607	CLA	CHB-C4A	2.29	1.36	1.33
25	3	608	CHL	CMC-C2C	2.30	1.49	1.45
26	5	604	CLA	CHC-C1C	2.30	1.42	1.35
26	R	613	CLA	CHC-C1C	2.30	1.42	1.35
26	a	410	CLA	CHC-C1C	2.30	1.42	1.35
26	C	512	CLA	CHC-C1C	2.31	1.42	1.35
26	S	614	CLA	CHC-C1C	2.31	1.42	1.35
26	r	613	CLA	CHC-C1C	2.31	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	509	CLA	CHC-C1C	2.31	1.42	1.35
26	C	509	CLA	CHC-C1C	2.31	1.42	1.35
26	s	614	CLA	CHC-C1C	2.31	1.42	1.35
26	2	603	CLA	CHC-C1C	2.31	1.42	1.35
26	g	604	CLA	CHC-C1C	2.31	1.42	1.35
26	1	604	CLA	CHC-C1C	2.32	1.42	1.35
26	S	613	CLA	CHC-C1C	2.32	1.42	1.35
26	s	613	CLA	CHC-C1C	2.32	1.42	1.35
26	c	508	CLA	CHB-C4A	2.32	1.36	1.33
26	1	611	CLA	CHC-C1C	2.32	1.42	1.35
26	s	609	CLA	CHC-C1C	2.32	1.42	1.35
26	5	611	CLA	CHC-C1C	2.33	1.42	1.35
26	C	508	CLA	CHB-C4A	2.33	1.36	1.33
26	c	503	CLA	CHB-C4A	2.33	1.36	1.33
26	d	403	CLA	CHC-C1C	2.33	1.42	1.35
26	D	403	CLA	CHC-C1C	2.33	1.42	1.35
26	2	604	CLA	CHC-C1C	2.33	1.42	1.35
26	n	604	CLA	CHC-C1C	2.33	1.42	1.35
26	N	604	CLA	CHC-C1C	2.33	1.42	1.35
26	S	609	CLA	CHC-C1C	2.33	1.42	1.35
26	R	609	CLA	CHC-C1C	2.33	1.42	1.35
26	B	612	CLA	CHB-C4A	2.33	1.36	1.33
26	b	612	CLA	CHB-C4A	2.33	1.36	1.33
26	r	601	CLA	CHC-C1C	2.33	1.42	1.35
26	R	601	CLA	CHC-C1C	2.33	1.42	1.35
26	b	609	CLA	CHC-C1C	2.33	1.42	1.35
26	B	609	CLA	CHC-C1C	2.33	1.42	1.35
26	r	609	CLA	CHC-C1C	2.33	1.42	1.35
26	6	604	CLA	CHC-C1C	2.34	1.42	1.35
26	B	607	CLA	CHB-C4A	2.34	1.36	1.33
26	y	612	CLA	CHC-C1C	2.34	1.42	1.35
26	6	602	CLA	CHC-C1C	2.34	1.42	1.35
26	2	602	CLA	CHC-C1C	2.34	1.42	1.35
26	n	603	CLA	CHC-C1C	2.34	1.42	1.35
26	N	603	CLA	CHC-C1C	2.34	1.42	1.35
26	s	604	CLA	CHC-C1C	2.34	1.42	1.35
26	4	612	CLA	CHC-C1C	2.35	1.42	1.35
26	8	612	CLA	CHC-C1C	2.35	1.42	1.35
26	6	603	CLA	CHC-C1C	2.35	1.42	1.35
26	N	612	CLA	CHC-C1C	2.35	1.42	1.35
26	n	612	CLA	CHC-C1C	2.35	1.42	1.35
26	Y	612	CLA	CHC-C1C	2.35	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	603	CLA	CHC-C1C	2.35	1.42	1.35
25	g	609	CHL	CMC-C2C	2.36	1.49	1.45
26	8	611	CLA	CHC-C1C	2.36	1.42	1.35
26	S	604	CLA	CHC-C1C	2.36	1.42	1.35
25	G	609	CHL	CMC-C2C	2.36	1.49	1.45
26	4	611	CLA	CHC-C1C	2.36	1.42	1.35
26	5	610	CLA	CHC-C1C	2.37	1.42	1.35
26	C	503	CLA	CHB-C4A	2.37	1.36	1.33
26	C	501	CLA	CHC-C1C	2.37	1.42	1.35
26	c	501	CLA	CHC-C1C	2.37	1.42	1.35
26	C	510	CLA	CHC-C1C	2.37	1.42	1.35
26	c	510	CLA	CHC-C1C	2.37	1.42	1.35
26	y	614	CLA	CHC-C1C	2.37	1.42	1.35
26	Y	614	CLA	CHC-C1C	2.37	1.42	1.35
26	1	610	CLA	CHC-C1C	2.37	1.42	1.35
26	r	604	CLA	CHC-C1C	2.37	1.42	1.35
26	R	604	CLA	CHC-C1C	2.37	1.42	1.35
26	G	603	CLA	CHC-C1C	2.37	1.42	1.35
26	g	603	CLA	CHC-C1C	2.37	1.42	1.35
26	g	610	CLA	CHC-C1C	2.38	1.42	1.35
26	8	603	CLA	CHC-C1C	2.38	1.42	1.35
26	n	614	CLA	CHC-C1C	2.38	1.42	1.35
26	G	610	CLA	CHC-C1C	2.38	1.42	1.35
26	s	612	CLA	CHC-C1C	2.38	1.42	1.35
26	S	612	CLA	CHC-C1C	2.38	1.42	1.35
26	c	511	CLA	CHC-C1C	2.38	1.42	1.35
26	6	613	CLA	CHC-C1C	2.38	1.42	1.35
26	N	614	CLA	CHC-C1C	2.38	1.42	1.35
25	Y	601	CHL	CMC-C2C	2.38	1.49	1.45
25	y	601	CHL	CMC-C2C	2.38	1.49	1.45
26	y	611	CLA	CHC-C1C	2.38	1.42	1.35
26	C	511	CLA	CHC-C1C	2.38	1.42	1.35
26	Y	611	CLA	CHC-C1C	2.38	1.42	1.35
26	N	603	CLA	CHB-C4A	2.38	1.36	1.33
26	Y	602	CLA	CHC-C1C	2.38	1.42	1.35
26	3	602	CLA	CHC-C1C	2.39	1.42	1.35
26	2	613	CLA	CHC-C1C	2.39	1.42	1.35
26	7	602	CLA	CHC-C1C	2.39	1.42	1.35
26	g	612	CLA	CHC-C1C	2.40	1.42	1.35
26	G	612	CLA	CHC-C1C	2.40	1.42	1.35
26	G	602	CLA	CHC-C1C	2.40	1.42	1.35
26	n	603	CLA	CHB-C4A	2.40	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	602	CLA	CHC-C1C	2.40	1.42	1.35
26	g	602	CLA	CHC-C1C	2.40	1.42	1.35
26	b	613	CLA	CHC-C1C	2.41	1.42	1.35
26	1	614	CLA	CHC-C1C	2.41	1.42	1.35
26	y	602	CLA	CHC-C1C	2.41	1.42	1.35
26	2	610	CLA	CHC-C1C	2.41	1.42	1.35
26	D	402	CLA	CHC-C1C	2.41	1.42	1.35
26	d	402	CLA	CHC-C1C	2.41	1.42	1.35
26	6	610	CLA	CHC-C1C	2.42	1.42	1.35
26	5	614	CLA	CHC-C1C	2.42	1.42	1.35
26	6	611	CLA	CHC-C1C	2.42	1.42	1.35
26	2	611	CLA	CHC-C1C	2.42	1.42	1.35
26	B	602	CLA	CHC-C1C	2.42	1.42	1.35
26	B	613	CLA	CHC-C1C	2.42	1.42	1.35
26	n	602	CLA	CHC-C1C	2.43	1.42	1.35
26	N	602	CLA	CHC-C1C	2.43	1.42	1.35
26	Y	603	CLA	CHC-C1C	2.43	1.42	1.35
26	b	603	CLA	CHC-C1C	2.43	1.42	1.35
26	y	603	CLA	CHC-C1C	2.44	1.42	1.35
26	b	606	CLA	CHB-C4A	2.44	1.36	1.33
26	N	611	CLA	CHC-C1C	2.44	1.42	1.35
26	n	611	CLA	CHC-C1C	2.44	1.42	1.35
26	b	609	CLA	CHB-C4A	2.44	1.36	1.33
26	B	609	CLA	CHB-C4A	2.44	1.36	1.33
26	b	617	CLA	CHC-C1C	2.45	1.42	1.35
26	B	617	CLA	CHC-C1C	2.45	1.42	1.35
26	5	602	CLA	CHC-C1C	2.45	1.42	1.35
26	C	503	CLA	CHC-C1C	2.45	1.42	1.35
26	b	615	CLA	CHC-C1C	2.46	1.42	1.35
26	B	615	CLA	CHC-C1C	2.46	1.42	1.35
26	B	603	CLA	CHC-C1C	2.46	1.42	1.35
26	c	503	CLA	CHC-C1C	2.46	1.42	1.35
26	1	602	CLA	CHC-C1C	2.46	1.42	1.35
35	A	408	PHO	CHC-C1C	2.46	1.43	1.38
26	3	604	CLA	CHC-C1C	2.46	1.42	1.35
26	y	610	CLA	CHC-C1C	2.47	1.42	1.35
26	2	614	CLA	CHC-C1C	2.47	1.42	1.35
26	6	614	CLA	CHC-C1C	2.47	1.42	1.35
26	g	614	CLA	CHC-C1C	2.47	1.42	1.35
26	G	614	CLA	CHC-C1C	2.47	1.42	1.35
26	7	604	CLA	CHC-C1C	2.47	1.42	1.35
26	4	610	CLA	CHC-C1C	2.48	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	610	CLA	CHC-C1C	2.48	1.42	1.35
35	a	408	PHO	CHC-C1C	2.48	1.43	1.38
26	Y	610	CLA	CHC-C1C	2.48	1.42	1.35
26	8	602	CLA	CHC-C1C	2.49	1.42	1.35
26	4	602	CLA	CHC-C1C	2.49	1.42	1.35
26	y	603	CLA	CHB-C4A	2.49	1.36	1.33
26	Y	603	CLA	CHB-C4A	2.49	1.36	1.33
26	G	603	CLA	CHB-C4A	2.49	1.36	1.33
26	g	603	CLA	CHB-C4A	2.49	1.36	1.33
26	7	610	CLA	CHC-C1C	2.50	1.42	1.35
26	B	606	CLA	CHB-C4A	2.51	1.36	1.33
26	s	610	CLA	CHC-C1C	2.51	1.42	1.35
26	C	510	CLA	CHB-C4A	2.51	1.36	1.33
26	S	610	CLA	CHC-C1C	2.51	1.42	1.35
26	c	510	CLA	CHB-C4A	2.51	1.36	1.33
26	3	610	CLA	CHC-C1C	2.52	1.42	1.35
26	1	610	CLA	CHB-C4A	2.52	1.36	1.33
26	r	610	CLA	CHC-C1C	2.52	1.42	1.35
26	R	610	CLA	CHC-C1C	2.54	1.42	1.35
26	R	612	CLA	CHC-C1C	2.54	1.42	1.35
37	Z	101	LMG	C7-C8	2.54	1.57	1.50
37	z	101	LMG	C7-C8	2.54	1.57	1.50
26	R	602	CLA	CHC-C1C	2.55	1.42	1.35
36	a	412	SQD	O47-C7	2.55	1.41	1.34
26	r	612	CLA	CHC-C1C	2.56	1.42	1.35
36	A	412	SQD	O47-C7	2.56	1.41	1.34
26	b	611	CLA	CHB-C4A	2.56	1.36	1.33
26	B	611	CLA	CHB-C4A	2.56	1.36	1.33
26	5	610	CLA	CHB-C4A	2.57	1.36	1.33
26	r	602	CLA	CHC-C1C	2.58	1.42	1.35
26	7	610	CLA	CHB-C4A	2.59	1.36	1.33
26	3	610	CLA	CHB-C4A	2.60	1.36	1.33
26	G	613	CLA	CHC-C1C	2.62	1.42	1.35
26	Y	611	CLA	CHB-C4A	2.63	1.36	1.33
26	g	613	CLA	CHC-C1C	2.63	1.43	1.35
26	b	604	CLA	CHB-C4A	2.64	1.36	1.33
26	B	604	CLA	CHB-C4A	2.64	1.36	1.33
26	y	611	CLA	CHB-C4A	2.66	1.36	1.33
35	A	408	PHO	C3B-C4B	2.66	1.49	1.43
26	N	604	CLA	CHB-C4A	2.67	1.37	1.33
26	S	602	CLA	CHC-C1C	2.67	1.43	1.35
26	3	602	CLA	CHB-C4A	2.67	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	602	CLA	CHB-C4A	2.67	1.37	1.33
26	s	602	CLA	CHC-C1C	2.67	1.43	1.35
26	b	615	CLA	CHB-C4A	2.68	1.37	1.33
26	B	615	CLA	CHB-C4A	2.68	1.37	1.33
35	a	408	PHO	C3B-C4B	2.68	1.49	1.43
26	n	604	CLA	CHB-C4A	2.69	1.37	1.33
26	C	502	CLA	CHB-C4A	2.70	1.37	1.33
26	c	502	CLA	CHB-C4A	2.70	1.37	1.33
26	G	611	CLA	CHC-C1C	2.70	1.43	1.35
26	g	611	CLA	CHC-C1C	2.70	1.43	1.35
26	A	410	CLA	CHB-C4A	2.71	1.37	1.33
26	1	604	CLA	CHB-C4A	2.71	1.37	1.33
26	a	410	CLA	CHB-C4A	2.71	1.37	1.33
26	d	403	CLA	CHB-C4A	2.72	1.37	1.33
36	a	412	SQD	O48-C23	2.72	1.41	1.33
36	A	412	SQD	O48-C23	2.72	1.41	1.33
26	y	614	CLA	CHB-C4A	2.73	1.37	1.33
26	Y	614	CLA	CHB-C4A	2.73	1.37	1.33
26	D	403	CLA	CHB-C4A	2.73	1.37	1.33
26	R	610	CLA	CHB-C4A	2.73	1.37	1.33
26	3	613	CLA	CHB-C4A	2.74	1.37	1.33
26	s	614	CLA	CHB-C4A	2.76	1.37	1.33
26	5	604	CLA	CHB-C4A	2.76	1.37	1.33
26	7	613	CLA	CHB-C4A	2.77	1.37	1.33
26	d	402	CLA	CHB-C4A	2.77	1.37	1.33
36	B	621	SQD	O48-C23	2.78	1.41	1.33
26	S	614	CLA	CHB-C4A	2.78	1.37	1.33
26	r	610	CLA	CHB-C4A	2.78	1.37	1.33
26	A	406	CLA	CHB-C4A	2.79	1.37	1.33
26	a	406	CLA	CHB-C4A	2.79	1.37	1.33
36	b	621	SQD	O48-C23	2.79	1.41	1.33
26	b	608	CLA	CHB-C4A	2.80	1.37	1.33
26	6	610	CLA	CHB-C4A	2.82	1.37	1.33
26	2	610	CLA	CHB-C4A	2.83	1.37	1.33
26	B	617	CLA	CHB-C4A	2.84	1.37	1.33
26	D	402	CLA	CHB-C4A	2.84	1.37	1.33
36	a	418	SQD	O48-C23	2.85	1.41	1.33
26	B	613	CLA	CHB-C4A	2.86	1.37	1.33
26	b	613	CLA	CHB-C4A	2.86	1.37	1.33
26	C	504	CLA	CHB-C4A	2.86	1.37	1.33
26	B	608	CLA	CHB-C4A	2.86	1.37	1.33
36	A	418	SQD	O48-C23	2.86	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	617	CLA	CHB-C4A	2.87	1.37	1.33
35	A	409	PHO	CHC-C1C	2.88	1.44	1.38
36	A	418	SQD	O47-C7	2.88	1.42	1.34
36	a	418	SQD	O47-C7	2.88	1.42	1.34
35	a	409	PHO	CHC-C1C	2.88	1.44	1.38
26	c	501	CLA	CHB-C4A	2.89	1.37	1.33
26	c	504	CLA	CHB-C4A	2.89	1.37	1.33
26	n	614	CLA	CHB-C4A	2.90	1.37	1.33
26	7	612	CLA	CHB-C4A	2.92	1.37	1.33
26	G	602	CLA	CHB-C4A	2.92	1.37	1.33
26	g	602	CLA	CHB-C4A	2.92	1.37	1.33
26	N	614	CLA	CHB-C4A	2.93	1.37	1.33
26	A	407	CLA	CHB-C4A	2.94	1.37	1.33
26	a	407	CLA	CHB-C4A	2.94	1.37	1.33
26	3	612	CLA	CHB-C4A	2.95	1.37	1.33
26	3	604	CLA	CHB-C4A	2.95	1.37	1.33
26	C	501	CLA	CHB-C4A	2.95	1.37	1.33
26	n	602	CLA	CHB-C4A	2.96	1.37	1.33
26	c	509	CLA	CHB-C4A	2.96	1.37	1.33
26	N	602	CLA	CHB-C4A	2.98	1.37	1.33
26	C	509	CLA	CHB-C4A	2.99	1.37	1.33
36	b	623	SQD	O47-C7	2.99	1.43	1.34
36	b	621	SQD	O47-C7	2.99	1.43	1.34
36	B	623	SQD	O47-C7	3.00	1.43	1.34
26	C	511	CLA	CHB-C4A	3.01	1.37	1.33
26	c	511	CLA	CHB-C4A	3.01	1.37	1.33
26	7	604	CLA	CHB-C4A	3.01	1.37	1.33
36	B	621	SQD	O47-C7	3.01	1.43	1.34
26	1	602	CLA	CHB-C4A	3.02	1.37	1.33
26	5	602	CLA	CHB-C4A	3.02	1.37	1.33
26	6	603	CLA	CHB-C4A	3.03	1.37	1.33
26	2	603	CLA	CHB-C4A	3.03	1.37	1.33
26	g	611	CLA	CHB-C4A	3.04	1.37	1.33
26	y	612	CLA	CHB-C4A	3.05	1.37	1.33
26	G	604	CLA	CHB-C4A	3.05	1.37	1.33
26	g	604	CLA	CHB-C4A	3.05	1.37	1.33
26	3	603	CLA	CHB-C4A	3.06	1.37	1.33
26	4	610	CLA	CHB-C4A	3.06	1.37	1.33
26	b	616	CLA	CHB-C4A	3.06	1.37	1.33
26	Y	612	CLA	CHB-C4A	3.06	1.37	1.33
26	B	616	CLA	CHB-C4A	3.06	1.37	1.33
25	y	608	CHL	OBD-CAD	3.06	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	603	CLA	CHB-C4A	3.07	1.37	1.33
26	2	613	CLA	CHB-C4A	3.07	1.37	1.33
25	Y	608	CHL	OBD-CAD	3.07	1.26	1.21
26	8	604	CLA	CHB-C4A	3.07	1.37	1.33
26	8	610	CLA	CHB-C4A	3.08	1.37	1.33
26	1	613	CLA	CHB-C4A	3.09	1.37	1.33
26	5	613	CLA	CHB-C4A	3.09	1.37	1.33
26	G	611	CLA	CHB-C4A	3.09	1.37	1.33
26	6	613	CLA	CHB-C4A	3.09	1.37	1.33
26	4	604	CLA	CHB-C4A	3.09	1.37	1.33
26	2	614	CLA	CHB-C4A	3.10	1.37	1.33
26	B	605	CLA	CHB-C4A	3.11	1.37	1.33
26	4	603	CLA	CHB-C4A	3.11	1.37	1.33
26	1	612	CLA	CHB-C4A	3.11	1.37	1.33
26	5	612	CLA	CHB-C4A	3.11	1.37	1.33
26	8	602	CLA	CHB-C4A	3.12	1.37	1.33
26	n	610	CLA	CHB-C4A	3.12	1.37	1.33
26	b	605	CLA	CHB-C4A	3.12	1.37	1.33
26	6	614	CLA	CHB-C4A	3.14	1.37	1.33
26	r	603	CLA	CHB-C4A	3.14	1.37	1.33
26	R	603	CLA	CHB-C4A	3.14	1.37	1.33
26	8	603	CLA	CHB-C4A	3.15	1.37	1.33
26	N	610	CLA	CHB-C4A	3.16	1.37	1.33
26	2	611	CLA	CHB-C4A	3.16	1.37	1.33
26	6	602	CLA	CHB-C4A	3.16	1.37	1.33
25	G	601	CHL	OBD-CAD	3.16	1.26	1.21
25	g	601	CHL	OBD-CAD	3.16	1.26	1.21
25	Y	606	CHL	OBD-CAD	3.17	1.27	1.21
26	c	513	CLA	CHB-C4A	3.17	1.37	1.33
25	y	606	CHL	OBD-CAD	3.17	1.27	1.21
26	6	611	CLA	CHB-C4A	3.17	1.37	1.33
26	4	602	CLA	CHB-C4A	3.17	1.37	1.33
26	2	602	CLA	CHB-C4A	3.19	1.37	1.33
36	B	623	SQD	O48-C23	3.19	1.42	1.33
26	C	513	CLA	CHB-C4A	3.19	1.37	1.33
36	b	623	SQD	O48-C23	3.20	1.42	1.33
26	c	507	CLA	CHB-C4A	3.20	1.37	1.33
26	C	507	CLA	CHB-C4A	3.20	1.37	1.33
26	s	603	CLA	CHB-C4A	3.21	1.37	1.33
26	3	614	CLA	CHB-C4A	3.21	1.37	1.33
26	7	614	CLA	CHB-C4A	3.21	1.37	1.33
26	y	613	CLA	CHB-C4A	3.22	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	613	CLA	CHB-C4A	3.23	1.37	1.33
26	b	603	CLA	CHB-C4A	3.23	1.37	1.33
26	B	603	CLA	CHB-C4A	3.23	1.37	1.33
35	A	409	PHO	C3B-C4B	3.23	1.50	1.43
25	3	608	CHL	OBD-CAD	3.24	1.27	1.21
26	r	609	CLA	CHB-C4A	3.24	1.37	1.33
26	s	612	CLA	CHB-C4A	3.24	1.37	1.33
26	S	612	CLA	CHB-C4A	3.24	1.37	1.33
26	8	612	CLA	CHB-C4A	3.24	1.37	1.33
26	C	506	CLA	CHB-C4A	3.25	1.37	1.33
25	7	608	CHL	OBD-CAD	3.25	1.27	1.21
26	4	612	CLA	CHB-C4A	3.26	1.37	1.33
26	S	603	CLA	CHB-C4A	3.26	1.37	1.33
25	8	608	CHL	OBD-CAD	3.26	1.27	1.21
35	a	409	PHO	C3B-C4B	3.27	1.50	1.43
26	Y	604	CLA	CHB-C4A	3.27	1.37	1.33
26	N	612	CLA	CHB-C4A	3.27	1.37	1.33
26	n	612	CLA	CHB-C4A	3.27	1.37	1.33
25	4	608	CHL	OBD-CAD	3.27	1.27	1.21
26	S	613	CLA	CHB-C4A	3.28	1.37	1.33
26	s	613	CLA	CHB-C4A	3.28	1.37	1.33
26	R	609	CLA	CHB-C4A	3.28	1.37	1.33
26	R	612	CLA	CHB-C4A	3.28	1.37	1.33
26	c	506	CLA	CHB-C4A	3.28	1.37	1.33
26	y	604	CLA	CHB-C4A	3.31	1.37	1.33
26	r	612	CLA	CHB-C4A	3.31	1.37	1.33
26	6	604	CLA	CHB-C4A	3.31	1.37	1.33
26	g	613	CLA	CHB-C4A	3.31	1.37	1.33
26	G	613	CLA	CHB-C4A	3.31	1.37	1.33
26	5	603	CLA	CHB-C4A	3.31	1.37	1.33
25	N	608	CHL	OBD-CAD	3.33	1.27	1.21
25	n	608	CHL	OBD-CAD	3.33	1.27	1.21
26	a	405	CLA	CHB-C4A	3.33	1.37	1.33
26	2	604	CLA	CHB-C4A	3.33	1.37	1.33
26	B	602	CLA	CHB-C4A	3.33	1.37	1.33
26	b	602	CLA	CHB-C4A	3.33	1.37	1.33
26	5	614	CLA	CHB-C4A	3.34	1.37	1.33
26	1	611	CLA	CHB-C4A	3.35	1.37	1.33
26	5	611	CLA	CHB-C4A	3.35	1.37	1.33
26	G	612	CLA	CHB-C4A	3.35	1.37	1.33
26	s	609	CLA	CHB-C4A	3.35	1.37	1.33
25	Y	601	CHL	OBD-CAD	3.36	1.27	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	609	CLA	CHB-C4A	3.36	1.37	1.33
26	A	405	CLA	CHB-C4A	3.36	1.37	1.33
26	l	614	CLA	CHB-C4A	3.36	1.37	1.33
25	y	601	CHL	OBD-CAD	3.36	1.27	1.21
26	c	505	CLA	CHB-C4A	3.37	1.37	1.33
26	l	603	CLA	CHB-C4A	3.37	1.37	1.33
26	g	612	CLA	CHB-C4A	3.38	1.37	1.33
26	R	602	CLA	CHB-C4A	3.39	1.37	1.33
26	r	602	CLA	CHB-C4A	3.39	1.37	1.33
25	g	608	CHL	OBD-CAD	3.39	1.27	1.21
26	S	604	CLA	CHB-C4A	3.39	1.37	1.33
25	G	608	CHL	OBD-CAD	3.40	1.27	1.21
25	n	601	CHL	OBD-CAD	3.40	1.27	1.21
25	N	601	CHL	OBD-CAD	3.41	1.27	1.21
26	G	610	CLA	CHB-C4A	3.41	1.37	1.33
26	g	610	CLA	CHB-C4A	3.41	1.37	1.33
26	C	505	CLA	CHB-C4A	3.43	1.37	1.33
26	2	612	CLA	CHB-C4A	3.43	1.37	1.33
26	6	612	CLA	CHB-C4A	3.43	1.37	1.33
26	s	604	CLA	CHB-C4A	3.43	1.37	1.33
26	B	614	CLA	CHB-C4A	3.45	1.37	1.33
26	g	614	CLA	CHB-C4A	3.45	1.37	1.33
26	4	611	CLA	CHB-C4A	3.45	1.37	1.33
26	8	611	CLA	CHB-C4A	3.46	1.37	1.33
26	R	611	CLA	CHB-C4A	3.46	1.37	1.33
26	r	613	CLA	CHB-C4A	3.47	1.38	1.33
26	R	604	CLA	CHB-C4A	3.48	1.38	1.33
26	b	614	CLA	CHB-C4A	3.48	1.38	1.33
26	y	602	CLA	CHB-C4A	3.48	1.38	1.33
26	Y	602	CLA	CHB-C4A	3.48	1.38	1.33
26	r	611	CLA	CHB-C4A	3.49	1.38	1.33
26	G	614	CLA	CHB-C4A	3.50	1.38	1.33
26	S	602	CLA	CHB-C4A	3.50	1.38	1.33
26	R	613	CLA	CHB-C4A	3.52	1.38	1.33
26	r	604	CLA	CHB-C4A	3.52	1.38	1.33
26	B	610	CLA	CHB-C4A	3.53	1.38	1.33
25	S	601	CHL	OBD-CAD	3.55	1.27	1.21
25	s	601	CHL	OBD-CAD	3.55	1.27	1.21
26	s	602	CLA	CHB-C4A	3.55	1.38	1.33
26	b	610	CLA	CHB-C4A	3.57	1.38	1.33
25	2	608	CHL	OBD-CAD	3.61	1.27	1.21
25	6	608	CHL	OBD-CAD	3.61	1.27	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	608	CHL	OBD-CAD	3.63	1.27	1.21
25	1	608	CHL	OBD-CAD	3.63	1.27	1.21
25	3	601	CHL	OBD-CAD	3.68	1.27	1.21
25	7	601	CHL	OBD-CAD	3.68	1.27	1.21
25	2	601	CHL	OBD-CAD	3.68	1.27	1.21
25	6	601	CHL	OBD-CAD	3.68	1.27	1.21
25	3	606	CHL	OBD-CAD	3.70	1.27	1.21
25	N	606	CHL	OBD-CAD	3.70	1.27	1.21
26	n	613	CLA	CHB-C4A	3.72	1.38	1.33
25	y	609	CHL	OBD-CAD	3.72	1.27	1.21
25	7	606	CHL	OBD-CAD	3.73	1.27	1.21
25	Y	609	CHL	OBD-CAD	3.73	1.27	1.21
26	7	611	CLA	CHB-C4A	3.73	1.38	1.33
25	n	606	CHL	OBD-CAD	3.74	1.27	1.21
26	N	613	CLA	CHB-C4A	3.74	1.38	1.33
26	3	611	CLA	CHB-C4A	3.76	1.38	1.33
26	r	601	CLA	CHB-C4A	3.77	1.38	1.33
26	R	601	CLA	CHB-C4A	3.77	1.38	1.33
25	y	607	CHL	O2A-CGA	3.82	1.44	1.33
25	Y	607	CHL	O2A-CGA	3.82	1.44	1.33
25	Y	607	CHL	OBD-CAD	3.85	1.28	1.21
25	Y	605	CHL	OBD-CAD	3.85	1.28	1.21
26	r	616	CLA	CHB-C4A	3.86	1.38	1.33
25	5	601	CHL	OBD-CAD	3.86	1.28	1.21
25	y	605	CHL	OBD-CAD	3.87	1.28	1.21
25	y	607	CHL	OBD-CAD	3.87	1.28	1.21
26	R	616	CLA	CHB-C4A	3.89	1.38	1.33
26	N	611	CLA	CHB-C4A	3.90	1.38	1.33
26	n	611	CLA	CHB-C4A	3.90	1.38	1.33
25	S	608	CHL	OBD-CAD	3.91	1.28	1.21
25	s	608	CHL	OBD-CAD	3.91	1.28	1.21
25	4	609	CHL	OBD-CAD	3.92	1.28	1.21
25	1	601	CHL	OBD-CAD	3.92	1.28	1.21
25	y	608	CHL	O2A-CGA	3.93	1.44	1.33
25	Y	608	CHL	O2A-CGA	3.93	1.44	1.33
25	N	609	CHL	OBD-CAD	3.93	1.28	1.21
25	8	609	CHL	OBD-CAD	3.95	1.28	1.21
25	N	608	CHL	O2A-CGA	3.95	1.45	1.33
25	G	601	CHL	O2A-CGA	3.95	1.45	1.33
25	g	601	CHL	O2A-CGA	3.96	1.45	1.33
25	G	609	CHL	OBD-CAD	3.96	1.28	1.21
25	5	609	CHL	OBD-CAD	3.96	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	609	CHL	OBD-CAD	3.96	1.28	1.21
25	n	609	CHL	OBD-CAD	3.96	1.28	1.21
25	n	608	CHL	O2A-CGA	3.97	1.45	1.33
25	g	609	CHL	OBD-CAD	3.97	1.28	1.21
25	N	607	CHL	OBD-CAD	3.99	1.28	1.21
25	n	607	CHL	OBD-CAD	3.99	1.28	1.21
25	R	606	CHL	OBD-CAD	4.00	1.28	1.21
25	1	606	CHL	OBD-CAD	4.00	1.28	1.21
25	5	606	CHL	OBD-CAD	4.00	1.28	1.21
26	s	611	CLA	CHB-C4A	4.02	1.38	1.33
26	S	611	CLA	CHB-C4A	4.02	1.38	1.33
25	5	605	CHL	OBD-CAD	4.02	1.28	1.21
25	r	606	CHL	OBD-CAD	4.03	1.28	1.21
25	1	607	CHL	OBD-CAD	4.04	1.28	1.21
25	1	605	CHL	OBD-CAD	4.04	1.28	1.21
25	5	607	CHL	OBD-CAD	4.04	1.28	1.21
25	6	607	CHL	OBD-CAD	4.05	1.28	1.21
41	f	101	HEM	C3C-CAC	4.07	1.55	1.47
41	F	101	HEM	C3C-CAC	4.07	1.55	1.47
25	5	607	CHL	O2A-CGA	4.08	1.45	1.33
25	7	601	CHL	O2A-CGA	4.09	1.45	1.33
25	G	607	CHL	O2A-CGA	4.09	1.45	1.33
25	g	607	CHL	O2A-CGA	4.09	1.45	1.33
25	1	607	CHL	O2A-CGA	4.09	1.45	1.33
25	3	609	CHL	OBD-CAD	4.09	1.28	1.21
25	7	609	CHL	OBD-CAD	4.09	1.28	1.21
25	Y	601	CHL	O2A-CGA	4.10	1.45	1.33
25	2	607	CHL	OBD-CAD	4.10	1.28	1.21
25	y	601	CHL	O2A-CGA	4.10	1.45	1.33
25	3	607	CHL	OBD-CAD	4.11	1.28	1.21
25	g	608	CHL	O2A-CGA	4.11	1.45	1.33
25	3	601	CHL	O2A-CGA	4.12	1.45	1.33
25	g	607	CHL	OBD-CAD	4.12	1.28	1.21
25	7	605	CHL	OBD-CAD	4.12	1.28	1.21
25	G	608	CHL	O2A-CGA	4.13	1.45	1.33
25	n	601	CHL	O2A-CGA	4.13	1.45	1.33
25	8	607	CHL	OBD-CAD	4.13	1.28	1.21
25	G	607	CHL	OBD-CAD	4.14	1.28	1.21
25	N	601	CHL	O2A-CGA	4.14	1.45	1.33
25	7	607	CHL	OBD-CAD	4.14	1.28	1.21
25	2	606	CHL	OBD-CAD	4.15	1.28	1.21
25	6	605	CHL	OBD-CAD	4.15	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	606	CHL	O2A-CGA	4.15	1.45	1.33
25	4	607	CHL	OBD-CAD	4.15	1.28	1.21
25	4	606	CHL	OBD-CAD	4.15	1.28	1.21
25	8	606	CHL	OBD-CAD	4.15	1.28	1.21
25	R	606	CHL	O2A-CGA	4.16	1.45	1.33
41	f	101	HEM	C3B-CAB	4.17	1.56	1.47
25	s	607	CHL	OBD-CAD	4.18	1.28	1.21
25	y	609	CHL	O2A-CGA	4.18	1.45	1.33
25	Y	609	CHL	O2A-CGA	4.18	1.45	1.33
41	F	101	HEM	C3B-CAB	4.18	1.56	1.47
25	S	606	CHL	OBD-CAD	4.18	1.28	1.21
25	s	606	CHL	OBD-CAD	4.18	1.28	1.21
25	R	608	CHL	O2A-CGA	4.18	1.45	1.33
25	r	608	CHL	O2A-CGA	4.18	1.45	1.33
25	S	607	CHL	OBD-CAD	4.18	1.28	1.21
25	2	609	CHL	O2A-CGA	4.18	1.45	1.33
25	6	609	CHL	O2A-CGA	4.18	1.45	1.33
25	3	605	CHL	OBD-CAD	4.19	1.28	1.21
25	8	601	CHL	OBD-CAD	4.19	1.28	1.21
25	6	606	CHL	OBD-CAD	4.19	1.28	1.21
25	4	601	CHL	OBD-CAD	4.19	1.28	1.21
25	2	605	CHL	OBD-CAD	4.19	1.28	1.21
25	6	607	CHL	O2A-CGA	4.20	1.45	1.33
25	2	607	CHL	O2A-CGA	4.21	1.45	1.33
25	N	607	CHL	O2A-CGA	4.22	1.45	1.33
25	n	607	CHL	O2A-CGA	4.22	1.45	1.33
25	r	607	CHL	O2A-CGA	4.23	1.45	1.33
25	2	609	CHL	OBD-CAD	4.24	1.28	1.21
25	6	609	CHL	OBD-CAD	4.24	1.28	1.21
25	R	607	CHL	O2A-CGA	4.24	1.45	1.33
25	G	609	CHL	O2A-CGA	4.25	1.45	1.33
25	R	607	CHL	OBD-CAD	4.27	1.28	1.21
25	N	609	CHL	O2A-CGA	4.28	1.45	1.33
25	g	609	CHL	O2A-CGA	4.28	1.45	1.33
25	5	609	CHL	O2A-CGA	4.28	1.45	1.33
25	r	607	CHL	OBD-CAD	4.28	1.28	1.21
25	n	609	CHL	O2A-CGA	4.30	1.46	1.33
25	1	609	CHL	O2A-CGA	4.30	1.46	1.33
25	G	606	CHL	OBD-CAD	4.30	1.28	1.21
25	g	606	CHL	OBD-CAD	4.30	1.28	1.21
25	N	606	CHL	O2A-CGA	4.34	1.46	1.33
25	n	606	CHL	O2A-CGA	4.35	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	605	CHL	O2A-CGA	4.35	1.46	1.33
25	Y	605	CHL	O2A-CGA	4.35	1.46	1.33
25	Y	606	CHL	O2A-CGA	4.41	1.46	1.33
25	y	606	CHL	O2A-CGA	4.41	1.46	1.33
25	3	609	CHL	O2A-CGA	4.43	1.46	1.33
25	7	609	CHL	O2A-CGA	4.43	1.46	1.33
25	S	607	CHL	O2A-CGA	4.44	1.46	1.33
25	s	607	CHL	O2A-CGA	4.44	1.46	1.33
25	S	608	CHL	O2D-CGD	4.44	1.44	1.33
25	s	608	CHL	O2D-CGD	4.45	1.44	1.33
25	G	605	CHL	OBD-CAD	4.45	1.29	1.21
25	G	606	CHL	O2A-CGA	4.46	1.46	1.33
25	g	606	CHL	O2A-CGA	4.46	1.46	1.33
25	N	605	CHL	OBD-CAD	4.47	1.29	1.21
25	n	605	CHL	OBD-CAD	4.47	1.29	1.21
25	N	607	CHL	O2D-CGD	4.49	1.44	1.33
25	n	607	CHL	O2D-CGD	4.49	1.44	1.33
25	Y	608	CHL	O2D-CGD	4.50	1.44	1.33
25	g	605	CHL	OBD-CAD	4.50	1.29	1.21
25	Y	607	CHL	O2D-CGD	4.51	1.44	1.33
25	N	605	CHL	O2A-CGA	4.51	1.46	1.33
25	n	605	CHL	O2A-CGA	4.51	1.46	1.33
25	r	614	CHL	O2D-CGD	4.51	1.44	1.33
25	R	614	CHL	O2D-CGD	4.51	1.44	1.33
25	Y	601	CHL	O2D-CGD	4.51	1.44	1.33
25	y	608	CHL	O2D-CGD	4.52	1.44	1.33
25	y	601	CHL	O2D-CGD	4.53	1.44	1.33
25	y	607	CHL	O2D-CGD	4.54	1.44	1.33
25	Y	609	CHL	O2D-CGD	4.56	1.44	1.33
25	g	607	CHL	O2D-CGD	4.58	1.44	1.33
25	y	609	CHL	O2D-CGD	4.58	1.44	1.33
25	g	605	CHL	O2D-CGD	4.58	1.44	1.33
25	R	606	CHL	O2D-CGD	4.59	1.44	1.33
25	r	614	CHL	OBD-CAD	4.59	1.29	1.21
25	R	614	CHL	OBD-CAD	4.59	1.29	1.21
25	5	609	CHL	O2D-CGD	4.59	1.44	1.33
25	G	605	CHL	O2D-CGD	4.60	1.44	1.33
25	1	609	CHL	O2D-CGD	4.61	1.44	1.33
25	G	607	CHL	O2D-CGD	4.61	1.44	1.33
25	r	606	CHL	O2D-CGD	4.62	1.44	1.33
25	7	608	CHL	O2D-CGD	4.62	1.44	1.33
25	3	608	CHL	O2D-CGD	4.63	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	608	CHL	O2D-CGD	4.64	1.45	1.33
25	5	608	CHL	O2D-CGD	4.64	1.45	1.33
25	1	608	CHL	O2D-CGD	4.64	1.45	1.33
25	Y	605	CHL	O2D-CGD	4.65	1.45	1.33
25	Y	606	CHL	O2D-CGD	4.65	1.45	1.33
25	y	606	CHL	O2D-CGD	4.65	1.45	1.33
25	y	605	CHL	O2D-CGD	4.66	1.45	1.33
25	g	609	CHL	O2D-CGD	4.66	1.45	1.33
25	2	608	CHL	O2D-CGD	4.66	1.45	1.33
25	G	609	CHL	O2D-CGD	4.67	1.45	1.33
25	5	607	CHL	O2D-CGD	4.67	1.45	1.33
25	1	607	CHL	O2D-CGD	4.69	1.45	1.33
25	7	609	CHL	O2D-CGD	4.73	1.45	1.33
25	2	609	CHL	O2D-CGD	4.73	1.45	1.33
25	6	609	CHL	O2D-CGD	4.73	1.45	1.33
25	3	609	CHL	O2D-CGD	4.75	1.45	1.33
25	8	609	CHL	O2D-CGD	4.76	1.45	1.33
25	1	605	CHL	O2D-CGD	4.79	1.45	1.33
25	4	609	CHL	O2D-CGD	4.79	1.45	1.33
25	5	605	CHL	O2D-CGD	4.79	1.45	1.33
25	7	601	CHL	O2D-CGD	4.80	1.45	1.33
25	3	601	CHL	O2D-CGD	4.80	1.45	1.33
25	7	607	CHL	O2A-CGA	4.80	1.47	1.33
25	3	607	CHL	O2A-CGA	4.80	1.47	1.33
25	4	608	CHL	O2D-CGD	4.80	1.45	1.33
25	g	608	CHL	O2D-CGD	4.81	1.45	1.33
25	G	608	CHL	O2D-CGD	4.81	1.45	1.33
25	S	606	CHL	O2D-CGD	4.81	1.45	1.33
25	8	606	CHL	O2D-CGD	4.81	1.45	1.33
25	s	606	CHL	O2D-CGD	4.81	1.45	1.33
25	N	609	CHL	O2D-CGD	4.81	1.45	1.33
25	g	601	CHL	O2D-CGD	4.81	1.45	1.33
25	8	608	CHL	O2D-CGD	4.82	1.45	1.33
25	N	605	CHL	O2D-CGD	4.82	1.45	1.33
25	n	605	CHL	O2D-CGD	4.82	1.45	1.33
25	6	607	CHL	O2D-CGD	4.82	1.45	1.33
25	R	608	CHL	O2D-CGD	4.82	1.45	1.33
25	r	608	CHL	O2D-CGD	4.82	1.45	1.33
25	4	606	CHL	O2D-CGD	4.82	1.45	1.33
25	2	607	CHL	O2D-CGD	4.83	1.45	1.33
25	G	601	CHL	O2D-CGD	4.83	1.45	1.33
25	N	608	CHL	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	606	CHL	O2D-CGD	4.84	1.45	1.33
25	n	609	CHL	O2D-CGD	4.84	1.45	1.33
25	3	606	CHL	O2D-CGD	4.85	1.45	1.33
25	7	607	CHL	O2D-CGD	4.86	1.45	1.33
25	3	607	CHL	O2D-CGD	4.86	1.45	1.33
25	N	606	CHL	O2D-CGD	4.86	1.45	1.33
25	n	608	CHL	O2D-CGD	4.86	1.45	1.33
25	n	606	CHL	O2D-CGD	4.88	1.45	1.33
25	1	606	CHL	O2D-CGD	4.89	1.45	1.33
25	R	607	CHL	O2D-CGD	4.89	1.45	1.33
25	5	606	CHL	O2D-CGD	4.89	1.45	1.33
25	r	607	CHL	O2D-CGD	4.91	1.45	1.33
25	2	606	CHL	O2D-CGD	4.91	1.45	1.33
25	6	601	CHL	O2D-CGD	4.91	1.45	1.33
25	S	607	CHL	O2D-CGD	4.91	1.45	1.33
25	s	607	CHL	O2D-CGD	4.91	1.45	1.33
25	6	606	CHL	O2D-CGD	4.91	1.45	1.33
25	1	601	CHL	O2D-CGD	4.92	1.45	1.33
25	6	605	CHL	O2D-CGD	4.92	1.45	1.33
25	N	601	CHL	O2D-CGD	4.92	1.45	1.33
25	4	607	CHL	O2D-CGD	4.92	1.45	1.33
25	8	607	CHL	O2D-CGD	4.92	1.45	1.33
25	S	601	CHL	O2D-CGD	4.94	1.45	1.33
25	2	601	CHL	O2D-CGD	4.94	1.45	1.33
25	n	601	CHL	O2D-CGD	4.94	1.45	1.33
25	5	601	CHL	O2D-CGD	4.95	1.45	1.33
25	2	605	CHL	O2D-CGD	4.95	1.45	1.33
25	s	601	CHL	O2D-CGD	4.95	1.45	1.33
25	3	605	CHL	O2D-CGD	4.96	1.45	1.33
25	7	605	CHL	O2D-CGD	4.96	1.45	1.33
25	g	606	CHL	O2D-CGD	5.08	1.46	1.33
25	G	606	CHL	O2D-CGD	5.12	1.46	1.33
25	3	606	CHL	C3C-C2C	8.43	1.44	1.34
25	7	606	CHL	C3C-C2C	8.48	1.45	1.34
25	s	607	CHL	C3C-C2C	8.61	1.45	1.34
25	n	601	CHL	C3C-C2C	8.64	1.45	1.34
25	N	601	CHL	C3C-C2C	8.64	1.45	1.34
25	Y	601	CHL	C3C-C2C	8.64	1.45	1.34
25	S	607	CHL	C3C-C2C	8.65	1.45	1.34
25	y	601	CHL	C3C-C2C	8.65	1.45	1.34
25	y	608	CHL	C3C-C2C	8.67	1.45	1.34
25	Y	608	CHL	C3C-C2C	8.70	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	606	CHL	C3C-C2C	8.71	1.45	1.34
25	Y	606	CHL	C3C-C2C	8.72	1.45	1.34
25	G	601	CHL	C3C-C2C	8.87	1.45	1.34
25	g	601	CHL	C3C-C2C	8.87	1.45	1.34
25	n	608	CHL	C3C-C2C	8.87	1.45	1.34
25	7	601	CHL	C3C-C2C	8.88	1.45	1.34
25	3	601	CHL	C3C-C2C	8.89	1.45	1.34
25	N	608	CHL	C3C-C2C	8.93	1.45	1.34
25	Y	607	CHL	C3C-C2C	9.04	1.45	1.34
25	y	607	CHL	C3C-C2C	9.05	1.45	1.34
25	1	605	CHL	C3C-C2C	9.10	1.45	1.34
25	4	608	CHL	C3C-C2C	9.10	1.45	1.34
25	5	605	CHL	C3C-C2C	9.10	1.45	1.34
25	6	601	CHL	C3C-C2C	9.11	1.45	1.34
25	2	601	CHL	C3C-C2C	9.12	1.45	1.34
25	1	608	CHL	C3C-C2C	9.12	1.45	1.34
25	N	607	CHL	C3C-C2C	9.15	1.45	1.34
25	n	607	CHL	C3C-C2C	9.15	1.45	1.34
25	8	608	CHL	C3C-C2C	9.16	1.45	1.34
25	5	608	CHL	C3C-C2C	9.16	1.45	1.34
25	r	607	CHL	C3C-C2C	9.19	1.45	1.34
25	R	607	CHL	C3C-C2C	9.22	1.45	1.34
25	g	605	CHL	C3C-C2C	9.23	1.45	1.34
25	G	605	CHL	C3C-C2C	9.28	1.46	1.34
25	1	606	CHL	C3C-C2C	9.29	1.46	1.34
25	5	606	CHL	C3C-C2C	9.29	1.46	1.34
25	r	608	CHL	C3C-C2C	9.31	1.46	1.34
25	6	607	CHL	C3C-C2C	9.32	1.46	1.34
25	Y	605	CHL	C3C-C2C	9.34	1.46	1.34
25	R	608	CHL	C3C-C2C	9.34	1.46	1.34
25	6	608	CHL	C3C-C2C	9.37	1.46	1.34
25	y	605	CHL	C3C-C2C	9.37	1.46	1.34
25	2	607	CHL	C3C-C2C	9.39	1.46	1.34
25	3	608	CHL	C3C-C2C	9.39	1.46	1.34
25	N	609	CHL	C3C-C2C	9.40	1.46	1.34
25	2	608	CHL	C3C-C2C	9.40	1.46	1.34
25	7	608	CHL	C3C-C2C	9.42	1.46	1.34
25	n	609	CHL	C3C-C2C	9.43	1.46	1.34
25	s	606	CHL	C3C-C2C	9.44	1.46	1.34
25	y	609	CHL	C3C-C2C	9.44	1.46	1.34
25	4	609	CHL	C3C-C2C	9.45	1.46	1.34
25	N	605	CHL	C3C-C2C	9.45	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	605	CHL	C3C-C2C	9.45	1.46	1.34
25	G	608	CHL	C3C-C2C	9.45	1.46	1.34
25	Y	609	CHL	C3C-C2C	9.45	1.46	1.34
25	8	609	CHL	C3C-C2C	9.45	1.46	1.34
25	S	606	CHL	C3C-C2C	9.46	1.46	1.34
25	g	608	CHL	C3C-C2C	9.47	1.46	1.34
25	G	606	CHL	C3C-C2C	9.48	1.46	1.34
25	g	606	CHL	C3C-C2C	9.48	1.46	1.34
25	5	607	CHL	C3C-C2C	9.49	1.46	1.34
25	5	609	CHL	C3C-C2C	9.51	1.46	1.34
25	1	609	CHL	C3C-C2C	9.51	1.46	1.34
25	5	601	CHL	C3C-C2C	9.51	1.46	1.34
25	1	607	CHL	C3C-C2C	9.52	1.46	1.34
25	1	601	CHL	C3C-C2C	9.53	1.46	1.34
25	8	607	CHL	C3C-C2C	9.55	1.46	1.34
25	3	605	CHL	C3C-C2C	9.56	1.46	1.34
25	7	605	CHL	C3C-C2C	9.57	1.46	1.34
25	G	607	CHL	C3C-C2C	9.58	1.46	1.34
25	g	607	CHL	C3C-C2C	9.58	1.46	1.34
25	4	607	CHL	C3C-C2C	9.58	1.46	1.34
25	8	606	CHL	C3C-C2C	9.67	1.46	1.34
25	N	606	CHL	C3C-C2C	9.67	1.46	1.34
25	n	606	CHL	C3C-C2C	9.67	1.46	1.34
25	G	609	CHL	C3C-C2C	9.70	1.46	1.34
25	S	608	CHL	C3C-C2C	9.71	1.46	1.34
25	s	608	CHL	C3C-C2C	9.71	1.46	1.34
25	g	609	CHL	C3C-C2C	9.71	1.46	1.34
25	4	606	CHL	C3C-C2C	9.72	1.46	1.34
25	2	609	CHL	C3C-C2C	9.72	1.46	1.34
25	R	606	CHL	C3C-C2C	9.73	1.46	1.34
25	6	609	CHL	C3C-C2C	9.74	1.46	1.34
25	2	606	CHL	C3C-C2C	9.75	1.46	1.34
25	6	605	CHL	C3C-C2C	9.76	1.46	1.34
25	2	605	CHL	C3C-C2C	9.76	1.46	1.34
25	3	609	CHL	C3C-C2C	9.79	1.46	1.34
25	R	614	CHL	C3C-C2C	9.79	1.46	1.34
25	6	606	CHL	C3C-C2C	9.80	1.46	1.34
25	7	609	CHL	C3C-C2C	9.81	1.46	1.34
25	r	606	CHL	C3C-C2C	9.81	1.46	1.34
25	r	614	CHL	C3C-C2C	9.82	1.46	1.34
25	7	607	CHL	C3C-C2C	9.98	1.46	1.34
25	3	607	CHL	C3C-C2C	10.02	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	601	CHL	C3C-C2C	10.14	1.47	1.34
25	S	601	CHL	C3C-C2C	10.16	1.47	1.34
25	s	601	CHL	C3C-C2C	10.16	1.47	1.34
25	4	601	CHL	C3C-C2C	10.18	1.47	1.34

All (5551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	601	CHL	C1C-C2C-C3C	-8.18	103.37	111.52
25	Y	601	CHL	C1C-C2C-C3C	-8.16	103.39	111.52
25	g	609	CHL	C1C-C2C-C3C	-8.13	103.41	111.52
25	G	609	CHL	C1C-C2C-C3C	-8.10	103.45	111.52
25	g	601	CHL	C1C-C2C-C3C	-8.08	103.47	111.52
25	G	601	CHL	C1C-C2C-C3C	-8.05	103.49	111.52
25	Y	609	CHL	C1C-C2C-C3C	-7.59	103.96	111.52
25	y	609	CHL	C1C-C2C-C3C	-7.55	103.99	111.52
31	8	623	BCR	C24-C23-C22	-7.53	114.90	126.21
25	n	601	CHL	C1C-C2C-C3C	-7.53	104.02	111.52
31	4	623	BCR	C24-C23-C22	-7.53	114.91	126.21
25	N	601	CHL	C1C-C2C-C3C	-7.51	104.03	111.52
28	y	1622	XAT	C6-C7-C8	-7.37	110.40	125.99
28	Y	1622	XAT	C6-C7-C8	-7.37	110.41	125.99
25	6	601	CHL	C1C-C2C-C3C	-7.32	104.23	111.52
25	2	601	CHL	C1C-C2C-C3C	-7.30	104.24	111.52
25	7	609	CHL	C1C-C2C-C3C	-7.10	104.44	111.52
25	3	609	CHL	C1C-C2C-C3C	-7.10	104.45	111.52
25	5	609	CHL	C1C-C2C-C3C	-7.06	104.48	111.52
26	C	508	CLA	CMB-C2B-C1B	-7.05	117.62	128.46
25	1	609	CHL	C1C-C2C-C3C	-7.05	104.50	111.52
26	c	508	CLA	CMB-C2B-C1B	-7.04	117.64	128.46
28	N	1622	XAT	C15-C14-C13	-7.02	117.29	127.31
28	n	1622	XAT	C15-C14-C13	-7.02	117.30	127.31
31	t	101	BCR	C24-C23-C22	-6.94	115.78	126.21
25	3	601	CHL	C1C-C2C-C3C	-6.94	104.61	111.52
31	T	101	BCR	C24-C23-C22	-6.92	115.81	126.21
25	r	614	CHL	C1C-C2C-C3C	-6.90	104.64	111.52
25	7	601	CHL	C1C-C2C-C3C	-6.89	104.65	111.52
25	6	609	CHL	C1C-C2C-C3C	-6.89	104.65	111.52
25	R	614	CHL	C1C-C2C-C3C	-6.88	104.66	111.52
25	2	609	CHL	C1C-C2C-C3C	-6.88	104.66	111.52
25	4	607	CHL	C1C-C2C-C3C	-6.69	104.86	111.52
25	1	601	CHL	C1C-C2C-C3C	-6.67	104.87	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	605	CHL	C1C-C2C-C3C	-6.66	104.88	111.52
25	n	609	CHL	C1C-C2C-C3C	-6.65	104.89	111.52
25	8	607	CHL	C1C-C2C-C3C	-6.65	104.89	111.52
25	N	609	CHL	C1C-C2C-C3C	-6.64	104.90	111.52
25	7	605	CHL	C1C-C2C-C3C	-6.64	104.90	111.52
25	5	601	CHL	C1C-C2C-C3C	-6.64	104.90	111.52
25	6	605	CHL	C1C-C2C-C3C	-6.63	104.91	111.52
25	4	601	CHL	C1C-C2C-C3C	-6.63	104.91	111.52
25	3	605	CHL	C1C-C2C-C3C	-6.62	104.92	111.52
25	6	606	CHL	C1C-C2C-C3C	-6.62	104.92	111.52
25	s	607	CHL	C1C-C2C-C3C	-6.60	104.94	111.52
25	2	606	CHL	C1C-C2C-C3C	-6.59	104.95	111.52
25	8	601	CHL	C1C-C2C-C3C	-6.59	104.95	111.52
25	S	607	CHL	C1C-C2C-C3C	-6.57	104.97	111.52
25	2	608	CHL	C1C-C2C-C3C	-6.56	104.98	111.52
25	6	608	CHL	C1C-C2C-C3C	-6.53	105.01	111.52
25	4	606	CHL	C1C-C2C-C3C	-6.52	105.02	111.52
26	n	604	CLA	CMB-C2B-C1B	-6.51	118.46	128.46
28	g	1622	XAT	C6-C7-C8	-6.50	112.24	125.99
25	1	605	CHL	C1C-C2C-C3C	-6.50	105.04	111.52
25	8	606	CHL	C1C-C2C-C3C	-6.50	105.04	111.52
25	7	608	CHL	C1C-C2C-C3C	-6.50	105.04	111.52
25	3	608	CHL	C1C-C2C-C3C	-6.49	105.05	111.52
25	G	608	CHL	C1C-C2C-C3C	-6.49	105.05	111.52
25	g	608	CHL	C1C-C2C-C3C	-6.49	105.06	111.52
28	G	1622	XAT	C6-C7-C8	-6.48	112.28	125.99
25	5	605	CHL	C1C-C2C-C3C	-6.48	105.06	111.52
26	N	604	CLA	CMB-C2B-C1B	-6.47	118.52	128.46
25	n	606	CHL	C1C-C2C-C3C	-6.46	105.08	111.52
25	N	606	CHL	C1C-C2C-C3C	-6.44	105.10	111.52
25	N	608	CHL	C1C-C2C-C3C	-6.43	105.11	111.52
31	C	516	BCR	C24-C23-C22	-6.42	116.56	126.21
31	c	516	BCR	C24-C23-C22	-6.42	116.56	126.21
31	T	101	BCR	C20-C21-C22	-6.41	118.16	127.31
25	G	606	CHL	C1C-C2C-C3C	-6.41	105.13	111.52
25	g	606	CHL	C1C-C2C-C3C	-6.40	105.14	111.52
25	n	608	CHL	C1C-C2C-C3C	-6.39	105.15	111.52
31	t	101	BCR	C20-C21-C22	-6.39	118.19	127.31
25	N	605	CHL	C1C-C2C-C3C	-6.39	105.15	111.52
25	n	605	CHL	C1C-C2C-C3C	-6.38	105.17	111.52
25	1	606	CHL	C1C-C2C-C3C	-6.33	105.21	111.52
25	5	606	CHL	C1C-C2C-C3C	-6.33	105.21	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	t	101	BCR	C16-C17-C18	-6.32	118.29	127.31
25	8	609	CHL	C1C-C2C-C3C	-6.32	105.22	111.52
31	T	101	BCR	C16-C17-C18	-6.31	118.30	127.31
25	4	609	CHL	C1C-C2C-C3C	-6.31	105.23	111.52
25	R	608	CHL	C1C-C2C-C3C	-6.31	105.23	111.52
25	r	608	CHL	C1C-C2C-C3C	-6.30	105.24	111.52
26	b	613	CLA	CMB-C2B-C1B	-6.26	118.84	128.46
26	y	604	CLA	CMB-C2B-C1B	-6.26	118.84	128.46
26	Y	604	CLA	CMB-C2B-C1B	-6.24	118.87	128.46
26	B	613	CLA	CMB-C2B-C1B	-6.22	118.90	128.46
28	R	622	XAT	C26-C27-C28	-6.19	112.90	125.99
28	r	622	XAT	C26-C27-C28	-6.18	112.92	125.99
25	3	607	CHL	C1C-C2C-C3C	-6.17	105.37	111.52
28	n	1622	XAT	C31-C30-C29	-6.17	118.51	127.31
25	7	607	CHL	C1C-C2C-C3C	-6.16	105.38	111.52
28	N	1622	XAT	C31-C30-C29	-6.16	118.52	127.31
31	8	623	BCR	C11-C10-C9	-6.13	118.56	127.31
25	4	608	CHL	C1C-C2C-C3C	-6.13	105.41	111.52
25	8	608	CHL	C1C-C2C-C3C	-6.13	105.41	111.52
25	S	601	CHL	C1C-C2C-C3C	-6.13	105.41	111.52
25	s	601	CHL	C1C-C2C-C3C	-6.13	105.41	111.52
26	G	604	CLA	CMB-C2B-C1B	-6.12	119.06	128.46
26	g	604	CLA	CMB-C2B-C1B	-6.12	119.06	128.46
31	4	623	BCR	C11-C10-C9	-6.11	118.59	127.31
27	3	1620	LUT	C23-C24-C25	-6.07	119.53	125.22
27	8	620	LUT	C23-C24-C25	-6.07	119.54	125.22
27	7	1620	LUT	C23-C24-C25	-6.06	119.54	125.22
25	y	606	CHL	C1C-C2C-C3C	-6.04	105.50	111.52
25	Y	606	CHL	C1C-C2C-C3C	-6.03	105.50	111.52
27	4	620	LUT	C23-C24-C25	-6.02	119.58	125.22
26	b	609	CLA	CMB-C2B-C1B	-6.00	119.24	128.46
26	B	609	CLA	CMB-C2B-C1B	-5.99	119.25	128.46
28	y	1622	XAT	C15-C14-C13	-5.98	118.77	127.31
28	Y	1622	XAT	C15-C14-C13	-5.98	118.77	127.31
25	y	605	CHL	C1C-C2C-C3C	-5.96	105.57	111.52
25	Y	605	CHL	C1C-C2C-C3C	-5.95	105.59	111.52
25	5	608	CHL	C1C-C2C-C3C	-5.93	105.61	111.52
26	B	605	CLA	CAA-C2A-C3A	-5.92	96.58	112.81
26	B	612	CLA	CMB-C2B-C1B	-5.92	119.37	128.46
26	b	605	CLA	CAA-C2A-C3A	-5.91	96.61	112.81
26	b	612	CLA	CMB-C2B-C1B	-5.90	119.39	128.46
25	1	608	CHL	C1C-C2C-C3C	-5.89	105.65	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	1622	XAT	C15-C14-C13	-5.89	118.91	127.31
26	C	504	CLA	CMB-C2B-C1B	-5.87	119.44	128.46
25	1	606	CHL	CBA-CAA-C2A	-5.87	107.21	115.66
31	d	404	BCR	C7-C8-C9	-5.86	117.41	126.21
26	c	504	CLA	CMB-C2B-C1B	-5.86	119.46	128.46
31	c	517	BCR	C24-C23-C22	-5.86	117.41	126.21
28	g	1622	XAT	C15-C14-C13	-5.85	118.95	127.31
25	5	606	CHL	CBA-CAA-C2A	-5.85	107.23	115.66
31	c	517	BCR	C7-C8-C9	-5.85	117.42	126.21
29	Y	1623	NEX	C35-C34-C33	-5.85	118.96	127.31
31	D	404	BCR	C7-C8-C9	-5.85	117.42	126.21
26	C	506	CLA	CMB-C2B-C1B	-5.85	119.47	128.46
31	C	517	BCR	C7-C8-C9	-5.85	117.42	126.21
29	y	1623	NEX	C35-C34-C33	-5.85	118.97	127.31
26	n	602	CLA	CMB-C2B-C1B	-5.83	119.50	128.46
26	N	602	CLA	CMB-C2B-C1B	-5.83	119.50	128.46
26	c	506	CLA	CMB-C2B-C1B	-5.83	119.50	128.46
31	C	517	BCR	C24-C23-C22	-5.83	117.45	126.21
25	R	607	CHL	C1C-C2C-C3C	-5.83	105.71	111.52
26	s	612	CLA	CMB-C2B-C1B	-5.82	119.52	128.46
26	S	612	CLA	CMB-C2B-C1B	-5.81	119.54	128.46
29	3	1623	NEX	C15-C14-C13	-5.81	119.03	127.31
25	S	606	CHL	C1C-C2C-C3C	-5.80	105.74	111.52
25	s	606	CHL	C1C-C2C-C3C	-5.80	105.74	111.52
25	r	606	CHL	C1C-C2C-C3C	-5.80	105.74	111.52
25	y	608	CHL	C1C-C2C-C3C	-5.80	105.74	111.52
29	7	1623	NEX	C15-C14-C13	-5.79	119.05	127.31
25	2	607	CHL	C1C-C2C-C3C	-5.78	105.76	111.52
25	r	607	CHL	C1C-C2C-C3C	-5.77	105.77	111.52
25	G	605	CHL	C1C-C2C-C3C	-5.76	105.78	111.52
25	Y	608	CHL	C1C-C2C-C3C	-5.76	105.78	111.52
25	6	607	CHL	C1C-C2C-C3C	-5.76	105.78	111.52
25	R	606	CHL	C1C-C2C-C3C	-5.76	105.78	111.52
25	g	605	CHL	C1C-C2C-C3C	-5.75	105.78	111.52
25	7	606	CHL	C1C-C2C-C3C	-5.71	105.83	111.52
25	3	606	CHL	C1C-C2C-C3C	-5.71	105.83	111.52
28	7	1622	XAT	C6-C7-C8	-5.69	113.96	125.99
28	3	1622	XAT	C6-C7-C8	-5.69	113.96	125.99
31	t	101	BCR	C11-C10-C9	-5.69	119.19	127.31
31	T	101	BCR	C11-C10-C9	-5.65	119.25	127.31
28	y	1622	XAT	C31-C30-C29	-5.65	119.25	127.31
28	Y	1622	XAT	C31-C30-C29	-5.63	119.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	621	SQD	C5-C6-S	-5.62	106.51	114.34
31	h	101	BCR	C11-C10-C9	-5.61	119.30	127.31
31	H	101	BCR	C11-C10-C9	-5.61	119.31	127.31
36	b	621	SQD	C5-C6-S	-5.60	106.54	114.34
25	G	607	CHL	C1C-C2C-C3C	-5.55	105.99	111.52
25	g	607	CHL	C1C-C2C-C3C	-5.55	105.99	111.52
28	r	622	XAT	C38-C25-C26	-5.53	112.95	122.31
28	4	622	XAT	C6-C7-C8	-5.53	114.30	125.99
28	8	622	XAT	C6-C7-C8	-5.53	114.30	125.99
28	R	622	XAT	C38-C25-C26	-5.53	112.96	122.31
31	C	515	BCR	C7-C8-C9	-5.52	117.92	126.21
25	y	607	CHL	C1C-C2C-C3C	-5.52	106.02	111.52
28	n	1622	XAT	C6-C7-C8	-5.50	114.37	125.99
25	Y	607	CHL	C1C-C2C-C3C	-5.49	106.04	111.52
31	c	515	BCR	C7-C8-C9	-5.49	117.96	126.21
28	N	1622	XAT	C6-C7-C8	-5.48	114.41	125.99
28	7	1622	XAT	C31-C30-C29	-5.47	119.51	127.31
28	3	1622	XAT	C31-C30-C29	-5.47	119.51	127.31
26	n	614	CLA	CMB-C2B-C1B	-5.46	120.07	128.46
26	1	604	CLA	CMB-C2B-C1B	-5.46	120.08	128.46
26	N	614	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
26	5	604	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
31	8	623	BCR	C16-C17-C18	-5.44	119.54	127.31
27	1	1620	LUT	C23-C24-C25	-5.44	120.12	125.22
31	4	623	BCR	C16-C17-C18	-5.44	119.55	127.31
26	R	603	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
26	r	603	CLA	CMB-C2B-C1B	-5.43	120.12	128.46
25	s	608	CHL	C1C-C2C-C3C	-5.43	106.11	111.52
29	r	623	NEX	C15-C14-C13	-5.42	119.57	127.31
26	c	509	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
26	C	509	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
27	5	1620	LUT	C23-C24-C25	-5.41	120.15	125.22
28	y	1622	XAT	C11-C10-C9	-5.40	119.61	127.31
25	S	608	CHL	C1C-C2C-C3C	-5.39	106.14	111.52
28	Y	1622	XAT	C11-C10-C9	-5.39	119.61	127.31
29	R	623	NEX	C15-C14-C13	-5.39	119.62	127.31
26	S	604	CLA	CMB-C2B-C1B	-5.38	120.19	128.46
26	A	405	CLA	CMB-C2B-C1B	-5.38	120.20	128.46
26	s	604	CLA	CMB-C2B-C1B	-5.37	120.21	128.46
26	a	405	CLA	CMB-C2B-C1B	-5.37	120.22	128.46
26	B	604	CLA	CMB-C2B-C1B	-5.33	120.27	128.46
31	b	618	BCR	C15-C14-C13	-5.31	119.73	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	T	101	BCR	C7-C8-C9	-5.31	118.23	126.21
31	B	618	BCR	C15-C14-C13	-5.31	119.73	127.31
26	b	604	CLA	CMB-C2B-C1B	-5.30	120.32	128.46
26	S	613	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
26	s	613	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
26	G	602	CLA	CMB-C2B-C1B	-5.28	120.34	128.46
26	D	403	CLA	CMB-C2B-C1B	-5.28	120.34	128.46
26	D	402	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
26	d	402	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
25	2	601	CHL	CBA-CAA-C2A	-5.28	108.05	115.66
25	6	601	CHL	CBA-CAA-C2A	-5.28	108.05	115.66
29	r	623	NEX	C11-C10-C9	-5.28	119.77	127.31
28	3	1622	XAT	C15-C14-C13	-5.27	119.79	127.31
29	R	623	NEX	C11-C10-C9	-5.27	119.79	127.31
31	t	101	BCR	C7-C8-C9	-5.27	118.30	126.21
26	g	602	CLA	CMB-C2B-C1B	-5.27	120.37	128.46
28	N	1622	XAT	C38-C25-C26	-5.26	113.41	122.31
25	Y	609	CHL	CBC-CAC-C3C	-5.26	104.96	112.95
26	C	510	CLA	CMB-C2B-C1B	-5.26	120.38	128.46
25	y	609	CHL	CBC-CAC-C3C	-5.26	104.97	112.95
28	5	1622	XAT	C31-C30-C29	-5.26	119.81	127.31
28	3	1622	XAT	C38-C25-C26	-5.26	113.42	122.31
28	n	1622	XAT	C38-C25-C26	-5.25	113.42	122.31
26	d	403	CLA	CMB-C2B-C1B	-5.25	120.39	128.46
28	7	1622	XAT	C15-C14-C13	-5.25	119.82	127.31
28	7	1622	XAT	C38-C25-C26	-5.24	113.44	122.31
36	B	623	SQD	C5-C6-S	-5.24	107.03	114.34
26	g	611	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
26	c	510	CLA	CMB-C2B-C1B	-5.24	120.42	128.46
28	1	1622	XAT	C31-C30-C29	-5.23	119.84	127.31
36	b	623	SQD	C5-C6-S	-5.22	107.06	114.34
26	G	611	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
28	4	622	XAT	C18-C5-C6	-5.20	113.51	122.31
28	8	622	XAT	C18-C5-C6	-5.20	113.52	122.31
28	5	1622	XAT	C15-C14-C13	-5.19	119.90	127.31
28	G	1622	XAT	C31-C30-C29	-5.18	119.91	127.31
31	4	623	BCR	C28-C27-C26	-5.18	104.87	113.78
28	1	1622	XAT	C15-C14-C13	-5.18	119.92	127.31
31	8	623	BCR	C28-C27-C26	-5.17	104.89	113.78
26	R	602	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
29	Y	1623	NEX	C17-C1-C6	-5.17	105.84	110.47
26	c	513	CLA	CMB-C2B-C1B	-5.15	120.54	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	602	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
28	g	1622	XAT	C31-C30-C29	-5.15	119.96	127.31
29	y	1623	NEX	C17-C1-C6	-5.13	105.88	110.47
26	C	513	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
29	n	1623	NEX	C35-C34-C33	-5.13	119.99	127.31
29	N	1623	NEX	C35-C34-C33	-5.12	120.00	127.31
29	6	1623	NEX	C15-C14-C13	-5.12	120.00	127.31
29	2	1623	NEX	C15-C14-C13	-5.11	120.02	127.31
26	b	608	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
26	S	614	CLA	CMB-C2B-C1B	-5.09	120.65	128.46
29	3	1623	NEX	C38-C25-C26	-5.08	113.71	122.31
26	s	614	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
28	1	1622	XAT	C38-C25-C26	-5.08	113.72	122.31
28	5	1622	XAT	C38-C25-C26	-5.07	113.73	122.31
28	r	622	XAT	C6-C7-C8	-5.07	115.27	125.99
26	B	608	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
28	R	622	XAT	C6-C7-C8	-5.06	115.29	125.99
25	5	607	CHL	C1C-C2C-C3C	-5.06	106.48	111.52
29	7	1623	NEX	C38-C25-C26	-5.06	113.75	122.31
25	1	607	CHL	C1C-C2C-C3C	-5.05	106.48	111.52
29	y	1623	NEX	C27-C28-C29	-5.04	117.71	125.53
29	Y	1623	NEX	C27-C28-C29	-5.04	117.71	125.53
29	R	623	NEX	C27-C28-C29	-5.03	117.73	125.53
29	r	623	NEX	C27-C28-C29	-5.03	117.73	125.53
29	5	1623	NEX	C27-C28-C29	-5.02	117.73	125.53
29	1	1623	NEX	C27-C28-C29	-5.02	117.74	125.53
25	s	607	CHL	CBC-CAC-C3C	-5.02	105.33	112.95
25	S	607	CHL	CBC-CAC-C3C	-5.01	105.34	112.95
31	8	623	BCR	C15-C14-C13	-5.00	120.18	127.31
31	4	623	BCR	C15-C14-C13	-4.97	120.21	127.31
29	s	1623	NEX	C11-C10-C9	-4.97	120.21	127.31
29	n	1623	NEX	C27-C28-C29	-4.97	117.82	125.53
29	S	1623	NEX	C11-C10-C9	-4.97	120.22	127.31
26	A	406	CLA	CMB-C2B-C1B	-4.96	120.83	128.46
26	a	406	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
29	g	1623	NEX	C11-C10-C9	-4.95	120.25	127.31
29	N	1623	NEX	C27-C28-C29	-4.95	117.86	125.53
28	y	1622	XAT	C15-C35-C34	-4.94	112.92	123.46
28	g	1622	XAT	C38-C25-C26	-4.93	113.97	122.31
29	G	1623	NEX	C38-C25-C26	-4.93	113.97	122.31
26	B	603	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
28	Y	1622	XAT	C15-C35-C34	-4.92	112.95	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	1623	NEX	C38-C25-C26	-4.92	113.98	122.31
27	s	1621	LUT	C23-C24-C25	-4.92	120.61	125.22
29	G	1623	NEX	C11-C10-C9	-4.92	120.29	127.31
28	G	1622	XAT	C38-C25-C26	-4.91	114.00	122.31
27	S	1621	LUT	C23-C24-C25	-4.90	120.62	125.22
26	b	603	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
26	Y	602	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
31	c	515	BCR	C21-C20-C19	-4.88	108.25	123.23
26	B	610	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
31	C	515	BCR	C21-C20-C19	-4.88	108.27	123.23
26	y	602	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
26	b	610	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
37	D	411	LMG	C1-C2-C3	-4.87	100.92	109.98
28	g	1622	XAT	C15-C35-C34	-4.87	113.07	123.46
28	4	622	XAT	C26-C27-C28	-4.86	115.72	125.99
27	2	1620	LUT	C35-C34-C33	-4.86	120.38	127.31
26	c	512	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
28	G	1622	XAT	C15-C35-C34	-4.85	113.10	123.46
29	2	1623	NEX	C38-C25-C26	-4.85	114.10	122.31
37	d	411	LMG	C1-C2-C3	-4.85	100.97	109.98
26	C	512	CLA	CMB-C2B-C1B	-4.85	121.02	128.46
29	6	1623	NEX	C38-C25-C26	-4.85	114.11	122.31
26	r	604	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
26	R	604	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
28	8	622	XAT	C26-C27-C28	-4.84	115.76	125.99
27	6	1620	LUT	C35-C34-C33	-4.84	120.40	127.31
31	b	620	BCR	C7-C8-C9	-4.84	118.95	126.21
28	Y	1622	XAT	C38-C25-C26	-4.84	114.13	122.31
28	y	1622	XAT	C38-C25-C26	-4.83	114.15	122.31
26	s	610	CLA	CMB-C2B-C1B	-4.82	121.05	128.46
31	B	620	BCR	C7-C8-C9	-4.82	118.97	126.21
26	B	607	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
29	3	1623	NEX	C11-C10-C9	-4.82	120.43	127.31
26	R	601	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
26	r	601	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
39	C	518	DGD	O3G-C3G-C2G	-4.81	99.55	110.99
39	c	518	DGD	O3G-C3G-C2G	-4.80	99.56	110.99
26	S	610	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
26	b	607	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
29	7	1623	NEX	C11-C10-C9	-4.79	120.47	127.31
27	G	1621	LUT	C15-C14-C13	-4.78	120.50	127.31
28	1	1622	XAT	C6-C7-C8	-4.76	115.92	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	5	1622	XAT	C6-C7-C8	-4.76	115.93	125.99
27	n	1621	LUT	C23-C24-C25	-4.76	120.76	125.22
27	S	1621	LUT	C35-C34-C33	-4.75	120.53	127.31
31	4	623	BCR	C7-C8-C9	-4.75	119.08	126.21
27	s	1621	LUT	C35-C34-C33	-4.75	120.54	127.31
29	n	1623	NEX	C38-C25-C26	-4.74	114.29	122.31
29	N	1623	NEX	C38-C25-C26	-4.74	114.29	122.31
28	2	1622	XAT	C38-C25-C26	-4.74	114.29	122.31
27	g	1621	LUT	C15-C14-C13	-4.74	120.55	127.31
28	6	1622	XAT	C38-C25-C26	-4.73	114.30	122.31
31	8	623	BCR	C7-C8-C9	-4.73	119.10	126.21
28	N	1622	XAT	C27-C28-C29	-4.73	118.19	125.53
28	n	1622	XAT	C15-C35-C34	-4.73	113.36	123.46
29	s	1623	NEX	C38-C25-C26	-4.72	114.33	122.31
28	n	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
28	N	1622	XAT	C15-C35-C34	-4.72	113.40	123.46
28	2	1622	XAT	C31-C30-C29	-4.71	120.58	127.31
27	N	1621	LUT	C23-C24-C25	-4.71	120.80	125.22
31	C	514	BCR	C15-C14-C13	-4.71	120.59	127.31
31	c	514	BCR	C15-C14-C13	-4.70	120.60	127.31
28	6	1622	XAT	C31-C30-C29	-4.69	120.61	127.31
29	S	1623	NEX	C38-C25-C26	-4.69	114.37	122.31
29	n	1623	NEX	C15-C14-C13	-4.68	120.63	127.31
29	1	1623	NEX	C38-C25-C26	-4.67	114.41	122.31
31	c	517	BCR	C15-C14-C13	-4.67	120.65	127.31
31	C	517	BCR	C15-C14-C13	-4.66	120.65	127.31
29	5	1623	NEX	C38-C25-C26	-4.64	114.45	122.31
29	N	1623	NEX	C15-C14-C13	-4.63	120.70	127.31
28	3	1622	XAT	C18-C5-C6	-4.63	114.48	122.31
31	H	101	BCR	C16-C17-C18	-4.63	120.71	127.31
28	7	1622	XAT	C18-C5-C6	-4.62	114.50	122.31
26	7	604	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
28	2	1622	XAT	C18-C5-C6	-4.61	114.51	122.31
26	3	604	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
31	h	101	BCR	C16-C17-C18	-4.60	120.74	127.31
29	1	1623	NEX	C31-C30-C29	-4.60	120.75	127.31
39	C	519	DGD	O3G-C3G-C2G	-4.59	100.06	110.99
28	6	1622	XAT	C18-C5-C6	-4.59	114.55	122.31
29	y	1623	NEX	C11-C10-C9	-4.59	120.76	127.31
39	c	519	DGD	O3G-C3G-C2G	-4.59	100.08	110.99
29	Y	1623	NEX	C11-C10-C9	-4.58	120.77	127.31
29	5	1623	NEX	C31-C30-C29	-4.58	120.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	517	BCR	C11-C10-C9	-4.57	120.78	127.31
28	g	1622	XAT	C27-C28-C29	-4.57	118.44	125.53
31	C	517	BCR	C11-C10-C9	-4.55	120.82	127.31
28	G	1622	XAT	C27-C28-C29	-4.54	118.48	125.53
31	B	619	BCR	C15-C14-C13	-4.54	120.83	127.31
26	S	602	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
26	C	508	CLA	O2D-CGD-O1D	-4.53	114.70	123.82
29	7	1623	NEX	C27-C28-C29	-4.52	118.51	125.53
26	s	602	CLA	CMB-C2B-C1B	-4.52	121.51	128.46
31	c	515	BCR	C15-C14-C13	-4.52	120.86	127.31
29	3	1623	NEX	C27-C28-C29	-4.51	118.53	125.53
28	8	622	XAT	C38-C25-C26	-4.51	114.69	122.31
26	b	614	CLA	CMB-C2B-C1B	-4.51	121.54	128.46
29	R	623	NEX	C38-C25-C26	-4.50	114.69	122.31
26	c	508	CLA	O2D-CGD-O1D	-4.50	114.76	123.82
28	1	1622	XAT	C18-C5-C6	-4.50	114.69	122.31
26	n	610	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
26	N	610	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
31	T	101	BCR	C20-C19-C18	-4.50	113.78	126.42
29	r	623	NEX	C38-C25-C26	-4.50	114.70	122.31
31	b	619	BCR	C15-C14-C13	-4.50	120.89	127.31
31	t	101	BCR	C20-C19-C18	-4.49	113.80	126.42
28	4	622	XAT	C38-C25-C26	-4.49	114.72	122.31
26	B	614	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
28	5	1622	XAT	C18-C5-C6	-4.48	114.74	122.31
31	C	515	BCR	C15-C14-C13	-4.48	120.92	127.31
28	r	622	XAT	C35-C34-C33	-4.47	120.93	127.31
29	1	1623	NEX	C35-C34-C33	-4.47	120.93	127.31
28	r	622	XAT	C18-C5-C6	-4.47	114.75	122.31
27	S	1620	LUT	C35-C34-C33	-4.47	120.94	127.31
28	R	622	XAT	C18-C5-C6	-4.46	114.76	122.31
27	s	1620	LUT	C35-C34-C33	-4.46	120.95	127.31
26	6	602	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
28	R	622	XAT	C35-C34-C33	-4.45	120.96	127.31
29	5	1623	NEX	C35-C34-C33	-4.45	120.96	127.31
31	H	101	BCR	C24-C23-C22	-4.45	119.53	126.21
31	C	516	BCR	C16-C17-C18	-4.45	120.97	127.31
31	h	101	BCR	C24-C23-C22	-4.44	119.53	126.21
29	Y	1623	NEX	C38-C25-C26	-4.44	114.80	122.31
29	y	1623	NEX	C38-C25-C26	-4.44	114.81	122.31
26	2	602	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
29	Y	1623	NEX	C15-C14-C13	-4.43	120.99	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	1622	XAT	C18-C5-C6	-4.42	114.83	122.31
28	y	1622	XAT	C18-C5-C6	-4.42	114.83	122.31
31	c	516	BCR	C16-C17-C18	-4.41	121.02	127.31
29	y	1623	NEX	C15-C14-C13	-4.41	121.02	127.31
27	l	1620	LUT	C35-C34-C33	-4.41	121.02	127.31
25	n	609	CHL	CBC-CAC-C3C	-4.41	106.26	112.95
31	b	618	BCR	C16-C17-C18	-4.40	121.03	127.31
31	B	618	BCR	C16-C17-C18	-4.38	121.05	127.31
25	N	609	CHL	CBC-CAC-C3C	-4.38	106.30	112.95
25	r	614	CHL	CBC-CAC-C3C	-4.38	106.31	112.95
27	5	1620	LUT	C35-C34-C33	-4.38	121.06	127.31
28	6	1622	XAT	C15-C14-C13	-4.38	121.06	127.31
29	S	1623	NEX	C27-C28-C29	-4.37	118.75	125.53
27	Y	1621	LUT	C15-C14-C13	-4.37	121.08	127.31
29	s	1623	NEX	C27-C28-C29	-4.36	118.76	125.53
27	n	1621	LUT	C15-C14-C13	-4.36	121.09	127.31
25	N	606	CHL	CBA-CAA-C2A	-4.36	109.75	115.76
25	n	606	CHL	CBA-CAA-C2A	-4.36	109.75	115.76
25	R	614	CHL	CBC-CAC-C3C	-4.35	106.34	112.95
31	c	517	BCR	C33-C5-C6	-4.35	119.64	124.51
26	B	617	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
28	2	1622	XAT	C15-C14-C13	-4.35	121.10	127.31
27	y	1621	LUT	C15-C14-C13	-4.35	121.11	127.31
27	N	1621	LUT	C15-C14-C13	-4.33	121.13	127.31
26	b	617	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
29	G	1623	NEX	C15-C14-C13	-4.33	121.14	127.31
29	g	1623	NEX	C15-C14-C13	-4.32	121.14	127.31
31	C	517	BCR	C33-C5-C6	-4.31	119.68	124.51
29	r	623	NEX	C35-C34-C33	-4.31	121.16	127.31
27	Y	1621	LUT	C35-C34-C33	-4.30	121.17	127.31
29	6	1623	NEX	C27-C28-C29	-4.30	118.86	125.53
29	2	1623	NEX	C27-C28-C29	-4.30	118.86	125.53
29	R	623	NEX	C35-C34-C33	-4.30	121.17	127.31
31	B	619	BCR	C11-C10-C9	-4.30	121.18	127.31
28	l	1622	XAT	C11-C10-C9	-4.29	121.19	127.31
31	b	619	BCR	C11-C10-C9	-4.29	121.19	127.31
28	5	1622	XAT	C11-C10-C9	-4.28	121.20	127.31
31	C	516	BCR	C28-C27-C26	-4.27	106.43	113.78
31	c	515	BCR	C11-C10-C9	-4.27	121.22	127.31
27	y	1621	LUT	C35-C34-C33	-4.26	121.23	127.31
31	c	516	BCR	C28-C27-C26	-4.24	106.48	113.78
31	C	515	BCR	C11-C10-C9	-4.24	121.25	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	607	CHL	C1C-C2C-C3C	-4.24	107.29	111.52
25	n	607	CHL	C1C-C2C-C3C	-4.24	107.29	111.52
26	Y	610	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
26	y	610	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
25	G	609	CHL	CBC-CAC-C3C	-4.23	106.52	112.95
25	2	606	CHL	CBA-CAA-C2A	-4.22	109.58	115.66
25	6	606	CHL	CBA-CAA-C2A	-4.22	109.58	115.66
25	N	605	CHL	O2D-CGD-O1D	-4.22	115.34	123.82
25	n	605	CHL	O2D-CGD-O1D	-4.22	115.34	123.82
29	S	1623	NEX	C15-C14-C13	-4.21	121.30	127.31
39	C	520	DGD	O3G-C3G-C2G	-4.21	100.97	110.99
35	a	409	PHO	CMB-C2B-C1B	-4.21	118.49	125.04
25	g	609	CHL	CBC-CAC-C3C	-4.20	106.57	112.95
26	c	504	CLA	O2D-CGD-O1D	-4.20	115.37	123.82
26	C	504	CLA	O2D-CGD-O1D	-4.20	115.37	123.82
39	c	520	DGD	O3G-C3G-C2G	-4.20	100.99	110.99
26	c	511	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
35	A	409	PHO	CMB-C2B-C1B	-4.20	118.50	125.04
31	b	620	BCR	C16-C17-C18	-4.20	121.32	127.31
31	B	620	BCR	C16-C17-C18	-4.20	121.32	127.31
29	s	1623	NEX	C15-C14-C13	-4.20	121.32	127.31
31	t	101	BCR	C15-C14-C13	-4.19	121.33	127.31
31	T	101	BCR	C15-C14-C13	-4.19	121.33	127.31
26	a	410	CLA	C1-C2-C3	-4.18	118.25	125.96
26	C	511	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
25	N	601	CHL	CBC-CAC-C3C	-4.17	106.62	112.95
26	y	612	CLA	OBD-CAD-CBD	-4.17	119.64	125.94
26	Y	612	CLA	OBD-CAD-CBD	-4.17	119.65	125.94
27	7	1621	LUT	C23-C24-C25	-4.16	121.32	125.22
29	6	1623	NEX	C11-C10-C9	-4.16	121.37	127.31
26	A	410	CLA	C1-C2-C3	-4.16	118.29	125.96
25	n	601	CHL	CBC-CAC-C3C	-4.16	106.63	112.95
26	g	614	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
26	4	602	CLA	O2D-CGD-O1D	-4.15	115.46	123.82
31	A	411	BCR	C7-C8-C9	-4.15	119.97	126.21
29	2	1623	NEX	C11-C10-C9	-4.15	121.39	127.31
27	G	1621	LUT	C35-C34-C33	-4.15	121.39	127.31
26	d	403	CLA	O2D-CGD-O1D	-4.14	115.48	123.82
26	G	614	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
28	7	1622	XAT	C15-C35-C34	-4.13	114.64	123.46
27	g	1621	LUT	C35-C34-C33	-4.13	121.41	127.31
27	3	1621	LUT	C23-C24-C25	-4.13	121.34	125.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	1621	LUT	C15-C14-C13	-4.13	121.41	127.31
28	3	1622	XAT	C15-C35-C34	-4.13	114.64	123.46
26	8	602	CLA	O2D-CGD-O1D	-4.13	115.51	123.82
26	D	403	CLA	O2D-CGD-O1D	-4.13	115.51	123.82
31	a	411	BCR	C7-C8-C9	-4.11	120.03	126.21
27	5	1621	LUT	C15-C14-C13	-4.11	121.44	127.31
26	B	606	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
26	b	606	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
28	r	622	XAT	C15-C14-C13	-4.09	121.47	127.31
25	1	607	CHL	CBA-CAA-C2A	-4.09	110.12	115.76
31	c	515	BCR	C16-C17-C18	-4.09	121.48	127.31
25	G	605	CHL	C4A-C3A-C2A	-4.08	97.61	103.86
27	2	1621	LUT	C15-C14-C13	-4.08	121.48	127.31
31	D	404	BCR	C11-C10-C9	-4.08	121.49	127.31
31	d	404	BCR	C11-C10-C9	-4.08	121.49	127.31
27	5	1621	LUT	C23-C24-C25	-4.08	121.40	125.22
25	g	605	CHL	C4A-C3A-C2A	-4.08	97.63	103.86
26	3	602	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
26	7	602	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
25	G	605	CHL	O2D-CGD-O1D	-4.07	115.63	123.82
25	g	605	CHL	O2D-CGD-O1D	-4.07	115.64	123.82
25	5	607	CHL	CBA-CAA-C2A	-4.07	110.15	115.76
28	R	622	XAT	C15-C14-C13	-4.07	121.50	127.31
31	C	515	BCR	C16-C17-C18	-4.07	121.51	127.31
25	7	606	CHL	OMC-CMC-C2C	-4.07	119.10	124.29
27	6	1621	LUT	C15-C14-C13	-4.06	121.51	127.31
26	b	611	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
25	3	606	CHL	OMC-CMC-C2C	-4.06	119.11	124.29
26	5	610	CLA	C1B-CHB-C4A	-4.06	122.08	130.12
29	R	623	NEX	C26-C27-C28	-4.06	117.41	125.99
29	r	623	NEX	C26-C27-C28	-4.06	117.41	125.99
26	N	612	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
26	n	612	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
26	1	610	CLA	C1B-CHB-C4A	-4.05	122.11	130.12
27	1	1621	LUT	C23-C24-C25	-4.04	121.43	125.22
26	6	604	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
26	B	611	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
28	3	1622	XAT	C27-C28-C29	-4.02	119.30	125.53
28	7	1622	XAT	C27-C28-C29	-4.02	119.30	125.53
26	s	614	CLA	O2D-CGD-O1D	-4.01	115.75	123.82
26	2	604	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
26	G	610	CLA	CMB-C2B-C1B	-4.01	122.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	404	BCR	C24-C23-C22	-3.99	120.21	126.21
26	S	614	CLA	O2D-CGD-O1D	-3.99	115.79	123.82
26	g	610	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
31	D	404	BCR	C24-C23-C22	-3.99	120.22	126.21
25	g	606	CHL	CBA-CAA-C2A	-3.99	110.26	115.76
25	G	606	CHL	CBA-CAA-C2A	-3.98	110.27	115.76
29	N	1623	NEX	C17-C1-C6	-3.97	106.92	110.47
26	A	407	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
28	N	1622	XAT	C11-C10-C9	-3.96	121.65	127.31
31	H	101	BCR	C15-C14-C13	-3.96	121.66	127.31
31	h	101	BCR	C15-C14-C13	-3.96	121.66	127.31
27	2	1620	LUT	C35-C15-C14	-3.96	115.02	123.46
26	N	613	CLA	CMB-C2B-C1B	-3.96	122.39	128.46
26	a	407	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
28	Y	1622	XAT	C27-C28-C29	-3.94	119.42	125.53
28	n	1622	XAT	C11-C10-C9	-3.94	121.69	127.31
26	c	507	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
27	6	1620	LUT	C35-C15-C14	-3.93	115.06	123.46
28	y	1622	XAT	C27-C28-C29	-3.93	119.42	125.53
26	y	614	CLA	O2D-CGD-O1D	-3.93	115.91	123.82
29	n	1623	NEX	C17-C1-C6	-3.93	106.95	110.47
26	C	507	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
27	N	1620	LUT	C35-C34-C33	-3.93	121.71	127.31
26	G	612	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
26	g	612	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
26	n	613	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
26	Y	614	CLA	O2D-CGD-O1D	-3.91	115.95	123.82
26	8	603	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
27	n	1620	LUT	C35-C34-C33	-3.91	121.74	127.31
31	c	517	BCR	C16-C17-C18	-3.90	121.74	127.31
26	y	613	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	a	410	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	r	610	CLA	C1B-CHB-C4A	-3.90	122.40	130.12
31	H	101	BCR	C7-C8-C9	-3.90	120.36	126.21
26	b	615	CLA	O2D-CGD-O1D	-3.89	115.98	123.82
26	R	610	CLA	C1B-CHB-C4A	-3.89	122.40	130.12
31	h	101	BCR	C7-C8-C9	-3.89	120.37	126.21
26	Y	613	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
26	4	603	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
28	8	622	XAT	C35-C34-C33	-3.89	121.76	127.31
31	B	620	BCR	C11-C10-C9	-3.88	121.77	127.31
31	b	620	BCR	C11-C10-C9	-3.88	121.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	608	CHL	OMC-CMC-C2C	-3.88	119.34	124.29
25	Y	606	CHL	CBA-CAA-C2A	-3.88	110.41	115.76
28	4	622	XAT	C35-C34-C33	-3.88	121.77	127.31
25	R	606	CHL	CBA-CAA-C2A	-3.88	110.41	115.76
31	C	517	BCR	C16-C17-C18	-3.87	121.78	127.31
26	A	410	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
36	A	418	SQD	O9-S-O7	-3.87	100.44	113.86
36	a	418	SQD	O9-S-O7	-3.87	100.44	113.86
25	S	606	CHL	OMC-CMC-C2C	-3.87	119.35	124.29
28	y	1622	XAT	C35-C34-C33	-3.87	121.79	127.31
26	B	615	CLA	O2D-CGD-O1D	-3.86	116.05	123.82
27	r	620	LUT	C30-C31-C32	-3.85	111.41	123.23
27	R	620	LUT	C30-C31-C32	-3.85	111.41	123.23
31	T	101	BCR	C33-C5-C6	-3.85	120.20	124.51
36	b	623	SQD	O9-S-O7	-3.85	100.52	113.86
25	r	606	CHL	CBA-CAA-C2A	-3.85	110.45	115.76
25	s	606	CHL	OMC-CMC-C2C	-3.85	119.38	124.29
25	y	606	CHL	CBA-CAA-C2A	-3.85	110.46	115.76
25	4	608	CHL	OMC-CMC-C2C	-3.84	119.38	124.29
25	2	609	CHL	CBC-CAC-C3C	-3.84	107.11	112.95
36	B	623	SQD	O9-S-O7	-3.84	100.54	113.86
31	c	516	BCR	C20-C21-C22	-3.84	121.83	127.31
28	G	1622	XAT	C4-C3-C2	-3.84	102.85	110.68
28	Y	1622	XAT	C35-C34-C33	-3.84	121.83	127.31
27	7	1621	LUT	C15-C14-C13	-3.84	121.83	127.31
27	3	1621	LUT	C15-C14-C13	-3.84	121.83	127.31
25	7	606	CHL	CBA-CAA-C2A	-3.84	110.13	115.66
25	3	606	CHL	CBA-CAA-C2A	-3.83	110.14	115.66
26	Y	603	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
26	a	410	CLA	O2D-CGD-O1D	-3.82	116.12	123.82
26	y	603	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
28	3	1622	XAT	C26-C27-C28	-3.82	117.92	125.99
25	6	609	CHL	CBC-CAC-C3C	-3.82	107.16	112.95
31	b	620	BCR	C15-C14-C13	-3.82	121.86	127.31
27	1	1620	LUT	C30-C31-C32	-3.82	111.53	123.23
27	2	1620	LUT	C23-C24-C25	-3.81	121.64	125.22
28	g	1622	XAT	C4-C3-C2	-3.81	102.91	110.68
31	B	620	BCR	C15-C14-C13	-3.81	121.87	127.31
26	A	410	CLA	O2D-CGD-O1D	-3.81	116.15	123.82
28	g	1622	XAT	C18-C5-C6	-3.81	115.86	122.31
31	C	516	BCR	C20-C21-C22	-3.81	121.87	127.31
26	5	614	CLA	CMB-C2B-C1B	-3.81	122.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	CLA	CAA-CBA-CGA	-3.81	101.87	113.35
28	G	1622	XAT	C18-C5-C6	-3.81	115.87	122.31
26	g	603	CLA	OBD-CAD-CBD	-3.80	120.20	125.94
26	d	402	CLA	CAA-CBA-CGA	-3.80	101.89	113.35
27	5	1620	LUT	C30-C31-C32	-3.80	111.57	123.23
31	t	101	BCR	C33-C5-C6	-3.80	120.25	124.51
28	7	1622	XAT	C26-C27-C28	-3.80	117.96	125.99
26	1	614	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
39	C	518	DGD	O6D-C1D-O3G	-3.79	101.02	110.02
26	8	602	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
28	y	1622	XAT	C10-C11-C12	-3.79	111.60	123.23
28	Y	1622	XAT	C10-C11-C12	-3.79	111.62	123.23
29	G	1623	NEX	C35-C34-C33	-3.79	121.91	127.31
26	G	603	CLA	OBD-CAD-CBD	-3.78	120.23	125.94
26	4	602	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
29	g	1623	NEX	C35-C34-C33	-3.78	121.91	127.31
27	6	1620	LUT	C23-C24-C25	-3.78	121.68	125.22
26	s	603	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
39	c	518	DGD	O6D-C1D-O3G	-3.78	101.05	110.02
31	T	101	BCR	C28-C27-C26	-3.78	107.28	113.78
27	G	1620	LUT	C35-C34-C33	-3.78	121.92	127.31
31	C	514	BCR	C20-C21-C22	-3.77	121.93	127.31
26	5	603	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
26	1	603	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
39	C	520	DGD	O6D-C1D-O3G	-3.77	101.08	110.02
26	C	505	CLA	O2D-CGD-O1D	-3.76	116.25	123.82
26	7	610	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
28	G	1622	XAT	C10-C11-C12	-3.76	111.70	123.23
26	6	614	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
26	7	613	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
39	c	520	DGD	O6D-C1D-O3G	-3.75	101.11	110.02
31	t	101	BCR	C28-C27-C26	-3.75	107.32	113.78
39	h	102	DGD	O3G-C3G-C2G	-3.75	102.06	110.99
25	s	608	CHL	C4A-C3A-C2A	-3.75	98.12	103.86
31	c	514	BCR	C20-C21-C22	-3.75	121.95	127.31
28	n	1622	XAT	C18-C5-C6	-3.75	115.96	122.31
26	2	614	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
28	N	1622	XAT	C18-C5-C6	-3.75	115.97	122.31
26	S	603	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
26	3	610	CLA	C1B-CHB-C4A	-3.75	122.70	130.12
28	g	1622	XAT	C10-C11-C12	-3.74	111.74	123.23
26	c	505	CLA	O2D-CGD-O1D	-3.74	116.29	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	611	CLA	O2D-CGD-O1D	-3.74	116.29	123.82
26	r	609	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
39	H	102	DGD	O3G-C3G-C2G	-3.74	102.10	110.99
27	g	1620	LUT	C35-C34-C33	-3.74	121.98	127.31
25	S	608	CHL	C4A-C3A-C2A	-3.73	98.15	103.86
26	C	503	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	c	503	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
36	b	621	SQD	O9-S-O7	-3.73	100.94	113.86
26	3	613	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
26	N	604	CLA	O2D-CGD-O1D	-3.72	116.33	123.82
26	Y	614	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
26	y	614	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
31	C	516	BCR	C33-C5-C6	-3.72	120.34	124.51
27	N	1621	LUT	C10-C11-C12	-3.72	111.83	123.23
28	5	1622	XAT	C27-C28-C29	-3.72	119.76	125.53
31	D	404	BCR	C16-C17-C18	-3.72	122.01	127.31
26	R	609	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
29	g	1623	NEX	C27-C28-C29	-3.71	119.77	125.53
36	B	621	SQD	O9-S-O7	-3.71	100.98	113.86
27	n	1621	LUT	C10-C11-C12	-3.71	111.84	123.23
26	y	611	CLA	O2D-CGD-O1D	-3.71	116.35	123.82
31	a	411	BCR	C15-C14-C13	-3.71	122.02	127.31
26	R	610	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
26	r	610	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
26	n	604	CLA	O2D-CGD-O1D	-3.71	116.36	123.82
31	C	514	BCR	C10-C11-C12	-3.71	111.86	123.23
26	C	502	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
31	d	404	BCR	C16-C17-C18	-3.70	122.03	127.31
31	c	516	BCR	C33-C5-C6	-3.70	120.37	124.51
27	4	620	LUT	C15-C14-C13	-3.70	122.03	127.31
28	1	1622	XAT	C27-C28-C29	-3.70	119.79	125.53
29	G	1623	NEX	C27-C28-C29	-3.70	119.80	125.53
31	c	514	BCR	C10-C11-C12	-3.70	111.89	123.23
27	S	1620	LUT	C35-C15-C14	-3.69	115.59	123.46
31	A	411	BCR	C15-C14-C13	-3.69	122.05	127.31
27	s	1620	LUT	C35-C15-C14	-3.69	115.59	123.46
25	6	601	CHL	CBC-CAC-C3C	-3.69	107.35	112.95
27	3	1620	LUT	C35-C34-C33	-3.68	122.05	127.31
27	4	620	LUT	C7-C8-C9	-3.68	120.68	126.21
25	2	601	CHL	CBC-CAC-C3C	-3.68	107.36	112.95
26	c	502	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
26	b	613	CLA	O2D-CGD-O1D	-3.68	116.42	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	1620	LUT	C35-C34-C33	-3.67	122.07	127.31
27	3	1620	LUT	C15-C14-C13	-3.67	122.08	127.31
28	6	1622	XAT	C11-C10-C9	-3.67	122.08	127.31
27	Y	1620	LUT	C10-C11-C12	-3.67	111.98	123.23
27	8	620	LUT	C15-C14-C13	-3.67	122.08	127.31
28	2	1622	XAT	C11-C10-C9	-3.67	122.08	127.31
27	8	620	LUT	C7-C8-C9	-3.67	120.70	126.21
27	y	1620	LUT	C10-C11-C12	-3.66	111.99	123.23
27	6	1621	LUT	C35-C34-C33	-3.66	122.08	127.31
27	2	1621	LUT	C35-C34-C33	-3.66	122.08	127.31
26	r	612	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	y	604	CLA	C1B-CHB-C4A	-3.66	122.87	130.12
27	3	1620	LUT	C10-C11-C12	-3.66	112.01	123.23
27	7	1620	LUT	C10-C11-C12	-3.66	112.02	123.23
26	B	606	CLA	O2D-CGD-O1D	-3.66	116.47	123.82
26	B	613	CLA	O2D-CGD-O1D	-3.65	116.47	123.82
25	1	609	CHL	CHA-CBD-CGD	-3.65	106.53	115.00
26	c	505	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
26	C	505	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
26	8	604	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
25	5	609	CHL	CHA-CBD-CGD	-3.65	106.53	115.00
27	7	1620	LUT	C15-C14-C13	-3.65	122.10	127.31
25	g	609	CHL	CBA-CAA-C2A	-3.65	110.73	115.76
26	R	612	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
29	6	1623	NEX	C31-C30-C29	-3.64	122.11	127.31
26	7	610	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
26	Y	604	CLA	C1B-CHB-C4A	-3.64	122.90	130.12
26	3	610	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
26	b	606	CLA	O2D-CGD-O1D	-3.64	116.50	123.82
29	2	1623	NEX	C31-C30-C29	-3.64	122.12	127.31
25	G	609	CHL	CBA-CAA-C2A	-3.63	110.75	115.76
31	A	411	BCR	C20-C21-C22	-3.63	122.13	127.31
26	4	604	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	1	613	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
37	A	413	LMG	O6-C1-O1	-3.63	101.41	110.02
31	A	411	BCR	C16-C17-C18	-3.63	122.13	127.31
31	C	514	BCR	C15-C16-C17	-3.63	115.72	123.46
26	6	613	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
26	C	509	CLA	O2D-CGD-O1D	-3.63	116.53	123.82
26	s	610	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
37	a	413	LMG	O6-C1-O1	-3.62	101.43	110.02
31	a	411	BCR	C20-C21-C22	-3.62	122.14	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	610	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
31	a	411	BCR	C16-C17-C18	-3.62	122.14	127.31
31	a	411	BCR	C11-C10-C9	-3.61	122.15	127.31
26	c	512	CLA	O2D-CGD-O1D	-3.61	116.55	123.82
31	c	514	BCR	C15-C16-C17	-3.61	115.75	123.46
26	c	509	CLA	O2D-CGD-O1D	-3.61	116.55	123.82
25	Y	607	CHL	C3B-CAB-CBB	-3.61	117.09	125.20
31	c	514	BCR	C16-C17-C18	-3.61	122.16	127.31
27	G	1621	LUT	C10-C11-C12	-3.61	112.17	123.23
31	A	411	BCR	C11-C10-C9	-3.61	122.17	127.31
29	1	1623	NEX	C15-C14-C13	-3.60	122.17	127.31
27	g	1621	LUT	C10-C11-C12	-3.60	112.18	123.23
26	5	613	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
31	C	514	BCR	C16-C17-C18	-3.60	122.17	127.31
36	A	412	SQD	O9-S-O7	-3.60	101.38	113.86
26	G	611	CLA	O2D-CGD-O1D	-3.60	116.58	123.82
26	C	512	CLA	O2D-CGD-O1D	-3.60	116.58	123.82
26	C	508	CLA	C1B-CHB-C4A	-3.60	123.00	130.12
25	y	607	CHL	C3B-CAB-CBB	-3.60	117.13	125.20
26	2	613	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
36	a	412	SQD	O9-S-O7	-3.59	101.40	113.86
26	g	611	CLA	O2D-CGD-O1D	-3.59	116.59	123.82
25	6	607	CHL	CBA-CAA-C2A	-3.59	110.81	115.76
29	5	1623	NEX	C15-C14-C13	-3.59	122.19	127.31
26	y	610	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
26	c	508	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
26	8	610	CLA	C1B-CHB-C4A	-3.58	123.02	130.12
27	6	1620	LUT	C30-C31-C32	-3.58	112.26	123.23
27	G	1620	LUT	C15-C14-C13	-3.58	122.20	127.31
26	N	604	CLA	C1B-CHB-C4A	-3.58	123.03	130.12
25	2	607	CHL	CBA-CAA-C2A	-3.57	110.83	115.76
26	7	612	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
31	B	619	BCR	C16-C17-C18	-3.57	122.21	127.31
31	b	619	BCR	C16-C17-C18	-3.57	122.21	127.31
26	Y	610	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
27	2	1620	LUT	C30-C31-C32	-3.57	112.28	123.23
26	6	612	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
26	2	612	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
26	c	501	CLA	O2D-CGD-O1D	-3.57	116.64	123.82
26	c	513	CLA	O2D-CGD-O1D	-3.57	116.64	123.82
26	n	604	CLA	C1B-CHB-C4A	-3.56	123.07	130.12
26	4	610	CLA	C1B-CHB-C4A	-3.56	123.07	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	501	CLA	O2D-CGD-O1D	-3.56	116.66	123.82
26	4	612	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
27	g	1621	LUT	C7-C8-C9	-3.56	120.87	126.21
26	G	603	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
26	g	603	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
27	S	1620	LUT	C15-C14-C13	-3.56	122.24	127.31
26	C	513	CLA	O2D-CGD-O1D	-3.55	116.67	123.82
26	B	605	CLA	CAA-CBA-CGA	-3.55	102.65	113.35
27	s	1620	LUT	C15-C14-C13	-3.55	122.24	127.31
26	8	612	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	b	605	CLA	CAA-CBA-CGA	-3.54	102.67	113.35
26	3	612	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
27	G	1621	LUT	C7-C8-C9	-3.54	120.89	126.21
27	N	1620	LUT	C35-C15-C14	-3.54	115.91	123.46
27	g	1620	LUT	C15-C14-C13	-3.54	122.26	127.31
26	b	603	CLA	O2D-CGD-O1D	-3.53	116.72	123.82
26	3	613	CLA	C1B-CHB-C4A	-3.53	123.13	130.12
26	5	611	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
27	n	1620	LUT	C35-C15-C14	-3.52	115.94	123.46
26	7	602	CLA	C1B-CHB-C4A	-3.52	123.14	130.12
26	1	611	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
27	5	1620	LUT	C10-C11-C12	-3.52	112.44	123.23
29	g	1623	NEX	C31-C30-C29	-3.51	122.30	127.31
26	3	602	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
26	b	617	CLA	OBD-CAD-CBD	-3.51	120.64	125.94
26	B	603	CLA	O2D-CGD-O1D	-3.51	116.76	123.82
26	7	613	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
27	1	1620	LUT	C10-C11-C12	-3.51	112.47	123.23
27	r	620	LUT	C35-C34-C33	-3.51	122.30	127.31
25	G	601	CHL	CBC-CAC-C3C	-3.51	107.62	112.95
25	g	601	CHL	CBC-CAC-C3C	-3.51	107.63	112.95
27	N	1621	LUT	C16-C1-C6	-3.50	104.63	110.31
26	2	610	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
31	b	619	BCR	C28-C27-C26	-3.50	107.77	113.78
31	B	619	BCR	C28-C27-C26	-3.49	107.77	113.78
31	B	620	BCR	C28-C27-C26	-3.49	107.77	113.78
29	G	1623	NEX	C31-C30-C29	-3.49	122.33	127.31
26	B	607	CLA	O2D-CGD-O1D	-3.49	116.80	123.82
27	n	1621	LUT	C16-C1-C6	-3.49	104.65	110.31
26	R	603	CLA	O2D-CGD-O1D	-3.49	116.80	123.82
28	N	1622	XAT	C10-C11-C12	-3.49	112.54	123.23
25	S	606	CHL	CMA-C3A-C2A	-3.48	104.25	115.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	n	1622	XAT	C10-C11-C12	-3.48	112.55	123.23
25	Y	608	CHL	C4A-C3A-C2A	-3.48	98.53	103.86
26	b	607	CLA	O2D-CGD-O1D	-3.48	116.82	123.82
26	6	610	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
26	B	617	CLA	OBD-CAD-CBD	-3.48	120.69	125.94
26	8	611	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
31	c	517	BCR	C15-C16-C17	-3.48	116.04	123.46
26	B	604	CLA	O2D-CGD-O1D	-3.48	116.83	123.82
31	C	517	BCR	C15-C16-C17	-3.47	116.05	123.46
31	b	620	BCR	C28-C27-C26	-3.47	107.81	113.78
26	r	603	CLA	O2D-CGD-O1D	-3.47	116.83	123.82
25	y	608	CHL	C4A-C3A-C2A	-3.47	98.55	103.86
27	R	620	LUT	C35-C34-C33	-3.47	122.36	127.31
25	s	606	CHL	CMA-C3A-C2A	-3.47	104.30	115.84
26	b	604	CLA	O2D-CGD-O1D	-3.46	116.85	123.82
28	n	1622	XAT	C35-C34-C33	-3.46	122.37	127.31
26	4	611	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
27	N	1621	LUT	C7-C8-C9	-3.45	121.03	126.21
25	3	601	CHL	CBA-CAA-C2A	-3.45	111.00	115.76
26	B	611	CLA	O2D-CGD-O1D	-3.45	116.89	123.82
26	g	613	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
26	G	613	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
26	C	513	CLA	CAA-C2A-C3A	-3.44	103.37	112.81
26	b	611	CLA	O2D-CGD-O1D	-3.44	116.91	123.82
25	7	601	CHL	CBA-CAA-C2A	-3.44	111.02	115.76
26	6	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	5	601	CHL	CBA-CAA-C2A	-3.43	110.72	115.66
28	N	1622	XAT	C35-C34-C33	-3.43	122.41	127.31
26	2	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	c	513	CLA	CAA-C2A-C3A	-3.43	103.41	112.81
26	Y	603	CLA	OBD-CAD-CBD	-3.43	120.77	125.94
26	R	613	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
26	y	603	CLA	OBD-CAD-CBD	-3.42	120.77	125.94
26	2	603	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
39	B	626	DGD	O6D-C1D-O3G	-3.42	101.90	110.02
27	n	1621	LUT	C7-C8-C9	-3.42	121.08	126.21
25	1	601	CHL	CBA-CAA-C2A	-3.41	110.74	115.66
28	7	1622	XAT	C4-C3-C2	-3.41	103.72	110.68
26	6	603	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
26	r	613	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	y	605	CHL	OMC-CMC-C2C	-3.41	119.93	124.29
38	d	405	PL9	C7-C8-C9	-3.41	121.01	126.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	608	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
39	b	626	DGD	O6D-C1D-O3G	-3.40	101.94	110.02
26	r	616	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
28	Y	1622	XAT	C26-C27-C28	-3.40	118.80	125.99
26	b	608	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
38	D	405	PL9	C7-C8-C9	-3.40	121.03	126.71
28	y	1622	XAT	C26-C27-C28	-3.40	118.81	125.99
26	5	610	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
26	1	610	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
28	3	1622	XAT	C4-C3-C2	-3.40	103.75	110.68
26	1	612	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
29	N	1623	NEX	C11-C10-C9	-3.39	122.47	127.31
26	R	616	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
31	b	619	BCR	C20-C21-C22	-3.39	122.47	127.31
26	G	604	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
26	A	407	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
26	5	602	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	s	609	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
27	3	1620	LUT	C30-C31-C32	-3.39	112.84	123.23
26	B	605	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
26	C	502	CLA	O2D-CGD-O1D	-3.39	117.00	123.82
26	c	502	CLA	O2D-CGD-O1D	-3.39	117.00	123.82
31	B	619	BCR	C20-C21-C22	-3.39	122.48	127.31
26	r	602	CLA	O2D-CGD-O1D	-3.39	117.01	123.82
27	7	1620	LUT	C30-C31-C32	-3.38	112.85	123.23
26	N	610	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
29	n	1623	NEX	C11-C10-C9	-3.38	122.48	127.31
37	B	2633	LMG	O2-C2-C1	-3.38	102.95	110.03
26	a	407	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
26	5	612	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
25	Y	605	CHL	OMC-CMC-C2C	-3.38	119.98	124.29
26	A	406	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
26	5	604	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
26	g	604	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
27	r	620	LUT	C35-C15-C14	-3.38	116.26	123.46
25	2	605	CHL	C4A-C3A-C2A	-3.38	98.70	103.86
37	b	2633	LMG	O2-C2-C1	-3.38	102.97	110.03
26	S	609	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
27	5	1621	LUT	C35-C34-C33	-3.38	122.49	127.31
26	R	602	CLA	O2D-CGD-O1D	-3.37	117.03	123.82
26	a	406	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
27	S	1621	LUT	C30-C31-C32	-3.37	112.89	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	g	1620	LUT	C10-C11-C12	-3.37	112.89	123.23
26	l	602	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
26	n	610	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
26	b	605	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
25	6	605	CHL	C4A-C3A-C2A	-3.37	98.71	103.86
27	s	1621	LUT	C30-C31-C32	-3.37	112.90	123.23
26	B	612	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
26	b	612	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
26	A	410	CLA	C1B-CHB-C4A	-3.36	123.45	130.12
26	l	604	CLA	C1B-CHB-C4A	-3.36	123.45	130.12
27	R	620	LUT	C35-C15-C14	-3.36	116.28	123.46
27	l	1621	LUT	C35-C34-C33	-3.36	122.51	127.31
28	N	1622	XAT	C4-C3-C2	-3.36	103.84	110.68
27	G	1620	LUT	C10-C11-C12	-3.36	112.93	123.23
28	R	622	XAT	C10-C11-C12	-3.36	112.93	123.23
29	7	1623	NEX	C39-C29-C30	-3.36	118.22	122.92
26	G	611	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
28	r	622	XAT	C10-C11-C12	-3.35	112.94	123.23
26	a	410	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
28	n	1622	XAT	C4-C3-C2	-3.35	103.86	110.68
39	C	519	DGD	O6D-C1D-O3G	-3.35	102.07	110.02
25	4	606	CHL	C4A-C3A-C2A	-3.35	98.74	103.86
26	5	613	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
31	B	620	BCR	C1-C6-C5	-3.35	117.89	122.59
39	c	519	DGD	O6D-C1D-O3G	-3.34	102.08	110.02
31	b	620	BCR	C1-C6-C5	-3.34	117.89	122.59
26	n	603	CLA	OBD-CAD-CBD	-3.34	120.89	125.94
27	r	620	LUT	C23-C24-C25	-3.34	122.09	125.22
26	B	609	CLA	O2D-CGD-O1D	-3.34	117.10	123.82
26	6	611	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
26	B	606	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
26	2	611	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
26	y	604	CLA	O2D-CGD-O1D	-3.34	117.11	123.82
26	8	610	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
26	g	611	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
26	b	606	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
29	3	1623	NEX	C39-C29-C30	-3.33	118.26	122.92
27	R	620	LUT	C23-C24-C25	-3.33	122.10	125.22
26	l	613	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
26	s	609	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
26	b	609	CLA	O2D-CGD-O1D	-3.32	117.14	123.82
26	b	616	CLA	O2D-CGD-O1D	-3.32	117.14	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	623	NEX	C15-C35-C34	-3.32	116.37	123.46
29	R	623	NEX	C15-C35-C34	-3.32	116.38	123.46
25	6	609	CHL	CHA-CBD-CGD	-3.32	107.30	115.00
26	4	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
26	B	616	CLA	O2D-CGD-O1D	-3.32	117.15	123.82
31	B	620	BCR	C24-C23-C22	-3.32	121.23	126.21
26	3	612	CLA	OBD-CAD-CBD	-3.32	120.93	125.94
26	N	603	CLA	OBD-CAD-CBD	-3.32	120.93	125.94
25	2	609	CHL	CHA-CBD-CGD	-3.31	107.31	115.00
31	b	619	BCR	C8-C7-C6	-3.31	117.98	127.25
25	8	606	CHL	C4A-C3A-C2A	-3.31	98.79	103.86
37	C	521	LMG	C1-C2-C3	-3.31	103.82	109.98
25	S	606	CHL	O2D-CGD-O1D	-3.31	117.16	123.82
26	S	609	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
26	Y	604	CLA	O2D-CGD-O1D	-3.31	117.16	123.82
31	b	620	BCR	C24-C23-C22	-3.31	121.24	126.21
27	s	1621	LUT	C35-C15-C14	-3.31	116.41	123.46
26	B	602	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
31	B	619	BCR	C8-C7-C6	-3.30	118.01	127.25
29	3	1623	NEX	C11-C12-C13	-3.30	117.14	126.42
26	b	611	CLA	CAA-CBA-CGA	-3.30	103.40	113.35
29	7	1623	NEX	C11-C12-C13	-3.30	117.15	126.42
26	S	611	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	s	606	CHL	O2D-CGD-O1D	-3.30	117.18	123.82
26	B	611	CLA	CAA-CBA-CGA	-3.30	103.42	113.35
26	b	602	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
26	7	612	CLA	OBD-CAD-CBD	-3.29	120.97	125.94
37	c	521	LMG	C1-C2-C3	-3.29	103.86	109.98
27	S	1621	LUT	C35-C15-C14	-3.29	116.44	123.46
28	6	1622	XAT	C27-C28-C29	-3.29	120.43	125.53
27	4	620	LUT	C11-C10-C9	-3.29	122.62	127.31
28	2	1622	XAT	C27-C28-C29	-3.29	120.43	125.53
28	2	1622	XAT	C7-C8-C9	-3.29	120.43	125.53
26	G	610	CLA	C1B-CHB-C4A	-3.28	123.61	130.12
26	7	612	CLA	O2D-CGD-O1D	-3.28	117.22	123.82
25	8	601	CHL	CBC-CAC-C3C	-3.28	107.97	112.95
27	1	1620	LUT	C35-C15-C14	-3.28	116.46	123.46
27	s	1621	LUT	C10-C11-C12	-3.28	113.17	123.23
26	s	611	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
26	3	612	CLA	O2D-CGD-O1D	-3.28	117.23	123.82
27	8	620	LUT	C11-C10-C9	-3.27	122.64	127.31
28	5	1622	XAT	C35-C34-C33	-3.27	122.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	1620	LUT	C10-C11-C12	-3.27	113.20	123.23
27	n	1620	LUT	C10-C11-C12	-3.27	113.20	123.23
27	S	1621	LUT	C10-C11-C12	-3.27	113.20	123.23
27	5	1620	LUT	C35-C15-C14	-3.27	116.48	123.46
28	1	1622	XAT	C35-C34-C33	-3.27	122.65	127.31
25	3	609	CHL	CBC-CAC-C3C	-3.26	108.00	112.95
29	r	623	NEX	C31-C30-C29	-3.26	122.65	127.31
27	r	620	LUT	C10-C11-C12	-3.26	113.22	123.23
25	4	601	CHL	CBC-CAC-C3C	-3.26	108.00	112.95
26	D	403	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
26	a	406	CLA	O2D-CGD-O1D	-3.26	117.27	123.82
27	Y	1620	LUT	C15-C14-C13	-3.26	122.66	127.31
26	g	610	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
26	G	603	CLA	CAA-C2A-C3A	-3.25	103.90	112.81
26	g	603	CLA	CAA-C2A-C3A	-3.25	103.90	112.81
28	6	1622	XAT	C7-C8-C9	-3.25	120.49	125.53
25	1	607	CHL	C3B-CAB-CBB	-3.25	117.91	125.20
27	R	620	LUT	C10-C11-C12	-3.25	113.27	123.23
28	G	1622	XAT	C11-C10-C9	-3.25	122.68	127.31
26	r	610	CLA	O2D-CGD-O1D	-3.25	117.29	123.82
25	3	605	CHL	CBC-CAC-C3C	-3.24	108.03	112.95
26	B	615	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
25	7	607	CHL	CBA-CAA-C2A	-3.24	111.29	115.76
29	R	623	NEX	C31-C30-C29	-3.24	122.68	127.31
26	c	508	CLA	CMC-C2C-C1C	-3.24	120.11	125.02
27	r	620	LUT	C15-C14-C13	-3.24	122.68	127.31
26	d	403	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
26	A	406	CLA	O2D-CGD-O1D	-3.24	117.30	123.82
29	S	1623	NEX	C26-C27-C28	-3.24	119.14	125.99
25	7	609	CHL	CBC-CAC-C3C	-3.24	108.03	112.95
26	b	615	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
27	R	620	LUT	C15-C14-C13	-3.23	122.69	127.31
25	n	608	CHL	CBC-CAC-C3C	-3.23	108.04	112.95
31	C	515	BCR	C15-C16-C17	-3.23	116.56	123.46
31	c	515	BCR	C15-C16-C17	-3.23	116.57	123.46
25	3	607	CHL	CBA-CAA-C2A	-3.23	111.31	115.76
26	R	610	CLA	O2D-CGD-O1D	-3.23	117.32	123.82
26	n	602	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
25	5	607	CHL	C3B-CAB-CBB	-3.22	117.96	125.20
26	N	602	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
26	3	603	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
27	y	1620	LUT	C15-C14-C13	-3.22	122.71	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	605	CHL	CBC-CAC-C3C	-3.22	108.06	112.95
27	N	1621	LUT	C35-C34-C33	-3.22	122.72	127.31
25	N	608	CHL	CBC-CAC-C3C	-3.22	108.07	112.95
26	g	614	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
27	8	620	LUT	C18-C5-C6	-3.22	120.91	124.51
29	s	1623	NEX	C26-C27-C28	-3.22	119.19	125.99
26	C	508	CLA	CMC-C2C-C1C	-3.21	120.15	125.02
25	8	601	CHL	C4A-C3A-C2A	-3.21	98.94	103.86
28	g	1622	XAT	C11-C10-C9	-3.21	122.73	127.31
25	4	601	CHL	C4A-C3A-C2A	-3.21	98.95	103.86
26	7	602	CLA	O2D-CGD-O1D	-3.21	117.36	123.82
28	g	1622	XAT	C35-C34-C33	-3.21	122.73	127.31
27	n	1621	LUT	C35-C34-C33	-3.21	122.73	127.31
26	G	614	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
27	Y	1620	LUT	C30-C31-C32	-3.20	113.40	123.23
26	2	611	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
26	b	617	CLA	O2D-CGD-O1D	-3.20	117.39	123.82
25	5	605	CHL	CBC-CAC-C3C	-3.20	108.10	112.95
28	y	1622	XAT	C4-C3-C2	-3.20	104.17	110.68
26	r	604	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
26	B	617	CLA	O2D-CGD-O1D	-3.19	117.40	123.82
26	7	603	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
28	Y	1622	XAT	C4-C3-C2	-3.19	104.18	110.68
27	y	1620	LUT	C30-C31-C32	-3.19	113.44	123.23
31	a	411	BCR	C24-C23-C22	-3.19	121.42	126.21
27	4	620	LUT	C18-C5-C6	-3.19	120.94	124.51
26	6	611	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
29	S	1623	NEX	C35-C34-C33	-3.19	122.76	127.31
29	1	1623	NEX	C11-C10-C9	-3.18	122.77	127.31
26	6	611	CLA	O2D-CGD-O1D	-3.18	117.41	123.82
26	c	501	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
25	1	605	CHL	CBC-CAC-C3C	-3.18	108.12	112.95
28	8	622	XAT	C15-C14-C13	-3.18	122.77	127.31
26	C	501	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
29	5	1623	NEX	C11-C10-C9	-3.18	122.77	127.31
25	S	601	CHL	C4A-C3A-C2A	-3.18	99.00	103.86
26	n	613	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
28	4	622	XAT	C15-C14-C13	-3.18	122.77	127.31
29	s	1623	NEX	C35-C34-C33	-3.18	122.77	127.31
26	r	611	CLA	O2D-CGD-O1D	-3.18	117.42	123.82
28	G	1622	XAT	C35-C34-C33	-3.17	122.78	127.31
26	R	611	CLA	O2D-CGD-O1D	-3.17	117.44	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	613	CLA	O2D-CGD-O1D	-3.17	117.44	123.82
26	N	603	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
26	3	602	CLA	O2D-CGD-O1D	-3.17	117.44	123.82
25	n	605	CHL	C4A-C3A-C2A	-3.17	99.01	103.86
26	B	611	CLA	CAA-C2A-C3A	-3.17	104.12	112.81
26	N	613	CLA	O2D-CGD-O1D	-3.17	117.45	123.82
25	4	606	CHL	CBC-CAC-C3C	-3.17	108.14	112.95
26	Y	602	CLA	O2D-CGD-O1D	-3.17	117.45	123.82
26	2	611	CLA	O2D-CGD-O1D	-3.17	117.45	123.82
26	R	604	CLA	C1B-CHB-C4A	-3.17	123.85	130.12
26	n	603	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
26	2	613	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
26	b	611	CLA	CAA-C2A-C3A	-3.16	104.14	112.81
25	8	606	CHL	CBC-CAC-C3C	-3.16	108.15	112.95
26	4	604	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
27	8	620	LUT	C30-C31-C32	-3.16	113.53	123.23
27	4	620	LUT	C35-C34-C33	-3.16	122.80	127.31
27	4	620	LUT	C30-C31-C32	-3.16	113.54	123.23
28	3	1622	XAT	C11-C10-C9	-3.16	122.80	127.31
26	6	613	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
26	r	609	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
26	R	609	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
31	A	411	BCR	C24-C23-C22	-3.16	121.47	126.21
27	8	620	LUT	C35-C34-C33	-3.16	122.81	127.31
25	3	605	CHL	C4A-C3A-C2A	-3.15	99.03	103.86
26	N	613	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
26	b	607	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
25	7	605	CHL	C4A-C3A-C2A	-3.15	99.04	103.86
31	C	515	BCR	C24-C23-C22	-3.15	121.48	126.21
26	y	602	CLA	O2D-CGD-O1D	-3.15	117.48	123.82
26	g	602	CLA	C1-C2-C3	-3.15	120.16	125.96
26	y	611	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
26	G	602	CLA	C1-C2-C3	-3.15	120.16	125.96
25	N	605	CHL	C4A-C3A-C2A	-3.15	99.05	103.86
25	s	601	CHL	C4A-C3A-C2A	-3.15	99.05	103.86
25	Y	601	CHL	O2D-CGD-O1D	-3.15	117.49	123.82
26	8	604	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
26	B	607	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
25	y	601	CHL	O2D-CGD-O1D	-3.14	117.49	123.82
27	S	1620	LUT	C10-C11-C12	-3.14	113.59	123.23
26	C	501	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
27	Y	1620	LUT	C35-C15-C14	-3.14	116.75	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	1622	XAT	C35-C34-C33	-3.14	122.82	127.31
26	c	501	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
31	c	515	BCR	C24-C23-C22	-3.14	121.49	126.21
26	r	611	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
26	C	502	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
31	B	618	BCR	C7-C8-C9	-3.14	121.50	126.21
38	d	405	PL9	C7-C3-C2	-3.14	118.77	123.23
27	n	1620	LUT	C15-C14-C13	-3.14	122.83	127.31
26	Y	611	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
38	D	405	PL9	C7-C3-C2	-3.14	118.77	123.23
26	g	603	CLA	O2D-CGD-O1D	-3.13	117.52	123.82
27	s	1620	LUT	C10-C11-C12	-3.13	113.62	123.23
26	B	604	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
28	2	1622	XAT	C35-C34-C33	-3.13	122.84	127.31
27	N	1620	LUT	C15-C14-C13	-3.13	122.85	127.31
27	y	1620	LUT	C35-C15-C14	-3.12	116.80	123.46
28	7	1622	XAT	C11-C10-C9	-3.12	122.85	127.31
26	C	507	CLA	O2D-CGD-O1D	-3.12	117.54	123.82
31	d	404	BCR	C38-C26-C25	-3.12	121.01	124.51
31	b	618	BCR	C7-C8-C9	-3.12	121.52	126.21
26	c	507	CLA	O2D-CGD-O1D	-3.12	117.54	123.82
26	6	603	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
26	c	502	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
26	R	611	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
26	3	614	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
26	G	603	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
26	r	603	CLA	OBD-CAD-CBD	-3.12	121.23	125.94
28	3	1622	XAT	C24-C23-C22	-3.12	104.33	110.68
26	b	609	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
26	R	603	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
31	b	618	BCR	C21-C20-C19	-3.11	113.68	123.23
26	b	604	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
31	B	618	BCR	C21-C20-C19	-3.11	113.69	123.23
26	A	405	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
28	r	622	XAT	C35-C15-C14	-3.11	116.82	123.46
26	2	603	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
26	s	604	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
26	8	602	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
26	a	405	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
31	c	517	BCR	C21-C20-C19	-3.10	113.71	123.23
28	7	1622	XAT	C24-C23-C22	-3.10	104.36	110.68
26	7	614	CLA	O2D-CGD-O1D	-3.10	117.58	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	g	1621	LUT	C23-C24-C25	-3.10	122.31	125.22
28	R	622	XAT	C35-C15-C14	-3.10	116.85	123.46
31	D	404	BCR	C38-C26-C25	-3.10	121.04	124.51
31	C	517	BCR	C21-C20-C19	-3.09	113.74	123.23
25	y	608	CHL	CBC-CAC-C3C	-3.09	108.25	112.95
26	B	609	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
26	Y	612	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
26	4	602	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
26	S	604	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
26	y	603	CLA	O2D-CGD-O1D	-3.09	117.61	123.82
31	8	623	BCR	C11-C12-C13	-3.09	117.74	126.42
26	1	614	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
26	S	602	CLA	O2D-CGD-O1D	-3.08	117.62	123.82
31	4	623	BCR	C11-C12-C13	-3.08	117.76	126.42
27	n	1620	LUT	C30-C31-C32	-3.08	113.78	123.23
41	f	101	HEM	CBA-CAA-C2A	-3.08	106.60	112.48
27	N	1620	LUT	C30-C31-C32	-3.08	113.79	123.23
29	6	1623	NEX	C15-C35-C34	-3.08	116.89	123.46
31	T	101	BCR	C16-C15-C14	-3.08	116.89	123.46
27	G	1621	LUT	C23-C24-C25	-3.08	122.33	125.22
31	t	101	BCR	C16-C15-C14	-3.08	116.89	123.46
25	Y	608	CHL	CBC-CAC-C3C	-3.08	108.28	112.95
26	s	602	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
26	2	604	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	Y	605	CHL	C4A-C3A-C2A	-3.07	99.16	103.86
26	Y	603	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
39	c	519	DGD	O5D-C6D-C5D	-3.07	103.81	108.94
26	1	611	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
26	5	611	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
26	n	603	CLA	O2D-CGD-O1D	-3.07	117.65	123.82
31	H	101	BCR	C20-C21-C22	-3.07	122.93	127.31
25	S	606	CHL	CBA-CAA-C2A	-3.07	111.24	115.66
25	y	605	CHL	C4A-C3A-C2A	-3.07	99.17	103.86
26	N	611	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
26	n	611	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
31	h	101	BCR	C20-C21-C22	-3.07	122.93	127.31
38	A	414	PL9	C7-C3-C2	-3.06	118.87	123.23
26	c	506	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
26	C	506	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
26	y	612	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
29	3	1623	NEX	C24-C23-C22	-3.06	104.44	110.68
27	4	620	LUT	C8-C7-C6	-3.06	118.68	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	604	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
41	F	101	HEM	CBA-CAA-C2A	-3.06	106.63	112.48
29	2	1623	NEX	C15-C35-C34	-3.06	116.93	123.46
38	a	414	PL9	C7-C3-C2	-3.06	118.88	123.23
26	N	603	CLA	O2D-CGD-O1D	-3.06	117.67	123.82
26	B	611	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
26	5	614	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
26	6	604	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
27	8	620	LUT	C8-C7-C6	-3.05	118.71	127.25
26	7	604	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
31	d	404	BCR	C15-C14-C13	-3.05	122.96	127.31
31	b	620	BCR	C4-C5-C6	-3.05	118.27	122.74
27	G	1621	LUT	C30-C31-C32	-3.05	113.88	123.23
29	7	1623	NEX	C24-C23-C22	-3.05	104.47	110.68
25	s	606	CHL	CBA-CAA-C2A	-3.05	111.27	115.66
26	2	602	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
26	6	602	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
27	g	1621	LUT	C18-C5-C6	-3.04	121.10	124.51
29	S	1623	NEX	C31-C30-C29	-3.04	122.97	127.31
39	C	519	DGD	O5D-C6D-C5D	-3.04	103.86	108.94
31	D	404	BCR	C15-C14-C13	-3.04	122.97	127.31
26	b	611	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
29	s	1623	NEX	C31-C30-C29	-3.03	122.98	127.31
27	G	1621	LUT	C18-C5-C6	-3.03	121.11	124.51
27	7	1621	LUT	C15-C35-C34	-3.03	116.99	123.46
31	B	620	BCR	C4-C5-C6	-3.03	118.29	122.74
27	s	1620	LUT	C30-C31-C32	-3.03	113.94	123.23
27	S	1620	LUT	C30-C31-C32	-3.03	113.94	123.23
27	g	1621	LUT	C30-C31-C32	-3.03	113.94	123.23
26	R	604	CLA	CAA-C2A-C3A	-3.03	104.51	112.81
26	2	610	CLA	O2D-CGD-O1D	-3.03	117.73	123.82
28	3	1622	XAT	C31-C32-C33	-3.03	117.91	126.42
26	r	604	CLA	CAA-C2A-C3A	-3.03	104.52	112.81
27	N	1620	LUT	C38-C25-C24	-3.03	117.17	123.68
27	2	1620	LUT	C10-C11-C12	-3.02	113.96	123.23
26	S	603	CLA	O2D-CGD-O1D	-3.02	117.74	123.82
26	b	610	CLA	C7-C6-C5	-3.02	104.71	113.11
27	r	620	LUT	C28-C29-C30	-3.02	114.31	118.94
26	B	610	CLA	C7-C6-C5	-3.02	104.72	113.11
27	6	1620	LUT	C10-C11-C12	-3.02	113.98	123.23
26	N	602	CLA	O2D-CGD-O1D	-3.01	117.75	123.82
28	7	1622	XAT	C31-C32-C33	-3.01	117.95	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	618	BCR	C20-C21-C22	-3.01	123.01	127.31
26	g	604	CLA	C1-C2-C3	-3.01	121.93	126.68
26	c	505	CLA	C7-C6-C5	-3.01	104.75	113.11
26	C	505	CLA	C7-C6-C5	-3.01	104.75	113.11
27	3	1621	LUT	C15-C35-C34	-3.01	117.04	123.46
26	B	610	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
26	6	610	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
26	b	610	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
26	4	611	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
26	8	611	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
26	R	613	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	6	614	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	G	603	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	s	603	CLA	O2D-CGD-O1D	-3.00	117.78	123.82
26	G	604	CLA	C1-C2-C3	-3.00	121.94	126.68
27	Y	1620	LUT	C35-C34-C33	-3.00	123.02	127.31
25	r	606	CHL	CBC-CAC-C3C	-3.00	108.39	112.95
26	7	603	CLA	CBC-CAC-C3C	-3.00	103.89	112.41
26	3	603	CLA	CBC-CAC-C3C	-3.00	103.90	112.41
27	y	1620	LUT	C35-C34-C33	-3.00	123.03	127.31
39	C	518	DGD	O3E-C3E-C2E	-3.00	103.83	110.36
39	c	518	DGD	O3E-C3E-C2E	-3.00	103.83	110.36
26	r	613	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
26	n	602	CLA	O2D-CGD-O1D	-2.99	117.80	123.82
36	a	418	SQD	C5-C6-S	-2.99	110.17	114.34
27	R	620	LUT	C28-C29-C30	-2.99	114.35	118.94
25	R	606	CHL	CBC-CAC-C3C	-2.99	108.41	112.95
25	7	606	CHL	CBC-CAC-C3C	-2.99	108.41	112.95
27	n	1620	LUT	C38-C25-C24	-2.99	117.24	123.68
25	G	605	CHL	OMC-CMC-C2C	-2.99	120.47	124.29
26	2	614	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
27	2	1621	LUT	C10-C11-C12	-2.99	114.07	123.23
26	R	611	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
25	3	606	CHL	CBC-CAC-C3C	-2.99	108.42	112.95
31	C	516	BCR	C10-C11-C12	-2.98	114.08	123.23
31	c	516	BCR	C10-C11-C12	-2.98	114.08	123.23
28	4	622	XAT	C4-C3-C2	-2.98	104.61	110.68
35	A	408	PHO	CAA-CBA-CGA	-2.98	104.36	113.35
28	8	622	XAT	C4-C3-C2	-2.98	104.61	110.68
26	g	613	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
35	a	408	PHO	CAA-CBA-CGA	-2.98	104.37	113.35
26	g	603	CLA	C1B-CHB-C4A	-2.98	124.22	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	618	BCR	C20-C21-C22	-2.98	123.06	127.31
39	B	626	DGD	CDB-CCB-CBB	-2.98	99.12	114.45
26	y	614	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
31	A	411	BCR	C38-C26-C25	-2.97	121.18	124.51
39	b	626	DGD	CDB-CCB-CBB	-2.97	99.13	114.45
26	G	613	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
27	7	1621	LUT	C10-C11-C12	-2.97	114.11	123.23
36	A	418	SQD	C5-C6-S	-2.97	110.20	114.34
27	6	1621	LUT	C10-C11-C12	-2.97	114.12	123.23
26	Y	614	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	g	605	CHL	OMC-CMC-C2C	-2.96	120.51	124.29
26	1	602	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
26	n	603	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
31	a	411	BCR	C38-C26-C25	-2.96	121.19	124.51
26	5	602	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
27	7	1621	LUT	C35-C34-C33	-2.96	123.09	127.31
27	3	1621	LUT	C10-C11-C12	-2.96	114.16	123.23
26	r	611	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
26	s	611	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
28	2	1622	XAT	C6-C7-C8	-2.95	119.75	125.99
39	C	520	DGD	O5D-C6D-C5D	-2.95	104.00	108.94
28	4	622	XAT	C10-C11-C12	-2.95	114.18	123.23
31	b	618	BCR	C15-C16-C17	-2.95	117.17	123.46
26	N	603	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
39	c	520	DGD	O5D-C6D-C5D	-2.95	104.01	108.94
26	B	603	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
26	N	602	CLA	C1-C2-C3	-2.95	120.53	125.96
27	G	1620	LUT	C38-C25-C24	-2.95	117.33	123.68
31	B	618	BCR	C15-C16-C17	-2.95	117.17	123.46
26	S	602	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
26	b	603	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
28	8	622	XAT	C10-C11-C12	-2.94	114.21	123.23
26	B	613	CLA	CMA-C3A-C4A	-2.94	103.87	111.77
26	n	602	CLA	C1-C2-C3	-2.94	120.54	125.96
26	s	602	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	Y	602	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	b	605	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
26	b	610	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
39	h	102	DGD	O6D-C1D-O3G	-2.94	103.05	110.02
25	5	609	CHL	CBC-CAC-C3C	-2.94	108.49	112.95
39	B	626	DGD	C3G-C2G-C1G	-2.93	105.24	111.86
27	g	1620	LUT	C38-C25-C24	-2.93	117.36	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	1622	XAT	C31-C32-C33	-2.93	118.17	126.42
26	b	613	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
39	H	102	DGD	O6D-C1D-O3G	-2.93	103.06	110.02
28	5	1622	XAT	C31-C32-C33	-2.93	118.18	126.42
28	6	1622	XAT	C6-C7-C8	-2.93	119.80	125.99
26	S	611	CLA	O2D-CGD-O1D	-2.93	117.93	123.82
27	g	1620	LUT	C30-C31-C32	-2.93	114.25	123.23
26	y	602	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
27	G	1620	LUT	C30-C31-C32	-2.93	114.25	123.23
27	5	1621	LUT	C18-C5-C6	-2.93	121.23	124.51
39	b	626	DGD	C3G-C2G-C1G	-2.92	105.26	111.86
26	n	614	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
27	3	1621	LUT	C35-C34-C33	-2.92	123.14	127.31
26	3	611	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
26	R	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
26	C	504	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
27	S	1620	LUT	C11-C10-C9	-2.92	123.14	127.31
26	c	504	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
27	s	1620	LUT	C11-C10-C9	-2.92	123.15	127.31
26	N	614	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	Y	613	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	B	610	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
31	a	411	BCR	C16-C15-C14	-2.91	117.24	123.46
26	c	511	CLA	O2D-CGD-O1D	-2.91	117.96	123.82
26	y	613	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	G	602	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	7	611	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
37	c	521	LMG	O1-C7-C8	-2.91	104.06	110.99
31	c	517	BCR	C20-C21-C22	-2.91	123.16	127.31
25	G	607	CHL	CBA-CAA-C2A	-2.91	111.75	115.76
26	r	602	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
26	C	511	CLA	O2D-CGD-O1D	-2.91	117.97	123.82
37	C	521	LMG	O1-C7-C8	-2.91	104.07	110.99
31	b	619	BCR	C24-C23-C22	-2.91	121.84	126.21
31	A	411	BCR	C16-C15-C14	-2.91	117.26	123.46
25	1	609	CHL	CBC-CAC-C3C	-2.90	108.54	112.95
25	s	601	CHL	CBA-CAA-C2A	-2.90	111.48	115.66
26	g	604	CLA	O2D-CGD-O1D	-2.90	117.98	123.82
31	B	619	BCR	C24-C23-C22	-2.90	121.86	126.21
26	y	602	CLA	C1-C2-C3	-2.90	120.61	125.96
28	r	622	XAT	C4-C3-C2	-2.90	104.77	110.68
26	B	605	CLA	CMB-C2B-C1B	-2.90	124.01	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	1623	NEX	C26-C27-C28	-2.90	119.86	125.99
29	1	1623	NEX	C26-C27-C28	-2.90	119.87	125.99
31	C	517	BCR	C20-C21-C22	-2.90	123.18	127.31
26	g	602	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
25	g	607	CHL	CBA-CAA-C2A	-2.89	111.77	115.76
27	Y	1621	LUT	C10-C11-C12	-2.89	114.36	123.23
28	8	622	XAT	C24-C23-C22	-2.89	104.79	110.68
31	T	101	BCR	C11-C12-C13	-2.89	118.29	126.42
26	2	612	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
31	B	618	BCR	C11-C10-C9	-2.89	123.18	127.31
26	y	612	CLA	O2D-CGD-O1D	-2.89	118.00	123.82
27	y	1621	LUT	C10-C11-C12	-2.89	114.37	123.23
26	R	604	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
28	R	622	XAT	C4-C3-C2	-2.89	104.80	110.68
27	1	1621	LUT	C22-C23-C24	-2.89	108.46	111.73
31	t	101	BCR	C11-C12-C13	-2.89	118.30	126.42
25	r	614	CHL	O2D-CGD-O1D	-2.89	118.01	123.82
25	2	608	CHL	CBC-CAC-C3C	-2.89	108.57	112.95
27	G	1620	LUT	C23-C24-C25	-2.89	122.51	125.22
26	Y	612	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
27	8	620	LUT	C31-C30-C29	-2.88	123.19	127.31
26	r	604	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
27	1	1621	LUT	C18-C5-C6	-2.88	121.28	124.51
26	G	604	CLA	O2D-CGD-O1D	-2.88	118.02	123.82
25	6	608	CHL	CBC-CAC-C3C	-2.88	108.58	112.95
26	Y	602	CLA	C1-C2-C3	-2.88	120.66	125.96
26	6	612	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
31	C	514	BCR	C21-C20-C19	-2.88	114.41	123.23
27	g	1620	LUT	C23-C24-C25	-2.88	122.52	125.22
25	S	601	CHL	CBA-CAA-C2A	-2.88	111.52	115.66
25	Y	606	CHL	O2D-CGD-O1D	-2.88	118.03	123.82
25	y	606	CHL	O2D-CGD-O1D	-2.88	118.03	123.82
25	R	614	CHL	O2D-CGD-O1D	-2.88	118.03	123.82
27	S	1621	LUT	C8-C9-C10	-2.88	114.53	118.94
27	5	1621	LUT	C22-C23-C24	-2.87	108.48	111.73
26	7	603	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
26	A	407	CLA	O2D-CGD-O1D	-2.87	118.04	123.82
27	s	1621	LUT	C8-C9-C10	-2.87	114.53	118.94
31	c	514	BCR	C21-C20-C19	-2.87	114.42	123.23
25	g	606	CHL	C3B-CAB-CBB	-2.87	118.76	125.20
26	1	604	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
29	g	1623	NEX	C39-C29-C30	-2.87	118.91	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	622	XAT	C24-C23-C22	-2.87	104.84	110.68
25	5	607	CHL	OMC-CMC-C2C	-2.87	120.63	124.29
25	G	606	CHL	C3B-CAB-CBB	-2.87	118.77	125.20
37	z	101	LMG	O8-C28-O10	-2.86	116.44	123.55
31	B	619	BCR	C15-C16-C17	-2.86	117.35	123.46
26	N	614	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
37	Z	101	LMG	O8-C28-O10	-2.86	116.44	123.55
26	n	614	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
31	b	619	BCR	C15-C16-C17	-2.86	117.36	123.46
25	R	607	CHL	CBA-CAA-C2A	-2.86	111.81	115.76
27	y	1620	LUT	C38-C25-C24	-2.86	117.52	123.68
26	8	603	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
26	5	604	CLA	O2D-CGD-O1D	-2.86	118.07	123.82
27	3	1621	LUT	C22-C23-C24	-2.86	108.50	111.73
26	4	603	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
26	a	407	CLA	O2D-CGD-O1D	-2.86	118.08	123.82
28	Y	1622	XAT	C24-C23-C22	-2.85	104.86	110.68
26	B	602	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	b	602	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	C	506	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
29	G	1623	NEX	C39-C29-C30	-2.85	118.93	122.92
27	4	620	LUT	C31-C30-C29	-2.85	123.24	127.31
26	3	614	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	C	509	CLA	CAA-C2A-C3A	-2.85	105.00	112.81
31	8	623	BCR	C3-C4-C5	-2.85	108.88	113.78
25	1	605	CHL	C4A-C3A-C2A	-2.85	99.50	103.86
25	r	607	CHL	CBA-CAA-C2A	-2.85	111.83	115.76
26	3	603	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
37	C	521	LMG	O6-C1-O1	-2.85	103.26	110.02
31	b	618	BCR	C11-C10-C9	-2.85	123.25	127.31
27	7	1621	LUT	C22-C23-C24	-2.84	108.51	111.73
37	d	411	LMG	O6-C1-O1	-2.84	103.27	110.02
37	D	411	LMG	O6-C1-O1	-2.84	103.27	110.02
27	2	1620	LUT	C15-C14-C13	-2.84	123.25	127.31
25	1	607	CHL	OMC-CMC-C2C	-2.84	120.66	124.29
26	5	614	CLA	O2D-CGD-O1D	-2.84	118.10	123.82
26	7	614	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
26	1	614	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
35	a	409	PHO	O2D-CGD-O1D	-2.84	118.11	123.82
29	1	1623	NEX	C24-C23-C22	-2.84	104.90	110.68
28	y	1622	XAT	C24-C23-C22	-2.84	104.90	110.68
26	B	602	CLA	O2D-CGD-O1D	-2.84	118.11	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	509	CLA	CAA-C2A-C3A	-2.83	105.04	112.81
31	4	623	BCR	C3-C4-C5	-2.83	108.91	113.78
27	6	1620	LUT	C15-C14-C13	-2.83	123.27	127.31
26	3	612	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
29	N	1623	NEX	C39-C29-C30	-2.83	118.96	122.92
26	g	612	CLA	O2D-CGD-O1D	-2.83	118.12	123.82
26	c	506	CLA	O2D-CGD-O1D	-2.83	118.12	123.82
39	h	102	DGD	C1D-C2D-C3D	-2.83	104.72	109.98
37	c	521	LMG	O6-C1-O1	-2.83	103.30	110.02
27	y	1620	LUT	C23-C24-C25	-2.83	122.57	125.22
26	G	614	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
26	5	612	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
27	Y	1620	LUT	C38-C25-C24	-2.82	117.60	123.68
26	b	602	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
25	5	605	CHL	C4A-C3A-C2A	-2.82	99.54	103.86
27	g	1620	LUT	C35-C15-C14	-2.82	117.44	123.46
26	s	604	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
29	n	1623	NEX	C39-C29-C30	-2.82	118.97	122.92
27	G	1620	LUT	C35-C15-C14	-2.82	117.44	123.46
27	n	1621	LUT	C30-C31-C32	-2.82	114.58	123.23
26	c	509	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
26	l	612	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
26	c	510	CLA	O2D-CGD-O1D	-2.82	118.15	123.82
26	G	612	CLA	O2D-CGD-O1D	-2.82	118.15	123.82
26	R	601	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
26	r	601	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
29	5	1623	NEX	C24-C23-C22	-2.81	104.95	110.68
26	7	612	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
26	d	402	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
26	g	614	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
35	A	409	PHO	O2D-CGD-O1D	-2.81	118.16	123.82
39	H	102	DGD	C1D-C2D-C3D	-2.81	104.75	109.98
26	C	509	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
26	S	604	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
26	N	603	CLA	CAA-C2A-C3A	-2.81	105.10	112.81
26	l	612	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
26	g	610	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
27	N	1621	LUT	C30-C31-C32	-2.81	114.62	123.23
26	5	612	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
26	C	510	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
29	g	1623	NEX	C26-C27-C28	-2.81	120.06	125.99
26	G	610	CLA	O2D-CGD-O1D	-2.80	118.18	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	603	CLA	CAA-C2A-C3A	-2.80	105.13	112.81
39	h	102	DGD	O3E-C3E-C2E	-2.80	104.26	110.36
39	c	519	DGD	O3E-C3E-C2E	-2.80	104.26	110.36
27	N	1621	LUT	C22-C23-C24	-2.80	108.56	111.73
25	N	601	CHL	O2D-CGD-O1D	-2.80	118.19	123.82
29	r	623	NEX	C39-C29-C30	-2.80	119.00	122.92
25	N	601	CHL	C1-C2-C3	-2.80	120.80	125.96
27	Y	1621	LUT	C30-C31-C32	-2.80	114.65	123.23
39	h	102	DGD	C3D-C4D-C5D	-2.80	105.29	110.22
25	G	608	CHL	C1-C2-C3	-2.80	120.80	125.96
26	C	507	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
26	S	603	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
26	a	406	CLA	CAC-C3C-C4C	-2.80	120.89	124.83
27	y	1621	LUT	C30-C31-C32	-2.79	114.66	123.23
39	H	102	DGD	O3E-C3E-C2E	-2.79	104.28	110.36
31	c	516	BCR	C16-C15-C14	-2.79	117.50	123.46
25	n	601	CHL	C1-C2-C3	-2.79	120.81	125.96
29	G	1623	NEX	C26-C27-C28	-2.79	120.09	125.99
26	b	608	CLA	O2D-CGD-O1D	-2.79	118.20	123.82
26	G	603	CLA	CBC-CAC-C3C	-2.79	104.49	112.41
26	g	603	CLA	CBC-CAC-C3C	-2.79	104.49	112.41
26	s	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
26	r	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
26	R	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
31	c	516	BCR	C15-C14-C13	-2.79	123.33	127.31
25	g	608	CHL	C1-C2-C3	-2.79	120.82	125.96
29	y	1623	NEX	C26-C27-C28	-2.79	120.10	125.99
26	B	606	CLA	C1-C2-C3	-2.79	120.82	125.96
27	3	1620	LUT	C7-C8-C9	-2.78	122.03	126.21
26	B	608	CLA	O2D-CGD-O1D	-2.78	118.22	123.82
29	S	1623	NEX	O4-C5-C18	-2.78	104.63	109.51
29	s	1623	NEX	O4-C5-C18	-2.78	104.63	109.51
25	n	601	CHL	O2D-CGD-O1D	-2.78	118.22	123.82
38	a	414	PL9	O2-C1-C2	-2.78	117.26	121.39
31	C	516	BCR	C16-C15-C14	-2.78	117.52	123.46
39	C	519	DGD	O3E-C3E-C2E	-2.78	104.30	110.36
26	b	606	CLA	C1-C2-C3	-2.78	120.83	125.96
26	2	612	CLA	CAA-C2A-C3A	-2.78	105.18	112.81
26	D	402	CLA	O2D-CGD-O1D	-2.78	118.22	123.82
38	A	414	PL9	O2-C1-C2	-2.78	117.26	121.39
25	3	601	CHL	CBC-CAC-C3C	-2.78	108.73	112.95
26	c	507	CLA	C1B-CHB-C4A	-2.78	124.62	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	406	CLA	CAC-C3C-C4C	-2.78	120.91	124.83
39	H	102	DGD	C3D-C4D-C5D	-2.78	105.33	110.22
29	r	623	NEX	C30-C31-C32	-2.78	114.72	123.23
25	7	601	CHL	CBC-CAC-C3C	-2.78	108.74	112.95
26	8	612	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
27	n	1621	LUT	C22-C23-C24	-2.77	108.59	111.73
26	S	614	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
29	R	623	NEX	C30-C31-C32	-2.77	114.73	123.23
29	Y	1623	NEX	C26-C27-C28	-2.77	120.14	125.99
26	6	612	CLA	CAA-C2A-C3A	-2.77	105.22	112.81
26	C	513	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
37	Z	101	LMG	C1-C2-C3	-2.77	104.83	109.98
26	N	610	CLA	O2A-CGA-O1A	-2.77	116.68	123.55
25	r	608	CHL	O1D-CGD-CBD	-2.77	118.82	124.53
29	R	623	NEX	C39-C29-C30	-2.77	119.05	122.92
26	s	613	CLA	O2D-CGD-O1D	-2.77	118.25	123.82
25	R	608	CHL	O1D-CGD-CBD	-2.76	118.82	124.53
26	s	614	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
27	7	1620	LUT	C7-C8-C9	-2.76	122.06	126.21
26	S	612	CLA	O2D-CGD-O1D	-2.76	118.26	123.82
26	8	604	CLA	O2D-CGD-O1D	-2.76	118.27	123.82
26	s	612	CLA	O2D-CGD-O1D	-2.76	118.27	123.82
31	C	516	BCR	C15-C14-C13	-2.76	123.37	127.31
31	b	618	BCR	C33-C5-C6	-2.76	121.42	124.51
31	B	618	BCR	C33-C5-C6	-2.76	121.42	124.51
26	c	513	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
37	z	101	LMG	C1-C2-C3	-2.76	104.85	109.98
27	4	620	LUT	C10-C11-C12	-2.76	114.78	123.23
29	n	1623	NEX	C26-C27-C28	-2.75	120.17	125.99
25	g	608	CHL	CBC-CAC-C3C	-2.75	108.77	112.95
25	G	608	CHL	CBC-CAC-C3C	-2.75	108.77	112.95
26	6	613	CLA	O2D-CGD-O1D	-2.75	118.28	123.82
26	4	612	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
26	2	602	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
26	S	613	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
26	n	610	CLA	O2A-CGA-O1A	-2.75	116.72	123.55
27	Y	1620	LUT	C23-C24-C25	-2.75	122.64	125.22
28	3	1622	XAT	C10-C11-C12	-2.75	114.81	123.23
26	B	616	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
26	6	602	CLA	O2D-CGD-O1D	-2.75	118.30	123.82
39	B	626	DGD	C1D-C2D-C3D	-2.75	104.88	109.98
31	B	618	BCR	C10-C11-C12	-2.74	114.81	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	514	BCR	C8-C9-C10	-2.74	114.73	118.94
26	N	612	CLA	O2D-CGD-O1D	-2.74	118.30	123.82
26	4	604	CLA	O2D-CGD-O1D	-2.74	118.30	123.82
31	B	619	BCR	C39-C30-C25	-2.74	105.86	110.31
28	7	1622	XAT	C10-C11-C12	-2.74	114.81	123.23
26	3	614	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
26	3	613	CLA	O2D-CGD-O1D	-2.74	118.30	123.82
27	8	620	LUT	C10-C11-C12	-2.74	114.82	123.23
29	N	1623	NEX	C26-C27-C28	-2.74	120.20	125.99
31	c	514	BCR	C8-C9-C10	-2.74	114.73	118.94
26	2	613	CLA	O2D-CGD-O1D	-2.74	118.31	123.82
39	b	626	DGD	C1D-C2D-C3D	-2.74	104.89	109.98
26	b	609	CLA	OBD-CAD-CBD	-2.74	121.80	125.94
26	B	609	CLA	OBD-CAD-CBD	-2.74	121.80	125.94
26	N	612	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
28	r	622	XAT	C8-C9-C10	-2.74	114.74	118.94
26	5	603	CLA	O2D-CGD-O1D	-2.74	118.31	123.82
26	8	603	CLA	CAA-C2A-C3A	-2.74	105.31	112.81
26	y	603	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
26	Y	603	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
26	n	612	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
26	y	611	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
26	7	613	CLA	O2D-CGD-O1D	-2.73	118.32	123.82
26	Y	611	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
31	b	620	BCR	C20-C21-C22	-2.73	123.41	127.31
26	5	602	CLA	O2D-CGD-O1D	-2.73	118.32	123.82
31	B	620	BCR	C20-C21-C22	-2.73	123.41	127.31
26	y	604	CLA	C1-C2-C3	-2.73	122.37	126.68
31	b	619	BCR	C39-C30-C25	-2.73	105.88	110.31
31	b	618	BCR	C10-C11-C12	-2.73	114.87	123.23
29	Y	1623	NEX	C39-C29-C30	-2.73	119.10	122.92
26	Y	604	CLA	C1-C2-C3	-2.73	122.37	126.68
25	6	609	CHL	CBA-CAA-C2A	-2.73	112.00	115.76
28	R	622	XAT	C8-C9-C10	-2.73	114.76	118.94
26	4	603	CLA	CAA-C2A-C3A	-2.73	105.34	112.81
27	S	1620	LUT	C7-C8-C9	-2.72	122.12	126.21
28	2	1622	XAT	C26-C27-C28	-2.72	120.23	125.99
31	a	411	BCR	C21-C20-C19	-2.72	114.88	123.23
26	1	603	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
26	n	612	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
27	s	1620	LUT	C7-C8-C9	-2.72	122.12	126.21
26	D	402	CLA	C2C-C1C-NC	-2.72	108.36	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	613	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
26	3	603	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
26	7	603	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
27	G	1621	LUT	C28-C29-C30	-2.72	114.77	118.94
25	G	606	CHL	C4A-C3A-C2A	-2.72	99.70	103.86
26	7	614	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
27	g	1621	LUT	C28-C29-C30	-2.72	114.77	118.94
26	b	616	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	g	606	CHL	C4A-C3A-C2A	-2.72	99.71	103.86
26	G	602	CLA	O2D-CGD-O1D	-2.72	118.36	123.82
31	A	411	BCR	C21-C20-C19	-2.72	114.90	123.23
25	2	609	CHL	CBA-CAA-C2A	-2.71	112.02	115.76
26	6	603	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
26	g	602	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
26	b	616	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
26	G	612	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
31	c	515	BCR	C3-C4-C5	-2.71	109.12	113.78
28	n	1622	XAT	C24-C23-C22	-2.71	105.16	110.68
28	N	1622	XAT	C24-C23-C22	-2.71	105.16	110.68
31	C	515	BCR	C3-C4-C5	-2.71	109.12	113.78
29	y	1623	NEX	C39-C29-C30	-2.71	119.13	122.92
26	1	602	CLA	O2D-CGD-O1D	-2.71	118.37	123.82
28	6	1622	XAT	C26-C27-C28	-2.71	120.27	125.99
28	7	1622	XAT	C35-C34-C33	-2.70	123.45	127.31
39	c	518	DGD	CDB-CCB-CBB	-2.70	100.53	114.45
28	1	1622	XAT	C4-C3-C2	-2.70	105.17	110.68
26	g	612	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
26	1	603	CLA	CBC-CAC-C3C	-2.70	104.74	112.41
26	S	613	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
29	s	1623	NEX	C24-C23-C22	-2.70	105.18	110.68
39	C	518	DGD	CDB-CCB-CBB	-2.70	100.53	114.45
26	B	616	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
26	1	603	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
26	5	603	CLA	CBC-CAC-C3C	-2.70	104.75	112.41
26	6	612	CLA	O2D-CGD-O1D	-2.70	118.39	123.82
26	5	603	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
39	h	102	DGD	CDB-CCB-CBB	-2.70	100.56	114.45
29	S	1623	NEX	C24-C23-C22	-2.70	105.19	110.68
25	3	607	CHL	OMC-CMC-C2C	-2.70	120.85	124.29
28	3	1622	XAT	C35-C34-C33	-2.70	123.46	127.31
26	2	603	CLA	O2D-CGD-O1D	-2.70	118.40	123.82
28	r	622	XAT	C31-C32-C33	-2.69	118.85	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	503	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
31	C	515	BCR	C38-C26-C25	-2.69	121.49	124.51
26	d	402	CLA	C2C-C1C-NC	-2.69	108.37	110.22
28	R	622	XAT	C31-C32-C33	-2.69	118.85	126.42
26	r	610	CLA	O2A-CGA-O1A	-2.69	116.86	123.55
26	c	503	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
28	5	1622	XAT	C4-C3-C2	-2.69	105.20	110.68
26	7	612	CLA	CAA-C2A-C3A	-2.69	105.44	112.81
26	2	612	CLA	O2D-CGD-O1D	-2.69	118.41	123.82
25	7	607	CHL	OMC-CMC-C2C	-2.69	120.86	124.29
39	H	102	DGD	CDB-CCB-CBB	-2.69	100.61	114.45
26	B	605	CLA	C1-C2-C3	-2.69	121.01	125.96
26	s	610	CLA	OBD-CAD-CBD	-2.69	121.89	125.94
25	N	606	CHL	OMC-CMC-C2C	-2.69	120.86	124.29
25	n	605	CHL	OMC-CMC-C2C	-2.69	120.86	124.29
26	3	612	CLA	CAA-C2A-C3A	-2.68	105.46	112.81
26	b	605	CLA	C1-C2-C3	-2.68	121.02	125.96
26	r	611	CLA	C1C-NC-C4C	-2.68	105.52	107.06
27	2	1620	LUT	C11-C10-C9	-2.68	123.49	127.31
25	g	601	CHL	O2D-CGD-O1D	-2.68	118.43	123.82
26	R	610	CLA	O2A-CGA-O1A	-2.68	116.91	123.55
37	A	413	LMG	O3-C3-C2	-2.67	104.54	110.36
26	S	610	CLA	OBD-CAD-CBD	-2.67	121.90	125.94
25	n	606	CHL	OMC-CMC-C2C	-2.67	120.88	124.29
26	r	609	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
25	N	605	CHL	OMC-CMC-C2C	-2.67	120.88	124.29
29	7	1623	NEX	C30-C31-C32	-2.67	115.04	123.23
36	a	412	SQD	O48-C23-O10	-2.67	116.93	123.55
35	A	408	PHO	O2A-CGA-O1A	-2.67	116.93	123.55
29	3	1623	NEX	C30-C31-C32	-2.67	115.05	123.23
26	R	611	CLA	C1C-NC-C4C	-2.67	105.52	107.06
25	Y	607	CHL	CAA-CBA-CGA	-2.67	105.31	113.35
25	G	601	CHL	O2D-CGD-O1D	-2.67	118.46	123.82
26	n	610	CLA	OBD-CAD-CBD	-2.66	121.92	125.94
27	n	1621	LUT	C15-C35-C34	-2.66	117.77	123.46
26	s	610	CLA	O2D-CGD-O1D	-2.66	118.46	123.82
26	S	610	CLA	O2D-CGD-O1D	-2.66	118.46	123.82
29	7	1623	NEX	C15-C35-C34	-2.66	117.78	123.46
31	H	101	BCR	C3-C4-C5	-2.66	109.20	113.78
31	c	515	BCR	C38-C26-C25	-2.66	121.53	124.51
26	a	410	CLA	CAA-CBA-CGA	-2.66	105.33	113.35
25	y	607	CHL	CAA-CBA-CGA	-2.66	105.33	113.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	408	PHO	O2A-CGA-O1A	-2.66	116.95	123.55
26	n	611	CLA	O2D-CGD-O1D	-2.66	118.47	123.82
27	N	1621	LUT	C15-C35-C34	-2.66	117.79	123.46
31	c	515	BCR	C23-C22-C21	-2.66	114.86	118.94
26	N	610	CLA	OBD-CAD-CBD	-2.66	121.93	125.94
37	a	413	LMG	O3-C3-C2	-2.66	104.58	110.36
25	R	606	CHL	O2D-CGD-O1D	-2.66	118.48	123.82
31	h	101	BCR	C3-C4-C5	-2.66	109.22	113.78
26	C	507	CLA	CAA-C2A-C3A	-2.65	105.54	112.81
29	6	1623	NEX	C26-C27-C28	-2.65	120.38	125.99
30	N	2630	LHG	C20-C19-C18	-2.65	100.79	114.45
26	A	410	CLA	CAA-CBA-CGA	-2.65	105.36	113.35
36	A	412	SQD	O48-C23-O10	-2.65	116.97	123.55
26	c	507	CLA	CAA-C2A-C3A	-2.65	105.54	112.81
29	3	1623	NEX	C15-C35-C34	-2.65	117.81	123.46
25	r	606	CHL	O2D-CGD-O1D	-2.65	118.49	123.82
29	2	1623	NEX	C26-C27-C28	-2.65	120.40	125.99
26	R	609	CLA	O2D-CGD-O1D	-2.65	118.50	123.82
31	C	515	BCR	C23-C22-C21	-2.65	114.88	118.94
30	n	2630	LHG	C20-C19-C18	-2.64	100.83	114.45
26	6	603	CLA	CBC-CAC-C3C	-2.64	104.90	112.41
26	2	614	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
26	4	611	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
28	1	1622	XAT	C26-C27-C28	-2.64	120.41	125.99
28	5	1622	XAT	C26-C27-C28	-2.64	120.41	125.99
35	A	408	PHO	CMC-C2C-C1C	-2.64	120.93	125.04
26	N	611	CLA	O2D-CGD-O1D	-2.64	118.51	123.82
31	D	404	BCR	C21-C20-C19	-2.64	115.14	123.23
31	d	404	BCR	C21-C20-C19	-2.64	115.14	123.23
26	2	603	CLA	CBC-CAC-C3C	-2.64	104.92	112.41
35	A	408	PHO	CBD-CHA-C4D	-2.64	105.57	108.54
25	8	607	CHL	OMC-CMC-C2C	-2.64	120.92	124.29
27	6	1621	LUT	C23-C24-C25	-2.64	122.75	125.22
37	D	411	LMG	C6-C5-C4	-2.64	106.83	113.00
27	6	1620	LUT	C11-C10-C9	-2.64	123.55	127.31
25	8	608	CHL	CBC-CAC-C3C	-2.64	108.95	112.95
27	R	620	LUT	C38-C25-C24	-2.64	118.01	123.68
27	r	620	LUT	C38-C25-C24	-2.63	118.02	123.68
31	H	101	BCR	C38-C26-C25	-2.63	121.57	124.51
26	6	604	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
30	C	2630	LHG	O8-C6-C5	-2.63	102.06	108.66
25	g	606	CHL	CBC-CAC-C3C	-2.63	108.96	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	611	CLA	O2A-CGA-O1A	-2.63	117.03	123.55
26	n	611	CLA	O2A-CGA-O1A	-2.63	117.03	123.55
26	8	611	CLA	O2D-CGD-O1D	-2.62	118.54	123.82
26	6	614	CLA	O2D-CGD-O1D	-2.62	118.54	123.82
25	4	608	CHL	CBC-CAC-C3C	-2.62	108.97	112.95
27	5	1621	LUT	C10-C11-C12	-2.62	115.19	123.23
26	5	603	CLA	CAA-C2A-C3A	-2.62	105.62	112.81
26	1	603	CLA	CAA-C2A-C3A	-2.62	105.62	112.81
37	d	411	LMG	C6-C5-C4	-2.62	106.87	113.00
39	c	518	DGD	C3G-C2G-C1G	-2.62	105.95	111.86
27	1	1621	LUT	C10-C11-C12	-2.62	115.20	123.23
35	a	408	PHO	CMC-C2C-C1C	-2.62	120.96	125.04
25	G	606	CHL	CBC-CAC-C3C	-2.62	108.97	112.95
39	C	518	DGD	C3G-C2G-C1G	-2.62	105.95	111.86
25	4	607	CHL	OMC-CMC-C2C	-2.62	120.95	124.29
31	h	101	BCR	C38-C26-C25	-2.62	121.58	124.51
26	n	603	CLA	C3C-C4C-NC	-2.62	107.56	110.21
30	L	101	LHG	C11-C10-C9	-2.61	100.98	114.45
30	l	101	LHG	C11-C10-C9	-2.61	100.98	114.45
25	3	606	CHL	C4A-C3A-C2A	-2.61	99.86	103.86
30	c	2630	LHG	O8-C6-C5	-2.61	102.09	108.66
26	2	604	CLA	O2D-CGD-O1D	-2.61	118.57	123.82
25	G	601	CHL	C1-C2-C3	-2.61	121.15	125.96
26	s	611	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
26	S	611	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
35	a	408	PHO	CBD-CHA-C4D	-2.61	105.60	108.54
25	5	608	CHL	C4A-C3A-C2A	-2.61	99.87	103.86
25	1	608	CHL	C4A-C3A-C2A	-2.61	99.87	103.86
26	Y	612	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
26	7	610	CLA	O2D-CGD-O1D	-2.61	118.58	123.82
26	3	610	CLA	O2D-CGD-O1D	-2.61	118.58	123.82
26	y	612	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
26	C	505	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
26	N	603	CLA	C3C-C4C-NC	-2.60	107.58	110.21
27	7	1621	LUT	C38-C25-C24	-2.60	118.08	123.68
31	b	620	BCR	C33-C5-C6	-2.60	121.60	124.51
25	7	606	CHL	C4A-C3A-C2A	-2.60	99.89	103.86
27	2	1621	LUT	C23-C24-C25	-2.60	122.78	125.22
25	2	605	CHL	CBC-CAC-C3C	-2.60	109.01	112.95
26	5	613	CLA	O2D-CGD-O1D	-2.60	118.60	123.82
28	g	1622	XAT	C24-C23-C22	-2.60	105.39	110.68
26	c	505	CLA	C1B-CHB-C4A	-2.60	124.98	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	404	BCR	C10-C11-C12	-2.59	115.27	123.23
31	d	404	BCR	C10-C11-C12	-2.59	115.27	123.23
30	c	2630	LHG	C18-C17-C16	-2.59	101.09	114.45
30	n	2630	LHG	C11-C10-C9	-2.59	101.09	114.45
25	6	605	CHL	CBC-CAC-C3C	-2.59	109.01	112.95
30	N	2630	LHG	C11-C10-C9	-2.59	101.11	114.45
31	B	620	BCR	C33-C5-C6	-2.59	121.61	124.51
27	2	1620	LUT	C38-C25-C24	-2.59	118.11	123.68
25	G	609	CHL	O2D-CGD-O1D	-2.59	118.61	123.82
25	g	601	CHL	C1-C2-C3	-2.59	121.19	125.96
30	C	2630	LHG	C18-C17-C16	-2.58	101.14	114.45
39	c	518	DGD	O6E-C5E-C6E	-2.58	100.22	106.41
25	g	609	CHL	O2D-CGD-O1D	-2.58	118.62	123.82
39	C	518	DGD	O6E-C5E-C6E	-2.58	100.22	106.41
27	3	1621	LUT	C38-C25-C24	-2.58	118.12	123.68
26	C	511	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
39	c	519	DGD	O2D-C2D-C1D	-2.58	104.63	110.03
39	C	519	DGD	O2D-C2D-C1D	-2.58	104.63	110.03
26	3	611	CLA	CAA-C2A-C3A	-2.58	105.74	112.81
26	n	602	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
26	N	602	CLA	OBD-CAD-CBD	-2.58	122.04	125.94
28	G	1622	XAT	C24-C23-C22	-2.58	105.43	110.68
26	7	611	CLA	CAA-C2A-C3A	-2.58	105.74	112.81
29	y	1623	NEX	C31-C30-C29	-2.58	123.63	127.31
26	c	511	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
29	R	623	NEX	C17-C1-C6	-2.58	108.17	110.47
27	6	1620	LUT	C38-C25-C24	-2.58	118.13	123.68
31	C	516	BCR	C8-C7-C6	-2.58	120.04	127.25
26	b	612	CLA	O2D-CGD-O1D	-2.57	118.64	123.82
31	c	516	BCR	C8-C7-C6	-2.57	120.05	127.25
27	G	1621	LUT	C31-C30-C29	-2.57	123.64	127.31
29	Y	1623	NEX	C31-C30-C29	-2.57	123.64	127.31
25	r	607	CHL	C5-C3-C2	-2.57	115.84	121.10
28	6	1622	XAT	C15-C35-C34	-2.57	117.98	123.46
26	1	613	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
26	B	612	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
26	S	612	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
26	b	606	CLA	CMC-C2C-C1C	-2.57	121.13	125.02
26	B	607	CLA	OBD-CAD-CBD	-2.57	122.07	125.94
28	2	1622	XAT	C15-C35-C34	-2.57	117.99	123.46
26	g	603	CLA	C3C-C4C-NC	-2.56	107.61	110.21
26	y	602	CLA	C6-C7-C8	-2.56	107.32	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	2630	LHG	C20-C19-C18	-2.56	101.25	114.45
25	R	607	CHL	C5-C3-C2	-2.56	115.86	121.10
26	N	603	CLA	CBC-CAC-C3C	-2.56	105.14	112.41
28	2	1622	XAT	C4-C3-C2	-2.56	105.46	110.68
35	a	409	PHO	CBD-CHA-C4D	-2.56	105.66	108.54
26	b	607	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
26	Y	602	CLA	C6-C7-C8	-2.56	107.33	115.73
30	C	2630	LHG	C20-C19-C18	-2.56	101.28	114.45
27	N	1621	LUT	C8-C9-C10	-2.56	115.02	118.94
29	N	1623	NEX	C31-C30-C29	-2.56	123.66	127.31
29	r	623	NEX	C17-C1-C6	-2.56	108.19	110.47
29	N	1623	NEX	C24-C23-C22	-2.56	105.47	110.68
26	n	603	CLA	CBC-CAC-C3C	-2.56	105.16	112.41
26	s	612	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
28	6	1622	XAT	C4-C3-C2	-2.55	105.48	110.68
27	g	1621	LUT	C31-C30-C29	-2.55	123.67	127.31
26	G	603	CLA	C3C-C4C-NC	-2.55	107.63	110.21
27	5	1621	LUT	C38-C25-C24	-2.55	118.19	123.68
30	b	2630	LHG	C11-C10-C9	-2.55	101.32	114.45
28	5	1622	XAT	C11-C12-C13	-2.55	119.26	126.42
31	b	618	BCR	C3-C4-C5	-2.55	109.40	113.78
35	A	409	PHO	CBD-CHA-C4D	-2.55	105.67	108.54
26	B	606	CLA	CMC-C2C-C1C	-2.55	121.16	125.02
29	n	1623	NEX	C24-C23-C22	-2.55	105.49	110.68
26	3	604	CLA	O2D-CGD-O1D	-2.55	118.70	123.82
27	1	1621	LUT	C38-C25-C24	-2.54	118.20	123.68
30	B	2630	LHG	C11-C10-C9	-2.54	101.35	114.45
26	5	611	CLA	O2D-CGD-O1D	-2.54	118.70	123.82
31	B	618	BCR	C3-C4-C5	-2.54	109.41	113.78
27	s	1620	LUT	C38-C25-C24	-2.54	118.21	123.68
27	S	1620	LUT	C38-C25-C24	-2.54	118.21	123.68
29	7	1623	NEX	C20-C13-C14	-2.54	119.36	122.92
30	3	2630	LHG	C11-C10-C9	-2.54	101.36	114.45
27	n	1621	LUT	C8-C9-C10	-2.54	115.04	118.94
30	7	2630	LHG	C11-C10-C9	-2.54	101.37	114.45
25	6	609	CHL	C1-C2-C3	-2.54	121.28	125.96
39	c	519	DGD	C3G-C2G-C1G	-2.54	106.13	111.86
28	1	1622	XAT	C11-C12-C13	-2.54	119.29	126.42
25	N	606	CHL	O2D-CGD-O1D	-2.54	118.71	123.82
29	6	1623	NEX	C39-C29-C30	-2.54	119.37	122.92
26	y	613	CLA	C16-C15-C13	-2.54	107.40	115.73
30	g	2630	LHG	C11-C10-C9	-2.54	101.39	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	606	CHL	CBC-CAC-C3C	-2.54	109.10	112.95
25	r	606	CHL	C4A-C3A-C2A	-2.54	99.98	103.86
26	B	613	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
26	b	613	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
25	n	606	CHL	O2D-CGD-O1D	-2.53	118.72	123.82
26	g	602	CLA	OBD-CAD-CBD	-2.53	122.12	125.94
30	G	2630	LHG	C11-C10-C9	-2.53	101.41	114.45
26	7	604	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
25	5	606	CHL	CBC-CAC-C3C	-2.53	109.11	112.95
29	2	1623	NEX	C39-C29-C30	-2.53	119.38	122.92
39	c	519	DGD	CDB-CCB-CBB	-2.53	101.43	114.45
26	Y	613	CLA	C16-C15-C13	-2.53	107.44	115.73
29	n	1623	NEX	C31-C30-C29	-2.53	123.70	127.31
39	C	519	DGD	CDB-CCB-CBB	-2.52	101.45	114.45
39	C	519	DGD	C3G-C2G-C1G	-2.52	106.17	111.86
27	1	1620	LUT	C15-C14-C13	-2.52	123.71	127.31
26	r	612	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
29	3	1623	NEX	C20-C13-C14	-2.52	119.40	122.92
31	H	101	BCR	C16-C15-C14	-2.52	118.09	123.46
25	R	606	CHL	C4A-C3A-C2A	-2.52	100.01	103.86
37	b	622	LMG	O6-C1-O1	-2.51	104.05	110.02
25	7	605	CHL	OMC-CMC-C2C	-2.51	121.08	124.29
26	R	612	CLA	O2D-CGD-O1D	-2.51	118.76	123.82
26	1	611	CLA	O2D-CGD-O1D	-2.51	118.76	123.82
26	n	611	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
25	3	605	CHL	OMC-CMC-C2C	-2.51	121.08	124.29
26	R	616	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
25	2	609	CHL	C1-C2-C3	-2.51	121.33	125.96
26	g	612	CLA	CAA-C2A-C3A	-2.51	105.93	112.81
26	G	612	CLA	CAA-C2A-C3A	-2.51	105.93	112.81
29	6	1623	NEX	C11-C12-C13	-2.51	119.38	126.42
25	n	609	CHL	O2D-CGD-O1D	-2.51	118.78	123.82
25	1	608	CHL	CBC-CAC-C3C	-2.50	109.15	112.95
27	5	1621	LUT	C30-C31-C32	-2.50	115.55	123.23
39	H	102	DGD	C3G-C2G-C1G	-2.50	106.21	111.86
25	y	606	CHL	OMC-CMC-C2C	-2.50	121.09	124.29
31	B	620	BCR	C16-C15-C14	-2.50	118.12	123.46
26	r	616	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
27	5	1620	LUT	C15-C14-C13	-2.50	123.74	127.31
25	y	609	CHL	O2D-CGD-O1D	-2.50	118.79	123.82
26	N	611	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
37	B	622	LMG	O6-C1-O1	-2.50	104.08	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	101	BCR	C16-C15-C14	-2.50	118.13	123.46
25	Y	606	CHL	OMC-CMC-C2C	-2.50	121.10	124.29
39	C	518	DGD	O3D-C3D-C4D	-2.50	104.92	110.36
29	2	1623	NEX	C11-C12-C13	-2.50	119.41	126.42
26	G	612	CLA	OBD-CAD-CBD	-2.50	122.17	125.94
31	b	620	BCR	C16-C15-C14	-2.50	118.14	123.46
29	Y	1623	NEX	C24-C23-C22	-2.50	105.60	110.68
25	N	609	CHL	O2D-CGD-O1D	-2.49	118.80	123.82
39	h	102	DGD	C3G-C2G-C1G	-2.49	106.23	111.86
25	y	608	CHL	O2D-CGD-O1D	-2.49	118.81	123.82
27	G	1620	LUT	C28-C29-C30	-2.49	115.12	118.94
39	c	518	DGD	O3D-C3D-C4D	-2.49	104.94	110.36
29	5	1623	NEX	C15-C35-C34	-2.49	118.15	123.46
26	G	602	CLA	OBD-CAD-CBD	-2.49	122.18	125.94
37	D	411	LMG	O1-C7-C8	-2.49	105.07	110.99
31	a	411	BCR	C33-C5-C6	-2.49	121.72	124.51
29	y	1623	NEX	C24-C23-C22	-2.49	105.62	110.68
25	Y	608	CHL	O2D-CGD-O1D	-2.48	118.82	123.82
27	3	1620	LUT	C35-C15-C14	-2.48	118.16	123.46
27	1	1621	LUT	C30-C31-C32	-2.48	115.62	123.23
27	1	1621	LUT	C7-C8-C9	-2.48	122.48	126.21
29	6	1623	NEX	C35-C34-C33	-2.48	123.77	127.31
27	Y	1621	LUT	C37-C21-C22	-2.48	104.68	109.42
37	d	411	LMG	O1-C7-C8	-2.48	105.09	110.99
31	A	411	BCR	C33-C5-C6	-2.48	121.73	124.51
25	Y	609	CHL	O2D-CGD-O1D	-2.48	118.83	123.82
29	1	1623	NEX	C15-C35-C34	-2.48	118.17	123.46
26	8	612	CLA	CAA-C2A-C3A	-2.48	106.02	112.81
27	4	620	LUT	C15-C35-C34	-2.47	118.18	123.46
26	B	612	CLA	OBD-CAD-CBD	-2.47	122.20	125.94
26	b	612	CLA	OBD-CAD-CBD	-2.47	122.20	125.94
30	g	2630	LHG	C20-C19-C18	-2.47	101.71	114.45
30	G	2630	LHG	C20-C19-C18	-2.47	101.72	114.45
27	n	1620	LUT	C8-C9-C10	-2.47	115.15	118.94
26	g	612	CLA	OBD-CAD-CBD	-2.47	122.21	125.94
27	7	1620	LUT	C35-C15-C14	-2.47	118.19	123.46
26	4	612	CLA	CAA-C2A-C3A	-2.47	106.04	112.81
25	5	608	CHL	CBC-CAC-C3C	-2.47	109.20	112.95
27	8	620	LUT	C15-C35-C34	-2.47	118.19	123.46
26	4	603	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
28	7	1622	XAT	C32-C33-C34	-2.47	115.15	118.94
28	3	1622	XAT	C32-C33-C34	-2.47	115.15	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	y	1621	LUT	C37-C21-C22	-2.47	104.71	109.42
27	g	1620	LUT	C28-C29-C30	-2.47	115.16	118.94
39	c	520	DGD	C3G-C2G-C1G	-2.47	106.29	111.86
26	a	406	CLA	C3C-C4C-NC	-2.46	107.71	110.21
27	6	1620	LUT	C7-C8-C9	-2.46	122.51	126.21
26	B	608	CLA	CMC-C2C-C1C	-2.46	121.28	125.02
26	c	510	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
27	2	1620	LUT	C7-C8-C9	-2.46	122.51	126.21
27	3	1620	LUT	C15-C35-C34	-2.46	118.21	123.46
27	N	1620	LUT	C8-C9-C10	-2.46	115.16	118.94
26	Y	610	CLA	O2A-CGA-O1A	-2.46	117.44	123.55
26	C	510	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
26	c	510	CLA	C6-C7-C8	-2.46	107.66	115.73
26	C	510	CLA	C6-C7-C8	-2.46	107.66	115.73
28	4	622	XAT	C35-C15-C14	-2.46	118.22	123.46
26	R	610	CLA	C1-C2-C3	-2.46	121.43	125.96
26	r	616	CLA	O2D-CGD-O1D	-2.46	118.88	123.82
30	c	522	LHG	C11-C10-C9	-2.46	101.80	114.45
26	y	610	CLA	O2A-CGA-O1A	-2.46	117.45	123.55
39	C	520	DGD	C3G-C2G-C1G	-2.45	106.32	111.86
29	2	1623	NEX	C35-C34-C33	-2.45	123.81	127.31
31	c	515	BCR	C11-C12-C13	-2.45	119.52	126.42
27	5	1621	LUT	C7-C8-C9	-2.45	122.53	126.21
28	8	622	XAT	C35-C15-C14	-2.45	118.23	123.46
26	g	610	CLA	OBD-CAD-CBD	-2.45	122.24	125.94
27	4	620	LUT	C35-C15-C14	-2.45	118.23	123.46
30	C	522	LHG	C11-C10-C9	-2.45	101.83	114.45
26	8	603	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
27	7	1620	LUT	C15-C35-C34	-2.45	118.24	123.46
25	R	614	CHL	CAA-C2A-C3A	-2.45	110.40	115.37
25	5	605	CHL	OMC-CMC-C2C	-2.44	121.17	124.29
27	6	1621	LUT	C16-C1-C6	-2.44	106.34	110.31
26	s	614	CLA	OBD-CAD-CBD	-2.44	122.25	125.94
39	c	520	DGD	O3E-C3E-C2E	-2.44	105.04	110.36
26	b	608	CLA	CMC-C2C-C1C	-2.44	121.32	125.02
31	C	515	BCR	C11-C12-C13	-2.44	119.55	126.42
37	A	415	LMG	O3-C3-C2	-2.44	105.04	110.36
37	a	415	LMG	O3-C3-C2	-2.44	105.04	110.36
26	b	614	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
39	C	520	DGD	O3E-C3E-C2E	-2.44	105.04	110.36
29	S	1623	NEX	C39-C29-C30	-2.44	119.50	122.92
26	R	616	CLA	O2D-CGD-O1D	-2.44	118.91	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	610	CLA	C1-C2-C3	-2.44	121.46	125.96
31	t	101	BCR	C7-C6-C5	-2.44	115.72	121.54
26	B	614	CLA	O2D-CGD-O1D	-2.44	118.92	123.82
27	3	1621	LUT	C31-C30-C29	-2.44	123.83	127.31
29	s	1623	NEX	C39-C29-C30	-2.44	119.51	122.92
26	A	406	CLA	C3C-C4C-NC	-2.43	107.75	110.21
25	r	614	CHL	CAA-C2A-C3A	-2.43	110.43	115.37
27	8	620	LUT	C35-C15-C14	-2.43	118.27	123.46
31	T	101	BCR	C7-C6-C5	-2.43	115.74	121.54
26	C	508	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
31	B	619	BCR	C21-C20-C19	-2.43	115.77	123.23
27	Y	1620	LUT	C28-C29-C30	-2.43	115.21	118.94
28	4	622	XAT	C30-C31-C32	-2.43	115.77	123.23
31	b	619	BCR	C21-C20-C19	-2.43	115.77	123.23
26	S	614	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
31	c	515	BCR	C16-C15-C14	-2.43	118.27	123.46
27	S	1621	LUT	C38-C25-C24	-2.43	118.45	123.68
26	G	610	CLA	OBD-CAD-CBD	-2.43	122.27	125.94
28	8	622	XAT	C30-C31-C32	-2.43	115.78	123.23
26	b	605	CLA	C16-C17-C18	-2.43	104.37	115.96
25	5	605	CHL	O2D-CGD-O1D	-2.43	118.93	123.82
31	4	623	BCR	C20-C19-C18	-2.43	119.59	126.42
26	B	605	CLA	C16-C17-C18	-2.43	104.38	115.96
25	1	608	CHL	OMC-CMC-C2C	-2.43	121.19	124.29
27	2	1621	LUT	C16-C1-C6	-2.43	106.37	110.31
31	8	623	BCR	C20-C19-C18	-2.43	119.60	126.42
30	1	2630	LHG	C11-C10-C9	-2.43	101.96	114.45
27	7	1621	LUT	C31-C30-C29	-2.43	123.85	127.31
25	1	605	CHL	OMC-CMC-C2C	-2.42	121.19	124.29
26	B	617	CLA	CAA-C2A-C3A	-2.42	106.17	112.81
25	5	608	CHL	OMC-CMC-C2C	-2.42	121.20	124.29
28	N	1622	XAT	C39-C29-C30	-2.42	119.53	122.92
37	z	101	LMG	O2-C2-C1	-2.42	104.96	110.03
26	b	617	CLA	CAA-C2A-C3A	-2.42	106.17	112.81
30	5	2630	LHG	C11-C10-C9	-2.42	101.97	114.45
26	b	607	CLA	CAA-CBA-CGA	-2.42	106.06	113.35
27	y	1620	LUT	C28-C29-C30	-2.42	115.23	118.94
26	5	610	CLA	OBD-CAD-CBD	-2.42	122.29	125.94
25	1	609	CHL	OMC-CMC-C2C	-2.42	121.20	124.29
26	1	610	CLA	OBD-CAD-CBD	-2.42	122.29	125.94
26	n	610	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
37	c	521	LMG	O3-C3-C2	-2.42	105.10	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	607	CLA	CAA-CBA-CGA	-2.42	106.07	113.35
31	D	404	BCR	C33-C5-C6	-2.42	121.80	124.51
39	B	626	DGD	O3G-C3G-C2G	-2.42	105.24	110.99
31	C	515	BCR	C16-C15-C14	-2.41	118.31	123.46
30	C	2630	LHG	C11-C10-C9	-2.41	102.01	114.45
30	c	2630	LHG	C11-C10-C9	-2.41	102.02	114.45
25	l	605	CHL	O2D-CGD-O1D	-2.41	118.96	123.82
37	C	521	LMG	O3-C3-C2	-2.41	105.11	110.36
26	B	605	CLA	C6-C5-C3	-2.41	107.19	112.66
39	b	626	DGD	O3G-C3G-C2G	-2.41	105.25	110.99
27	6	1621	LUT	C38-C25-C24	-2.41	118.49	123.68
26	c	508	CLA	OBD-CAD-CBD	-2.41	122.30	125.94
25	6	607	CHL	O1D-CGD-CBD	-2.41	119.55	124.53
37	Z	101	LMG	O2-C2-C1	-2.41	104.99	110.03
27	s	1621	LUT	C38-C25-C24	-2.41	118.49	123.68
31	t	101	BCR	C39-C30-C25	-2.41	106.40	110.31
28	n	1622	XAT	C39-C29-C30	-2.41	119.55	122.92
25	5	609	CHL	OMC-CMC-C2C	-2.41	121.22	124.29
26	R	611	CLA	O2A-CGA-O1A	-2.41	117.58	123.55
30	D	408	LHG	C11-C10-C9	-2.41	102.06	114.45
31	T	101	BCR	C39-C30-C25	-2.40	106.41	110.31
30	d	408	LHG	C11-C10-C9	-2.40	102.07	114.45
37	a	415	LMG	O6-C1-O1	-2.40	104.31	110.02
31	H	101	BCR	C31-C1-C6	-2.40	106.41	110.31
25	2	607	CHL	O1D-CGD-CBD	-2.40	119.57	124.53
26	g	610	CLA	C1-C2-C3	-2.40	121.53	125.96
27	2	1621	LUT	C38-C25-C24	-2.40	118.51	123.68
27	s	1621	LUT	C15-C14-C13	-2.40	123.88	127.31
26	4	612	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
31	d	404	BCR	C33-C5-C6	-2.40	121.82	124.51
25	2	609	CHL	O1D-CGD-CBD	-2.40	119.58	124.53
26	8	612	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
25	6	609	CHL	O1D-CGD-CBD	-2.40	119.58	124.53
29	G	1623	NEX	C15-C35-C34	-2.40	118.35	123.46
26	N	610	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
26	b	605	CLA	C6-C5-C3	-2.40	107.23	112.66
27	2	1620	LUT	C28-C29-C30	-2.39	115.27	118.94
26	r	611	CLA	O2A-CGA-O1A	-2.39	117.60	123.55
26	6	603	CLA	CAA-C2A-C3A	-2.39	106.25	112.81
26	2	603	CLA	CAA-C2A-C3A	-2.39	106.25	112.81
37	A	415	LMG	O6-C1-O1	-2.39	104.34	110.02
25	2	605	CHL	CBA-CAA-C2A	-2.39	112.22	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	606	CHL	O2D-CGD-O1D	-2.39	119.01	123.82
25	2	606	CHL	CBC-CAC-C3C	-2.39	109.32	112.95
25	6	606	CHL	CBC-CAC-C3C	-2.39	109.33	112.95
30	Y	2630	LHG	C11-C10-C9	-2.39	102.16	114.45
26	G	610	CLA	C1-C2-C3	-2.39	121.56	125.96
30	y	2630	LHG	C11-C10-C9	-2.39	102.16	114.45
27	S	1621	LUT	C15-C14-C13	-2.39	123.91	127.31
25	6	605	CHL	CBA-CAA-C2A	-2.38	112.22	115.66
25	8	606	CHL	O2D-CGD-O1D	-2.38	119.02	123.82
31	h	101	BCR	C31-C1-C6	-2.38	106.44	110.31
31	8	623	BCR	C27-C26-C25	-2.38	119.24	122.74
25	5	609	CHL	C1-C2-C3	-2.38	121.56	125.96
26	3	610	CLA	OBD-CAD-CBD	-2.38	122.34	125.94
29	g	1623	NEX	C24-C23-C22	-2.38	105.83	110.68
27	6	1620	LUT	C28-C29-C30	-2.38	115.29	118.94
26	3	611	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
28	1	1622	XAT	C15-C35-C34	-2.38	118.38	123.46
28	5	1622	XAT	C15-C35-C34	-2.38	118.38	123.46
29	G	1623	NEX	C24-C23-C22	-2.38	105.83	110.68
37	B	622	LMG	C38-C37-C36	-2.38	102.19	114.45
37	A	413	LMG	C6-C5-C4	-2.38	107.44	113.00
26	5	610	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
30	1	2630	LHG	C20-C19-C18	-2.38	102.20	114.45
26	7	610	CLA	O2A-CGA-O1A	-2.38	117.65	123.55
30	R	2630	LHG	C20-C19-C18	-2.38	102.21	114.45
26	R	601	CLA	CAC-C3C-C2C	-2.38	123.37	127.49
30	r	2630	LHG	C20-C19-C18	-2.38	102.21	114.45
37	b	622	LMG	C38-C37-C36	-2.38	102.22	114.45
26	c	512	CLA	OBD-CAD-CBD	-2.37	122.35	125.94
25	8	607	CHL	CBC-CAC-C3C	-2.37	109.34	112.95
29	g	1623	NEX	C15-C35-C34	-2.37	118.39	123.46
37	a	413	LMG	C6-C5-C4	-2.37	107.45	113.00
26	s	611	CLA	O2A-CGA-O1A	-2.37	117.66	123.55
26	b	617	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
37	b	2633	LMG	C1-O6-C5	-2.37	109.25	113.72
30	5	2630	LHG	C20-C19-C18	-2.37	102.24	114.45
26	r	601	CLA	CAC-C3C-C2C	-2.37	123.39	127.49
27	Y	1620	LUT	C31-C30-C29	-2.37	123.93	127.31
25	1	609	CHL	C1-C2-C3	-2.37	121.59	125.96
27	Y	1621	LUT	C7-C8-C9	-2.37	122.65	126.21
29	r	623	NEX	C11-C12-C13	-2.37	119.76	126.42
26	1	610	CLA	O2D-CGD-O1D	-2.37	119.06	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	611	CLA	O2A-CGA-O1A	-2.37	117.67	123.55
25	g	608	CHL	O2D-CGD-O1D	-2.37	119.06	123.82
26	C	512	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
30	D	409	LHG	C18-C17-C16	-2.37	102.26	114.45
26	R	613	CLA	O2A-CGA-O1A	-2.37	117.68	123.55
25	4	606	CHL	OMC-CMC-C2C	-2.37	121.27	124.29
26	7	611	CLA	O2D-CGD-O1D	-2.37	119.06	123.82
29	R	623	NEX	C11-C12-C13	-2.37	119.77	126.42
27	y	1621	LUT	C7-C8-C9	-2.36	122.66	126.21
25	y	601	CHL	CBC-CAC-C3C	-2.36	109.36	112.95
29	7	1623	NEX	C26-C27-C28	-2.36	120.99	125.99
25	r	606	CHL	O2A-CGA-O1A	-2.36	117.68	123.55
26	r	612	CLA	CAA-C2A-C3A	-2.36	106.33	112.81
27	s	1621	LUT	C11-C10-C9	-2.36	123.94	127.31
26	3	610	CLA	O2A-CGA-O1A	-2.36	117.68	123.55
25	4	607	CHL	CBC-CAC-C3C	-2.36	109.36	112.95
30	d	409	LHG	C18-C17-C16	-2.36	102.29	114.45
26	7	610	CLA	OBD-CAD-CBD	-2.36	122.38	125.94
41	F	101	HEM	CMD-C2D-C1D	-2.36	124.84	128.46
37	B	2633	LMG	C1-O6-C5	-2.36	109.27	113.72
27	y	1620	LUT	C31-C30-C29	-2.36	123.95	127.31
27	y	1620	LUT	C8-C9-C10	-2.36	115.32	118.94
29	n	1623	NEX	C15-C35-C34	-2.36	118.43	123.46
25	3	609	CHL	O2D-CGD-O1D	-2.36	119.08	123.82
29	2	1623	NEX	C24-C23-C22	-2.36	105.88	110.68
25	8	606	CHL	OMC-CMC-C2C	-2.36	121.28	124.29
25	Y	601	CHL	CBC-CAC-C3C	-2.36	109.37	112.95
27	Y	1620	LUT	C8-C9-C10	-2.36	115.33	118.94
26	r	603	CLA	CAA-C2A-C3A	-2.36	106.35	112.81
31	4	623	BCR	C27-C26-C25	-2.36	119.28	122.74
26	1	603	CLA	OBD-CAD-CBD	-2.35	122.38	125.94
26	r	613	CLA	O2A-CGA-O1A	-2.35	117.71	123.55
26	R	603	CLA	CAA-C2A-C3A	-2.35	106.36	112.81
25	R	606	CHL	O2A-CGA-O1A	-2.35	117.71	123.55
25	G	608	CHL	O2D-CGD-O1D	-2.35	119.09	123.82
29	3	1623	NEX	C26-C27-C28	-2.35	121.02	125.99
37	a	413	LMG	C40-C39-C38	-2.35	102.34	114.45
37	A	413	LMG	C40-C39-C38	-2.35	102.34	114.45
37	z	101	LMG	C1-O6-C5	-2.35	109.29	113.72
26	5	603	CLA	OBD-CAD-CBD	-2.35	122.39	125.94
29	3	1623	NEX	C35-C34-C33	-2.35	123.96	127.31
29	7	1623	NEX	C35-C34-C33	-2.35	123.96	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	1623	NEX	C15-C35-C34	-2.35	118.45	123.46
30	b	2631	LHG	C20-C19-C18	-2.35	102.36	114.45
29	6	1623	NEX	C24-C23-C22	-2.35	105.90	110.68
28	Y	1622	XAT	C31-C32-C33	-2.35	119.82	126.42
26	R	612	CLA	CAA-C2A-C3A	-2.35	106.38	112.81
30	B	2631	LHG	C20-C19-C18	-2.34	102.37	114.45
26	B	617	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
25	7	609	CHL	O2D-CGD-O1D	-2.34	119.10	123.82
28	y	1622	XAT	C31-C32-C33	-2.34	119.83	126.42
26	n	603	CLA	C1-C2-C3	-2.34	121.64	125.96
30	D	409	LHG	C11-C10-C9	-2.34	102.39	114.45
39	C	518	DGD	CAB-C9B-C8B	-2.34	102.39	114.45
28	2	1622	XAT	C31-C32-C33	-2.34	119.84	126.42
27	Y	1621	LUT	C23-C24-C25	-2.34	123.03	125.22
26	B	615	CLA	O2A-CGA-O1A	-2.34	117.74	123.55
27	6	1620	LUT	C12-C13-C14	-2.34	115.35	118.94
27	S	1621	LUT	C11-C10-C9	-2.34	123.97	127.31
26	2	610	CLA	C1-C2-C3	-2.34	122.98	126.68
30	d	409	LHG	C11-C10-C9	-2.34	102.40	114.45
26	a	405	CLA	C6-C7-C8	-2.34	108.06	115.73
27	G	1620	LUT	C7-C8-C9	-2.34	122.70	126.21
30	N	2630	LHG	C27-C26-C25	-2.34	102.41	114.45
27	2	1620	LUT	C12-C13-C14	-2.34	115.36	118.94
41	f	101	HEM	CMD-C2D-C1D	-2.34	124.87	128.46
26	A	405	CLA	C6-C7-C8	-2.34	108.06	115.73
37	a	415	LMG	O2-C2-C1	-2.33	105.14	110.03
25	n	609	CHL	CBA-CAA-C2A	-2.33	112.54	115.76
39	c	518	DGD	CAB-C9B-C8B	-2.33	102.42	114.45
25	3	606	CHL	CHA-CBD-CGD	-2.33	109.59	115.00
25	G	606	CHL	O2D-CGD-O1D	-2.33	119.13	123.82
27	Y	1621	LUT	C38-C25-C24	-2.33	118.66	123.68
30	n	2630	LHG	C27-C26-C25	-2.33	102.44	114.45
26	2	602	CLA	C1-C2-C3	-2.33	121.67	125.96
30	d	409	LHG	C27-C26-C25	-2.33	102.45	114.45
30	D	409	LHG	C27-C26-C25	-2.33	102.47	114.45
28	6	1622	XAT	C31-C32-C33	-2.33	119.88	126.42
27	g	1620	LUT	C7-C8-C9	-2.33	122.72	126.21
37	A	415	LMG	O2-C2-C1	-2.33	105.16	110.03
27	G	1621	LUT	C38-C25-C24	-2.33	118.67	123.68
26	R	610	CLA	CAA-CBA-CGA	-2.33	106.34	113.35
30	N	2630	LHG	C18-C17-C16	-2.33	102.47	114.45
27	2	1621	LUT	C30-C31-C32	-2.33	116.10	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	615	CLA	O2A-CGA-O1A	-2.33	117.78	123.55
26	r	602	CLA	O2A-CGA-O1A	-2.33	117.78	123.55
25	G	607	CHL	C11-C10-C8	-2.32	108.10	115.73
27	Y	1621	LUT	C31-C30-C29	-2.32	123.99	127.31
25	7	606	CHL	CHA-CBD-CGD	-2.32	109.61	115.00
26	N	603	CLA	C1-C2-C3	-2.32	121.67	125.96
27	r	620	LUT	C15-C35-C34	-2.32	118.50	123.46
39	c	519	DGD	CBB-CAB-C9B	-2.32	102.48	114.45
37	Z	101	LMG	C1-O6-C5	-2.32	109.34	113.72
26	b	615	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
28	g	1622	XAT	C39-C29-C30	-2.32	119.67	122.92
25	2	609	CHL	O2D-CGD-O1D	-2.32	119.15	123.82
25	6	609	CHL	O2D-CGD-O1D	-2.32	119.15	123.82
30	Y	2630	LHG	C20-C19-C18	-2.32	102.50	114.45
26	6	602	CLA	C1-C2-C3	-2.32	121.68	125.96
27	S	1621	LUT	C16-C1-C6	-2.32	106.55	110.31
26	r	610	CLA	CAA-CBA-CGA	-2.32	106.36	113.35
27	6	1621	LUT	C30-C31-C32	-2.32	116.12	123.23
26	b	604	CLA	OBD-CAD-CBD	-2.32	122.44	125.94
25	g	607	CHL	C11-C10-C8	-2.32	108.12	115.73
25	7	605	CHL	O2D-CGD-O1D	-2.32	119.16	123.82
25	3	605	CHL	O2D-CGD-O1D	-2.32	119.16	123.82
26	y	613	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
39	C	519	DGD	CBB-CAB-C9B	-2.32	102.52	114.45
30	y	2630	LHG	C20-C19-C18	-2.32	102.52	114.45
28	n	1622	XAT	C7-C8-C9	-2.32	121.94	125.53
30	n	2630	LHG	C18-C17-C16	-2.32	102.52	114.45
26	B	615	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
25	N	609	CHL	CBA-CAA-C2A	-2.31	112.57	115.76
26	6	610	CLA	C1-C2-C3	-2.31	123.02	126.68
27	2	1621	LUT	C18-C5-C6	-2.31	121.92	124.51
26	g	604	CLA	OBD-CAD-CBD	-2.31	122.45	125.94
25	g	606	CHL	O2D-CGD-O1D	-2.31	119.17	123.82
25	n	608	CHL	C1-C2-C3	-2.31	121.70	125.96
26	r	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
26	R	602	CLA	O2A-CGA-O1A	-2.31	117.81	123.55
26	2	603	CLA	OBD-CAD-CBD	-2.31	122.45	125.94
39	B	626	DGD	O2D-C2D-C3D	-2.31	105.33	110.36
39	b	626	DGD	O2D-C2D-C3D	-2.31	105.33	110.36
28	y	1622	XAT	O4-C5-C6	-2.31	57.00	58.94
25	n	608	CHL	O2D-CGD-O1D	-2.31	119.17	123.82
26	G	604	CLA	OBD-CAD-CBD	-2.31	122.45	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	g	1621	LUT	C38-C25-C24	-2.31	118.71	123.68
27	s	1621	LUT	C16-C1-C6	-2.31	106.57	110.31
25	4	608	CHL	C4A-C3A-C2A	-2.31	100.33	103.86
26	S	602	CLA	O2A-CGA-O1A	-2.31	117.82	123.55
30	B	2630	LHG	C20-C19-C18	-2.31	102.57	114.45
27	y	1621	LUT	C31-C30-C29	-2.31	124.02	127.31
26	3	602	CLA	OBD-CAD-CBD	-2.31	122.46	125.94
26	7	602	CLA	OBD-CAD-CBD	-2.31	122.46	125.94
27	y	1621	LUT	C38-C25-C24	-2.30	118.72	123.68
25	5	609	CHL	O1D-CGD-CBD	-2.30	119.77	124.53
26	s	602	CLA	O2A-CGA-O1A	-2.30	117.83	123.55
27	8	620	LUT	C1-C6-C5	-2.30	119.35	122.59
26	a	405	CLA	C2C-C1C-NC	-2.30	108.64	110.22
37	a	415	LMG	C40-C39-C38	-2.30	102.59	114.45
28	G	1622	XAT	C39-C29-C30	-2.30	119.70	122.92
30	b	2630	LHG	C20-C19-C18	-2.30	102.59	114.45
37	A	415	LMG	C40-C39-C38	-2.30	102.59	114.45
27	4	620	LUT	C1-C6-C5	-2.30	119.36	122.59
27	y	1621	LUT	C23-C24-C25	-2.30	123.06	125.22
25	N	608	CHL	O2D-CGD-O1D	-2.30	119.19	123.82
26	C	513	CLA	O2A-CGA-O1A	-2.30	117.84	123.55
26	B	604	CLA	OBD-CAD-CBD	-2.30	122.47	125.94
30	l	101	LHG	C20-C19-C18	-2.30	102.61	114.45
27	R	620	LUT	C15-C35-C34	-2.30	118.56	123.46
25	8	608	CHL	C4A-C3A-C2A	-2.30	100.35	103.86
26	y	610	CLA	OBD-CAD-CBD	-2.30	122.47	125.94
27	6	1621	LUT	C18-C5-C6	-2.30	121.94	124.51
26	b	612	CLA	CMC-C2C-C1C	-2.30	121.54	125.02
26	B	604	CLA	O2A-CGA-O1A	-2.30	117.85	123.55
26	Y	610	CLA	OBD-CAD-CBD	-2.30	122.47	125.94
26	B	612	CLA	CMC-C2C-C1C	-2.30	121.54	125.02
30	s	2630	LHG	C11-C10-C9	-2.29	102.63	114.45
27	y	1620	LUT	C8-C7-C6	-2.29	120.83	127.25
30	L	101	LHG	C20-C19-C18	-2.29	102.64	114.45
25	N	608	CHL	C1-C2-C3	-2.29	121.73	125.96
28	N	1622	XAT	C7-C8-C9	-2.29	121.97	125.53
26	Y	613	CLA	O2D-CGD-O1D	-2.29	119.21	123.82
30	g	2630	LHG	C27-C26-C25	-2.29	102.65	114.45
30	S	2630	LHG	C11-C10-C9	-2.29	102.65	114.45
29	Y	1623	NEX	C15-C35-C34	-2.29	118.57	123.46
29	r	623	NEX	O24-C25-C26	-2.29	57.02	58.94
26	6	603	CLA	OBD-CAD-CBD	-2.29	122.48	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	1623	NEX	C15-C35-C34	-2.29	118.57	123.46
25	7	606	CHL	O2D-CGD-O1D	-2.29	119.21	123.82
31	A	411	BCR	C10-C11-C12	-2.29	116.21	123.23
30	G	2630	LHG	C27-C26-C25	-2.29	102.66	114.45
26	c	513	CLA	O2A-CGA-O1A	-2.29	117.87	123.55
25	3	606	CHL	O2D-CGD-O1D	-2.29	119.22	123.82
26	R	612	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
35	a	408	PHO	O2D-CGD-O1D	-2.28	119.22	123.82
27	6	1621	LUT	C8-C9-C10	-2.28	115.44	118.94
31	b	618	BCR	C23-C22-C21	-2.28	115.44	118.94
26	B	617	CLA	C2C-C1C-NC	-2.28	108.66	110.22
31	a	411	BCR	C10-C11-C12	-2.28	116.23	123.23
26	b	604	CLA	O2A-CGA-O1A	-2.28	117.88	123.55
25	1	609	CHL	O1D-CGD-CBD	-2.28	119.82	124.53
26	B	616	CLA	CAA-C2A-C3A	-2.28	106.55	112.81
26	b	616	CLA	CAA-C2A-C3A	-2.28	106.56	112.81
25	Y	605	CHL	O2D-CGD-O1D	-2.28	119.23	123.82
39	c	519	DGD	C5B-C4B-C3B	-2.28	102.70	114.45
27	Y	1620	LUT	C8-C7-C6	-2.28	120.87	127.25
27	2	1621	LUT	C8-C9-C10	-2.28	115.44	118.94
28	2	1622	XAT	C10-C11-C12	-2.28	116.24	123.23
28	n	1622	XAT	C5-C4-C3	-2.28	108.27	112.64
28	6	1622	XAT	C10-C11-C12	-2.28	116.25	123.23
28	Y	1622	XAT	O4-C5-C6	-2.28	57.03	58.94
37	b	622	LMG	C40-C39-C38	-2.28	102.73	114.45
26	g	603	CLA	C1-C2-C3	-2.28	121.76	125.96
31	C	516	BCR	C8-C9-C10	-2.28	115.45	118.94
39	C	519	DGD	C5B-C4B-C3B	-2.28	102.73	114.45
26	A	405	CLA	C2C-C1C-NC	-2.27	108.66	110.22
37	C	521	LMG	C40-C39-C38	-2.27	102.74	114.45
28	N	1622	XAT	C5-C4-C3	-2.27	108.28	112.64
31	B	618	BCR	C23-C22-C21	-2.27	115.45	118.94
26	c	503	CLA	O2D-CGD-O1D	-2.27	119.25	123.82
26	c	511	CLA	C1-C2-C3	-2.27	121.77	125.96
27	1	1621	LUT	C8-C7-C6	-2.27	120.89	127.25
26	C	511	CLA	C1-C2-C3	-2.27	121.77	125.96
25	1	605	CHL	CHA-CBD-CGD	-2.27	109.73	115.00
25	r	608	CHL	CHA-CBD-CGD	-2.27	109.73	115.00
25	y	605	CHL	O2D-CGD-O1D	-2.27	119.25	123.82
37	c	521	LMG	C40-C39-C38	-2.27	102.76	114.45
37	B	622	LMG	C40-C39-C38	-2.27	102.76	114.45
25	y	608	CHL	C1-C2-C3	-2.27	121.78	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A	413	LMG	C38-C37-C36	-2.27	102.77	114.45
26	d	402	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
30	d	409	LHG	C20-C19-C18	-2.27	102.77	114.45
26	d	403	CLA	C7-C6-C5	-2.27	106.81	113.11
37	B	2633	LMG	C40-C39-C38	-2.27	102.78	114.45
26	D	403	CLA	C7-C6-C5	-2.27	106.81	113.11
26	g	612	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
35	A	408	PHO	O2D-CGD-O1D	-2.27	119.26	123.82
26	c	513	CLA	CAA-CBA-CGA	-2.27	106.52	113.35
26	G	603	CLA	C1-C2-C3	-2.26	121.78	125.96
26	c	507	CLA	CBC-CAC-C3C	-2.26	105.98	112.41
30	D	409	LHG	C20-C19-C18	-2.26	102.79	114.45
26	C	507	CLA	CBC-CAC-C3C	-2.26	105.99	112.41
37	a	413	LMG	C38-C37-C36	-2.26	102.80	114.45
29	R	623	NEX	O24-C25-C26	-2.26	57.04	58.94
31	c	516	BCR	C8-C9-C10	-2.26	115.47	118.94
25	5	605	CHL	CHA-CBD-CGD	-2.26	109.76	115.00
26	C	503	CLA	O2D-CGD-O1D	-2.26	119.27	123.82
31	4	623	BCR	C20-C21-C22	-2.26	124.08	127.31
37	b	2633	LMG	C40-C39-C38	-2.26	102.81	114.45
27	5	1621	LUT	C8-C7-C6	-2.26	120.93	127.25
37	B	622	LMG	O3-C3-C2	-2.26	105.44	110.36
31	B	619	BCR	C10-C11-C12	-2.26	116.31	123.23
26	A	406	CLA	C11-C12-C13	-2.26	108.32	115.73
26	N	604	CLA	OBD-CAD-CBD	-2.26	122.53	125.94
37	B	2633	LMG	C38-C37-C36	-2.26	102.83	114.45
37	b	2633	LMG	C38-C37-C36	-2.26	102.83	114.45
29	S	1623	NEX	O24-C25-C26	-2.25	57.05	58.94
26	c	501	CLA	C7-C6-C5	-2.25	106.85	113.11
25	R	608	CHL	CHA-CBD-CGD	-2.25	109.78	115.00
26	G	612	CLA	O2A-CGA-O1A	-2.25	117.96	123.55
26	1	602	CLA	OBD-CAD-CBD	-2.25	122.54	125.94
25	Y	608	CHL	C1-C2-C3	-2.25	121.81	125.96
31	b	619	BCR	C10-C11-C12	-2.25	116.33	123.23
25	R	607	CHL	CAA-CBA-CGA	-2.25	106.57	113.35
26	N	612	CLA	CAA-C2A-C3A	-2.25	106.64	112.81
26	C	501	CLA	C7-C6-C5	-2.25	106.86	113.11
26	D	402	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
25	G	606	CHL	OMC-CMC-C2C	-2.25	121.42	124.29
26	a	406	CLA	C11-C12-C13	-2.25	108.35	115.73
30	2	2630	LHG	C11-C10-C9	-2.25	102.87	114.45
30	6	2630	LHG	C11-C10-C9	-2.25	102.88	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	410	LHG	C11-C10-C9	-2.25	102.88	114.45
26	y	603	CLA	C1-C2-C3	-2.24	121.82	125.96
26	7	603	CLA	CHA-C1A-NA	-2.24	120.97	126.18
26	C	513	CLA	CAA-CBA-CGA	-2.24	106.58	113.35
26	C	505	CLA	OBD-CAD-CBD	-2.24	122.55	125.94
39	C	518	DGD	C1D-C2D-C3D	-2.24	105.81	109.98
26	n	604	CLA	OBD-CAD-CBD	-2.24	122.55	125.94
27	2	1621	LUT	C8-C7-C6	-2.24	120.98	127.25
26	R	613	CLA	O2D-CGD-O1D	-2.24	119.31	123.82
25	g	606	CHL	OMC-CMC-C2C	-2.24	121.43	124.29
26	B	607	CLA	O2A-CGA-O1A	-2.24	117.99	123.55
30	d	410	LHG	C11-C10-C9	-2.24	102.91	114.45
37	b	622	LMG	O3-C3-C2	-2.24	105.48	110.36
38	D	405	PL9	C22-C23-C24	-2.24	122.05	127.68
38	d	405	PL9	C22-C23-C24	-2.24	122.05	127.68
29	s	1623	NEX	O24-C25-C26	-2.24	57.06	58.94
26	b	614	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
30	d	408	LHG	O8-C23-O10	-2.24	117.99	123.55
25	Y	608	CHL	O2A-CGA-O1A	-2.24	118.00	123.55
29	y	1623	NEX	C11-C12-C13	-2.24	120.13	126.42
25	r	607	CHL	CAA-CBA-CGA	-2.24	106.61	113.35
26	3	603	CLA	CHA-C1A-NA	-2.24	120.98	126.18
26	B	616	CLA	O2A-CGA-O1A	-2.24	118.00	123.55
25	N	608	CHL	C4A-C3A-C2A	-2.24	100.44	103.86
29	Y	1623	NEX	C11-C12-C13	-2.23	120.14	126.42
30	r	2630	LHG	C11-C10-C9	-2.23	102.94	114.45
26	b	617	CLA	C2C-C1C-NC	-2.23	108.69	110.22
26	n	612	CLA	CAA-C2A-C3A	-2.23	106.69	112.81
27	G	1620	LUT	C16-C1-C6	-2.23	106.69	110.31
26	B	614	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
35	A	408	PHO	C6-C7-C8	-2.23	108.41	115.73
31	8	623	BCR	C20-C21-C22	-2.23	124.13	127.31
26	5	602	CLA	OBD-CAD-CBD	-2.23	122.57	125.94
27	Y	1621	LUT	C8-C9-C10	-2.23	115.52	118.94
30	D	409	LHG	O8-C23-O10	-2.23	118.02	123.55
37	B	622	LMG	C1-C2-C3	-2.23	105.84	109.98
35	a	408	PHO	C6-C7-C8	-2.23	108.42	115.73
26	r	613	CLA	O2D-CGD-O1D	-2.23	119.34	123.82
30	R	2630	LHG	C11-C10-C9	-2.23	102.98	114.45
25	y	608	CHL	O2A-CGA-O1A	-2.23	118.02	123.55
26	Y	603	CLA	O2A-CGA-O1A	-2.23	118.02	123.55
28	8	622	XAT	C25-C24-C23	-2.23	108.37	112.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	505	CLA	OBD-CAD-CBD	-2.23	122.58	125.94
26	r	602	CLA	OBD-CAD-CBD	-2.23	122.58	125.94
30	g	2630	LHG	C18-C17-C16	-2.22	102.99	114.45
27	y	1621	LUT	C8-C9-C10	-2.22	115.53	118.94
30	D	408	LHG	O8-C23-O10	-2.22	118.03	123.55
28	r	622	XAT	C24-C23-C22	-2.22	106.15	110.68
25	n	608	CHL	C4A-C3A-C2A	-2.22	100.46	103.86
27	6	1621	LUT	C8-C7-C6	-2.22	121.03	127.25
27	r	620	LUT	C12-C13-C14	-2.22	115.53	118.94
30	5	2630	LHG	C27-C26-C25	-2.22	103.01	114.45
26	b	616	CLA	O2A-CGA-O1A	-2.22	118.04	123.55
28	4	622	XAT	C25-C24-C23	-2.22	108.38	112.64
26	D	402	CLA	CMA-C3A-C2A	-2.22	104.76	113.77
26	d	402	CLA	CMA-C3A-C2A	-2.22	104.76	113.77
39	B	626	DGD	O2G-C1B-O1B	-2.22	118.14	123.68
26	b	607	CLA	O2A-CGA-O1A	-2.22	118.04	123.55
28	1	1622	XAT	C5-C4-C3	-2.22	108.38	112.64
27	n	1621	LUT	C35-C15-C14	-2.22	118.73	123.46
26	b	605	CLA	O2D-CGD-O1D	-2.22	119.36	123.82
39	c	518	DGD	C1D-C2D-C3D	-2.22	105.86	109.98
27	n	1621	LUT	C31-C30-C29	-2.22	124.14	127.31
26	R	602	CLA	OBD-CAD-CBD	-2.22	122.59	125.94
27	Y	1620	LUT	C15-C35-C34	-2.22	118.73	123.46
26	y	603	CLA	O2A-CGA-O1A	-2.22	118.05	123.55
26	7	603	CLA	O2A-CGA-O1A	-2.22	118.05	123.55
25	R	614	CHL	C3B-CAB-CBB	-2.22	120.22	125.20
25	s	601	CHL	O2D-CGD-O1D	-2.22	119.36	123.82
30	d	409	LHG	O8-C23-O10	-2.22	118.05	123.55
30	1	2630	LHG	C18-C17-C16	-2.22	103.04	114.45
30	1	2630	LHG	C27-C26-C25	-2.22	103.04	114.45
39	C	520	DGD	O6E-C1E-O5D	-2.22	104.76	110.02
26	C	507	CLA	O2A-CGA-O1A	-2.21	118.05	123.55
26	Y	611	CLA	O2A-CGA-O1A	-2.21	118.05	123.55
26	6	603	CLA	O2A-CGA-O1A	-2.21	118.05	123.55
28	5	1622	XAT	C24-C23-C22	-2.21	106.17	110.68
30	C	523	LHG	C20-C19-C18	-2.21	103.05	114.45
25	g	608	CHL	C4A-C3A-C2A	-2.21	100.48	103.86
26	Y	603	CLA	C1-C2-C3	-2.21	121.88	125.96
30	G	2630	LHG	C18-C17-C16	-2.21	103.06	114.45
25	G	608	CHL	C4A-C3A-C2A	-2.21	100.48	103.86
27	y	1620	LUT	C15-C35-C34	-2.21	118.74	123.46
25	4	609	CHL	C4A-C3A-C2A	-2.21	100.48	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	1621	LUT	C31-C30-C29	-2.21	124.16	127.31
39	b	626	DGD	O2G-C1B-O1B	-2.21	118.16	123.68
26	c	507	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
26	b	602	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
30	c	523	LHG	C20-C19-C18	-2.21	103.07	114.45
39	c	520	DGD	O6E-C1E-O5D	-2.21	104.78	110.02
27	R	620	LUT	C12-C13-C14	-2.21	115.55	118.94
27	G	1621	LUT	C15-C35-C34	-2.21	118.75	123.46
37	b	622	LMG	C1-C2-C3	-2.21	105.87	109.98
30	5	2630	LHG	C18-C17-C16	-2.21	103.08	114.45
26	B	605	CLA	O2D-CGD-O1D	-2.21	119.38	123.82
30	d	410	LHG	C27-C26-C25	-2.21	103.09	114.45
39	c	518	DGD	O6D-C5D-C6D	-2.20	102.23	106.64
27	g	1620	LUT	C16-C1-C6	-2.20	106.73	110.31
30	2	2630	LHG	C27-C26-C25	-2.20	103.10	114.45
27	N	1621	LUT	C35-C15-C14	-2.20	118.76	123.46
26	y	611	CLA	O2A-CGA-O1A	-2.20	118.08	123.55
27	5	1620	LUT	C28-C29-C30	-2.20	115.56	118.94
28	5	1622	XAT	C5-C4-C3	-2.20	108.41	112.64
30	D	410	LHG	C27-C26-C25	-2.20	103.11	114.45
26	2	603	CLA	O2A-CGA-O1A	-2.20	118.08	123.55
27	g	1621	LUT	C15-C35-C34	-2.20	118.76	123.46
26	3	611	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
39	C	518	DGD	O6D-C5D-C6D	-2.20	102.24	106.64
27	7	1620	LUT	C18-C5-C6	-2.20	122.04	124.51
25	3	609	CHL	CHA-CBD-CGD	-2.20	109.89	115.00
30	6	2630	LHG	C27-C26-C25	-2.20	103.12	114.45
26	3	603	CLA	O2A-CGA-O1A	-2.20	118.09	123.55
30	S	2630	LHG	C5-O7-C7	-2.20	112.68	117.88
30	s	2630	LHG	C5-O7-C7	-2.20	112.68	117.88
25	r	614	CHL	C3B-CAB-CBB	-2.20	120.26	125.20
27	N	1620	LUT	C28-C29-C30	-2.20	115.57	118.94
25	S	601	CHL	O2D-CGD-O1D	-2.20	119.39	123.82
25	8	609	CHL	C4A-C3A-C2A	-2.20	100.50	103.86
26	1	612	CLA	CAA-C2A-C3A	-2.20	106.78	112.81
28	1	1622	XAT	C24-C23-C22	-2.20	106.21	110.68
25	Y	609	CHL	O1D-CGD-CBD	-2.20	120.00	124.53
26	C	501	CLA	O2A-CGA-O1A	-2.20	118.10	123.55
26	7	611	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
30	b	2631	LHG	C11-C10-C9	-2.19	103.15	114.45
27	G	1620	LUT	C8-C9-C10	-2.19	115.57	118.94
28	R	622	XAT	C24-C23-C22	-2.19	106.21	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	612	CLA	CAA-C2A-C3A	-2.19	106.80	112.81
26	R	603	CLA	C3C-C4C-NC	-2.19	107.99	110.21
25	8	607	CHL	O1D-CGD-CBD	-2.19	120.00	124.53
25	7	609	CHL	O1D-CGD-CBD	-2.19	120.00	124.53
27	g	1620	LUT	C8-C9-C10	-2.19	115.58	118.94
27	1	1620	LUT	C28-C29-C30	-2.19	115.58	118.94
30	B	2631	LHG	C11-C10-C9	-2.19	103.16	114.45
38	D	405	PL9	C31-C32-C33	-2.19	104.45	111.97
27	3	1620	LUT	C18-C5-C6	-2.19	122.06	124.51
25	3	608	CHL	O2D-CGD-O1D	-2.19	119.41	123.82
25	y	609	CHL	CBA-CAA-C2A	-2.19	112.74	115.76
25	4	607	CHL	O1D-CGD-CBD	-2.19	120.01	124.53
30	r	2630	LHG	C18-C17-C16	-2.19	103.17	114.45
30	b	2630	LHG	C18-C17-C16	-2.19	103.17	114.45
38	d	405	PL9	C31-C32-C33	-2.19	104.45	111.97
25	7	609	CHL	CHA-CBD-CGD	-2.19	109.93	115.00
27	n	1620	LUT	C28-C29-C30	-2.19	115.59	118.94
30	B	2630	LHG	C18-C17-C16	-2.19	103.19	114.45
30	R	2630	LHG	C18-C17-C16	-2.18	103.20	114.45
26	B	602	CLA	O2A-CGA-O1A	-2.18	118.13	123.55
29	1	1623	NEX	C11-C12-C13	-2.18	120.28	126.42
35	A	409	PHO	C1-C2-C3	-2.18	121.94	125.96
26	B	610	CLA	O2A-CGA-O1A	-2.18	118.14	123.55
25	7	608	CHL	C4A-C3A-C2A	-2.18	100.53	103.86
25	y	609	CHL	O1D-CGD-CBD	-2.18	120.03	124.53
26	Y	610	CLA	C1-C2-C3	-2.18	121.95	125.96
26	c	501	CLA	O2A-CGA-O1A	-2.18	118.15	123.55
25	7	608	CHL	O2D-CGD-O1D	-2.18	119.44	123.82
25	Y	609	CHL	CBA-CAA-C2A	-2.18	112.76	115.76
26	1	612	CLA	CHA-C1A-NA	-2.18	121.13	126.18
25	1	601	CHL	OMC-CMC-C2C	-2.17	121.51	124.29
30	c	2630	LHG	C27-C26-C25	-2.17	103.26	114.45
27	1	1620	LUT	C8-C7-C6	-2.17	121.17	127.25
26	r	603	CLA	C3C-C4C-NC	-2.17	108.01	110.21
30	R	2630	LHG	C27-C26-C25	-2.17	103.27	114.45
25	3	609	CHL	O1D-CGD-CBD	-2.17	120.05	124.53
39	c	519	DGD	C1D-C2D-C3D	-2.17	105.94	109.98
30	C	2630	LHG	C27-C26-C25	-2.17	103.27	114.45
25	5	601	CHL	O2D-CGD-O1D	-2.17	119.45	123.82
29	5	1623	NEX	C11-C12-C13	-2.17	120.32	126.42
25	5	601	CHL	OMC-CMC-C2C	-2.17	121.52	124.29
26	b	610	CLA	O2A-CGA-O1A	-2.17	118.16	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	s	1621	LUT	C15-C35-C34	-2.17	118.83	123.46
26	G	613	CLA	O2D-CGD-O1D	-2.17	119.46	123.82
27	S	1621	LUT	C15-C35-C34	-2.17	118.83	123.46
25	2	607	CHL	OMC-CMC-C2C	-2.17	121.52	124.29
35	A	408	PHO	C2B-C1B-NB	-2.17	106.61	109.82
30	r	2630	LHG	C27-C26-C25	-2.17	103.29	114.45
26	y	610	CLA	C1-C2-C3	-2.17	121.97	125.96
26	5	612	CLA	CHA-C1A-NA	-2.17	121.15	126.18
26	a	406	CLA	C1C-C2C-C3C	-2.16	104.52	106.92
29	G	1623	NEX	C30-C31-C32	-2.16	116.60	123.23
39	c	518	DGD	O2D-C2D-C1D	-2.16	105.51	110.03
26	R	610	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
39	b	626	DGD	O1G-C1A-O1A	-2.16	118.19	123.55
39	C	519	DGD	C1D-C2D-C3D	-2.16	105.96	109.98
27	5	1620	LUT	C8-C7-C6	-2.16	121.20	127.25
26	c	503	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
26	B	616	CLA	C6-C7-C8	-2.16	108.65	115.73
29	g	1623	NEX	C30-C31-C32	-2.16	116.61	123.23
25	3	608	CHL	C4A-C3A-C2A	-2.16	100.56	103.86
35	a	409	PHO	C1-C2-C3	-2.16	121.98	125.96
27	G	1621	LUT	C35-C15-C14	-2.16	118.86	123.46
26	d	403	CLA	O2A-CGA-O1A	-2.16	118.20	123.55
31	b	619	BCR	C33-C5-C6	-2.16	122.09	124.51
38	D	405	PL9	C27-C28-C29	-2.16	122.27	127.68
38	d	405	PL9	C27-C28-C29	-2.15	122.27	127.68
30	4	2630	LHG	O8-C6-C5	-2.15	103.24	108.66
39	h	102	DGD	O5D-C6D-C5D	-2.15	105.34	108.94
39	H	102	DGD	O5D-C6D-C5D	-2.15	105.34	108.94
37	C	521	LMG	C38-C37-C36	-2.15	103.36	114.45
27	s	1620	LUT	C8-C7-C6	-2.15	121.23	127.25
27	S	1620	LUT	C8-C7-C6	-2.15	121.23	127.25
37	A	415	LMG	C38-C37-C36	-2.15	103.37	114.45
37	a	415	LMG	C38-C37-C36	-2.15	103.37	114.45
27	g	1621	LUT	C35-C15-C14	-2.15	118.87	123.46
39	C	518	DGD	O2D-C2D-C1D	-2.15	105.53	110.03
26	b	611	CLA	O2A-CGA-O1A	-2.15	118.21	123.55
26	r	610	CLA	OBD-CAD-CBD	-2.15	122.69	125.94
25	1	601	CHL	O2D-CGD-O1D	-2.15	119.50	123.82
28	R	622	XAT	C31-C30-C29	-2.15	124.24	127.31
26	b	616	CLA	C6-C7-C8	-2.15	108.68	115.73
25	7	607	CHL	O2D-CGD-O1D	-2.15	119.50	123.82
25	3	607	CHL	O2D-CGD-O1D	-2.15	119.50	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	610	CLA	C1-C2-C3	-2.14	122.00	125.96
25	N	608	CHL	O1D-CGD-CBD	-2.14	120.10	124.53
31	c	514	BCR	C40-C30-C25	-2.14	106.83	110.31
26	B	611	CLA	O2A-CGA-O1A	-2.14	118.23	123.55
35	A	408	PHO	C3C-C4C-NC	-2.14	106.69	110.19
37	c	521	LMG	C38-C37-C36	-2.14	103.41	114.45
26	C	503	CLA	O2A-CGA-O1A	-2.14	118.23	123.55
25	2	601	CHL	C4A-C3A-C2A	-2.14	100.58	103.86
25	2	606	CHL	C4A-C3A-C2A	-2.14	100.58	103.86
35	a	408	PHO	C2B-C1B-NB	-2.14	106.65	109.82
26	g	613	CLA	O2D-CGD-O1D	-2.14	119.51	123.82
31	C	514	BCR	C40-C30-C25	-2.14	106.84	110.31
39	B	626	DGD	O1G-C1A-O1A	-2.14	118.24	123.55
30	Y	2630	LHG	C27-C26-C25	-2.14	103.43	114.45
27	S	1621	LUT	C31-C30-C29	-2.14	124.26	127.31
26	D	403	CLA	O2A-CGA-O1A	-2.14	118.24	123.55
26	d	403	CLA	CAA-CBA-CGA	-2.14	106.91	113.35
25	6	607	CHL	OMC-CMC-C2C	-2.14	121.56	124.29
26	G	602	CLA	O2A-CGA-O1A	-2.14	118.25	123.55
31	c	517	BCR	C11-C12-C13	-2.14	120.42	126.42
26	s	602	CLA	C1-C2-C3	-2.14	122.02	125.96
30	y	2630	LHG	C27-C26-C25	-2.14	103.45	114.45
27	s	1621	LUT	C28-C29-C30	-2.13	115.67	118.94
31	C	517	BCR	C11-C12-C13	-2.13	120.42	126.42
30	8	2630	LHG	O8-C6-C5	-2.13	103.29	108.66
30	b	2631	LHG	C18-C17-C16	-2.13	103.47	114.45
30	c	522	LHG	C27-C26-C25	-2.13	103.47	114.45
27	5	1620	LUT	C8-C9-C10	-2.13	115.67	118.94
30	s	2630	LHG	C27-C26-C25	-2.13	103.48	114.45
26	A	406	CLA	C1C-C2C-C3C	-2.13	104.56	106.92
26	S	610	CLA	C1-C2-C3	-2.13	122.03	125.96
30	S	2630	LHG	C27-C26-C25	-2.13	103.48	114.45
26	d	403	CLA	OBD-CAD-CBD	-2.13	122.72	125.94
30	s	2630	LHG	O8-C23-O10	-2.13	118.26	123.55
26	y	602	CLA	OBD-CAD-CBD	-2.13	122.72	125.94
28	r	622	XAT	C31-C30-C29	-2.13	124.27	127.31
30	S	2630	LHG	O8-C23-O10	-2.13	118.27	123.55
26	Y	602	CLA	OBD-CAD-CBD	-2.13	122.73	125.94
25	n	608	CHL	O1D-CGD-CBD	-2.13	120.14	124.53
29	1	1623	NEX	C10-C11-C12	-2.13	116.71	123.23
37	b	2633	LMG	C3-C4-C5	-2.13	106.47	110.22
25	6	601	CHL	C4A-C3A-C2A	-2.13	100.61	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	522	LHG	C27-C26-C25	-2.13	103.50	114.45
26	n	612	CLA	OBD-CAD-CBD	-2.13	122.73	125.94
25	7	606	CHL	O1D-CGD-CBD	-2.13	120.14	124.53
26	D	403	CLA	CAA-CBA-CGA	-2.13	106.94	113.35
26	a	407	CLA	O2A-CGA-O1A	-2.13	118.27	123.55
27	s	1621	LUT	C31-C30-C29	-2.13	124.28	127.31
27	7	1620	LUT	C8-C9-C10	-2.13	115.68	118.94
26	g	602	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
37	B	2633	LMG	C3-C4-C5	-2.12	106.47	110.22
30	B	2631	LHG	C18-C17-C16	-2.12	103.51	114.45
26	C	505	CLA	C1-C2-C3	-2.12	122.04	125.96
26	Y	603	CLA	CAA-C2A-C3A	-2.12	106.99	112.81
27	S	1621	LUT	C28-C29-C30	-2.12	115.68	118.94
28	6	1622	XAT	C39-C29-C30	-2.12	119.95	122.92
39	c	519	DGD	CAB-C9B-C8B	-2.12	103.53	114.45
26	A	406	CLA	C16-C15-C13	-2.12	108.77	115.73
25	2	608	CHL	C4A-C3A-C2A	-2.12	100.62	103.86
26	S	602	CLA	C1-C2-C3	-2.12	122.05	125.96
35	a	408	PHO	C3C-C4C-NC	-2.12	106.73	110.19
25	8	609	CHL	CBC-CAC-C3C	-2.12	109.73	112.95
26	y	603	CLA	CBC-CAC-C3C	-2.12	106.39	112.41
25	6	606	CHL	C4A-C3A-C2A	-2.12	100.62	103.86
26	N	612	CLA	OBD-CAD-CBD	-2.12	122.74	125.94
31	c	516	BCR	C31-C1-C6	-2.12	106.87	110.31
25	4	609	CHL	CBC-CAC-C3C	-2.12	109.73	112.95
27	3	1620	LUT	C8-C9-C10	-2.12	115.69	118.94
31	B	619	BCR	C11-C12-C13	-2.12	120.47	126.42
30	C	522	LHG	C18-C17-C16	-2.12	103.55	114.45
26	a	406	CLA	C16-C15-C13	-2.12	108.78	115.73
30	c	522	LHG	C18-C17-C16	-2.12	103.55	114.45
39	C	520	DGD	O3D-C3D-C4D	-2.12	105.75	110.36
39	c	520	DGD	O3D-C3D-C4D	-2.12	105.75	110.36
26	Y	603	CLA	CBC-CAC-C3C	-2.12	106.40	112.41
25	R	607	CHL	O2D-CGD-O1D	-2.12	119.56	123.82
26	A	407	CLA	O2A-CGA-O1A	-2.12	118.30	123.55
29	R	623	NEX	C4-C3-C2	-2.11	106.37	110.68
29	5	1623	NEX	C10-C11-C12	-2.11	116.75	123.23
25	3	606	CHL	O1D-CGD-CBD	-2.11	120.17	124.53
36	A	418	SQD	O47-C7-O49	-2.11	118.40	123.68
39	C	519	DGD	CAB-C9B-C8B	-2.11	103.56	114.45
36	a	418	SQD	O47-C7-O49	-2.11	118.40	123.68
26	n	602	CLA	C6-C7-C8	-2.11	108.80	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	b	626	DGD	O3E-C3E-C2E	-2.11	105.76	110.36
27	6	1620	LUT	C8-C7-C6	-2.11	121.34	127.25
25	6	608	CHL	C4A-C3A-C2A	-2.11	100.63	103.86
27	2	1620	LUT	C8-C7-C6	-2.11	121.34	127.25
31	B	619	BCR	C33-C5-C6	-2.11	122.14	124.51
31	b	619	BCR	C11-C12-C13	-2.11	120.49	126.42
26	C	506	CLA	CMC-C2C-C1C	-2.11	121.82	125.02
31	C	515	BCR	C4-C5-C6	-2.11	119.64	122.74
25	y	601	CHL	C4A-C3A-C2A	-2.11	100.64	103.86
29	S	1623	NEX	C11-C12-C13	-2.11	120.49	126.42
28	g	1622	XAT	O4-C5-C6	-2.11	57.17	58.94
28	g	1622	XAT	C26-C27-C28	-2.11	121.53	125.99
26	b	605	CLA	C11-C10-C8	-2.11	108.81	115.73
25	y	608	CHL	CHA-CBD-CGD	-2.11	110.11	115.00
26	c	505	CLA	C1-C2-C3	-2.11	122.07	125.96
26	c	506	CLA	CMC-C2C-C1C	-2.11	121.83	125.02
39	c	520	DGD	CAB-C9B-C8B	-2.11	103.59	114.45
29	s	1623	NEX	C11-C12-C13	-2.11	120.50	126.42
27	Y	1621	LUT	C35-C15-C14	-2.11	118.96	123.46
25	2	606	CHL	O2D-CGD-O1D	-2.11	119.58	123.82
39	C	520	DGD	CAB-C9B-C8B	-2.11	103.60	114.45
27	l	1620	LUT	C8-C9-C10	-2.11	115.71	118.94
28	G	1622	XAT	C26-C27-C28	-2.11	121.54	125.99
26	y	603	CLA	CAA-C2A-C3A	-2.11	107.04	112.81
29	n	1623	NEX	C4-C3-C2	-2.11	106.39	110.68
25	r	607	CHL	O2D-CGD-O1D	-2.11	119.58	123.82
39	B	626	DGD	O3E-C3E-C2E	-2.11	105.78	110.36
29	S	1623	NEX	C15-C35-C34	-2.11	118.97	123.46
29	s	1623	NEX	C15-C35-C34	-2.11	118.97	123.46
25	6	606	CHL	O2D-CGD-O1D	-2.11	119.58	123.82
26	B	605	CLA	C11-C10-C8	-2.11	108.82	115.73
30	C	522	LHG	C20-C19-C18	-2.11	103.61	114.45
27	G	1621	LUT	C37-C21-C22	-2.10	105.40	109.42
25	6	609	CHL	OMC-CMC-C2C	-2.10	121.60	124.29
25	8	609	CHL	O1D-CGD-CBD	-2.10	120.19	124.53
26	3	614	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
39	B	626	DGD	O6E-C5E-C6E	-2.10	101.37	106.41
30	c	522	LHG	C20-C19-C18	-2.10	103.62	114.45
25	Y	608	CHL	CHA-CBD-CGD	-2.10	110.12	115.00
36	B	621	SQD	O47-C7-O49	-2.10	118.43	123.68
27	7	1621	LUT	C30-C31-C32	-2.10	116.78	123.23
29	r	623	NEX	C4-C3-C2	-2.10	106.40	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	C	520	DGD	C7B-C6B-C5B	-2.10	103.63	114.45
26	7	611	CLA	C1C-NC-C4C	-2.10	105.85	107.06
26	7	614	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
27	N	1620	LUT	C7-C8-C9	-2.10	123.06	126.21
25	Y	601	CHL	C4A-C3A-C2A	-2.10	100.65	103.86
25	2	609	CHL	OMC-CMC-C2C	-2.10	121.61	124.29
25	3	605	CHL	O1D-CGD-CBD	-2.10	120.20	124.53
39	c	520	DGD	C7B-C6B-C5B	-2.10	103.64	114.45
29	N	1623	NEX	C4-C3-C2	-2.10	106.41	110.68
27	3	1621	LUT	C30-C31-C32	-2.10	116.79	123.23
31	T	101	BCR	C1-C6-C5	-2.10	119.64	122.59
39	c	520	DGD	CBB-CAB-C9B	-2.10	103.64	114.45
31	C	516	BCR	C31-C1-C6	-2.10	106.91	110.31
25	7	605	CHL	CHA-CBD-CGD	-2.10	110.14	115.00
27	r	620	LUT	C18-C5-C6	-2.10	122.16	124.51
27	R	620	LUT	C18-C5-C6	-2.10	122.16	124.51
26	1	604	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
27	6	1621	LUT	C28-C29-C30	-2.10	115.72	118.94
31	c	515	BCR	C4-C5-C6	-2.10	119.66	122.74
26	1	610	CLA	O2A-CGA-O1A	-2.10	118.35	123.55
31	d	404	BCR	C3-C4-C5	-2.10	110.18	113.78
26	N	602	CLA	C6-C7-C8	-2.10	108.85	115.73
25	3	605	CHL	CHA-CBD-CGD	-2.10	110.14	115.00
39	C	520	DGD	CBB-CAB-C9B	-2.09	103.66	114.45
25	r	606	CHL	C1-C2-C3	-2.09	122.10	125.96
26	5	610	CLA	O2A-CGA-O1A	-2.09	118.35	123.55
25	4	606	CHL	O1D-CGD-CBD	-2.09	120.21	124.53
30	s	2630	LHG	C18-C17-C16	-2.09	103.66	114.45
30	S	2630	LHG	C18-C17-C16	-2.09	103.67	114.45
27	y	1621	LUT	C35-C15-C14	-2.09	118.99	123.46
28	2	1622	XAT	C39-C29-C30	-2.09	119.99	122.92
39	c	520	DGD	C5B-C4B-C3B	-2.09	103.67	114.45
39	C	520	DGD	C5B-C4B-C3B	-2.09	103.68	114.45
27	5	1621	LUT	C31-C30-C29	-2.09	124.33	127.31
26	R	601	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
39	b	626	DGD	O6E-C5E-C6E	-2.09	101.40	106.41
37	b	622	LMG	O2-C2-C1	-2.09	105.66	110.03
26	c	503	CLA	C7-C6-C5	-2.09	107.30	113.11
26	5	604	CLA	O2A-CGA-O1A	-2.09	118.36	123.55
36	b	621	SQD	O47-C7-O49	-2.09	118.47	123.68
27	6	1621	LUT	C35-C15-C14	-2.09	119.00	123.46
26	C	503	CLA	C7-C6-C5	-2.09	107.31	113.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	622	LMG	O2-C2-C1	-2.09	105.66	110.03
26	G	602	CLA	C6-C7-C8	-2.09	108.88	115.73
25	8	606	CHL	O1D-CGD-CBD	-2.09	120.22	124.53
25	R	608	CHL	C4A-C3A-C2A	-2.09	100.67	103.86
27	N	1620	LUT	C23-C24-C25	-2.09	123.26	125.22
25	1	601	CHL	CBC-CAC-C3C	-2.09	109.78	112.95
26	g	602	CLA	C6-C7-C8	-2.09	108.89	115.73
25	R	606	CHL	C1-C2-C3	-2.09	122.11	125.96
27	g	1621	LUT	C37-C21-C22	-2.09	105.44	109.42
25	4	609	CHL	O1D-CGD-CBD	-2.08	120.23	124.53
25	r	608	CHL	C4A-C3A-C2A	-2.08	100.67	103.86
27	n	1620	LUT	C7-C8-C9	-2.08	123.08	126.21
27	2	1621	LUT	C35-C15-C14	-2.08	119.02	123.46
26	3	611	CLA	CHA-C1A-NA	-2.08	121.34	126.18
39	c	520	DGD	O2D-C2D-C1D	-2.08	105.68	110.03
31	t	101	BCR	C1-C6-C5	-2.08	119.67	122.59
39	C	518	DGD	O3G-C1D-C2D	-2.08	104.84	108.23
27	1	1621	LUT	C31-C30-C29	-2.08	124.34	127.31
26	c	510	CLA	CAA-C2A-C3A	-2.08	107.11	112.81
27	2	1621	LUT	C28-C29-C30	-2.08	115.75	118.94
27	5	1620	LUT	C11-C10-C9	-2.08	124.34	127.31
26	b	609	CLA	C1-C2-C3	-2.08	122.13	125.96
27	5	1620	LUT	C38-C25-C24	-2.08	119.21	123.68
37	Z	101	LMG	C38-C37-C36	-2.08	103.75	114.45
30	7	2630	LHG	C18-C17-C16	-2.08	103.75	114.45
30	3	2630	LHG	C18-C17-C16	-2.08	103.75	114.45
39	C	519	DGD	C7B-C6B-C5B	-2.08	103.75	114.45
31	d	404	BCR	C15-C16-C17	-2.08	119.03	123.46
26	D	403	CLA	OBD-CAD-CBD	-2.08	122.80	125.94
25	7	605	CHL	O1D-CGD-CBD	-2.08	120.25	124.53
28	g	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
26	B	609	CLA	O2A-CGA-O1A	-2.07	118.40	123.55
31	D	404	BCR	C3-C4-C5	-2.07	110.21	113.78
39	C	520	DGD	C3D-C4D-C5D	-2.07	106.56	110.22
39	c	520	DGD	C3D-C4D-C5D	-2.07	106.56	110.22
39	C	519	DGD	C3D-C4D-C5D	-2.07	106.56	110.22
31	B	619	BCR	C16-C15-C14	-2.07	119.04	123.46
30	C	522	LHG	C5-O7-C7	-2.07	112.98	117.88
39	c	519	DGD	C7B-C6B-C5B	-2.07	103.77	114.45
26	6	610	CLA	O2A-CGA-O1A	-2.07	118.40	123.55
28	G	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
37	z	101	LMG	C38-C37-C36	-2.07	103.78	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	602	CLA	CAA-CBA-CGA	-2.07	107.11	113.35
39	c	520	DGD	C1D-C2D-C3D	-2.07	106.13	109.98
26	C	501	CLA	OBD-CAD-CBD	-2.07	122.81	125.94
26	R	601	CLA	O2A-CGA-O1A	-2.07	118.41	123.55
26	r	603	CLA	O2A-CGA-O1A	-2.07	118.41	123.55
26	B	610	CLA	OBD-CAD-CBD	-2.07	122.81	125.94
26	b	610	CLA	OBD-CAD-CBD	-2.07	122.81	125.94
26	7	611	CLA	CHA-C1A-NA	-2.07	121.37	126.18
37	d	411	LMG	C9-C8-C7	-2.07	107.19	111.86
26	r	601	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
39	c	519	DGD	C3D-C4D-C5D	-2.07	106.57	110.22
26	Y	602	CLA	CAA-CBA-CGA	-2.07	107.11	113.35
27	n	1621	LUT	C28-C29-C30	-2.07	115.77	118.94
27	N	1621	LUT	C28-C29-C30	-2.07	115.77	118.94
31	D	404	BCR	C15-C16-C17	-2.07	119.05	123.46
30	Y	2630	LHG	C18-C17-C16	-2.07	103.80	114.45
26	1	604	CLA	C1-C2-C3	-2.07	123.41	126.68
25	3	609	CHL	C1-C2-C3	-2.07	122.15	125.96
26	C	510	CLA	CAA-C2A-C3A	-2.07	107.14	112.81
39	C	520	DGD	O2D-C2D-C1D	-2.07	105.71	110.03
25	6	607	CHL	C3B-CAB-CBB	-2.07	120.56	125.20
30	y	2630	LHG	C18-C17-C16	-2.07	103.81	114.45
26	8	610	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
26	4	610	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
37	D	411	LMG	C9-C8-C7	-2.07	107.20	111.86
25	S	607	CHL	O2D-CGD-O1D	-2.07	119.66	123.82
25	2	607	CHL	C3B-CAB-CBB	-2.06	120.56	125.20
39	C	520	DGD	C1D-C2D-C3D	-2.06	106.14	109.98
26	R	603	CLA	O2A-CGA-O1A	-2.06	118.43	123.55
26	5	604	CLA	C1-C2-C3	-2.06	123.42	126.68
27	5	1620	LUT	C7-C8-C9	-2.06	123.11	126.21
26	Y	614	CLA	O2A-CGA-O1A	-2.06	118.43	123.55
27	1	1620	LUT	C38-C25-C24	-2.06	119.24	123.68
27	1	1620	LUT	C7-C8-C9	-2.06	123.11	126.21
39	c	518	DGD	O5D-C6D-C5D	-2.06	105.50	108.94
37	B	2633	LMG	C42-C41-C40	-2.06	103.84	114.45
26	B	609	CLA	C1-C2-C3	-2.06	122.16	125.96
26	r	601	CLA	O2A-CGA-O1A	-2.06	118.44	123.55
31	b	619	BCR	C16-C15-C14	-2.06	119.07	123.46
26	c	506	CLA	C1-C2-C3	-2.06	122.17	125.96
26	b	609	CLA	O2A-CGA-O1A	-2.06	118.44	123.55
26	y	614	CLA	O2A-CGA-O1A	-2.06	118.44	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	t	101	BCR	C4-C5-C6	-2.06	119.72	122.74
30	R	2630	LHG	O8-C6-C5	-2.06	103.49	108.66
30	c	522	LHG	C5-O7-C7	-2.06	113.02	117.88
39	C	518	DGD	C5B-C4B-C3B	-2.06	103.86	114.45
31	4	623	BCR	C35-C13-C14	-2.06	120.04	122.92
39	c	518	DGD	O3G-C1D-C2D	-2.06	104.88	108.23
25	6	601	CHL	O2D-CGD-O1D	-2.06	119.68	123.82
27	5	1621	LUT	C15-C35-C34	-2.05	119.08	123.46
39	C	518	DGD	O5D-C6D-C5D	-2.05	105.51	108.94
30	D	408	LHG	C27-C26-C25	-2.05	103.87	114.45
27	Y	1621	LUT	C15-C35-C34	-2.05	119.08	123.46
26	A	405	CLA	O2D-CGD-O1D	-2.05	119.69	123.82
39	c	518	DGD	C5B-C4B-C3B	-2.05	103.88	114.45
25	r	607	CHL	C4A-C3A-C2A	-2.05	100.72	103.86
27	n	1620	LUT	C23-C24-C25	-2.05	123.30	125.22
37	b	2633	LMG	C42-C41-C40	-2.05	103.88	114.45
26	B	605	CLA	CAC-C3C-C2C	-2.05	123.94	127.49
25	s	607	CHL	O2D-CGD-O1D	-2.05	119.69	123.82
25	5	607	CHL	C1-C2-C3	-2.05	122.18	125.96
28	R	622	XAT	O24-C25-C26	-2.05	57.22	58.94
28	r	622	XAT	O24-C25-C26	-2.05	57.22	58.94
29	6	1623	NEX	C19-C9-C10	-2.05	120.05	122.92
25	4	601	CHL	OMC-CMC-C2C	-2.05	121.67	124.29
30	d	408	LHG	C27-C26-C25	-2.05	103.89	114.45
27	1	1621	LUT	C15-C35-C34	-2.05	119.09	123.46
25	2	601	CHL	O2D-CGD-O1D	-2.05	119.70	123.82
27	3	1621	LUT	C8-C7-C6	-2.05	121.52	127.25
31	4	623	BCR	C2-C3-C4	-2.05	106.46	111.34
25	5	601	CHL	CBC-CAC-C3C	-2.05	109.84	112.95
26	2	610	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
27	1	1620	LUT	C11-C10-C9	-2.05	124.39	127.31
35	A	409	PHO	C3C-C4C-NC	-2.05	106.85	110.19
26	3	611	CLA	C1C-NC-C4C	-2.05	105.88	107.06
25	2	608	CHL	CMA-C3A-C2A	-2.05	109.03	115.84
26	7	613	CLA	OBD-CAD-CBD	-2.05	122.85	125.94
26	N	604	CLA	C1-C2-C3	-2.05	123.45	126.68
37	A	413	LMG	C1-C2-C3	-2.04	106.18	109.98
27	7	1621	LUT	C8-C7-C6	-2.04	121.53	127.25
26	Y	604	CLA	OBD-CAD-CBD	-2.04	122.85	125.94
26	c	501	CLA	OBD-CAD-CBD	-2.04	122.85	125.94
25	7	609	CHL	C1-C2-C3	-2.04	122.19	125.96
29	2	1623	NEX	C19-C9-C10	-2.04	120.06	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	606	CHL	CHA-CBD-CGD	-2.04	110.26	115.00
37	a	413	LMG	C1-C2-C3	-2.04	106.18	109.98
30	r	2630	LHG	O8-C6-C5	-2.04	103.52	108.66
28	N	1622	XAT	C26-C27-C28	-2.04	121.67	125.99
30	c	523	LHG	C18-C17-C16	-2.04	103.93	114.45
30	C	523	LHG	C18-C17-C16	-2.04	103.93	114.45
26	C	506	CLA	C1-C2-C3	-2.04	122.19	125.96
25	n	608	CHL	C11-C12-C13	-2.04	109.03	115.73
26	3	613	CLA	OBD-CAD-CBD	-2.04	122.86	125.94
26	N	610	CLA	CHA-C1A-NA	-2.04	121.44	126.18
28	G	1622	XAT	O4-C5-C6	-2.04	57.23	58.94
25	r	606	CHL	CHA-CBD-CGD	-2.04	110.27	115.00
25	6	608	CHL	CMA-C3A-C2A	-2.04	109.06	115.84
26	s	612	CLA	OBD-CAD-CBD	-2.04	122.86	125.94
26	a	405	CLA	O2D-CGD-O1D	-2.04	119.72	123.82
26	C	512	CLA	CAA-C2A-C3A	-2.04	107.23	112.81
26	b	605	CLA	CAC-C3C-C2C	-2.04	123.96	127.49
25	1	607	CHL	C1-C2-C3	-2.04	122.20	125.96
25	2	605	CHL	O2D-CGD-O1D	-2.04	119.72	123.82
26	S	609	CLA	O2D-CGD-O1D	-2.04	119.72	123.82
25	y	606	CHL	C4A-C3A-C2A	-2.03	100.75	103.86
26	c	512	CLA	CAA-C2A-C3A	-2.03	107.23	112.81
31	T	101	BCR	C4-C5-C6	-2.03	119.76	122.74
28	n	1622	XAT	C26-C27-C28	-2.03	121.70	125.99
26	n	610	CLA	CHA-C1A-NA	-2.03	121.46	126.18
26	y	613	CLA	OBD-CAD-CBD	-2.03	122.87	125.94
26	y	612	CLA	O2A-CGA-O1A	-2.03	118.51	123.55
39	b	626	DGD	O6E-C1E-O5D	-2.03	105.20	110.02
25	N	608	CHL	C11-C12-C13	-2.03	109.07	115.73
30	L	101	LHG	C27-C26-C25	-2.03	103.99	114.45
30	l	101	LHG	C27-C26-C25	-2.03	103.99	114.45
25	4	609	CHL	CHA-CBD-CGD	-2.03	110.29	115.00
31	c	515	BCR	C10-C11-C12	-2.03	117.00	123.23
31	8	623	BCR	C2-C3-C4	-2.03	106.51	111.34
39	B	626	DGD	O6E-C1E-O5D	-2.03	105.20	110.02
27	y	1621	LUT	C15-C35-C34	-2.03	119.13	123.46
26	n	604	CLA	C1-C2-C3	-2.03	123.48	126.68
26	Y	613	CLA	OBD-CAD-CBD	-2.03	122.88	125.94
25	8	601	CHL	OMC-CMC-C2C	-2.03	121.70	124.29
25	6	605	CHL	OMC-CMC-C2C	-2.03	121.70	124.29
29	y	1623	NEX	C30-C31-C32	-2.03	117.02	123.23
25	6	605	CHL	O2D-CGD-O1D	-2.03	119.74	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	621	SQD	O48-C23-O10	-2.03	118.52	123.55
25	R	607	CHL	C4A-C3A-C2A	-2.02	100.77	103.86
25	4	609	CHL	CMA-C3A-C2A	-2.02	109.11	115.84
30	B	2630	LHG	C27-C26-C25	-2.02	104.03	114.45
31	C	514	BCR	C7-C8-C9	-2.02	123.17	126.21
31	8	623	BCR	C35-C13-C14	-2.02	120.09	122.92
26	s	609	CLA	O2D-CGD-O1D	-2.02	119.75	123.82
26	S	602	CLA	OBD-CAD-CBD	-2.02	122.89	125.94
26	C	502	CLA	CAA-C2A-C3A	-2.02	107.27	112.81
35	a	409	PHO	C3C-C4C-NC	-2.02	106.89	110.19
27	8	620	LUT	C38-C25-C24	-2.02	119.33	123.68
36	B	621	SQD	O48-C23-O10	-2.02	118.53	123.55
26	6	603	CLA	C3C-C4C-NC	-2.02	108.16	110.21
31	c	514	BCR	C8-C7-C6	-2.02	121.59	127.25
30	c	522	LHG	O8-C6-C5	-2.02	103.58	108.66
30	C	522	LHG	O8-C6-C5	-2.02	103.58	108.66
26	b	607	CLA	CMC-C2C-C1C	-2.02	121.96	125.02
29	N	1623	NEX	C30-C31-C32	-2.02	117.04	123.23
25	5	606	CHL	OMC-CMC-C2C	-2.02	121.71	124.29
25	G	607	CHL	O2A-CGA-O1A	-2.02	118.54	123.55
30	b	2630	LHG	C27-C26-C25	-2.02	104.05	114.45
31	C	515	BCR	C10-C11-C12	-2.02	117.04	123.23
31	C	516	BCR	C37-C22-C21	-2.02	120.09	122.92
30	L	101	LHG	C18-C17-C16	-2.02	104.05	114.45
25	2	605	CHL	OMC-CMC-C2C	-2.02	121.71	124.29
29	Y	1623	NEX	C30-C31-C32	-2.02	117.04	123.23
31	c	514	BCR	C7-C8-C9	-2.02	123.18	126.21
27	n	1621	LUT	C38-C25-C24	-2.02	119.34	123.68
31	C	514	BCR	C8-C7-C6	-2.02	121.61	127.25
27	3	1620	LUT	C38-C25-C24	-2.02	119.34	123.68
35	a	408	PHO	C2A-C1A-NA	-2.02	109.46	111.91
29	3	1623	NEX	O4-C5-C18	-2.01	105.98	109.51
30	C	523	LHG	C11-C10-C9	-2.01	104.07	114.45
26	y	604	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
30	l	101	LHG	C18-C17-C16	-2.01	104.07	114.45
26	B	617	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
25	3	601	CHL	O2D-CGD-O1D	-2.01	119.77	123.82
26	1	611	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
25	1	606	CHL	OMC-CMC-C2C	-2.01	121.72	124.29
26	Y	612	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
25	7	601	CHL	O2D-CGD-O1D	-2.01	119.77	123.82
25	g	607	CHL	O2A-CGA-O1A	-2.01	118.55	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	603	CLA	C3C-C4C-NC	-2.01	108.17	110.21
26	b	617	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
26	s	603	CLA	CHA-C1A-NA	-2.01	121.51	126.18
26	S	603	CLA	CHA-C1A-NA	-2.01	121.51	126.18
30	b	2631	LHG	C29-C28-C27	-2.01	104.09	114.45
30	c	523	LHG	C11-C10-C9	-2.01	104.09	114.45
35	A	408	PHO	C2A-C1A-NA	-2.01	109.46	111.91
25	8	609	CHL	CMA-C3A-C2A	-2.01	109.15	115.84
26	r	612	CLA	OBD-CAD-CBD	-2.01	122.90	125.94
27	7	1620	LUT	C38-C25-C24	-2.01	119.35	123.68
27	4	620	LUT	C38-C25-C24	-2.01	119.35	123.68
26	B	608	CLA	CHC-C1C-C2C	-2.01	121.17	126.65
31	c	516	BCR	C37-C22-C21	-2.01	120.11	122.92
30	3	2630	LHG	C27-C26-C25	-2.01	104.10	114.45
26	c	502	CLA	CAA-C2A-C3A	-2.01	107.30	112.81
30	B	2631	LHG	C29-C28-C27	-2.01	104.10	114.45
31	B	620	BCR	C21-C20-C19	-2.01	117.07	123.23
25	Y	606	CHL	C4A-C3A-C2A	-2.01	100.79	103.86
26	S	612	CLA	OBD-CAD-CBD	-2.01	122.91	125.94
29	n	1623	NEX	O24-C25-C26	-2.01	57.25	58.94
26	c	504	CLA	OBD-CAD-CBD	-2.01	122.91	125.94
27	N	1621	LUT	C38-C25-C24	-2.01	119.36	123.68
26	s	604	CLA	C1-C2-C3	-2.01	123.51	126.68
25	8	609	CHL	CHA-CBD-CGD	-2.01	110.34	115.00
26	b	608	CLA	CHC-C1C-C2C	-2.01	121.18	126.65
38	d	405	PL9	C36-C37-C38	-2.01	105.08	111.97
29	7	1623	NEX	O4-C5-C18	-2.01	106.00	109.51
38	D	405	PL9	C36-C34-C33	-2.01	117.00	121.10
25	n	607	CHL	O2D-CGD-O1D	-2.01	119.78	123.82
29	n	1623	NEX	C30-C31-C32	-2.01	117.08	123.23
31	C	514	BCR	C16-C15-C14	-2.01	119.18	123.46
28	3	1622	XAT	O24-C25-C26	-2.00	57.26	58.94
39	C	519	DGD	O5E-C6E-C5E	-2.00	104.60	111.34
30	7	2630	LHG	C27-C26-C25	-2.00	104.13	114.45
38	D	405	PL9	C36-C37-C38	-2.00	105.09	111.97
31	b	620	BCR	C21-C20-C19	-2.00	117.09	123.23
26	N	610	CLA	C1-C2-C3	-2.00	122.27	125.96
26	5	611	CLA	OBD-CAD-CBD	-2.00	122.92	125.94
26	C	512	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
26	R	612	CLA	OBD-CAD-CBD	-2.00	122.92	125.94
26	N	602	CLA	CMD-C2D-C3D	2.00	128.60	124.89
26	b	614	CLA	C1D-CHD-C4C	2.00	125.22	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	607	CHL	CHB-C1B-C2B	2.00	122.53	116.99
25	G	606	CHL	CED-O2D-CGD	2.00	120.66	115.97
28	3	1622	XAT	C38-C25-C24	2.00	116.57	114.28
31	C	515	BCR	C2-C1-C6	2.00	113.61	110.48
26	N	612	CLA	C4A-NA-C1A	2.00	108.94	106.45
26	n	612	CLA	C4A-NA-C1A	2.00	108.94	106.45
26	B	603	CLA	C1C-NC-C4C	2.00	108.21	107.06
36	a	412	SQD	C1-O5-C5	2.00	117.49	113.72
26	B	611	CLA	C2A-C1A-CHA	2.00	127.47	123.92
26	c	506	CLA	CHB-C4A-NA	2.01	127.29	124.51
26	B	612	CLA	O1D-CGD-CBD	2.01	128.21	124.60
27	8	620	LUT	C40-C33-C32	2.01	121.30	118.10
26	G	603	CLA	C1D-CHD-C4C	2.01	125.23	122.48
26	A	407	CLA	C1C-NC-C4C	2.01	108.21	107.06
31	B	619	BCR	C37-C22-C23	2.01	121.30	118.10
31	C	516	BCR	C35-C13-C12	2.01	121.30	118.10
25	Y	609	CHL	OMC-CMC-C2C	2.01	126.85	124.29
26	n	614	CLA	O1D-CGD-CBD	2.01	128.21	124.60
26	g	602	CLA	C4A-NA-C1A	2.01	108.95	106.45
25	s	601	CHL	CED-O2D-CGD	2.01	120.69	115.97
25	N	601	CHL	CBA-CAA-C2A	2.01	118.53	115.76
25	2	601	CHL	CED-O2D-CGD	2.01	120.69	115.97
26	B	605	CLA	CMB-C2B-C3B	2.01	128.63	124.89
26	C	506	CLA	CMC-C2C-C3C	2.01	131.66	126.09
26	c	511	CLA	C2A-C1A-CHA	2.01	127.49	123.92
26	Y	604	CLA	O1D-CGD-CBD	2.01	128.22	124.60
31	b	619	BCR	C37-C22-C23	2.01	121.31	118.10
26	7	611	CLA	CAA-C2A-C1A	2.01	118.58	111.97
26	3	611	CLA	CAA-C2A-C1A	2.01	118.58	111.97
25	g	606	CHL	CED-O2D-CGD	2.02	120.70	115.97
26	n	602	CLA	CMD-C2D-C3D	2.02	128.63	124.89
26	b	608	CLA	CHC-C1C-NC	2.02	127.88	124.08
31	B	619	BCR	C34-C9-C8	2.02	121.31	118.10
26	N	604	CLA	O2D-CGD-CBD	2.02	114.90	111.30
31	c	516	BCR	C35-C13-C12	2.02	121.31	118.10
26	7	613	CLA	C4A-NA-C1A	2.02	108.96	106.45
31	8	623	BCR	C2-C1-C6	2.02	113.63	110.48
31	c	515	BCR	C2-C1-C6	2.02	113.63	110.48
26	s	609	CLA	CHB-C4A-NA	2.02	127.30	124.51
26	d	402	CLA	O2D-CGD-CBD	2.02	114.91	111.30
26	b	612	CLA	O1D-CGD-CBD	2.02	128.23	124.60
26	g	603	CLA	C1D-CHD-C4C	2.02	125.25	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	603	CLA	CMD-C2D-C3D	2.02	128.65	124.89
26	5	602	CLA	CHB-C4A-NA	2.02	127.31	124.51
27	5	1620	LUT	C20-C13-C12	2.02	121.32	118.10
26	b	611	CLA	C2A-C1A-CHA	2.02	127.51	123.92
26	b	616	CLA	C2A-C1A-CHA	2.03	127.51	123.92
25	6	601	CHL	CED-O2D-CGD	2.03	120.72	115.97
26	B	614	CLA	C1D-CHD-C4C	2.03	125.26	122.48
27	6	1621	LUT	C1-C2-C3	2.03	117.79	113.40
26	C	502	CLA	C1D-CHD-C4C	2.03	125.26	122.48
26	b	605	CLA	CMB-C2B-C3B	2.03	128.66	124.89
26	C	506	CLA	CHB-C4A-NA	2.03	127.32	124.51
26	S	609	CLA	CHB-C4A-NA	2.03	127.32	124.51
26	5	604	CLA	O1D-CGD-CBD	2.03	128.25	124.60
26	y	604	CLA	O1D-CGD-CBD	2.03	128.25	124.60
31	T	101	BCR	C29-C30-C25	2.03	113.66	110.48
35	a	409	PHO	CMB-C2B-C3B	2.03	133.62	128.47
26	n	603	CLA	C1D-CHD-C4C	2.03	125.26	122.48
27	8	620	LUT	C19-C9-C8	2.03	121.34	118.10
26	c	506	CLA	C2A-C1A-CHA	2.03	127.52	123.92
26	1	602	CLA	CHB-C4A-NA	2.03	127.33	124.51
26	c	502	CLA	C1D-CHD-C4C	2.03	125.27	122.48
26	b	603	CLA	CMD-C2D-C3D	2.04	128.67	124.89
26	C	511	CLA	C2A-C1A-CHA	2.04	127.53	123.92
25	n	601	CHL	CBA-CAA-C2A	2.04	118.57	115.76
26	r	613	CLA	C4A-NA-C1A	2.04	108.98	106.45
25	R	608	CHL	CHB-C1B-C2B	2.04	122.64	116.99
26	c	513	CLA	C2A-C1A-CHA	2.04	127.53	123.92
26	C	513	CLA	C2A-C1A-CHA	2.04	127.53	123.92
26	b	616	CLA	CMB-C2B-C3B	2.04	128.68	124.89
26	B	608	CLA	CHC-C1C-NC	2.04	127.92	124.08
26	G	602	CLA	C4A-NA-C1A	2.04	108.98	106.45
27	2	1621	LUT	C1-C2-C3	2.04	117.82	113.40
26	C	506	CLA	C2A-C1A-CHA	2.04	127.54	123.92
26	B	616	CLA	C2A-C1A-CHA	2.04	127.54	123.92
26	8	602	CLA	C4A-NA-C1A	2.04	108.99	106.45
27	s	1621	LUT	C20-C13-C12	2.05	121.36	118.10
25	6	607	CHL	C4-C3-C5	2.05	118.84	115.29
25	1	605	CHL	CHB-C1B-C2B	2.05	122.65	116.99
35	A	409	PHO	CMB-C2B-C3B	2.05	133.66	128.47
26	1	604	CLA	O1D-CGD-CBD	2.05	128.28	124.60
25	r	608	CHL	CHB-C1B-C2B	2.05	122.66	116.99
25	2	607	CHL	C4-C3-C5	2.05	118.84	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	408	PHO	CBD-CHA-C1A	2.05	131.18	126.36
25	y	606	CHL	CHB-C1B-C2B	2.05	122.67	116.99
27	4	620	LUT	C19-C9-C8	2.05	121.37	118.10
25	5	605	CHL	CHB-C1B-C2B	2.05	122.67	116.99
27	S	1621	LUT	C20-C13-C12	2.05	121.37	118.10
35	a	408	PHO	CBD-CHA-C1A	2.05	131.20	126.36
26	C	509	CLA	C2A-C3A-C4A	2.05	105.19	101.87
26	r	603	CLA	C1C-NC-C4C	2.05	108.24	107.06
27	2	1620	LUT	C19-C9-C8	2.06	121.37	118.10
26	b	617	CLA	CAC-C3C-C4C	2.06	127.73	124.83
26	N	603	CLA	C1D-CHD-C4C	2.06	125.30	122.48
27	1	1620	LUT	C20-C13-C12	2.06	121.38	118.10
26	b	616	CLA	C3A-C2A-C1A	2.06	104.42	101.34
26	B	616	CLA	C3A-C2A-C1A	2.06	104.42	101.34
26	n	602	CLA	O2D-CGD-CBD	2.06	114.98	111.30
26	y	604	CLA	C1D-CHD-C4C	2.06	125.30	122.48
25	Y	606	CHL	CHB-C1B-C2B	2.06	122.70	116.99
26	6	611	CLA	O2D-CGD-CBD	2.07	114.99	111.30
37	Z	101	LMG	O8-C28-C29	2.07	117.91	111.90
25	y	605	CHL	CHB-C1B-C2B	2.07	122.71	116.99
26	c	509	CLA	C2A-C3A-C4A	2.07	105.21	101.87
25	2	608	CHL	CHB-C1B-C2B	2.07	122.72	116.99
26	B	616	CLA	CMB-C2B-C3B	2.07	128.73	124.89
25	7	609	CHL	C4D-C3D-CAD	2.07	109.52	104.71
26	B	613	CLA	C2A-C3A-C4A	2.07	105.21	101.87
26	3	603	CLA	O1D-CGD-CBD	2.07	128.32	124.60
26	c	508	CLA	CGD-CBD-CAD	2.07	117.65	110.71
26	N	602	CLA	O2D-CGD-CBD	2.07	115.00	111.30
26	C	502	CLA	CMC-C2C-C3C	2.07	131.82	126.09
25	3	609	CHL	C4D-C3D-CAD	2.07	109.52	104.71
26	n	610	CLA	O2A-CGA-CBA	2.07	117.93	111.90
27	6	1620	LUT	C19-C9-C8	2.07	121.40	118.10
26	R	609	CLA	O1D-CGD-CBD	2.07	128.33	124.60
26	B	617	CLA	CAC-C3C-C4C	2.07	127.75	124.83
26	Y	604	CLA	C1D-CHD-C4C	2.07	125.32	122.48
26	a	407	CLA	C1C-NC-C4C	2.07	108.25	107.06
26	2	611	CLA	O2D-CGD-CBD	2.07	115.00	111.30
26	a	405	CLA	C1C-C2C-C3C	2.08	109.23	106.92
26	s	609	CLA	CMD-C2D-C3D	2.08	128.75	124.89
26	y	611	CLA	O1D-CGD-CBD	2.08	128.33	124.60
26	r	609	CLA	O1D-CGD-CBD	2.08	128.33	124.60
26	N	610	CLA	O2A-CGA-CBA	2.08	117.94	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	608	CHL	CHB-C1B-C2B	2.08	122.74	116.99
25	2	606	CHL	CHB-C1B-C2B	2.08	122.75	116.99
26	2	602	CLA	CHB-C4A-NA	2.08	127.39	124.51
26	N	614	CLA	CMD-C2D-C3D	2.08	128.75	124.89
26	C	508	CLA	CGD-CBD-CAD	2.08	117.68	110.71
25	S	601	CHL	CMD-C2D-C3D	2.08	119.53	114.27
25	s	601	CHL	CMD-C2D-C3D	2.08	119.53	114.27
26	2	612	CLA	C2A-C1A-CHA	2.08	127.61	123.92
26	6	612	CLA	C2A-C1A-CHA	2.08	127.61	123.92
31	b	618	BCR	C33-C5-C4	2.08	117.40	113.45
25	Y	605	CHL	CHB-C1B-C2B	2.08	122.76	116.99
37	z	101	LMG	O8-C28-C29	2.08	117.96	111.90
26	7	603	CLA	O1D-CGD-CBD	2.08	128.35	124.60
26	c	502	CLA	CMC-C2C-C3C	2.08	131.86	126.09
26	R	603	CLA	C1C-NC-C4C	2.08	108.25	107.06
35	a	408	PHO	CHB-C4A-NA	2.09	128.55	124.99
26	b	612	CLA	C1D-CHD-C4C	2.09	125.34	122.48
25	g	601	CHL	C1-O2A-CGA	2.09	121.78	116.77
26	A	405	CLA	C1C-C2C-C3C	2.09	109.24	106.92
26	B	617	CLA	C3A-C2A-C1A	2.09	104.47	101.34
25	6	606	CHL	CHB-C1B-C2B	2.09	122.78	116.99
26	n	604	CLA	CHB-C4A-NA	2.09	127.40	124.51
25	5	607	CHL	CHB-C1B-C2B	2.09	122.78	116.99
25	2	601	CHL	CHB-C1B-C2B	2.09	122.78	116.99
26	b	613	CLA	C2A-C3A-C4A	2.09	105.25	101.87
26	G	610	CLA	CAA-C2A-C1A	2.09	118.84	111.97
28	R	622	XAT	C20-C13-C12	2.09	121.44	118.10
28	r	622	XAT	C20-C13-C12	2.09	121.44	118.10
26	g	604	CLA	CHB-C4A-NA	2.10	127.41	124.51
31	d	404	BCR	C38-C26-C27	2.10	117.43	113.45
26	G	603	CLA	O2D-CGD-CBD	2.10	115.04	111.30
31	D	404	BCR	C38-C26-C27	2.10	117.43	113.45
31	B	618	BCR	C33-C5-C4	2.10	117.43	113.45
25	g	607	CHL	C1-O2A-CGA	2.10	121.80	116.77
25	1	607	CHL	CHB-C1B-C2B	2.10	122.80	116.99
26	Y	602	CLA	C4A-NA-C1A	2.10	109.06	106.45
25	3	609	CHL	C4-C3-C5	2.10	118.93	115.29
25	7	609	CHL	C4-C3-C5	2.10	118.93	115.29
26	1	602	CLA	CAC-C3C-C4C	2.10	127.79	124.83
26	s	612	CLA	C4A-NA-C1A	2.10	109.06	106.45
26	b	617	CLA	C3A-C2A-C1A	2.10	104.48	101.34
35	A	408	PHO	CHB-C4A-NA	2.10	128.58	124.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	609	CLA	CMD-C2D-C3D	2.10	128.79	124.89
26	n	614	CLA	CMD-C2D-C3D	2.10	128.80	124.89
28	R	622	XAT	C38-C25-C24	2.10	116.69	114.28
26	B	612	CLA	C1D-CHD-C4C	2.10	125.36	122.48
25	G	601	CHL	C1-O2A-CGA	2.10	121.82	116.77
25	N	608	CHL	C4D-C3D-CAD	2.11	109.60	104.71
25	n	608	CHL	C4D-C3D-CAD	2.11	109.60	104.71
26	6	602	CLA	CHB-C4A-NA	2.11	127.42	124.51
25	s	606	CHL	CHB-C1B-C2B	2.11	122.82	116.99
26	g	610	CLA	CAA-C2A-C1A	2.11	118.88	111.97
25	S	606	CHL	CHB-C1B-C2B	2.11	122.83	116.99
26	r	609	CLA	C2C-C1C-NC	2.11	111.67	110.22
25	6	601	CHL	CHB-C1B-C2B	2.11	122.83	116.99
26	Y	611	CLA	O1D-CGD-CBD	2.11	128.39	124.60
26	N	603	CLA	O2D-CGD-CBD	2.11	115.07	111.30
26	G	602	CLA	CMD-C2D-C3D	2.11	128.81	124.89
26	N	604	CLA	CHB-C4A-NA	2.11	127.43	124.51
26	R	603	CLA	C4A-NA-C1A	2.11	109.08	106.45
25	4	608	CHL	C4D-C3D-CAD	2.11	109.62	104.71
25	G	607	CHL	C1-O2A-CGA	2.12	121.85	116.77
26	g	603	CLA	O2D-CGD-CBD	2.12	115.08	111.30
26	r	603	CLA	C4A-NA-C1A	2.12	109.08	106.45
26	S	612	CLA	C4A-NA-C1A	2.12	109.08	106.45
25	7	608	CHL	C4D-C3D-CAD	2.12	109.63	104.71
31	b	620	BCR	C37-C22-C23	2.12	121.48	118.10
25	G	601	CHL	CED-O2D-CGD	2.12	120.94	115.97
26	y	602	CLA	C4A-NA-C1A	2.12	109.09	106.45
26	B	605	CLA	O2D-CGD-CBD	2.12	115.09	111.30
28	r	622	XAT	C38-C25-C24	2.12	116.71	114.28
25	g	601	CHL	CHB-C1B-C2B	2.12	122.87	116.99
25	5	606	CHL	CHB-C1B-C2B	2.12	122.87	116.99
26	C	502	CLA	O2D-CGD-CBD	2.12	115.09	111.30
26	c	502	CLA	O2D-CGD-CBD	2.12	115.09	111.30
26	s	602	CLA	O1D-CGD-CBD	2.12	128.42	124.60
26	R	616	CLA	CMB-C2B-C3B	2.13	128.84	124.89
26	5	602	CLA	CAC-C3C-C4C	2.13	127.83	124.83
25	8	608	CHL	C4D-C3D-CAD	2.13	109.65	104.71
25	G	601	CHL	CHB-C1B-C2B	2.13	122.88	116.99
26	b	605	CLA	O2D-CGD-CBD	2.13	115.10	111.30
27	3	1621	LUT	C1-C2-C3	2.13	118.01	113.40
25	1	606	CHL	CHB-C1B-C2B	2.13	122.89	116.99
26	G	604	CLA	CHB-C4A-NA	2.13	127.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	613	CLA	CMD-C2D-C3D	2.13	128.85	124.89
25	Y	608	CHL	C4D-C3D-CAD	2.13	109.67	104.71
25	3	608	CHL	C4D-C3D-CAD	2.13	109.67	104.71
26	Y	611	CLA	C2A-C1A-CHA	2.13	127.70	123.92
26	A	405	CLA	CBC-CAC-C3C	2.14	118.48	112.41
31	B	620	BCR	C37-C22-C23	2.14	121.50	118.10
26	a	405	CLA	CBC-CAC-C3C	2.14	118.48	112.41
26	n	603	CLA	O2D-CGD-CBD	2.14	115.12	111.30
25	g	601	CHL	CED-O2D-CGD	2.14	120.98	115.97
25	R	608	CHL	C4-C3-C5	2.14	119.00	115.29
29	y	1623	NEX	C28-C29-C30	2.14	122.22	118.94
25	4	606	CHL	C4D-C3D-CAD	2.14	109.68	104.71
26	S	610	CLA	O2D-CGD-CBD	2.14	115.12	111.30
26	y	611	CLA	C2A-C1A-CHA	2.14	127.71	123.92
26	a	405	CLA	O2D-CGD-CBD	2.14	115.12	111.30
26	y	612	CLA	C4A-NA-C1A	2.14	109.11	106.45
28	4	622	XAT	C39-C29-C28	2.14	121.51	118.10
26	s	610	CLA	O2D-CGD-CBD	2.15	115.13	111.30
28	n	1622	XAT	C40-C33-C32	2.15	121.52	118.10
26	5	604	CLA	CHB-C4A-NA	2.15	127.48	124.51
26	S	602	CLA	O1D-CGD-CBD	2.15	128.46	124.60
25	y	608	CHL	C4D-C3D-CAD	2.15	109.70	104.71
25	n	606	CHL	CHC-C4B-C3B	2.15	123.31	118.23
25	N	606	CHL	CHB-C1B-C2B	2.15	122.94	116.99
27	7	1621	LUT	C1-C2-C3	2.15	118.05	113.40
29	Y	1623	NEX	C28-C29-C30	2.15	122.24	118.94
26	B	607	CLA	CAC-C3C-C4C	2.15	127.86	124.83
26	R	616	CLA	C4A-NA-C1A	2.15	109.12	106.45
26	N	612	CLA	C2A-C1A-CHA	2.15	127.73	123.92
26	Y	612	CLA	C4A-NA-C1A	2.15	109.12	106.45
26	g	602	CLA	CMD-C2D-C3D	2.15	128.88	124.89
26	r	616	CLA	CMB-C2B-C3B	2.15	128.88	124.89
26	R	609	CLA	C2C-C1C-NC	2.15	111.70	110.22
25	N	606	CHL	CHC-C4B-C3B	2.15	123.33	118.23
26	A	405	CLA	O2D-CGD-CBD	2.15	115.14	111.30
25	r	608	CHL	C4-C3-C5	2.16	119.03	115.29
31	c	516	BCR	C34-C9-C8	2.16	121.53	118.10
26	7	614	CLA	CMB-C2B-C3B	2.16	128.90	124.89
25	n	606	CHL	CHB-C1B-C2B	2.16	122.97	116.99
26	b	607	CLA	CAC-C3C-C4C	2.16	127.88	124.83
26	c	509	CLA	CGD-CBD-CAD	2.16	117.95	110.71
26	C	509	CLA	CGD-CBD-CAD	2.16	117.96	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	8	622	XAT	C39-C29-C28	2.16	121.54	118.10
25	1	605	CHL	C4D-C3D-CAD	2.16	109.73	104.71
26	N	613	CLA	CMD-C2D-C3D	2.16	128.91	124.89
26	y	603	CLA	C2A-C1A-CHA	2.17	127.76	123.92
25	8	606	CHL	C4D-C3D-CAD	2.17	109.74	104.71
39	B	626	DGD	C1E-O6E-C5E	2.17	117.80	113.72
26	n	612	CLA	C2A-C1A-CHA	2.17	127.76	123.92
26	C	503	CLA	O1D-CGD-CBD	2.17	128.50	124.60
26	Y	603	CLA	C2A-C1A-CHA	2.17	127.76	123.92
39	h	102	DGD	O6E-C5E-C4E	2.17	113.66	109.66
31	C	516	BCR	C34-C9-C8	2.17	121.56	118.10
26	1	604	CLA	CHB-C4A-NA	2.17	127.51	124.51
28	N	1622	XAT	C40-C33-C32	2.17	121.56	118.10
39	H	102	DGD	O6E-C5E-C4E	2.17	113.66	109.66
26	b	608	CLA	CMC-C2C-C3C	2.17	132.11	126.09
26	C	508	CLA	CMC-C2C-C3C	2.17	132.11	126.09
26	1	611	CLA	CHB-C4A-NA	2.18	127.52	124.51
26	5	611	CLA	CHB-C4A-NA	2.18	127.52	124.51
25	5	605	CHL	C4D-C3D-CAD	2.18	109.76	104.71
35	A	408	PHO	CMC-C2C-C3C	2.18	132.11	126.09
26	c	508	CLA	CMC-C2C-C3C	2.18	132.12	126.09
26	r	616	CLA	C4A-NA-C1A	2.18	109.16	106.45
26	y	603	CLA	C1D-CHD-C4C	2.18	125.46	122.48
26	d	402	CLA	CAC-C3C-C4C	2.18	127.90	124.83
30	L	101	LHG	O8-C23-C24	2.18	118.24	111.90
26	G	604	CLA	CMD-C2D-C3D	2.18	128.94	124.89
27	5	1621	LUT	C39-C29-C28	2.18	121.57	118.10
35	a	408	PHO	CMC-C2C-C3C	2.18	132.12	126.09
26	8	603	CLA	C4A-NA-C1A	2.18	109.16	106.45
25	7	608	CHL	CHB-C1B-C2B	2.18	123.03	116.99
26	s	603	CLA	O1D-CGD-CBD	2.18	128.52	124.60
26	Y	611	CLA	CMB-C2B-C3B	2.18	128.94	124.89
28	8	622	XAT	C20-C13-C12	2.18	121.58	118.10
25	3	608	CHL	CHB-C1B-C2B	2.18	123.03	116.99
39	b	626	DGD	C1E-O6E-C5E	2.18	117.83	113.72
26	c	513	CLA	O2D-CGD-CBD	2.18	115.20	111.30
25	S	601	CHL	C4D-C3D-CAD	2.18	109.78	104.71
26	Y	603	CLA	C1D-CHD-C4C	2.19	125.47	122.48
28	5	1622	XAT	C19-C9-C8	2.19	121.58	118.10
26	3	614	CLA	CMB-C2B-C3B	2.19	128.95	124.89
26	D	402	CLA	CAC-C3C-C4C	2.19	127.92	124.83
25	g	609	CHL	O2A-CGA-CBA	2.19	118.27	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	608	CLA	CMC-C2C-C3C	2.19	132.15	126.09
25	s	601	CHL	C4D-C3D-CAD	2.19	109.80	104.71
26	b	616	CLA	O2D-CGD-CBD	2.19	115.21	111.30
38	d	405	PL9	C20-C19-C21	2.19	119.09	115.29
26	g	604	CLA	CMD-C2D-C3D	2.19	128.96	124.89
25	g	607	CHL	C4D-C3D-CAD	2.19	109.80	104.71
26	C	513	CLA	O2D-CGD-CBD	2.19	115.22	111.30
26	S	603	CLA	O1D-CGD-CBD	2.19	128.54	124.60
25	G	609	CHL	O2A-CGA-CBA	2.19	118.28	111.90
26	4	604	CLA	CMD-C2D-C3D	2.19	128.96	124.89
26	C	511	CLA	C1D-CHD-C4C	2.19	125.48	122.48
26	3	610	CLA	CHB-C4A-NA	2.19	127.55	124.51
25	N	606	CHL	C4D-C3D-CAD	2.19	109.81	104.71
25	n	606	CHL	C4D-C3D-CAD	2.19	109.81	104.71
38	D	405	PL9	C20-C19-C21	2.19	119.09	115.29
25	G	607	CHL	C4D-C3D-CAD	2.19	109.81	104.71
25	s	607	CHL	C4D-C3D-CAD	2.20	109.81	104.71
27	1	1621	LUT	C39-C29-C28	2.20	121.60	118.10
27	R	620	LUT	C2-C3-C4	2.20	113.35	110.32
28	4	622	XAT	C20-C13-C12	2.20	121.60	118.10
30	l	101	LHG	O8-C23-C24	2.20	118.29	111.90
26	c	511	CLA	C1D-CHD-C4C	2.20	125.49	122.48
26	c	503	CLA	O1D-CGD-CBD	2.20	128.55	124.60
26	y	611	CLA	CMB-C2B-C3B	2.20	128.97	124.89
27	5	1621	LUT	C19-C9-C8	2.20	121.60	118.10
25	r	607	CHL	CED-O2D-CGD	2.20	121.12	115.97
26	B	616	CLA	O2D-CGD-CBD	2.20	115.23	111.30
25	N	601	CHL	CHB-C1B-C2B	2.20	123.08	116.99
25	y	601	CHL	CHB-C1B-C2B	2.20	123.09	116.99
25	S	607	CHL	C4D-C3D-CAD	2.20	109.83	104.71
25	y	607	CHL	C4D-C3D-CAD	2.20	109.83	104.71
28	n	1622	XAT	C28-C29-C30	2.20	122.32	118.94
26	G	603	CLA	CMD-C2D-C3D	2.20	128.98	124.89
26	4	603	CLA	C4A-NA-C1A	2.21	109.19	106.45
25	n	601	CHL	CHB-C1B-C2B	2.21	123.10	116.99
26	8	604	CLA	CMD-C2D-C3D	2.21	128.99	124.89
26	g	614	CLA	O2D-CGD-CBD	2.21	115.24	111.30
27	n	1620	LUT	C17-C1-C6	2.21	113.89	110.31
26	y	614	CLA	C4A-NA-C1A	2.21	109.19	106.45
27	N	1620	LUT	C17-C1-C6	2.21	113.89	110.31
26	Y	614	CLA	C4A-NA-C1A	2.21	109.19	106.45
28	1	1622	XAT	C19-C9-C8	2.21	121.62	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	601	CHL	CHB-C1B-C2B	2.21	123.11	116.99
26	G	604	CLA	C1D-CHD-C4C	2.21	125.51	122.48
28	G	1622	XAT	C18-C5-C4	2.21	116.81	114.28
36	B	623	SQD	O5-C5-C4	2.21	113.73	109.66
36	b	623	SQD	O5-C5-C4	2.21	113.73	109.66
25	Y	607	CHL	C4D-C3D-CAD	2.21	109.85	104.71
25	g	609	CHL	C4D-C3D-CAD	2.21	109.85	104.71
27	r	620	LUT	C2-C3-C4	2.21	113.38	110.32
26	y	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	Y	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	g	603	CLA	CMD-C2D-C3D	2.22	129.01	124.89
26	7	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
31	4	623	BCR	C38-C26-C27	2.22	117.66	113.45
25	R	607	CHL	CED-O2D-CGD	2.22	121.17	115.97
26	G	614	CLA	O2D-CGD-CBD	2.22	115.27	111.30
27	1	1621	LUT	C19-C9-C8	2.22	121.64	118.10
26	Y	612	CLA	OBD-CAD-C3D	2.22	132.12	128.03
25	G	609	CHL	C4D-C3D-CAD	2.22	109.88	104.71
25	r	606	CHL	C4D-C3D-CAD	2.22	109.88	104.71
36	b	621	SQD	O48-C23-C24	2.22	118.37	111.90
25	2	609	CHL	C4D-C3D-CAD	2.22	109.88	104.71
25	R	606	CHL	C4D-C3D-CAD	2.23	109.88	104.71
36	B	621	SQD	O48-C23-C24	2.23	118.38	111.90
26	s	604	CLA	CMD-C2D-C3D	2.23	129.02	124.89
26	y	602	CLA	CAC-C3C-C4C	2.23	127.97	124.83
28	N	1622	XAT	C28-C29-C30	2.23	122.36	118.94
27	G	1621	LUT	C19-C9-C8	2.23	121.65	118.10
26	B	611	CLA	O2D-CGD-CBD	2.23	115.28	111.30
26	3	603	CLA	C4A-NA-C1A	2.23	109.22	106.45
26	3	610	CLA	CMD-C2D-C3D	2.23	129.03	124.89
26	y	612	CLA	OBD-CAD-C3D	2.23	132.14	128.03
27	g	1621	LUT	C19-C9-C8	2.23	121.66	118.10
28	g	1622	XAT	C18-C5-C4	2.23	116.84	114.28
26	b	611	CLA	O2D-CGD-CBD	2.23	115.29	111.30
25	Y	606	CHL	C4D-C3D-CAD	2.24	109.90	104.71
25	1	609	CHL	CHC-C4B-C3B	2.24	123.53	118.23
26	7	610	CLA	CMD-C2D-C3D	2.24	129.04	124.89
25	s	607	CHL	CHB-C1B-C2B	2.24	123.19	116.99
31	8	623	BCR	C38-C26-C27	2.24	117.70	113.45
26	7	603	CLA	C4A-NA-C1A	2.24	109.23	106.45
27	N	1620	LUT	C19-C9-C8	2.24	121.67	118.10
27	n	1620	LUT	C19-C9-C8	2.24	121.67	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	601	CHL	C4D-C3D-CAD	2.24	109.92	104.71
26	R	616	CLA	CMD-C2D-C3D	2.24	129.05	124.89
25	8	607	CHL	C4D-C3D-CAD	2.24	109.92	104.71
25	S	607	CHL	CHB-C1B-C2B	2.24	123.20	116.99
26	Y	602	CLA	CAC-C3C-C4C	2.24	127.99	124.83
26	c	501	CLA	CMB-C2B-C3B	2.24	129.06	124.89
26	Y	611	CLA	O2D-CGD-CBD	2.25	115.31	111.30
25	N	601	CHL	C4D-C3D-CAD	2.25	109.93	104.71
25	y	606	CHL	C4D-C3D-CAD	2.25	109.93	104.71
25	3	606	CHL	C4D-C3D-CAD	2.25	109.93	104.71
26	y	611	CLA	O2D-CGD-CBD	2.25	115.31	111.30
26	r	603	CLA	C1D-CHD-C4C	2.25	125.56	122.48
39	C	520	DGD	C1E-O6E-C5E	2.25	117.95	113.72
39	c	520	DGD	C1E-O6E-C5E	2.25	117.95	113.72
26	S	604	CLA	CMD-C2D-C3D	2.25	129.07	124.89
26	N	614	CLA	C4A-NA-C1A	2.25	109.25	106.45
25	7	606	CHL	C4D-C3D-CAD	2.25	109.94	104.71
25	5	609	CHL	CHC-C4B-C3B	2.25	123.56	118.23
26	g	604	CLA	C1D-CHD-C4C	2.25	125.56	122.48
25	4	607	CHL	C4D-C3D-CAD	2.25	109.94	104.71
26	g	610	CLA	CHB-C4A-NA	2.25	127.63	124.51
31	D	404	BCR	C35-C13-C12	2.25	121.69	118.10
31	d	404	BCR	C35-C13-C12	2.25	121.69	118.10
26	G	611	CLA	O2D-CGD-CBD	2.25	115.33	111.30
26	R	603	CLA	C1D-CHD-C4C	2.25	125.57	122.48
25	6	609	CHL	C4D-C3D-CAD	2.26	109.95	104.71
26	A	406	CLA	C1C-NC-C4C	2.26	108.35	107.06
25	Y	601	CHL	O2A-CGA-CBA	2.26	118.47	111.90
28	4	622	XAT	C19-C9-C8	2.26	121.70	118.10
25	N	607	CHL	CHC-C4B-C3B	2.26	123.59	118.23
28	8	622	XAT	C19-C9-C8	2.27	121.71	118.10
26	C	501	CLA	CMB-C2B-C3B	2.27	129.10	124.89
27	7	1620	LUT	C20-C13-C12	2.27	121.71	118.10
26	c	512	CLA	C4A-NA-C1A	2.27	109.27	106.45
26	r	616	CLA	CMD-C2D-C3D	2.27	129.10	124.89
25	G	609	CHL	OMC-CMC-C2C	2.27	127.18	124.29
25	2	605	CHL	C4D-C3D-CAD	2.27	109.98	104.71
31	c	515	BCR	C36-C18-C19	2.27	121.71	118.10
31	C	515	BCR	C36-C18-C19	2.27	121.71	118.10
26	n	610	CLA	CHB-C4A-NA	2.27	127.65	124.51
26	g	611	CLA	O2D-CGD-CBD	2.27	115.35	111.30
25	1	606	CHL	CED-O2D-CGD	2.27	121.29	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	610	CLA	C1D-CHD-C4C	2.27	125.59	122.48
26	r	611	CLA	O1D-CGD-CBD	2.27	128.68	124.60
26	R	611	CLA	O1D-CGD-CBD	2.27	128.68	124.60
26	b	605	CLA	C4A-NA-C1A	2.27	109.27	106.45
26	B	605	CLA	C4A-NA-C1A	2.27	109.27	106.45
36	a	418	SQD	O48-C23-C24	2.27	118.52	111.90
26	7	612	CLA	OBD-CAD-C3D	2.28	132.22	128.03
36	A	418	SQD	O48-C23-C24	2.28	118.52	111.90
26	3	612	CLA	OBD-CAD-C3D	2.28	132.22	128.03
25	g	609	CHL	OMC-CMC-C2C	2.28	127.19	124.29
26	C	505	CLA	CHB-C4A-NA	2.28	127.66	124.51
25	y	601	CHL	O2A-CGA-CBA	2.28	118.52	111.90
26	s	613	CLA	CMD-C2D-C3D	2.28	129.12	124.89
25	6	605	CHL	C4D-C3D-CAD	2.28	110.00	104.71
26	C	512	CLA	C4A-NA-C1A	2.28	109.28	106.45
25	n	607	CHL	CHC-C4B-C3B	2.28	123.63	118.23
31	4	623	BCR	C37-C22-C23	2.28	121.73	118.10
25	g	605	CHL	C4D-C3D-CAD	2.28	110.01	104.71
26	r	604	CLA	C4A-NA-C1A	2.28	109.28	106.45
26	R	604	CLA	C4A-NA-C1A	2.28	109.28	106.45
26	c	508	CLA	C4A-NA-C1A	2.28	109.28	106.45
26	S	613	CLA	CMD-C2D-C3D	2.28	129.13	124.89
27	5	1620	LUT	C19-C9-C8	2.28	121.73	118.10
26	n	610	CLA	C1D-CHD-C4C	2.28	125.60	122.48
26	G	610	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	6	610	CLA	CMD-C2D-C3D	2.29	129.13	124.89
25	2	607	CHL	C4D-C3D-CAD	2.29	110.02	104.71
27	1	1620	LUT	C19-C9-C8	2.29	121.74	118.10
26	3	602	CLA	O2D-CGD-CBD	2.29	115.38	111.30
25	G	605	CHL	C4D-C3D-CAD	2.29	110.03	104.71
26	c	503	CLA	CMD-C2D-C3D	2.29	129.14	124.89
26	N	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	n	614	CLA	C4A-NA-C1A	2.29	109.29	106.45
27	g	1621	LUT	C1-C2-C3	2.29	118.35	113.40
26	N	611	CLA	CMB-C2B-C3B	2.29	129.14	124.89
26	n	611	CLA	CMB-C2B-C3B	2.29	129.14	124.89
26	C	508	CLA	C4A-NA-C1A	2.29	109.30	106.45
25	5	606	CHL	CED-O2D-CGD	2.29	121.34	115.97
26	2	610	CLA	CMD-C2D-C3D	2.29	129.14	124.89
25	S	606	CHL	C4D-C3D-CAD	2.29	110.03	104.71
25	5	607	CHL	C4-C3-C5	2.29	119.27	115.29
25	s	606	CHL	C4D-C3D-CAD	2.29	110.04	104.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	607	CHL	C4D-C3D-CAD	2.29	110.04	104.71
26	G	603	CLA	C1C-NC-C4C	2.29	108.38	107.06
31	A	411	BCR	C37-C22-C23	2.29	121.75	118.10
27	3	1620	LUT	C20-C13-C12	2.30	121.76	118.10
27	G	1621	LUT	C1-C2-C3	2.30	118.37	113.40
29	R	623	NEX	C28-C29-C30	2.30	122.47	118.94
25	1	607	CHL	C4-C3-C5	2.30	119.27	115.29
29	3	1623	NEX	C12-C13-C14	2.30	122.47	118.94
26	c	505	CLA	CHB-C4A-NA	2.30	127.69	124.51
26	3	602	CLA	CMD-C2D-C3D	2.30	129.16	124.89
26	6	611	CLA	C4A-NA-C1A	2.30	109.31	106.45
26	B	607	CLA	C4A-NA-C1A	2.30	109.31	106.45
31	8	623	BCR	C37-C22-C23	2.30	121.76	118.10
26	Y	610	CLA	CMD-C2D-C3D	2.30	129.16	124.89
26	7	602	CLA	O2D-CGD-CBD	2.30	115.41	111.30
25	g	608	CHL	C4D-C3D-CAD	2.30	110.06	104.71
25	G	607	CHL	CED-O2D-CGD	2.30	121.37	115.97
25	6	608	CHL	C4D-C3D-CAD	2.30	110.06	104.71
26	c	503	CLA	C1D-CHD-C4C	2.31	125.64	122.48
26	a	407	CLA	C4A-NA-C1A	2.31	109.31	106.45
26	B	605	CLA	C2A-C3A-C4A	2.31	105.59	101.87
25	3	605	CHL	C4D-C3D-CAD	2.31	110.07	104.71
25	y	606	CHL	CHC-C4B-C3B	2.31	123.70	118.23
27	8	620	LUT	C39-C29-C28	2.31	121.78	118.10
26	2	611	CLA	C4A-NA-C1A	2.31	109.32	106.45
25	Y	606	CHL	CHC-C4B-C3B	2.31	123.70	118.23
26	C	503	CLA	CMD-C2D-C3D	2.31	129.18	124.89
25	5	609	CHL	C4D-C3D-CAD	2.31	110.08	104.71
26	r	603	CLA	O1D-CGD-CBD	2.31	128.75	124.60
26	R	603	CLA	O1D-CGD-CBD	2.31	128.75	124.60
26	Y	614	CLA	CMD-C2D-C3D	2.31	129.18	124.89
25	2	608	CHL	C4D-C3D-CAD	2.31	110.08	104.71
29	7	1623	NEX	C12-C13-C14	2.31	122.49	118.94
27	g	1621	LUT	C39-C29-C28	2.31	121.78	118.10
26	5	603	CLA	C4A-NA-C1A	2.31	109.32	106.45
26	1	603	CLA	C4A-NA-C1A	2.31	109.32	106.45
26	7	602	CLA	CMD-C2D-C3D	2.31	129.19	124.89
26	a	406	CLA	C1C-NC-C4C	2.31	108.39	107.06
27	G	1621	LUT	C39-C29-C28	2.31	121.79	118.10
26	n	603	CLA	C4A-NA-C1A	2.31	109.33	106.45
29	r	623	NEX	C28-C29-C30	2.31	122.49	118.94
25	n	605	CHL	CHB-C1B-C2B	2.32	123.41	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	608	CHL	C4D-C3D-CAD	2.32	110.09	104.71
26	N	604	CLA	O1D-CGD-CBD	2.32	128.76	124.60
27	4	620	LUT	C39-C29-C28	2.32	121.79	118.10
26	r	604	CLA	CMD-C2D-C3D	2.32	129.19	124.89
26	b	611	CLA	C3A-C2A-C1A	2.32	104.81	101.34
25	l	605	CHL	CHC-C4B-C3B	2.32	123.72	118.23
26	c	512	CLA	CHB-C4A-NA	2.32	127.72	124.51
26	B	616	CLA	CMD-C2D-C3D	2.32	129.20	124.89
26	y	610	CLA	CMD-C2D-C3D	2.32	129.20	124.89
26	c	513	CLA	O2A-CGA-CBA	2.32	118.65	111.90
26	S	604	CLA	C2A-C1A-CHA	2.32	128.03	123.92
26	n	604	CLA	O1D-CGD-CBD	2.32	128.77	124.60
26	b	615	CLA	C4A-NA-C1A	2.32	109.33	106.45
31	a	411	BCR	C37-C22-C23	2.32	121.80	118.10
25	2	606	CHL	C4D-C3D-CAD	2.32	110.10	104.71
26	g	603	CLA	C1C-NC-C4C	2.32	108.39	107.06
26	B	611	CLA	C3A-C2A-C1A	2.32	104.82	101.34
26	y	614	CLA	CMD-C2D-C3D	2.32	129.21	124.89
26	s	613	CLA	C4A-NA-C1A	2.32	109.34	106.45
25	g	607	CHL	CED-O2D-CGD	2.32	121.42	115.97
25	5	605	CHL	CHC-C4B-C3B	2.33	123.74	118.23
26	B	615	CLA	C4A-NA-C1A	2.33	109.34	106.45
26	B	614	CLA	O1D-CGD-CBD	2.33	128.78	124.60
26	s	602	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	S	613	CLA	C4A-NA-C1A	2.33	109.34	106.45
25	l	609	CHL	C4D-C3D-CAD	2.33	110.12	104.71
25	N	605	CHL	CHB-C1B-C2B	2.33	123.44	116.99
25	G	608	CHL	CMD-C2D-C3D	2.33	120.16	114.27
26	b	616	CLA	CMD-C2D-C3D	2.33	129.21	124.89
25	s	608	CHL	C4D-C3D-CAD	2.33	110.12	104.71
25	l	607	CHL	C4D-C3D-CAD	2.33	110.12	104.71
27	7	1620	LUT	C39-C29-C28	2.33	121.81	118.10
25	3	608	CHL	CHC-C4B-C3B	2.33	123.75	118.23
28	n	1622	XAT	C18-C5-C4	2.33	116.95	114.28
26	R	604	CLA	CMD-C2D-C3D	2.33	129.22	124.89
26	C	503	CLA	C1D-CHD-C4C	2.33	125.67	122.48
26	b	605	CLA	C2A-C3A-C4A	2.33	105.63	101.87
26	5	612	CLA	C2A-C1A-CHA	2.33	128.05	123.92
26	l	612	CLA	C2A-C1A-CHA	2.33	128.05	123.92
26	b	607	CLA	C4A-NA-C1A	2.33	109.35	106.45
25	g	608	CHL	CMD-C2D-C3D	2.33	120.17	114.27
26	C	512	CLA	CHB-C4A-NA	2.33	127.74	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	601	CHL	O2A-CGA-CBA	2.33	118.69	111.90
27	n	1621	LUT	C19-C9-C8	2.33	121.81	118.10
25	6	606	CHL	C4D-C3D-CAD	2.33	110.13	104.71
25	r	614	CHL	C4D-C3D-CAD	2.33	110.13	104.71
25	R	614	CHL	C4D-C3D-CAD	2.33	110.13	104.71
26	C	513	CLA	O2A-CGA-CBA	2.33	118.69	111.90
26	N	603	CLA	C4A-NA-C1A	2.33	109.35	106.45
26	S	604	CLA	C3A-C2A-C1A	2.33	104.84	101.34
27	3	1620	LUT	C39-C29-C28	2.34	121.82	118.10
25	5	607	CHL	C4D-C3D-CAD	2.34	110.14	104.71
25	7	605	CHL	C4D-C3D-CAD	2.34	110.14	104.71
25	N	601	CHL	O2A-CGA-CBA	2.34	118.70	111.90
38	d	405	PL9	C8-C7-C3	2.34	118.65	111.73
26	C	505	CLA	CMD-C2D-C3D	2.34	129.24	124.89
26	A	407	CLA	C4A-NA-C1A	2.34	109.36	106.45
26	C	513	CLA	C4A-NA-C1A	2.34	109.36	106.45
26	C	503	CLA	C4A-NA-C1A	2.34	109.36	106.45
26	c	503	CLA	C4A-NA-C1A	2.34	109.36	106.45
28	N	1622	XAT	C18-C5-C4	2.35	116.97	114.28
25	S	608	CHL	C4D-C3D-CAD	2.35	110.17	104.71
26	S	602	CLA	CHB-C4A-NA	2.35	127.76	124.51
26	y	613	CLA	C4A-NA-C1A	2.35	109.37	106.45
38	D	405	PL9	C8-C7-C3	2.35	118.68	111.73
26	8	610	CLA	CMD-C2D-C3D	2.35	129.25	124.89
26	b	614	CLA	O1D-CGD-CBD	2.35	128.82	124.60
26	s	604	CLA	C2A-C1A-CHA	2.35	128.09	123.92
26	c	513	CLA	C4A-NA-C1A	2.35	109.37	106.45
25	7	608	CHL	CHC-C4B-C3B	2.35	123.80	118.23
26	n	611	CLA	CMD-C2D-C3D	2.35	129.26	124.89
25	1	601	CHL	CHB-C1B-C2B	2.35	123.51	116.99
26	b	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	Y	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	8	604	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	y	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	4	610	CLA	CMD-C2D-C3D	2.36	129.27	124.89
26	7	614	CLA	CMD-C2D-C3D	2.36	129.27	124.89
26	3	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	7	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
25	S	607	CHL	C4-C3-C5	2.36	119.39	115.29
25	s	607	CHL	C4-C3-C5	2.36	119.39	115.29
25	5	601	CHL	CHB-C1B-C2B	2.36	123.53	116.99
26	d	403	CLA	CMD-C2D-C3D	2.36	129.28	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	516	BCR	C32-C1-C6	2.36	114.14	110.31
31	C	516	BCR	C32-C1-C6	2.36	114.14	110.31
26	s	614	CLA	CHB-C4A-NA	2.36	127.78	124.51
27	N	1621	LUT	C19-C9-C8	2.36	121.86	118.10
25	G	606	CHL	CHC-C4B-C3B	2.36	123.83	118.23
26	c	505	CLA	CMD-C2D-C3D	2.36	129.28	124.89
26	N	611	CLA	CMD-C2D-C3D	2.37	129.28	124.89
26	s	604	CLA	C3A-C2A-C1A	2.37	104.88	101.34
26	B	610	CLA	CHB-C4A-NA	2.37	127.78	124.51
25	g	606	CHL	CHC-C4B-C3B	2.37	123.83	118.23
26	7	611	CLA	C2A-C1A-CHA	2.37	128.11	123.92
26	3	611	CLA	C2A-C1A-CHA	2.37	128.11	123.92
30	n	2630	LHG	O8-C23-C24	2.37	118.78	111.90
25	G	601	CHL	C4D-C3D-CAD	2.37	110.21	104.71
25	g	601	CHL	C4D-C3D-CAD	2.37	110.21	104.71
26	G	614	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	Y	613	CLA	C4A-NA-C1A	2.37	109.39	106.45
25	r	606	CHL	CMD-C2D-C3D	2.37	120.27	114.27
26	y	604	CLA	C4A-NA-C1A	2.37	109.39	106.45
26	A	407	CLA	O2D-CGD-CBD	2.37	115.53	111.30
27	1	1620	LUT	C39-C29-C28	2.37	121.88	118.10
25	R	606	CHL	CMD-C2D-C3D	2.37	120.28	114.27
30	N	2630	LHG	O8-C23-C24	2.37	118.81	111.90
26	3	614	CLA	CMD-C2D-C3D	2.38	129.30	124.89
29	7	1623	NEX	C28-C29-C30	2.38	122.59	118.94
26	D	403	CLA	CMD-C2D-C3D	2.38	129.30	124.89
27	n	1620	LUT	C39-C29-C28	2.38	121.89	118.10
26	Y	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	R	612	CLA	CMD-C2D-C3D	2.38	129.31	124.89
26	y	612	CLA	CMB-C2B-C3B	2.38	129.31	124.89
26	6	604	CLA	CHB-C4A-NA	2.38	127.80	124.51
26	B	603	CLA	C4A-NA-C1A	2.38	109.41	106.45
25	7	607	CHL	C1-O2A-CGA	2.38	122.48	116.77
25	Y	609	CHL	O2A-CGA-CBA	2.38	118.83	111.90
31	c	516	BCR	C33-C5-C4	2.38	117.97	113.45
26	N	611	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	n	611	CLA	CHB-C4A-NA	2.38	127.81	124.51
28	3	1622	XAT	C19-C9-C8	2.38	121.90	118.10
26	g	614	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	Y	604	CLA	C4A-NA-C1A	2.39	109.41	106.45
25	N	609	CHL	O2A-CGA-CBA	2.39	118.84	111.90
25	3	607	CHL	C1-O2A-CGA	2.39	122.50	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	405	CLA	CMD-C2D-C3D	2.39	129.32	124.89
28	7	1622	XAT	C19-C9-C8	2.39	121.90	118.10
25	5	608	CHL	CHB-C1B-C2B	2.39	123.61	116.99
25	1	608	CHL	CHB-C1B-C2B	2.39	123.61	116.99
27	N	1620	LUT	C39-C29-C28	2.39	121.91	118.10
25	Y	607	CHL	CED-O2D-CGD	2.39	121.57	115.97
25	n	609	CHL	O2A-CGA-CBA	2.39	118.85	111.90
26	a	407	CLA	O2D-CGD-CBD	2.39	115.57	111.30
26	y	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	G	603	CLA	C4A-NA-C1A	2.39	109.42	106.45
25	Y	608	CHL	C4-C3-C5	2.39	119.44	115.29
27	5	1620	LUT	C39-C29-C28	2.39	121.91	118.10
26	r	612	CLA	CMD-C2D-C3D	2.39	129.33	124.89
26	g	613	CLA	C4A-NA-C1A	2.39	109.42	106.45
26	G	613	CLA	C4A-NA-C1A	2.39	109.42	106.45
26	4	604	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	5	608	CHL	C4D-C3D-CAD	2.39	110.27	104.71
25	1	608	CHL	C4D-C3D-CAD	2.39	110.27	104.71
26	S	614	CLA	CHB-C4A-NA	2.39	127.82	124.51
25	y	607	CHL	CED-O2D-CGD	2.39	121.58	115.97
26	C	510	CLA	C1D-CHD-C4C	2.39	125.76	122.48
31	C	516	BCR	C33-C5-C4	2.39	117.99	113.45
29	3	1623	NEX	C28-C29-C30	2.39	122.62	118.94
26	R	611	CLA	C2A-C1A-CHA	2.40	128.16	123.92
26	b	603	CLA	C4A-NA-C1A	2.40	109.43	106.45
26	g	603	CLA	C4A-NA-C1A	2.40	109.43	106.45
25	y	609	CHL	O2A-CGA-CBA	2.40	118.87	111.90
25	4	609	CHL	CHB-C1B-C2B	2.40	123.63	116.99
25	R	607	CHL	C4D-C3D-CAD	2.40	110.28	104.71
25	8	609	CHL	CHB-C1B-C2B	2.40	123.63	116.99
26	r	611	CLA	C2A-C1A-CHA	2.40	128.17	123.92
36	a	418	SQD	O5-C5-C4	2.40	114.08	109.66
35	A	409	PHO	CHB-C1B-NB	2.40	129.35	124.64
26	C	501	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	7	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	r	614	CHL	CHC-C4B-C3B	2.40	123.92	118.23
25	R	614	CHL	CHC-C4B-C3B	2.41	123.93	118.23
25	y	608	CHL	C4-C3-C5	2.41	119.46	115.29
26	2	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	Y	607	CHL	O2A-CGA-CBA	2.41	118.90	111.90
26	d	403	CLA	C4A-NA-C1A	2.41	109.44	106.45
26	c	501	CLA	CHB-C4A-NA	2.41	127.84	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	615	CLA	C4-C3-C5	2.41	119.47	115.29
25	y	607	CHL	O2A-CGA-CBA	2.41	118.91	111.90
25	r	607	CHL	C4D-C3D-CAD	2.41	110.31	104.71
35	a	409	PHO	CHB-C1B-NB	2.41	129.37	124.64
28	G	1622	XAT	C40-C33-C32	2.41	121.94	118.10
26	Y	612	CLA	CMB-C2B-C3B	2.41	129.37	124.89
25	l	609	CHL	C4-C3-C5	2.41	119.47	115.29
26	b	616	CLA	C4A-NA-C1A	2.41	109.45	106.45
26	a	405	CLA	CMD-C2D-C3D	2.41	129.37	124.89
26	r	610	CLA	CMD-C2D-C3D	2.42	129.37	124.89
36	A	418	SQD	O5-C5-C4	2.42	114.11	109.66
26	5	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	y	601	CHL	C4D-C3D-CAD	2.42	110.33	104.71
26	B	616	CLA	C4A-NA-C1A	2.42	109.45	106.45
26	R	610	CLA	CMD-C2D-C3D	2.42	129.38	124.89
27	S	1621	LUT	C39-C29-C28	2.42	121.96	118.10
26	3	614	CLA	CHB-C4A-NA	2.42	127.86	124.51
31	B	619	BCR	C29-C30-C25	2.42	114.27	110.48
26	B	615	CLA	C4-C3-C5	2.42	119.49	115.29
26	l	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
26	c	510	CLA	C1D-CHD-C4C	2.42	125.80	122.48
25	5	609	CHL	C4-C3-C5	2.42	119.49	115.29
26	R	602	CLA	O2D-CGD-CBD	2.43	115.63	111.30
25	5	606	CHL	C4D-C3D-CAD	2.43	110.35	104.71
25	Y	601	CHL	C4D-C3D-CAD	2.43	110.35	104.71
25	N	605	CHL	C4D-C3D-CAD	2.43	110.35	104.71
28	g	1622	XAT	C40-C33-C32	2.43	121.97	118.10
27	s	1621	LUT	C39-C29-C28	2.43	121.97	118.10
26	3	604	CLA	CMD-C2D-C3D	2.43	129.40	124.89
26	7	604	CLA	CMD-C2D-C3D	2.43	129.40	124.89
26	g	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
30	Y	2630	LHG	O8-C23-C24	2.43	118.97	111.90
30	y	2630	LHG	O8-C23-C24	2.43	118.97	111.90
28	6	1622	XAT	C18-C5-C4	2.43	117.06	114.28
28	2	1622	XAT	C18-C5-C4	2.43	117.06	114.28
26	r	602	CLA	O2D-CGD-CBD	2.43	115.64	111.30
38	A	414	PL9	C7-C3-C4	2.43	121.74	118.29
26	b	615	CLA	CHB-C4A-NA	2.43	127.88	124.51
26	B	615	CLA	CHB-C4A-NA	2.43	127.88	124.51
25	n	605	CHL	C4D-C3D-CAD	2.43	110.36	104.71
27	y	1621	LUT	C19-C9-C8	2.44	121.98	118.10
26	R	612	CLA	CHB-C4A-NA	2.44	127.88	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	606	CHL	C4D-C3D-CAD	2.44	110.37	104.71
26	3	611	CLA	C4A-NA-C1A	2.44	109.48	106.45
26	c	509	CLA	CMD-C2D-C3D	2.44	129.41	124.89
36	B	621	SQD	C1-O5-C5	2.44	118.31	113.72
26	D	403	CLA	C4A-NA-C1A	2.44	109.48	106.45
31	b	619	BCR	C29-C30-C25	2.44	114.29	110.48
26	b	607	CLA	O2D-CGD-CBD	2.44	115.66	111.30
36	b	621	SQD	C1-O5-C5	2.44	118.31	113.72
31	b	620	BCR	C29-C30-C25	2.44	114.30	110.48
36	b	621	SQD	C45-O47-C7	2.44	123.65	117.88
26	B	607	CLA	O2D-CGD-CBD	2.44	115.67	111.30
26	c	506	CLA	C4A-NA-C1A	2.44	109.49	106.45
26	C	506	CLA	C4A-NA-C1A	2.44	109.49	106.45
36	B	621	SQD	C45-O47-C7	2.44	123.65	117.88
26	A	410	CLA	C4A-NA-C1A	2.45	109.49	106.45
26	y	603	CLA	O2D-CGD-CBD	2.45	115.67	111.30
26	b	603	CLA	O2D-CGD-CBD	2.45	115.67	111.30
26	Y	603	CLA	O2D-CGD-CBD	2.45	115.67	111.30
26	r	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	1	606	CHL	CHC-C4B-C3B	2.45	124.03	118.23
27	Y	1621	LUT	C19-C9-C8	2.45	122.00	118.10
26	c	510	CLA	C4A-NA-C1A	2.45	109.49	106.45
26	B	603	CLA	O2D-CGD-CBD	2.45	115.68	111.30
35	a	408	PHO	C1B-NB-C4B	2.45	111.38	106.52
35	A	408	PHO	C1B-NB-C4B	2.45	111.38	106.52
25	7	609	CHL	CHB-C1B-C2B	2.46	123.80	116.99
26	7	611	CLA	C4A-NA-C1A	2.46	109.50	106.45
25	3	609	CHL	CHB-C1B-C2B	2.46	123.80	116.99
26	C	509	CLA	CMD-C2D-C3D	2.46	129.46	124.89
30	s	2630	LHG	O8-C23-C24	2.46	119.06	111.90
31	B	620	BCR	C29-C30-C25	2.46	114.32	110.48
26	3	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
26	7	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
26	a	410	CLA	C4A-NA-C1A	2.46	109.51	106.45
26	G	602	CLA	CHB-C4A-NA	2.46	127.92	124.51
30	S	2630	LHG	O8-C23-C24	2.46	119.07	111.90
25	2	609	CHL	C4-C3-C5	2.47	119.57	115.29
38	a	414	PL9	C7-C3-C4	2.47	121.79	118.29
26	C	510	CLA	C4A-NA-C1A	2.47	109.52	106.45
25	5	606	CHL	CHC-C4B-C3B	2.47	124.08	118.23
26	S	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	y	614	CLA	CHB-C4A-NA	2.47	127.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	8	602	CLA	CMD-C2D-C3D	2.47	129.48	124.89
26	S	610	CLA	CMD-C2D-C3D	2.48	129.49	124.89
31	t	101	BCR	C35-C13-C12	2.48	122.05	118.10
26	R	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
26	1	610	CLA	CMD-C2D-C3D	2.48	129.50	124.89
26	Y	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	7	601	CHL	C4D-C3D-CAD	2.48	110.48	104.71
26	Y	603	CLA	C4A-NA-C1A	2.48	109.54	106.45
26	y	603	CLA	C4A-NA-C1A	2.49	109.54	106.45
26	4	602	CLA	CMD-C2D-C3D	2.49	129.51	124.89
25	6	609	CHL	C4-C3-C5	2.49	119.60	115.29
25	4	608	CHL	CHB-C1B-C2B	2.49	123.88	116.99
25	Y	607	CHL	C1-O2A-CGA	2.49	122.74	116.77
26	s	610	CLA	CMD-C2D-C3D	2.49	129.51	124.89
25	S	608	CHL	CMD-C2D-C3D	2.49	120.58	114.27
26	g	604	CLA	O1D-CGD-CBD	2.49	129.08	124.60
25	G	601	CHL	C4-C3-C5	2.49	119.62	115.29
25	R	608	CHL	CMD-C2D-C3D	2.50	120.59	114.27
26	r	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	5	612	CLA	CMD-C2D-C3D	2.50	129.53	124.89
26	1	612	CLA	CMD-C2D-C3D	2.50	129.53	124.89
25	8	608	CHL	CHB-C1B-C2B	2.50	123.91	116.99
25	s	608	CHL	CMD-C2D-C3D	2.50	120.60	114.27
26	s	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	r	608	CHL	CMD-C2D-C3D	2.50	120.60	114.27
25	4	606	CHL	CHB-C1B-C2B	2.50	123.92	116.99
25	y	607	CHL	C1-O2A-CGA	2.50	122.78	116.77
25	g	601	CHL	C4-C3-C5	2.50	119.63	115.29
26	y	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
26	5	610	CLA	CMD-C2D-C3D	2.50	129.54	124.89
25	3	601	CHL	C4D-C3D-CAD	2.50	110.53	104.71
26	N	603	CLA	C1C-NC-C4C	2.51	108.50	107.06
25	N	607	CHL	CHD-C1D-C2D	2.51	123.94	116.99
25	5	601	CHL	C4D-C3D-CAD	2.51	110.54	104.71
25	n	607	CHL	CHD-C1D-C2D	2.51	123.94	116.99
25	G	606	CHL	C4D-C3D-CAD	2.51	110.54	104.71
31	T	101	BCR	C35-C13-C12	2.51	122.10	118.10
25	g	606	CHL	C4D-C3D-CAD	2.51	110.55	104.71
26	2	612	CLA	CMB-C2B-C3B	2.51	129.55	124.89
26	G	604	CLA	O1D-CGD-CBD	2.51	129.12	124.60
25	8	606	CHL	CHB-C1B-C2B	2.51	123.95	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	614	CHL	CMD-C2D-C3D	2.52	120.64	114.27
25	R	614	CHL	CMD-C2D-C3D	2.52	120.65	114.27
26	1	602	CLA	CMD-C2D-C3D	2.52	129.57	124.89
25	6	607	CHL	CHB-C1B-C2B	2.52	123.97	116.99
26	6	612	CLA	CMB-C2B-C3B	2.52	129.57	124.89
26	N	602	CLA	CHB-C4A-NA	2.53	128.00	124.51
26	3	611	CLA	C2C-C1C-NC	2.53	111.96	110.22
25	1	601	CHL	C4D-C3D-CAD	2.53	110.58	104.71
30	r	2630	LHG	O8-C23-C24	2.53	119.26	111.90
25	y	607	CHL	CHC-C4B-C3B	2.53	124.22	118.23
26	8	603	CLA	CMD-C2D-C3D	2.53	129.59	124.89
26	7	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	C	513	CLA	CBA-CAA-C2A	2.53	121.37	113.80
25	2	607	CHL	CHB-C1B-C2B	2.53	124.00	116.99
25	Y	607	CHL	CHC-C4B-C3B	2.53	124.23	118.23
26	7	611	CLA	C2C-C1C-NC	2.53	111.97	110.22
26	n	602	CLA	CHB-C4A-NA	2.53	128.02	124.51
26	n	603	CLA	C1C-NC-C4C	2.53	108.51	107.06
26	6	613	CLA	CHB-C4A-NA	2.54	128.02	124.51
26	c	513	CLA	CBA-CAA-C2A	2.54	121.39	113.80
31	b	618	BCR	C37-C22-C23	2.54	122.14	118.10
25	g	609	CHL	CHC-C4B-C3B	2.54	124.25	118.23
26	5	602	CLA	CMD-C2D-C3D	2.54	129.61	124.89
28	y	1622	XAT	C40-C33-C32	2.54	122.15	118.10
30	R	2630	LHG	O8-C23-C24	2.54	119.30	111.90
26	6	610	CLA	CHB-C4A-NA	2.54	128.03	124.51
26	n	610	CLA	C2A-C1A-CHA	2.55	128.43	123.92
26	B	603	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	4	603	CLA	CMD-C2D-C3D	2.55	129.62	124.89
26	2	610	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	2	613	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	s	607	CHL	CHC-C4B-C3B	2.55	124.26	118.23
25	G	606	CHL	CMD-C2D-C3D	2.55	120.72	114.27
26	2	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
36	B	621	SQD	O8-S-C6	2.55	109.12	106.01
25	G	609	CHL	CHC-C4B-C3B	2.55	124.27	118.23
30	g	2630	LHG	O8-C23-C24	2.55	119.33	111.90
26	y	611	CLA	C4A-NA-C1A	2.55	109.62	106.45
25	S	607	CHL	CHC-C4B-C3B	2.55	124.28	118.23
25	R	607	CHL	CMD-C2D-C3D	2.55	120.73	114.27
25	r	607	CHL	CMD-C2D-C3D	2.55	120.73	114.27
28	Y	1622	XAT	C40-C33-C32	2.55	122.17	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	611	CLA	CMD-C2D-C3D	2.55	129.63	124.89
28	7	1622	XAT	C18-C5-C4	2.56	117.21	114.28
26	1	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	6	614	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	N	608	CHL	C7-C6-C5	2.56	120.22	113.11
26	7	611	CLA	CMD-C2D-C3D	2.56	129.64	124.89
26	5	611	CLA	CMD-C2D-C3D	2.56	129.64	124.89
26	1	603	CLA	CMD-C2D-C3D	2.56	129.64	124.89
26	3	604	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	g	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	G	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	g	606	CHL	CMD-C2D-C3D	2.56	120.74	114.27
31	B	618	BCR	C37-C22-C23	2.56	122.17	118.10
25	n	608	CHL	C7-C6-C5	2.56	120.22	113.11
26	b	603	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	8	611	CLA	CMD-C2D-C3D	2.56	129.64	124.89
30	G	2630	LHG	O8-C23-C24	2.56	119.35	111.90
26	5	603	CLA	CMD-C2D-C3D	2.56	129.65	124.89
26	N	610	CLA	C2A-C1A-CHA	2.56	128.46	123.92
30	B	2631	LHG	O8-C23-C24	2.56	119.36	111.90
31	c	514	BCR	C34-C9-C8	2.56	122.19	118.10
27	R	620	LUT	C19-C9-C8	2.57	122.19	118.10
25	n	607	CHL	O2A-CGA-CBA	2.57	119.36	111.90
39	h	102	DGD	C1E-O6E-C5E	2.57	118.55	113.72
25	2	601	CHL	C4D-C3D-CAD	2.57	110.67	104.71
36	b	621	SQD	O8-S-C6	2.57	109.14	106.01
26	4	611	CLA	CMD-C2D-C3D	2.57	129.66	124.89
25	N	607	CHL	O2A-CGA-CBA	2.57	119.37	111.90
27	r	620	LUT	C20-C13-C12	2.57	122.19	118.10
30	3	2630	LHG	O8-C23-C24	2.57	119.38	111.90
25	G	601	CHL	O2A-CGA-CBA	2.57	119.38	111.90
25	6	601	CHL	C4D-C3D-CAD	2.57	110.68	104.71
28	3	1622	XAT	C18-C5-C4	2.57	117.23	114.28
31	c	516	BCR	C29-C30-C25	2.57	114.50	110.48
26	Y	611	CLA	C4A-NA-C1A	2.57	109.65	106.45
30	b	2631	LHG	O8-C23-C24	2.57	119.39	111.90
27	r	620	LUT	C19-C9-C8	2.57	122.20	118.10
25	g	601	CHL	O2A-CGA-CBA	2.58	119.39	111.90
39	H	102	DGD	C1E-O6E-C5E	2.58	118.57	113.72
30	5	2630	LHG	O8-C23-C24	2.58	119.40	111.90
25	6	605	CHL	CHB-C1B-C2B	2.58	124.13	116.99
25	2	605	CHL	CHB-C1B-C2B	2.58	124.13	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	611	CLA	CMD-C2D-C3D	2.58	129.68	124.89
25	y	605	CHL	O2A-CGA-CBA	2.58	119.40	111.90
25	4	608	CHL	CHC-C4B-C3B	2.58	124.34	118.23
27	R	620	LUT	C20-C13-C12	2.58	122.21	118.10
25	Y	605	CHL	O2A-CGA-CBA	2.58	119.41	111.90
30	1	2630	LHG	O8-C23-C24	2.58	119.41	111.90
27	2	1621	LUT	C39-C29-C28	2.58	122.21	118.10
30	7	2630	LHG	O8-C23-C24	2.58	119.41	111.90
27	6	1621	LUT	C39-C29-C28	2.58	122.22	118.10
26	5	613	CLA	CHB-C4A-NA	2.58	128.09	124.51
36	A	418	SQD	O47-C45-C44	2.58	117.83	108.44
31	C	514	BCR	C34-C9-C8	2.58	122.22	118.10
36	a	418	SQD	O47-C45-C44	2.59	117.83	108.44
26	5	614	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	2	609	CHL	CHC-C4B-C3B	2.59	124.36	118.23
26	r	601	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	b	604	CLA	O2D-CGD-CBD	2.59	115.92	111.30
25	8	608	CHL	CHC-C4B-C3B	2.59	124.37	118.23
26	N	602	CLA	CAC-C3C-C4C	2.59	128.48	124.83
25	6	609	CHL	CHC-C4B-C3B	2.59	124.37	118.23
26	S	603	CLA	CMD-C2D-C3D	2.59	129.71	124.89
26	1	614	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	s	603	CLA	CMD-C2D-C3D	2.60	129.72	124.89
30	C	2630	LHG	O8-C23-C24	2.60	119.47	111.90
30	c	2630	LHG	O8-C23-C24	2.60	119.47	111.90
27	6	1620	LUT	C39-C29-C28	2.60	122.24	118.10
26	c	504	CLA	C4A-NA-C1A	2.60	109.68	106.45
26	B	604	CLA	O2D-CGD-CBD	2.60	115.95	111.30
26	8	603	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	R	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
31	C	516	BCR	C29-C30-C25	2.61	114.55	110.48
26	S	611	CLA	C4A-NA-C1A	2.61	109.69	106.45
27	2	1620	LUT	C39-C29-C28	2.61	122.25	118.10
26	b	602	CLA	CMB-C2B-C3B	2.61	129.73	124.89
26	n	602	CLA	CAC-C3C-C4C	2.61	128.51	124.83
38	A	414	PL9	C8-C7-C3	2.61	119.46	111.73
26	B	602	CLA	CMB-C2B-C3B	2.62	129.75	124.89
26	g	613	CLA	CMD-C2D-C3D	2.62	129.75	124.89
25	6	609	CHL	O2A-CGA-CBA	2.62	119.51	111.90
25	2	609	CHL	O2A-CGA-CBA	2.62	119.52	111.90
26	G	613	CLA	CMD-C2D-C3D	2.62	129.75	124.89
25	3	607	CHL	C4-C3-C5	2.62	119.83	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	607	CHL	CHD-C1D-C2D	2.62	124.25	116.99
26	N	610	CLA	CMD-C2D-C3D	2.62	129.76	124.89
26	n	610	CLA	CMD-C2D-C3D	2.62	129.76	124.89
26	R	612	CLA	CMB-C2B-C3B	2.62	129.76	124.89
27	g	1620	LUT	C39-C29-C28	2.62	122.28	118.10
26	4	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	5	612	CLA	CHB-C4A-NA	2.63	128.14	124.51
25	N	607	CHL	CED-O2D-CGD	2.63	122.13	115.97
26	y	602	CLA	CMD-C2D-C3D	2.63	129.77	124.89
26	R	601	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	7	607	CHL	C4-C3-C5	2.63	119.85	115.29
38	a	414	PL9	C8-C7-C3	2.63	119.51	111.73
26	r	609	CLA	CHB-C4A-NA	2.63	128.15	124.51
26	Y	613	CLA	CMD-C2D-C3D	2.63	129.78	124.89
26	y	613	CLA	CMD-C2D-C3D	2.63	129.78	124.89
27	6	1621	LUT	C19-C9-C8	2.63	122.29	118.10
27	G	1620	LUT	C39-C29-C28	2.63	122.29	118.10
25	y	607	CHL	CHD-C1D-C2D	2.63	124.28	116.99
26	r	611	CLA	C4A-NA-C1A	2.64	109.72	106.45
26	C	504	CLA	C4A-NA-C1A	2.64	109.72	106.45
26	G	602	CLA	CAC-C3C-C4C	2.64	128.55	124.83
26	R	613	CLA	CMB-C2B-C3B	2.64	129.79	124.89
26	r	613	CLA	CMB-C2B-C3B	2.64	129.79	124.89
25	n	607	CHL	CED-O2D-CGD	2.64	122.16	115.97
26	s	611	CLA	C4A-NA-C1A	2.64	109.73	106.45
26	a	406	CLA	C4A-NA-C1A	2.64	109.73	106.45
26	6	611	CLA	CHB-C4A-NA	2.64	128.17	124.51
26	1	612	CLA	CHB-C4A-NA	2.64	128.17	124.51
27	2	1621	LUT	C19-C9-C8	2.64	122.31	118.10
26	D	402	CLA	C1C-NC-C4C	2.64	108.58	107.06
26	d	402	CLA	C1C-NC-C4C	2.64	108.58	107.06
25	5	609	CHL	CMD-C2D-C3D	2.65	120.96	114.27
26	2	611	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	1	607	CHL	O2A-CGA-CBA	2.65	119.61	111.90
25	4	609	CHL	CMD-C2D-C3D	2.65	120.97	114.27
25	8	609	CHL	CMD-C2D-C3D	2.65	120.97	114.27
26	Y	602	CLA	CMD-C2D-C3D	2.65	129.81	124.89
25	G	608	CHL	O2A-CGA-CBA	2.65	119.61	111.90
26	b	614	CLA	C4A-NA-C1A	2.65	109.74	106.45
26	2	611	CLA	CMD-C2D-C3D	2.65	129.81	124.89
26	r	612	CLA	CMB-C2B-C3B	2.65	129.81	124.89
25	g	608	CHL	O2A-CGA-CBA	2.65	119.61	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	607	CHL	CHC-C4B-C3B	2.65	124.51	118.23
26	g	602	CLA	CAC-C3C-C4C	2.66	128.58	124.83
26	B	609	CLA	C4A-NA-C1A	2.66	109.75	106.45
25	1	609	CHL	CMD-C2D-C3D	2.66	120.99	114.27
25	3	609	CHL	CMD-C2D-C3D	2.66	120.99	114.27
26	Y	604	CLA	CMD-C2D-C3D	2.66	129.82	124.89
26	y	604	CLA	CMD-C2D-C3D	2.66	129.82	124.89
25	G	605	CHL	CMD-C2D-C3D	2.66	121.00	114.27
25	5	607	CHL	CHC-C4B-C3B	2.66	124.53	118.23
26	R	611	CLA	C4A-NA-C1A	2.66	109.75	106.45
25	5	607	CHL	O2A-CGA-CBA	2.66	119.64	111.90
26	s	609	CLA	CMB-C2B-C3B	2.66	129.83	124.89
25	Y	609	CHL	CHC-C4B-C3B	2.66	124.54	118.23
26	A	406	CLA	C4A-NA-C1A	2.67	109.76	106.45
26	6	611	CLA	CMD-C2D-C3D	2.67	129.84	124.89
26	7	613	CLA	CMD-C2D-C3D	2.67	129.84	124.89
26	N	614	CLA	CHB-C4A-NA	2.67	128.20	124.51
26	b	612	CLA	C4A-NA-C1A	2.67	109.76	106.45
25	2	606	CHL	CMD-C2D-C3D	2.67	121.02	114.27
26	B	614	CLA	C4A-NA-C1A	2.67	109.76	106.45
26	r	601	CLA	C4A-NA-C1A	2.67	109.77	106.45
25	g	605	CHL	CMD-C2D-C3D	2.67	121.03	114.27
25	7	609	CHL	CMD-C2D-C3D	2.67	121.03	114.27
26	3	613	CLA	CMD-C2D-C3D	2.67	129.85	124.89
26	g	612	CLA	CHB-C4A-NA	2.67	128.21	124.51
27	3	1621	LUT	C19-C9-C8	2.67	122.36	118.10
26	4	604	CLA	CMB-C2B-C3B	2.67	129.85	124.89
28	7	1622	XAT	C40-C33-C32	2.67	122.36	118.10
35	A	408	PHO	C4A-NA-C1A	2.67	110.32	108.16
26	R	602	CLA	C4A-NA-C1A	2.67	109.77	106.45
25	7	607	CHL	CMD-C2D-C3D	2.67	121.04	114.27
26	4	611	CLA	CHB-C4A-NA	2.68	128.21	124.51
26	S	609	CLA	CMB-C2B-C3B	2.68	129.86	124.89
26	8	604	CLA	CMB-C2B-C3B	2.68	129.86	124.89
25	y	609	CHL	CHC-C4B-C3B	2.68	124.57	118.23
26	G	610	CLA	CMD-C2D-C3D	2.68	129.87	124.89
27	7	1621	LUT	C19-C9-C8	2.68	122.37	118.10
26	6	611	CLA	CMB-C2B-C3B	2.68	129.87	124.89
26	N	603	CLA	CMB-C2B-C3B	2.68	129.87	124.89
26	S	611	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	Y	612	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	G	612	CLA	CHB-C4A-NA	2.68	128.22	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	602	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	s	608	CHL	O2D-CGD-CBD	2.68	117.75	111.20
25	G	609	CHL	C4-C3-C5	2.68	119.94	115.29
26	R	610	CLA	O1D-CGD-CBD	2.68	129.42	124.60
26	R	601	CLA	C4A-NA-C1A	2.69	109.78	106.45
26	B	612	CLA	C4A-NA-C1A	2.69	109.78	106.45
26	b	609	CLA	C4A-NA-C1A	2.69	109.79	106.45
25	3	607	CHL	CMD-C2D-C3D	2.69	121.07	114.27
26	C	510	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	y	608	CHL	CMD-C2D-C3D	2.69	121.08	114.27
25	S	607	CHL	O2A-CGA-CBA	2.69	119.72	111.90
25	6	606	CHL	CMD-C2D-C3D	2.69	121.08	114.27
26	B	602	CLA	CHB-C4A-NA	2.69	128.23	124.51
35	A	409	PHO	C1B-NB-C4B	2.69	111.85	106.52
28	3	1622	XAT	C40-C33-C32	2.69	122.39	118.10
25	G	607	CHL	O2A-CGA-CBA	2.69	119.73	111.90
25	g	607	CHL	O2A-CGA-CBA	2.69	119.73	111.90
35	a	408	PHO	C4A-NA-C1A	2.69	110.34	108.16
26	8	611	CLA	CHB-C4A-NA	2.69	128.23	124.51
31	4	623	BCR	C29-C30-C25	2.69	114.69	110.48
25	g	609	CHL	C4-C3-C5	2.69	119.96	115.29
26	s	611	CLA	CHB-C4A-NA	2.69	128.24	124.51
26	7	603	CLA	C2A-C1A-CHA	2.69	128.69	123.92
26	2	611	CLA	CMB-C2B-C3B	2.69	129.89	124.89
25	g	607	CHL	CMD-C2D-C3D	2.69	121.09	114.27
26	n	614	CLA	CHB-C4A-NA	2.70	128.24	124.51
27	6	1620	LUT	C20-C13-C12	2.70	122.39	118.10
31	8	623	BCR	C29-C30-C25	2.70	114.69	110.48
25	r	608	CHL	O2A-CGA-CBA	2.70	119.75	111.90
26	g	610	CLA	CMD-C2D-C3D	2.70	129.90	124.89
26	r	610	CLA	O1D-CGD-CBD	2.70	129.45	124.60
25	S	608	CHL	O2D-CGD-CBD	2.70	117.78	111.20
31	c	515	BCR	C37-C22-C23	2.70	122.40	118.10
31	C	515	BCR	C37-C22-C23	2.70	122.40	118.10
26	C	508	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	s	607	CHL	O2A-CGA-CBA	2.70	119.75	111.90
25	Y	608	CHL	CMD-C2D-C3D	2.70	121.10	114.27
26	r	602	CLA	C4A-NA-C1A	2.70	109.80	106.45
25	y	606	CHL	CHD-C1D-C2D	2.70	124.47	116.99
25	r	608	CHL	CHC-C4B-C3B	2.70	124.63	118.23
26	b	614	CLA	C4-C3-C5	2.70	119.98	115.29
36	A	412	SQD	O48-C23-C24	2.70	119.77	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	612	CLA	CHB-C4A-NA	2.71	128.25	124.51
25	G	607	CHL	CMD-C2D-C3D	2.71	121.12	114.27
25	4	607	CHL	CMD-C2D-C3D	2.71	121.12	114.27
26	n	603	CLA	CMB-C2B-C3B	2.71	129.92	124.89
25	R	608	CHL	O2A-CGA-CBA	2.71	119.78	111.90
26	B	617	CLA	C4A-NA-C1A	2.71	109.81	106.45
25	7	605	CHL	CHB-C1B-C2B	2.71	124.49	116.99
35	a	409	PHO	C1B-NB-C4B	2.71	111.89	106.52
25	3	605	CHL	CHB-C1B-C2B	2.71	124.50	116.99
26	4	602	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	R	602	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	r	602	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	5	604	CLA	CMD-C2D-C3D	2.71	129.92	124.89
26	3	603	CLA	C2A-C1A-CHA	2.71	128.73	123.92
25	Y	606	CHL	CHD-C1D-C2D	2.71	124.51	116.99
26	c	510	CLA	CHB-C4A-NA	2.71	128.27	124.51
26	c	508	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	B	614	CLA	C4-C3-C5	2.72	120.00	115.29
26	R	609	CLA	C4A-NA-C1A	2.72	109.83	106.45
36	a	412	SQD	O48-C23-C24	2.72	119.81	111.90
26	6	604	CLA	CMD-C2D-C3D	2.72	129.94	124.89
25	8	607	CHL	CMD-C2D-C3D	2.72	121.16	114.27
26	b	617	CLA	C4A-NA-C1A	2.72	109.83	106.45
25	R	608	CHL	CHC-C4B-C3B	2.72	124.68	118.23
27	2	1620	LUT	C20-C13-C12	2.72	122.44	118.10
26	b	606	CLA	C4A-NA-C1A	2.72	109.83	106.45
25	6	607	CHL	O2A-CGA-CBA	2.73	119.83	111.90
28	5	1622	XAT	C18-C5-C4	2.73	117.40	114.28
26	r	609	CLA	C4A-NA-C1A	2.73	109.84	106.45
26	1	604	CLA	CMD-C2D-C3D	2.73	129.95	124.89
26	G	611	CLA	C4A-NA-C1A	2.73	109.84	106.45
25	2	607	CHL	CHC-C4B-C3B	2.73	124.69	118.23
26	s	612	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	R	609	CLA	CMD-C2D-C3D	2.73	129.96	124.89
26	y	611	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	y	607	CHL	O2D-CGD-CBD	2.73	117.86	111.20
25	Y	607	CHL	O2D-CGD-CBD	2.73	117.86	111.20
26	R	603	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	C	507	CLA	C2A-C1A-CHA	2.73	128.76	123.92
26	C	507	CLA	CMD-C2D-C3D	2.73	129.96	124.89
25	2	607	CHL	O2A-CGA-CBA	2.73	119.85	111.90
25	N	607	CHL	O2D-CGD-CBD	2.73	117.87	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	513	CLA	CHB-C4A-NA	2.73	128.29	124.51
35	A	409	PHO	O1D-CGD-CBD	2.73	129.51	124.60
30	b	2630	LHG	O8-C23-C24	2.73	119.86	111.90
35	a	409	PHO	C4A-NA-C1A	2.74	110.37	108.16
26	C	509	CLA	C4A-NA-C1A	2.74	109.85	106.45
26	2	604	CLA	CMD-C2D-C3D	2.74	129.97	124.89
26	c	507	CLA	CMD-C2D-C3D	2.74	129.97	124.89
26	7	613	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	Y	611	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	2	608	CHL	CHC-C4B-C3B	2.74	124.72	118.23
28	1	1622	XAT	C18-C5-C4	2.74	117.42	114.28
26	r	609	CLA	CMD-C2D-C3D	2.74	129.97	124.89
26	8	602	CLA	CHB-C4A-NA	2.74	128.30	124.51
29	R	623	NEX	O24-C25-C38	2.74	118.45	115.02
26	3	613	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	S	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
36	a	412	SQD	C3-C4-C5	2.74	115.05	110.22
30	B	2630	LHG	O8-C23-C24	2.74	119.88	111.90
26	c	513	CLA	CHB-C4A-NA	2.74	128.31	124.51
26	r	612	CLA	C4A-NA-C1A	2.74	109.86	106.45
26	c	507	CLA	C2A-C1A-CHA	2.74	128.78	123.92
26	c	501	CLA	O2D-CGD-CBD	2.75	116.20	111.30
26	B	606	CLA	C4A-NA-C1A	2.75	109.86	106.45
26	C	501	CLA	O2D-CGD-CBD	2.75	116.21	111.30
25	6	608	CHL	CHC-C4B-C3B	2.75	124.74	118.23
36	A	412	SQD	C3-C4-C5	2.75	115.06	110.22
26	r	611	CLA	CMB-C2B-C3B	2.75	129.99	124.89
26	6	612	CLA	CHB-C4A-NA	2.75	128.31	124.51
26	g	611	CLA	C4A-NA-C1A	2.75	109.86	106.45
25	n	607	CHL	O2D-CGD-CBD	2.75	117.91	111.20
25	6	607	CHL	CHC-C4B-C3B	2.75	124.75	118.23
26	r	602	CLA	CMD-C2D-C3D	2.75	130.00	124.89
26	B	613	CLA	O2D-CGD-CBD	2.75	116.21	111.30
26	r	601	CLA	CMD-C2D-C3D	2.75	130.00	124.89
26	B	605	CLA	CBA-CAA-C2A	2.75	122.03	113.80
26	c	509	CLA	C4A-NA-C1A	2.75	109.87	106.45
26	3	611	CLA	CHB-C4A-NA	2.75	128.32	124.51
26	d	402	CLA	C1D-CHD-C4C	2.76	126.25	122.48
35	A	409	PHO	C4A-NA-C1A	2.76	110.39	108.16
26	r	603	CLA	CHB-C4A-NA	2.76	128.32	124.51
26	s	603	CLA	C2A-C1A-CHA	2.76	128.81	123.92
25	n	608	CHL	CMD-C2D-C3D	2.76	121.25	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	612	CLA	CMD-C2D-C3D	2.76	130.01	124.89
25	N	608	CHL	CMD-C2D-C3D	2.76	121.25	114.27
35	a	409	PHO	O1D-CGD-CBD	2.76	129.56	124.60
29	r	623	NEX	O24-C25-C38	2.76	118.47	115.02
28	2	1622	XAT	O4-C5-C18	2.76	118.48	115.02
26	S	603	CLA	C2A-C1A-CHA	2.76	128.81	123.92
26	7	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	5	606	CHL	CMD-C2D-C3D	2.76	121.26	114.27
26	R	611	CLA	CMB-C2B-C3B	2.76	130.02	124.89
25	2	606	CHL	CHC-C4B-C3B	2.76	124.78	118.23
26	6	603	CLA	CMB-C2B-C3B	2.77	130.02	124.89
25	3	609	CHL	CHC-C4B-C3B	2.77	124.78	118.23
26	b	613	CLA	O2D-CGD-CBD	2.77	116.24	111.30
26	b	605	CLA	CBA-CAA-C2A	2.77	122.08	113.80
26	R	602	CLA	CMD-C2D-C3D	2.77	130.03	124.89
26	2	603	CLA	CMB-C2B-C3B	2.77	130.03	124.89
26	b	602	CLA	C4A-NA-C1A	2.77	109.89	106.45
26	5	613	CLA	CMD-C2D-C3D	2.77	130.03	124.89
26	b	612	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	D	402	CLA	C1D-CHD-C4C	2.77	126.27	122.48
26	R	612	CLA	C4A-NA-C1A	2.77	109.89	106.45
25	1	606	CHL	CMD-C2D-C3D	2.77	121.29	114.27
25	8	609	CHL	CHC-C4B-C3B	2.78	124.80	118.23
26	1	613	CLA	CMD-C2D-C3D	2.78	130.04	124.89
26	s	603	CLA	C4A-NA-C1A	2.78	109.90	106.45
26	S	603	CLA	C4A-NA-C1A	2.78	109.90	106.45
25	5	607	CHL	CMD-C2D-C3D	2.78	121.30	114.27
26	2	612	CLA	CMD-C2D-C3D	2.78	130.04	124.89
26	R	601	CLA	CMD-C2D-C3D	2.78	130.04	124.89
25	7	609	CHL	CHC-C4B-C3B	2.78	124.81	118.23
26	B	602	CLA	C4A-NA-C1A	2.78	109.90	106.45
25	6	606	CHL	CHC-C4B-C3B	2.78	124.82	118.23
26	N	612	CLA	CHB-C4A-NA	2.78	128.36	124.51
26	n	612	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	1	607	CHL	CMD-C2D-C3D	2.78	121.31	114.27
25	4	609	CHL	CHC-C4B-C3B	2.78	124.82	118.23
26	G	603	CLA	CMB-C2B-C3B	2.78	130.06	124.89
25	R	608	CHL	CHD-C1D-C2D	2.78	124.70	116.99
25	G	609	CHL	CMD-C2D-C3D	2.78	121.32	114.27
25	Y	601	CHL	C1-O2A-CGA	2.79	123.46	116.77
25	g	609	CHL	CMD-C2D-C3D	2.79	121.33	114.27
26	2	612	CLA	CHB-C4A-NA	2.79	128.37	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
26	R	609	CLA	CMB-C2B-C3B	2.79	130.07	124.89
26	Y	612	CLA	CMD-C2D-C3D	2.79	130.07	124.89
26	n	611	CLA	C4A-NA-C1A	2.79	109.92	106.45
25	7	605	CHL	CHC-C4B-C3B	2.79	124.84	118.23
25	y	601	CHL	C1-O2A-CGA	2.79	123.47	116.77
26	6	612	CLA	CMD-C2D-C3D	2.79	130.07	124.89
25	r	608	CHL	CHD-C1D-C2D	2.79	124.73	116.99
28	6	1622	XAT	O4-C5-C18	2.79	118.52	115.02
26	b	609	CLA	C1D-CHD-C4C	2.79	126.31	122.48
26	B	609	CLA	C1D-CHD-C4C	2.79	126.31	122.48
26	g	603	CLA	CMB-C2B-C3B	2.80	130.08	124.89
26	b	606	CLA	O2D-CGD-CBD	2.80	116.29	111.30
26	B	606	CLA	O2D-CGD-CBD	2.80	116.30	111.30
26	N	611	CLA	C4A-NA-C1A	2.80	109.92	106.45
25	n	609	CHL	CHC-C4B-C3B	2.80	124.86	118.23
25	N	601	CHL	C1-O2A-CGA	2.80	123.49	116.77
26	b	615	CLA	CMB-C2B-C3B	2.80	130.09	124.89
26	c	502	CLA	CMB-C2B-C3B	2.80	130.09	124.89
25	3	605	CHL	CHC-C4B-C3B	2.80	124.87	118.23
26	4	610	CLA	CMB-C2B-C3B	2.80	130.09	124.89
26	r	609	CLA	CMB-C2B-C3B	2.81	130.10	124.89
30	c	522	LHG	O8-C23-C24	2.81	120.07	111.90
25	n	601	CHL	C1-O2A-CGA	2.81	123.52	116.77
28	6	1622	XAT	O24-C25-C38	2.81	118.54	115.02
30	C	522	LHG	O8-C23-C24	2.81	120.09	111.90
28	8	622	XAT	C38-C25-C24	2.81	117.50	114.28
25	6	605	CHL	CHC-C4B-C3B	2.82	124.90	118.23
36	b	623	SQD	C44-O6-C1	2.82	119.54	113.76
28	r	622	XAT	C19-C9-C8	2.82	122.59	118.10
26	4	611	CLA	CMB-C2B-C3B	2.82	130.12	124.89
28	2	1622	XAT	O24-C25-C38	2.82	118.55	115.02
26	8	610	CLA	CMB-C2B-C3B	2.82	130.13	124.89
28	4	622	XAT	C38-C25-C24	2.82	117.51	114.28
26	N	613	CLA	CHB-C4A-NA	2.82	128.42	124.51
25	N	609	CHL	CHC-C4B-C3B	2.83	124.92	118.23
36	B	623	SQD	C44-O6-C1	2.83	119.55	113.76
26	2	603	CLA	CMD-C2D-C3D	2.83	130.14	124.89
26	C	502	CLA	CMB-C2B-C3B	2.83	130.14	124.89
26	s	611	CLA	CMB-C2B-C3B	2.83	130.14	124.89
26	C	505	CLA	CGD-CBD-CAD	2.83	120.19	110.71
26	6	603	CLA	CMD-C2D-C3D	2.83	130.14	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	609	CHL	O2A-CGA-CBA	2.83	120.14	111.90
25	5	609	CHL	CHB-C1B-C2B	2.83	124.83	116.99
25	5	609	CHL	O2A-CGA-CBA	2.83	120.14	111.90
25	1	605	CHL	CMD-C2D-C3D	2.83	121.44	114.27
25	2	605	CHL	CHC-C4B-C3B	2.83	124.94	118.23
26	c	505	CLA	CGD-CBD-CAD	2.83	120.21	110.71
26	B	615	CLA	CMB-C2B-C3B	2.84	130.15	124.89
25	8	608	CHL	O2D-CGD-CBD	2.84	118.12	111.20
26	s	612	CLA	CMD-C2D-C3D	2.84	130.15	124.89
26	S	612	CLA	CMD-C2D-C3D	2.84	130.15	124.89
26	N	613	CLA	C4A-NA-C1A	2.84	109.97	106.45
26	n	613	CLA	C4A-NA-C1A	2.84	109.97	106.45
26	B	617	CLA	CHB-C4A-NA	2.84	128.43	124.51
26	S	611	CLA	CMB-C2B-C3B	2.84	130.16	124.89
26	1	611	CLA	CMB-C2B-C3B	2.84	130.16	124.89
26	b	610	CLA	C4A-NA-C1A	2.84	109.98	106.45
25	3	606	CHL	CHC-C4B-C3B	2.84	124.96	118.23
25	5	608	CHL	O2D-CGD-CBD	2.84	118.13	111.20
25	1	608	CHL	O2D-CGD-CBD	2.84	118.13	111.20
25	4	608	CHL	O2D-CGD-CBD	2.84	118.13	111.20
28	R	622	XAT	C19-C9-C8	2.84	122.63	118.10
25	N	609	CHL	C4-C3-C5	2.84	120.22	115.29
25	7	606	CHL	CHC-C4B-C3B	2.84	124.97	118.23
25	1	609	CHL	CHB-C1B-C2B	2.84	124.87	116.99
25	2	607	CHL	CMD-C2D-C3D	2.85	121.47	114.27
26	5	611	CLA	CMB-C2B-C3B	2.85	130.17	124.89
26	7	603	CLA	CMB-C2B-C3B	2.85	130.18	124.89
26	b	617	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	8	611	CLA	CMB-C2B-C3B	2.85	130.18	124.89
25	5	605	CHL	CMD-C2D-C3D	2.85	121.48	114.27
27	y	1620	LUT	C39-C29-C28	2.85	122.64	118.10
25	6	607	CHL	CMD-C2D-C3D	2.86	121.50	114.27
39	b	626	DGD	O5D-C1E-C2E	2.86	112.90	108.23
25	N	605	CHL	CHC-C4B-C3B	2.86	125.00	118.23
26	4	612	CLA	CHB-C4A-NA	2.86	128.47	124.51
25	3	605	CHL	CMD-C2D-C3D	2.86	121.51	114.27
25	n	609	CHL	C4-C3-C5	2.86	120.25	115.29
39	B	626	DGD	O5D-C1E-C2E	2.86	112.90	108.23
26	B	610	CLA	C4A-NA-C1A	2.87	110.01	106.45
25	s	606	CHL	CMD-C2D-C3D	2.87	121.53	114.27
26	8	612	CLA	CMD-C2D-C3D	2.87	130.22	124.89
25	n	605	CHL	CHC-C4B-C3B	2.87	125.03	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	612	CLA	CMB-C2B-C3B	2.87	130.22	124.89
25	4	607	CHL	CHC-C4B-C3B	2.87	125.03	118.23
25	7	605	CHL	CMD-C2D-C3D	2.87	121.53	114.27
25	N	606	CHL	O2A-CGA-CBA	2.87	120.25	111.90
26	R	604	CLA	CHB-C4A-NA	2.87	128.49	124.51
25	s	608	CHL	CHB-C1B-C2B	2.87	124.95	116.99
26	n	613	CLA	CHB-C4A-NA	2.87	128.49	124.51
26	b	617	CLA	O2D-CGD-CBD	2.88	116.44	111.30
25	S	606	CHL	CMD-C2D-C3D	2.88	121.55	114.27
26	3	603	CLA	CMB-C2B-C3B	2.88	130.23	124.89
36	a	418	SQD	O47-C7-C8	2.88	117.53	111.55
26	1	612	CLA	CMB-C2B-C3B	2.88	130.24	124.89
25	8	607	CHL	CHC-C4B-C3B	2.88	125.06	118.23
26	B	609	CLA	CMD-C2D-C3D	2.88	130.24	124.89
25	n	606	CHL	O2A-CGA-CBA	2.88	120.29	111.90
26	C	503	CLA	CHB-C4A-NA	2.88	128.50	124.51
26	c	504	CLA	O2D-CGD-CBD	2.89	116.45	111.30
25	6	608	CHL	CMD-C2D-C3D	2.89	121.57	114.27
25	S	608	CHL	CHB-C1B-C2B	2.89	124.98	116.99
26	B	617	CLA	O2D-CGD-CBD	2.89	116.46	111.30
25	4	601	CHL	CMD-C2D-C3D	2.89	121.58	114.27
25	6	609	CHL	CMD-C2D-C3D	2.89	121.59	114.27
25	3	609	CHL	O2A-CGA-CBA	2.89	120.32	111.90
25	8	601	CHL	CMD-C2D-C3D	2.89	121.59	114.27
25	2	608	CHL	CMD-C2D-C3D	2.89	121.59	114.27
26	r	604	CLA	CHB-C4A-NA	2.89	128.51	124.51
27	Y	1620	LUT	C39-C29-C28	2.89	122.71	118.10
25	2	609	CHL	CMD-C2D-C3D	2.89	121.60	114.27
25	7	609	CHL	O2A-CGA-CBA	2.90	120.32	111.90
26	C	504	CLA	O2D-CGD-CBD	2.90	116.47	111.30
25	Y	606	CHL	O2A-CGA-CBA	2.90	120.33	111.90
25	R	607	CHL	O2A-CGA-CBA	2.90	120.33	111.90
36	A	418	SQD	O47-C7-C8	2.90	117.57	111.55
26	4	612	CLA	CMD-C2D-C3D	2.90	130.27	124.89
26	N	612	CLA	CMD-C2D-C3D	2.90	130.28	124.89
26	b	609	CLA	CMD-C2D-C3D	2.90	130.28	124.89
26	2	613	CLA	CMB-C2B-C3B	2.90	130.28	124.89
25	y	606	CHL	O2A-CGA-CBA	2.91	120.36	111.90
26	s	610	CLA	CHB-C4A-NA	2.91	128.53	124.51
26	3	612	CLA	CMB-C2B-C3B	2.91	130.29	124.89
26	b	611	CLA	C4A-NA-C1A	2.91	110.06	106.45
26	8	612	CLA	CHB-C4A-NA	2.91	128.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	607	CHL	O2A-CGA-CBA	2.91	120.37	111.90
26	c	503	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	6	613	CLA	CMB-C2B-C3B	2.91	130.30	124.89
26	8	612	CLA	CMB-C2B-C3B	2.91	130.30	124.89
26	y	603	CLA	CMB-C2B-C3B	2.91	130.30	124.89
41	F	101	HEM	CMC-C2C-C3C	2.92	130.31	124.89
26	b	606	CLA	CHB-C4A-NA	2.92	128.55	124.51
26	c	505	CLA	CMB-C2B-C3B	2.92	130.31	124.89
26	2	604	CLA	CMB-C2B-C3B	2.92	130.31	124.89
41	f	101	HEM	CMC-C2C-C3C	2.92	130.31	124.89
26	6	604	CLA	CMB-C2B-C3B	2.92	130.31	124.89
26	S	610	CLA	CHB-C4A-NA	2.92	128.55	124.51
26	n	612	CLA	CMD-C2D-C3D	2.92	130.31	124.89
25	R	614	CHL	O2D-CGD-CBD	2.92	118.33	111.20
29	R	623	NEX	C38-C25-C24	2.92	117.63	114.28
29	r	623	NEX	C38-C25-C24	2.92	117.63	114.28
26	B	606	CLA	CHB-C4A-NA	2.92	128.56	124.51
26	C	505	CLA	CMB-C2B-C3B	2.93	130.32	124.89
27	s	1621	LUT	C19-C9-C8	2.93	122.76	118.10
26	6	610	CLA	CMB-C2B-C3B	2.93	130.33	124.89
26	4	612	CLA	CMB-C2B-C3B	2.93	130.33	124.89
26	7	612	CLA	CMB-C2B-C3B	2.93	130.33	124.89
26	Y	603	CLA	CMB-C2B-C3B	2.93	130.33	124.89
25	Y	609	CHL	C4-C3-C5	2.93	120.37	115.29
27	S	1621	LUT	C19-C9-C8	2.93	122.77	118.10
26	B	611	CLA	C4A-NA-C1A	2.93	110.09	106.45
25	5	608	CHL	CMD-C2D-C3D	2.93	121.69	114.27
26	b	604	CLA	CMD-C2D-C3D	2.93	130.33	124.89
26	B	604	CLA	CMD-C2D-C3D	2.93	130.33	124.89
26	a	406	CLA	CHB-C4A-NA	2.93	128.57	124.51
26	A	406	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	1	608	CHL	CMD-C2D-C3D	2.94	121.70	114.27
25	r	614	CHL	O2D-CGD-CBD	2.94	118.37	111.20
26	B	607	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	4	606	CHL	CMD-C2D-C3D	2.94	121.71	114.27
30	2	2630	LHG	O8-C23-C24	2.94	120.45	111.90
30	6	2630	LHG	O8-C23-C24	2.94	120.45	111.90
26	a	405	CLA	C4A-NA-C1A	2.94	110.10	106.45
36	B	621	SQD	C44-O6-C1	2.94	119.79	113.76
26	c	513	CLA	CMD-C2D-C3D	2.94	130.35	124.89
26	c	511	CLA	C4A-NA-C1A	2.94	110.11	106.45
36	b	621	SQD	C44-O6-C1	2.95	119.80	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	606	CHL	CMD-C2D-C3D	2.95	121.73	114.27
26	b	607	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	y	609	CHL	C4-C3-C5	2.95	120.41	115.29
26	g	613	CLA	O2D-CGD-CBD	2.95	116.57	111.30
26	C	513	CLA	CMD-C2D-C3D	2.95	130.37	124.89
26	C	512	CLA	O2D-CGD-CBD	2.95	116.57	111.30
26	a	410	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	5	608	CHL	CHD-C1D-C2D	2.95	125.17	116.99
25	1	608	CHL	CHD-C1D-C2D	2.95	125.17	116.99
25	N	605	CHL	CMD-C2D-C3D	2.95	121.75	114.27
26	2	610	CLA	CMB-C2B-C3B	2.96	130.38	124.89
25	8	607	CHL	CHB-C1B-C2B	2.96	125.18	116.99
31	C	517	BCR	C33-C5-C4	2.96	119.06	113.45
26	A	410	CLA	CHB-C4A-NA	2.96	128.60	124.51
25	n	605	CHL	CMD-C2D-C3D	2.96	121.76	114.27
25	4	607	CHL	CHB-C1B-C2B	2.96	125.19	116.99
26	C	511	CLA	C4A-NA-C1A	2.97	110.14	106.45
26	5	613	CLA	CMB-C2B-C3B	2.97	130.40	124.89
26	c	512	CLA	O2D-CGD-CBD	2.97	116.61	111.30
26	1	613	CLA	CMB-C2B-C3B	2.97	130.40	124.89
25	N	605	CHL	O2A-CGA-CBA	2.97	120.55	111.90
25	3	601	CHL	O2A-CGA-CBA	2.97	120.55	111.90
26	b	612	CLA	CMD-C2D-C3D	2.97	130.41	124.89
26	G	613	CLA	O2D-CGD-CBD	2.98	116.62	111.30
36	a	418	SQD	O6-C1-C2	2.98	113.09	108.23
36	A	418	SQD	O6-C1-C2	2.98	113.09	108.23
25	7	601	CHL	O2A-CGA-CBA	2.98	120.58	111.90
26	B	612	CLA	CMD-C2D-C3D	2.98	130.43	124.89
31	c	517	BCR	C33-C5-C4	2.98	119.11	113.45
35	a	408	PHO	O1D-CGD-CBD	2.98	129.96	124.60
25	n	605	CHL	O2A-CGA-CBA	2.99	120.59	111.90
26	G	613	CLA	CMB-C2B-C3B	2.99	130.43	124.89
35	A	408	PHO	O1D-CGD-CBD	2.99	129.97	124.60
26	A	405	CLA	C4A-NA-C1A	2.99	110.17	106.45
25	N	608	CHL	CHD-C1D-C2D	2.99	125.28	116.99
25	3	606	CHL	CMD-C2D-C3D	2.99	121.84	114.27
25	y	601	CHL	CHC-C4B-C3B	2.99	125.32	118.23
26	B	613	CLA	C4A-NA-C1A	3.00	110.17	106.45
25	n	608	CHL	CHD-C1D-C2D	3.00	125.30	116.99
26	g	613	CLA	CMB-C2B-C3B	3.00	130.46	124.89
25	Y	601	CHL	CHC-C4B-C3B	3.00	125.34	118.23
26	Y	614	CLA	O2D-CGD-CBD	3.00	116.66	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	418	SQD	C4-C3-C2	3.00	116.13	110.84
25	8	608	CHL	CMD-C2D-C3D	3.00	121.87	114.27
26	5	610	CLA	CMB-C2B-C3B	3.00	130.47	124.89
25	7	606	CHL	CMD-C2D-C3D	3.00	121.87	114.27
26	1	610	CLA	CMB-C2B-C3B	3.01	130.47	124.89
36	a	418	SQD	C4-C3-C2	3.01	116.14	110.84
26	G	611	CLA	CMB-C2B-C3B	3.01	130.47	124.89
26	B	609	CLA	CHB-C4A-NA	3.01	128.67	124.51
26	g	611	CLA	CMB-C2B-C3B	3.01	130.47	124.89
26	b	613	CLA	C4A-NA-C1A	3.01	110.19	106.45
26	G	611	CLA	CHB-C4A-NA	3.01	128.67	124.51
26	y	614	CLA	O2D-CGD-CBD	3.01	116.68	111.30
27	S	1621	LUT	C17-C1-C6	3.01	115.19	110.31
25	4	608	CHL	CMD-C2D-C3D	3.01	121.90	114.27
25	8	601	CHL	CHC-C4B-C3B	3.01	125.37	118.23
25	4	601	CHL	CHC-C4B-C3B	3.01	125.37	118.23
26	g	611	CLA	CHB-C4A-NA	3.02	128.68	124.51
25	n	608	CHL	O2A-CGA-CBA	3.02	120.68	111.90
25	2	605	CHL	CMD-C2D-C3D	3.02	121.91	114.27
25	6	605	CHL	CMD-C2D-C3D	3.02	121.91	114.27
25	N	608	CHL	O2A-CGA-CBA	3.02	120.69	111.90
25	7	608	CHL	CHD-C1D-C2D	3.02	125.36	116.99
27	s	1621	LUT	C17-C1-C6	3.03	115.22	110.31
26	Y	613	CLA	O2D-CGD-CBD	3.03	116.72	111.30
25	3	608	CHL	CHD-C1D-C2D	3.04	125.40	116.99
26	b	609	CLA	CHB-C4A-NA	3.04	128.71	124.51
25	g	609	CHL	C1-O2A-CGA	3.04	124.06	116.77
26	y	613	CLA	O2D-CGD-CBD	3.04	116.73	111.30
27	r	620	LUT	C39-C29-C28	3.04	122.94	118.10
25	g	606	CHL	O2A-CGA-CBA	3.04	120.75	111.90
26	r	603	CLA	CMD-C2D-C3D	3.04	130.54	124.89
27	R	620	LUT	C39-C29-C28	3.04	122.95	118.10
25	5	608	CHL	CHC-C4B-C3B	3.04	125.44	118.23
25	s	607	CHL	CHD-C1D-C2D	3.04	125.42	116.99
25	7	607	CHL	O2A-CGA-CBA	3.05	120.77	111.90
25	S	607	CHL	CHD-C1D-C2D	3.05	125.43	116.99
26	4	603	CLA	CMB-C2B-C3B	3.05	130.55	124.89
36	B	623	SQD	O5-C1-C2	3.05	116.18	110.30
26	8	603	CLA	CMB-C2B-C3B	3.05	130.55	124.89
26	c	506	CLA	CMD-C2D-C3D	3.05	130.56	124.89
26	R	603	CLA	CMD-C2D-C3D	3.05	130.56	124.89
26	b	616	CLA	CHB-C4A-NA	3.05	128.73	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	616	CLA	CHB-C4A-NA	3.05	128.73	124.51
36	b	623	SQD	O5-C1-C2	3.05	116.19	110.30
26	C	506	CLA	CMD-C2D-C3D	3.05	130.56	124.89
26	B	608	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	G	609	CHL	C1-O2A-CGA	3.06	124.11	116.77
26	b	609	CLA	O2D-CGD-CBD	3.06	116.76	111.30
26	a	405	CLA	CHB-C4A-NA	3.06	128.74	124.51
38	D	405	PL9	C40-C39-C41	3.06	120.59	115.29
25	G	606	CHL	O2A-CGA-CBA	3.06	120.80	111.90
25	1	608	CHL	CHC-C4B-C3B	3.06	125.48	118.23
25	3	607	CHL	O2A-CGA-CBA	3.06	120.81	111.90
25	r	606	CHL	CHC-C4B-C3B	3.07	125.50	118.23
30	d	409	LHG	O8-C23-C24	3.07	120.83	111.90
36	B	623	SQD	O48-C23-C24	3.07	120.84	111.90
25	y	609	CHL	CMD-C2D-C3D	3.07	122.04	114.27
25	Y	609	CHL	CMD-C2D-C3D	3.07	122.04	114.27
26	r	611	CLA	CHB-C4A-NA	3.07	128.76	124.51
26	A	405	CLA	CHB-C4A-NA	3.07	128.76	124.51
36	b	623	SQD	O48-C23-C24	3.07	120.84	111.90
30	D	409	LHG	O8-C23-C24	3.07	120.84	111.90
26	B	615	CLA	O2D-CGD-CBD	3.07	116.79	111.30
38	d	405	PL9	C40-C39-C41	3.08	120.63	115.29
26	3	610	CLA	CMB-C2B-C3B	3.08	130.60	124.89
26	G	611	CLA	CMD-C2D-C3D	3.08	130.60	124.89
26	7	610	CLA	CMB-C2B-C3B	3.08	130.60	124.89
26	B	609	CLA	O2D-CGD-CBD	3.08	116.80	111.30
26	S	611	CLA	CMD-C2D-C3D	3.08	130.61	124.89
26	b	615	CLA	O2D-CGD-CBD	3.08	116.80	111.30
26	b	608	CLA	CHB-C4A-NA	3.08	128.77	124.51
26	g	611	CLA	CMD-C2D-C3D	3.08	130.61	124.89
25	N	609	CHL	C1-O2A-CGA	3.08	124.17	116.77
26	3	603	CLA	CMD-C2D-C3D	3.08	130.61	124.89
26	B	617	CLA	CMD-C2D-C3D	3.08	130.62	124.89
26	s	611	CLA	CMD-C2D-C3D	3.08	130.62	124.89
30	C	523	LHG	O8-C23-C24	3.09	120.88	111.90
26	a	406	CLA	O2D-CGD-CBD	3.09	116.81	111.30
25	R	606	CHL	CHC-C4B-C3B	3.09	125.55	118.23
25	R	614	CHL	CHB-C1B-C2B	3.09	125.55	116.99
25	n	609	CHL	C1-O2A-CGA	3.09	124.19	116.77
30	c	523	LHG	O8-C23-C24	3.09	120.90	111.90
26	7	603	CLA	CMD-C2D-C3D	3.09	130.63	124.89
25	r	614	CHL	CHB-C1B-C2B	3.10	125.56	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	607	CLA	CMD-C2D-C3D	3.10	130.64	124.89
26	1	603	CLA	CHB-C4A-NA	3.10	128.80	124.51
25	6	608	CHL	CHD-C1D-C2D	3.10	125.58	116.99
25	G	601	CHL	CHC-C4B-C3B	3.10	125.58	118.23
25	4	608	CHL	CHD-C1D-C2D	3.10	125.59	116.99
25	y	607	CHL	CMD-C2D-C3D	3.11	122.13	114.27
26	c	508	CLA	CMD-C2D-C3D	3.11	130.66	124.89
26	A	406	CLA	O2D-CGD-CBD	3.11	116.85	111.30
26	R	610	CLA	CMB-C2B-C3B	3.11	130.66	124.89
26	S	614	CLA	O2D-CGD-CBD	3.11	116.86	111.30
26	5	603	CLA	CHB-C4A-NA	3.11	128.81	124.51
26	R	611	CLA	CHB-C4A-NA	3.11	128.82	124.51
25	8	608	CHL	CHD-C1D-C2D	3.11	125.61	116.99
25	y	605	CHL	O2D-CGD-CBD	3.11	118.80	111.20
25	2	608	CHL	CHD-C1D-C2D	3.11	125.62	116.99
26	Y	603	CLA	CHB-C4A-NA	3.11	128.82	124.51
26	a	407	CLA	CHB-C4A-NA	3.12	128.82	124.51
26	s	614	CLA	O2D-CGD-CBD	3.12	116.87	111.30
25	Y	607	CHL	CMD-C2D-C3D	3.12	122.17	114.27
26	b	617	CLA	CMD-C2D-C3D	3.12	130.68	124.89
26	r	610	CLA	CMB-C2B-C3B	3.12	130.69	124.89
26	B	607	CLA	CMD-C2D-C3D	3.12	130.69	124.89
25	Y	605	CHL	O2D-CGD-CBD	3.12	118.82	111.20
26	3	613	CLA	CMB-C2B-C3B	3.12	130.69	124.89
25	g	601	CHL	CHC-C4B-C3B	3.13	125.64	118.23
26	C	508	CLA	CMD-C2D-C3D	3.13	130.69	124.89
25	Y	605	CHL	CHC-C4B-C3B	3.13	125.64	118.23
36	B	623	SQD	O8-S-C6	3.13	109.83	106.01
25	5	601	CHL	CHC-C4B-C3B	3.13	125.64	118.23
25	1	601	CHL	CHC-C4B-C3B	3.13	125.64	118.23
25	n	606	CHL	CHD-C1D-C2D	3.13	125.66	116.99
25	7	606	CHL	CHD-C1D-C2D	3.13	125.66	116.99
26	1	603	CLA	CMB-C2B-C3B	3.13	130.71	124.89
26	y	603	CLA	CHB-C4A-NA	3.14	128.85	124.51
25	n	605	CHL	CHD-C1D-C2D	3.14	125.68	116.99
25	3	606	CHL	CHD-C1D-C2D	3.14	125.68	116.99
25	N	606	CHL	CHD-C1D-C2D	3.14	125.70	116.99
26	g	612	CLA	CMD-C2D-C3D	3.14	130.73	124.89
26	G	612	CLA	CMD-C2D-C3D	3.14	130.73	124.89
26	7	613	CLA	CMB-C2B-C3B	3.15	130.73	124.89
25	y	605	CHL	CHC-C4B-C3B	3.15	125.68	118.23
26	c	504	CLA	CHB-C4A-NA	3.15	128.86	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	603	CLA	CMB-C2B-C3B	3.15	130.73	124.89
25	n	606	CHL	CMD-C2D-C3D	3.15	122.24	114.27
30	D	410	LHG	O8-C23-C24	3.15	121.06	111.90
26	A	407	CLA	CHB-C4A-NA	3.15	128.87	124.51
25	N	605	CHL	CHD-C1D-C2D	3.15	125.72	116.99
31	t	101	BCR	C1-C6-C7	3.16	124.60	115.73
25	N	606	CHL	CMD-C2D-C3D	3.16	122.26	114.27
30	d	408	LHG	O8-C23-C24	3.16	121.09	111.90
26	y	614	CLA	CMB-C2B-C3B	3.16	130.75	124.89
31	T	101	BCR	C1-C6-C7	3.16	124.61	115.73
30	D	408	LHG	O8-C23-C24	3.16	121.10	111.90
25	1	607	CHL	O2D-CGD-CBD	3.17	118.93	111.20
36	b	623	SQD	O8-S-C6	3.17	109.88	106.01
25	y	605	CHL	CMD-C2D-C3D	3.17	122.29	114.27
30	d	410	LHG	O8-C23-C24	3.17	121.12	111.90
26	D	402	CLA	C4A-NA-C1A	3.17	110.39	106.45
25	R	607	CHL	CHD-C1D-C2D	3.17	125.77	116.99
25	5	607	CHL	O2D-CGD-CBD	3.17	118.94	111.20
26	n	604	CLA	CMD-C2D-C3D	3.17	130.78	124.89
26	Y	614	CLA	CMB-C2B-C3B	3.17	130.78	124.89
25	G	608	CHL	CHC-C4B-C3B	3.18	125.75	118.23
25	y	605	CHL	CHD-C1D-C2D	3.18	125.79	116.99
26	N	604	CLA	CMD-C2D-C3D	3.18	130.79	124.89
25	7	608	CHL	CMD-C2D-C3D	3.18	122.31	114.27
25	s	607	CHL	CMD-C2D-C3D	3.18	122.31	114.27
25	r	607	CHL	CHD-C1D-C2D	3.18	125.80	116.99
25	Y	605	CHL	CMD-C2D-C3D	3.18	122.32	114.27
26	5	614	CLA	CMB-C2B-C3B	3.18	130.79	124.89
26	1	614	CLA	CMB-C2B-C3B	3.18	130.79	124.89
26	C	504	CLA	CHB-C4A-NA	3.18	128.91	124.51
25	g	608	CHL	CHC-C4B-C3B	3.18	125.77	118.23
25	S	607	CHL	CMD-C2D-C3D	3.18	122.33	114.27
25	Y	605	CHL	CHD-C1D-C2D	3.19	125.83	116.99
25	3	608	CHL	CMD-C2D-C3D	3.19	122.35	114.27
26	d	402	CLA	C4A-NA-C1A	3.20	110.42	106.45
36	A	412	SQD	O7-S-C6	3.20	109.56	106.83
28	4	622	XAT	O24-C25-C38	3.20	119.02	115.02
26	b	605	CLA	CAC-C3C-C4C	3.20	129.35	124.83
26	a	410	CLA	CMD-C2D-C3D	3.20	130.84	124.89
28	8	622	XAT	O24-C25-C38	3.21	119.03	115.02
25	8	606	CHL	CHC-C4B-C3B	3.21	125.83	118.23
25	r	607	CHL	CHC-C4B-C3B	3.21	125.83	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	603	CLA	CHB-C4A-NA	3.21	128.95	124.51
25	G	608	CHL	CHD-C1D-C2D	3.21	125.89	116.99
26	B	608	CLA	C4A-NA-C1A	3.22	110.44	106.45
26	c	502	CLA	CHB-C4A-NA	3.22	128.96	124.51
25	4	606	CHL	CHC-C4B-C3B	3.22	125.85	118.23
26	g	610	CLA	CMB-C2B-C3B	3.22	130.87	124.89
25	g	608	CHL	CHD-C1D-C2D	3.22	125.91	116.99
26	A	410	CLA	CMD-C2D-C3D	3.22	130.87	124.89
26	B	605	CLA	CAC-C3C-C4C	3.22	129.37	124.83
25	S	601	CHL	CHC-C4B-C3B	3.22	125.86	118.23
25	s	601	CHL	CHC-C4B-C3B	3.22	125.87	118.23
26	G	610	CLA	CMB-C2B-C3B	3.23	130.88	124.89
25	6	605	CHL	CHD-C1D-C2D	3.23	125.92	116.99
25	2	605	CHL	CHD-C1D-C2D	3.23	125.92	116.99
25	R	607	CHL	CHC-C4B-C3B	3.23	125.87	118.23
36	a	412	SQD	O7-S-C6	3.23	109.59	106.83
39	c	518	DGD	C1E-O6E-C5E	3.23	119.80	113.72
26	b	608	CLA	C4A-NA-C1A	3.23	110.46	106.45
25	Y	601	CHL	C4-C3-C5	3.23	120.90	115.29
26	6	603	CLA	CHB-C4A-NA	3.24	128.99	124.51
25	n	609	CHL	CHD-C1D-C2D	3.24	125.96	116.99
25	S	608	CHL	CHD-C1D-C2D	3.24	125.96	116.99
25	N	609	CHL	CHD-C1D-C2D	3.24	125.97	116.99
25	8	601	CHL	CHB-C1B-C2B	3.24	125.97	116.99
26	2	614	CLA	CMB-C2B-C3B	3.24	130.91	124.89
26	1	602	CLA	CMB-C2B-C3B	3.25	130.92	124.89
26	Y	611	CLA	CMD-C2D-C3D	3.25	130.92	124.89
26	C	512	CLA	CMD-C2D-C3D	3.25	130.92	124.89
25	G	607	CHL	O2D-CGD-CBD	3.25	119.13	111.20
25	s	608	CHL	CHD-C1D-C2D	3.25	125.99	116.99
25	y	608	CHL	CHD-C1D-C2D	3.25	126.00	116.99
25	Y	608	CHL	CHD-C1D-C2D	3.25	126.00	116.99
27	4	620	LUT	C18-C5-C4	3.26	120.28	114.33
39	C	518	DGD	C1E-O6E-C5E	3.26	119.85	113.72
25	4	601	CHL	CHB-C1B-C2B	3.26	126.01	116.99
25	6	608	CHL	O2D-CGD-CBD	3.26	119.15	111.20
26	C	502	CLA	CHB-C4A-NA	3.26	129.02	124.51
26	c	512	CLA	CMD-C2D-C3D	3.26	130.94	124.89
26	R	604	CLA	CBA-CAA-C2A	3.26	123.55	113.80
25	y	601	CHL	C4-C3-C5	3.26	120.95	115.29
26	r	604	CLA	CBA-CAA-C2A	3.26	123.56	113.80
25	y	608	CHL	O2A-CGA-CBA	3.26	121.39	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	608	CHL	O2A-CGA-CBA	3.26	121.39	111.90
25	g	607	CHL	O2D-CGD-CBD	3.26	119.17	111.20
25	s	606	CHL	CHD-C1D-C2D	3.27	126.03	116.99
25	2	608	CHL	O2D-CGD-CBD	3.27	119.17	111.20
25	N	609	CHL	CMD-C2D-C3D	3.27	122.54	114.27
26	6	614	CLA	CMB-C2B-C3B	3.27	130.96	124.89
25	S	608	CHL	CHC-C4B-C3B	3.27	125.97	118.23
26	y	611	CLA	CMD-C2D-C3D	3.27	130.96	124.89
25	G	606	CHL	O2D-CGD-CBD	3.27	119.19	111.20
25	n	609	CHL	CMD-C2D-C3D	3.28	122.56	114.27
25	g	606	CHL	O2D-CGD-CBD	3.28	119.20	111.20
27	8	620	LUT	C18-C5-C4	3.28	120.32	114.33
25	r	607	CHL	C4-C3-C5	3.28	120.98	115.29
26	c	511	CLA	CHB-C4A-NA	3.28	129.05	124.51
26	5	602	CLA	CMB-C2B-C3B	3.28	130.98	124.89
25	s	608	CHL	CHC-C4B-C3B	3.28	126.00	118.23
25	S	606	CHL	CHD-C1D-C2D	3.28	126.08	116.99
26	C	511	CLA	CHB-C4A-NA	3.28	129.05	124.51
26	c	509	CLA	O2D-CGD-CBD	3.29	117.17	111.30
26	r	610	CLA	CHB-C4A-NA	3.29	129.06	124.51
25	1	607	CHL	CHD-C1D-C2D	3.29	126.10	116.99
25	g	609	CHL	CHD-C1D-C2D	3.29	126.10	116.99
26	G	612	CLA	CMB-C2B-C3B	3.29	131.00	124.89
26	c	504	CLA	CMD-C2D-C3D	3.29	131.00	124.89
25	5	607	CHL	CHD-C1D-C2D	3.29	126.11	116.99
26	c	502	CLA	C4A-NA-C1A	3.29	110.54	106.45
26	C	509	CLA	O2D-CGD-CBD	3.29	117.19	111.30
25	R	607	CHL	C4-C3-C5	3.29	121.00	115.29
26	d	403	CLA	CHB-C4A-NA	3.30	129.07	124.51
25	G	609	CHL	CHD-C1D-C2D	3.30	126.12	116.99
26	C	504	CLA	CMD-C2D-C3D	3.30	131.02	124.89
26	B	608	CLA	CMB-C2B-C3B	3.30	131.02	124.89
26	b	608	CLA	CMB-C2B-C3B	3.30	131.02	124.89
26	g	612	CLA	CMB-C2B-C3B	3.31	131.03	124.89
26	A	410	CLA	O2D-CGD-CBD	3.31	117.21	111.30
26	R	610	CLA	CHB-C4A-NA	3.31	129.09	124.51
26	C	502	CLA	C4A-NA-C1A	3.31	110.56	106.45
25	2	601	CHL	O2D-CGD-CBD	3.31	119.28	111.20
26	C	505	CLA	C4A-NA-C1A	3.31	110.56	106.45
25	S	607	CHL	O2D-CGD-CBD	3.31	119.29	111.20
25	R	606	CHL	O2A-CGA-CBA	3.31	121.55	111.90
26	B	614	CLA	CMB-C2B-C3B	3.31	131.04	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	611	CLA	CHB-C4A-NA	3.32	129.10	124.51
26	b	614	CLA	CMB-C2B-C3B	3.32	131.05	124.89
25	2	601	CHL	CHC-C4B-C3B	3.32	126.10	118.23
25	S	601	CHL	O2D-CGD-CBD	3.32	119.31	111.20
26	D	403	CLA	CHB-C4A-NA	3.32	129.11	124.51
26	c	505	CLA	C4A-NA-C1A	3.32	110.58	106.45
25	s	607	CHL	O2D-CGD-CBD	3.32	119.31	111.20
25	s	601	CHL	O2D-CGD-CBD	3.32	119.31	111.20
25	r	606	CHL	O2A-CGA-CBA	3.33	121.58	111.90
26	a	410	CLA	O2D-CGD-CBD	3.33	117.24	111.30
25	6	601	CHL	O2D-CGD-CBD	3.33	119.32	111.20
26	4	602	CLA	CMB-C2B-C3B	3.33	131.07	124.89
25	Y	606	CHL	CMD-C2D-C3D	3.33	122.70	114.27
25	y	606	CHL	CMD-C2D-C3D	3.33	122.70	114.27
25	5	606	CHL	CHD-C1D-C2D	3.33	126.22	116.99
36	b	621	SQD	O6-C1-C2	3.33	113.67	108.23
25	6	601	CHL	CHC-C4B-C3B	3.33	126.13	118.23
25	N	608	CHL	CHC-C4B-C3B	3.33	126.13	118.23
25	n	608	CHL	CHC-C4B-C3B	3.33	126.13	118.23
26	B	611	CLA	CHB-C4A-NA	3.34	129.12	124.51
28	1	1622	XAT	O24-C25-C38	3.34	119.20	115.02
41	F	101	HEM	CMB-C2B-C3B	3.34	131.09	124.89
36	B	621	SQD	O6-C1-C2	3.34	113.69	108.23
26	S	603	CLA	CHB-C4A-NA	3.34	129.13	124.51
25	1	606	CHL	CHD-C1D-C2D	3.34	126.25	116.99
36	a	412	SQD	O5-C5-C4	3.34	115.82	109.66
25	6	609	CHL	CHB-C1B-C2B	3.34	126.25	116.99
25	2	609	CHL	CHB-C1B-C2B	3.35	126.26	116.99
41	f	101	HEM	CMB-C2B-C3B	3.35	131.10	124.89
26	8	602	CLA	CMB-C2B-C3B	3.35	131.11	124.89
26	3	603	CLA	CHB-C4A-NA	3.35	129.14	124.51
25	n	601	CHL	CHC-C4B-C3B	3.35	126.17	118.23
25	1	606	CHL	O2D-CGD-CBD	3.35	119.38	111.20
26	a	407	CLA	CMB-C2B-C3B	3.35	131.11	124.89
26	s	603	CLA	CHB-C4A-NA	3.36	129.16	124.51
25	N	601	CHL	CHC-C4B-C3B	3.36	126.19	118.23
29	6	1623	NEX	C16-C1-C6	3.36	113.48	110.47
25	5	606	CHL	O2D-CGD-CBD	3.36	119.40	111.20
25	g	607	CHL	CHC-C4B-C3B	3.36	126.19	118.23
26	n	603	CLA	CHB-C4A-NA	3.36	129.16	124.51
26	N	603	CLA	CHB-C4A-NA	3.36	129.16	124.51
28	5	1622	XAT	O24-C25-C38	3.36	119.23	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	407	CLA	CMB-C2B-C3B	3.37	131.14	124.89
36	A	412	SQD	O5-C5-C4	3.37	115.86	109.66
26	c	502	CLA	CMD-C2D-C3D	3.37	131.14	124.89
25	3	605	CHL	CHD-C1D-C2D	3.37	126.33	116.99
26	C	502	CLA	CMD-C2D-C3D	3.37	131.15	124.89
25	G	607	CHL	CHC-C4B-C3B	3.38	126.23	118.23
25	r	607	CHL	O2D-CGD-CBD	3.38	119.45	111.20
25	7	605	CHL	CHD-C1D-C2D	3.38	126.36	116.99
26	7	603	CLA	CHB-C4A-NA	3.39	129.20	124.51
25	R	607	CHL	O2D-CGD-CBD	3.39	119.47	111.20
26	c	507	CLA	C4A-NA-C1A	3.39	110.66	106.45
26	S	603	CLA	CMB-C2B-C3B	3.39	131.18	124.89
25	2	606	CHL	CHD-C1D-C2D	3.39	126.38	116.99
28	7	1622	XAT	O4-C5-C18	3.39	119.26	115.02
25	6	606	CHL	CHD-C1D-C2D	3.39	126.38	116.99
25	6	606	CHL	O2D-CGD-CBD	3.40	119.49	111.20
26	B	611	CLA	CMB-C2B-C3B	3.40	131.20	124.89
25	G	605	CHL	CHC-C4B-C3B	3.40	126.29	118.23
29	y	1623	NEX	O24-C25-C38	3.40	119.28	115.02
26	C	503	CLA	CMB-C2B-C3B	3.40	131.21	124.89
25	2	606	CHL	O2D-CGD-CBD	3.40	119.50	111.20
25	2	607	CHL	CHD-C1D-C2D	3.41	126.42	116.99
26	c	503	CLA	CMB-C2B-C3B	3.41	131.21	124.89
26	s	603	CLA	CMB-C2B-C3B	3.41	131.21	124.89
26	b	606	CLA	CMB-C2B-C3B	3.41	131.22	124.89
26	B	606	CLA	CMB-C2B-C3B	3.41	131.22	124.89
29	2	1623	NEX	C16-C1-C6	3.41	113.52	110.47
26	8	602	CLA	O2D-CGD-CBD	3.41	117.39	111.30
25	6	607	CHL	CHD-C1D-C2D	3.41	126.44	116.99
26	d	402	CLA	CMB-C2B-C3B	3.41	131.23	124.89
25	g	605	CHL	CHC-C4B-C3B	3.41	126.32	118.23
26	b	611	CLA	CMB-C2B-C3B	3.42	131.23	124.89
28	3	1622	XAT	O4-C5-C18	3.42	119.30	115.02
25	2	605	CHL	O2D-CGD-CBD	3.42	119.54	111.20
26	C	507	CLA	C4A-NA-C1A	3.42	110.70	106.45
25	7	608	CHL	O2D-CGD-CBD	3.42	119.55	111.20
26	D	402	CLA	CMB-C2B-C3B	3.42	131.24	124.89
25	6	605	CHL	O2D-CGD-CBD	3.42	119.55	111.20
26	g	603	CLA	CHB-C4A-NA	3.43	129.25	124.51
29	Y	1623	NEX	O24-C25-C38	3.43	119.31	115.02
26	Y	610	CLA	CMB-C2B-C3B	3.43	131.25	124.89
25	G	606	CHL	CHD-C1D-C2D	3.43	126.49	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	605	CHL	CHD-C1D-C2D	3.43	126.50	116.99
29	1	1623	NEX	O24-C25-C38	3.43	119.32	115.02
26	4	602	CLA	O2D-CGD-CBD	3.44	117.44	111.30
31	B	620	BCR	C33-C5-C4	3.44	119.98	113.45
28	N	1622	XAT	O4-C5-C18	3.44	119.32	115.02
25	1	605	CHL	CHD-C1D-C2D	3.44	126.52	116.99
28	n	1622	XAT	O4-C5-C18	3.44	119.32	115.02
25	3	608	CHL	O2D-CGD-CBD	3.44	119.59	111.20
25	g	606	CHL	CHD-C1D-C2D	3.44	126.52	116.99
29	G	1623	NEX	C16-C1-C6	3.44	113.55	110.47
25	g	605	CHL	CHD-C1D-C2D	3.44	126.52	116.99
25	Y	609	CHL	CHD-C1D-C2D	3.44	126.53	116.99
29	g	1623	NEX	C16-C1-C6	3.44	113.56	110.47
26	y	610	CLA	CMB-C2B-C3B	3.45	131.28	124.89
25	G	605	CHL	CHD-C1D-C2D	3.45	126.54	116.99
26	G	603	CLA	CHB-C4A-NA	3.45	129.28	124.51
29	5	1623	NEX	O24-C25-C38	3.45	119.34	115.02
26	c	505	CLA	O2D-CGD-CBD	3.45	117.47	111.30
25	y	609	CHL	CHD-C1D-C2D	3.45	126.56	116.99
31	b	620	BCR	C33-C5-C4	3.46	120.02	113.45
25	5	601	CHL	O2D-CGD-CBD	3.46	119.64	111.20
25	1	601	CHL	O2D-CGD-CBD	3.46	119.65	111.20
26	C	505	CLA	O2D-CGD-CBD	3.46	117.49	111.30
36	A	412	SQD	C4-C3-C2	3.46	116.94	110.84
31	t	101	BCR	C33-C5-C4	3.46	120.02	113.45
25	3	607	CHL	CHB-C1B-C2B	3.46	126.59	116.99
26	a	410	CLA	CMB-C2B-C3B	3.47	131.33	124.89
25	7	607	CHL	CHB-C1B-C2B	3.47	126.61	116.99
31	T	101	BCR	C33-C5-C4	3.48	120.05	113.45
25	4	609	CHL	O2D-CGD-CBD	3.48	119.68	111.20
26	A	410	CLA	CMB-C2B-C3B	3.48	131.34	124.89
25	8	609	CHL	O2D-CGD-CBD	3.48	119.70	111.20
36	A	418	SQD	O8-S-C6	3.48	110.26	106.01
36	a	412	SQD	C4-C3-C2	3.49	116.99	110.84
36	a	418	SQD	O8-S-C6	3.49	110.27	106.01
26	C	507	CLA	CMB-C2B-C3B	3.49	131.37	124.89
25	7	601	CHL	O2D-CGD-CBD	3.50	119.73	111.20
25	3	601	CHL	O2D-CGD-CBD	3.50	119.73	111.20
26	R	611	CLA	CMD-C2D-C3D	3.50	131.38	124.89
26	c	507	CLA	CMB-C2B-C3B	3.50	131.39	124.89
25	8	606	CHL	CHD-C1D-C2D	3.51	126.70	116.99
26	n	613	CLA	CMB-C2B-C3B	3.51	131.40	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	507	CLA	CHB-C4A-NA	3.51	129.37	124.51
26	C	509	CLA	CHB-C4A-NA	3.51	129.37	124.51
26	N	612	CLA	CMB-C2B-C3B	3.51	131.41	124.89
29	6	1623	NEX	O24-C25-C38	3.51	119.42	115.02
25	4	606	CHL	CHD-C1D-C2D	3.52	126.73	116.99
26	r	611	CLA	CMD-C2D-C3D	3.52	131.43	124.89
29	G	1623	NEX	O24-C25-C38	3.52	119.43	115.02
26	N	613	CLA	CMB-C2B-C3B	3.52	131.43	124.89
26	n	612	CLA	CMB-C2B-C3B	3.53	131.43	124.89
27	1	1621	LUT	C2-C3-C4	3.53	115.20	110.32
26	B	613	CLA	CHB-C4A-NA	3.53	129.40	124.51
26	Y	613	CLA	CMB-C2B-C3B	3.54	131.45	124.89
26	y	613	CLA	CMB-C2B-C3B	3.54	131.45	124.89
25	G	607	CHL	CHD-C1D-C2D	3.54	126.78	116.99
25	g	607	CHL	CHD-C1D-C2D	3.54	126.79	116.99
26	c	509	CLA	CHB-C4A-NA	3.54	129.40	124.51
26	C	507	CLA	CHB-C4A-NA	3.54	129.41	124.51
25	6	609	CHL	CHD-C1D-C2D	3.54	126.79	116.99
26	7	602	CLA	CMB-C2B-C3B	3.54	131.47	124.89
25	G	601	CHL	O2D-CGD-CBD	3.54	119.85	111.20
26	3	604	CLA	CMB-C2B-C3B	3.54	131.47	124.89
26	3	602	CLA	CMB-C2B-C3B	3.54	131.47	124.89
26	B	607	CLA	CMB-C2B-C3B	3.54	131.47	124.89
29	g	1623	NEX	O24-C25-C38	3.55	119.46	115.02
29	2	1623	NEX	O24-C25-C38	3.55	119.46	115.02
26	S	604	CLA	C4A-NA-C1A	3.55	110.86	106.45
25	R	606	CHL	CHD-C1D-C2D	3.55	126.82	116.99
25	r	606	CHL	CHD-C1D-C2D	3.55	126.82	116.99
25	7	601	CHL	CHC-C4B-C3B	3.55	126.64	118.23
25	Y	608	CHL	CHC-C4B-C3B	3.55	126.64	118.23
25	2	609	CHL	CHD-C1D-C2D	3.55	126.83	116.99
26	G	614	CLA	CMB-C2B-C3B	3.55	131.49	124.89
26	b	607	CLA	CMB-C2B-C3B	3.56	131.49	124.89
26	b	613	CLA	CHB-C4A-NA	3.56	129.43	124.51
26	D	403	CLA	O2D-CGD-CBD	3.56	117.66	111.30
27	5	1621	LUT	C2-C3-C4	3.56	115.23	110.32
26	s	604	CLA	C4A-NA-C1A	3.56	110.88	106.45
25	g	601	CHL	O2D-CGD-CBD	3.57	119.90	111.20
25	3	601	CHL	CHC-C4B-C3B	3.57	126.68	118.23
25	y	608	CHL	CHC-C4B-C3B	3.57	126.68	118.23
26	g	614	CLA	CMB-C2B-C3B	3.57	131.52	124.89
25	4	607	CHL	O2D-CGD-CBD	3.57	119.91	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	604	CLA	CMB-C2B-C3B	3.57	131.52	124.89
25	g	608	CHL	O2D-CGD-CBD	3.57	119.92	111.20
25	G	608	CHL	O2D-CGD-CBD	3.57	119.92	111.20
28	g	1622	XAT	O24-C25-C38	3.57	119.49	115.02
26	d	403	CLA	O2D-CGD-CBD	3.57	117.69	111.30
25	3	607	CHL	CHC-C4B-C3B	3.58	126.70	118.23
25	8	607	CHL	O2D-CGD-CBD	3.59	119.95	111.20
26	S	604	CLA	CHB-C4A-NA	3.59	129.47	124.51
26	2	602	CLA	CMB-C2B-C3B	3.59	131.54	124.89
26	C	511	CLA	CMB-C2B-C3B	3.59	131.55	124.89
25	3	607	CHL	O2D-CGD-CBD	3.59	119.96	111.20
25	7	607	CHL	CHC-C4B-C3B	3.59	126.74	118.23
25	S	606	CHL	CHC-C4B-C3B	3.59	126.74	118.23
25	7	607	CHL	O2D-CGD-CBD	3.59	119.97	111.20
25	s	606	CHL	CHC-C4B-C3B	3.60	126.75	118.23
26	s	604	CLA	CHB-C4A-NA	3.60	129.49	124.51
28	G	1622	XAT	O24-C25-C38	3.60	119.52	115.02
26	c	511	CLA	CMB-C2B-C3B	3.60	131.58	124.89
26	6	602	CLA	CMB-C2B-C3B	3.60	131.58	124.89
26	b	604	CLA	CMB-C2B-C3B	3.63	131.63	124.89
26	g	604	CLA	CMB-C2B-C3B	3.63	131.63	124.89
25	5	609	CHL	CHD-C1D-C2D	3.64	127.07	116.99
25	1	609	CHL	CHD-C1D-C2D	3.64	127.08	116.99
26	B	604	CLA	CMB-C2B-C3B	3.66	131.68	124.89
26	1	604	CLA	CMB-C2B-C3B	3.66	131.69	124.89
26	G	604	CLA	CMB-C2B-C3B	3.67	131.69	124.89
25	n	606	CHL	O2D-CGD-CBD	3.68	120.17	111.20
25	1	605	CHL	O2D-CGD-CBD	3.68	120.17	111.20
25	N	606	CHL	O2D-CGD-CBD	3.68	120.18	111.20
25	1	609	CHL	O2D-CGD-CBD	3.68	120.18	111.20
26	5	604	CLA	CMB-C2B-C3B	3.68	131.72	124.89
26	b	605	CLA	CBC-CAC-C3C	3.68	122.87	112.41
25	5	605	CHL	O2D-CGD-CBD	3.69	120.20	111.20
26	b	605	CLA	CHB-C4A-NA	3.69	129.62	124.51
25	g	609	CHL	O2D-CGD-CBD	3.70	120.22	111.20
26	B	605	CLA	CBC-CAC-C3C	3.70	122.92	112.41
25	G	609	CHL	O2D-CGD-CBD	3.70	120.23	111.20
25	5	609	CHL	O2D-CGD-CBD	3.70	120.23	111.20
25	n	609	CHL	O2D-CGD-CBD	3.71	120.24	111.20
26	B	605	CLA	CHB-C4A-NA	3.71	129.65	124.51
25	N	609	CHL	O2D-CGD-CBD	3.72	120.27	111.20
26	n	613	CLA	O2D-CGD-CBD	3.72	117.94	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	605	CLA	CAA-C2A-C1A	3.73	124.18	111.97
25	n	607	CHL	CMD-C2D-C3D	3.74	123.72	114.27
26	N	613	CLA	O2D-CGD-CBD	3.74	117.98	111.30
26	s	602	CLA	CMB-C2B-C3B	3.74	131.83	124.89
36	B	621	SQD	C4-C3-C2	3.74	117.43	110.84
26	S	602	CLA	CMB-C2B-C3B	3.74	131.83	124.89
26	B	605	CLA	CAA-C2A-C1A	3.74	124.23	111.97
36	a	418	SQD	C45-O47-C7	3.74	126.72	117.88
36	A	418	SQD	C45-O47-C7	3.74	126.72	117.88
25	N	607	CHL	CMD-C2D-C3D	3.75	123.77	114.27
36	b	621	SQD	C4-C3-C2	3.76	117.47	110.84
25	N	601	CHL	CHD-C1D-C2D	3.76	127.41	116.99
25	n	601	CHL	CHD-C1D-C2D	3.76	127.41	116.99
25	y	601	CHL	O2D-CGD-CBD	3.77	120.39	111.20
25	Y	601	CHL	O2D-CGD-CBD	3.78	120.43	111.20
26	N	604	CLA	CMB-C2B-C3B	3.78	131.91	124.89
26	r	611	CLA	C2C-C1C-NC	3.79	112.83	110.22
26	r	604	CLA	CMB-C2B-C3B	3.79	131.93	124.89
28	5	1622	XAT	O4-C5-C18	3.80	119.77	115.02
26	y	604	CLA	CMB-C2B-C3B	3.80	131.94	124.89
28	1	1622	XAT	O4-C5-C18	3.80	119.78	115.02
26	R	611	CLA	C2C-C1C-NC	3.80	112.84	110.22
25	4	607	CHL	CHD-C1D-C2D	3.80	127.52	116.99
25	8	607	CHL	CHD-C1D-C2D	3.80	127.52	116.99
26	n	604	CLA	CMB-C2B-C3B	3.81	131.96	124.89
26	R	604	CLA	CMB-C2B-C3B	3.81	131.96	124.89
25	S	601	CHL	CHD-C1D-C2D	3.81	127.56	116.99
26	Y	604	CLA	CMB-C2B-C3B	3.82	131.97	124.89
36	A	412	SQD	O47-C7-C8	3.82	119.48	111.55
25	Y	606	CHL	O2D-CGD-CBD	3.82	120.52	111.20
25	6	607	CHL	O2D-CGD-CBD	3.82	120.53	111.20
25	s	601	CHL	CHD-C1D-C2D	3.82	127.58	116.99
25	y	606	CHL	O2D-CGD-CBD	3.82	120.53	111.20
36	a	412	SQD	O47-C7-C8	3.83	119.50	111.55
25	2	607	CHL	O2D-CGD-CBD	3.83	120.55	111.20
26	R	601	CLA	C1D-CHD-C4C	3.83	127.72	122.48
25	s	606	CHL	O2D-CGD-CBD	3.84	120.58	111.20
25	7	605	CHL	O2D-CGD-CBD	3.85	120.60	111.20
25	r	614	CHL	CHD-C1D-C2D	3.85	127.66	116.99
25	R	614	CHL	CHD-C1D-C2D	3.85	127.66	116.99
25	y	608	CHL	O2D-CGD-CBD	3.85	120.60	111.20
25	S	606	CHL	O2D-CGD-CBD	3.86	120.61	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	606	CHL	O2D-CGD-CBD	3.86	120.61	111.20
25	2	601	CHL	CHD-C1D-C2D	3.86	127.67	116.99
25	3	606	CHL	O2D-CGD-CBD	3.86	120.61	111.20
25	Y	608	CHL	O2D-CGD-CBD	3.86	120.62	111.20
26	B	617	CLA	CMB-C2B-C3B	3.86	132.06	124.89
26	r	601	CLA	C1D-CHD-C4C	3.86	127.76	122.48
25	R	606	CHL	O2D-CGD-CBD	3.86	120.63	111.20
25	6	601	CHL	CHD-C1D-C2D	3.87	127.70	116.99
25	7	606	CHL	O2D-CGD-CBD	3.87	120.64	111.20
25	3	605	CHL	O2D-CGD-CBD	3.87	120.64	111.20
26	b	617	CLA	CMB-C2B-C3B	3.87	132.07	124.89
30	3	2630	LHG	O4-P-O5	3.88	132.36	112.28
26	N	610	CLA	CMB-C2B-C3B	3.88	132.09	124.89
25	n	608	CHL	O2D-CGD-CBD	3.88	120.67	111.20
25	n	601	CHL	O2D-CGD-CBD	3.89	120.68	111.20
30	7	2630	LHG	O4-P-O5	3.89	132.40	112.28
25	N	608	CHL	O2D-CGD-CBD	3.89	120.69	111.20
26	S	610	CLA	CMB-C2B-C3B	3.89	132.12	124.89
26	n	610	CLA	CMB-C2B-C3B	3.90	132.13	124.89
25	N	601	CHL	O2D-CGD-CBD	3.90	120.73	111.20
25	3	601	CHL	CHD-C1D-C2D	3.91	127.81	116.99
26	s	610	CLA	CMB-C2B-C3B	3.91	132.15	124.89
25	8	606	CHL	O2D-CGD-CBD	3.91	120.75	111.20
25	7	601	CHL	CHD-C1D-C2D	3.92	127.84	116.99
25	G	601	CHL	CHD-C1D-C2D	3.92	127.85	116.99
26	b	610	CLA	CMB-C2B-C3B	3.92	132.17	124.89
25	4	606	CHL	O2D-CGD-CBD	3.92	120.77	111.20
25	g	605	CHL	O2D-CGD-CBD	3.93	120.78	111.20
26	r	601	CLA	CMB-C2B-C3B	3.93	132.18	124.89
25	G	605	CHL	O2D-CGD-CBD	3.93	120.78	111.20
30	b	2631	LHG	O4-P-O5	3.93	132.61	112.28
30	B	2631	LHG	O4-P-O5	3.93	132.61	112.28
26	B	610	CLA	CMB-C2B-C3B	3.93	132.19	124.89
30	6	2630	LHG	O4-P-O5	3.94	132.67	112.28
30	2	2630	LHG	O4-P-O5	3.94	132.67	112.28
25	g	601	CHL	CHD-C1D-C2D	3.94	127.90	116.99
26	R	601	CLA	CMB-C2B-C3B	3.94	132.21	124.89
30	b	2630	LHG	O4-P-O5	3.95	132.71	112.28
25	7	609	CHL	CHD-C1D-C2D	3.95	127.93	116.99
26	y	602	CLA	CMB-C2B-C3B	3.95	132.22	124.89
30	B	2630	LHG	O4-P-O5	3.95	132.74	112.28
25	3	609	CHL	CHD-C1D-C2D	3.96	127.96	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	609	CHL	O2D-CGD-CBD	3.96	120.87	111.20
30	c	2630	LHG	O4-P-O5	3.97	132.84	112.28
26	Y	602	CLA	CMB-C2B-C3B	3.97	132.26	124.89
25	7	609	CHL	O2D-CGD-CBD	3.97	120.89	111.20
30	C	2630	LHG	O4-P-O5	3.97	132.85	112.28
26	c	506	CLA	CMB-C2B-C3B	3.99	132.30	124.89
30	G	2630	LHG	O4-P-O5	3.99	132.96	112.28
30	D	410	LHG	O4-P-O5	4.00	132.97	112.28
30	d	410	LHG	O4-P-O5	4.00	132.99	112.28
26	C	506	CLA	CMB-C2B-C3B	4.00	132.32	124.89
30	g	2630	LHG	O4-P-O5	4.00	133.00	112.28
30	5	2630	LHG	O4-P-O5	4.01	133.01	112.28
30	l	2630	LHG	O4-P-O5	4.01	133.02	112.28
30	c	522	LHG	O4-P-O5	4.01	133.06	112.28
30	R	2630	LHG	O4-P-O5	4.02	133.08	112.28
30	C	522	LHG	O4-P-O5	4.02	133.08	112.28
29	n	1623	NEX	O24-C25-C38	4.02	120.05	115.02
30	r	2630	LHG	O4-P-O5	4.02	133.11	112.28
26	c	512	CLA	CMB-C2B-C3B	4.03	132.37	124.89
26	C	512	CLA	CMB-C2B-C3B	4.03	132.37	124.89
30	N	2630	LHG	O4-P-O5	4.04	133.20	112.28
29	N	1623	NEX	O24-C25-C38	4.04	120.08	115.02
30	n	2630	LHG	O4-P-O5	4.05	133.22	112.28
26	r	604	CLA	O2D-CGD-CBD	4.05	118.54	111.30
30	d	409	LHG	O4-P-O5	4.05	133.25	112.28
30	D	409	LHG	O4-P-O5	4.05	133.25	112.28
30	Y	2630	LHG	O4-P-O5	4.05	133.25	112.28
30	y	2630	LHG	O4-P-O5	4.05	133.25	112.28
36	b	621	SQD	O7-S-C6	4.06	110.30	106.83
28	R	622	XAT	O24-C25-C38	4.06	120.10	115.02
26	R	604	CLA	O2D-CGD-CBD	4.06	118.56	111.30
30	S	2630	LHG	O4-P-O5	4.06	133.31	112.28
28	n	1622	XAT	O24-C25-C38	4.07	120.11	115.02
28	N	1622	XAT	O24-C25-C38	4.07	120.11	115.02
30	s	2630	LHG	O4-P-O5	4.07	133.33	112.28
30	d	408	LHG	O4-P-O5	4.07	133.36	112.28
36	B	621	SQD	O7-S-C6	4.08	110.31	106.83
30	D	408	LHG	O4-P-O5	4.08	133.39	112.28
27	G	1621	LUT	C2-C3-C4	4.08	115.95	110.32
26	B	603	CLA	CMB-C2B-C3B	4.08	132.47	124.89
25	Y	609	CHL	O2D-CGD-CBD	4.08	121.16	111.20
28	r	622	XAT	O24-C25-C38	4.08	120.13	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	603	CLA	CMB-C2B-C3B	4.09	132.47	124.89
25	y	609	CHL	O2D-CGD-CBD	4.09	121.18	111.20
26	3	612	CLA	CMD-C2D-C3D	4.09	132.48	124.89
27	g	1621	LUT	C2-C3-C4	4.09	115.97	110.32
25	8	601	CHL	CHD-C1D-C2D	4.10	128.34	116.99
26	S	604	CLA	CMB-C2B-C3B	4.10	132.50	124.89
25	4	601	CHL	CHD-C1D-C2D	4.10	128.34	116.99
30	8	2630	LHG	O4-P-O5	4.10	133.50	112.28
30	C	523	LHG	O4-P-O5	4.10	133.51	112.28
30	c	523	LHG	O4-P-O5	4.10	133.52	112.28
25	1	601	CHL	CHD-C1D-C2D	4.11	128.37	116.99
30	4	2630	LHG	O4-P-O5	4.11	133.55	112.28
30	l	101	LHG	O4-P-O5	4.11	133.56	112.28
30	L	101	LHG	O4-P-O5	4.11	133.57	112.28
28	Y	1622	XAT	O24-C25-C38	4.11	120.17	115.02
25	y	601	CHL	CHD-C1D-C2D	4.11	128.38	116.99
25	5	601	CHL	CHD-C1D-C2D	4.12	128.39	116.99
26	s	604	CLA	CMB-C2B-C3B	4.12	132.53	124.89
26	7	612	CLA	CMD-C2D-C3D	4.12	132.53	124.89
26	r	602	CLA	CMB-C2B-C3B	4.12	132.54	124.89
25	6	609	CHL	O2D-CGD-CBD	4.13	121.27	111.20
25	2	609	CHL	O2D-CGD-CBD	4.13	121.27	111.20
25	r	608	CHL	O2D-CGD-CBD	4.13	121.27	111.20
26	S	613	CLA	CMB-C2B-C3B	4.13	132.56	124.89
25	Y	601	CHL	CHD-C1D-C2D	4.13	128.44	116.99
36	A	412	SQD	O8-S-C6	4.13	111.06	106.01
36	a	412	SQD	O8-S-C6	4.14	111.06	106.01
25	R	608	CHL	O2D-CGD-CBD	4.14	121.30	111.20
26	R	602	CLA	CMB-C2B-C3B	4.14	132.58	124.89
26	s	613	CLA	CMB-C2B-C3B	4.15	132.59	124.89
25	8	609	CHL	CHD-C1D-C2D	4.15	128.49	116.99
28	y	1622	XAT	O24-C25-C38	4.16	120.22	115.02
25	4	609	CHL	CHD-C1D-C2D	4.16	128.51	116.99
25	N	605	CHL	O2D-CGD-CBD	4.16	121.35	111.20
25	n	605	CHL	O2D-CGD-CBD	4.16	121.35	111.20
26	r	601	CLA	CAC-C3C-C4C	4.18	130.72	124.83
26	R	601	CLA	CAC-C3C-C4C	4.19	130.74	124.83
26	b	612	CLA	CMB-C2B-C3B	4.19	132.68	124.89
26	B	612	CLA	CMB-C2B-C3B	4.20	132.69	124.89
26	r	601	CLA	CBC-CAC-C3C	4.21	124.36	112.41
26	R	601	CLA	CBC-CAC-C3C	4.21	124.37	112.41
29	3	1623	NEX	O24-C25-C38	4.22	120.30	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	508	CLA	O2D-CGD-CBD	4.22	118.85	111.30
29	7	1623	NEX	O24-C25-C38	4.23	120.31	115.02
26	C	508	CLA	O2D-CGD-CBD	4.23	118.86	111.30
29	y	1623	NEX	C2-C1-C6	4.25	113.34	109.21
29	Y	1623	NEX	C2-C1-C6	4.25	113.34	109.21
26	c	509	CLA	CMB-C2B-C3B	4.27	132.82	124.89
26	g	602	CLA	CMB-C2B-C3B	4.27	132.82	124.89
26	a	405	CLA	CMB-C2B-C3B	4.29	132.84	124.89
25	3	607	CHL	CHD-C1D-C2D	4.29	128.87	116.99
26	C	509	CLA	CMB-C2B-C3B	4.29	132.86	124.89
25	7	607	CHL	CHD-C1D-C2D	4.30	128.89	116.99
26	G	602	CLA	CMB-C2B-C3B	4.30	132.87	124.89
26	A	405	CLA	CMB-C2B-C3B	4.31	132.88	124.89
26	A	406	CLA	CMB-C2B-C3B	4.32	132.91	124.89
29	S	1623	NEX	O24-C25-C38	4.32	120.43	115.02
29	s	1623	NEX	O24-C25-C38	4.32	120.43	115.02
26	a	406	CLA	CMB-C2B-C3B	4.33	132.92	124.89
36	B	621	SQD	O47-C7-C8	4.34	120.56	111.55
36	b	621	SQD	O47-C7-C8	4.35	120.58	111.55
26	s	614	CLA	CMB-C2B-C3B	4.37	133.00	124.89
26	S	614	CLA	CMB-C2B-C3B	4.37	133.00	124.89
36	B	623	SQD	O47-C7-C8	4.37	120.63	111.55
36	b	623	SQD	O47-C7-C8	4.38	120.65	111.55
36	b	623	SQD	C1-O5-C5	4.39	121.99	113.72
25	r	614	CHL	C1D-CHD-C4C	4.41	121.76	112.37
26	b	610	CLA	CMD-C2D-C3D	4.41	133.07	124.89
26	B	610	CLA	CMD-C2D-C3D	4.41	133.07	124.89
36	B	623	SQD	C1-O5-C5	4.41	122.03	113.72
25	R	614	CHL	C1D-CHD-C4C	4.42	121.79	112.37
28	g	1622	XAT	O4-C5-C18	4.45	120.59	115.02
28	G	1622	XAT	O4-C5-C18	4.45	120.59	115.02
25	8	609	CHL	C1D-CHD-C4C	4.46	121.89	112.37
25	4	609	CHL	C1D-CHD-C4C	4.48	121.91	112.37
26	D	403	CLA	CMB-C2B-C3B	4.48	133.20	124.89
28	r	622	XAT	O4-C5-C18	4.48	120.63	115.02
26	d	403	CLA	CMB-C2B-C3B	4.48	133.21	124.89
26	c	513	CLA	CMB-C2B-C3B	4.48	133.21	124.89
26	C	513	CLA	CMB-C2B-C3B	4.48	133.21	124.89
28	R	622	XAT	O4-C5-C18	4.52	120.67	115.02
25	3	607	CHL	C1D-CHD-C4C	4.52	122.01	112.37
25	7	607	CHL	C1D-CHD-C4C	4.53	122.02	112.37
26	c	510	CLA	CMB-C2B-C3B	4.55	133.34	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	601	CHL	C1D-CHD-C4C	4.56	122.08	112.37
25	4	601	CHL	C1D-CHD-C4C	4.58	122.12	112.37
28	3	1622	XAT	O24-C25-C38	4.58	120.75	115.02
26	C	510	CLA	CMB-C2B-C3B	4.58	133.39	124.89
28	7	1622	XAT	O24-C25-C38	4.59	120.76	115.02
26	s	602	CLA	CMD-C2D-C3D	4.61	133.44	124.89
26	S	602	CLA	CMD-C2D-C3D	4.61	133.44	124.89
26	c	504	CLA	CMB-C2B-C3B	4.61	133.45	124.89
26	C	504	CLA	CMB-C2B-C3B	4.63	133.48	124.89
26	N	614	CLA	CMB-C2B-C3B	4.66	133.53	124.89
26	r	603	CLA	CMB-C2B-C3B	4.66	133.53	124.89
36	A	412	SQD	O6-C1-C2	4.66	115.83	108.23
36	a	412	SQD	O6-C1-C2	4.67	115.85	108.23
26	R	603	CLA	CMB-C2B-C3B	4.68	133.57	124.89
26	n	614	CLA	CMB-C2B-C3B	4.68	133.57	124.89
25	6	609	CHL	C1D-CHD-C4C	4.69	122.37	112.37
25	2	609	CHL	C1D-CHD-C4C	4.71	122.41	112.37
25	S	608	CHL	C1D-CHD-C4C	4.71	122.41	112.37
38	d	405	PL9	C7-C3-C4	4.72	120.72	116.88
25	s	608	CHL	C1D-CHD-C4C	4.73	122.44	112.37
26	n	602	CLA	CMB-C2B-C3B	4.74	133.68	124.89
26	N	602	CLA	CMB-C2B-C3B	4.75	133.71	124.89
26	b	609	CLA	CMB-C2B-C3B	4.76	133.72	124.89
26	B	609	CLA	CMB-C2B-C3B	4.76	133.72	124.89
28	8	622	XAT	O4-C5-C18	4.76	120.98	115.02
28	4	622	XAT	O4-C5-C18	4.76	120.98	115.02
38	D	405	PL9	C7-C3-C4	4.77	120.75	116.88
25	n	607	CHL	C1D-CHD-C4C	4.88	122.77	112.37
25	N	607	CHL	C1D-CHD-C4C	4.89	122.79	112.37
25	2	606	CHL	C1D-CHD-C4C	4.89	122.79	112.37
25	R	608	CHL	C1D-CHD-C4C	4.90	122.82	112.37
25	Y	606	CHL	C1D-CHD-C4C	4.91	122.83	112.37
25	y	606	CHL	C1D-CHD-C4C	4.91	122.83	112.37
25	6	606	CHL	C1D-CHD-C4C	4.91	122.84	112.37
25	7	606	CHL	C1D-CHD-C4C	4.92	122.85	112.37
25	r	608	CHL	C1D-CHD-C4C	4.92	122.86	112.37
26	S	612	CLA	CMB-C2B-C3B	4.93	134.03	124.89
25	3	606	CHL	C1D-CHD-C4C	4.93	122.87	112.37
28	y	1622	XAT	O4-C5-C18	4.93	121.19	115.02
28	Y	1622	XAT	O4-C5-C18	4.93	121.19	115.02
36	b	623	SQD	O7-S-C6	4.93	111.04	106.83
25	Y	607	CHL	C1D-CHD-C4C	4.93	122.88	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	612	CLA	CMB-C2B-C3B	4.93	134.04	124.89
36	B	623	SQD	O7-S-C6	4.93	111.04	106.83
25	1	609	CHL	C1D-CHD-C4C	4.94	122.90	112.37
25	5	608	CHL	C1D-CHD-C4C	4.94	122.90	112.37
25	1	608	CHL	C1D-CHD-C4C	4.94	122.90	112.37
25	5	609	CHL	C1D-CHD-C4C	4.95	122.92	112.37
25	4	608	CHL	C1D-CHD-C4C	4.96	122.93	112.37
25	Y	608	CHL	C1D-CHD-C4C	4.96	122.93	112.37
25	y	607	CHL	C1D-CHD-C4C	4.96	122.93	112.37
25	y	608	CHL	C1D-CHD-C4C	4.96	122.94	112.37
25	8	608	CHL	C1D-CHD-C4C	4.97	122.96	112.37
25	s	606	CHL	C3B-C4B-NB	5.03	112.31	103.55
26	C	508	CLA	CMB-C2B-C3B	5.05	134.26	124.89
25	S	606	CHL	C3B-C4B-NB	5.05	112.36	103.55
26	c	508	CLA	CMB-C2B-C3B	5.05	134.27	124.89
25	2	608	CHL	C1D-CHD-C4C	5.06	123.16	112.37
25	6	608	CHL	C1D-CHD-C4C	5.06	123.16	112.37
25	S	607	CHL	C1D-CHD-C4C	5.06	123.16	112.37
25	s	607	CHL	C1D-CHD-C4C	5.07	123.17	112.37
26	B	613	CLA	CMD-C2D-C3D	5.07	134.30	124.89
25	r	607	CHL	C1D-CHD-C4C	5.09	123.22	112.37
25	n	608	CHL	C1D-CHD-C4C	5.09	123.23	112.37
25	R	607	CHL	C1D-CHD-C4C	5.09	123.23	112.37
25	N	608	CHL	C1D-CHD-C4C	5.10	123.24	112.37
26	b	613	CLA	CMD-C2D-C3D	5.10	134.36	124.89
25	7	609	CHL	C1D-CHD-C4C	5.11	123.26	112.37
25	8	607	CHL	C1D-CHD-C4C	5.11	123.26	112.37
25	3	609	CHL	C1D-CHD-C4C	5.12	123.28	112.37
25	5	607	CHL	C1D-CHD-C4C	5.12	123.28	112.37
25	5	606	CHL	C1D-CHD-C4C	5.12	123.29	112.37
25	G	608	CHL	C1D-CHD-C4C	5.13	123.29	112.37
25	4	607	CHL	C1D-CHD-C4C	5.13	123.29	112.37
25	2	607	CHL	C1D-CHD-C4C	5.13	123.30	112.37
25	1	607	CHL	C1D-CHD-C4C	5.13	123.30	112.37
25	5	605	CHL	C1D-CHD-C4C	5.13	123.30	112.37
25	g	608	CHL	C1D-CHD-C4C	5.13	123.31	112.37
25	1	606	CHL	C1D-CHD-C4C	5.14	123.31	112.37
25	6	607	CHL	C1D-CHD-C4C	5.14	123.33	112.37
25	S	601	CHL	C1D-CHD-C4C	5.15	123.35	112.37
26	B	613	CLA	CMB-C2B-C3B	5.15	134.45	124.89
25	1	605	CHL	C1D-CHD-C4C	5.15	123.35	112.37
25	s	601	CHL	C1D-CHD-C4C	5.15	123.36	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	607	CHL	C1D-CHD-C4C	5.16	123.37	112.37
25	g	607	CHL	C1D-CHD-C4C	5.18	123.41	112.37
26	b	613	CLA	CMB-C2B-C3B	5.18	134.51	124.89
25	n	606	CHL	C1D-CHD-C4C	5.23	123.53	112.37
25	G	607	CHL	C3B-C4B-NB	5.24	112.69	103.55
25	g	609	CHL	C1D-CHD-C4C	5.25	123.56	112.37
25	N	606	CHL	C1D-CHD-C4C	5.25	123.56	112.37
25	g	607	CHL	C3B-C4B-NB	5.26	112.72	103.55
25	2	605	CHL	C1D-CHD-C4C	5.27	123.60	112.37
25	6	605	CHL	C1D-CHD-C4C	5.28	123.61	112.37
25	G	609	CHL	C1D-CHD-C4C	5.28	123.61	112.37
25	g	605	CHL	C3B-C4B-NB	5.29	112.78	103.55
25	r	606	CHL	C1D-CHD-C4C	5.30	123.66	112.37
25	G	605	CHL	C3B-C4B-NB	5.31	112.81	103.55
25	7	608	CHL	C1D-CHD-C4C	5.31	123.69	112.37
25	R	606	CHL	C1D-CHD-C4C	5.31	123.69	112.37
25	3	608	CHL	C1D-CHD-C4C	5.34	123.75	112.37
25	G	606	CHL	C1D-CHD-C4C	5.37	123.81	112.37
25	g	606	CHL	C1D-CHD-C4C	5.38	123.84	112.37
25	y	605	CHL	C3B-C4B-NB	5.42	112.99	103.55
25	Y	605	CHL	C3B-C4B-NB	5.44	113.03	103.55
36	A	418	SQD	O9-S-C6	5.47	111.50	106.83
36	a	418	SQD	O9-S-C6	5.47	111.50	106.83
25	G	606	CHL	C3B-C4B-NB	5.50	113.13	103.55
25	g	606	CHL	C3B-C4B-NB	5.50	113.14	103.55
25	s	601	CHL	C3B-C4B-NB	5.51	113.16	103.55
25	n	609	CHL	C1D-CHD-C4C	5.52	124.13	112.37
25	N	609	CHL	C1D-CHD-C4C	5.52	124.14	112.37
25	S	601	CHL	C3B-C4B-NB	5.53	113.19	103.55
25	8	608	CHL	C3B-C4B-NB	5.53	113.19	103.55
25	4	608	CHL	C3B-C4B-NB	5.53	113.19	103.55
25	8	606	CHL	C3B-C4B-NB	5.54	113.21	103.55
25	4	606	CHL	C3B-C4B-NB	5.55	113.22	103.55
25	8	606	CHL	C1D-CHD-C4C	5.57	124.25	112.37
25	3	605	CHL	C1D-CHD-C4C	5.58	124.27	112.37
25	7	605	CHL	C1D-CHD-C4C	5.58	124.27	112.37
25	g	605	CHL	C1D-CHD-C4C	5.59	124.28	112.37
25	G	605	CHL	C1D-CHD-C4C	5.59	124.28	112.37
25	4	601	CHL	C3B-C4B-NB	5.59	113.30	103.55
25	4	606	CHL	C1D-CHD-C4C	5.59	124.29	112.37
36	B	623	SQD	O9-S-C6	5.60	111.61	106.83
25	4	609	CHL	C3B-C4B-NB	5.60	113.32	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	607	CHL	C3B-C4B-NB	5.61	113.34	103.55
25	8	601	CHL	C3B-C4B-NB	5.62	113.35	103.55
25	3	606	CHL	C3B-C4B-NB	5.62	113.35	103.55
36	b	623	SQD	O9-S-C6	5.62	111.63	106.83
25	6	605	CHL	C3B-C4B-NB	5.62	113.36	103.55
25	s	606	CHL	C1D-CHD-C4C	5.63	124.36	112.37
25	7	606	CHL	C3B-C4B-NB	5.63	113.36	103.55
25	1	601	CHL	C1D-CHD-C4C	5.63	124.37	112.37
25	2	605	CHL	C3B-C4B-NB	5.63	113.37	103.55
25	S	606	CHL	C1D-CHD-C4C	5.64	124.38	112.37
25	3	607	CHL	C3B-C4B-NB	5.64	113.38	103.55
25	8	609	CHL	C3B-C4B-NB	5.64	113.38	103.55
25	6	608	CHL	C3B-C4B-NB	5.64	113.39	103.55
25	5	601	CHL	C1D-CHD-C4C	5.65	124.42	112.37
25	2	601	CHL	C1D-CHD-C4C	5.66	124.42	112.37
25	2	608	CHL	C3B-C4B-NB	5.66	113.43	103.55
25	3	601	CHL	C3B-C4B-NB	5.67	113.43	103.55
25	6	601	CHL	C1D-CHD-C4C	5.67	124.45	112.37
25	R	606	CHL	C3B-C4B-NB	5.68	113.44	103.55
25	r	606	CHL	C3B-C4B-NB	5.68	113.45	103.55
25	7	601	CHL	C3B-C4B-NB	5.68	113.45	103.55
25	1	608	CHL	C3B-C4B-NB	5.69	113.47	103.55
25	5	608	CHL	C3B-C4B-NB	5.69	113.47	103.55
25	6	606	CHL	C3B-C4B-NB	5.69	113.47	103.55
25	2	606	CHL	C3B-C4B-NB	5.69	113.47	103.55
25	7	609	CHL	C3B-C4B-NB	5.70	113.49	103.55
25	Y	609	CHL	C1D-CHD-C4C	5.71	124.53	112.37
25	y	609	CHL	C1D-CHD-C4C	5.71	124.54	112.37
25	3	609	CHL	C3B-C4B-NB	5.72	113.52	103.55
25	4	607	CHL	C3B-C4B-NB	5.72	113.53	103.55
25	8	607	CHL	C3B-C4B-NB	5.73	113.55	103.55
25	n	606	CHL	C3B-C4B-NB	5.75	113.57	103.55
25	5	601	CHL	C3B-C4B-NB	5.75	113.58	103.55
25	1	601	CHL	C3B-C4B-NB	5.75	113.58	103.55
25	N	606	CHL	C3B-C4B-NB	5.76	113.59	103.55
25	n	605	CHL	C3B-C4B-NB	5.77	113.61	103.55
25	5	606	CHL	C3B-C4B-NB	5.77	113.62	103.55
25	y	608	CHL	C3B-C4B-NB	5.78	113.62	103.55
25	N	605	CHL	C3B-C4B-NB	5.78	113.63	103.55
25	1	606	CHL	C3B-C4B-NB	5.78	113.64	103.55
25	7	608	CHL	C3B-C4B-NB	5.79	113.64	103.55
25	6	607	CHL	C3B-C4B-NB	5.79	113.65	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	608	CHL	C3B-C4B-NB	5.79	113.65	103.55
25	2	609	CHL	C3B-C4B-NB	5.80	113.65	103.55
25	Y	608	CHL	C3B-C4B-NB	5.80	113.66	103.55
25	2	607	CHL	C3B-C4B-NB	5.81	113.67	103.55
25	7	605	CHL	C3B-C4B-NB	5.81	113.67	103.55
25	n	608	CHL	C3B-C4B-NB	5.81	113.68	103.55
25	6	609	CHL	C3B-C4B-NB	5.81	113.68	103.55
25	r	614	CHL	C3B-C4B-NB	5.81	113.68	103.55
25	N	608	CHL	C3B-C4B-NB	5.81	113.68	103.55
25	Y	606	CHL	C3B-C4B-NB	5.82	113.69	103.55
25	3	605	CHL	C3B-C4B-NB	5.82	113.69	103.55
25	R	614	CHL	C3B-C4B-NB	5.83	113.71	103.55
25	y	605	CHL	C1D-CHD-C4C	5.83	124.79	112.37
25	Y	605	CHL	C1D-CHD-C4C	5.83	124.80	112.37
25	y	606	CHL	C3B-C4B-NB	5.84	113.73	103.55
25	N	601	CHL	C3B-C4B-NB	5.85	113.75	103.55
25	G	608	CHL	C3B-C4B-NB	5.87	113.78	103.55
25	n	601	CHL	C3B-C4B-NB	5.87	113.79	103.55
25	R	614	CHL	CMB-C2B-C3B	5.88	127.37	113.69
25	r	614	CHL	CMB-C2B-C3B	5.88	127.37	113.69
28	Y	1622	XAT	O4-C5-C4	5.89	117.60	113.33
25	R	608	CHL	C3B-C4B-NB	5.89	113.81	103.55
25	g	608	CHL	C3B-C4B-NB	5.89	113.82	103.55
28	y	1622	XAT	O4-C5-C4	5.89	117.60	113.33
25	r	608	CHL	C3B-C4B-NB	5.91	113.85	103.55
25	Y	607	CHL	C3B-C4B-NB	5.91	113.85	103.55
25	N	601	CHL	C1D-CHD-C4C	5.91	124.97	112.37
25	n	601	CHL	C1D-CHD-C4C	5.91	124.97	112.37
25	S	608	CHL	C3B-C4B-NB	5.91	113.86	103.55
25	y	607	CHL	C3B-C4B-NB	5.92	113.87	103.55
25	s	608	CHL	C3B-C4B-NB	5.93	113.89	103.55
25	R	607	CHL	C3B-C4B-NB	5.93	113.89	103.55
25	5	605	CHL	C3B-C4B-NB	5.95	113.92	103.55
25	1	605	CHL	C3B-C4B-NB	5.95	113.93	103.55
25	r	607	CHL	C3B-C4B-NB	5.95	113.93	103.55
25	5	607	CHL	C3B-C4B-NB	5.97	113.96	103.55
25	6	601	CHL	C3B-C4B-NB	5.97	113.96	103.55
25	1	607	CHL	C3B-C4B-NB	5.98	113.97	103.55
25	2	601	CHL	C3B-C4B-NB	5.99	114.00	103.55
25	g	601	CHL	C3B-C4B-NB	6.00	114.00	103.55
25	n	605	CHL	C1D-CHD-C4C	6.02	125.21	112.37
25	G	601	CHL	C3B-C4B-NB	6.03	114.06	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	609	CHL	C3B-C4B-NB	6.03	114.06	103.55
36	b	621	SQD	O9-S-C6	6.03	111.98	106.83
25	1	609	CHL	C3B-C4B-NB	6.03	114.06	103.55
28	g	1622	XAT	O4-C5-C4	6.03	117.71	113.33
25	N	605	CHL	C1D-CHD-C4C	6.04	125.24	112.37
36	B	621	SQD	O9-S-C6	6.05	112.00	106.83
28	G	1622	XAT	O4-C5-C4	6.06	117.73	113.33
25	n	607	CHL	C3B-C4B-NB	6.07	114.14	103.55
25	N	607	CHL	C3B-C4B-NB	6.07	114.14	103.55
25	7	601	CHL	C1D-CHD-C4C	6.08	125.32	112.37
25	3	601	CHL	C1D-CHD-C4C	6.08	125.32	112.37
25	6	609	CHL	CMB-C2B-C3B	6.08	127.83	113.69
25	2	609	CHL	CMB-C2B-C3B	6.08	127.84	113.69
25	S	606	CHL	CMB-C2B-C3B	6.09	127.86	113.69
25	s	606	CHL	CMB-C2B-C3B	6.09	127.86	113.69
25	Y	601	CHL	C1D-CHD-C4C	6.12	125.41	112.37
25	y	601	CHL	C1D-CHD-C4C	6.12	125.41	112.37
25	Y	601	CHL	CMB-C2B-C3B	6.13	127.95	113.69
25	G	601	CHL	C1D-CHD-C4C	6.14	125.45	112.37
25	g	601	CHL	C1D-CHD-C4C	6.15	125.47	112.37
25	y	601	CHL	CMB-C2B-C3B	6.15	128.00	113.69
25	1	601	CHL	C4B-CHC-C1C	6.27	125.74	112.37
25	7	605	CHL	C4B-CHC-C1C	6.28	125.75	112.37
25	5	601	CHL	C4B-CHC-C1C	6.29	125.77	112.37
25	y	609	CHL	C3B-C4B-NB	6.29	114.52	103.55
25	Y	609	CHL	C3B-C4B-NB	6.29	114.52	103.55
25	3	605	CHL	C4B-CHC-C1C	6.29	125.78	112.37
25	1	606	CHL	C4B-CHC-C1C	6.32	125.84	112.37
25	5	606	CHL	C4B-CHC-C1C	6.33	125.86	112.37
25	Y	601	CHL	C3B-C4B-NB	6.34	114.61	103.55
25	s	601	CHL	C4B-CHC-C1C	6.35	125.89	112.37
25	y	601	CHL	C3B-C4B-NB	6.35	114.62	103.55
25	S	607	CHL	C3B-C4B-NB	6.36	114.63	103.55
25	4	607	CHL	C4B-CHC-C1C	6.36	125.92	112.37
25	S	601	CHL	C4B-CHC-C1C	6.36	125.92	112.37
25	s	607	CHL	C3B-C4B-NB	6.36	114.64	103.55
25	8	607	CHL	C4B-CHC-C1C	6.38	125.96	112.37
25	r	606	CHL	CMB-C2B-C3B	6.40	128.57	113.69
25	R	606	CHL	CMB-C2B-C3B	6.41	128.59	113.69
25	N	609	CHL	C3B-C4B-NB	6.41	114.73	103.55
25	n	609	CHL	C3B-C4B-NB	6.42	114.74	103.55
25	1	608	CHL	CMB-C2B-C3B	6.45	128.70	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	608	CHL	CMB-C2B-C3B	6.46	128.72	113.69
25	G	606	CHL	C4B-CHC-C1C	6.50	126.21	112.37
28	3	1622	XAT	O24-C25-C24	6.50	118.05	113.33
25	3	607	CHL	CMB-C2B-C3B	6.51	128.84	113.69
25	g	606	CHL	C4B-CHC-C1C	6.51	126.25	112.37
28	7	1622	XAT	O24-C25-C24	6.52	118.06	113.33
25	7	607	CHL	CMB-C2B-C3B	6.52	128.86	113.69
25	n	605	CHL	CMB-C2B-C3B	6.52	128.86	113.69
25	N	605	CHL	CMB-C2B-C3B	6.53	128.88	113.69
25	S	607	CHL	CMB-C2B-C3B	6.53	128.88	113.69
25	s	607	CHL	CMB-C2B-C3B	6.53	128.88	113.69
25	G	609	CHL	C3B-C4B-NB	6.54	114.96	103.55
25	n	606	CHL	C4B-CHC-C1C	6.54	126.31	112.37
28	8	622	XAT	O4-C5-C4	6.55	118.08	113.33
25	G	608	CHL	CMB-C2B-C3B	6.56	128.94	113.69
25	N	606	CHL	C4B-CHC-C1C	6.56	126.35	112.37
25	g	608	CHL	CMB-C2B-C3B	6.56	128.96	113.69
25	g	609	CHL	C3B-C4B-NB	6.57	115.00	103.55
25	4	607	CHL	CMB-C2B-C3B	6.57	128.98	113.69
25	5	609	CHL	CMB-C2B-C3B	6.58	128.99	113.69
25	8	607	CHL	CMB-C2B-C3B	6.59	129.02	113.69
25	G	601	CHL	CMB-C2B-C3B	6.59	129.02	113.69
25	g	601	CHL	CMB-C2B-C3B	6.59	129.02	113.69
25	1	609	CHL	CMB-C2B-C3B	6.59	129.03	113.69
25	2	607	CHL	C4B-CHC-C1C	6.59	126.42	112.37
28	4	622	XAT	O4-C5-C4	6.61	118.12	113.33
25	6	607	CHL	C4B-CHC-C1C	6.61	126.45	112.37
25	3	607	CHL	C4B-CHC-C1C	6.61	126.45	112.37
25	7	607	CHL	C4B-CHC-C1C	6.62	126.47	112.37
25	5	607	CHL	C4B-CHC-C1C	6.64	126.51	112.37
25	1	607	CHL	C4B-CHC-C1C	6.64	126.51	112.37
36	A	412	SQD	O9-S-C6	6.64	112.50	106.83
25	4	606	CHL	CMB-C2B-C3B	6.64	129.14	113.69
25	8	606	CHL	CMB-C2B-C3B	6.64	129.14	113.69
25	Y	606	CHL	C4B-CHC-C1C	6.65	126.54	112.37
36	a	412	SQD	O9-S-C6	6.65	112.51	106.83
25	y	606	CHL	C4B-CHC-C1C	6.66	126.56	112.37
25	2	609	CHL	C4B-CHC-C1C	6.66	126.56	112.37
25	8	606	CHL	C4B-CHC-C1C	6.66	126.56	112.37
28	5	1622	XAT	O4-C5-C4	6.66	118.16	113.33
25	6	609	CHL	C4B-CHC-C1C	6.67	126.58	112.37
25	4	606	CHL	C4B-CHC-C1C	6.67	126.58	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	1622	XAT	O4-C5-C4	6.68	118.17	113.33
25	3	601	CHL	CMB-C2B-C3B	6.68	129.23	113.69
25	4	601	CHL	C4B-CHC-C1C	6.68	126.61	112.37
25	8	601	CHL	C4B-CHC-C1C	6.70	126.64	112.37
25	7	601	CHL	CMB-C2B-C3B	6.70	129.27	113.69
25	N	607	CHL	C4B-CHC-C1C	6.70	126.65	112.37
25	7	605	CHL	CMB-C2B-C3B	6.71	129.29	113.69
25	5	607	CHL	CMB-C2B-C3B	6.71	129.30	113.69
25	1	607	CHL	CMB-C2B-C3B	6.71	129.30	113.69
25	8	609	CHL	C4B-CHC-C1C	6.71	126.67	112.37
25	2	605	CHL	C4B-CHC-C1C	6.71	126.67	112.37
25	3	605	CHL	CMB-C2B-C3B	6.71	129.31	113.69
25	6	605	CHL	C4B-CHC-C1C	6.72	126.68	112.37
25	4	608	CHL	CMB-C2B-C3B	6.72	129.31	113.69
25	n	607	CHL	C4B-CHC-C1C	6.72	126.69	112.37
25	4	609	CHL	C4B-CHC-C1C	6.72	126.69	112.37
25	2	607	CHL	CMB-C2B-C3B	6.72	129.33	113.69
25	8	608	CHL	CMB-C2B-C3B	6.73	129.34	113.69
25	2	606	CHL	CMB-C2B-C3B	6.73	129.34	113.69
25	8	608	CHL	C4B-CHC-C1C	6.73	126.71	112.37
25	6	606	CHL	CMB-C2B-C3B	6.73	129.35	113.69
25	6	607	CHL	CMB-C2B-C3B	6.74	129.36	113.69
25	n	601	CHL	CMB-C2B-C3B	6.74	129.37	113.69
25	4	608	CHL	C4B-CHC-C1C	6.74	126.74	112.37
25	1	609	CHL	C4B-CHC-C1C	6.75	126.75	112.37
25	5	609	CHL	C4B-CHC-C1C	6.75	126.75	112.37
25	N	601	CHL	CMB-C2B-C3B	6.76	129.41	113.69
25	3	609	CHL	C4B-CHC-C1C	6.76	126.77	112.37
25	r	607	CHL	CMB-C2B-C3B	6.76	129.42	113.69
25	7	609	CHL	C4B-CHC-C1C	6.77	126.79	112.37
25	R	607	CHL	CMB-C2B-C3B	6.77	129.45	113.69
25	n	608	CHL	CMB-C2B-C3B	6.83	129.58	113.69
25	2	601	CHL	CMB-C2B-C3B	6.83	129.59	113.69
25	N	608	CHL	CMB-C2B-C3B	6.84	129.59	113.69
25	R	608	CHL	CMB-C2B-C3B	6.84	129.59	113.69
25	r	608	CHL	CMB-C2B-C3B	6.84	129.59	113.69
25	3	608	CHL	CMB-C2B-C3B	6.84	129.59	113.69
25	Y	608	CHL	CMB-C2B-C3B	6.84	129.60	113.69
25	y	605	CHL	CMB-C2B-C3B	6.85	129.61	113.69
25	7	608	CHL	CMB-C2B-C3B	6.85	129.62	113.69
25	6	601	CHL	CMB-C2B-C3B	6.85	129.63	113.69
25	y	608	CHL	CMB-C2B-C3B	6.86	129.64	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	605	CHL	CMB-C2B-C3B	6.86	129.65	113.69
36	A	418	SQD	O7-S-C6	6.86	112.69	106.83
25	8	609	CHL	CMB-C2B-C3B	6.87	129.68	113.69
25	6	605	CHL	CMB-C2B-C3B	6.87	129.68	113.69
25	4	609	CHL	CMB-C2B-C3B	6.87	129.68	113.69
25	2	605	CHL	CMB-C2B-C3B	6.89	129.71	113.69
25	5	605	CHL	CMB-C2B-C3B	6.90	129.75	113.69
36	a	418	SQD	O7-S-C6	6.91	112.73	106.83
25	1	605	CHL	CMB-C2B-C3B	6.91	129.76	113.69
25	S	608	CHL	CMB-C2B-C3B	6.95	129.85	113.69
25	s	608	CHL	CMB-C2B-C3B	6.95	129.85	113.69
25	3	609	CHL	CMB-C2B-C3B	6.96	129.87	113.69
25	7	609	CHL	CMB-C2B-C3B	6.96	129.89	113.69
25	r	606	CHL	C4B-CHC-C1C	6.97	127.21	112.37
25	2	606	CHL	C4B-CHC-C1C	6.97	127.22	112.37
25	2	608	CHL	CMB-C2B-C3B	6.97	129.90	113.69
25	6	608	CHL	CMB-C2B-C3B	6.97	129.91	113.69
25	R	606	CHL	C4B-CHC-C1C	6.98	127.24	112.37
25	8	601	CHL	CMB-C2B-C3B	6.98	129.93	113.69
25	6	606	CHL	C4B-CHC-C1C	6.99	127.26	112.37
25	3	606	CHL	CMB-C2B-C3B	6.99	129.94	113.69
25	G	605	CHL	CMB-C2B-C3B	6.99	129.95	113.69
25	3	606	CHL	C4B-CHC-C1C	6.99	127.27	112.37
25	4	601	CHL	CMB-C2B-C3B	6.99	129.96	113.69
25	7	606	CHL	C4B-CHC-C1C	7.00	127.28	112.37
25	5	601	CHL	CMB-C2B-C3B	7.00	129.98	113.69
25	1	601	CHL	CMB-C2B-C3B	7.00	129.98	113.69
25	g	605	CHL	CMB-C2B-C3B	7.00	129.98	113.69
25	7	606	CHL	CMB-C2B-C3B	7.01	129.99	113.69
25	S	607	CHL	C4B-CHC-C1C	7.01	127.31	112.37
25	g	607	CHL	CMB-C2B-C3B	7.01	130.00	113.69
25	1	606	CHL	CMB-C2B-C3B	7.01	130.00	113.69
25	s	607	CHL	C4B-CHC-C1C	7.02	127.32	112.37
25	1	605	CHL	C4B-CHC-C1C	7.02	127.33	112.37
25	5	606	CHL	CMB-C2B-C3B	7.02	130.03	113.69
25	G	607	CHL	CMB-C2B-C3B	7.03	130.03	113.69
25	5	605	CHL	C4B-CHC-C1C	7.03	127.35	112.37
25	s	606	CHL	C4B-CHC-C1C	7.09	127.47	112.37
25	S	606	CHL	C4B-CHC-C1C	7.10	127.49	112.37
25	r	614	CHL	C4B-CHC-C1C	7.13	127.56	112.37
25	R	614	CHL	C4B-CHC-C1C	7.13	127.56	112.37
25	y	609	CHL	CMB-C2B-C3B	7.19	130.42	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	601	CHL	CMB-C2B-C3B	7.20	130.43	113.69
25	s	601	CHL	CMB-C2B-C3B	7.20	130.43	113.69
25	G	605	CHL	C4B-CHC-C1C	7.20	127.71	112.37
25	7	601	CHL	C4B-CHC-C1C	7.20	127.72	112.37
25	g	607	CHL	C4B-CHC-C1C	7.20	127.72	112.37
29	S	1623	NEX	O24-C25-C24	7.21	118.56	113.33
25	Y	609	CHL	CMB-C2B-C3B	7.21	130.46	113.69
25	g	605	CHL	C4B-CHC-C1C	7.21	127.74	112.37
29	s	1623	NEX	O24-C25-C24	7.22	118.57	113.33
25	3	601	CHL	C4B-CHC-C1C	7.22	127.75	112.37
25	Y	607	CHL	CMB-C2B-C3B	7.22	130.49	113.69
25	G	607	CHL	C4B-CHC-C1C	7.22	127.76	112.37
25	y	607	CHL	CMB-C2B-C3B	7.24	130.53	113.69
25	Y	605	CHL	C4B-CHC-C1C	7.26	127.85	112.37
25	y	605	CHL	C4B-CHC-C1C	7.26	127.85	112.37
25	G	601	CHL	C4B-CHC-C1C	7.28	127.88	112.37
25	N	609	CHL	CMB-C2B-C3B	7.28	130.63	113.69
25	3	608	CHL	C4B-CHC-C1C	7.29	127.89	112.37
25	g	601	CHL	C4B-CHC-C1C	7.29	127.90	112.37
25	n	609	CHL	CMB-C2B-C3B	7.29	130.65	113.69
25	n	607	CHL	CMB-C2B-C3B	7.29	130.66	113.69
25	7	608	CHL	C4B-CHC-C1C	7.30	127.92	112.37
25	6	608	CHL	C4B-CHC-C1C	7.30	127.93	112.37
25	N	607	CHL	CMB-C2B-C3B	7.30	130.68	113.69
25	2	608	CHL	C4B-CHC-C1C	7.30	127.93	112.37
25	2	601	CHL	C4B-CHC-C1C	7.30	127.94	112.37
25	n	609	CHL	C4B-CHC-C1C	7.31	127.94	112.37
25	6	601	CHL	C4B-CHC-C1C	7.31	127.94	112.37
25	5	608	CHL	C4B-CHC-C1C	7.32	127.96	112.37
25	N	605	CHL	C4B-CHC-C1C	7.32	127.97	112.37
25	G	609	CHL	CMB-C2B-C3B	7.32	130.72	113.69
25	g	609	CHL	CMB-C2B-C3B	7.33	130.75	113.69
25	1	608	CHL	C4B-CHC-C1C	7.33	128.00	112.37
25	Y	606	CHL	CMB-C2B-C3B	7.33	130.75	113.69
25	N	609	CHL	C4B-CHC-C1C	7.34	128.00	112.37
25	n	605	CHL	C4B-CHC-C1C	7.34	128.01	112.37
25	y	606	CHL	CMB-C2B-C3B	7.34	130.77	113.69
25	y	609	CHL	C4B-CHC-C1C	7.41	128.15	112.37
25	Y	609	CHL	C4B-CHC-C1C	7.41	128.15	112.37
25	n	606	CHL	CMB-C2B-C3B	7.41	130.92	113.69
25	y	607	CHL	C4B-CHC-C1C	7.41	128.16	112.37
25	Y	607	CHL	C4B-CHC-C1C	7.42	128.19	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	606	CHL	CMB-C2B-C3B	7.43	130.97	113.69
25	y	601	CHL	C4B-CHC-C1C	7.49	128.33	112.37
25	Y	601	CHL	C4B-CHC-C1C	7.50	128.35	112.37
25	N	601	CHL	C4B-CHC-C1C	7.51	128.37	112.37
25	n	601	CHL	C4B-CHC-C1C	7.51	128.38	112.37
28	r	622	XAT	O24-C25-C24	7.52	118.79	113.33
28	R	622	XAT	O24-C25-C24	7.55	118.81	113.33
25	s	608	CHL	C4B-CHC-C1C	7.60	128.57	112.37
25	S	608	CHL	C4B-CHC-C1C	7.61	128.58	112.37
25	G	606	CHL	CMB-C2B-C3B	7.64	131.47	113.69
25	g	606	CHL	CMB-C2B-C3B	7.66	131.50	113.69
25	g	609	CHL	C4B-CHC-C1C	7.70	128.77	112.37
25	G	609	CHL	C4B-CHC-C1C	7.71	128.80	112.37
28	3	1622	XAT	O4-C5-C4	7.73	118.94	113.33
25	R	608	CHL	C4B-CHC-C1C	7.76	128.91	112.37
25	r	608	CHL	C4B-CHC-C1C	7.76	128.91	112.37
28	7	1622	XAT	O4-C5-C4	7.77	118.97	113.33
28	y	1622	XAT	O24-C25-C24	7.80	118.99	113.33
25	g	608	CHL	C4B-CHC-C1C	7.82	129.02	112.37
25	G	608	CHL	C4B-CHC-C1C	7.82	129.03	112.37
29	N	1623	NEX	O24-C25-C24	7.83	119.01	113.33
29	n	1623	NEX	O24-C25-C24	7.84	119.02	113.33
28	Y	1622	XAT	O24-C25-C24	7.85	119.03	113.33
28	4	622	XAT	O24-C25-C24	7.86	119.03	113.33
29	7	1623	NEX	O24-C25-C24	7.88	119.05	113.33
28	8	622	XAT	O24-C25-C24	7.91	119.07	113.33
28	N	1622	XAT	O24-C25-C24	7.92	119.08	113.33
28	n	1622	XAT	O24-C25-C24	7.96	119.10	113.33
29	3	1623	NEX	O24-C25-C24	7.96	119.11	113.33
28	R	622	XAT	O4-C5-C4	7.96	119.11	113.33
28	n	1622	XAT	O4-C5-C4	7.99	119.13	113.33
29	r	623	NEX	O24-C25-C24	8.00	119.13	113.33
29	R	623	NEX	O24-C25-C24	8.00	119.14	113.33
28	N	1622	XAT	O4-C5-C4	8.01	119.14	113.33
28	r	622	XAT	O4-C5-C4	8.02	119.15	113.33
25	n	608	CHL	C4B-CHC-C1C	8.10	129.63	112.37
25	N	608	CHL	C4B-CHC-C1C	8.11	129.66	112.37
25	Y	608	CHL	C4B-CHC-C1C	8.12	129.68	112.37
25	y	608	CHL	C4B-CHC-C1C	8.13	129.69	112.37
25	R	607	CHL	C4B-CHC-C1C	8.18	129.79	112.37
25	r	607	CHL	C4B-CHC-C1C	8.18	129.81	112.37
29	y	1623	NEX	O24-C25-C24	8.63	119.59	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	1623	NEX	O24-C25-C24	8.65	119.60	113.33
28	G	1622	XAT	O24-C25-C24	8.97	119.83	113.33
28	g	1622	XAT	O24-C25-C24	9.06	119.90	113.33
29	G	1623	NEX	O24-C25-C24	9.23	120.02	113.33
29	g	1623	NEX	O24-C25-C24	9.24	120.03	113.33
29	6	1623	NEX	O24-C25-C24	9.30	120.08	113.33
29	2	1623	NEX	O24-C25-C24	9.34	120.11	113.33
28	6	1622	XAT	O4-C5-C4	9.38	120.14	113.33
28	2	1622	XAT	O4-C5-C4	9.44	120.17	113.33
28	5	1622	XAT	O24-C25-C24	9.51	120.23	113.33
28	1	1622	XAT	O24-C25-C24	9.52	120.24	113.33
29	5	1623	NEX	O24-C25-C24	9.55	120.25	113.33
29	1	1623	NEX	O24-C25-C24	9.59	120.29	113.33
28	6	1622	XAT	O24-C25-C24	10.68	121.08	113.33
28	2	1622	XAT	O24-C25-C24	10.76	121.14	113.33

All (626) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
26	R	613	CLA	NC
26	R	613	CLA	ND
26	R	613	CLA	NA
26	3	612	CLA	NC
26	3	612	CLA	ND
26	3	612	CLA	NA
26	r	601	CLA	NC
26	r	601	CLA	ND
26	r	601	CLA	NA
26	1	613	CLA	NC
26	1	613	CLA	NA
26	6	611	CLA	NC
26	6	611	CLA	NA
26	c	511	CLA	NC
26	c	511	CLA	ND
26	c	511	CLA	NA
26	s	610	CLA	NC
26	s	610	CLA	ND
26	s	610	CLA	NA
26	g	612	CLA	NC
26	g	612	CLA	ND
26	g	612	CLA	NA
26	6	613	CLA	NC

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Mol	Chain	Res	Type	Atom
26	6	613	CLA	NA
26	b	605	CLA	NC
26	b	605	CLA	ND
26	b	605	CLA	NA
26	4	602	CLA	NC
26	4	602	CLA	ND
26	4	602	CLA	NA
26	b	615	CLA	NC
26	b	615	CLA	ND
26	b	615	CLA	NA
26	B	617	CLA	NC
26	B	617	CLA	ND
26	B	617	CLA	NA
26	N	613	CLA	NC
26	N	613	CLA	ND
26	N	613	CLA	NA
26	B	615	CLA	NC
26	B	615	CLA	ND
26	B	615	CLA	NA
26	b	603	CLA	NC
26	b	603	CLA	ND
26	b	603	CLA	NA
26	b	609	CLA	NC
26	b	609	CLA	NA
26	Y	610	CLA	NC
26	Y	610	CLA	NA
26	Y	610	CLA	ND
26	A	410	CLA	NC
26	A	410	CLA	ND
26	A	410	CLA	NA
26	2	612	CLA	NC
26	2	612	CLA	ND
26	2	612	CLA	NA
26	3	610	CLA	NC
26	3	610	CLA	ND
26	3	610	CLA	NA
26	s	612	CLA	NC
26	s	612	CLA	ND
26	s	612	CLA	NA
26	y	603	CLA	NC
26	y	603	CLA	ND
26	y	603	CLA	NA

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Mol	Chain	Res	Type	Atom
26	6	603	CLA	NC
26	6	603	CLA	ND
26	6	603	CLA	NA
26	s	602	CLA	NC
26	s	602	CLA	ND
26	s	602	CLA	NA
26	s	611	CLA	NC
26	s	611	CLA	ND
26	s	611	CLA	NA
26	1	604	CLA	NC
26	1	604	CLA	NA
26	N	611	CLA	NC
26	N	611	CLA	ND
26	N	611	CLA	NA
26	4	611	CLA	NC
26	4	611	CLA	ND
26	4	611	CLA	NA
26	8	604	CLA	NC
26	8	604	CLA	NA
26	5	614	CLA	NC
26	5	614	CLA	ND
26	5	614	CLA	NA
26	y	611	CLA	NC
26	y	611	CLA	ND
26	y	611	CLA	NA
26	7	611	CLA	NC
26	7	611	CLA	ND
26	7	611	CLA	NA
26	6	612	CLA	NC
26	6	612	CLA	ND
26	6	612	CLA	NA
26	b	614	CLA	NC
26	b	614	CLA	ND
26	b	614	CLA	NA
26	n	604	CLA	NC
26	n	604	CLA	ND
26	n	604	CLA	NA
26	1	611	CLA	NC
26	1	611	CLA	ND
26	1	611	CLA	NA
26	n	603	CLA	NC
26	n	603	CLA	ND

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Mol	Chain	Res	Type	Atom
26	n	603	CLA	NA
26	Y	603	CLA	NC
26	Y	603	CLA	ND
26	Y	603	CLA	NA
26	A	405	CLA	NC
26	A	405	CLA	ND
26	A	405	CLA	NA
26	1	602	CLA	NC
26	1	602	CLA	ND
26	1	602	CLA	NA
26	5	611	CLA	NC
26	5	611	CLA	ND
26	5	611	CLA	NA
26	3	604	CLA	NC
26	3	604	CLA	ND
26	3	604	CLA	NA
26	S	602	CLA	NC
26	S	602	CLA	ND
26	S	602	CLA	NA
26	G	603	CLA	NC
26	G	603	CLA	ND
26	G	603	CLA	NA
26	B	610	CLA	NC
26	B	610	CLA	NA
26	C	502	CLA	NC
26	C	502	CLA	ND
26	C	502	CLA	NA
26	s	614	CLA	NC
26	s	614	CLA	ND
26	s	614	CLA	NA
26	2	604	CLA	NC
26	2	604	CLA	ND
26	2	604	CLA	NA
26	5	603	CLA	NC
26	5	603	CLA	NA
26	5	603	CLA	ND
26	B	603	CLA	NC
26	B	603	CLA	ND
26	B	603	CLA	NA
26	S	610	CLA	NC
26	S	610	CLA	ND
26	S	610	CLA	NA

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Mol	Chain	Res	Type	Atom
26	G	612	CLA	NC
26	G	612	CLA	ND
26	G	612	CLA	NA
26	A	407	CLA	NC
26	A	407	CLA	NA
26	C	511	CLA	NC
26	C	511	CLA	ND
26	C	511	CLA	NA
26	n	611	CLA	NC
26	n	611	CLA	ND
26	n	611	CLA	NA
26	S	613	CLA	NC
26	S	613	CLA	ND
26	S	613	CLA	NA
26	4	612	CLA	NC
26	4	612	CLA	ND
26	4	612	CLA	NA
26	3	614	CLA	NC
26	3	614	CLA	ND
26	3	614	CLA	NA
26	y	612	CLA	NC
26	y	612	CLA	ND
26	y	612	CLA	NA
26	B	613	CLA	NC
26	B	613	CLA	ND
26	B	613	CLA	NA
26	N	614	CLA	NC
26	N	614	CLA	ND
26	N	614	CLA	NA
26	5	613	CLA	NC
26	5	613	CLA	NA
26	Y	604	CLA	NC
26	Y	604	CLA	ND
26	Y	604	CLA	NA
26	2	603	CLA	NC
26	2	603	CLA	NA
26	2	603	CLA	ND
26	D	402	CLA	NC
26	D	402	CLA	ND
26	D	402	CLA	NA
26	3	611	CLA	NC
26	3	611	CLA	ND

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Mol	Chain	Res	Type	Atom
26	3	611	CLA	NA
26	3	613	CLA	NC
26	3	613	CLA	ND
26	3	613	CLA	NA
26	b	606	CLA	NC
26	b	606	CLA	ND
26	b	606	CLA	NA
26	y	602	CLA	NC
26	y	602	CLA	ND
26	y	602	CLA	NA
26	R	610	CLA	NC
26	R	610	CLA	ND
26	R	610	CLA	NA
26	6	610	CLA	NC
26	6	610	CLA	ND
26	6	610	CLA	NA
26	r	603	CLA	NC
26	r	603	CLA	ND
26	r	603	CLA	NA
26	G	614	CLA	NC
26	G	614	CLA	ND
26	G	614	CLA	NA
26	B	602	CLA	NC
26	B	602	CLA	ND
26	B	602	CLA	NA
26	C	503	CLA	NC
26	C	503	CLA	ND
26	C	503	CLA	NA
26	7	614	CLA	NC
26	7	614	CLA	ND
26	7	614	CLA	NA
26	r	613	CLA	NC
26	r	613	CLA	ND
26	r	613	CLA	NA
26	R	611	CLA	NC
26	R	611	CLA	ND
26	R	611	CLA	NA
26	3	603	CLA	NC
26	3	603	CLA	NA
26	3	603	CLA	ND
26	N	604	CLA	NC
26	N	604	CLA	ND

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Mol	Chain	Res	Type	Atom
26	N	604	CLA	NA
26	5	610	CLA	NC
26	5	610	CLA	ND
26	5	610	CLA	NA
26	b	607	CLA	NC
26	b	607	CLA	ND
26	b	607	CLA	NA
26	8	610	CLA	NC
26	8	610	CLA	ND
26	8	610	CLA	NA
26	4	604	CLA	NC
26	4	604	CLA	NA
26	6	604	CLA	NC
26	6	604	CLA	ND
26	6	604	CLA	NA
26	R	601	CLA	NC
26	R	601	CLA	ND
26	R	601	CLA	NA
26	8	602	CLA	NC
26	8	602	CLA	ND
26	8	602	CLA	NA
26	G	604	CLA	NC
26	G	604	CLA	ND
26	G	604	CLA	NA
26	n	602	CLA	NC
26	n	602	CLA	ND
26	n	602	CLA	NA
26	b	604	CLA	NC
26	b	604	CLA	ND
26	b	604	CLA	NA
26	y	614	CLA	NC
26	y	614	CLA	ND
26	y	614	CLA	NA
26	r	609	CLA	NC
26	r	609	CLA	ND
26	r	609	CLA	NA
26	2	610	CLA	NC
26	2	610	CLA	ND
26	2	610	CLA	NA
26	a	407	CLA	NC
26	a	407	CLA	NA
26	r	612	CLA	NC

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Mol	Chain	Res	Type	Atom
26	r	612	CLA	ND
26	r	612	CLA	NA
26	2	611	CLA	NC
26	2	611	CLA	NA
26	4	610	CLA	NC
26	4	610	CLA	ND
26	4	610	CLA	NA
26	y	610	CLA	NC
26	y	610	CLA	NA
26	y	610	CLA	ND
26	S	609	CLA	NC
26	S	609	CLA	ND
26	S	609	CLA	NA
26	N	610	CLA	NC
26	N	610	CLA	NA
26	N	610	CLA	ND
26	c	509	CLA	NC
26	c	509	CLA	ND
26	c	509	CLA	NA
26	g	613	CLA	NC
26	g	613	CLA	ND
26	g	613	CLA	NA
26	c	507	CLA	NC
26	c	507	CLA	ND
26	c	507	CLA	NA
26	B	609	CLA	NC
26	B	609	CLA	NA
26	N	602	CLA	NC
26	N	602	CLA	ND
26	N	602	CLA	NA
26	g	614	CLA	NC
26	g	614	CLA	ND
26	g	614	CLA	NA
26	B	605	CLA	NC
26	B	605	CLA	ND
26	B	605	CLA	NA
26	C	501	CLA	NC
26	C	501	CLA	ND
26	C	501	CLA	NA
26	b	610	CLA	NC
26	b	610	CLA	NA
26	c	504	CLA	NC

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Mol	Chain	Res	Type	Atom
26	c	504	CLA	ND
26	c	504	CLA	NA
26	3	602	CLA	NC
26	3	602	CLA	ND
26	3	602	CLA	NA
26	R	616	CLA	NC
26	R	616	CLA	NA
26	1	610	CLA	NC
26	1	610	CLA	ND
26	1	610	CLA	NA
26	S	614	CLA	NC
26	S	614	CLA	ND
26	S	614	CLA	NA
26	b	613	CLA	NC
26	b	613	CLA	ND
26	b	613	CLA	NA
26	5	602	CLA	NC
26	5	602	CLA	ND
26	5	602	CLA	NA
26	b	616	CLA	NC
26	b	616	CLA	ND
26	b	616	CLA	NA
26	d	403	CLA	NC
26	d	403	CLA	NA
26	7	602	CLA	NC
26	7	602	CLA	ND
26	7	602	CLA	NA
26	R	602	CLA	NC
26	R	602	CLA	ND
26	R	602	CLA	NA
26	S	611	CLA	NC
26	S	611	CLA	ND
26	S	611	CLA	NA
26	R	612	CLA	NC
26	R	612	CLA	ND
26	R	612	CLA	NA
26	B	612	CLA	NC
26	B	612	CLA	ND
26	B	612	CLA	NA
26	8	603	CLA	NC
26	8	603	CLA	NA
26	8	603	CLA	ND

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Mol	Chain	Res	Type	Atom
26	c	506	CLA	NC
26	c	506	CLA	ND
26	c	506	CLA	NA
26	c	503	CLA	NC
26	c	503	CLA	ND
26	c	503	CLA	NA
26	b	611	CLA	NC
26	b	611	CLA	ND
26	b	611	CLA	NA
26	5	612	CLA	NC
26	5	612	CLA	NA
26	5	612	CLA	ND
26	n	614	CLA	NC
26	n	614	CLA	ND
26	n	614	CLA	NA
26	1	603	CLA	NC
26	1	603	CLA	NA
26	1	603	CLA	ND
26	G	611	CLA	NC
26	G	611	CLA	ND
26	G	611	CLA	NA
26	g	603	CLA	NC
26	g	603	CLA	ND
26	g	603	CLA	NA
26	c	505	CLA	NC
26	c	505	CLA	ND
26	c	505	CLA	NA
26	Y	614	CLA	NC
26	Y	614	CLA	ND
26	Y	614	CLA	NA
26	R	609	CLA	NC
26	R	609	CLA	ND
26	R	609	CLA	NA
26	A	406	CLA	NC
26	A	406	CLA	ND
26	A	406	CLA	NA
26	Y	613	CLA	NC
26	Y	613	CLA	ND
26	Y	613	CLA	NA
26	N	612	CLA	NC
26	N	612	CLA	ND
26	N	612	CLA	NA

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Mol	Chain	Res	Type	Atom
26	C	512	CLA	NC
26	C	512	CLA	ND
26	C	512	CLA	NA
26	c	501	CLA	NC
26	c	501	CLA	ND
26	c	501	CLA	NA
26	s	603	CLA	NC
26	s	603	CLA	ND
26	s	603	CLA	NA
26	r	610	CLA	NC
26	r	610	CLA	ND
26	r	610	CLA	NA
26	c	502	CLA	NC
26	c	502	CLA	ND
26	c	502	CLA	NA
26	r	611	CLA	NC
26	r	611	CLA	ND
26	r	611	CLA	NA
26	C	508	CLA	NC
26	C	508	CLA	ND
26	C	508	CLA	NA
26	7	610	CLA	NC
26	7	610	CLA	ND
26	7	610	CLA	NA
26	Y	611	CLA	NC
26	Y	611	CLA	ND
26	Y	611	CLA	NA
26	B	614	CLA	NC
26	B	614	CLA	ND
26	B	614	CLA	NA
26	c	513	CLA	NC
26	c	513	CLA	NA
26	c	512	CLA	NC
26	c	512	CLA	ND
26	c	512	CLA	NA
26	y	613	CLA	NC
26	y	613	CLA	ND
26	y	613	CLA	NA
26	r	604	CLA	NC
26	r	604	CLA	ND
26	r	604	CLA	NA
26	b	602	CLA	NC

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Mol	Chain	Res	Type	Atom
26	b	602	CLA	ND
26	b	602	CLA	NA
26	8	611	CLA	NC
26	8	611	CLA	ND
26	8	611	CLA	NA
26	g	602	CLA	NC
26	g	602	CLA	ND
26	g	602	CLA	NA
26	5	604	CLA	NC
26	5	604	CLA	NA
26	7	603	CLA	NC
26	7	603	CLA	NA
26	7	603	CLA	ND
26	G	610	CLA	NC
26	G	610	CLA	NA
26	G	610	CLA	ND
26	B	608	CLA	NC
26	B	608	CLA	ND
26	B	608	CLA	NA
26	g	611	CLA	NC
26	g	611	CLA	ND
26	g	611	CLA	NA
26	C	513	CLA	NC
26	C	513	CLA	NA
26	C	510	CLA	NC
26	C	510	CLA	ND
26	C	510	CLA	NA
26	Y	602	CLA	NC
26	Y	602	CLA	ND
26	Y	602	CLA	NA
26	c	508	CLA	NC
26	c	508	CLA	ND
26	c	508	CLA	NA
26	4	603	CLA	NC
26	4	603	CLA	NA
26	4	603	CLA	ND
26	2	614	CLA	NC
26	2	614	CLA	ND
26	2	614	CLA	NA
26	B	611	CLA	NC
26	B	611	CLA	ND
26	B	611	CLA	NA

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Mol	Chain	Res	Type	Atom
26	n	612	CLA	NC
26	n	612	CLA	ND
26	n	612	CLA	NA
26	y	604	CLA	NC
26	y	604	CLA	ND
26	y	604	CLA	NA
26	R	603	CLA	NC
26	R	603	CLA	ND
26	R	603	CLA	NA
26	1	614	CLA	NC
26	1	614	CLA	ND
26	1	614	CLA	NA
26	a	406	CLA	NC
26	a	406	CLA	ND
26	a	406	CLA	NA
26	C	507	CLA	NC
26	C	507	CLA	ND
26	C	507	CLA	NA
26	Y	612	CLA	NC
26	Y	612	CLA	ND
26	Y	612	CLA	NA
26	2	602	CLA	NC
26	2	602	CLA	ND
26	2	602	CLA	NA
26	G	602	CLA	NC
26	G	602	CLA	ND
26	G	602	CLA	NA
26	7	612	CLA	NC
26	7	612	CLA	ND
26	7	612	CLA	NA
26	N	603	CLA	NC
26	N	603	CLA	ND
26	N	603	CLA	NA
26	c	510	CLA	NC
26	c	510	CLA	ND
26	c	510	CLA	NA
26	s	609	CLA	NC
26	s	609	CLA	ND
26	s	609	CLA	NA
26	a	405	CLA	NC
26	a	405	CLA	ND
26	a	405	CLA	NA

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Mol	Chain	Res	Type	Atom
26	n	610	CLA	NC
26	n	610	CLA	NA
26	n	610	CLA	ND
26	6	602	CLA	NC
26	6	602	CLA	ND
26	6	602	CLA	NA
26	B	616	CLA	NC
26	B	616	CLA	ND
26	B	616	CLA	NA
26	2	613	CLA	NC
26	2	613	CLA	NA
26	C	506	CLA	NC
26	C	506	CLA	ND
26	C	506	CLA	NA
26	g	610	CLA	NC
26	g	610	CLA	NA
26	g	610	CLA	ND
26	b	608	CLA	NC
26	b	608	CLA	ND
26	b	608	CLA	NA
26	1	612	CLA	NC
26	1	612	CLA	NA
26	1	612	CLA	ND
26	S	603	CLA	NC
26	S	603	CLA	ND
26	S	603	CLA	NA
26	6	614	CLA	NC
26	6	614	CLA	ND
26	6	614	CLA	NA
26	G	613	CLA	NC
26	G	613	CLA	ND
26	G	613	CLA	NA
26	C	505	CLA	NC
26	C	505	CLA	ND
26	C	505	CLA	NA
26	a	410	CLA	NC
26	a	410	CLA	ND
26	a	410	CLA	NA
26	B	606	CLA	NC
26	B	606	CLA	ND
26	B	606	CLA	NA
26	S	612	CLA	NC

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Mol	Chain	Res	Type	Atom
26	S	612	CLA	ND
26	S	612	CLA	NA
26	D	403	CLA	NC
26	D	403	CLA	NA
26	7	604	CLA	NC
26	7	604	CLA	ND
26	7	604	CLA	NA
26	b	612	CLA	NC
26	b	612	CLA	ND
26	b	612	CLA	NA
26	C	504	CLA	NC
26	C	504	CLA	ND
26	C	504	CLA	NA
26	g	604	CLA	NC
26	g	604	CLA	ND
26	g	604	CLA	NA
26	C	509	CLA	NC
26	C	509	CLA	ND
26	C	509	CLA	NA
26	r	616	CLA	NC
26	r	616	CLA	NA
26	R	604	CLA	NC
26	R	604	CLA	ND
26	R	604	CLA	NA
26	B	607	CLA	NC
26	B	607	CLA	ND
26	B	607	CLA	NA
26	s	604	CLA	NC
26	s	604	CLA	ND
26	s	604	CLA	NA
26	d	402	CLA	NC
26	d	402	CLA	ND
26	d	402	CLA	NA
26	s	613	CLA	NC
26	s	613	CLA	ND
26	s	613	CLA	NA
26	8	612	CLA	NC
26	8	612	CLA	ND
26	8	612	CLA	NA
26	S	604	CLA	NC
26	S	604	CLA	ND
26	S	604	CLA	NA

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Mol	Chain	Res	Type	Atom
26	7	613	CLA	NC
26	7	613	CLA	ND
26	7	613	CLA	NA
26	b	617	CLA	NC
26	b	617	CLA	ND
26	b	617	CLA	NA
26	B	604	CLA	NC
26	B	604	CLA	ND
26	B	604	CLA	NA
26	r	602	CLA	NC
26	r	602	CLA	ND
26	r	602	CLA	NA
26	n	613	CLA	NC
26	n	613	CLA	ND
26	n	613	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	a	412	SQD	C45-O47-C7-C8
36	A	412	SQD	C45-O47-C7-C8

There are no ring outliers.

278 monomers are involved in 746 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	1620	LUT	4	0
27	1	1621	LUT	5	0
28	1	1622	XAT	4	0
29	1	1623	NEX	2	0
30	1	2630	LHG	2	0
25	1	601	CHL	1	0
26	1	602	CLA	4	0
26	1	603	CLA	3	0
26	1	604	CLA	1	0
25	1	606	CHL	1	0
25	1	607	CHL	5	0
25	1	608	CHL	1	0
25	1	609	CHL	5	0
26	1	610	CLA	1	0
26	1	613	CLA	2	0
26	1	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	2	1620	LUT	5	0
27	2	1621	LUT	3	0
28	2	1622	XAT	6	0
29	2	1623	NEX	1	0
30	2	2630	LHG	1	0
26	2	602	CLA	2	0
26	2	603	CLA	1	0
26	2	604	CLA	1	0
25	2	605	CHL	1	0
25	2	606	CHL	2	0
25	2	607	CHL	1	0
25	2	609	CHL	2	0
26	2	611	CLA	1	0
26	2	612	CLA	2	0
26	2	613	CLA	2	0
27	3	1620	LUT	4	0
27	3	1621	LUT	3	0
28	3	1622	XAT	3	0
29	3	1623	NEX	3	0
30	3	2630	LHG	2	0
25	3	601	CHL	1	0
26	3	602	CLA	2	0
26	3	603	CLA	5	0
25	3	605	CHL	1	0
25	3	606	CHL	4	0
25	3	607	CHL	4	0
25	3	608	CHL	4	0
25	3	609	CHL	6	0
26	3	611	CLA	3	0
26	3	612	CLA	1	0
26	3	613	CLA	1	0
26	3	614	CLA	1	0
30	4	2630	LHG	1	0
25	4	601	CHL	2	0
25	4	606	CHL	2	0
25	4	608	CHL	2	0
25	4	609	CHL	1	0
26	4	610	CLA	1	0
26	4	611	CLA	1	0
26	4	612	CLA	3	0
27	4	620	LUT	2	0
28	4	622	XAT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	4	623	BCR	7	0
27	5	1620	LUT	3	0
27	5	1621	LUT	5	0
28	5	1622	XAT	3	0
29	5	1623	NEX	2	0
30	5	2630	LHG	2	0
25	5	601	CHL	1	0
26	5	602	CLA	3	0
26	5	603	CLA	3	0
26	5	604	CLA	1	0
25	5	606	CHL	1	0
25	5	607	CHL	6	0
25	5	608	CHL	1	0
25	5	609	CHL	4	0
26	5	610	CLA	1	0
26	5	613	CLA	2	0
26	5	614	CLA	1	0
27	6	1620	LUT	3	0
27	6	1621	LUT	3	0
28	6	1622	XAT	4	0
30	6	2630	LHG	1	0
26	6	602	CLA	2	0
26	6	603	CLA	1	0
26	6	604	CLA	1	0
25	6	605	CHL	1	0
25	6	606	CHL	2	0
25	6	607	CHL	1	0
25	6	609	CHL	3	0
26	6	611	CLA	1	0
26	6	612	CLA	2	0
26	6	613	CLA	2	0
26	6	614	CLA	1	0
27	7	1620	LUT	3	0
27	7	1621	LUT	2	0
28	7	1622	XAT	3	0
29	7	1623	NEX	3	0
30	7	2630	LHG	1	0
25	7	601	CHL	2	0
26	7	602	CLA	3	0
26	7	603	CLA	4	0
25	7	606	CHL	4	0
25	7	607	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	7	608	CHL	4	0
25	7	609	CHL	7	0
26	7	611	CLA	2	0
26	7	612	CLA	1	0
26	7	614	CLA	1	0
30	8	2630	LHG	1	0
25	8	601	CHL	2	0
25	8	606	CHL	2	0
25	8	608	CHL	2	0
25	8	609	CHL	1	0
26	8	610	CLA	1	0
26	8	611	CLA	1	0
26	8	612	CLA	2	0
27	8	620	LUT	3	0
28	8	622	XAT	3	0
31	8	623	BCR	8	0
26	A	405	CLA	11	0
26	A	406	CLA	5	0
26	A	407	CLA	1	0
35	A	408	PHO	8	0
35	A	409	PHO	3	0
26	A	410	CLA	5	0
31	A	411	BCR	6	0
36	A	412	SQD	2	0
37	A	413	LMG	2	0
38	A	414	PL9	1	0
36	A	418	SQD	11	0
30	B	2630	LHG	2	0
30	B	2631	LHG	4	0
37	B	2633	LMG	3	0
26	B	602	CLA	5	0
26	B	603	CLA	8	0
26	B	604	CLA	3	0
26	B	605	CLA	7	0
26	B	606	CLA	5	0
26	B	607	CLA	6	0
26	B	608	CLA	2	0
26	B	609	CLA	2	0
26	B	610	CLA	2	0
26	B	611	CLA	4	0
26	B	612	CLA	5	0
26	B	613	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	B	614	CLA	7	0
26	B	615	CLA	3	0
26	B	616	CLA	3	0
26	B	617	CLA	4	0
31	B	618	BCR	5	0
31	B	619	BCR	6	0
31	B	620	BCR	5	0
36	B	621	SQD	5	0
37	B	622	LMG	5	0
36	B	623	SQD	4	0
39	B	626	DGD	5	0
30	C	2630	LHG	6	0
26	C	501	CLA	6	0
26	C	502	CLA	6	0
26	C	503	CLA	4	0
26	C	504	CLA	2	0
26	C	505	CLA	4	0
26	C	506	CLA	3	0
26	C	507	CLA	4	0
26	C	508	CLA	3	0
26	C	509	CLA	2	0
26	C	510	CLA	9	0
26	C	511	CLA	3	0
26	C	512	CLA	5	0
26	C	513	CLA	5	0
31	C	514	BCR	6	0
31	C	515	BCR	4	0
31	C	516	BCR	6	0
31	C	517	BCR	8	0
39	C	518	DGD	2	0
39	C	519	DGD	3	0
39	C	520	DGD	1	0
37	C	521	LMG	1	0
30	C	522	LHG	4	0
30	C	523	LHG	2	0
26	D	402	CLA	7	0
26	D	403	CLA	3	0
31	D	404	BCR	3	0
38	D	405	PL9	2	0
30	D	408	LHG	1	0
30	D	409	LHG	13	0
30	D	410	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	D	411	LMG	2	0
27	G	1620	LUT	8	0
27	G	1621	LUT	6	0
28	G	1622	XAT	6	0
29	G	1623	NEX	5	0
30	G	2630	LHG	5	0
25	G	601	CHL	6	0
26	G	602	CLA	4	0
26	G	603	CLA	4	0
26	G	604	CLA	2	0
25	G	605	CHL	2	0
25	G	606	CHL	5	0
25	G	607	CHL	9	0
25	G	608	CHL	2	0
25	G	609	CHL	6	0
26	G	610	CLA	5	0
26	G	611	CLA	3	0
26	G	613	CLA	6	0
26	G	614	CLA	3	0
31	H	101	BCR	7	0
39	H	102	DGD	4	0
30	L	101	LHG	3	0
27	N	1620	LUT	5	0
27	N	1621	LUT	6	0
28	N	1622	XAT	7	0
29	N	1623	NEX	2	0
30	N	2630	LHG	4	0
25	N	601	CHL	3	0
26	N	602	CLA	8	0
26	N	603	CLA	6	0
26	N	604	CLA	1	0
25	N	605	CHL	1	0
25	N	606	CHL	1	0
25	N	607	CHL	4	0
25	N	608	CHL	1	0
25	N	609	CHL	4	0
26	N	610	CLA	8	0
26	N	611	CLA	1	0
26	N	612	CLA	3	0
26	N	613	CLA	4	0
30	R	2630	LHG	5	0
26	R	601	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	R	602	CLA	4	0
26	R	603	CLA	3	0
26	R	604	CLA	3	0
25	R	606	CHL	5	0
25	R	607	CHL	1	0
25	R	608	CHL	4	0
26	R	609	CLA	3	0
26	R	610	CLA	1	0
26	R	611	CLA	6	0
26	R	612	CLA	2	0
26	R	613	CLA	6	0
25	R	614	CHL	3	0
26	R	616	CLA	3	0
27	R	620	LUT	5	0
28	R	622	XAT	5	0
29	R	623	NEX	6	0
27	S	1620	LUT	4	0
27	S	1621	LUT	3	0
29	S	1623	NEX	3	0
30	S	2630	LHG	5	0
26	S	603	CLA	1	0
26	S	604	CLA	3	0
25	S	606	CHL	1	0
25	S	607	CHL	4	0
25	S	608	CHL	1	0
26	S	609	CLA	8	0
26	S	610	CLA	4	0
26	S	611	CLA	1	0
26	S	612	CLA	1	0
26	S	613	CLA	2	0
26	S	614	CLA	3	0
31	T	101	BCR	10	0
27	Y	1620	LUT	6	0
27	Y	1621	LUT	4	0
28	Y	1622	XAT	7	0
29	Y	1623	NEX	3	0
30	Y	2630	LHG	4	0
25	Y	601	CHL	3	0
26	Y	602	CLA	7	0
26	Y	603	CLA	10	0
26	Y	604	CLA	1	0
25	Y	605	CHL	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	606	CHL	2	0
25	Y	607	CHL	4	0
25	Y	608	CHL	2	0
25	Y	609	CHL	3	0
26	Y	610	CLA	1	0
26	Y	611	CLA	1	0
26	Y	612	CLA	2	0
26	Y	613	CLA	5	0
26	Y	614	CLA	1	0
37	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.