



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 13, 2017 – 08:26 AM EDT

PDB ID : 5XNM  
EMDB ID: : EMD-6742  
Title : Structure of unstacked 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 : 3.20 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](mailto: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.

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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

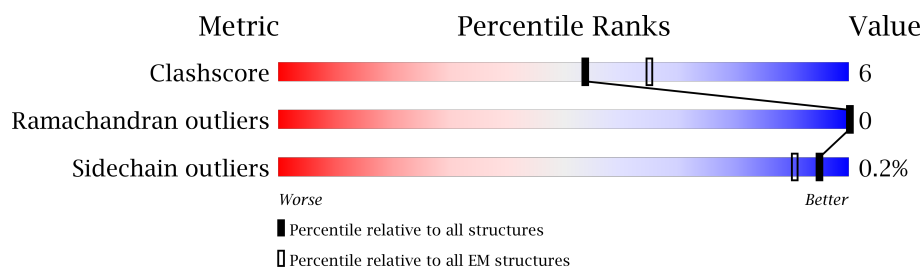
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









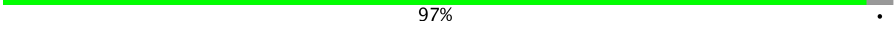

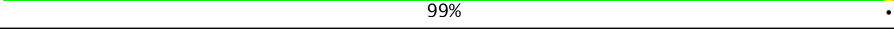

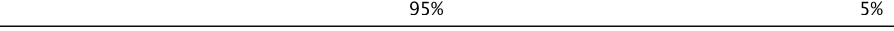
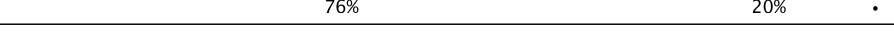
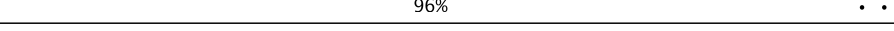






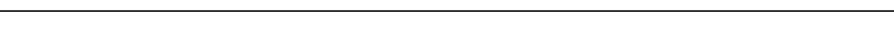

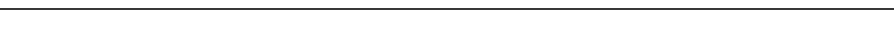
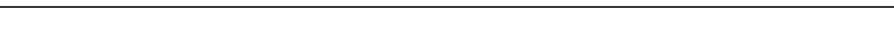


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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  $\geq 3$ , 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	













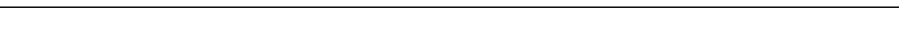



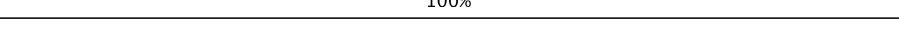



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Mol	Chain	Length	Quality of chain
1	y	232	 94% 6%
2	3	243	 75% 15% 9%
2	7	243	 74% 16% 9%
3	4	210	 76% 18% 6%
3	8	210	 73% 20% 6%
4	A	344	 81% 15% .
4	a	344	 97% .
5	B	507	 80% 19% .
5	b	507	 99% ..
6	C	473	 79% 16% 5%
6	c	473	 95% 5%
7	D	353	 76% 20% .
7	d	353	 96% ..
8	E	83	 81% 10% 10%
8	e	83	 90% 10%
9	F	39	 74% . 23%
9	f	39	 77% 23%
10	H	73	 71% 10% . 18%
10	h	73	 81% . 18%
11	I	36	 78% 17% 6%
11	i	36	 94% 6%
12	J	40	 80% 5% 15%
12	j	40	 85% 15%
13	K	61	 46% 15% 39%
13	k	61	 61% 39%

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Mol	Chain	Length	Quality of chain
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	248	
16	o	248	
17	R	246	
17	r	246	
18	S	244	
18	s	244	
19	T	35	
19	t	35	
20	U	99	
20	u	99	
21	W	54	
21	w	54	
22	X	86	
22	x	86	
23	Z	62	
23	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	1	610	X	-	-	-
25	CLA	1	611	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	613	X	-	-	-
25	CLA	1	614	X	-	-	-
25	CLA	2	602	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	613	X	-	-	-
25	CLA	2	614	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	603	X	-	-	-
25	CLA	3	604	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	611	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	613	X	-	-	-
25	CLA	3	614	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	5	611	X	-	-	-
25	CLA	5	612	X	-	-	-
25	CLA	5	613	X	-	-	-
25	CLA	5	614	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	604	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-
25	CLA	6	612	X	-	-	-
25	CLA	6	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	6	614	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	611	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	7	613	X	-	-	-
25	CLA	7	614	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	603	X	-	-	-
25	CLA	8	604	X	-	-	-
25	CLA	8	610	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	407	X	-	-	-
25	CLA	A	410	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	607	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	B	617	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	614	X	-	-	-
25	CLA	Y	602	X	-	-	-
25	CLA	Y	603	X	-	-	-
25	CLA	Y	604	X	-	-	-
25	CLA	Y	610	X	-	-	-
25	CLA	Y	611	X	-	-	-
25	CLA	Y	612	X	-	-	-
25	CLA	Y	613	X	-	-	-
25	CLA	Y	614	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	407	X	-	-	-
25	CLA	a	410	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	607	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-

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

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

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 92842 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	340	Total	C	N	O	S	0	0
			2703	1784	443	464	12		
7	d	340	Total	C	N	O	S	0	0
			2703	1784	443	464	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	34	Total	C	N	O	0	0
			247	168	38	41		
12	j	34	Total	C	N	O	0	0
			247	168	38	41		

- 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	214	Total	C	N	O	S	0	0
			1631	1039	260	329	3		
16	o	214	Total	C	N	O	S	0	0
			1631	1039	260	329	3		

- Molecule 17 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

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

- Molecule 18 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

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

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

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

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

- Molecule 20 is a protein called Photosystem II luminal extrinsic protein Tn, PsbTn.

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

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

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

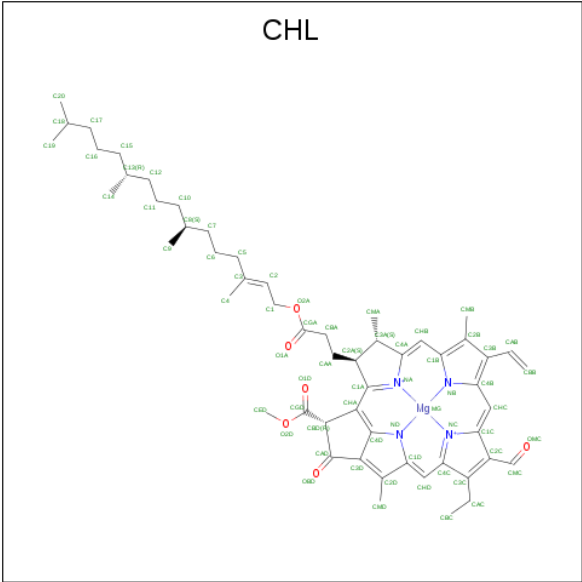
- Molecule 22 is a protein called Photosystem II reaction center protein X.

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

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

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

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

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

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Mol	Chain	Residues	Atoms					AltConf
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	R	1	Total	C	Mg	N	O	0
			225	183	4	16	22	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	S	1	Total	C	Mg	N	O	0
			196	152	4	16	24	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	Y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	5	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	

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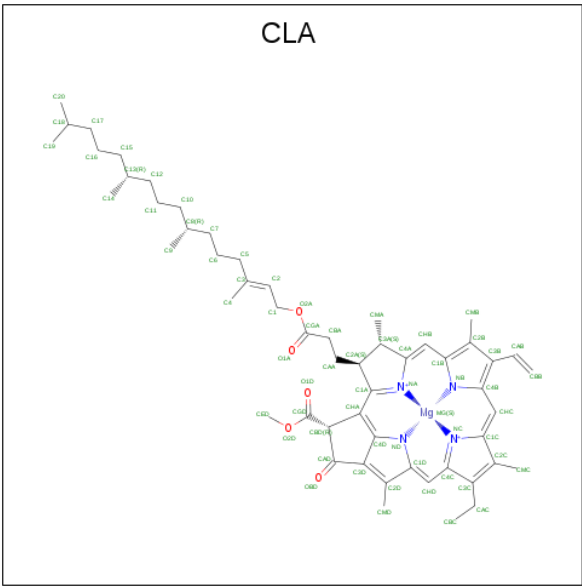
Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	6	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
24	7	1	Total	C	Mg	N	O	0
			316	250	6	24	36	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

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

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
			Total	C	Mg	N	O	
			412	332	8	32	40	
			Total	C	Mg	N	O	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
			Total	C	Mg	N	O	
			412	332	8	32	40	
			Total	C	Mg	N	O	
25	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
			Total	C	Mg	N	O	
			412	332	8	32	40	
			Total	C	Mg	N	O	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
			Total	C	Mg	N	O	
			391	311	8	32	40	
			Total	C	Mg	N	O	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
			Total	C	Mg	N	O	
			391	311	8	32	40	
			Total	C	Mg	N	O	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
			Total	C	Mg	N	O	
			391	311	8	32	40	
			Total	C	Mg	N	O	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	G	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	
25	N	1	Total	C	Mg	N	O	0
			473	393	8	32	40	

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

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
25	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
25	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
25	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
25	6	1	Total 391	C 311	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	6	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	7	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
25	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	

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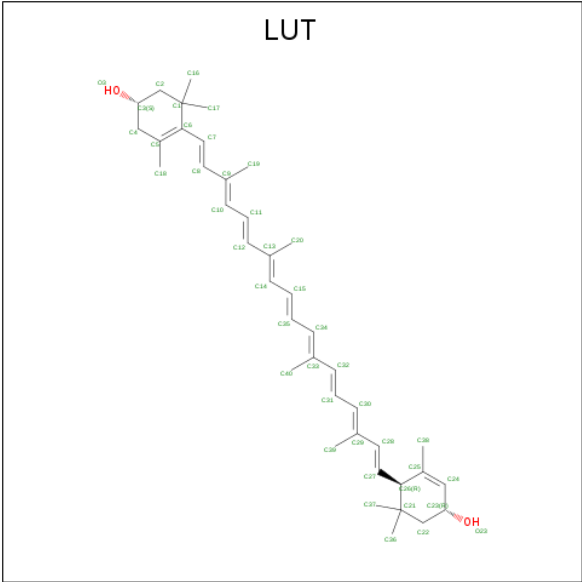
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
25	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
25	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
25	s	1	Total 465	C 375	Mg 9	N 36	O 45	0

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

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			84	80	4	
26	1	1	Total	C	O	0
			84	80	4	
26	2	1	Total	C	O	0
			84	80	4	
26	2	1	Total	C	O	0
			84	80	4	
26	3	1	Total	C	O	0
			84	80	4	
26	3	1	Total	C	O	0
			84	80	4	
26	4	1	Total	C	O	0
			42	40	2	
26	G	1	Total	C	O	0
			84	80	4	
26	G	1	Total	C	O	0
			84	80	4	
26	N	1	Total	C	O	0
			84	80	4	
26	N	1	Total	C	O	0
			84	80	4	
26	R	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			84	80	4	
26	S	1	Total	C	O	0
			84	80	4	

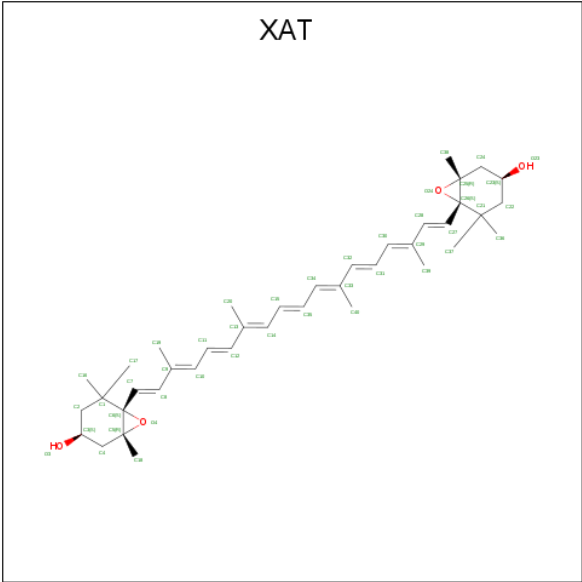
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Mol	Chain	Residues	Atoms			AltConf
26	Y	1	Total	C	O	0
			84	80	4	
26	Y	1	Total	C	O	0
			84	80	4	
26	5	1	Total	C	O	0
			84	80	4	
26	5	1	Total	C	O	0
			84	80	4	
26	6	1	Total	C	O	0
			84	80	4	
26	6	1	Total	C	O	0
			84	80	4	
26	7	1	Total	C	O	0
			84	80	4	
26	7	1	Total	C	O	0
			84	80	4	
26	8	1	Total	C	O	0
			42	40	2	
26	g	1	Total	C	O	0
			84	80	4	
26	g	1	Total	C	O	0
			84	80	4	
26	n	1	Total	C	O	0
			84	80	4	
26	n	1	Total	C	O	0
			84	80	4	
26	r	1	Total	C	O	0
			42	40	2	
26	s	1	Total	C	O	0
			84	80	4	
26	s	1	Total	C	O	0
			84	80	4	
26	y	1	Total	C	O	0
			84	80	4	
26	y	1	Total	C	O	0
			84	80	4	

- Molecule 27 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: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



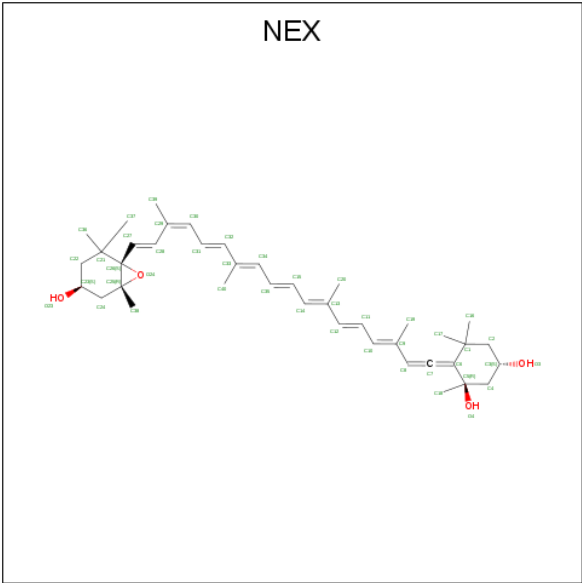
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	
27	G	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	Y	1	Total	C	O	0
			44	40	4	
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	
27	g	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	

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

- Molecule 28 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1, 3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



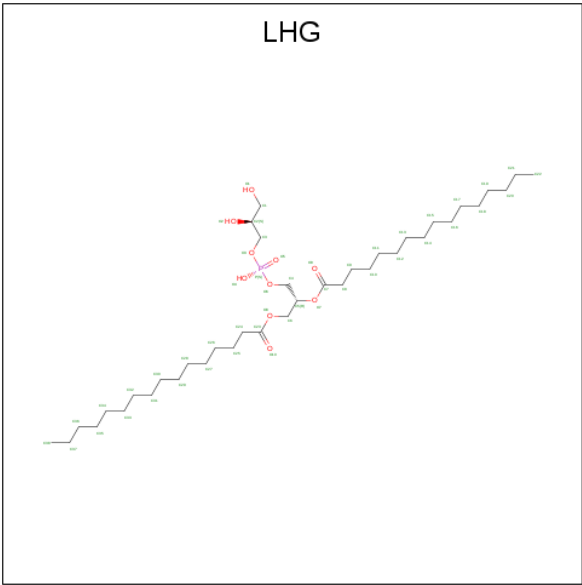
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	R	1	Total	C	O	0
			44	40	4	
28	S	1	Total	C	O	0
			44	40	4	
28	Y	1	Total	C	O	0
			44	40	4	

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

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
29	1	1	Total	C	O	P	0
			41	30	10	1	
29	2	1	Total	C	O	P	0
			37	26	10	1	
29	3	1	Total	C	O	P	0
			47	36	10	1	

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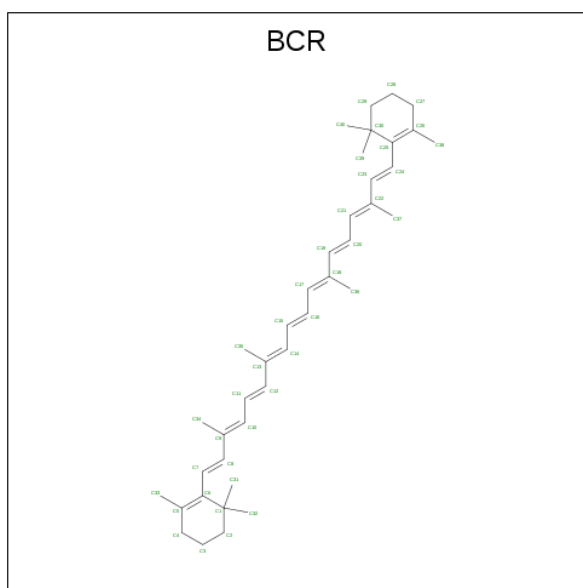
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total	C	O	P	0
			21	10	10	1	
29	B	1	Total	C	O	P	0
			96	74	20	2	
29	B	1	Total	C	O	P	0
			96	74	20	2	
29	C	1	Total	C	O	P	0
			147	114	30	3	
29	C	1	Total	C	O	P	0
			147	114	30	3	
29	C	1	Total	C	O	P	0
			147	114	30	3	
29	D	1	Total	C	O	P	0
			138	105	30	3	
29	D	1	Total	C	O	P	0
			138	105	30	3	
29	D	1	Total	C	O	P	0
			138	105	30	3	
29	G	1	Total	C	O	P	0
			49	38	10	1	
29	L	1	Total	C	O	P	0
			49	38	10	1	
29	N	1	Total	C	O	P	0
			49	38	10	1	
29	R	1	Total	C	O	P	0
			42	31	10	1	
29	S	1	Total	C	O	P	0
			49	38	10	1	
29	Y	1	Total	C	O	P	0
			49	38	10	1	
29	5	1	Total	C	O	P	0
			41	30	10	1	
29	6	1	Total	C	O	P	0
			37	26	10	1	
29	7	1	Total	C	O	P	0
			47	36	10	1	
29	8	1	Total	C	O	P	0
			21	10	10	1	
29	b	1	Total	C	O	P	0
			96	74	20	2	
29	b	1	Total	C	O	P	0
			96	74	20	2	

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

- Molecule 30 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



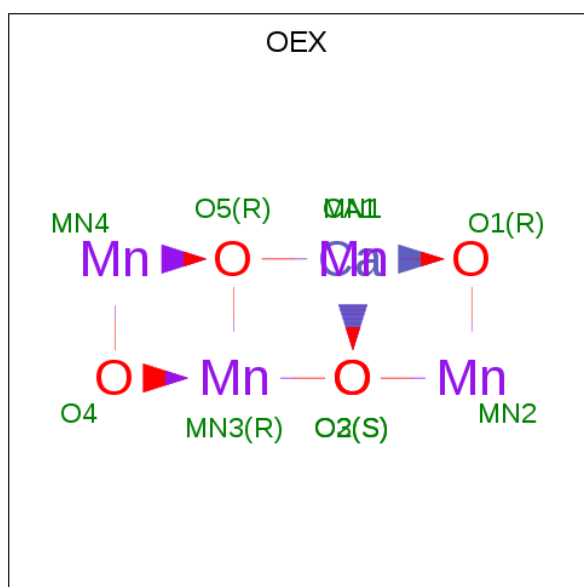
Mol	Chain	Residues	Atoms	AltConf
30	4	1	Total C 40 40	0
30	A	1	Total C 40 40	0
30	B	1	Total C 120 120	0
30	B	1	Total C 120 120	0
30	B	1	Total C 120 120	0
30	C	1	Total C 160 160	0
30	C	1	Total C 160 160	0
30	C	1	Total C 160 160	0
30	C	1	Total C 160 160	0
30	D	1	Total C 40 40	0
30	H	1	Total C 40 40	0
30	T	1	Total C 40 40	0
30	8	1	Total C 40 40	0
30	a	1	Total C 40 40	0
30	b	1	Total C 120 120	0
30	b	1	Total C 120 120	0
30	b	1	Total C 120 120	0
30	c	1	Total C 160 160	0
30	c	1	Total C 160 160	0
30	c	1	Total C 160 160	0
30	c	1	Total C 160 160	0
30	d	1	Total C 40 40	0

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

- Molecule 31 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



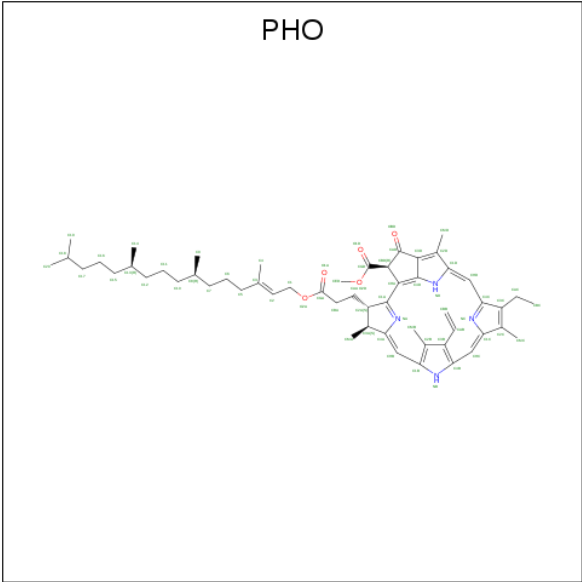
Mol	Chain	Residues	Atoms				AltConf
31	A	1	Total	Ca	Mn	O	0
			10	1	4	5	
31	a	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 32 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

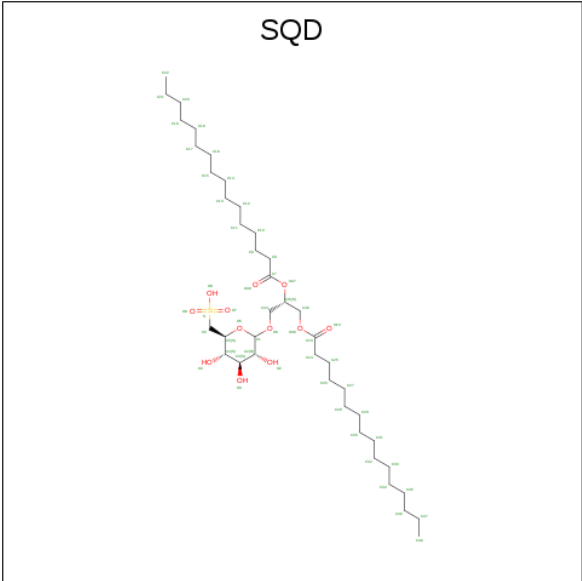
- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_5$ ).





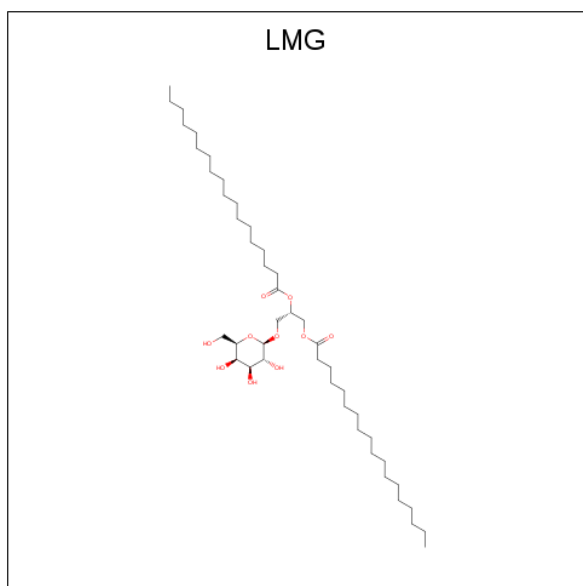
Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	N	O	0
			128	110	8	10	
33	A	1	Total	C	N	O	0
			128	110	8	10	
33	a	1	Total	C	N	O	0
			128	110	8	10	
33	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



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

- Molecule 35 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



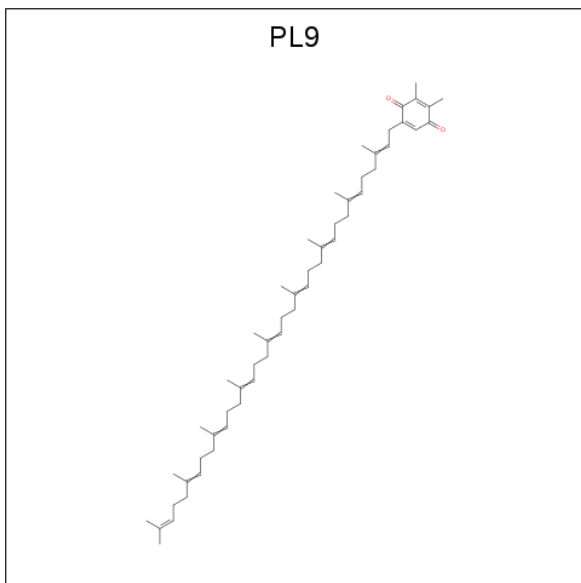
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			88	68	20	
35	A	1	Total	C	O	0
			88	68	20	
35	B	1	Total	C	O	0
			106	86	20	

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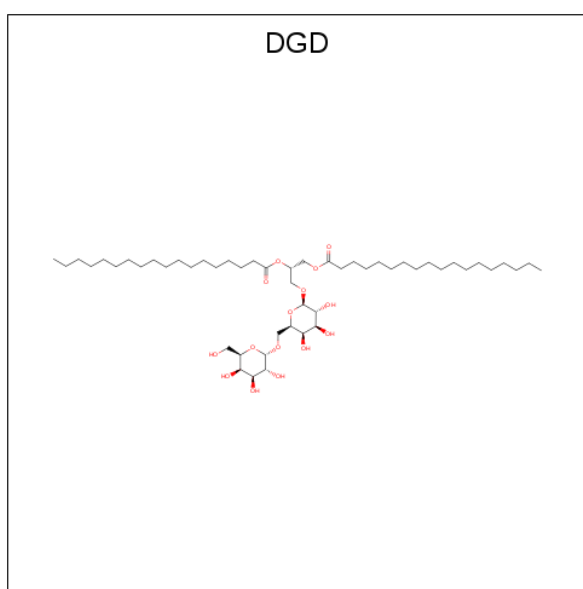
Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			106	86	20	
35	C	1	Total	C	O	0
			51	41	10	
35	D	1	Total	C	O	0
			46	36	10	
35	Z	1	Total	C	O	0
			51	41	10	
35	a	1	Total	C	O	0
			88	68	20	
35	a	1	Total	C	O	0
			88	68	20	
35	b	1	Total	C	O	0
			106	86	20	
35	b	1	Total	C	O	0
			106	86	20	
35	c	1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

- Molecule 36 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
36	A	1	Total	C	O	0
			13	11	2	
36	D	1	Total	C	O	0
			55	53	2	
36	a	1	Total	C	O	0
			13	11	2	
36	d	1	Total	C	O	0
			55	53	2	

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



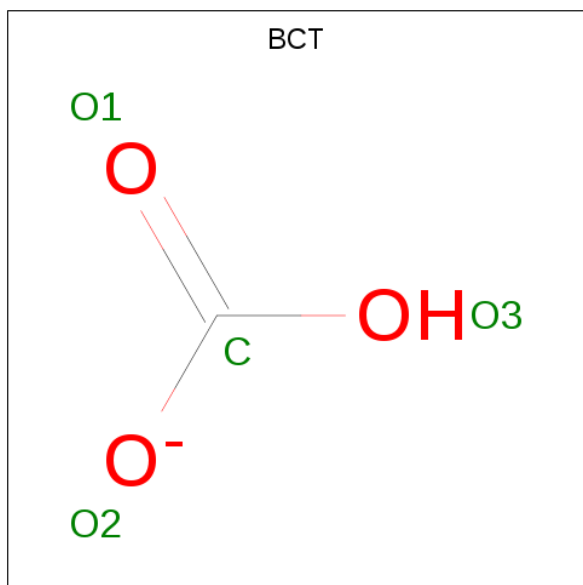
Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			59	44	15	
37	C	1	Total	C	O	0
			177	132	45	
37	C	1	Total	C	O	0
			177	132	45	
37	C	1	Total	C	O	0
			177	132	45	
37	H	1	Total	C	O	0
			62	47	15	
37	b	1	Total	C	O	0
			59	44	15	
37	c	1	Total	C	O	0
			177	132	45	

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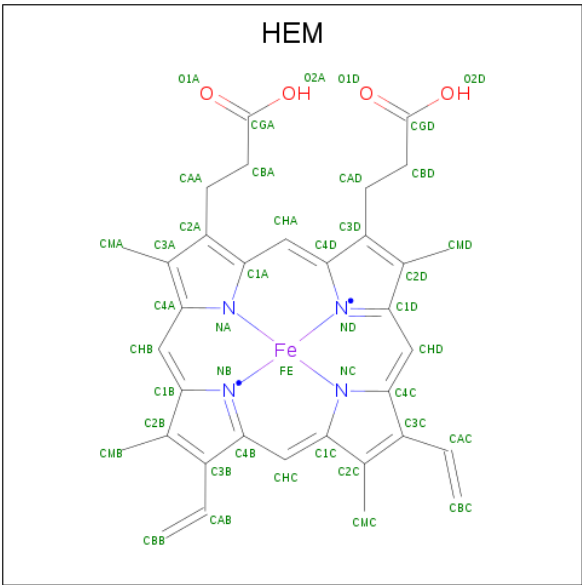
Mol	Chain	Residues	Atoms			AltConf
37	c	1	Total	C	O	0
			177	132	45	
37	c	1	Total	C	O	0
			177	132	45	
37	h	1	Total	C	O	0
			62	47	15	

- Molecule 38 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).

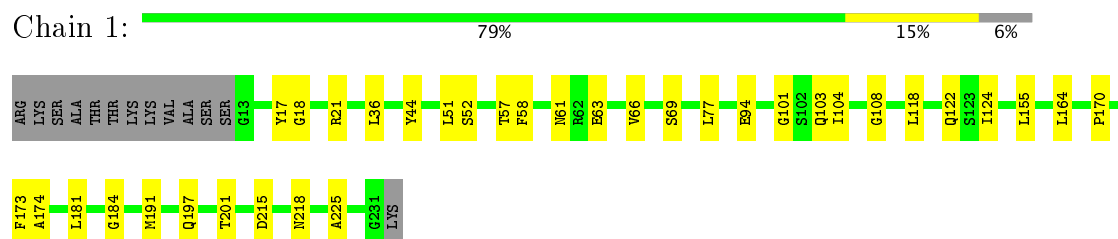


Mol	Chain	Residues	Atoms					AltConf
39	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
39	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

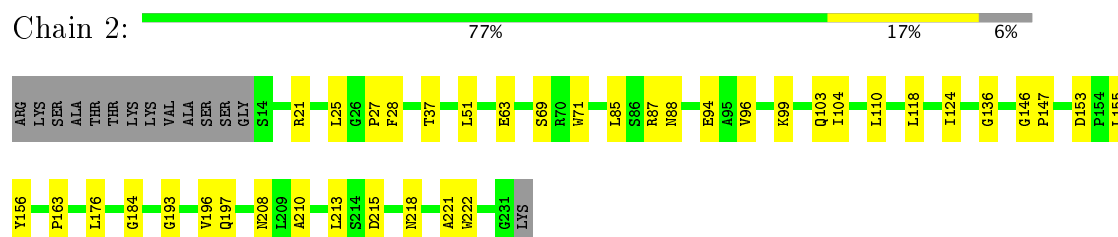
### 3 Residue-property plots [i](#)

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.

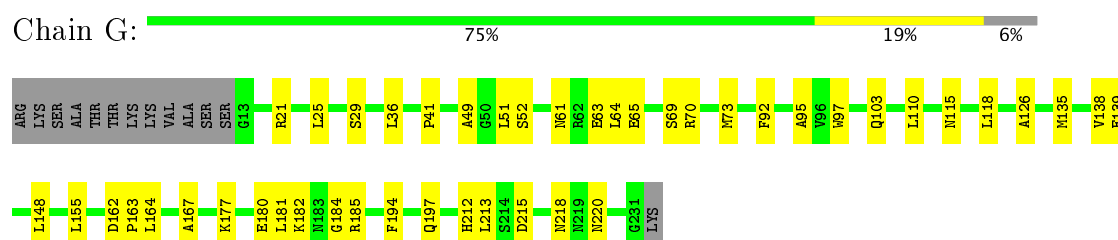
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



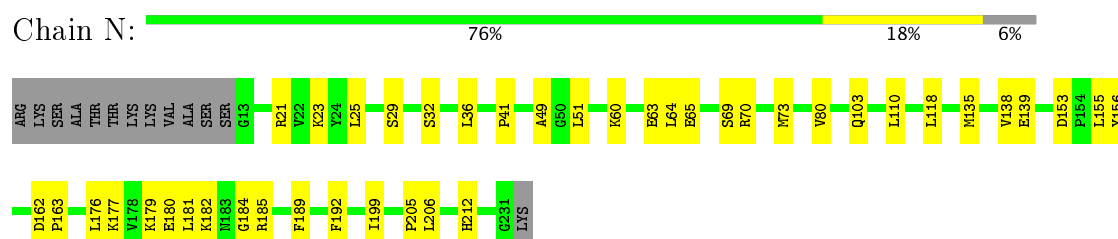
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



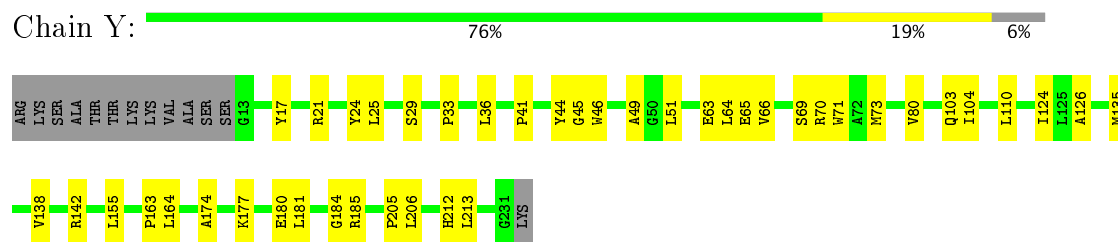
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



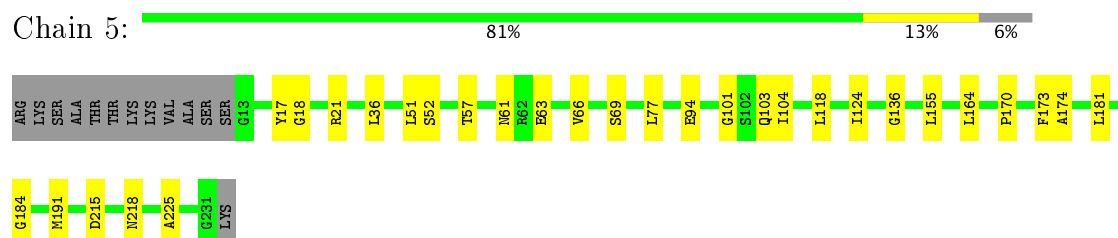
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



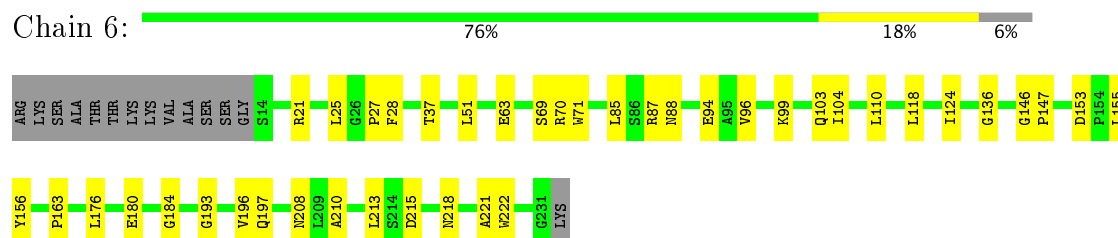
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



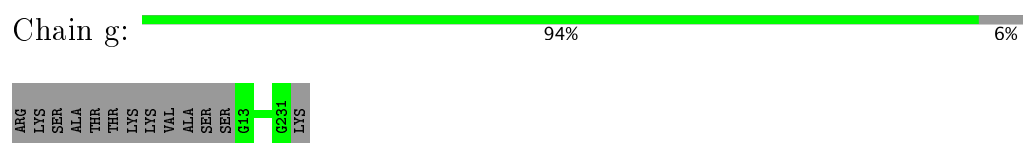
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



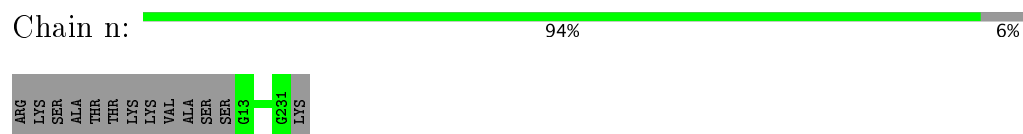
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



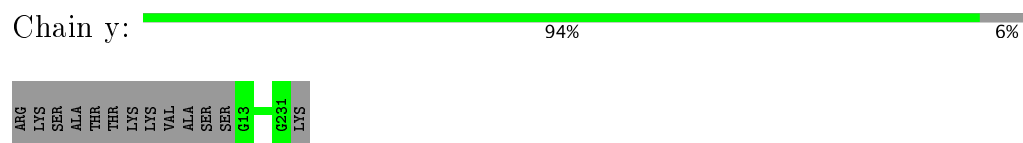
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



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

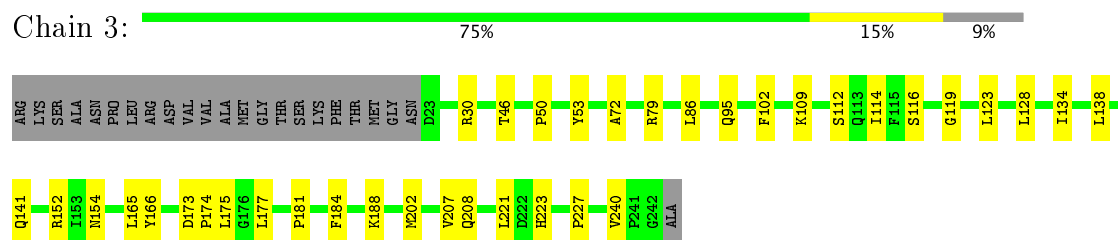


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

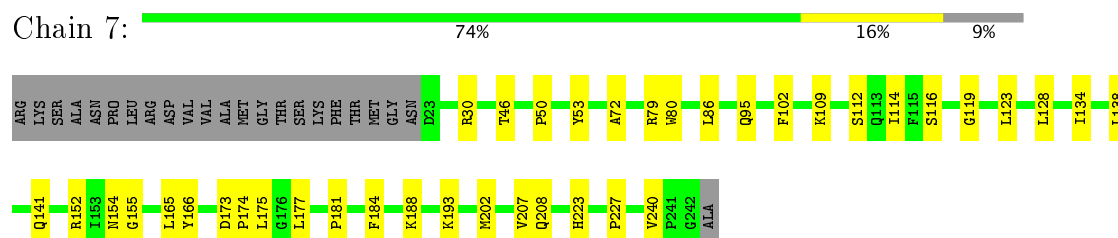


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

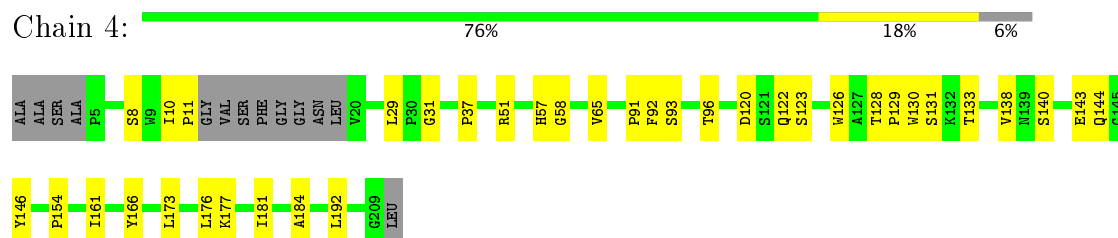




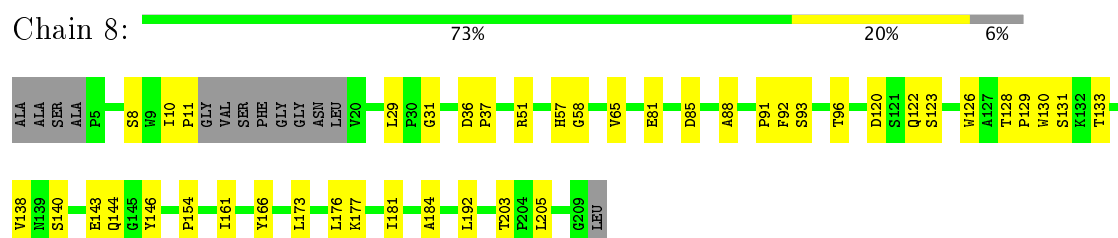
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



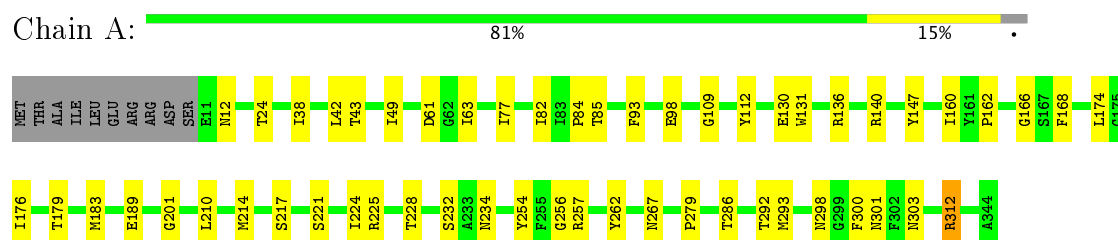
- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24



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

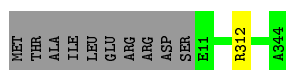


- Molecule 4: Photosystem II protein D1



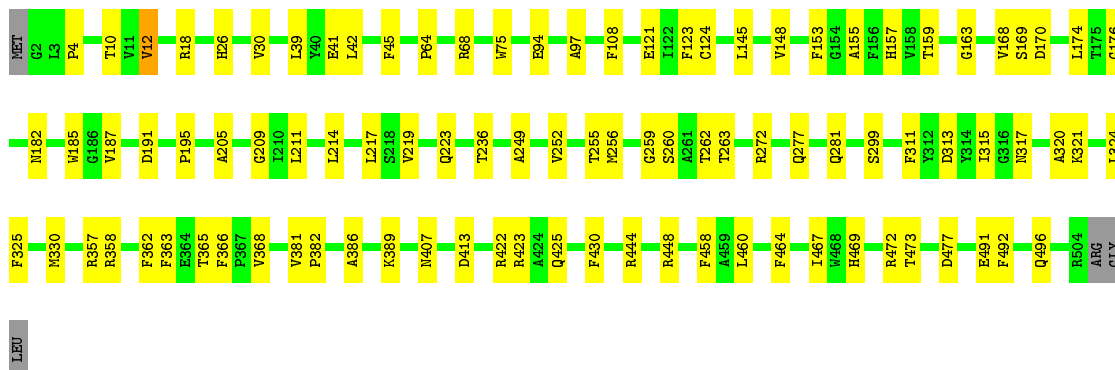
- Molecule 4: Photosystem II protein D1





• Molecule 5: Photosystem II CP47 reaction center protein

Chain B: 80% 19%



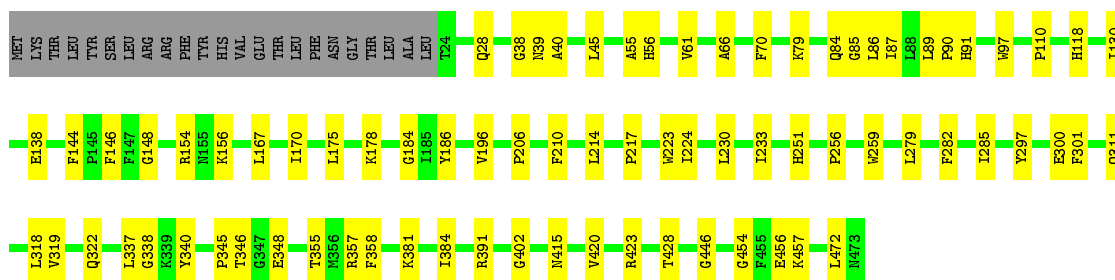
• Molecule 5: Photosystem II CP47 reaction center protein

Chain b: 99%



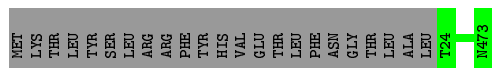
• Molecule 6: Photosystem II CP43 reaction center protein

Chain C: 79% 16% 5%



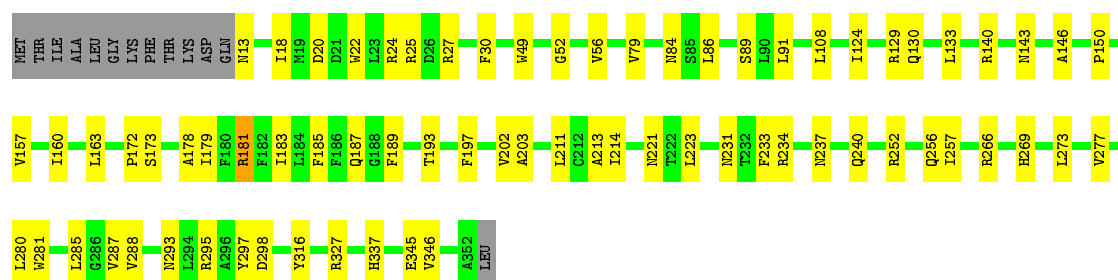
• Molecule 6: Photosystem II CP43 reaction center protein

Chain c: 95% 5%



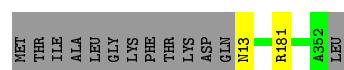
• Molecule 7: Photosystem II D2 protein

Chain D: 76% 20%



- Molecule 7: Photosystem II D2 protein

Chain d: 96%



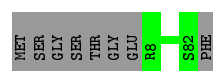
- Molecule 8: Cytochrome b559 subunit alpha

Chain E: 81%



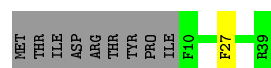
- Molecule 8: Cytochrome b559 subunit alpha

Chain e: 90%



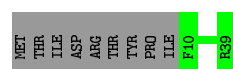
- Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain F: 74%



- Molecule 9: Cytochrome b559 subunit beta, PsbF

Chain f: 77%




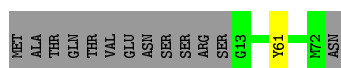
- Molecule 10: Photosystem II reaction center protein H

Chain H: 71%



- Molecule 10: Photosystem II reaction center protein H

Chain h:  81% 18%



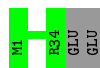
- Molecule 11: Photosystem II reaction center protein I, PsbI

Chain I:  78% 17% 6%




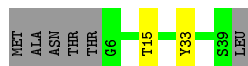
- Molecule 11: Photosystem II reaction center protein I, PsbI

Chain i:  94% 6%




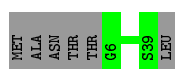
- Molecule 12: Photosystem II reaction center protein J

Chain J:  80% 5% 15%



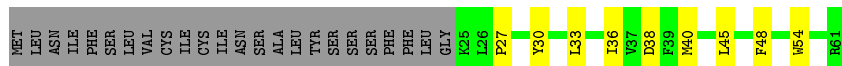
- Molecule 12: Photosystem II reaction center protein J

Chain j:  85% 15%



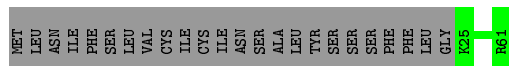
- Molecule 13: Photosystem II reaction center protein K

Chain K:  46% 15% 39%



- Molecule 13: Photosystem II reaction center protein K

Chain k:  61% 39%



- Molecule 14: Photosystem II reaction center protein L

Chain L:  61% 37%



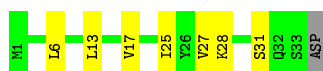
- Molecule 14: Photosystem II reaction center protein L

Chain l: 97%



- Molecule 15: Photosystem II reaction center protein M

Chain M: 76%



- Molecule 15: Photosystem II reaction center protein M

Chain m: 97%



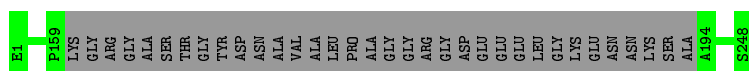
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain O: 71%



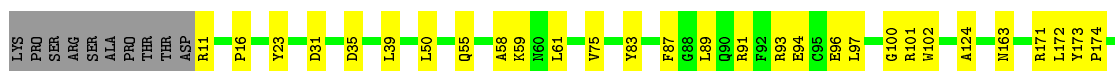
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

Chain o: 86%



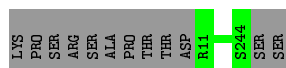
- Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain R: 77%



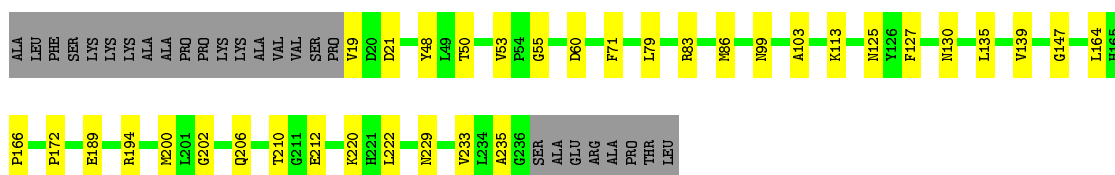
- Molecule 17: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

Chain r:  95% 5%




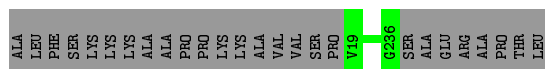
- Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain S:  75% 14% 11%



- Molecule 18: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

Chain s:  89% 11%



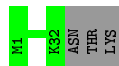
- Molecule 19: Photosystem II reaction center protein T

Chain T:  71% 20% 9%



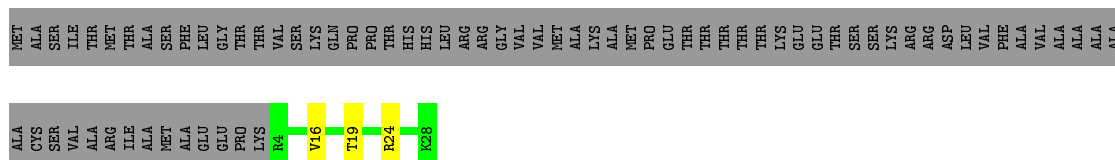
- Molecule 19: Photosystem II reaction center protein T

Chain t:  91% 9%



- Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn

Chain U:  22% 75%




- Molecule 20: Photosystem II luminal extrinsic protein Tn, PsbTn

Chain u:  25% 75%

MET ALA ALA SER ILE THR MET THR ALA SER PHE LEU GLY THR VAL SER LYS GLN PRO PRO THR THR HIS HIS LEU ARG ARG GLY VAL VAL MET MET LYS ALA MET PRO GLU THR THR THR THR LYS LYS GLU GLU THR THR SER SER LYS ARG ARG ASP LEU VAL PHE ALA VAL ALA ALA ALA

ALA CYS SER VAL ALA ARG ILE ALA MET ALA ALA GLU PRO LYS R4 R28

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

Chain W:  85% 15%


L3 V2 T8 E9 F15 G16 L17 L22 G31 Y40 L54

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

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 22: Photosystem II reaction center protein X

Chain X:  41% 5% 55%

SER ILE GLY ARG ALA SER SER LYS SER ASN GLY ARG PHE GLN VAL VAL LYS LYS LYS LYS VAL VAL THR THR GLY LEU THR ALA ALA ALA ALA LEU THR THR GLN MET MET VAL ILE PRO ASP VAL ALA ALA ALA A45 S76 V81 R32 R83 GLY SER GLN

- Molecule 22: Photosystem II reaction center protein X

Chain x:  45% 55%

SER ILE GLY ARG ALA SER SER LYS SER ASN GLY ARG PHE GLN VAL VAL LYS LYS LYS LYS VAL VAL THR THR GLY LEU THR ALA ALA ALA ALA LEU THR THR GLN MET MET VAL ILE PRO ASP VAL ALA ALA ALA A45 R83 GLY SER GLN

- Molecule 23: Photosystem II reaction center protein Z

Chain Z:  87% 13%

H1 V9 L12 I13 L20 P24 L57 R58 S59 L60 T61 S62

- Molecule 23: Photosystem II reaction center protein Z

Chain z:  100%

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	50237	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, 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	0.48	0/1720	0.55	0/2342
1	2	0.43	0/1716	0.54	0/2337
1	5	0.48	0/1720	0.55	0/2342
1	6	0.43	0/1716	0.54	0/2337
1	G	0.44	0/1720	0.53	0/2342
1	N	0.45	0/1720	0.53	0/2342
1	Y	0.52	0/1720	0.55	0/2342
1	g	0.44	0/1720	0.53	0/2342
1	n	0.45	0/1720	0.53	0/2342
1	y	0.52	0/1720	0.55	0/2342
10	H	0.47	0/461	0.58	0/626
10	h	0.47	0/461	0.58	0/626
11	I	0.61	0/286	0.69	0/386
11	i	0.61	0/286	0.69	0/386
12	J	0.30	0/253	0.59	0/343
12	j	0.30	0/253	0.60	0/343
13	K	0.55	0/318	0.64	0/434
13	k	0.55	0/318	0.64	0/434
14	L	0.48	0/319	0.56	0/434
14	l	0.48	0/319	0.56	0/434
15	M	0.54	0/260	0.65	0/355
15	m	0.54	0/260	0.65	0/355
16	O	0.41	0/1664	0.56	0/2250
16	o	0.41	0/1664	0.56	0/2250
17	R	0.43	0/1886	0.57	0/2569
17	r	0.43	0/1886	0.57	0/2569
18	S	0.32	0/1736	0.54	0/2359
18	s	0.32	0/1736	0.54	0/2359
19	T	0.51	0/269	0.50	0/365
19	t	0.51	0/269	0.50	0/365
2	3	0.49	0/1759	0.59	1/2396 (0.0%)
2	7	0.49	0/1759	0.59	1/2396 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
20	U	0.36	0/197	0.56	0/264
20	u	0.36	0/197	0.57	0/264
21	W	0.48	0/429	0.60	0/581
21	w	0.48	0/429	0.60	0/581
22	X	0.49	0/279	0.56	0/380
22	x	0.48	0/279	0.56	0/380
23	Z	0.42	0/474	0.53	0/648
23	z	0.42	0/474	0.53	0/648
3	4	0.42	0/1586	0.59	0/2158
3	8	0.42	0/1586	0.59	0/2158
4	A	0.47	0/2697	0.57	0/3677
4	a	0.47	0/2697	0.57	0/3677
5	B	0.56	0/4081	0.59	0/5556
5	b	0.56	0/4081	0.59	0/5556
6	C	0.36	0/3614	0.54	0/4922
6	c	0.36	0/3614	0.54	0/4922
7	D	0.62	0/2795	0.65	0/3812
7	d	0.62	0/2795	0.65	0/3812
8	E	0.33	0/630	0.50	0/857
8	e	0.33	0/630	0.50	0/857
9	F	0.34	0/248	0.51	0/335
9	f	0.34	0/248	0.51	0/335
All	All	0.47	0/69674	0.57	2/94824 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	123	LEU	CA-CB-CG	6.24	129.66	115.30
2	3	123	LEU	CA-CB-CG	6.24	129.64	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	24	0
1	2	1664	0	1593	29	0
1	5	1668	0	1596	23	0
1	6	1664	0	1593	29	0
1	G	1668	0	1596	40	0
1	N	1668	0	1596	39	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	30	0
2	7	1707	0	1659	33	0
3	4	1534	0	1486	31	0
3	8	1534	0	1486	35	0
4	A	2616	0	2522	55	0
4	a	2616	0	2522	0	0
5	B	3948	0	3818	84	0
5	b	3948	0	3818	0	0
6	C	3497	0	3422	63	0
6	c	3497	0	3422	0	0
7	D	2703	0	2593	62	0
7	d	2703	0	2593	0	0
8	E	612	0	595	7	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	13	0
10	h	452	0	473	0	0
11	I	278	0	291	7	0
11	i	278	0	291	0	0
12	J	247	0	258	2	0
12	j	247	0	258	0	0
13	K	306	0	313	13	0
13	k	306	0	313	0	0
14	L	311	0	299	19	0
14	l	311	0	299	0	0
15	M	256	0	284	6	0
15	m	256	0	284	0	0
16	O	1631	0	1625	25	0
16	o	1631	0	1625	0	0
17	R	1835	0	1801	52	0
17	r	1835	0	1801	0	0
18	S	1689	0	1670	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	s	1689	0	1670	0	0
19	T	261	0	280	9	0
19	t	261	0	280	0	0
20	U	193	0	205	4	0
20	u	193	0	205	0	0
21	W	419	0	402	8	0
21	w	419	0	402	0	0
22	X	276	0	301	4	0
22	x	276	0	301	0	0
23	Z	464	0	493	7	0
23	z	464	0	493	0	0
24	1	309	0	244	9	0
24	2	306	0	238	12	0
24	3	316	0	254	16	0
24	4	229	0	152	3	0
24	5	309	0	244	12	0
24	6	306	0	238	13	0
24	7	316	0	254	19	0
24	8	229	0	152	3	0
24	G	355	0	335	18	0
24	N	362	0	350	17	0
24	R	225	0	201	7	0
24	S	196	0	144	5	0
24	Y	362	0	350	22	0
24	g	355	0	335	0	0
24	n	362	0	350	0	0
24	r	225	0	201	0	0
24	s	196	0	144	0	0
24	y	362	0	350	0	0
25	1	412	0	348	14	0
25	2	391	0	314	16	0
25	3	426	0	373	19	0
25	4	270	0	198	4	0
25	5	412	0	348	13	0
25	6	391	0	314	16	0
25	7	426	0	373	21	0
25	8	270	0	198	5	0
25	A	240	0	242	18	0
25	B	1040	0	1152	69	0
25	C	845	0	936	39	0
25	D	130	0	144	10	0
25	G	477	0	477	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	N	473	0	468	26	0
25	R	543	0	490	28	0
25	S	465	0	393	10	0
25	Y	473	0	468	29	0
25	a	240	0	242	0	0
25	b	1040	0	1152	0	0
25	c	845	0	936	0	0
25	d	130	0	144	0	0
25	g	477	0	477	0	0
25	n	473	0	468	0	0
25	r	543	0	490	0	0
25	s	465	0	393	0	0
25	y	473	0	468	0	0
26	1	84	0	112	10	0
26	2	84	0	112	6	0
26	3	84	0	112	12	0
26	4	42	0	56	4	0
26	5	84	0	112	11	0
26	6	84	0	112	6	0
26	7	84	0	112	10	0
26	8	42	0	56	3	0
26	G	84	0	112	13	0
26	N	84	0	112	8	0
26	R	42	0	56	4	0
26	S	84	0	112	8	0
26	Y	84	0	112	8	0
26	g	84	0	112	0	0
26	n	84	0	112	0	0
26	r	42	0	56	0	0
26	s	84	0	112	0	0
26	y	84	0	112	0	0
27	1	44	0	56	4	0
27	2	44	0	56	6	0
27	3	44	0	56	4	0
27	4	44	0	56	4	0
27	5	44	0	56	4	0
27	6	44	0	56	5	0
27	7	44	0	56	7	0
27	8	44	0	56	6	0
27	G	44	0	56	4	0
27	N	44	0	56	7	0
27	R	44	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Y	44	0	56	6	0
27	g	44	0	56	0	0
27	n	44	0	56	0	0
27	r	44	0	56	0	0
27	y	44	0	56	0	0
28	1	44	0	56	3	0
28	2	44	0	56	2	0
28	3	44	0	56	2	0
28	5	44	0	56	3	0
28	6	44	0	56	0	0
28	7	44	0	56	2	0
28	G	44	0	56	4	0
28	N	44	0	56	5	0
28	R	44	0	56	4	0
28	S	44	0	56	2	0
28	Y	44	0	56	4	0
28	g	44	0	56	0	0
28	n	44	0	56	0	0
28	r	44	0	56	0	0
28	s	44	0	56	0	0
28	y	44	0	56	0	0
29	1	41	0	55	0	0
29	2	37	0	44	2	0
29	3	47	0	67	5	0
29	4	21	0	12	1	0
29	5	41	0	55	0	0
29	6	37	0	44	2	0
29	7	47	0	67	6	0
29	8	21	0	12	1	0
29	B	96	0	141	6	0
29	C	147	0	222	9	0
29	D	138	0	195	19	0
29	G	49	0	74	5	0
29	L	49	0	74	8	0
29	N	49	0	74	4	0
29	R	42	0	57	3	0
29	S	49	0	74	2	0
29	Y	49	0	74	4	0
29	b	96	0	141	0	0
29	c	147	0	222	0	0
29	d	138	0	195	0	0
29	g	49	0	74	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	l	49	0	74	0	0
29	n	49	0	74	0	0
29	r	42	0	57	0	0
29	s	49	0	74	0	0
29	y	49	0	74	0	0
30	4	40	0	56	3	0
30	8	40	0	56	3	0
30	A	40	0	56	4	0
30	B	120	0	168	19	0
30	C	160	0	224	17	0
30	D	40	0	56	7	0
30	H	40	0	56	6	0
30	T	40	0	56	8	0
30	a	40	0	56	0	0
30	b	120	0	168	0	0
30	c	160	0	224	0	0
30	d	40	0	56	0	0
30	h	40	0	56	0	0
30	t	40	0	56	0	0
31	A	10	0	0	2	0
31	a	10	0	0	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	A	128	0	148	14	0
33	a	128	0	148	0	0
34	A	104	0	144	8	0
34	B	96	0	126	8	0
34	a	104	0	145	0	0
34	b	96	0	125	0	0
35	A	88	0	116	2	0
35	B	106	0	158	6	0
35	C	51	0	72	1	0
35	D	46	0	62	3	0
35	Z	51	0	72	6	0
35	a	88	0	116	0	0
35	b	106	0	158	0	0
35	c	51	0	72	0	0
35	d	46	0	62	0	0
35	z	51	0	72	0	0
36	A	13	0	7	0	0
36	D	55	0	80	6	0
36	a	13	0	7	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	d	55	0	80	0	0
37	B	59	0	76	1	0
37	C	177	0	228	8	0
37	H	62	0	80	6	0
37	b	59	0	76	0	0
37	c	177	0	228	0	0
37	h	62	0	80	0	0
38	D	4	0	0	1	0
38	d	4	0	0	0	0
39	F	43	0	30	0	0
39	f	43	0	30	0	0
All	All	92842	0	92620	1174	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 (1174) 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)
24:7:606:CHL:HBB2	24:7:607:CHL:HBB1	1.57	0.86
24:3:606:CHL:HBB2	24:3:607:CHL:HBB1	1.57	0.85
25:B:603:CLA:H12	10:H:61:TYR:HD2	1.46	0.80
25:1:602:CLA:HAB	26:1:1621:LUT:H32	1.66	0.77
16:O:128:PHE:HA	16:O:222:GLN:HE22	1.50	0.76
25:5:602:CLA:HAB	26:5:1621:LUT:H32	1.66	0.76
7:D:86:LEU:HD13	7:D:91:LEU:HD11	1.70	0.74
25:2:610:CLA:H2	26:2:1620:LUT:H28	1.72	0.72
25:6:610:CLA:H2	26:6:1620:LUT:H28	1.72	0.71
30:C:516:BCR:HC21	23:Z:13:ILE:HG23	1.74	0.70
30:C:517:BCR:H332	23:Z:12:LEU:HD23	1.74	0.70
2:3:95:GLN:HE22	2:3:102:PHE:H	1.39	0.69
2:7:95:GLN:HE22	2:7:102:PHE:H	1.39	0.69
1:G:70:ARG:NE	1:G:180:GLU:OE2	2.24	0.69
33:A:409:PHO:H3A	25:D:402:CLA:H142	1.75	0.68
6:C:456:GLU:OE2	6:C:457:LYS:NZ	2.26	0.68
17:R:163:ASN:HD22	25:R:616:CLA:HBC3	1.59	0.67
5:B:313:ASP:OD2	5:B:358:ARG:NH2	2.27	0.67
7:D:187:GLN:HB2	25:D:402:CLA:HBC1	1.76	0.67
5:B:18:ARG:NH1	14:L:5:ASN:HD22	1.91	0.67
17:R:235:LEU:HD22	3:8:91:PRO:HB2	180.03	0.67
3:4:91:PRO:HB2	17:R:235:LEU:HD22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:C:517:BCR:H333	23:Z:9:VAL:HG13	1.77	0.67
18:S:200:MET:HG2	26:S:1621:LUT:H14	1.76	0.67
5:B:187:VAL:HG23	25:B:602:CLA:HMD3	1.77	0.66
5:B:145:LEU:HB3	25:B:605:CLA:H162	1.77	0.66
18:S:139:VAL:HG22	24:S:607:CHL:HBC1	1.77	0.66
7:D:193:THR:HG23	25:D:402:CLA:HBC2	1.78	0.66
25:C:503:CLA:HMA1	35:Z:101:LMG:H191	1.78	0.65
14:L:20:TRP:CZ3	14:L:23:LEU:HD23	2.32	0.65
18:S:147:GLY:HA2	25:S:609:CLA:HAB	1.79	0.64
25:B:603:CLA:H12	10:H:61:TYR:CD2	2.30	0.64
25:A:410:CLA:HAA2	35:A:413:LMG:H112	1.79	0.64
4:A:221:SER:HA	7:D:140:ARG:HB2	1.80	0.64
2:7:208:GLN:HE22	26:7:1620:LUT:H41	1.62	0.64
2:3:208:GLN:HE22	26:3:1620:LUT:H41	1.62	0.64
24:R:606:CHL:HBA2	28:R:623:NEX:H403	1.80	0.64
17:R:93:ARG:NH1	17:R:96:GLU:OE2	2.31	0.64
25:5:610:CLA:H2	26:5:1620:LUT:H28	1.81	0.63
10:H:61:TYR:HD1	10:H:61:TYR:O	1.82	0.63
4:A:82:ILE:HB	4:A:174:LEU:HB2	1.80	0.63
34:B:621:SQD:H141	34:B:623:SQD:H122	1.81	0.63
25:G:610:CLA:H52	26:G:1620:LUT:H28	1.81	0.63
3:8:138:VAL:HG22	3:8:140:SER:H	1.63	0.62
16:O:117:GLN:HE21	16:O:121:GLY:HA2	1.64	0.62
25:B:608:CLA:H2	35:B:622:LMG:H151	1.81	0.62
3:4:138:VAL:HG22	3:4:140:SER:H	1.63	0.62
27:N:1622:XAT:H363	29:N:2630:LHG:HC41	1.81	0.62
7:D:20:ASP:OD2	7:D:24:ARG:NH1	2.28	0.62
5:B:423:ARG:NH1	5:B:430:PHE:O	2.33	0.62
4:A:140:ARG:HB2	7:D:221:ASN:HA	1.82	0.62
1:N:118:LEU:HG	18:S:127:PHE:HZ	1.65	0.62
5:B:12:VAL:HG12	25:B:613:CLA:HMC2	1.82	0.62
25:1:610:CLA:H2	26:1:1620:LUT:H28	1.81	0.61
25:B:603:CLA:H202	37:H:102:DGD:HA72	1.81	0.61
25:A:410:CLA:H2	11:I:12:VAL:HG11	1.83	0.61
25:1:602:CLA:HBA1	26:1:1621:LUT:H382	1.83	0.61
22:X:81:VAL:HG12	22:X:83:ARG:H	1.65	0.61
24:6:606:CHL:HMB1	24:6:609:CHL:HAC1	1.82	0.61
6:C:402:GLY:HA3	6:C:420:VAL:HG22	1.83	0.61
25:R:602:CLA:H72	27:R:622:XAT:H28	1.83	0.61
7:D:298:ASP:HA	7:D:316:TYR:OH	2.00	0.61
6:C:86:LEU:HD13	6:C:89:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:511:CLA:H141	23:Z:20:LEU:HD22	1.83	0.61
1:6:163:PRO:HD2	26:6:1620:LUT:H23	1.83	0.60
27:7:1622:XAT:H12	29:7:2630:LHG:H191	1.83	0.60
24:2:606:CHL:HMB1	24:2:609:CHL:HAC1	1.82	0.60
3:4:93:SER:N	17:R:235:LEU:O	2.35	0.60
25:G:613:CLA:H162	25:G:614:CLA:H2	1.83	0.60
25:C:511:CLA:HBA1	30:C:517:BCR:H271	1.84	0.60
1:Y:164:LEU:HD12	26:Y:1620:LUT:H222	1.84	0.60
6:C:45:LEU:HD22	6:C:138:GLU:HB3	1.84	0.60
1:G:115:ASN:HB3	1:G:118:LEU:HD12	1.84	0.60
2:7:50:PRO:HG3	2:7:188:LYS:HD3	1.83	0.60
5:B:311:PHE:O	5:B:317:ASN:ND2	2.35	0.60
1:G:103:GLN:NE2	25:G:604:CLA:O1D	2.34	0.60
1:2:104:ILE:HG21	1:2:124:ILE:HD13	1.83	0.59
1:6:104:ILE:HG21	1:6:124:ILE:HD13	1.83	0.59
27:3:1622:XAT:H12	29:3:2630:LHG:H191	1.83	0.59
4:A:24:THR:O	7:D:256:GLN:NE2	2.30	0.59
1:2:163:PRO:HD2	26:2:1620:LUT:H23	1.83	0.59
1:2:21:ARG:NH1	1:2:37:THR:O	2.35	0.59
1:6:21:ARG:NH1	1:6:37:THR:O	2.35	0.59
5:B:124:CYS:O	10:H:24:LYS:NZ	2.36	0.59
25:5:602:CLA:HBA1	26:5:1621:LUT:H382	1.83	0.59
17:R:97:LEU:HB3	17:R:172:LEU:HD11	1.85	0.59
5:B:18:ARG:NH2	34:B:621:SQD:O8	2.36	0.59
1:1:103:GLN:HE22	25:1:604:CLA:HED3	1.67	0.59
17:R:23:TYR:HD2	17:R:89:LEU:HD11	1.68	0.59
30:D:404:BCR:H14C	9:F:27:PHE:CD2	2.38	0.59
5:B:389:LYS:N	7:D:345:GLU:OE2	2.36	0.59
1:1:66:VAL:HG22	1:1:181:LEU:HD21	1.85	0.59
2:3:50:PRO:HG3	2:3:188:LYS:HD3	1.83	0.58
1:N:139:GLU:OE1	24:N:609:CHL:NA	2.36	0.58
16:O:227:ASP:HB3	16:O:230:ALA:HB3	1.85	0.58
17:R:59:LYS:HE2	17:R:61:LEU:HD21	1.85	0.58
1:Y:70:ARG:NE	1:Y:180:GLU:OE2	2.36	0.58
16:O:207:THR:HG22	16:O:214:VAL:HG22	1.84	0.58
17:R:235:LEU:O	3:8:93:SER:N	169.31	0.58
30:C:517:BCR:H312	13:K:33:LEU:HD13	1.84	0.58
17:R:16:PRO:HA	3:8:126:TRP:CH2	161.12	0.58
25:Y:603:CLA:HMD3	24:Y:607:CHL:H193	1.85	0.58
6:C:472:LEU:HD21	7:D:256:GLN:HE21	1.68	0.58
2:3:79:ARG:NH1	24:3:608:CHL:OBD	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5:603:CLA:HMD1	24:5:609:CHL:HBA2	1.86	0.58
17:R:236:HIS:HA	3:8:93:SER:HB2	165.24	0.58
1:5:66:VAL:HG22	1:5:181:LEU:HD21	1.85	0.58
6:C:346:THR:OG1	6:C:348:GLU:OE1	2.21	0.58
7:D:108:LEU:HD23	8:E:66:ILE:HD13	1.85	0.58
17:R:101:ARG:NH2	24:R:608:CHL:OBD	2.36	0.58
2:7:141:GLN:HE22	24:7:607:CHL:HMC	1.69	0.58
1:N:23:LYS:NZ	1:N:32:SER:HB3	2.19	0.58
4:A:77:ILE:HD11	19:T:6:TYR:HB3	1.85	0.58
25:3:603:CLA:HMD1	24:3:609:CHL:HBA2	1.85	0.58
2:7:79:ARG:NH1	24:7:608:CHL:OBD	2.36	0.58
3:4:126:TRP:CH2	17:R:16:PRO:HA	2.39	0.57
1:5:103:GLN:HE22	25:5:604:CLA:HED3	1.67	0.57
4:A:201:GLY:HA3	4:A:286:THR:HG23	1.86	0.57
33:A:409:PHO:OBD	7:D:130:GLN:NE2	2.37	0.57
25:3:611:CLA:HAB	27:3:1622:XAT:H221	1.86	0.57
29:C:522:LHG:H181	21:W:31:GLY:HA3	1.86	0.57
3:4:93:SER:HB2	17:R:236:HIS:HA	1.85	0.57
4:A:43:THR:HG23	30:A:411:BCR:H362	1.87	0.57
25:7:603:CLA:HMD1	24:7:609:CHL:HBA2	1.85	0.57
4:A:166:GLY:HA3	6:C:358:PHE:HE1	1.70	0.57
1:N:64:LEU:HD11	1:Y:49:ALA:HA	1.87	0.57
25:7:611:CLA:HAB	27:7:1622:XAT:H221	1.86	0.57
30:D:404:BCR:H372	35:D:411:LMG:H292	1.87	0.57
16:O:51:LEU:HB3	16:O:89:ILE:HB	1.86	0.57
1:Y:51:LEU:HD13	25:Y:602:CLA:H42	1.87	0.57
1:5:94:GLU:N	1:5:103:GLN:OE1	2.38	0.56
5:B:256:MET:HA	5:B:263:THR:HG21	1.87	0.56
6:C:282:PHE:HE1	25:C:501:CLA:H111	1.70	0.56
25:C:511:CLA:C4D	13:K:54:TRP:HH2	2.18	0.56
5:B:30:VAL:HG11	25:B:613:CLA:H112	1.87	0.56
5:B:30:VAL:HG12	25:B:606:CLA:HHD	1.87	0.56
17:R:235:LEU:HB3	3:8:92:PHE:HA	173.58	0.56
2:3:109:LYS:HA	24:3:607:CHL:HED3	1.87	0.56
2:3:141:GLN:HE22	24:3:607:CHL:HMC	1.69	0.56
25:4:611:CLA:HBA2	25:4:612:CLA:HMD1	1.87	0.56
1:N:110:LEU:HD22	24:N:606:CHL:HMD2	1.88	0.56
17:R:124:ALA:HB1	25:R:604:CLA:HED1	1.86	0.56
1:N:70:ARG:NH1	24:N:608:CHL:OBD	2.33	0.56
1:2:213:LEU:HD21	25:2:614:CLA:HMC3	1.86	0.56
2:7:175:LEU:HD13	26:7:1620:LUT:H222	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:213:LEU:HD21	25:6:614:CLA:HMC3	1.86	0.56
4:A:136:ARG:NH1	11:I:27:ASP:OD1	2.39	0.56
29:D:408:LHG:H152	29:L:101:LHG:H272	1.87	0.56
25:B:606:CLA:HMA1	25:B:607:CLA:H3A	1.88	0.56
37:C:519:DGD:HAT2	37:C:520:DGD:HBE1	1.88	0.56
29:C:2630:LHG:H101	25:S:611:CLA:HAB	1.87	0.56
25:1:603:CLA:HMD1	24:1:609:CHL:HBA2	1.86	0.56
25:N:603:CLA:HMD1	24:N:609:CHL:HBA2	1.88	0.56
17:R:91:ARG:NH1	25:R:603:CLA:O1A	2.38	0.56
1:1:21:ARG:NH2	1:1:36:LEU:O	2.39	0.55
4:A:140:ARG:NH2	29:D:410:LHG:O5	2.39	0.55
1:N:21:ARG:NH2	1:N:36:LEU:O	2.38	0.55
25:Y:602:CLA:H92	25:Y:603:CLA:HMA1	1.87	0.55
4:A:42:LEU:HD23	34:A:418:SQD:H212	1.88	0.55
3:4:92:PHE:HA	17:R:235:LEU:HB3	1.87	0.55
4:A:303:ASN:O	6:C:415:ASN:ND2	2.39	0.55
24:G:606:CHL:HMB1	24:G:609:CHL:HAC1	1.89	0.55
1:G:69:SER:HB3	1:G:184:GLY:HA3	1.89	0.55
2:7:109:LYS:HA	24:7:607:CHL:HED3	1.87	0.55
29:D:409:LHG:O1	29:L:101:LHG:O4	2.25	0.55
18:S:202:GLY:O	18:S:206:GLN:HB3	2.07	0.55
25:C:501:CLA:H171	25:C:507:CLA:H122	1.89	0.55
1:1:94:GLU:N	1:1:103:GLN:OE1	2.38	0.55
1:2:193:GLY:O	1:2:197:GLN:HG2	2.07	0.55
25:G:603:CLA:H12	1:N:51:LEU:HD11	1.88	0.55
21:W:17:LEU:HA	21:W:22:LEU:HD23	1.89	0.55
6:C:311:GLN:OE1	6:C:355:THR:OG1	2.25	0.55
5:B:191:ASP:HB2	10:H:70:ILE:HG12	1.89	0.55
1:N:103:GLN:NE2	25:N:604:CLA:O1D	2.40	0.55
1:2:215:ASP:OD2	1:2:218:ASN:ND2	2.40	0.55
1:5:21:ARG:NH2	1:5:36:LEU:O	2.39	0.55
1:6:193:GLY:O	1:6:197:GLN:HG2	2.07	0.55
25:8:611:CLA:HBA2	25:8:612:CLA:HMD1	1.87	0.55
25:C:513:CLA:H71	29:C:2630:LHG:H122	1.89	0.55
16:O:65:VAL:HA	16:O:71:LEU:HD21	1.90	0.55
16:O:81:ARG:NH1	21:W:9:GLU:OE2	2.40	0.55
1:2:27:PRO:O	2:3:154:ASN:ND2	2.40	0.54
2:3:175:LEU:HD13	26:3:1620:LUT:H222	1.88	0.54
24:1:607:CHL:HBB1	24:3:601:CHL:H141	1.90	0.54
29:B:2631:LHG:H242	29:B:2631:LHG:HC91	1.90	0.54
5:B:357:ARG:NH1	5:B:358:ARG:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:410:CLA:H2	11:I:12:VAL:CG1	2.37	0.54
1:N:70:ARG:NE	1:N:180:GLU:OE2	2.38	0.54
1:Y:104:ILE:HG21	1:Y:124:ILE:HD13	1.90	0.54
6:C:297:TYR:O	6:C:423:ARG:NH2	2.38	0.54
1:1:164:LEU:HD13	26:1:1620:LUT:H222	1.90	0.54
1:6:27:PRO:O	2:7:154:ASN:ND2	2.40	0.54
25:7:603:CLA:HMA2	25:7:603:CLA:H2	1.90	0.54
29:8:2630:LHG:O1	29:8:2630:LHG:O3	2.24	0.54
5:B:256:MET:O	5:B:448:ARG:NH1	2.39	0.54
17:R:182:LEU:HD12	26:R:620:LUT:H222	1.90	0.54
25:3:603:CLA:HMA2	25:3:603:CLA:H2	1.90	0.54
4:A:293:MET:HG2	4:A:298:ASN:HA	1.90	0.54
1:6:85:LEU:HD23	1:6:88:ASN:HD22	1.73	0.54
25:7:611:CLA:H3A	3:8:131:SER:HA	1.90	0.54
14:L:20:TRP:HA	14:L:20:TRP:CE3	2.43	0.54
3:4:161:ILE:HA	3:4:166:TYR:HA	1.90	0.54
1:6:215:ASP:OD2	1:6:218:ASN:ND2	2.40	0.54
25:C:511:CLA:CHA	13:K:54:TRP:HH2	2.21	0.54
6:C:130:ILE:HD11	30:C:517:BCR:H21C	1.90	0.54
24:G:608:CHL:H152	28:G:1623:NEX:H402	1.90	0.54
24:5:607:CHL:HBB1	24:7:601:CHL:H141	1.89	0.54
30:B:618:BCR:H322	35:B:622:LMG:H111	1.90	0.54
17:R:204:LEU:HD13	25:R:611:CLA:HBC1	1.90	0.54
1:2:85:LEU:HD23	1:2:88:ASN:HD22	1.73	0.54
3:4:31:GLY:HA3	3:4:181:ILE:HG21	1.90	0.54
1:5:164:LEU:HD13	26:5:1620:LUT:H222	1.90	0.54
3:8:161:ILE:HA	3:8:166:TYR:HA	1.90	0.54
5:B:358:ARG:HG3	20:U:19:THR:HB	1.90	0.54
6:C:154:ARG:HB3	6:C:256:PRO:HG2	1.90	0.54
1:N:135:MET:HA	1:N:138:VAL:HG22	1.90	0.54
2:3:202:MET:HE2	26:3:1621:LUT:H10	1.88	0.53
6:C:223:TRP:HZ3	6:C:285:ILE:CD1	2.22	0.53
29:C:523:LHG:HC5	25:Y:611:CLA:H11	1.90	0.53
17:R:39:LEU:HD12	27:R:622:XAT:H23	1.90	0.53
18:S:125:ASN:ND2	18:S:130:ASN:OD1	2.41	0.53
25:3:611:CLA:H3A	3:4:131:SER:HA	1.90	0.53
1:6:63:GLU:HA	1:6:155:LEU:HD21	1.91	0.53
2:7:112:SER:HB3	24:7:607:CHL:HED2	1.90	0.53
25:G:602:CLA:H92	25:G:603:CLA:HMA1	1.90	0.53
29:S:2630:LHG:H282	29:S:2630:LHG:HC91	1.90	0.53
27:2:1622:XAT:H14	29:2:2630:LHG:H171	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:131:TRP:CZ3	25:C:505:CLA:HAA2	2.44	0.53
36:D:405:PL9:H111	29:D:409:LHG:HC92	1.91	0.53
25:2:603:CLA:HED2	24:2:609:CHL:H93	1.90	0.53
3:8:65:VAL:HG21	26:8:620:LUT:H12	1.91	0.53
16:O:145:GLU:HB3	16:O:197:LYS:HE2	1.91	0.53
1:Y:80:VAL:HG13	1:Y:206:LEU:HD11	1.90	0.53
1:1:18:GLY:O	1:1:21:ARG:NH1	2.40	0.53
33:A:409:PHO:HBC3	7:D:280:LEU:HD22	1.91	0.53
33:A:408:PHO:H51	34:A:418:SQD:H201	1.91	0.53
30:D:404:BCR:H21C	35:D:411:LMG:H372	1.90	0.53
24:N:608:CHL:HBB1	24:N:608:CHL:HHC	1.91	0.53
16:O:111:TYR:HD2	16:O:127:LEU:HD11	1.74	0.53
1:Y:126:ALA:HB3	24:Y:605:CHL:HMC	1.91	0.53
24:G:601:CHL:HHC	24:G:601:CHL:HBB1	1.91	0.53
3:8:31:GLY:HA3	3:8:181:ILE:HG21	1.90	0.52
34:B:623:SQD:H62	14:L:8:GLU:HB2	1.91	0.52
25:N:602:CLA:H203	26:N:1621:LUT:H391	1.90	0.52
1:Y:103:GLN:HE22	25:Y:604:CLA:HED2	1.74	0.52
5:B:153:PHE:HB2	25:B:607:CLA:HBB1	1.91	0.52
6:C:79:LYS:HB3	6:C:84:GLN:HE21	1.75	0.52
4:A:279:PRO:HG2	7:D:213:ALA:HB2	1.91	0.52
18:S:99:ASN:ND2	18:S:103:ALA:O	2.42	0.52
1:Y:212:HIS:CG	25:Y:613:CLA:HAA2	2.44	0.52
24:1:608:CHL:HBB1	24:1:608:CHL:HHC	1.92	0.52
2:3:174:PRO:HD2	26:3:1620:LUT:H23	1.91	0.52
25:6:603:CLA:HED2	24:6:609:CHL:H93	1.91	0.52
5:B:169:SER:HA	5:B:176:GLY:HA2	1.92	0.52
5:B:255:THR:HG21	25:B:603:CLA:HED1	1.91	0.52
6:C:345:PRO:HB3	16:O:81:ARG:HD3	1.91	0.52
6:C:223:TRP:HE3	37:C:518:DGD:HB21	1.73	0.52
1:Y:44:TYR:HE2	24:Y:601:CHL:HBC2	1.74	0.52
1:1:52:SER:OG	1:1:61:ASN:ND2	2.43	0.52
1:2:221:ALA:N	25:2:613:CLA:O1A	2.43	0.52
27:6:1622:XAT:H14	29:6:2630:LHG:H171	1.91	0.52
5:B:18:ARG:HH11	14:L:5:ASN:HD22	1.56	0.52
1:2:25:LEU:HB3	1:2:28:PHE:HB2	1.91	0.52
2:7:174:PRO:HD2	26:7:1620:LUT:H23	1.91	0.52
4:A:162:PRO:HB3	4:A:168:PHE:HA	1.91	0.52
24:N:601:CHL:HHC	24:N:601:CHL:HBB1	1.92	0.52
1:N:69:SER:HB3	1:N:184:GLY:HA3	1.91	0.52
16:O:32:ILE:HG23	16:O:208:LYS:HE2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:50:THR:O	18:S:50:THR:HG22	2.09	0.52
27:G:1622:XAT:H1	29:G:2630:LHG:HO1	1.56	0.52
14:L:17:SER:HB3	29:L:101:LHG:HC62	1.91	0.52
17:R:75:VAL:HG22	17:R:83:TYR:HE1	1.75	0.52
3:8:131:SER:O	3:8:133:THR:OG1	2.24	0.52
1:G:51:LEU:HD13	25:G:602:CLA:H42	1.92	0.52
4:A:85:THR:HA	4:A:109:GLY:HA3	1.91	0.52
6:C:251:HIS:HE1	25:C:506:CLA:NA	2.08	0.52
17:R:96:GLU:HB2	25:R:602:CLA:C1B	2.40	0.52
5:B:214:LEU:CD1	25:R:609:CLA:H93	2.40	0.52
3:4:65:VAL:HG21	26:4:620:LUT:H12	1.91	0.52
1:6:25:LEU:HB3	1:6:28:PHE:HB2	1.91	0.52
25:B:615:CLA:H43	34:B:621:SQD:H122	1.91	0.52
27:Y:1622:XAT:H10	29:Y:2630:LHG:H212	1.92	0.52
24:5:608:CHL:HBB1	24:5:608:CHL:HHC	1.92	0.52
6:C:322:GLN:HE22	6:C:381:LYS:HA	1.75	0.52
1:N:51:LEU:HD13	25:N:602:CLA:H42	1.90	0.52
1:1:69:SER:HB3	1:1:184:GLY:HA3	1.92	0.51
1:2:63:GLU:HA	1:2:155:LEU:HD21	1.91	0.51
5:B:155:ALA:O	5:B:159:THR:OG1	2.28	0.51
5:B:75:TRP:HB3	37:B:626:DGD:HD5	1.91	0.51
6:C:454:GLY:O	11:I:34:ARG:NH2	2.43	0.51
25:C:503:CLA:HAB	25:C:512:CLA:H41	1.92	0.51
2:3:112:SER:HB3	24:3:607:CHL:HED2	1.90	0.51
3:8:10:ILE:HG23	3:8:11:PRO:HD3	1.92	0.51
4:A:257:ARG:NH2	5:B:491:GLU:O	2.43	0.51
25:C:511:CLA:C4D	13:K:54:TRP:CH2	2.93	0.51
1:6:221:ALA:N	25:6:613:CLA:O1A	2.43	0.51
1:G:213:LEU:HD21	25:G:614:CLA:HMC3	1.92	0.51
29:C:2630:LHG:H152	29:S:2630:LHG:H111	1.92	0.51
1:Y:69:SER:HB3	1:Y:184:GLY:HA3	1.92	0.51
4:A:189:GLU:OE2	31:A:401:OEX:O5	2.29	0.51
34:A:412:SQD:H442	7:D:233:PHE:CD2	2.46	0.51
25:B:604:CLA:HAB	25:B:606:CLA:H152	1.92	0.51
30:B:619:BCR:HC42	35:B:622:LMG:H341	1.93	0.51
1:G:51:LEU:HD11	25:Y:603:CLA:H12	1.93	0.51
24:Y:606:CHL:HMB1	24:Y:609:CHL:HAC1	1.93	0.51
24:Y:608:CHL:HBB1	24:Y:608:CHL:HHC	1.92	0.51
1:1:77:LEU:HD13	25:1:612:CLA:HBB2	1.92	0.51
2:3:114:ILE:HG21	2:3:134:ILE:HD13	1.91	0.51
5:B:223:GLN:N	10:H:34:ALA:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:94:GLU:N	1:2:103:GLN:OE1	2.43	0.51
25:3:602:CLA:H72	26:3:1621:LUT:H30	1.93	0.51
1:G:21:ARG:NH2	1:G:36:LEU:O	2.41	0.51
16:O:138:LYS:HG2	16:O:140:ASP:H	1.75	0.51
1:5:77:LEU:HD13	25:5:612:CLA:HBB2	1.92	0.51
3:8:58:GLY:HA3	3:8:184:ALA:HB1	1.93	0.51
1:N:118:LEU:HG	18:S:127:PHE:CZ	2.46	0.51
25:Y:603:CLA:HMA2	25:Y:603:CLA:H2	1.92	0.51
25:2:602:CLA:HBA1	26:2:1621:LUT:H382	1.93	0.51
3:4:58:GLY:HA3	3:4:184:ALA:HB1	1.93	0.51
1:5:52:SER:OG	1:5:61:ASN:ND2	2.43	0.51
1:5:69:SER:HB3	1:5:184:GLY:HA3	1.92	0.51
1:6:94:GLU:N	1:6:103:GLN:OE1	2.43	0.51
34:A:412:SQD:H131	29:D:410:LHG:H142	1.93	0.51
6:C:40:ALA:HB2	25:C:508:CLA:H2A	1.93	0.51
1:Y:41:PRO:HG3	1:Y:177:LYS:HB3	1.93	0.51
1:1:51:LEU:HD13	25:1:602:CLA:H42	1.93	0.51
3:8:120:ASP:O	3:8:123:SER:OG	2.28	0.51
19:T:15:GLY:HA2	30:T:101:BCR:H12C	1.92	0.51
1:Y:135:MET:HA	1:Y:138:VAL:HG22	1.93	0.51
1:5:51:LEU:HD13	25:5:602:CLA:H42	1.93	0.51
2:7:114:ILE:HG21	2:7:134:ILE:HD13	1.91	0.51
2:7:175:LEU:HB3	2:7:177:LEU:HD13	1.93	0.51
25:7:602:CLA:H72	26:7:1621:LUT:H30	1.93	0.51
25:A:405:CLA:H122	33:A:408:PHO:H3A	1.94	0.51
11:I:5:LYS:HE2	21:W:22:LEU:HD21	1.94	0.50
19:T:17:ILE:HG22	30:T:101:BCR:H313	1.93	0.50
3:4:120:ASP:O	3:4:123:SER:OG	2.28	0.50
27:6:1622:XAT:H41	24:7:607:CHL:HAA2	1.93	0.50
17:R:100:GLY:HA3	17:R:202:ALA:HB1	1.93	0.50
25:B:605:CLA:H91	25:B:607:CLA:HAB	1.92	0.50
25:B:605:CLA:HBA1	25:B:605:CLA:HBD	1.93	0.50
24:Y:601:CHL:HHC	24:Y:601:CHL:HBB1	1.92	0.50
29:C:522:LHG:H192	25:Y:612:CLA:H101	1.93	0.50
5:B:281:GLN:NE2	20:U:19:THR:OG1	2.42	0.50
6:C:148:GLY:O	6:C:156:LYS:NZ	2.44	0.50
2:3:175:LEU:HB3	2:3:177:LEU:HD13	1.93	0.50
3:4:10:ILE:HG23	3:4:11:PRO:HD3	1.93	0.50
4:A:286:THR:HG21	25:A:405:CLA:HMA3	1.93	0.50
4:A:256:GLY:HA3	5:B:492:PHE:HZ	1.76	0.50
4:A:98:GLU:OE2	21:W:8:THR:OG1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:N:609:CHL:HBB1	24:Y:601:CHL:H51	1.93	0.50
6:C:38:GLY:HA3	25:C:511:CLA:HMD3	1.94	0.50
17:R:194:LEU:HB3	25:R:610:CLA:H3A	1.93	0.50
1:Y:103:GLN:NE2	25:Y:604:CLA:O1D	2.44	0.50
3:4:57:HIS:HD2	27:4:622:XAT:H15	1.77	0.50
24:8:608:CHL:HBB1	24:8:608:CHL:HHC	1.93	0.50
25:8:612:CLA:H2A	25:8:612:CLA:HED2	1.94	0.50
25:A:410:CLA:H13	35:A:413:LMG:H321	1.94	0.50
17:R:215:GLN:O	17:R:219:THR:OG1	2.25	0.50
18:S:166:PRO:HB3	24:S:608:CHL:HBC2	1.94	0.50
7:D:297:TYR:OH	7:D:327:ARG:NH1	2.42	0.50
1:N:153:ASP:OD2	1:N:156:TYR:N	2.43	0.50
25:S:603:CLA:H2A	25:S:603:CLA:HED2	1.94	0.50
2:3:152:ARG:NH2	24:3:609:CHL:O1D	2.45	0.50
25:4:612:CLA:HED2	25:4:612:CLA:H2A	1.94	0.50
3:4:154:PRO:HD2	26:4:620:LUT:H23	1.94	0.50
4:A:38:ILE:HG23	34:A:418:SQD:H151	1.94	0.50
30:B:618:BCR:HC41	15:M:6:LEU:HD23	1.94	0.50
7:D:30:PHE:O	7:D:129:ARG:NH1	2.37	0.50
1:G:73:MET:SD	25:G:610:CLA:HAB	2.52	0.50
1:Y:44:TYR:CE2	24:Y:601:CHL:HBC2	2.47	0.50
1:2:208:ASN:ND2	25:2:613:CLA:O1D	2.45	0.49
25:6:603:CLA:HMD1	24:6:609:CHL:HBA2	1.94	0.49
1:G:220:ASN:HB2	25:G:614:CLA:HED1	1.94	0.49
27:2:1622:XAT:H41	24:3:607:CHL:HAA2	1.93	0.49
24:4:608:CHL:HBB1	24:4:608:CHL:HHC	1.93	0.49
5:B:330:MET:HA	5:B:444:ARG:HB2	1.93	0.49
18:S:83:ARG:NE	18:S:189:GLU:OE2	2.44	0.49
24:3:606:CHL:HMB1	24:3:609:CHL:HAC1	1.94	0.49
6:C:110:PRO:HB3	35:Z:101:LMG:H142	1.94	0.49
6:C:230:LEU:HD23	6:C:233:ILE:HD12	1.94	0.49
8:E:57:THR:O	8:E:61:GLN:NE2	2.46	0.49
1:G:163:PRO:HD2	26:G:1620:LUT:H23	1.94	0.49
1:N:162:ASP:OD1	26:N:1620:LUT:O23	2.31	0.49
25:Y:611:CLA:HHC	25:Y:611:CLA:HBB1	1.94	0.49
25:6:602:CLA:HBA1	26:6:1621:LUT:H382	1.93	0.49
3:8:57:HIS:HD2	27:8:622:XAT:H15	1.77	0.49
4:A:267:ASN:ND2	7:D:233:PHE:O	2.45	0.49
5:B:362:PHE:HB3	7:D:189:PHE:CD2	2.48	0.49
8:E:60:ARG:NH1	8:E:62:GLY:O	2.45	0.49
24:G:607:CHL:HBB1	26:G:1621:LUT:H161	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:ARG:NH1	24:G:608:CHL:OBD	2.38	0.49
5:B:10:THR:OG1	17:R:55:GLN:NE2	2.45	0.49
24:1:607:CHL:HAA2	27:3:1622:XAT:H41	1.94	0.49
1:2:222:TRP:HZ2	2:3:138:LEU:HD22	1.78	0.49
25:2:603:CLA:HMD1	24:2:609:CHL:HBA2	1.94	0.49
24:5:607:CHL:HAA2	27:7:1622:XAT:H41	1.95	0.49
25:A:405:CLA:H102	33:A:408:PHO:HAA1	1.95	0.49
30:B:619:BCR:H14C	30:T:101:BCR:H383	32.43	0.49
25:G:603:CLA:H42	25:Y:603:CLA:H41	1.95	0.49
5:B:299:SER:HB3	5:B:407:ASN:HD21	1.78	0.49
1:5:18:GLY:O	1:5:21:ARG:NH1	2.40	0.49
25:A:407:CLA:HAB	25:D:402:CLA:H72	1.95	0.49
5:B:320:ALA:HB1	7:D:293:ASN:HD22	1.77	0.49
1:G:135:MET:HA	1:G:138:VAL:HG22	1.94	0.49
1:N:41:PRO:HG3	1:N:177:LYS:HD3	1.94	0.49
25:N:610:CLA:HBB1	25:N:612:CLA:H3A	1.95	0.49
17:R:187:ASP:N	17:R:187:ASP:OD1	2.37	0.49
17:R:23:TYR:OH	17:R:35:ASP:OD2	2.28	0.49
1:Y:73:MET:SD	25:Y:610:CLA:HAB	2.53	0.49
1:6:222:TRP:HZ2	2:7:138:LEU:HD22	1.78	0.49
25:B:615:CLA:H8	30:B:618:BCR:H362	1.95	0.49
1:N:65:GLU:OE2	1:N:185:ARG:NE	2.43	0.49
3:4:93:SER:CB	17:R:236:HIS:HA	2.43	0.49
17:R:39:LEU:HD13	25:R:602:CLA:H42	1.95	0.49
1:Y:142:ARG:NH2	24:Y:609:CHL:O1D	2.43	0.49
27:3:1622:XAT:H393	29:3:2630:LHG:H101	1.94	0.49
4:A:176:ILE:HD11	36:D:405:PL9:H452	1.95	0.49
4:A:254:TYR:HE2	7:D:143:ASN:HD22	1.61	0.49
5:B:321:LYS:NZ	5:B:363:PHE:O	2.46	0.49
1:G:64:LEU:HD11	1:N:49:ALA:HA	1.95	0.49
25:B:602:CLA:HAC1	30:H:101:BCR:H383	1.95	0.49
17:R:180:ASP:OD1	26:R:620:LUT:O23	2.29	0.49
1:6:176:LEU:HB3	25:6:610:CLA:H3A	1.95	0.48
17:R:236:HIS:HA	3:8:93:SER:CB	165.04	0.48
4:A:12:ASN:HD21	21:W:40:TYR:HA	1.78	0.48
6:C:28:GLN:NE2	7:D:234:ARG:HD3	2.28	0.48
5:B:362:PHE:HB3	7:D:189:PHE:HD2	1.78	0.48
25:B:603:CLA:C1	10:H:61:TYR:HD2	2.23	0.48
1:6:208:ASN:ND2	25:6:613:CLA:O1D	2.45	0.48
24:7:606:CHL:HMB1	24:7:609:CHL:HAC1	1.94	0.48
25:B:616:CLA:H172	25:B:616:CLA:H91	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:409:LHG:H131	14:L:20:TRP:HH2	1.78	0.48
7:D:25:ARG:NH2	22:X:81:VAL:HG22	2.28	0.48
2:7:152:ARG:NH2	24:7:609:CHL:O1D	2.45	0.48
1:G:162:ASP:OD1	26:G:1620:LUT:O23	2.32	0.48
1:G:139:GLU:OE1	24:G:609:CHL:NA	2.46	0.48
18:S:60:ASP:OD1	26:S:1621:LUT:O23	2.30	0.48
27:5:1622:XAT:H41	24:6:607:CHL:HAA2	1.95	0.48
2:7:202:MET:HE2	26:7:1621:LUT:H10	1.95	0.48
3:8:154:PRO:HD2	26:8:620:LUT:H23	1.94	0.48
6:C:223:TRP:CZ3	6:C:285:ILE:CD1	2.97	0.48
25:C:501:CLA:HBB1	25:C:507:CLA:H41	1.95	0.48
1:2:176:LEU:HB3	25:2:610:CLA:H3A	1.95	0.48
1:2:51:LEU:HD13	25:2:602:CLA:H42	1.95	0.48
3:4:143:GLU:H	3:4:146:TYR:HB2	1.79	0.48
27:6:1622:XAT:H31	27:6:1622:XAT:H391	1.71	0.48
25:7:611:CLA:HMB2	3:8:130:TRP:HB2	1.95	0.48
25:R:611:CLA:HAB	3:8:130:TRP:HD1	174.44	0.48
29:B:2630:LHG:H241	24:R:607:CHL:HMD2	1.95	0.48
1:2:103:GLN:HG3	1:2:110:LEU:HD13	1.96	0.48
1:6:96:VAL:HG12	1:6:99:LYS:H	1.78	0.48
4:A:131:TRP:HE1	6:C:446:GLY:HA2	1.79	0.48
31:A:401:OEX:O4	6:C:357:ARG:NH2	2.46	0.48
14:L:20:TRP:CZ3	29:L:101:LHG:H161	2.49	0.48
3:4:130:TRP:HD1	25:R:611:CLA:HAB	1.78	0.48
27:7:1622:XAT:H393	29:7:2630:LHG:H101	1.94	0.48
1:G:65:GLU:OE2	1:G:185:ARG:NE	2.43	0.48
29:D:408:LHG:O9	29:L:101:LHG:HC81	2.13	0.48
27:1:1622:XAT:H41	24:2:607:CHL:HAA2	1.95	0.48
25:C:507:CLA:H142	30:C:515:BCR:H362	1.96	0.48
14:L:24:LEU:HD23	29:L:101:LHG:H261	1.96	0.48
25:N:602:CLA:H92	25:N:603:CLA:HMA1	1.95	0.48
1:2:87:ARG:HH12	1:2:210:ALA:HB2	1.79	0.48
3:4:131:SER:O	3:4:133:THR:OG1	2.24	0.48
1:6:118:LEU:HD23	24:6:605:CHL:HED2	1.96	0.48
5:B:168:VAL:HG13	5:B:195:PRO:HG2	1.95	0.48
17:R:83:TYR:OH	17:R:94:GLU:OE1	2.25	0.48
18:S:210:THR:HG22	18:S:233:VAL:HG11	1.95	0.48
3:4:129:PRO:HB2	25:R:611:CLA:HMB1	1.96	0.48
5:B:41:GLU:O	5:B:45:PHE:N	2.46	0.48
25:B:614:CLA:H41	25:B:614:CLA:H61	1.61	0.48
7:D:157:VAL:HG22	7:D:287:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:52:GLY:HA3	7:D:79:VAL:HG22	1.96	0.48
1:G:194:PHE:HE1	26:G:1620:LUT:C5	2.27	0.48
18:S:222:LEU:HD11	25:S:614:CLA:HMC3	1.94	0.48
4:A:301:ASN:OD1	4:A:303:ASN:ND2	2.47	0.47
33:A:408:PHO:H51	34:A:418:SQD:H223	1.96	0.47
1:N:179:LYS:HD3	25:N:612:CLA:HAA2	1.96	0.47
25:N:610:CLA:H71	25:N:612:CLA:H101	1.96	0.47
1:6:69:SER:HB3	1:6:184:GLY:HA3	1.96	0.47
4:A:84:PRO:HA	4:A:112:TYR:CG	2.49	0.47
1:G:194:PHE:HE1	26:G:1620:LUT:H41	1.79	0.47
1:G:110:LEU:HD21	25:G:604:CLA:HAA1	1.96	0.47
24:S:606:CHL:HHC	24:S:606:CHL:HBB1	1.96	0.47
1:2:96:VAL:HG12	1:2:99:LYS:H	1.78	0.47
24:3:608:CHL:H2A	24:3:608:CHL:HED3	1.97	0.47
1:6:51:LEU:HD13	25:6:602:CLA:H42	1.95	0.47
16:O:89:ILE:HD13	16:O:130:ILE:HD11	1.96	0.47
2:3:53:TYR:HB2	25:3:602:CLA:HMD1	1.96	0.47
2:7:72:ALA:HA	2:7:165:LEU:HD11	1.96	0.47
3:8:37:PRO:HD2	27:8:622:XAT:H242	1.95	0.47
25:C:511:CLA:HBA2	13:K:54:TRP:CH2	2.50	0.47
16:O:202:LEU:HD23	16:O:218:PHE:HB3	1.96	0.47
28:1:1623:NEX:H22	25:R:612:CLA:H11	1.97	0.47
16:O:58:PHE:CE2	21:W:2:VAL:HG21	2.50	0.47
28:1:1623:NEX:H11	28:1:1623:NEX:H191	1.78	0.47
25:1:613:CLA:H2	25:1:613:CLA:H61	1.60	0.47
1:2:153:ASP:OD2	1:2:156:TYR:N	2.43	0.47
2:3:116:SER:OG	2:3:119:GLY:O	2.33	0.47
2:3:30:ARG:NH1	2:3:46:THR:O	2.48	0.47
25:R:612:CLA:H11	28:5:1623:NEX:H22	170.16	0.47
24:7:608:CHL:HED3	24:7:608:CHL:H2A	1.97	0.47
5:B:236:THR:HB	5:B:473:THR:HG21	1.96	0.47
25:C:508:CLA:HBC2	29:D:410:LHG:H341	1.97	0.47
15:M:28:LYS:HG3	15:M:31:SER:HB3	6.17	0.47
25:N:603:CLA:H91	24:N:609:CHL:H112	1.97	0.47
28:R:623:NEX:H22	1:Y:163:PRO:HB2	126.87	0.47
1:2:118:LEU:HD23	24:2:605:CHL:HED2	1.96	0.47
3:8:143:GLU:H	3:8:146:TYR:HB2	1.79	0.47
5:B:363:PHE:CD1	5:B:363:PHE:N	2.83	0.47
30:C:517:BCR:H281	13:K:54:TRP:CE3	2.50	0.47
25:G:613:CLA:H91	29:G:2630:LHG:H321	1.96	0.47
24:G:607:CHL:H62	24:G:607:CHL:H2	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:176:LEU:HD23	1:N:179:LYS:HD2	1.97	0.47
18:S:19:VAL:HG12	18:S:21:ASP:H	1.79	0.47
14:L:26:PHE:CD1	19:T:16:ILE:HD11	2.50	0.47
30:B:620:BCR:H271	19:T:22:PHE:HB3	46.31	0.47
25:3:611:CLA:HMB2	3:4:130:TRP:HB2	1.95	0.47
3:4:37:PRO:HD2	27:4:622:XAT:H242	1.95	0.47
25:5:613:CLA:H2	25:5:613:CLA:H61	1.60	0.47
2:7:53:TYR:HB2	25:7:602:CLA:HMD1	1.96	0.47
6:C:206:PRO:O	6:C:210:PHE:HB2	2.15	0.47
7:D:160:ILE:HG21	7:D:288:VAL:HG22	1.96	0.47
28:N:1623:NEX:H11	28:N:1623:NEX:H191	1.73	0.47
18:S:79:LEU:HD13	18:S:164:LEU:HD23	1.96	0.47
1:Y:205:PRO:O	26:Y:1620:LUT:O3	2.29	0.47
2:3:128:LEU:HD23	24:3:605:CHL:HED2	1.96	0.47
29:4:2630:LHG:O3	29:4:2630:LHG:O1	2.24	0.47
1:5:191:MET:HE2	26:5:1621:LUT:H12	1.96	0.47
1:6:103:GLN:HG3	1:6:110:LEU:HD13	1.96	0.47
30:B:618:BCR:H342	30:T:101:BCR:H402	24.04	0.47
6:C:259:TRP:HH2	25:C:507:CLA:H201	1.80	0.47
6:C:279:LEU:HD11	25:C:507:CLA:HBA1	1.97	0.47
27:G:1622:XAT:H201	27:G:1622:XAT:H15	1.67	0.47
18:S:113:LYS:HA	24:S:607:CHL:HED3	1.96	0.47
1:2:69:SER:HB3	1:2:184:GLY:HA3	1.96	0.47
4:A:61:ASP:HB2	4:A:63:ILE:HG12	1.97	0.47
5:B:219:VAL:HG22	17:R:87:PHE:HZ	1.80	0.47
25:B:605:CLA:HBB1	25:B:614:CLA:HBC2	1.96	0.47
7:D:163:LEU:HD13	37:H:102:DGD:HB92	1.97	0.47
35:B:2633:LMG:H272	25:R:609:CLA:H43	1.97	0.47
1:6:87:ARG:HH12	1:6:210:ALA:HB2	1.79	0.47
24:7:606:CHL:HBC2	24:7:607:CHL:HH2	1.97	0.47
30:A:411:BCR:H11C	30:A:411:BCR:H341	1.81	0.47
5:B:185:TRP:HD1	24:R:607:CHL:H93	1.80	0.47
25:D:403:CLA:H61	25:D:403:CLA:H102	1.72	0.47
28:R:623:NEX:H11	28:R:623:NEX:H191	1.74	0.47
3:4:29:LEU:HD11	3:4:51:ARG:HD3	1.97	0.47
30:C:517:BCR:H351	30:C:517:BCR:H15C	1.80	0.47
7:D:49:TRP:HA	7:D:79:VAL:HG21	1.96	0.47
27:N:1622:XAT:H15	27:N:1622:XAT:H201	1.62	0.47
27:Y:1622:XAT:H31	27:Y:1622:XAT:H391	1.78	0.47
25:2:610:CLA:H43	25:2:612:CLA:HBA1	1.97	0.46
25:6:610:CLA:H43	25:6:612:CLA:HBA1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:167:LEU:HD11	25:C:512:CLA:HMB2	1.97	0.46
24:G:601:CHL:H91	24:G:601:CHL:H112	1.79	0.46
25:C:510:CLA:H191	13:K:45:LEU:HD23	1.97	0.46
16:O:220:SER:O	16:O:237:LYS:HA	2.15	0.46
24:Y:609:CHL:HBB1	24:Y:609:CHL:HHC	1.97	0.46
2:7:30:ARG:NH1	2:7:46:THR:O	2.48	0.46
4:A:292:THR:HG22	6:C:428:THR:HB	1.97	0.46
5:B:148:VAL:HG11	29:B:2631:LHG:H201	1.97	0.46
30:C:514:BCR:H351	30:C:514:BCR:H15C	1.78	0.46
6:C:87:ILE:O	6:C:91:HIS:ND1	2.48	0.46
28:Y:1623:NEX:H191	28:Y:1623:NEX:H11	1.74	0.46
1:1:191:MET:HE2	26:1:1621:LUT:H12	1.96	0.46
1:5:17:TYR:HE2	1:5:174:ALA:HB1	1.81	0.46
33:A:408:PHO:H2	33:A:408:PHO:H61	1.56	0.46
1:N:25:LEU:HB2	1:N:29:SER:HA	1.98	0.46
25:N:613:CLA:H2	25:N:613:CLA:H61	1.67	0.46
26:Y:1621:LUT:H15	26:Y:1621:LUT:H201	1.82	0.46
24:Y:607:CHL:H2	24:Y:607:CHL:H62	1.55	0.46
2:7:116:SER:OG	2:7:119:GLY:O	2.33	0.46
27:8:622:XAT:H15	27:8:622:XAT:H201	1.82	0.46
25:B:611:CLA:H141	25:B:613:CLA:HBD	1.96	0.46
7:D:173:SER:HB2	7:D:178:ALA:HB1	1.98	0.46
27:G:1622:XAT:H391	27:G:1622:XAT:H31	1.73	0.46
26:N:1621:LUT:H401	26:N:1621:LUT:H35	1.79	0.46
1:N:205:PRO:O	26:N:1620:LUT:O3	2.28	0.46
25:R:611:CLA:HMB1	3:8:129:PRO:HB2	172.84	0.46
25:1:613:CLA:H2	25:1:614:CLA:HMD1	1.97	0.46
6:C:223:TRP:HZ3	6:C:285:ILE:HG12	1.80	0.46
6:C:91:HIS:NE2	25:C:502:CLA:O1D	2.40	0.46
16:O:201:THR:O	16:O:218:PHE:HA	2.15	0.46
16:O:60:VAL:HG22	16:O:236:VAL:HG22	1.97	0.46
25:R:613:CLA:H92	29:R:2630:LHG:H171	1.98	0.46
25:Y:602:CLA:H101	26:Y:1621:LUT:H371	1.97	0.46
1:1:215:ASP:OD2	1:1:218:ASN:ND2	2.46	0.46
2:7:128:LEU:HD23	24:7:605:CHL:HED2	1.96	0.46
30:C:515:BCR:H351	30:C:515:BCR:H15C	1.78	0.46
25:A:405:CLA:H191	29:D:409:LHG:H331	1.98	0.46
7:D:84:ASN:HD22	7:D:337:HIS:CD2	2.33	0.46
1:G:63:GLU:HA	1:G:155:LEU:HD21	1.98	0.46
25:G:613:CLA:H2	25:G:613:CLA:H61	1.72	0.46
10:H:30:TYR:HE2	17:R:50:LEU:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:23:LYS:HZ3	1:N:32:SER:HB3	1.79	0.46
1:1:17:TYR:HE2	1:1:174:ALA:HB1	1.81	0.46
4:A:224:ILE:O	7:D:266:ARG:NH2	2.43	0.46
25:A:406:CLA:H52	36:D:405:PL9:H151	1.98	0.46
4:A:130:GLU:HG2	7:D:257:ILE:HG21	1.98	0.46
25:B:610:CLA:CHC	30:H:101:BCR:HC8	2.45	0.46
7:D:124:ILE:HD11	37:H:102:DGD:HAE1	1.98	0.46
18:S:55:GLY:HA3	18:S:194:ARG:HH12	1.80	0.46
1:2:147:PRO:HB2	24:2:608:CHL:HBB2	1.98	0.46
2:3:72:ALA:HA	2:3:165:LEU:HD11	1.96	0.46
25:5:610:CLA:CBB	26:5:1620:LUT:H32	2.46	0.46
5:B:315:ILE:HG12	5:B:321:LYS:HG3	1.97	0.46
25:B:613:CLA:H61	25:B:613:CLA:H102	1.62	0.46
6:C:186:TYR:HA	6:C:196:VAL:HA	1.98	0.46
6:C:66:ALA:HB1	13:K:40:MET:HB3	1.98	0.46
1:G:148:LEU:HG	24:G:608:CHL:HBB1	1.97	0.46
1:G:52:SER:OG	1:G:61:ASN:ND2	2.48	0.46
1:N:63:GLU:HA	1:N:155:LEU:HD21	1.97	0.46
27:R:622:XAT:H35	27:R:622:XAT:H401	1.79	0.46
24:S:606:CHL:HMC	24:S:607:CHL:C1C	2.46	0.46
25:7:602:CLA:HBA1	26:7:1621:LUT:H382	1.98	0.46
5:B:157:HIS:HE1	25:B:607:CLA:NA	2.14	0.46
30:B:618:BCR:H351	30:B:618:BCR:H15C	1.79	0.46
30:B:620:BCR:H11C	30:B:620:BCR:H341	1.83	0.46
25:G:603:CLA:HBB1	25:G:603:CLA:HHC	1.98	0.46
6:C:338:GLY:HA2	16:O:111:TYR:OH	2.16	0.46
16:O:227:ASP:HB2	16:O:231:LYS:HE3	1.97	0.46
18:S:53:VAL:HG21	18:S:71:PHE:HE2	1.80	0.46
1:Y:21:ARG:NH2	1:Y:36:LEU:O	2.44	0.46
25:Y:613:CLA:H2	25:Y:613:CLA:H61	1.67	0.46
25:3:602:CLA:HBA1	26:3:1621:LUT:H382	1.98	0.46
4:A:140:ARG:NH1	7:D:223:LEU:HD12	2.30	0.46
7:D:211:LEU:HA	7:D:214:ILE:HG22	1.98	0.46
1:G:97:TRP:O	26:G:1621:LUT:O3	2.34	0.46
13:K:27:PRO:HB2	13:K:30:TYR:HD2	1.80	0.46
29:D:409:LHG:H321	19:T:21:ILE:HD11	1.97	0.46
27:1:1622:XAT:H31	27:1:1622:XAT:H391	1.74	0.45
3:4:173:LEU:HG	3:4:177:LYS:HE3	1.98	0.45
27:7:1622:XAT:H11	27:7:1622:XAT:H191	1.80	0.45
24:7:606:CHL:HHC	24:7:606:CHL:HBB1	1.98	0.45
4:A:228:THR:HA	17:R:58:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:49:ILE:HG12	36:D:405:PL9:H501	1.98	0.45
24:3:606:CHL:HBB1	24:3:606:CHL:HHC	1.98	0.45
24:5:609:CHL:H112	24:5:609:CHL:H91	1.83	0.45
27:7:1622:XAT:H201	27:7:1622:XAT:H15	1.78	0.45
4:A:312:ARG:NH1	8:E:56:PHE:HB2	2.32	0.45
3:4:96:THR:HG21	17:R:235:LEU:HA	1.99	0.45
25:S:604:CLA:HBA2	25:S:604:CLA:H3A	1.79	0.45
1:1:104:ILE:HG21	1:1:124:ILE:HD13	1.98	0.45
25:7:611:CLA:HMC1	29:7:2630:LHG:H311	1.98	0.45
29:B:2630:LHG:H152	29:B:2631:LHG:H162	1.99	0.45
7:D:237:ASN:HB3	7:D:240:GLN:HB3	1.98	0.45
25:R:602:CLA:H101	27:R:622:XAT:H371	1.98	0.45
25:2:614:CLA:HBA2	25:2:614:CLA:H3A	1.73	0.45
24:3:606:CHL:HBC2	24:3:607:CHL:HHD	1.97	0.45
25:3:611:CLA:HMB3	29:3:2630:LHG:HC11	1.99	0.45
24:7:609:CHL:H91	24:7:609:CHL:H112	1.83	0.45
4:A:147:TYR:OH	33:A:408:PHO:O1A	2.31	0.45
5:B:145:LEU:HD22	25:B:605:CLA:H18	1.98	0.45
25:C:512:CLA:HMB3	30:C:514:BCR:H391	1.99	0.45
5:B:460:LEU:HG	7:D:281:TRP:HZ3	1.82	0.45
26:G:1620:LUT:H35	26:G:1620:LUT:H401	1.78	0.45
25:G:610:CLA:HBB1	25:G:612:CLA:H3A	1.99	0.45
24:N:607:CHL:H2	24:N:607:CHL:H62	1.59	0.45
25:R:611:CLA:H3A	25:R:611:CLA:HBA2	1.54	0.45
26:R:620:LUT:H35	26:R:620:LUT:H401	1.84	0.45
25:N:603:CLA:H12	1:Y:51:LEU:HD11	1.98	0.45
25:G:602:CLA:H91	25:Y:603:CLA:H8	1.98	0.45
27:5:1622:XAT:H191	27:5:1622:XAT:H11	1.79	0.45
5:B:260:SER:HG	5:B:262:THR:HG1	1.61	0.45
5:B:362:PHE:CZ	7:D:185:PHE:HZ	2.34	0.45
6:C:61:VAL:HG13	6:C:118:HIS:HD2	1.82	0.45
30:C:516:BCR:H21C	12:J:15:THR:HG23	1.98	0.45
27:N:1622:XAT:H391	27:N:1622:XAT:H31	1.73	0.45
1:N:192:PHE:CD2	25:N:602:CLA:H171	2.51	0.45
5:B:211:LEU:HD22	25:R:603:CLA:H111	1.97	0.45
5:B:277:GLN:HB3	20:U:24:ARG:HG3	1.98	0.45
5:B:368:VAL:HG21	5:B:422:ARG:HG2	1.98	0.45
25:B:602:CLA:H92	25:B:602:CLA:H61	1.81	0.45
25:B:614:CLA:H102	25:B:614:CLA:H62	1.79	0.45
30:B:619:BCR:H24C	30:B:619:BCR:H371	1.84	0.45
6:C:223:TRP:CE3	6:C:224:ILE:HG12	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:318:LEU:HD12	6:C:340:TYR:HB3	1.99	0.45
24:Y:601:CHL:H102	27:Y:1622:XAT:H14	1.99	0.45
1:Y:71:TRP:CE2	24:Y:608:CHL:HED2	2.52	0.45
26:1:1621:LUT:H201	26:1:1621:LUT:H15	1.80	0.45
25:B:604:CLA:H62	25:B:604:CLA:H41	1.76	0.45
25:G:610:CLA:H62	25:G:610:CLA:H41	1.82	0.45
15:M:27:VAL:HG12	15:M:28:LYS:HB2	5.26	0.45
28:N:1623:NEX:H201	28:N:1623:NEX:H15	1.78	0.45
25:N:603:CLA:H61	25:N:603:CLA:H92	1.81	0.45
3:8:29:LEU:HD11	3:8:51:ARG:HD3	1.97	0.45
25:B:612:CLA:H72	25:B:612:CLA:H112	1.74	0.45
7:D:18:ILE:HG22	22:X:76:SER:HB3	1.99	0.45
7:D:183:ILE:HA	25:D:402:CLA:HMD2	1.99	0.45
25:A:410:CLA:HAB	11:I:15:PHE:CD2	2.52	0.45
24:G:609:CHL:HMB2	24:N:601:CHL:H3A	1.99	0.45
1:1:108:GLY:O	1:1:122:GLN:NE2	2.39	0.45
24:1:607:CHL:H91	24:1:607:CHL:H112	1.79	0.45
25:1:610:CLA:CBB	26:1:1620:LUT:H32	2.46	0.45
25:5:613:CLA:H2	25:5:614:CLA:HMD1	1.97	0.45
25:B:613:CLA:HBA2	25:B:613:CLA:H3A	1.58	0.45
25:B:616:CLA:H3A	25:B:616:CLA:HBA1	1.77	0.45
30:B:618:BCR:H11C	30:B:618:BCR:H341	1.87	0.45
6:C:85:GLY:HA3	37:C:519:DGD:HE2	1.99	0.45
7:D:181:ARG:HD3	7:D:181:ARG:C	2.37	0.45
30:H:101:BCR:H371	30:H:101:BCR:H24C	1.76	0.45
1:Y:65:GLU:OE2	1:Y:185:ARG:NE	2.47	0.45
24:7:601:CHL:HAC1	29:7:2630:LHG:HC2	1.99	0.45
34:B:621:SQD:H271	34:B:623:SQD:H102	1.99	0.45
29:D:409:LHG:C28	19:T:17:ILE:HG23	2.47	0.45
26:G:1621:LUT:H15	26:G:1621:LUT:H201	1.81	0.45
1:N:212:HIS:CG	25:N:613:CLA:HAA2	2.52	0.45
25:S:613:CLA:H61	25:S:613:CLA:H2	1.70	0.45
25:Y:612:CLA:H142	25:Y:612:CLA:H111	1.78	0.45
25:7:611:CLA:HMB3	29:7:2630:LHG:HC11	1.98	0.44
17:R:235:LEU:HA	3:8:96:THR:HG21	169.05	0.44
4:A:160:ILE:HD11	37:C:518:DGD:HBT2	1.99	0.44
7:D:91:LEU:HA	7:D:91:LEU:HD23	1.81	0.44
1:G:49:ALA:HA	1:Y:64:LEU:HD11	1.98	0.44
28:S:1623:NEX:H11	28:S:1623:NEX:H191	1.76	0.44
24:2:606:CHL:HBC2	24:2:607:CHL:HHD	1.98	0.44
3:8:173:LEU:HG	3:8:177:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:D:409:LHG:H272	29:D:409:LHG:H141	1.99	0.44
24:N:606:CHL:HBA2	28:N:1623:NEX:H31	1.99	0.44
1:Y:63:GLU:HA	1:Y:155:LEU:HD21	1.99	0.44
25:Y:603:CLA:H3A	25:Y:603:CLA:HBA1	1.64	0.44
24:Y:608:CHL:HMB2	24:Y:608:CHL:H111	2.00	0.44
1:5:104:ILE:HG21	1:5:124:ILE:HD13	1.98	0.44
4:A:42:LEU:CD2	34:A:418:SQD:H212	2.47	0.44
7:D:22:TRP:O	7:D:27:ARG:NH2	2.39	0.44
29:D:410:LHG:H121	29:D:410:LHG:H312	1.99	0.44
10:H:49:LEU:HB3	30:H:101:BCR:H14C	1.99	0.44
27:Y:1622:XAT:H15	27:Y:1622:XAT:H201	1.65	0.44
2:3:207:VAL:HG11	25:3:613:CLA:HAC2	2.00	0.44
24:6:606:CHL:HBC2	24:6:607:CHL:HHD	1.98	0.44
6:C:39:ASN:ND2	25:C:510:CLA:O1A	2.49	0.44
26:G:1621:LUT:H401	26:G:1621:LUT:H35	1.79	0.44
1:G:126:ALA:HB3	24:G:605:CHL:HMC	1.99	0.44
30:T:101:BCR:H11C	30:T:101:BCR:H341	1.77	0.44
6:C:214:LEU:HD22	21:W:15:PHE:CZ	2.53	0.44
28:Y:1623:NEX:H35	28:Y:1623:NEX:H401	1.72	0.44
1:6:136:GLY:HA2	24:6:609:CHL:HAB	2.00	0.44
1:6:147:PRO:HB2	24:6:608:CHL:HBB2	1.98	0.44
5:B:363:PHE:HB3	5:B:365:THR:O	2.18	0.44
25:B:611:CLA:H11	25:B:613:CLA:H191	1.99	0.44
25:G:611:CLA:H61	25:G:611:CLA:H41	1.86	0.44
25:N:611:CLA:H61	25:N:611:CLA:H92	1.81	0.44
25:N:613:CLA:H121	27:N:1622:XAT:H34	1.99	0.44
16:O:125:PRO:HG2	16:O:225:ASP:HB3	2.00	0.44
27:2:1622:XAT:H35	27:2:1622:XAT:H401	1.88	0.44
3:4:51:ARG:HH21	3:4:144:GLN:HB2	1.82	0.44
25:B:602:CLA:H52	25:B:602:CLA:H12	1.76	0.44
5:B:362:PHE:O	7:D:295:ARG:NH1	2.51	0.44
24:G:607:CHL:H143	24:G:607:CHL:H111	1.71	0.44
30:H:101:BCR:H15C	30:H:101:BCR:H351	1.79	0.44
14:L:30:VAL:O	14:L:34:ASN:ND2	2.51	0.44
35:Z:101:LMG:H291	35:Z:101:LMG:HC91	1.80	0.44
28:5:1623:NEX:H15	28:5:1623:NEX:H201	1.90	0.44
5:B:170:ASP:HB3	5:B:174:LEU:H	1.83	0.44
5:B:205:ALA:O	5:B:209:GLY:N	2.45	0.44
6:C:28:GLN:HE22	7:D:231:ASN:HD22	1.66	0.44
5:B:325:PHE:CG	14:L:35:TYR:HB3	2.53	0.44
16:O:47:ASN:HA	16:O:91:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:608:CHL:H11	26:Y:1620:LUT:H383	1.99	0.44
26:5:1621:LUT:H35	26:5:1621:LUT:H401	1.84	0.44
4:A:24:THR:O	7:D:252:ARG:NH2	2.47	0.44
25:C:510:CLA:H193	25:C:510:CLA:H162	1.80	0.44
27:N:1622:XAT:H361	29:N:2630:LHG:HC92	2.00	0.44
17:R:11:ARG:HH21	17:R:31:ASP:CG	2.21	0.44
17:R:187:ASP:HA	17:R:188:PRO:HD3	1.82	0.44
25:S:603:CLA:HBA1	25:S:603:CLA:H3A	1.87	0.44
28:2:1623:NEX:H201	28:2:1623:NEX:H15	1.71	0.44
24:4:601:CHL:H3A	24:4:601:CHL:HBA1	1.76	0.44
28:7:1623:NEX:H11	28:7:1623:NEX:H191	1.80	0.44
7:D:52:GLY:HA2	7:D:56:VAL:HB	1.99	0.44
1:N:199:ILE:HG13	24:N:607:CHL:H42	2.00	0.44
18:S:212:GLU:OE2	18:S:220:LYS:NZ	2.42	0.44
25:3:611:CLA:HMC1	29:3:2630:LHG:H311	1.98	0.43
24:3:601:CHL:HAC1	29:3:2630:LHG:HC2	1.99	0.43
1:5:215:ASP:OD2	1:5:218:ASN:ND2	2.46	0.43
24:8:606:CHL:HBA2	30:8:623:BCR:H19C	2.00	0.43
1:G:215:ASP:OD2	1:G:218:ASN:HB2	2.18	0.43
25:N:602:CLA:H13	25:N:602:CLA:H172	1.81	0.43
17:R:181:PRO:HD2	26:R:620:LUT:H23	1.99	0.43
4:A:225:ARG:HD3	17:R:58:ALA:HB1	1.99	0.43
26:7:1620:LUT:H35	26:7:1620:LUT:H401	1.86	0.43
4:A:42:LEU:HD23	34:A:418:SQD:C21	2.48	0.43
5:B:324:LEU:HD21	7:D:197:PHE:HE2	1.83	0.43
7:D:89:SER:HB3	8:E:69:ARG:NH2	2.33	0.43
24:N:606:CHL:HMB1	24:N:609:CHL:HAC1	2.00	0.43
24:N:607:CHL:H111	24:N:607:CHL:H143	1.74	0.43
18:S:172:PRO:HD2	26:S:1620:LUT:H23	2.00	0.43
27:Y:1622:XAT:H11	27:Y:1622:XAT:H191	1.81	0.43
1:Y:17:TYR:CE2	1:Y:174:ALA:HB1	2.54	0.43
4:A:217:SER:HA	7:D:273:LEU:HD12	1.99	0.43
25:B:604:CLA:H2	25:B:606:CLA:H91	2.00	0.43
25:B:615:CLA:H112	25:B:615:CLA:H91	1.86	0.43
25:D:403:CLA:H41	25:D:403:CLA:H62	1.79	0.43
29:D:409:LHG:HC2	14:L:14:ASN:HD21	1.84	0.43
1:G:148:LEU:N	24:G:608:CHL:OMC	2.52	0.43
25:G:611:CLA:H91	25:G:611:CLA:H112	1.79	0.43
29:D:409:LHG:H252	14:L:23:LEU:HD22	2.00	0.43
17:R:75:VAL:HG11	17:R:171:ARG:HD2	2.00	0.43
18:S:86:MET:SD	25:S:610:CLA:HAB	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:1622:XAT:H391	27:2:1622:XAT:H31	1.71	0.43
1:2:136:GLY:HA2	24:2:609:CHL:HAB	2.00	0.43
5:B:281:GLN:HG2	20:U:16:VAL:HG22	2.01	0.43
5:B:26:HIS:HB2	25:B:613:CLA:HMB2	2.00	0.43
4:A:254:TYR:CD1	7:D:133:LEU:HG	2.53	0.43
28:G:1623:NEX:H191	28:G:1623:NEX:H11	1.76	0.43
25:S:613:CLA:HMB3	26:S:1620:LUT:H162	2.01	0.43
26:4:620:LUT:H201	26:4:620:LUT:H15	1.79	0.43
24:4:606:CHL:HBA2	30:4:623:BCR:H19C	2.00	0.43
2:7:227:PRO:HG2	25:7:614:CLA:HMB3	2.01	0.43
25:B:611:CLA:H102	25:B:616:CLA:HAA1	2.00	0.43
25:C:506:CLA:H41	25:C:506:CLA:H62	1.81	0.43
25:C:510:CLA:HBA1	25:C:510:CLA:H11	1.76	0.43
17:R:185:ALA:HB1	17:R:191:LYS:HG3	2.00	0.43
26:S:1620:LUT:H401	26:S:1620:LUT:H35	1.79	0.43
28:5:1623:NEX:H191	28:5:1623:NEX:H11	1.78	0.43
1:5:170:PRO:HA	1:5:173:PHE:HB3	2.00	0.43
5:B:366:PHE:O	5:B:425:GLN:NE2	2.49	0.43
25:B:604:CLA:H162	25:B:604:CLA:H193	1.84	0.43
25:B:613:CLA:H122	25:B:613:CLA:H162	1.88	0.43
7:D:202:VAL:HG22	25:D:402:CLA:C1B	2.49	0.43
1:G:164:LEU:HD12	26:G:1620:LUT:H222	2.01	0.43
18:S:202:GLY:O	18:S:206:GLN:CB	2.66	0.43
25:5:602:CLA:H93	25:5:602:CLA:H111	1.85	0.43
25:A:406:CLA:HMA1	25:A:406:CLA:H121	2.01	0.43
1:G:181:LEU:HA	1:G:181:LEU:HD23	1.87	0.43
1:G:92:PHE:HB2	1:G:95:ALA:HB2	2.01	0.43
26:Y:1621:LUT:H401	26:Y:1621:LUT:H35	1.77	0.43
27:2:1622:XAT:H363	29:2:2630:LHG:HC41	2.01	0.43
5:B:413:ASP:OD1	5:B:413:ASP:N	2.51	0.43
6:C:217:PRO:HG3	37:C:518:DGD:HA71	2.01	0.43
1:1:44:TYR:N	25:1:602:CLA:OBD	2.40	0.43
26:3:1620:LUT:H35	26:3:1620:LUT:H401	1.86	0.43
26:8:620:LUT:H35	26:8:620:LUT:H401	1.80	0.43
5:B:249:ALA:HA	5:B:252:VAL:HG22	2.01	0.43
30:B:620:BCR:H351	30:B:620:BCR:H15C	1.85	0.43
4:A:63:ILE:HA	6:C:337:LEU:HD11	2.01	0.43
37:H:102:DGD:HB91	37:H:102:DGD:HB62	1.66	0.43
26:1:1620:LUT:H201	26:1:1620:LUT:H15	1.86	0.43
25:1:603:CLA:H3A	25:1:603:CLA:HBA1	1.78	0.43
2:3:227:PRO:HG2	25:3:614:CLA:HMB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:477:ASP:N	5:B:477:ASP:OD1	2.52	0.43
29:D:409:LHG:H281	19:T:17:ILE:HG23	2.01	0.43
27:G:1622:XAT:H11	27:G:1622:XAT:H191	1.93	0.43
17:R:16:PRO:HB2	3:8:122:GLN:H	166.49	0.43
26:Y:1620:LUT:H401	26:Y:1620:LUT:H35	1.86	0.43
1:Y:25:LEU:HB2	1:Y:29:SER:HA	2.01	0.43
24:G:601:CHL:H152	24:Y:607:CHL:HBB1	2.01	0.43
1:2:96:VAL:HB	1:2:99:LYS:HB2	2.01	0.42
25:3:613:CLA:HMB3	26:3:1620:LUT:H162	2.01	0.42
2:3:166:TYR:HB3	25:3:610:CLA:HED2	2.01	0.42
1:6:71:TRP:CE2	24:6:608:CHL:HED2	2.54	0.42
24:6:609:CHL:H61	24:6:609:CHL:H93	1.84	0.42
1:6:96:VAL:HB	1:6:99:LYS:HB2	2.01	0.42
28:7:1623:NEX:H15	28:7:1623:NEX:H201	1.67	0.42
2:7:181:PRO:HA	2:7:184:PHE:HB3	2.02	0.42
3:8:51:ARG:HH21	3:8:144:GLN:HB2	1.82	0.42
25:A:405:CLA:C3	33:A:408:PHO:HBB1	2.49	0.42
25:B:617:CLA:H11	25:B:617:CLA:H51	1.90	0.42
30:B:619:BCR:H351	30:B:619:BCR:H15C	1.79	0.42
30:B:619:BCR:H20C	30:B:619:BCR:H361	1.86	0.42
1:G:63:GLU:HA	1:G:155:LEU:HD11	2.01	0.42
25:B:608:CLA:H192	14:L:28:LEU:HD11	2.01	0.42
1:N:73:MET:SD	25:N:610:CLA:HAB	2.59	0.42
3:4:192:LEU:HD13	25:4:603:CLA:HBB2	2.01	0.42
6:C:223:TRP:CG	6:C:224:ILE:N	2.87	0.42
26:G:1621:LUT:H372	25:Y:603:CLA:HED3	2.01	0.42
25:N:610:CLA:H41	25:N:610:CLA:H62	1.86	0.42
25:2:604:CLA:HBA1	24:2:606:CHL:C1D	2.49	0.42
27:2:1622:XAT:H202	2:3:138:LEU:HD21	2.01	0.42
27:8:622:XAT:H401	27:8:622:XAT:H35	1.85	0.42
4:A:210:LEU:O	4:A:214:MET:HB2	2.20	0.42
6:C:319:VAL:HG22	6:C:384:ILE:HD13	2.02	0.42
1:G:212:HIS:CG	25:G:613:CLA:HAA2	2.55	0.42
30:H:101:BCR:H361	30:H:101:BCR:H20C	1.82	0.42
25:N:613:CLA:H91	29:N:2630:LHG:H321	2.01	0.42
1:Y:36:LEU:HD13	1:Y:45:GLY:HA2	2.01	0.42
25:Y:602:CLA:H13	25:Y:602:CLA:H172	1.84	0.42
25:Y:610:CLA:H111	25:Y:610:CLA:H91	1.89	0.42
1:1:170:PRO:HA	1:1:173:PHE:HB3	2.00	0.42
26:4:620:LUT:H401	26:4:620:LUT:H35	1.80	0.42
2:7:207:VAL:HG11	25:7:613:CLA:HAC2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:603:CLA:H62	25:B:603:CLA:H41	1.75	0.42
36:D:405:PL9:H401	29:D:409:LHG:H212	2.01	0.42
1:1:225:ALA:HA	27:1:1622:XAT:H42	2.02	0.42
1:2:71:TRP:CE2	24:2:608:CHL:HED2	2.54	0.42
29:B:2630:LHG:H131	29:B:2631:LHG:H162	2.01	0.42
25:B:607:CLA:H141	25:B:607:CLA:H161	1.85	0.42
25:B:611:CLA:H143	25:B:611:CLA:HBD	2.00	0.42
6:C:144:PHE:O	6:C:148:GLY:N	2.52	0.42
7:D:146:ALA:HA	7:D:277:VAL:HG21	2.02	0.42
7:D:172:PRO:HB3	7:D:179:ILE:HD12	2.01	0.42
26:G:1620:LUT:H15	26:G:1620:LUT:H201	1.88	0.42
28:G:1623:NEX:H201	28:G:1623:NEX:H15	1.81	0.42
25:Y:603:CLA:H61	25:Y:603:CLA:H2	1.81	0.42
25:3:613:CLA:H61	25:3:613:CLA:H2	1.81	0.42
24:6:601:CHL:H3A	24:7:609:CHL:HMB2	2.01	0.42
25:A:410:CLA:H72	25:A:410:CLA:H112	1.81	0.42
30:D:404:BCR:H351	30:D:404:BCR:H15C	1.91	0.42
7:D:203:ALA:HB2	36:D:405:PL9:H353	2.02	0.42
1:G:110:LEU:HD22	24:G:606:CHL:HMD2	2.02	0.42
14:L:27:VAL:HG11	29:L:101:LHG:H201	2.02	0.42
14:L:20:TRP:HZ3	14:L:23:LEU:HD23	1.78	0.42
25:N:602:CLA:HBA1	26:N:1621:LUT:H382	2.01	0.42
1:Y:44:TYR:HE2	24:Y:601:CHL:CBC	2.32	0.42
1:2:146:GLY:HA3	1:2:147:PRO:HD3	1.85	0.42
24:2:601:CHL:H3A	24:3:609:CHL:HMB2	2.01	0.42
3:4:8:SER:HB2	3:4:11:PRO:HD2	2.01	0.42
1:5:225:ALA:HA	27:5:1622:XAT:H42	2.02	0.42
25:5:602:CLA:H92	25:5:603:CLA:HMA1	2.02	0.42
5:B:382:PRO:HB3	5:B:386:ALA:HB3	2.01	0.42
25:B:605:CLA:H93	25:B:606:CLA:HAB	2.02	0.42
25:C:512:CLA:HMA1	25:C:513:CLA:H143	2.01	0.42
35:C:521:LMG:H361	13:K:45:LEU:HD11	2.01	0.42
35:B:622:LMG:H242	7:D:285:LEU:HD23	2.02	0.42
24:G:601:CHL:H62	24:G:601:CHL:H41	1.82	0.42
13:K:45:LEU:O	13:K:48:PHE:HB3	2.20	0.42
1:N:182:LYS:NZ	29:N:2630:LHG:O4	2.44	0.42
17:R:203:ARG:HB2	29:R:2630:LHG:H241	2.02	0.42
1:Y:181:LEU:HA	1:Y:181:LEU:HD23	1.81	0.42
1:Y:24:TYR:CG	1:Y:46:TRP:HB2	2.55	0.42
27:4:622:XAT:H401	27:4:622:XAT:H35	1.85	0.42
1:5:181:LEU:HD23	1:5:181:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:8:192:LEU:HD13	25:8:603:CLA:HBB2	2.01	0.42
3:8:8:SER:HB2	3:8:11:PRO:HD2	2.01	0.42
4:A:234:ASN:HD21	29:D:408:LHG:HC11	1.85	0.42
5:B:182:ASN:HA	35:B:2633:LMG:HC62	2.02	0.42
5:B:469:HIS:HE1	25:B:612:CLA:NA	2.18	0.42
25:B:603:CLA:H42	37:H:102:DGD:HB41	2.01	0.42
25:C:506:CLA:H71	11:I:20:ILE:HD13	2.02	0.42
1:N:65:GLU:O	1:N:69:SER:OG	2.30	0.42
16:O:80:THR:O	16:O:81:ARG:HB2	2.19	0.42
5:B:214:LEU:HD12	25:R:609:CLA:H93	2.02	0.42
27:Y:1622:XAT:H12	29:Y:2630:LHG:H191	2.02	0.42
1:1:118:LEU:HD23	1:1:118:LEU:HA	1.86	0.42
28:2:1623:NEX:H401	28:2:1623:NEX:H35	1.90	0.42
28:3:1623:NEX:H201	28:3:1623:NEX:H15	1.67	0.42
3:4:122:GLN:H	17:R:16:PRO:HB2	1.84	0.42
1:6:146:GLY:HA3	1:6:147:PRO:HD3	1.85	0.42
25:6:604:CLA:HBA1	24:6:606:CHL:C1D	2.49	0.42
25:7:613:CLA:HMB3	26:7:1620:LUT:H162	2.01	0.42
3:8:128:THR:OG1	3:8:133:THR:N	2.53	0.42
25:B:603:CLA:H93	25:B:603:CLA:H61	1.78	0.42
5:B:42:LEU:HD13	5:B:94:GLU:HG3	2.02	0.42
24:G:607:CHL:HAA2	27:N:1622:XAT:H41	2.01	0.42
25:R:613:CLA:H111	29:R:2630:LHG:H292	2.02	0.42
18:S:229:ASN:ND2	35:Z:101:LMG:H342	2.35	0.42
28:Y:1623:NEX:H15	28:Y:1623:NEX:H201	1.84	0.42
30:4:623:BCR:H351	30:4:623:BCR:H15C	1.76	0.42
1:5:63:GLU:HA	1:5:155:LEU:HD11	2.01	0.42
27:6:1622:XAT:H363	29:6:2630:LHG:HC41	2.01	0.42
2:7:166:TYR:HB3	25:7:610:CLA:HED2	2.01	0.42
30:8:623:BCR:H341	30:8:623:BCR:H11C	1.85	0.42
3:8:85:ASP:HB3	3:8:88:ALA:HB2	2.02	0.42
6:C:167:LEU:HD23	6:C:170:ILE:HD12	2.02	0.42
25:C:504:CLA:H42	37:C:519:DGD:HB32	2.02	0.42
30:C:517:BCR:H371	30:C:517:BCR:H24C	1.75	0.42
27:R:622:XAT:H201	27:R:622:XAT:H15	1.87	0.42
30:B:619:BCR:H14C	30:T:101:BCR:C38	33.14	0.42
5:B:496:GLN:HE22	22:X:82:LYS:HB2	1.85	0.42
26:2:1620:LUT:H201	26:2:1620:LUT:H15	1.85	0.41
1:2:196:VAL:HG12	25:2:613:CLA:HMD3	2.02	0.41
1:6:153:ASP:OD2	1:6:156:TYR:N	2.43	0.41
4:A:179:THR:O	4:A:183:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:467:ILE:HD13	5:B:467:ILE:HA	1.91	0.41
6:C:70:PHE:CD1	13:K:38:ASP:HA	2.55	0.41
6:C:97:TRP:NE1	35:Z:101:LMG:H151	2.35	0.41
1:G:197:GLN:HG3	25:G:613:CLA:C1D	2.50	0.41
10:H:58:LEU:HD11	37:H:102:DGD:HA31	2.02	0.41
26:N:1620:LUT:H35	26:N:1620:LUT:H401	1.80	0.41
1:N:189:PHE:HD1	25:N:602:CLA:H201	1.85	0.41
5:B:217:LEU:HB3	25:R:616:CLA:HBA2	2.02	0.41
5:B:458:PHE:HB3	25:B:605:CLA:HBC2	2.02	0.41
34:B:623:SQD:H312	15:M:17:VAL:HG13	2.01	0.41
5:B:64:PRO:O	5:B:68:ARG:HB2	2.20	0.41
6:C:175:LEU:HB2	25:C:501:CLA:HMD3	2.02	0.41
25:C:513:CLA:H161	25:C:513:CLA:H203	1.84	0.41
7:D:150:PRO:HB3	25:D:402:CLA:H41	2.02	0.41
26:S:1621:LUT:H35	26:S:1621:LUT:H401	1.81	0.41
26:3:1620:LUT:H31	26:3:1620:LUT:H391	1.94	0.41
2:3:181:PRO:HA	2:3:184:PHE:HB3	2.02	0.41
26:5:1620:LUT:H391	26:5:1620:LUT:H31	1.88	0.41
26:5:1620:LUT:H35	26:5:1620:LUT:H401	1.77	0.41
25:6:602:CLA:CBB	26:6:1621:LUT:H32	2.50	0.41
25:6:612:CLA:HBB1	26:6:1620:LUT:C13	2.50	0.41
30:8:623:BCR:H351	30:8:623:BCR:H15C	1.76	0.41
25:A:406:CLA:H111	25:A:406:CLA:H152	1.84	0.41
25:B:615:CLA:H61	25:B:615:CLA:H92	1.94	0.41
30:D:404:BCR:H11C	30:D:404:BCR:H341	1.94	0.41
25:G:610:CLA:H172	25:G:610:CLA:H13	1.86	0.41
13:K:33:LEU:HD22	13:K:36:ILE:HD11	2.02	0.41
14:L:17:SER:OG	29:L:101:LHG:HC42	2.21	0.41
26:S:1620:LUT:H391	26:S:1620:LUT:H31	1.94	0.41
25:B:608:CLA:HAC2	30:T:101:BCR:H272	30.57	0.41
1:1:57:THR:HG22	1:1:61:ASN:HD21	1.85	0.41
25:2:602:CLA:CBB	26:2:1621:LUT:H32	2.50	0.41
25:3:610:CLA:CBB	26:3:1620:LUT:H32	2.51	0.41
25:5:612:CLA:HBB1	26:5:1620:LUT:H35	2.03	0.41
24:5:601:CHL:HMB2	24:6:609:CHL:HMB1	2.03	0.41
25:A:407:CLA:HMB3	33:A:409:PHO:H172	2.03	0.41
30:A:411:BCR:H371	30:A:411:BCR:H24C	1.79	0.41
5:B:108:PHE:CE2	30:T:101:BCR:H353	40.88	0.41
5:B:157:HIS:HA	5:B:163:GLY:HA3	2.02	0.41
25:B:611:CLA:H51	25:B:611:CLA:H8	1.93	0.41
28:G:1623:NEX:H35	28:G:1623:NEX:H401	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:PRO:HG3	1:G:177:LYS:HB3	2.03	0.41
5:B:121:GLU:HG3	10:H:16:ARG:HD3	2.03	0.41
16:O:80:THR:HG23	16:O:115:THR:HB	2.03	0.41
17:R:173:TYR:HE1	17:R:198:GLU:OE2	2.03	0.41
26:S:1621:LUT:H15	26:S:1621:LUT:H201	1.93	0.41
18:S:235:ALA:HB2	23:Z:59:SER:HB3	2.03	0.41
1:Y:110:LEU:HD22	24:Y:606:CHL:HMD2	2.03	0.41
25:Y:602:CLA:H161	25:Y:602:CLA:H193	1.85	0.41
25:Y:603:CLA:HBB1	25:Y:603:CLA:HHC	2.03	0.41
6:C:110:PRO:HG3	35:Z:101:LMG:H121	2.03	0.41
25:1:612:CLA:HBB1	26:1:1620:LUT:H35	2.03	0.41
1:5:118:LEU:HD23	1:5:118:LEU:HA	1.86	0.41
30:A:411:BCR:H15C	30:A:411:BCR:H351	1.85	0.41
29:B:2631:LHG:H341	29:B:2631:LHG:H161	2.03	0.41
25:B:610:CLA:HAB	25:B:610:CLA:HHC	1.89	0.41
25:B:616:CLA:H61	25:B:616:CLA:H2	1.80	0.41
25:C:501:CLA:HBB1	25:C:501:CLA:HHC	2.02	0.41
37:C:520:DGD:O1B	12:J:33:TYR:OH	2.31	0.41
7:D:269:HIS:CE1	38:D:401:BCT:O3	2.73	0.41
29:C:2630:LHG:H223	25:S:614:CLA:H2	2.02	0.41
24:Y:601:CHL:HMA3	29:Y:2630:LHG:H121	2.03	0.41
26:1:1620:LUT:H35	26:1:1620:LUT:H401	1.77	0.41
1:1:63:GLU:HA	1:1:155:LEU:HD11	2.01	0.41
25:2:603:CLA:H3A	25:2:603:CLA:HBA1	1.80	0.41
25:2:612:CLA:HBB1	26:2:1620:LUT:C13	2.51	0.41
26:5:1620:LUT:H201	26:5:1620:LUT:H15	1.86	0.41
1:5:118:LEU:HD23	24:5:605:CHL:HED2	2.03	0.41
3:8:36:ASP:OD1	27:8:622:XAT:O23	2.32	0.41
25:B:606:CLA:H92	25:B:606:CLA:H61	1.93	0.41
7:D:89:SER:HB3	8:E:69:ARG:HH21	1.86	0.41
1:G:167:ALA:HB2	25:G:610:CLA:HAA1	2.01	0.41
1:G:41:PRO:HG3	1:G:177:LYS:HD3	2.03	0.41
25:G:612:CLA:H142	25:G:612:CLA:H111	1.85	0.41
1:N:163:PRO:HD2	26:N:1620:LUT:H23	2.03	0.41
27:N:1622:XAT:H191	27:N:1622:XAT:H11	1.87	0.41
1:1:52:SER:HB3	1:1:58:PHE:HD1	1.85	0.41
26:3:1621:LUT:H201	26:3:1621:LUT:H15	1.94	0.41
5:B:39:LEU:HG	5:B:97:ALA:HB1	2.03	0.41
25:B:605:CLA:H72	25:B:605:CLA:H111	1.92	0.41
5:B:464:PHE:HD2	25:B:612:CLA:HAC2	1.85	0.41
6:C:146:PHE:HB3	29:C:2630:LHG:HC12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:56:HIS:HB2	25:C:509:CLA:HMB2	2.03	0.41
14:L:11:VAL:HG11	15:M:25:ILE:HD12	2.02	0.41
28:N:1623:NEX:H401	28:N:1623:NEX:H35	1.90	0.41
1:N:192:PHE:CE2	25:N:602:CLA:H171	2.55	0.41
16:O:110:ASP:N	16:O:110:ASP:OD1	2.53	0.41
27:R:622:XAT:H173	27:R:622:XAT:H3	1.91	0.41
18:S:48:TYR:OH	18:S:60:ASP:OD2	2.38	0.41
25:Y:602:CLA:H203	26:Y:1621:LUT:H391	2.03	0.41
25:C:511:CLA:H8	23:Z:24:PRO:HB3	2.03	0.41
24:1:607:CHL:HED1	2:3:240:VAL:HG13	2.02	0.41
2:3:221:LEU:HD13	2:3:221:LEU:HA	1.95	0.41
24:5:607:CHL:H91	24:5:607:CHL:H112	1.79	0.41
1:5:136:GLY:HA2	24:5:609:CHL:HAB	2.03	0.41
27:6:1622:XAT:H202	2:7:138:LEU:HD21	2.01	0.41
25:7:610:CLA:CBB	26:7:1620:LUT:H32	2.51	0.41
2:7:86:LEU:HD23	25:7:604:CLA:HMC1	2.03	0.41
25:B:615:CLA:HMB2	30:B:618:BCR:H392	2.02	0.41
25:C:513:CLA:H11	30:C:514:BCR:H381	2.02	0.41
25:C:511:CLA:H93	30:C:517:BCR:H23C	2.03	0.41
4:A:300:PHE:HE1	37:C:520:DGD:HB31	1.85	0.41
1:N:63:GLU:HA	1:N:155:LEU:HD11	2.03	0.41
1:N:176:LEU:HB3	25:N:610:CLA:H3A	2.03	0.41
25:R:612:CLA:HBB1	25:R:612:CLA:HHC	2.03	0.41
24:Y:607:CHL:H91	24:Y:607:CHL:H111	1.95	0.41
24:1:601:CHL:HMB2	24:2:609:CHL:HMB1	2.03	0.41
2:3:223:HIS:CG	25:3:613:CLA:HAA2	2.56	0.41
1:6:70:ARG:NE	1:6:180:GLU:OE2	2.45	0.41
25:7:602:CLA:H111	25:7:602:CLA:H93	1.86	0.41
6:C:300:GLU:HG3	6:C:391:ARG:HH12	1.86	0.41
4:A:262:TYR:CE2	8:E:10:PHE:HD2	2.39	0.41
1:N:181:LEU:HA	1:N:181:LEU:HD23	1.88	0.41
24:N:608:CHL:H152	28:N:1623:NEX:H402	2.03	0.41
25:N:611:CLA:H62	25:N:612:CLA:C1D	2.51	0.41
1:N:80:VAL:HG13	1:N:206:LEU:HD11	2.03	0.41
25:R:602:CLA:H93	25:R:602:CLA:H111	1.95	0.41
1:Y:213:LEU:HD21	25:Y:614:CLA:HMC3	2.03	0.41
25:1:602:CLA:H92	25:1:603:CLA:HMA1	2.02	0.41
1:1:101:GLY:HA2	24:1:606:CHL:HAC2	2.03	0.41
1:2:155:LEU:HD23	1:2:155:LEU:HA	1.89	0.41
1:5:101:GLY:HA2	24:5:606:CHL:HAC2	2.03	0.41
2:7:223:HIS:CG	25:7:613:CLA:HAA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:123:PHE:HE1	25:B:616:CLA:HBC3	1.86	0.41
25:B:612:CLA:H2	25:B:612:CLA:H61	1.81	0.41
30:B:618:BCR:H282	34:B:621:SQD:H82	2.02	0.41
25:B:614:CLA:HMD3	30:B:619:BCR:H341	2.03	0.41
6:C:90:PRO:HB3	6:C:301:PHE:HB3	2.03	0.41
30:D:404:BCR:H382	35:D:411:LMG:H341	2.03	0.41
25:B:615:CLA:H192	15:M:13:LEU:HD21	2.03	0.41
1:1:197:GLN:O	1:1:201:THR:OG1	2.32	0.41
1:5:57:THR:HG22	1:5:61:ASN:HD21	1.85	0.41
25:7:603:CLA:H61	25:7:603:CLA:H92	1.93	0.41
3:8:176:LEU:HB3	25:8:610:CLA:H3A	2.02	0.41
6:C:178:LYS:NZ	6:C:184:GLY:O	2.54	0.41
24:R:606:CHL:HMB1	25:R:609:CLA:HBC2	2.03	0.41
19:T:28:LYS:HE2	19:T:28:LYS:HB2	1.90	0.41
24:Y:606:CHL:HBA2	28:Y:1623:NEX:H403	2.03	0.41
25:Y:612:CLA:H102	25:Y:612:CLA:H61	1.87	0.41
3:4:176:LEU:HB3	25:4:610:CLA:H3A	2.02	0.40
26:6:1620:LUT:H391	26:6:1620:LUT:H31	1.91	0.40
25:6:604:CLA:HBA2	25:6:604:CLA:H3A	1.85	0.40
2:7:173:ASP:OD1	26:7:1620:LUT:O23	2.24	0.40
25:7:610:CLA:HBB1	25:7:610:CLA:H52	2.03	0.40
2:7:80:TRP:CD1	24:7:609:CHL:HMD3	2.57	0.40
33:A:409:PHO:H61	33:A:409:PHO:H41	1.78	0.40
5:B:259:GLY:O	10:H:61:TYR:OH	2.39	0.40
25:B:614:CLA:HBA1	25:B:614:CLA:H3A	1.90	0.40
24:N:606:CHL:HMC	24:N:607:CHL:NC	2.36	0.40
25:R:616:CLA:H3A	25:R:616:CLA:HBA2	1.87	0.40
18:S:135:LEU:O	18:S:139:VAL:HG23	2.21	0.40
27:1:1622:XAT:H201	27:1:1622:XAT:H15	1.76	0.40
28:3:1623:NEX:H35	28:3:1623:NEX:H401	1.87	0.40
2:3:173:ASP:OD1	26:3:1620:LUT:O23	2.24	0.40
30:4:623:BCR:H11C	30:4:623:BCR:H341	1.85	0.40
1:6:196:VAL:HG12	25:6:613:CLA:HMD3	2.02	0.40
25:6:614:CLA:H3A	25:6:614:CLA:HBA2	1.73	0.40
27:7:1622:XAT:H35	27:7:1622:XAT:H401	1.86	0.40
3:8:203:THR:HG22	3:8:205:LEU:H	1.86	0.40
25:B:603:CLA:H111	25:B:603:CLA:H143	1.98	0.40
25:D:402:CLA:H143	25:D:402:CLA:H161	1.89	0.40
1:G:182:LYS:HZ1	29:G:2630:LHG:P	2.57	0.40
17:R:102:TRP:CE2	24:R:608:CHL:HED2	2.56	0.40
3:4:128:THR:OG1	3:4:133:THR:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:7:128:LEU:HA	2:7:128:LEU:HD23	1.90	0.40
4:A:93:PHE:HZ	25:A:410:CLA:HAA1	1.86	0.40
5:B:366:PHE:HD2	5:B:425:GLN:HE21	1.68	0.40
30:B:619:BCR:H341	30:B:619:BCR:H11C	1.89	0.40
6:C:55:ALA:HB1	30:C:517:BCR:H373	2.04	0.40
30:D:404:BCR:H12C	9:F:27:PHE:CE2	2.57	0.40
29:G:2630:LHG:H361	29:G:2630:LHG:H332	1.98	0.40
1:G:25:LEU:HB2	1:G:29:SER:HA	2.04	0.40
25:G:603:CLA:H61	25:G:603:CLA:H92	1.85	0.40
25:N:603:CLA:HMD3	24:N:607:CHL:H193	2.03	0.40
1:N:60:LYS:NZ	1:Y:33:PRO:HG3	2.37	0.40
28:S:1623:NEX:H35	28:S:1623:NEX:H401	1.85	0.40
1:Y:66:VAL:HG22	1:Y:181:LEU:HD21	2.03	0.40
25:Y:611:CLA:C1B	29:Y:2630:LHG:HC31	2.52	0.40
29:C:522:LHG:HC81	25:Y:611:CLA:H51	2.04	0.40
2:3:86:LEU:HD23	25:3:604:CLA:HMC1	2.03	0.40
27:5:1622:XAT:H391	27:5:1622:XAT:H31	1.74	0.40
2:7:193:LYS:HZ1	29:7:2630:LHG:P	2.45	0.40
24:5:609:CHL:H42	25:7:602:CLA:H143	2.02	0.40
3:8:81:GLU:HA	24:8:607:CHL:HED2	2.03	0.40
25:8:604:CLA:C2B	27:8:622:XAT:H183	2.52	0.40
33:A:409:PHO:HBA1	33:A:409:PHO:H3A	1.83	0.40
5:B:381:VAL:O	7:D:346:VAL:HG12	2.22	0.40
4:A:232:SER:HB2	5:B:4:PRO:HG3	2.04	0.40
25:B:615:CLA:H93	34:B:623:SQD:H292	2.03	0.40
25:C:510:CLA:H2	25:C:510:CLA:H61	1.93	0.40
7:D:298:ASP:OD1	7:D:298:ASP:N	2.52	0.40
4:A:234:ASN:ND2	29:D:408:LHG:HC11	2.37	0.40
1:Y:63:GLU:HA	1:Y:155:LEU:HD11	2.03	0.40
24:Y:601:CHL:H61	24:Y:601:CHL:H101	1.85	0.40
23:Z:57:LEU:HD23	23:Z:60:LEU:HD12	2.03	0.40
28:1:1623:NEX:H35	28:1:1623:NEX:H401	1.93	0.40
24:1:609:CHL:H42	25:3:602:CLA:H143	2.02	0.40
27:4:622:XAT:H201	27:4:622:XAT:H15	1.82	0.40
24:5:607:CHL:HED1	2:7:240:VAL:HG13	2.02	0.40
2:7:155:GLY:HA2	24:7:608:CHL:HAC1	2.04	0.40
25:A:406:CLA:HMB3	33:A:408:PHO:H172	2.03	0.40
5:B:10:THR:HG22	25:B:612:CLA:HMA2	2.03	0.40
25:B:613:CLA:H111	25:B:614:CLA:HAB	2.04	0.40
24:G:601:CHL:HMA3	29:G:2630:LHG:H121	2.02	0.40
10:H:30:TYR:CE2	17:R:50:LEU:HG	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:1620:LUT:H201	26:N:1620:LUT:H15	1.88	0.40
17:R:174:PRO:HD3	24:R:608:CHL:HMD2	2.03	0.40
25:R:609:CLA:HAA2	25:R:616:CLA:C1D	2.52	0.40
28:R:623:NEX:H35	28:R:623:NEX:H401	1.94	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	211 (97%)	6 (3%)	0	100	100
1	2	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	5	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	6	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
1	G	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	N	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	Y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	g	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	n	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
1	y	217/232 (94%)	215 (99%)	2 (1%)	0	100	100
2	3	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
2	7	218/243 (90%)	208 (95%)	10 (5%)	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%)	324 (98%)	8 (2%)	0	100	100
4	a	332/344 (96%)	324 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
5	b	501/507 (99%)	488 (97%)	13 (3%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
6	c	448/473 (95%)	441 (98%)	7 (2%)	0	100	100
7	D	338/353 (96%)	332 (98%)	6 (2%)	0	100	100
7	d	338/353 (96%)	332 (98%)	6 (2%)	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%)	57 (98%)	1 (2%)	0	100	100
10	h	58/73 (80%)	57 (98%)	1 (2%)	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	32/40 (80%)	32 (100%)	0	0	100	100
12	j	32/40 (80%)	32 (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%)	31 (100%)	0	0	100	100
15	m	31/34 (91%)	31 (100%)	0	0	100	100
16	O	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
16	o	210/248 (85%)	203 (97%)	7 (3%)	0	100	100
17	R	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
17	r	232/246 (94%)	226 (97%)	6 (3%)	0	100	100
18	S	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
18	s	216/244 (88%)	206 (95%)	10 (5%)	0	100	100
19	T	30/35 (86%)	30 (100%)	0	0	100	100
19	t	30/35 (86%)	30 (100%)	0	0	100	100
20	U	23/99 (23%)	22 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	u	23/99 (23%)	22 (96%)	1 (4%)	0	100	100
21	W	52/54 (96%)	52 (100%)	0	0	100	100
21	w	52/54 (96%)	52 (100%)	0	0	100	100
22	X	37/86 (43%)	37 (100%)	0	0	100	100
22	x	37/86 (43%)	37 (100%)	0	0	100	100
23	Z	60/62 (97%)	60 (100%)	0	0	100	100
23	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	8596/9536 (90%)	8394 (98%)	202 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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
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%)	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%)	171 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	270/279 (97%)	269 (100%)	1 (0%)	93	97
4	a	270/279 (97%)	269 (100%)	1 (0%)	93	97
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%)	352 (100%)	0	100	100
6	c	352/373 (94%)	352 (100%)	0	100	100
7	D	274/285 (96%)	272 (99%)	2 (1%)	87	96
7	d	274/285 (96%)	272 (99%)	2 (1%)	87	96
8	E	67/73 (92%)	67 (100%)	0	100	100
8	e	67/73 (92%)	67 (100%)	0	100	100
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	25/30 (83%)	25 (100%)	0	100	100
12	j	25/30 (83%)	25 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100
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	182/204 (89%)	182 (100%)	0	100	100
16	o	182/204 (89%)	182 (100%)	0	100	100
17	R	191/202 (95%)	191 (100%)	0	100	100
17	r	191/202 (95%)	191 (100%)	0	100	100
18	S	170/190 (90%)	170 (100%)	0	100	100
18	s	170/190 (90%)	170 (100%)	0	100	100
19	T	29/32 (91%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	t	29/32 (91%)	29 (100%)	0	100	100
20	U	21/80 (26%)	21 (100%)	0	100	100
20	u	21/80 (26%)	21 (100%)	0	100	100
21	W	44/44 (100%)	44 (100%)	0	100	100
21	w	44/44 (100%)	44 (100%)	0	100	100
22	X	32/67 (48%)	32 (100%)	0	100	100
22	x	32/67 (48%)	32 (100%)	0	100	100
23	Z	54/54 (100%)	54 (100%)	0	100	100
23	z	54/54 (100%)	54 (100%)	0	100	100
All	All	6992/7658 (91%)	6978 (100%)	14 (0%)	95	98

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	312	ARG
5	B	12	VAL
5	B	272	ARG
5	B	472	ARG
7	D	13	ASN
7	D	181	ARG
10	H	61	TYR
4	a	312	ARG
5	b	12	VAL
5	b	272	ARG
5	b	472	ARG
7	d	13	ASN
7	d	181	ARG
10	h	61	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) 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	219	ASN
3	4	72	GLN

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Mol	Chain	Res	Type
4	A	234	ASN
4	A	301	ASN
4	A	303	ASN
4	A	335	ASN
5	B	216	HIS
6	C	28	GLN
6	C	322	GLN
6	C	415	ASN
7	D	13	ASN
7	D	84	ASN
7	D	351	ASN
1	G	122	GLN
14	L	5	ASN
14	L	10	ASN
16	O	74	GLN
16	O	222	GLN
17	R	47	GLN
17	R	55	GLN
1	Y	88	ASN
1	5	61	ASN
1	6	61	ASN
1	6	88	ASN
2	7	95	GLN
2	7	219	ASN
3	8	72	GLN
4	a	234	ASN
4	a	301	ASN
4	a	303	ASN
4	a	335	ASN
5	b	216	HIS
6	c	28	GLN
6	c	322	GLN
6	c	415	ASN
7	d	13	ASN
7	d	84	ASN
7	d	351	ASN
1	g	122	GLN
14	l	5	ASN
14	l	10	ASN
16	o	74	GLN
16	o	222	GLN
17	r	47	GLN

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Mol	Chain	Res	Type
17	r	55	GLN
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 486 ligands modelled in this entry, 2 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	$\# Z  > 2$
26	LUT	1	1620	-	41,43,43	0.91	2 (4%)	50,60,60	2.04	15 (30%)
26	LUT	1	1621	-	41,43,43	1.02	3 (7%)	50,60,60	1.96	17 (34%)
27	XAT	1	1622	-	39,47,47	0.93	1 (2%)	54,74,74	2.88	21 (38%)
28	NEX	1	1623	-	38,46,46	1.11	4 (10%)	49,70,70	2.65	18 (36%)
29	LHG	1	2630	25	40,40,48	0.73	1 (2%)	41,46,54	1.36	6 (14%)
24	CHL	1	601	1	41,54,74	5.24	27 (65%)	24,90,114	3.44	14 (58%)
25	CLA	1	602	1	52,69,73	1.21	7 (13%)	60,108,113	1.39	9 (15%)
25	CLA	1	603	1	46,63,73	1.34	8 (17%)	53,101,113	1.52	11 (20%)
25	CLA	1	604	-	41,58,73	1.39	8 (19%)	47,95,113	1.53	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHL	1	605	1	41,54,74	5.12	24 (58%)	24,90,114	3.45	15 (62%)
24	CHL	1	606	-	41,54,74	5.21	27 (65%)	24,90,114	3.37	14 (58%)
24	CHL	1	607	-	61,71,74	4.29	27 (44%)	46,110,114	2.68	16 (34%)
24	CHL	1	608	-	41,54,74	5.25	27 (65%)	24,90,114	3.41	14 (58%)
24	CHL	1	609	1	60,70,74	4.43	28 (46%)	46,109,114	2.77	16 (34%)
25	CLA	1	610	1	47,64,73	1.22	6 (12%)	54,102,113	1.47	8 (14%)
25	CLA	1	611	29	33,53,73	1.40	7 (21%)	37,89,113	1.53	7 (18%)
25	CLA	1	612	1	33,53,73	1.42	7 (21%)	37,89,113	1.67	10 (27%)
25	CLA	1	613	1	46,63,73	1.22	8 (17%)	53,101,113	1.40	7 (13%)
25	CLA	1	614	1	33,53,73	1.37	7 (21%)	37,89,113	1.51	5 (13%)
26	LUT	2	1620	-	41,43,43	0.79	0	50,60,60	1.84	16 (32%)
26	LUT	2	1621	-	41,43,43	0.84	1 (2%)	50,60,60	1.83	16 (32%)
27	XAT	2	1622	-	39,47,47	1.00	0	54,74,74	3.01	21 (38%)
28	NEX	2	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.46	13 (26%)
29	LHG	2	2630	25	36,36,48	0.72	1 (2%)	37,42,54	1.30	5 (13%)
24	CHL	2	601	1	41,54,74	5.10	25 (60%)	24,90,114	3.52	12 (50%)
25	CLA	2	602	1	52,69,73	1.16	5 (9%)	60,108,113	1.42	10 (16%)
25	CLA	2	603	1	46,63,73	1.23	7 (15%)	53,101,113	1.50	9 (16%)
25	CLA	2	604	-	33,53,73	1.36	8 (24%)	37,89,113	1.69	6 (16%)
24	CHL	2	605	1	41,54,74	4.98	24 (58%)	24,90,114	3.58	17 (70%)
24	CHL	2	606	-	41,54,74	5.16	25 (60%)	24,90,114	3.47	14 (58%)
24	CHL	2	607	-	59,69,74	4.31	26 (44%)	45,108,114	2.76	18 (40%)
24	CHL	2	608	-	41,54,74	5.08	27 (65%)	24,90,114	3.31	12 (50%)
24	CHL	2	609	1	59,69,74	4.30	27 (45%)	45,108,114	2.82	20 (44%)
25	CLA	2	610	1	41,58,73	1.33	7 (17%)	47,95,113	1.31	7 (14%)
25	CLA	2	611	29	33,53,73	1.34	6 (18%)	37,89,113	1.61	8 (21%)
25	CLA	2	612	1	33,53,73	1.41	5 (15%)	37,89,113	1.68	10 (27%)
25	CLA	2	613	1	33,53,73	1.39	7 (21%)	37,89,113	1.51	6 (16%)
25	CLA	2	614	1	33,53,73	1.35	6 (18%)	37,89,113	1.55	6 (16%)
26	LUT	3	1620	-	41,43,43	0.96	3 (7%)	50,60,60	2.02	18 (36%)
26	LUT	3	1621	-	41,43,43	0.92	1 (2%)	50,60,60	1.68	12 (24%)
27	XAT	3	1622	-	39,47,47	1.17	4 (10%)	54,74,74	3.07	27 (50%)
28	NEX	3	1623	-	38,46,46	0.93	2 (5%)	49,70,70	2.51	16 (32%)
29	LHG	3	2630	25	46,46,48	0.77	1 (2%)	47,52,54	1.33	4 (8%)
24	CHL	3	601	2	62,72,74	4.36	27 (43%)	48,111,114	2.71	19 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	3	602	2	51,68,73	1.18	6 (11%)	59,107,113	1.41	7 (11%)
25	CLA	3	603	2	46,63,73	1.26	9 (19%)	53,101,113	1.50	11 (20%)
25	CLA	3	604	-	33,53,73	1.43	7 (21%)	37,89,113	1.46	7 (18%)
24	CHL	3	605	2	41,54,74	5.04	25 (60%)	24,90,114	3.52	16 (66%)
24	CHL	3	606	-	41,54,74	5.23	25 (60%)	24,90,114	3.67	15 (62%)
24	CHL	3	607	-	51,61,74	4.57	27 (52%)	35,98,114	2.93	16 (45%)
24	CHL	3	608	-	41,54,74	5.18	27 (65%)	24,90,114	3.40	13 (54%)
24	CHL	3	609	2	59,69,74	4.31	27 (45%)	45,108,114	2.78	19 (42%)
25	CLA	3	610	2	51,68,73	1.21	7 (13%)	59,107,113	1.33	8 (13%)
25	CLA	3	611	29	46,63,73	1.38	7 (15%)	53,101,113	1.42	11 (20%)
25	CLA	3	612	2	33,53,73	1.48	8 (24%)	37,89,113	1.78	10 (27%)
25	CLA	3	613	2	49,66,73	1.22	7 (14%)	56,104,113	1.33	7 (12%)
25	CLA	3	614	2	39,56,73	1.25	5 (12%)	45,92,113	1.40	7 (15%)
29	LHG	4	2630	25	20,20,48	0.86	0	21,26,54	1.35	1 (4%)
24	CHL	4	601	3	36,53,74	5.09	21 (58%)	19,89,114	3.73	13 (68%)
25	CLA	4	602	3	33,53,73	1.31	6 (18%)	37,89,113	1.79	7 (18%)
25	CLA	4	603	3	33,53,73	1.39	6 (18%)	37,89,113	1.58	8 (21%)
25	CLA	4	604	-	33,53,73	1.43	7 (21%)	37,89,113	1.56	6 (16%)
24	CHL	4	606	-	41,54,74	5.06	26 (63%)	24,90,114	3.37	14 (58%)
24	CHL	4	607	-	41,54,74	5.02	25 (60%)	24,90,114	3.44	15 (62%)
24	CHL	4	608	-	41,54,74	5.11	25 (60%)	24,90,114	3.50	16 (66%)
24	CHL	4	609	3	41,54,74	5.11	25 (60%)	24,90,114	3.46	15 (62%)
25	CLA	4	610	3	33,53,73	1.43	7 (21%)	37,89,113	1.51	5 (13%)
25	CLA	4	611	29	33,53,73	1.42	6 (18%)	37,89,113	1.38	6 (16%)
25	CLA	4	612	3	33,53,73	1.32	5 (15%)	37,89,113	1.70	8 (21%)
26	LUT	4	620	-	41,43,43	0.95	2 (4%)	50,60,60	2.23	15 (30%)
27	XAT	4	622	-	39,47,47	0.94	1 (2%)	54,74,74	2.70	20 (37%)
30	BCR	4	623	-	41,41,41	0.76	0	56,56,56	2.18	14 (25%)
26	LUT	5	1620	-	41,43,43	0.92	2 (4%)	50,60,60	2.04	15 (30%)
26	LUT	5	1621	-	41,43,43	1.02	3 (7%)	50,60,60	1.96	17 (34%)
27	XAT	5	1622	-	39,47,47	0.94	1 (2%)	54,74,74	2.88	21 (38%)
28	NEX	5	1623	-	38,46,46	1.10	3 (7%)	49,70,70	2.65	18 (36%)
29	LHG	5	2630	25	40,40,48	0.73	1 (2%)	41,46,54	1.36	6 (14%)
24	CHL	5	601	1	41,54,74	5.23	27 (65%)	24,90,114	3.43	14 (58%)
25	CLA	5	602	1	52,69,73	1.21	7 (13%)	60,108,113	1.38	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	5	603	1	46,63,73	1.34	8 (17%)	53,101,113	1.52	11 (20%)
25	CLA	5	604	-	41,58,73	1.39	8 (19%)	47,95,113	1.53	9 (19%)
24	CHL	5	605	1	41,54,74	5.12	25 (60%)	24,90,114	3.45	15 (62%)
24	CHL	5	606	-	41,54,74	5.20	27 (65%)	24,90,114	3.37	14 (58%)
24	CHL	5	607	-	61,71,74	4.29	27 (44%)	46,110,114	2.68	15 (32%)
24	CHL	5	608	-	41,54,74	5.26	27 (65%)	24,90,114	3.41	14 (58%)
24	CHL	5	609	1	60,70,74	4.44	28 (46%)	46,109,114	2.77	16 (34%)
25	CLA	5	610	1	47,64,73	1.22	7 (14%)	54,102,113	1.47	8 (14%)
25	CLA	5	611	29	33,53,73	1.40	7 (21%)	37,89,113	1.53	7 (18%)
25	CLA	5	612	1	33,53,73	1.42	7 (21%)	37,89,113	1.67	10 (27%)
25	CLA	5	613	1	46,63,73	1.22	8 (17%)	53,101,113	1.40	7 (13%)
25	CLA	5	614	1	33,53,73	1.37	6 (18%)	37,89,113	1.51	5 (13%)
26	LUT	6	1620	-	41,43,43	0.79	0	50,60,60	1.85	16 (32%)
26	LUT	6	1621	-	41,43,43	0.85	1 (2%)	50,60,60	1.83	16 (32%)
27	XAT	6	1622	-	39,47,47	1.00	0	54,74,74	3.00	22 (40%)
28	NEX	6	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.46	13 (26%)
29	LHG	6	2630	25	36,36,48	0.72	1 (2%)	37,42,54	1.30	5 (13%)
24	CHL	6	601	1	41,54,74	5.10	25 (60%)	24,90,114	3.53	12 (50%)
25	CLA	6	602	1	52,69,73	1.16	5 (9%)	60,108,113	1.42	10 (16%)
25	CLA	6	603	1	46,63,73	1.23	7 (15%)	53,101,113	1.50	10 (18%)
25	CLA	6	604	-	33,53,73	1.36	8 (24%)	37,89,113	1.70	6 (16%)
24	CHL	6	605	1	41,54,74	4.98	24 (58%)	24,90,114	3.59	17 (70%)
24	CHL	6	606	-	41,54,74	5.16	25 (60%)	24,90,114	3.47	14 (58%)
24	CHL	6	607	-	59,69,74	4.31	26 (44%)	45,108,114	2.77	18 (40%)
24	CHL	6	608	-	41,54,74	5.08	27 (65%)	24,90,114	3.31	12 (50%)
24	CHL	6	609	1	59,69,74	4.30	27 (45%)	45,108,114	2.81	20 (44%)
25	CLA	6	610	1	41,58,73	1.32	7 (17%)	47,95,113	1.31	7 (14%)
25	CLA	6	611	29	33,53,73	1.33	6 (18%)	37,89,113	1.61	8 (21%)
25	CLA	6	612	1	33,53,73	1.40	5 (15%)	37,89,113	1.68	10 (27%)
25	CLA	6	613	1	33,53,73	1.38	7 (21%)	37,89,113	1.50	6 (16%)
25	CLA	6	614	1	33,53,73	1.35	6 (18%)	37,89,113	1.55	6 (16%)
26	LUT	7	1620	-	41,43,43	0.96	3 (7%)	50,60,60	2.02	18 (36%)
26	LUT	7	1621	-	41,43,43	0.92	1 (2%)	50,60,60	1.68	12 (24%)
27	XAT	7	1622	-	39,47,47	1.17	5 (12%)	54,74,74	3.07	27 (50%)
28	NEX	7	1623	-	38,46,46	0.94	2 (5%)	49,70,70	2.50	16 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	LHG	7	2630	25	46,46,48	0.77	1 (2%)	47,52,54	1.33	4 (8%)
24	CHL	7	601	2	62,72,74	4.36	27 (43%)	48,111,114	2.72	18 (37%)
25	CLA	7	602	2	51,68,73	1.18	6 (11%)	59,107,113	1.41	7 (11%)
25	CLA	7	603	2	46,63,73	1.26	9 (19%)	53,101,113	1.49	11 (20%)
25	CLA	7	604	-	33,53,73	1.43	7 (21%)	37,89,113	1.46	7 (18%)
24	CHL	7	605	2	41,54,74	5.05	25 (60%)	24,90,114	3.52	16 (66%)
24	CHL	7	606	-	41,54,74	5.24	25 (60%)	24,90,114	3.68	15 (62%)
24	CHL	7	607	-	51,61,74	4.58	27 (52%)	35,98,114	2.93	16 (45%)
24	CHL	7	608	-	41,54,74	5.18	27 (65%)	24,90,114	3.39	13 (54%)
24	CHL	7	609	2	59,69,74	4.31	27 (45%)	45,108,114	2.77	19 (42%)
25	CLA	7	610	2	51,68,73	1.21	7 (13%)	59,107,113	1.33	8 (13%)
25	CLA	7	611	29	46,63,73	1.38	7 (15%)	53,101,113	1.42	11 (20%)
25	CLA	7	612	2	33,53,73	1.49	8 (24%)	37,89,113	1.78	10 (27%)
25	CLA	7	613	2	49,66,73	1.22	7 (14%)	56,104,113	1.33	7 (12%)
25	CLA	7	614	2	39,56,73	1.25	5 (12%)	45,92,113	1.40	7 (15%)
29	LHG	8	2630	25	20,20,48	0.85	0	21,26,54	1.35	1 (4%)
24	CHL	8	601	3	36,53,74	5.08	21 (58%)	19,89,114	3.73	14 (73%)
25	CLA	8	602	3	33,53,73	1.31	6 (18%)	37,89,113	1.79	7 (18%)
25	CLA	8	603	3	33,53,73	1.39	6 (18%)	37,89,113	1.58	8 (21%)
25	CLA	8	604	-	33,53,73	1.44	7 (21%)	37,89,113	1.56	6 (16%)
24	CHL	8	606	-	41,54,74	5.06	26 (63%)	24,90,114	3.37	14 (58%)
24	CHL	8	607	-	41,54,74	5.02	26 (63%)	24,90,114	3.44	15 (62%)
24	CHL	8	608	-	41,54,74	5.11	25 (60%)	24,90,114	3.50	16 (66%)
24	CHL	8	609	3	41,54,74	5.12	25 (60%)	24,90,114	3.46	15 (62%)
25	CLA	8	610	3	33,53,73	1.43	7 (21%)	37,89,113	1.51	5 (13%)
25	CLA	8	611	29	33,53,73	1.41	6 (18%)	37,89,113	1.37	6 (16%)
25	CLA	8	612	3	33,53,73	1.33	5 (15%)	37,89,113	1.71	7 (18%)
26	LUT	8	620	-	41,43,43	0.94	2 (4%)	50,60,60	2.23	15 (30%)
27	XAT	8	622	-	39,47,47	0.94	1 (2%)	54,74,74	2.70	20 (37%)
30	BCR	8	623	-	41,41,41	0.77	0	56,56,56	2.18	14 (25%)
31	OEX	A	401	4,6	0,15,15	0.00	-	0,32,32	0.00	-
25	CLA	A	405	4	56,73,73	1.16	5 (8%)	65,113,113	1.39	6 (9%)
25	CLA	A	406	-	56,73,73	1.14	6 (10%)	65,113,113	1.39	7 (10%)
25	CLA	A	407	-	41,58,73	1.32	7 (17%)	47,95,113	1.39	6 (12%)
33	PHO	A	408	-	67,69,69	1.21	9 (13%)	87,99,99	1.13	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	PHO	A	409	-	67,69,69	1.20	7 (10%)	87,99,99	1.26	8 (9%)
25	CLA	A	410	4	51,68,73	1.21	7 (13%)	59,107,113	1.37	10 (16%)
30	BCR	A	411	-	41,41,41	0.79	0	56,56,56	1.84	13 (23%)
34	SQD	A	412	-	49,50,54	0.97	6 (12%)	59,61,65	1.85	8 (13%)
35	LMG	A	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.32	4 (7%)
36	PL9	A	414	-	13,13,55	0.74	0	17,17,69	1.92	4 (23%)
35	LMG	A	415	-	40,40,55	0.88	0	48,48,63	1.34	6 (12%)
34	SQD	A	418	-	53,54,54	0.91	5 (9%)	63,65,65	1.90	14 (22%)
29	LHG	B	2630	-	46,46,48	0.68	2 (4%)	47,52,54	1.25	6 (12%)
29	LHG	B	2631	-	48,48,48	0.64	1 (2%)	49,54,54	1.25	6 (12%)
35	LMG	B	2633	-	55,55,55	0.75	2 (3%)	63,63,63	1.38	6 (9%)
25	CLA	B	602	-	56,73,73	1.13	7 (12%)	65,113,113	1.25	6 (9%)
25	CLA	B	603	5	56,73,73	1.16	7 (12%)	65,113,113	1.22	5 (7%)
25	CLA	B	604	5	56,73,73	1.23	8 (14%)	65,113,113	1.38	8 (12%)
25	CLA	B	605	5	56,73,73	1.28	8 (14%)	65,113,113	1.75	16 (24%)
25	CLA	B	606	5	56,73,73	1.27	8 (14%)	65,113,113	1.38	8 (12%)
25	CLA	B	607	5	56,73,73	1.20	6 (10%)	65,113,113	1.37	7 (10%)
25	CLA	B	608	-	56,73,73	1.19	8 (14%)	65,113,113	1.39	6 (9%)
25	CLA	B	609	5	56,73,73	1.07	5 (8%)	65,113,113	1.57	9 (13%)
25	CLA	B	610	5	56,73,73	1.15	7 (12%)	65,113,113	1.43	12 (18%)
25	CLA	B	611	-	56,73,73	1.19	7 (12%)	65,113,113	1.44	13 (20%)
25	CLA	B	612	5	56,73,73	1.33	6 (10%)	65,113,113	1.65	13 (20%)
25	CLA	B	613	5	56,73,73	1.27	8 (14%)	65,113,113	1.61	10 (15%)
25	CLA	B	614	5	56,73,73	1.23	8 (14%)	65,113,113	1.44	10 (15%)
25	CLA	B	615	5	56,73,73	1.16	7 (12%)	65,113,113	1.31	7 (10%)
25	CLA	B	616	5	56,73,73	1.18	8 (14%)	65,113,113	1.36	12 (18%)
25	CLA	B	617	5	56,73,73	1.17	7 (12%)	65,113,113	1.39	9 (13%)
30	BCR	B	618	-	41,41,41	1.03	3 (7%)	56,56,56	1.96	13 (23%)
30	BCR	B	619	-	41,41,41	0.86	1 (2%)	56,56,56	1.85	16 (28%)
30	BCR	B	620	-	41,41,41	0.88	1 (2%)	56,56,56	2.01	15 (26%)
34	SQD	B	621	-	53,54,54	0.92	5 (9%)	63,65,65	1.91	11 (17%)
35	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.42	6 (10%)
34	SQD	B	623	-	41,42,54	1.10	5 (12%)	51,53,65	2.07	12 (23%)
37	DGD	B	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.41	7 (9%)
29	LHG	C	2630	-	48,48,48	0.63	1 (2%)	49,54,54	1.32	7 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	C	501	6	56,73,73	1.08	6 (10%)	65,113,113	1.21	7 (10%)
25	CLA	C	502	6	56,73,73	1.08	4 (7%)	65,113,113	1.41	9 (13%)
25	CLA	C	503	6	56,73,73	1.08	4 (7%)	65,113,113	1.29	6 (9%)
25	CLA	C	504	-	56,73,73	1.05	5 (8%)	65,113,113	1.36	6 (9%)
25	CLA	C	505	6	56,73,73	1.09	5 (8%)	65,113,113	1.42	9 (13%)
25	CLA	C	506	6	56,73,73	1.13	6 (10%)	65,113,113	1.35	8 (12%)
25	CLA	C	507	-	56,73,73	1.10	4 (7%)	65,113,113	1.45	11 (16%)
25	CLA	C	508	6	56,73,73	1.09	5 (8%)	65,113,113	1.52	8 (12%)
25	CLA	C	509	6	56,73,73	1.11	4 (7%)	65,113,113	1.38	8 (12%)
25	CLA	C	510	6	56,73,73	1.08	4 (7%)	65,113,113	1.39	6 (9%)
25	CLA	C	511	6	56,73,73	1.08	4 (7%)	65,113,113	1.29	8 (12%)
25	CLA	C	512	6	56,73,73	1.04	4 (7%)	65,113,113	1.32	9 (13%)
25	CLA	C	513	6	56,73,73	1.04	5 (8%)	65,113,113	1.46	10 (15%)
30	BCR	C	514	-	41,41,41	0.77	0	56,56,56	1.71	11 (19%)
30	BCR	C	515	-	41,41,41	0.76	0	56,56,56	1.89	17 (30%)
30	BCR	C	516	-	41,41,41	0.67	0	56,56,56	1.93	14 (25%)
30	BCR	C	517	-	41,41,41	0.79	0	56,56,56	2.10	13 (23%)
37	DGD	C	518	-	56,56,67	1.00	4 (7%)	70,70,81	1.57	13 (18%)
37	DGD	C	519	-	63,63,67	0.99	4 (6%)	77,77,81	1.41	10 (12%)
37	DGD	C	520	-	61,61,67	0.99	2 (3%)	75,75,81	1.46	11 (14%)
35	LMG	C	521	-	51,51,55	0.76	0	59,59,63	1.33	7 (11%)
29	LHG	C	522	-	48,48,48	0.65	1 (2%)	49,54,54	1.29	7 (14%)
29	LHG	C	523	-	48,48,48	0.64	1 (2%)	49,54,54	1.26	6 (12%)
38	BCT	D	401	32	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	D	402	7	56,73,73	1.25	8 (14%)	65,113,113	1.52	12 (18%)
25	CLA	D	403	7	56,73,73	1.12	7 (12%)	65,113,113	1.40	8 (12%)
30	BCR	D	404	-	41,41,41	0.74	0	56,56,56	1.93	13 (23%)
36	PL9	D	405	-	55,55,55	2.22	17 (30%)	69,69,69	1.58	17 (24%)
29	LHG	D	408	-	45,45,48	0.81	1 (2%)	46,51,54	1.40	6 (13%)
29	LHG	D	409	-	48,48,48	0.77	1 (2%)	49,54,54	1.36	7 (14%)
29	LHG	D	410	-	42,42,48	0.65	0	43,48,54	1.26	4 (9%)
35	LMG	D	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.41	6 (11%)
39	HEM	F	101	9,8	28,50,50	1.81	4 (14%)	17,82,82	1.64	3 (17%)
26	LUT	G	1620	-	41,43,43	0.87	2 (4%)	50,60,60	1.81	12 (24%)
26	LUT	G	1621	-	41,43,43	1.02	4 (9%)	50,60,60	2.03	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	XAT	G	1622	-	39,47,47	1.00	1 (2%)	54,74,74	2.86	22 (40%)
28	NEX	G	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.58	17 (34%)
29	LHG	G	2630	25	48,48,48	0.75	1 (2%)	49,54,54	1.34	7 (14%)
24	CHL	G	601	1	64,74,74	4.17	27 (42%)	51,114,114	2.60	18 (35%)
25	CLA	G	602	1	56,73,73	1.18	6 (10%)	65,113,113	1.52	12 (18%)
25	CLA	G	603	1	56,73,73	1.14	7 (12%)	65,113,113	1.50	11 (16%)
25	CLA	G	604	-	41,58,73	1.36	7 (17%)	47,95,113	1.57	9 (19%)
24	CHL	G	605	1	41,54,74	4.92	24 (58%)	24,90,114	3.46	15 (62%)
24	CHL	G	606	-	48,58,74	4.79	26 (54%)	32,94,114	3.12	18 (56%)
24	CHL	G	607	-	64,74,74	4.11	26 (40%)	51,114,114	2.41	16 (31%)
24	CHL	G	608	-	64,74,74	4.03	25 (39%)	51,114,114	2.50	15 (29%)
24	CHL	G	609	1	59,69,74	4.36	26 (44%)	45,108,114	2.76	16 (35%)
25	CLA	G	610	1	55,72,73	1.11	7 (12%)	63,111,113	1.44	9 (14%)
25	CLA	G	611	29	51,68,73	1.16	7 (13%)	59,107,113	1.31	7 (11%)
25	CLA	G	612	1	51,68,73	1.13	6 (11%)	59,107,113	1.37	7 (11%)
25	CLA	G	613	1	56,73,73	1.08	8 (14%)	65,113,113	1.28	7 (10%)
25	CLA	G	614	1	39,56,73	1.33	7 (17%)	45,92,113	1.31	5 (11%)
30	BCR	H	101	-	41,41,41	0.90	1 (2%)	56,56,56	2.01	13 (23%)
37	DGD	H	102	-	63,63,67	1.22	7 (11%)	77,77,81	1.57	10 (12%)
29	LHG	L	101	-	48,48,48	0.74	1 (2%)	49,54,54	1.34	7 (14%)
26	LUT	N	1620	-	41,43,43	0.90	2 (4%)	50,60,60	1.82	16 (32%)
26	LUT	N	1621	-	41,43,43	1.00	2 (4%)	50,60,60	1.97	15 (30%)
27	XAT	N	1622	-	39,47,47	0.93	1 (2%)	54,74,74	3.01	23 (42%)
28	NEX	N	1623	-	38,46,46	1.06	3 (7%)	49,70,70	2.44	16 (32%)
29	LHG	N	2630	25	48,48,48	0.74	1 (2%)	49,54,54	1.34	7 (14%)
24	CHL	N	601	1	64,74,74	4.09	26 (40%)	51,114,114	2.57	18 (35%)
25	CLA	N	602	1	56,73,73	1.14	7 (12%)	65,113,113	1.41	11 (16%)
25	CLA	N	603	1	56,73,73	1.17	7 (12%)	65,113,113	1.43	11 (16%)
25	CLA	N	604	-	41,58,73	1.36	6 (14%)	47,95,113	1.67	10 (21%)
24	CHL	N	605	1	46,56,74	4.79	25 (54%)	30,92,114	3.22	17 (56%)
24	CHL	N	606	-	48,58,74	4.91	27 (56%)	32,94,114	3.13	16 (50%)
24	CHL	N	607	-	64,74,74	4.14	26 (40%)	51,114,114	2.39	15 (29%)
24	CHL	N	608	-	64,74,74	4.13	25 (39%)	51,114,114	2.53	16 (31%)
24	CHL	N	609	1	64,74,74	4.26	28 (43%)	51,114,114	2.62	16 (31%)
25	CLA	N	610	1	56,73,73	1.10	6 (10%)	65,113,113	1.45	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	N	611	29	51,68,73	1.17	7 (13%)	59,107,113	1.28	9 (15%)
25	CLA	N	612	1	51,68,73	1.16	6 (11%)	59,107,113	1.40	9 (15%)
25	CLA	N	613	1	51,68,73	1.12	4 (7%)	59,107,113	1.46	8 (13%)
25	CLA	N	614	1	39,56,73	1.26	5 (12%)	45,92,113	1.50	7 (15%)
29	LHG	R	2630	25	41,41,48	0.71	1 (2%)	42,47,54	1.36	7 (16%)
25	CLA	R	601	17	40,57,73	1.26	6 (15%)	46,93,113	1.85	11 (23%)
25	CLA	R	602	17	51,68,73	1.16	7 (13%)	59,107,113	1.51	10 (16%)
25	CLA	R	603	17	51,68,73	1.16	7 (13%)	59,107,113	1.45	10 (16%)
25	CLA	R	604	-	39,56,73	1.33	6 (15%)	45,92,113	1.70	9 (20%)
24	CHL	R	606	-	64,74,74	4.16	27 (42%)	51,114,114	2.59	19 (37%)
24	CHL	R	607	-	54,64,74	4.43	27 (50%)	39,102,114	2.89	20 (51%)
24	CHL	R	608	-	59,69,74	4.33	27 (45%)	45,108,114	2.59	15 (33%)
25	CLA	R	609	17	49,66,73	1.20	6 (12%)	56,104,113	1.45	8 (14%)
25	CLA	R	610	17	56,73,73	1.14	7 (12%)	65,113,113	1.37	7 (10%)
25	CLA	R	611	29	40,57,73	1.30	6 (15%)	46,93,113	1.43	10 (21%)
25	CLA	R	612	17	40,57,73	1.30	6 (15%)	46,93,113	1.46	8 (17%)
25	CLA	R	613	17	51,68,73	1.25	7 (13%)	59,107,113	1.38	9 (15%)
24	CHL	R	614	17	40,50,74	5.00	22 (55%)	25,85,114	3.35	15 (60%)
25	CLA	R	616	17	33,53,73	1.47	7 (21%)	37,89,113	1.42	6 (16%)
26	LUT	R	620	-	41,43,43	0.99	4 (9%)	50,60,60	1.98	18 (36%)
27	XAT	R	622	-	39,47,47	1.02	2 (5%)	54,74,74	2.73	19 (35%)
28	NEX	R	623	-	38,46,46	1.06	3 (7%)	49,70,70	2.53	19 (38%)
26	LUT	S	1620	-	41,43,43	0.78	0	50,60,60	1.78	13 (26%)
26	LUT	S	1621	-	41,43,43	0.79	0	50,60,60	1.78	15 (30%)
28	NEX	S	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.39	15 (30%)
29	LHG	S	2630	25	48,48,48	0.63	1 (2%)	49,54,54	1.29	7 (14%)
24	CHL	S	601	18	41,54,74	4.97	25 (60%)	24,90,114	3.44	14 (58%)
25	CLA	S	602	18	52,69,73	1.12	5 (9%)	60,108,113	1.39	8 (13%)
25	CLA	S	603	18	33,53,73	1.34	5 (15%)	37,89,113	1.54	8 (21%)
25	CLA	S	604	-	41,58,73	1.23	4 (9%)	47,95,113	1.58	10 (21%)
24	CHL	S	606	-	41,54,74	4.75	23 (56%)	24,90,114	3.47	14 (58%)
24	CHL	S	607	-	56,66,74	4.15	21 (37%)	40,104,114	2.86	17 (42%)
24	CHL	S	608	-	41,54,74	4.84	24 (58%)	24,90,114	3.47	14 (58%)
25	CLA	S	609	18	33,53,73	1.37	5 (15%)	37,89,113	1.52	7 (18%)
25	CLA	S	610	18	46,63,73	1.17	6 (13%)	53,101,113	1.44	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	S	611	29	47,64,73	1.17	5 (10%)	54,102,113	1.30	7 (12%)
25	CLA	S	612	18	40,57,73	1.22	5 (12%)	46,93,113	1.55	7 (15%)
25	CLA	S	613	18	46,63,73	1.18	4 (8%)	53,101,113	1.39	7 (13%)
25	CLA	S	614	18	40,57,73	1.20	4 (10%)	46,93,113	1.56	6 (13%)
30	BCR	T	101	-	41,41,41	0.85	1 (2%)	56,56,56	2.63	23 (41%)
26	LUT	Y	1620	-	41,43,43	1.08	5 (12%)	50,60,60	1.96	20 (40%)
26	LUT	Y	1621	-	41,43,43	1.06	4 (9%)	50,60,60	1.92	17 (34%)
27	XAT	Y	1622	-	39,47,47	1.11	4 (10%)	54,74,74	2.97	19 (35%)
28	NEX	Y	1623	-	38,46,46	1.10	2 (5%)	49,70,70	2.67	19 (38%)
29	LHG	Y	2630	25	48,48,48	0.80	2 (4%)	49,54,54	1.28	6 (12%)
24	CHL	Y	601	1	64,74,74	4.27	26 (40%)	51,114,114	2.56	17 (33%)
25	CLA	Y	602	1	56,73,73	1.21	7 (12%)	65,113,113	1.39	8 (12%)
25	CLA	Y	603	1	56,73,73	1.18	7 (12%)	65,113,113	1.46	12 (18%)
25	CLA	Y	604	-	41,58,73	1.37	6 (14%)	47,95,113	1.69	8 (17%)
24	CHL	Y	605	1	46,56,74	4.83	26 (56%)	30,92,114	3.15	16 (53%)
24	CHL	Y	606	-	48,58,74	4.90	30 (62%)	32,94,114	3.15	16 (50%)
24	CHL	Y	607	-	64,74,74	4.22	28 (43%)	51,114,114	2.37	13 (25%)
24	CHL	Y	608	-	64,74,74	4.17	27 (42%)	51,114,114	2.50	17 (33%)
24	CHL	Y	609	1	64,74,74	4.24	26 (40%)	51,114,114	2.65	20 (39%)
25	CLA	Y	610	1	51,68,73	1.25	7 (13%)	59,107,113	1.39	8 (13%)
25	CLA	Y	611	29	51,68,73	1.21	6 (11%)	59,107,113	1.36	9 (15%)
25	CLA	Y	612	1	51,68,73	1.26	7 (13%)	59,107,113	1.38	11 (18%)
25	CLA	Y	613	1	56,73,73	1.12	6 (10%)	65,113,113	1.45	10 (15%)
25	CLA	Y	614	1	39,56,73	1.39	7 (17%)	45,92,113	1.33	8 (17%)
35	LMG	Z	101	-	51,51,55	0.91	4 (7%)	59,59,63	1.31	7 (11%)
31	OEX	a	401	4,6	0,15,15	0.00	-	0,32,32	0.00	-
25	CLA	a	405	4	56,73,73	1.16	5 (8%)	65,113,113	1.39	6 (9%)
25	CLA	a	406	-	56,73,73	1.14	6 (10%)	65,113,113	1.39	8 (12%)
25	CLA	a	407	-	41,58,73	1.32	7 (17%)	47,95,113	1.38	6 (12%)
33	PHO	a	408	-	67,69,69	1.21	9 (13%)	87,99,99	1.14	9 (10%)
33	PHO	a	409	-	67,69,69	1.19	8 (11%)	87,99,99	1.26	8 (9%)
25	CLA	a	410	4	51,68,73	1.21	7 (13%)	59,107,113	1.37	10 (16%)
30	BCR	a	411	-	41,41,41	0.79	0	56,56,56	1.84	13 (23%)
34	SQD	a	412	-	49,50,54	0.97	6 (12%)	59,61,65	1.85	8 (13%)
35	LMG	a	413	-	48,48,55	0.78	1 (2%)	56,56,63	1.32	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	PL9	a	414	-	13,13,55	0.73	0	17,17,69	1.93	4 (23%)
35	LMG	a	415	-	40,40,55	0.88	0	48,48,63	1.34	6 (12%)
34	SQD	a	418	-	53,54,54	0.91	5 (9%)	63,65,65	1.90	14 (22%)
29	LHG	b	2630	-	46,46,48	0.68	2 (4%)	47,52,54	1.25	5 (10%)
29	LHG	b	2631	-	48,48,48	0.63	1 (2%)	49,54,54	1.25	6 (12%)
35	LMG	b	2633	-	55,55,55	0.75	2 (3%)	63,63,63	1.38	6 (9%)
25	CLA	b	602	-	56,73,73	1.13	7 (12%)	65,113,113	1.25	6 (9%)
25	CLA	b	603	5	56,73,73	1.16	7 (12%)	65,113,113	1.22	5 (7%)
25	CLA	b	604	5	56,73,73	1.23	8 (14%)	65,113,113	1.38	8 (12%)
25	CLA	b	605	5	56,73,73	1.28	8 (14%)	65,113,113	1.75	16 (24%)
25	CLA	b	606	5	56,73,73	1.27	8 (14%)	65,113,113	1.39	8 (12%)
25	CLA	b	607	5	56,73,73	1.20	6 (10%)	65,113,113	1.37	7 (10%)
25	CLA	b	608	-	56,73,73	1.19	8 (14%)	65,113,113	1.38	6 (9%)
25	CLA	b	609	5	56,73,73	1.07	6 (10%)	65,113,113	1.58	9 (13%)
25	CLA	b	610	5	56,73,73	1.15	7 (12%)	65,113,113	1.43	12 (18%)
25	CLA	b	611	-	56,73,73	1.19	7 (12%)	65,113,113	1.44	13 (20%)
25	CLA	b	612	5	56,73,73	1.33	6 (10%)	65,113,113	1.65	13 (20%)
25	CLA	b	613	5	56,73,73	1.27	8 (14%)	65,113,113	1.61	10 (15%)
25	CLA	b	614	5	56,73,73	1.23	8 (14%)	65,113,113	1.44	10 (15%)
25	CLA	b	615	5	56,73,73	1.17	7 (12%)	65,113,113	1.31	8 (12%)
25	CLA	b	616	5	56,73,73	1.18	8 (14%)	65,113,113	1.36	11 (16%)
25	CLA	b	617	5	56,73,73	1.17	7 (12%)	65,113,113	1.39	9 (13%)
30	BCR	b	618	-	41,41,41	1.03	3 (7%)	56,56,56	1.96	13 (23%)
30	BCR	b	619	-	41,41,41	0.85	2 (4%)	56,56,56	1.85	16 (28%)
30	BCR	b	620	-	41,41,41	0.88	1 (2%)	56,56,56	2.01	15 (26%)
34	SQD	b	621	-	53,54,54	0.92	4 (7%)	63,65,65	1.91	11 (17%)
35	LMG	b	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.42	6 (10%)
34	SQD	b	623	-	41,42,54	1.10	5 (12%)	51,53,65	2.07	12 (23%)
37	DGD	b	626	-	60,60,67	0.97	1 (1%)	74,74,81	1.41	8 (10%)
29	LHG	c	2630	-	48,48,48	0.63	1 (2%)	49,54,54	1.32	7 (14%)
25	CLA	c	501	6	56,73,73	1.08	6 (10%)	65,113,113	1.21	7 (10%)
25	CLA	c	502	6	56,73,73	1.08	4 (7%)	65,113,113	1.41	9 (13%)
25	CLA	c	503	6	56,73,73	1.08	4 (7%)	65,113,113	1.28	6 (9%)
25	CLA	c	504	-	56,73,73	1.05	5 (8%)	65,113,113	1.36	6 (9%)
25	CLA	c	505	6	56,73,73	1.10	6 (10%)	65,113,113	1.42	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	c	506	6	56,73,73	1.14	6 (10%)	65,113,113	1.35	8 (12%)
25	CLA	c	507	-	56,73,73	1.10	4 (7%)	65,113,113	1.45	11 (16%)
25	CLA	c	508	6	56,73,73	1.09	5 (8%)	65,113,113	1.52	8 (12%)
25	CLA	c	509	6	56,73,73	1.11	4 (7%)	65,113,113	1.37	8 (12%)
25	CLA	c	510	6	56,73,73	1.08	4 (7%)	65,113,113	1.39	7 (10%)
25	CLA	c	511	6	56,73,73	1.08	4 (7%)	65,113,113	1.29	8 (12%)
25	CLA	c	512	6	56,73,73	1.05	4 (7%)	65,113,113	1.33	9 (13%)
25	CLA	c	513	6	56,73,73	1.05	5 (8%)	65,113,113	1.46	10 (15%)
30	BCR	c	514	-	41,41,41	0.76	0	56,56,56	1.71	11 (19%)
30	BCR	c	515	-	41,41,41	0.76	0	56,56,56	1.90	17 (30%)
30	BCR	c	516	-	41,41,41	0.67	0	56,56,56	1.93	14 (25%)
30	BCR	c	517	-	41,41,41	0.78	0	56,56,56	2.11	13 (23%)
37	DGD	c	518	-	56,56,67	0.99	4 (7%)	70,70,81	1.57	13 (18%)
37	DGD	c	519	-	63,63,67	0.99	4 (6%)	77,77,81	1.42	10 (12%)
37	DGD	c	520	-	61,61,67	0.99	2 (3%)	75,75,81	1.46	11 (14%)
35	LMG	c	521	-	51,51,55	0.76	0	59,59,63	1.33	7 (11%)
29	LHG	c	522	-	48,48,48	0.65	1 (2%)	49,54,54	1.29	7 (14%)
29	LHG	c	523	-	48,48,48	0.65	1 (2%)	49,54,54	1.26	6 (12%)
38	BCT	d	401	32	0,3,3	0.00	-	0,3,3	0.00	-
25	CLA	d	402	7	56,73,73	1.25	8 (14%)	65,113,113	1.52	12 (18%)
25	CLA	d	403	7	56,73,73	1.11	7 (12%)	65,113,113	1.40	8 (12%)
30	BCR	d	404	-	41,41,41	0.74	0	56,56,56	1.93	14 (25%)
36	PL9	d	405	-	55,55,55	2.22	17 (30%)	69,69,69	1.58	17 (24%)
29	LHG	d	408	-	45,45,48	0.81	1 (2%)	46,51,54	1.39	6 (13%)
29	LHG	d	409	-	48,48,48	0.78	1 (2%)	49,54,54	1.36	7 (14%)
29	LHG	d	410	-	42,42,48	0.65	1 (2%)	43,48,54	1.26	4 (9%)
35	LMG	d	411	-	46,46,55	0.85	2 (4%)	54,54,63	1.41	6 (11%)
39	HEM	f	101	9,8	28,50,50	1.81	4 (14%)	17,82,82	1.63	3 (17%)
26	LUT	g	1620	-	41,43,43	0.87	1 (2%)	50,60,60	1.82	12 (24%)
26	LUT	g	1621	-	41,43,43	1.02	4 (9%)	50,60,60	2.03	19 (38%)
27	XAT	g	1622	-	39,47,47	1.00	1 (2%)	54,74,74	2.86	22 (40%)
28	NEX	g	1623	-	38,46,46	0.97	1 (2%)	49,70,70	2.57	17 (34%)
29	LHG	g	2630	25	48,48,48	0.75	1 (2%)	49,54,54	1.34	7 (14%)
24	CHL	g	601	1	64,74,74	4.17	27 (42%)	51,114,114	2.60	18 (35%)
25	CLA	g	602	1	56,73,73	1.18	6 (10%)	65,113,113	1.53	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	g	603	1	56,73,73	1.14	7 (12%)	65,113,113	1.49	11 (16%)
25	CLA	g	604	-	41,58,73	1.36	7 (17%)	47,95,113	1.57	9 (19%)
24	CHL	g	605	1	41,54,74	4.93	24 (58%)	24,90,114	3.47	15 (62%)
24	CHL	g	606	-	48,58,74	4.80	26 (54%)	32,94,114	3.13	18 (56%)
24	CHL	g	607	-	64,74,74	4.12	26 (40%)	51,114,114	2.41	16 (31%)
24	CHL	g	608	-	64,74,74	4.03	25 (39%)	51,114,114	2.50	15 (29%)
24	CHL	g	609	1	59,69,74	4.36	26 (44%)	45,108,114	2.75	16 (35%)
25	CLA	g	610	1	55,72,73	1.11	7 (12%)	63,111,113	1.44	9 (14%)
25	CLA	g	611	29	51,68,73	1.16	7 (13%)	59,107,113	1.31	7 (11%)
25	CLA	g	612	1	51,68,73	1.13	6 (11%)	59,107,113	1.37	7 (11%)
25	CLA	g	613	1	56,73,73	1.07	8 (14%)	65,113,113	1.28	7 (10%)
25	CLA	g	614	1	39,56,73	1.33	7 (17%)	45,92,113	1.31	5 (11%)
30	BCR	h	101	-	41,41,41	0.90	0	56,56,56	2.01	13 (23%)
37	DGD	h	102	-	63,63,67	1.23	7 (11%)	77,77,81	1.57	10 (12%)
29	LHG	l	101	-	48,48,48	0.74	1 (2%)	49,54,54	1.34	7 (14%)
26	LUT	n	1620	-	41,43,43	0.90	2 (4%)	50,60,60	1.82	16 (32%)
26	LUT	n	1621	-	41,43,43	1.01	2 (4%)	50,60,60	1.97	15 (30%)
27	XAT	n	1622	-	39,47,47	0.94	1 (2%)	54,74,74	3.02	23 (42%)
28	NEX	n	1623	-	38,46,46	1.06	3 (7%)	49,70,70	2.44	16 (32%)
29	LHG	n	2630	25	48,48,48	0.74	1 (2%)	49,54,54	1.34	7 (14%)
24	CHL	n	601	1	64,74,74	4.09	26 (40%)	51,114,114	2.57	18 (35%)
25	CLA	n	602	1	56,73,73	1.14	7 (12%)	65,113,113	1.41	11 (16%)
25	CLA	n	603	1	56,73,73	1.18	7 (12%)	65,113,113	1.44	11 (16%)
25	CLA	n	604	-	41,58,73	1.35	6 (14%)	47,95,113	1.66	10 (21%)
24	CHL	n	605	1	46,56,74	4.79	25 (54%)	30,92,114	3.22	17 (56%)
24	CHL	n	606	-	48,58,74	4.91	27 (56%)	32,94,114	3.13	16 (50%)
24	CHL	n	607	-	64,74,74	4.14	27 (42%)	51,114,114	2.39	15 (29%)
24	CHL	n	608	-	64,74,74	4.13	25 (39%)	51,114,114	2.53	17 (33%)
24	CHL	n	609	1	64,74,74	4.27	28 (43%)	51,114,114	2.62	17 (33%)
25	CLA	n	610	1	56,73,73	1.10	6 (10%)	65,113,113	1.45	9 (13%)
25	CLA	n	611	29	51,68,73	1.17	7 (13%)	59,107,113	1.27	9 (15%)
25	CLA	n	612	1	51,68,73	1.16	6 (11%)	59,107,113	1.40	9 (15%)
25	CLA	n	613	1	51,68,73	1.13	5 (9%)	59,107,113	1.46	8 (13%)
25	CLA	n	614	1	39,56,73	1.27	5 (12%)	45,92,113	1.50	7 (15%)
29	LHG	r	2630	25	41,41,48	0.71	1 (2%)	42,47,54	1.36	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CLA	r	601	17	40,57,73	1.27	6 (15%)	46,93,113	1.85	11 (23%)
25	CLA	r	602	17	51,68,73	1.16	7 (13%)	59,107,113	1.51	10 (16%)
25	CLA	r	603	17	51,68,73	1.16	7 (13%)	59,107,113	1.44	10 (16%)
25	CLA	r	604	-	39,56,73	1.33	6 (15%)	45,92,113	1.70	9 (20%)
24	CHL	r	606	-	64,74,74	4.17	27 (42%)	51,114,114	2.59	19 (37%)
24	CHL	r	607	-	54,64,74	4.43	27 (50%)	39,102,114	2.89	20 (51%)
24	CHL	r	608	-	59,69,74	4.33	27 (45%)	45,108,114	2.59	15 (33%)
25	CLA	r	609	17	49,66,73	1.20	6 (12%)	56,104,113	1.45	8 (14%)
25	CLA	r	610	17	56,73,73	1.14	7 (12%)	65,113,113	1.37	7 (10%)
25	CLA	r	611	29	40,57,73	1.30	6 (15%)	46,93,113	1.43	10 (21%)
25	CLA	r	612	17	40,57,73	1.31	6 (15%)	46,93,113	1.46	8 (17%)
25	CLA	r	613	17	51,68,73	1.25	7 (13%)	59,107,113	1.38	9 (15%)
24	CHL	r	614	17	40,50,74	5.00	22 (55%)	25,85,114	3.36	15 (60%)
25	CLA	r	616	17	33,53,73	1.48	7 (21%)	37,89,113	1.42	6 (16%)
26	LUT	r	620	-	41,43,43	0.98	4 (9%)	50,60,60	1.99	18 (36%)
27	XAT	r	622	-	39,47,47	1.02	2 (5%)	54,74,74	2.73	19 (35%)
28	NEX	r	623	-	38,46,46	1.06	3 (7%)	49,70,70	2.53	20 (40%)
26	LUT	s	1620	-	41,43,43	0.77	0	50,60,60	1.77	13 (26%)
26	LUT	s	1621	-	41,43,43	0.79	0	50,60,60	1.78	14 (28%)
28	NEX	s	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.39	14 (28%)
29	LHG	s	2630	25	48,48,48	0.64	1 (2%)	49,54,54	1.28	7 (14%)
24	CHL	s	601	18	41,54,74	4.97	24 (58%)	24,90,114	3.44	14 (58%)
25	CLA	s	602	18	52,69,73	1.12	5 (9%)	60,108,113	1.39	8 (13%)
25	CLA	s	603	18	33,53,73	1.34	5 (15%)	37,89,113	1.53	8 (21%)
25	CLA	s	604	-	41,58,73	1.23	4 (9%)	47,95,113	1.58	10 (21%)
24	CHL	s	606	-	41,54,74	4.75	23 (56%)	24,90,114	3.47	14 (58%)
24	CHL	s	607	-	56,66,74	4.16	21 (37%)	40,104,114	2.86	17 (42%)
24	CHL	s	608	-	41,54,74	4.84	25 (60%)	24,90,114	3.47	14 (58%)
25	CLA	s	609	18	33,53,73	1.37	5 (15%)	37,89,113	1.52	7 (18%)
25	CLA	s	610	18	46,63,73	1.18	6 (13%)	53,101,113	1.44	8 (15%)
25	CLA	s	611	29	47,64,73	1.17	5 (10%)	54,102,113	1.30	6 (11%)
25	CLA	s	612	18	40,57,73	1.22	4 (10%)	46,93,113	1.55	7 (15%)
25	CLA	s	613	18	46,63,73	1.18	4 (8%)	53,101,113	1.39	7 (13%)
25	CLA	s	614	18	40,57,73	1.19	4 (10%)	46,93,113	1.55	6 (13%)
30	BCR	t	101	-	41,41,41	0.84	1 (2%)	56,56,56	2.62	23 (41%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	LUT	y	1620	-	41,43,43	1.09	5 (12%)	50,60,60	1.96	20 (40%)
26	LUT	y	1621	-	41,43,43	1.07	4 (9%)	50,60,60	1.92	17 (34%)
27	XAT	y	1622	-	39,47,47	1.11	4 (10%)	54,74,74	2.97	19 (35%)
28	NEX	y	1623	-	38,46,46	1.10	3 (7%)	49,70,70	2.67	19 (38%)
29	LHG	y	2630	25	48,48,48	0.80	2 (4%)	49,54,54	1.28	6 (12%)
24	CHL	y	601	1	64,74,74	4.27	26 (40%)	51,114,114	2.56	17 (33%)
25	CLA	y	602	1	56,73,73	1.21	7 (12%)	65,113,113	1.39	8 (12%)
25	CLA	y	603	1	56,73,73	1.18	7 (12%)	65,113,113	1.46	12 (18%)
25	CLA	y	604	-	41,58,73	1.37	6 (14%)	47,95,113	1.69	8 (17%)
24	CHL	y	605	1	46,56,74	4.82	26 (56%)	30,92,114	3.14	16 (53%)
24	CHL	y	606	-	48,58,74	4.90	30 (62%)	32,94,114	3.15	16 (50%)
24	CHL	y	607	-	64,74,74	4.23	28 (43%)	51,114,114	2.37	13 (25%)
24	CHL	y	608	-	64,74,74	4.17	27 (42%)	51,114,114	2.49	17 (33%)
24	CHL	y	609	1	64,74,74	4.23	27 (42%)	51,114,114	2.65	20 (39%)
25	CLA	y	610	1	51,68,73	1.25	7 (13%)	59,107,113	1.38	8 (13%)
25	CLA	y	611	29	51,68,73	1.21	6 (11%)	59,107,113	1.36	9 (15%)
25	CLA	y	612	1	51,68,73	1.25	7 (13%)	59,107,113	1.39	11 (18%)
25	CLA	y	613	1	56,73,73	1.11	6 (10%)	65,113,113	1.45	10 (15%)
25	CLA	y	614	1	39,56,73	1.38	7 (17%)	45,92,113	1.33	8 (17%)
35	LMG	z	101	-	51,51,55	0.90	4 (7%)	59,59,63	1.31	7 (11%)

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
26	LUT	1	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	1	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	1	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	1	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	1	2630	25	-	0/45/45/53	0/0/0/0
24	CHL	1	601	1	-	0/15/153/177	0/0/9/9
25	CLA	1	602	1	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	1	603	1	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	1	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	1	605	1	-	0/15/153/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	1	606	-	-	0/15/153/177	0/0/9/9
24	CHL	1	607	-	-	0/38/174/177	0/0/9/9
24	CHL	1	608	-	-	0/15/153/177	0/0/9/9
24	CHL	1	609	1	-	0/37/173/177	0/0/9/9
25	CLA	1	610	1	3/3/18/25	0/27/125/135	0/0/9/9
25	CLA	1	611	29	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	1	612	1	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	1	613	1	2/2/18/25	0/25/123/135	0/0/9/9
25	CLA	1	614	1	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	2	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	2	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	2	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	2	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	2	2630	25	-	0/41/41/53	0/0/0/0
24	CHL	2	601	1	-	0/15/153/177	0/0/9/9
25	CLA	2	602	1	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	2	603	1	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	2	604	-	2/2/16/25	0/11/111/135	0/0/9/9
24	CHL	2	605	1	-	0/15/153/177	0/0/9/9
24	CHL	2	606	-	-	0/15/153/177	0/0/9/9
24	CHL	2	607	-	-	0/35/171/177	0/0/9/9
24	CHL	2	608	-	-	0/15/153/177	0/0/9/9
24	CHL	2	609	1	-	0/35/171/177	0/0/9/9
25	CLA	2	610	1	3/3/17/25	0/19/117/135	0/0/9/9
25	CLA	2	611	29	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	2	612	1	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	2	613	1	2/2/16/25	0/11/111/135	0/0/9/9
25	CLA	2	614	1	2/2/16/25	0/11/111/135	0/0/9/9
26	LUT	3	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	3	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	3	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	3	2630	25	-	0/51/51/53	0/0/0/0
24	CHL	3	601	2	-	0/39/175/177	0/0/9/9
25	CLA	3	602	2	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	3	603	2	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	3	604	-	3/3/16/25	0/11/111/135	0/0/9/9
24	CHL	3	605	2	-	0/15/153/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	3	606	-	-	0/15/153/177	0/0/9/9
24	CHL	3	607	-	-	0/26/162/177	0/0/9/9
24	CHL	3	608	-	-	0/15/153/177	0/0/9/9
24	CHL	3	609	2	-	0/35/171/177	0/0/9/9
25	CLA	3	610	2	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	3	611	29	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	3	612	2	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	3	613	2	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	3	614	2	3/3/16/25	0/17/115/135	0/0/9/9
29	LHG	4	2630	25	-	0/23/23/53	0/0/0/0
24	CHL	4	601	3	-	0/9/151/177	0/0/9/9
25	CLA	4	602	3	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	4	603	3	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	4	604	-	2/2/16/25	0/11/111/135	0/0/9/9
24	CHL	4	606	-	-	0/15/153/177	0/0/9/9
24	CHL	4	607	-	-	0/15/153/177	0/0/9/9
24	CHL	4	608	-	-	0/15/153/177	0/0/9/9
24	CHL	4	609	3	-	0/15/153/177	0/0/9/9
25	CLA	4	610	3	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	4	611	29	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	4	612	3	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	4	620	-	-	0/29/67/67	0/2/2/2
27	XAT	4	622	-	-	0/31/93/93	0/2/4/4
30	BCR	4	623	-	-	0/29/63/63	0/2/2/2
26	LUT	5	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	5	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	5	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	5	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	5	2630	25	-	0/45/45/53	0/0/0/0
24	CHL	5	601	1	-	0/15/153/177	0/0/9/9
25	CLA	5	602	1	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	5	603	1	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	5	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	5	605	1	-	0/15/153/177	0/0/9/9
24	CHL	5	606	-	-	0/15/153/177	0/0/9/9
24	CHL	5	607	-	-	0/38/174/177	0/0/9/9
24	CHL	5	608	-	-	0/15/153/177	0/0/9/9
24	CHL	5	609	1	-	0/37/173/177	0/0/9/9
25	CLA	5	610	1	3/3/18/25	0/27/125/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	5	611	29	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	5	612	1	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	5	613	1	2/2/18/25	0/25/123/135	0/0/9/9
25	CLA	5	614	1	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	6	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	6	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	6	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	6	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	6	2630	25	-	0/41/41/53	0/0/0/0
24	CHL	6	601	1	-	0/15/153/177	0/0/9/9
25	CLA	6	602	1	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	6	603	1	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	6	604	-	2/2/16/25	0/11/111/135	0/0/9/9
24	CHL	6	605	1	-	0/15/153/177	0/0/9/9
24	CHL	6	606	-	-	0/15/153/177	0/0/9/9
24	CHL	6	607	-	-	0/35/171/177	0/0/9/9
24	CHL	6	608	-	-	0/15/153/177	0/0/9/9
24	CHL	6	609	1	-	0/35/171/177	0/0/9/9
25	CLA	6	610	1	3/3/17/25	0/19/117/135	0/0/9/9
25	CLA	6	611	29	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	6	612	1	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	6	613	1	2/2/16/25	0/11/111/135	0/0/9/9
25	CLA	6	614	1	2/2/16/25	0/11/111/135	0/0/9/9
26	LUT	7	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	7	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	7	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	7	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	7	2630	25	-	0/51/51/53	0/0/0/0
24	CHL	7	601	2	-	0/39/175/177	0/0/9/9
25	CLA	7	602	2	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	7	603	2	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	7	604	-	3/3/16/25	0/11/111/135	0/0/9/9
24	CHL	7	605	2	-	0/15/153/177	0/0/9/9
24	CHL	7	606	-	-	0/15/153/177	0/0/9/9
24	CHL	7	607	-	-	0/26/162/177	0/0/9/9
24	CHL	7	608	-	-	0/15/153/177	0/0/9/9
24	CHL	7	609	2	-	0/35/171/177	0/0/9/9
25	CLA	7	610	2	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	CLA	7	611	29	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	7	612	2	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	7	613	2	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	7	614	2	3/3/16/25	0/17/115/135	0/0/9/9
29	LHG	8	2630	25	-	0/23/23/53	0/0/0/0
24	CHL	8	601	3	-	0/9/151/177	0/0/9/9
25	CLA	8	602	3	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	8	603	3	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	8	604	-	2/2/16/25	0/11/111/135	0/0/9/9
24	CHL	8	606	-	-	0/15/153/177	0/0/9/9
24	CHL	8	607	-	-	0/15/153/177	0/0/9/9
24	CHL	8	608	-	-	0/15/153/177	0/0/9/9
24	CHL	8	609	3	-	0/15/153/177	0/0/9/9
25	CLA	8	610	3	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	8	611	29	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	8	612	3	3/3/16/25	0/11/111/135	0/0/9/9
26	LUT	8	620	-	-	0/29/67/67	0/2/2/2
27	XAT	8	622	-	-	0/31/93/93	0/2/4/4
30	BCR	8	623	-	-	0/29/63/63	0/2/2/2
31	OEX	A	401	4,6	-	0/0/68/68	0/0/6/6
25	CLA	A	405	4	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	406	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	A	407	-	3/3/17/25	0/19/117/135	0/0/9/9
33	PHO	A	408	-	-	0/53/103/103	0/1/6/6
33	PHO	A	409	-	-	0/53/103/103	0/1/6/6
25	CLA	A	410	4	3/3/19/25	0/31/129/135	0/0/9/9
30	BCR	A	411	-	-	0/29/63/63	0/2/2/2
34	SQD	A	412	-	-	0/45/65/69	0/1/1/1
35	LMG	A	413	-	-	0/43/63/70	0/1/1/1
36	PL9	A	414	-	-	0/5/18/73	0/1/1/1
35	LMG	A	415	-	-	0/35/55/70	0/1/1/1
34	SQD	A	418	-	-	0/49/69/69	0/1/1/1
29	LHG	B	2630	-	-	0/51/51/53	0/0/0/0
29	LHG	B	2631	-	-	0/53/53/53	0/0/0/0
35	LMG	B	2633	-	-	0/50/70/70	0/1/1/1
25	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	603	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	604	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
25	CLA	B	605	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	606	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	607	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	609	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	610	5	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	612	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	613	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	614	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	615	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	616	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	B	617	5	3/3/20/25	0/37/135/135	0/0/9/9
30	BCR	B	618	-	-	0/29/63/63	0/2/2/2
30	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	BCR	B	620	-	-	0/29/63/63	0/2/2/2
34	SQD	B	621	-	-	0/49/69/69	0/1/1/1
35	LMG	B	622	-	-	0/46/66/70	0/1/1/1
34	SQD	B	623	-	-	0/37/57/69	0/1/1/1
37	DGD	B	626	-	-	0/48/88/95	0/2/2/2
29	LHG	C	2630	-	-	0/53/53/53	0/0/0/0
25	CLA	C	501	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	502	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	503	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	505	6	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	506	6	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	508	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	509	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	510	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	511	6	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	C	512	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	C	513	6	2/2/20/25	0/37/135/135	0/0/9/9
30	BCR	C	514	-	-	0/29/63/63	0/2/2/2
30	BCR	C	515	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	BCR	C	516	-	-	0/29/63/63	0/2/2/2
30	BCR	C	517	-	-	0/29/63/63	0/2/2/2
37	DGD	C	518	-	-	0/44/84/95	0/2/2/2
37	DGD	C	519	-	-	0/51/91/95	0/2/2/2
37	DGD	C	520	-	-	0/49/89/95	0/2/2/2
35	LMG	C	521	-	-	0/46/66/70	0/1/1/1
29	LHG	C	522	-	-	0/53/53/53	0/0/0/0
29	LHG	C	523	-	-	0/53/53/53	0/0/0/0
38	BCT	D	401	32	-	0/0/0/0	0/0/0/0
25	CLA	D	402	7	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	D	403	7	2/2/20/25	0/37/135/135	0/0/9/9
30	BCR	D	404	-	-	0/29/63/63	0/2/2/2
36	PL9	D	405	-	-	0/53/73/73	0/1/1/1
29	LHG	D	408	-	-	0/50/50/53	0/0/0/0
29	LHG	D	409	-	-	0/53/53/53	0/0/0/0
29	LHG	D	410	-	-	0/47/47/53	0/0/0/0
35	LMG	D	411	-	-	0/41/61/70	0/1/1/1
39	HEM	F	101	9,8	-	0/6/54/54	0/0/8/8
26	LUT	G	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	G	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	G	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	G	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	G	2630	25	-	0/53/53/53	0/0/0/0
24	CHL	G	601	1	-	0/41/177/177	0/0/9/9
25	CLA	G	602	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	G	603	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	G	604	-	2/2/17/25	0/19/117/135	0/0/9/9
24	CHL	G	605	1	-	0/15/153/177	0/0/9/9
24	CHL	G	606	-	-	0/22/158/177	0/0/9/9
24	CHL	G	607	-	-	0/41/177/177	0/0/9/9
24	CHL	G	608	-	-	0/41/177/177	0/0/9/9
24	CHL	G	609	1	-	0/35/171/177	0/0/9/9
25	CLA	G	610	1	3/3/19/25	0/36/134/135	0/0/9/9
25	CLA	G	611	29	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	G	612	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	G	613	1	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	G	614	1	3/3/16/25	0/17/115/135	0/0/9/9
30	BCR	H	101	-	-	0/29/63/63	0/2/2/2
37	DGD	H	102	-	-	0/51/91/95	0/2/2/2
29	LHG	L	101	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	N	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	N	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	N	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	N	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	N	2630	25	-	0/53/53/53	0/0/0/0
24	CHL	N	601	1	-	0/41/177/177	0/0/9/9
25	CLA	N	602	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	N	603	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	N	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	N	605	1	-	0/20/156/177	0/0/9/9
24	CHL	N	606	-	-	0/22/158/177	0/0/9/9
24	CHL	N	607	-	-	0/41/177/177	0/0/9/9
24	CHL	N	608	-	-	0/41/177/177	0/0/9/9
24	CHL	N	609	1	-	0/41/177/177	0/0/9/9
25	CLA	N	610	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	N	611	29	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	N	612	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	N	613	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	N	614	1	3/3/16/25	0/17/115/135	0/0/9/9
29	LHG	R	2630	25	-	0/46/46/53	0/0/0/0
25	CLA	R	601	17	3/3/16/25	0/18/116/135	0/0/9/9
25	CLA	R	602	17	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	R	603	17	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	R	604	-	3/3/16/25	0/17/115/135	0/0/9/9
24	CHL	R	606	-	-	0/41/177/177	0/0/9/9
24	CHL	R	607	-	-	0/29/165/177	0/0/9/9
24	CHL	R	608	-	-	0/35/171/177	0/0/9/9
25	CLA	R	609	17	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	R	610	17	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	R	611	29	3/3/16/25	0/18/116/135	0/0/9/9
25	CLA	R	612	17	3/3/16/25	0/18/116/135	0/0/9/9
25	CLA	R	613	17	3/3/19/25	0/31/129/135	0/0/9/9
24	CHL	R	614	17	-	0/12/148/177	0/0/9/9
25	CLA	R	616	17	2/2/16/25	0/11/111/135	0/0/9/9
26	LUT	R	620	-	-	0/29/67/67	0/2/2/2
27	XAT	R	622	-	-	0/31/93/93	0/2/4/4
28	NEX	R	623	-	-	0/27/83/83	0/2/3/3
26	LUT	S	1620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
28	NEX	S	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	S	2630	25	-	0/53/53/53	0/0/0/0
24	CHL	S	601	18	-	0/15/153/177	0/0/9/9
25	CLA	S	602	18	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	S	603	18	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	S	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	S	606	-	-	1/15/153/177	0/0/9/9
24	CHL	S	607	-	-	0/32/168/177	0/0/9/9
24	CHL	S	608	-	-	0/15/153/177	0/0/9/9
25	CLA	S	609	18	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	S	610	18	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	S	611	29	3/3/18/25	0/27/125/135	0/0/9/9
25	CLA	S	612	18	3/3/16/25	0/18/116/135	0/0/9/9
25	CLA	S	613	18	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	S	614	18	3/3/16/25	0/18/116/135	0/0/9/9
30	BCR	T	101	-	-	0/29/63/63	0/2/2/2
26	LUT	Y	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	Y	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	Y	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	Y	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	Y	2630	25	-	0/53/53/53	0/0/0/0
24	CHL	Y	601	1	-	0/41/177/177	0/0/9/9
25	CLA	Y	602	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	Y	603	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	Y	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	Y	605	1	-	0/20/156/177	0/0/9/9
24	CHL	Y	606	-	-	0/22/158/177	0/0/9/9
24	CHL	Y	607	-	-	0/41/177/177	0/0/9/9
24	CHL	Y	608	-	-	0/41/177/177	0/0/9/9
24	CHL	Y	609	1	-	0/41/177/177	0/0/9/9
25	CLA	Y	610	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	Y	611	29	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	Y	612	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	Y	613	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	Y	614	1	3/3/16/25	0/17/115/135	0/0/9/9
35	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
31	OEX	a	401	4,6	-	0/0/68/68	0/0/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	a	405	4	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	a	407	-	3/3/17/25	0/19/117/135	0/0/9/9
33	PHO	a	408	-	-	0/53/103/103	0/1/6/6
33	PHO	a	409	-	-	0/53/103/103	0/1/6/6
25	CLA	a	410	4	3/3/19/25	0/31/129/135	0/0/9/9
30	BCR	a	411	-	-	0/29/63/63	0/2/2/2
34	SQD	a	412	-	-	0/45/65/69	0/1/1/1
35	LMG	a	413	-	-	0/43/63/70	0/1/1/1
36	PL9	a	414	-	-	0/5/18/73	0/1/1/1
35	LMG	a	415	-	-	0/35/55/70	0/1/1/1
34	SQD	a	418	-	-	0/49/69/69	0/1/1/1
29	LHG	b	2630	-	-	0/51/51/53	0/0/0/0
29	LHG	b	2631	-	-	0/53/53/53	0/0/0/0
35	LMG	b	2633	-	-	0/50/70/70	0/1/1/1
25	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	603	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	604	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	605	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	606	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	607	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	609	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	610	5	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	612	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	613	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	614	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	615	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	616	5	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	b	617	5	3/3/20/25	0/37/135/135	0/0/9/9
30	BCR	b	618	-	-	0/29/63/63	0/2/2/2
30	BCR	b	619	-	-	0/29/63/63	0/2/2/2
30	BCR	b	620	-	-	0/29/63/63	0/2/2/2
34	SQD	b	621	-	-	0/49/69/69	0/1/1/1
35	LMG	b	622	-	-	0/46/66/70	0/1/1/1
34	SQD	b	623	-	-	0/37/57/69	0/1/1/1
37	DGD	b	626	-	-	0/48/88/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	c	2630	-	-	0/53/53/53	0/0/0/0
25	CLA	c	501	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	502	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	503	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	505	6	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	506	6	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	508	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	509	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	510	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	511	6	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	c	512	6	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	c	513	6	2/2/20/25	0/37/135/135	0/0/9/9
30	BCR	c	514	-	-	0/29/63/63	0/2/2/2
30	BCR	c	515	-	-	0/29/63/63	0/2/2/2
30	BCR	c	516	-	-	0/29/63/63	0/2/2/2
30	BCR	c	517	-	-	0/29/63/63	0/2/2/2
37	DGD	c	518	-	-	0/44/84/95	0/2/2/2
37	DGD	c	519	-	-	0/51/91/95	0/2/2/2
37	DGD	c	520	-	-	0/49/89/95	0/2/2/2
35	LMG	c	521	-	-	0/46/66/70	0/1/1/1
29	LHG	c	522	-	-	0/53/53/53	0/0/0/0
29	LHG	c	523	-	-	0/53/53/53	0/0/0/0
38	BCT	d	401	32	-	0/0/0/0	0/0/0/0
25	CLA	d	402	7	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	d	403	7	2/2/20/25	0/37/135/135	0/0/9/9
30	BCR	d	404	-	-	0/29/63/63	0/2/2/2
36	PL9	d	405	-	-	0/53/73/73	0/1/1/1
29	LHG	d	408	-	-	0/50/50/53	0/0/0/0
29	LHG	d	409	-	-	0/53/53/53	0/0/0/0
29	LHG	d	410	-	-	0/47/47/53	0/0/0/0
35	LMG	d	411	-	-	0/41/61/70	0/1/1/1
39	HEM	f	101	9,8	-	0/6/54/54	0/0/8/8
26	LUT	g	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	g	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	g	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	g	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	g	2630	25	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	g	601	1	-	0/41/177/177	0/0/9/9
25	CLA	g	602	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	g	603	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	g	604	-	2/2/17/25	0/19/117/135	0/0/9/9
24	CHL	g	605	1	-	0/15/153/177	0/0/9/9
24	CHL	g	606	-	-	0/22/158/177	0/0/9/9
24	CHL	g	607	-	-	0/41/177/177	0/0/9/9
24	CHL	g	608	-	-	0/41/177/177	0/0/9/9
24	CHL	g	609	1	-	0/35/171/177	0/0/9/9
25	CLA	g	610	1	3/3/19/25	0/36/134/135	0/0/9/9
25	CLA	g	611	29	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	g	612	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	g	613	1	2/2/20/25	0/37/135/135	0/0/9/9
25	CLA	g	614	1	3/3/16/25	0/17/115/135	0/0/9/9
30	BCR	h	101	-	-	0/29/63/63	0/2/2/2
37	DGD	h	102	-	-	0/51/91/95	0/2/2/2
29	LHG	l	101	-	-	0/53/53/53	0/0/0/0
26	LUT	n	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	n	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	n	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	n	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	n	2630	25	-	0/53/53/53	0/0/0/0
24	CHL	n	601	1	-	0/41/177/177	0/0/9/9
25	CLA	n	602	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	n	603	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	n	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	n	605	1	-	0/20/156/177	0/0/9/9
24	CHL	n	606	-	-	0/22/158/177	0/0/9/9
24	CHL	n	607	-	-	0/41/177/177	0/0/9/9
24	CHL	n	608	-	-	0/41/177/177	0/0/9/9
24	CHL	n	609	1	-	0/41/177/177	0/0/9/9
25	CLA	n	610	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	n	611	29	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	n	612	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	n	613	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	n	614	1	3/3/16/25	0/17/115/135	0/0/9/9
29	LHG	r	2630	25	-	0/46/46/53	0/0/0/0
25	CLA	r	601	17	3/3/16/25	0/18/116/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	r	602	17	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	r	603	17	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	r	604	-	3/3/16/25	0/17/115/135	0/0/9/9
24	CHL	r	606	-	-	0/41/177/177	0/0/9/9
24	CHL	r	607	-	-	0/29/165/177	0/0/9/9
24	CHL	r	608	-	-	0/35/171/177	0/0/9/9
25	CLA	r	609	17	3/3/18/25	0/29/127/135	0/0/9/9
25	CLA	r	610	17	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	r	611	29	3/3/16/25	0/18/116/135	0/0/9/9
25	CLA	r	612	17	3/3/16/25	0/18/116/135	0/0/9/9
25	CLA	r	613	17	3/3/19/25	0/31/129/135	0/0/9/9
24	CHL	r	614	17	-	0/12/148/177	0/0/9/9
25	CLA	r	616	17	2/2/16/25	0/11/111/135	0/0/9/9
26	LUT	r	620	-	-	0/29/67/67	0/2/2/2
27	XAT	r	622	-	-	0/31/93/93	0/2/4/4
28	NEX	r	623	-	-	0/27/83/83	0/2/3/3
26	LUT	s	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	s	1621	-	-	0/29/67/67	0/2/2/2
28	NEX	s	1623	-	-	0/27/83/83	0/2/3/3
29	LHG	s	2630	25	-	0/53/53/53	0/0/0/0
24	CHL	s	601	18	-	0/15/153/177	0/0/9/9
25	CLA	s	602	18	3/3/19/25	0/33/131/135	0/0/9/9
25	CLA	s	603	18	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	s	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	s	606	-	-	1/15/153/177	0/0/9/9
24	CHL	s	607	-	-	0/32/168/177	0/0/9/9
24	CHL	s	608	-	-	0/15/153/177	0/0/9/9
25	CLA	s	609	18	3/3/16/25	0/11/111/135	0/0/9/9
25	CLA	s	610	18	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	s	611	29	3/3/18/25	0/27/125/135	0/0/9/9
25	CLA	s	612	18	3/3/16/25	0/18/116/135	0/0/9/9
25	CLA	s	613	18	3/3/18/25	0/25/123/135	0/0/9/9
25	CLA	s	614	18	3/3/16/25	0/18/116/135	0/0/9/9
30	BCR	t	101	-	-	0/29/63/63	0/2/2/2
26	LUT	y	1620	-	-	0/29/67/67	0/2/2/2
26	LUT	y	1621	-	-	0/29/67/67	0/2/2/2
27	XAT	y	1622	-	-	0/31/93/93	0/2/4/4
28	NEX	y	1623	-	-	0/27/83/83	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	y	2630	25	-	0/53/53/53	0/0/0/0
24	CHL	y	601	1	-	0/41/177/177	0/0/9/9
25	CLA	y	602	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	y	603	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	y	604	-	3/3/17/25	0/19/117/135	0/0/9/9
24	CHL	y	605	1	-	0/20/156/177	0/0/9/9
24	CHL	y	606	-	-	0/22/158/177	0/0/9/9
24	CHL	y	607	-	-	0/41/177/177	0/0/9/9
24	CHL	y	608	-	-	0/41/177/177	0/0/9/9
24	CHL	y	609	1	-	0/41/177/177	0/0/9/9
25	CLA	y	610	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	y	611	29	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	y	612	1	3/3/19/25	0/31/129/135	0/0/9/9
25	CLA	y	613	1	3/3/20/25	0/37/135/135	0/0/9/9
25	CLA	y	614	1	3/3/16/25	0/17/115/135	0/0/9/9
35	LMG	z	101	-	-	0/46/66/70	0/1/1/1

All (4253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	601	CHL	C3D-C4D	-20.84	1.31	1.54
24	y	601	CHL	C3D-C4D	-20.83	1.31	1.54
24	7	606	CHL	C3D-C4D	-20.57	1.31	1.54
24	3	606	CHL	C3D-C4D	-20.50	1.31	1.54
24	Y	609	CHL	C3D-C4D	-20.50	1.31	1.54
24	1	601	CHL	C3D-C4D	-20.49	1.31	1.54
24	y	609	CHL	C3D-C4D	-20.47	1.31	1.54
24	3	601	CHL	C3D-C4D	-20.45	1.31	1.54
24	7	601	CHL	C3D-C4D	-20.44	1.31	1.54
24	5	601	CHL	C3D-C4D	-20.43	1.31	1.54
24	5	608	CHL	C3D-C4D	-20.39	1.31	1.54
24	g	601	CHL	C3D-C4D	-20.39	1.31	1.54
24	G	601	CHL	C3D-C4D	-20.39	1.31	1.54
24	1	608	CHL	C3D-C4D	-20.37	1.31	1.54
24	5	609	CHL	C3D-C4D	-20.33	1.31	1.54
24	1	609	CHL	C3D-C4D	-20.32	1.31	1.54
24	n	608	CHL	C3D-C4D	-20.26	1.31	1.54
24	n	606	CHL	C3D-C4D	-20.23	1.31	1.54
24	N	608	CHL	C3D-C4D	-20.20	1.31	1.54
24	N	606	CHL	C3D-C4D	-20.20	1.31	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	608	CHL	C3D-C4D	-20.16	1.31	1.54
24	4	608	CHL	C3D-C4D	-20.15	1.31	1.54
24	y	608	CHL	C3D-C4D	-20.15	1.31	1.54
24	y	606	CHL	C3D-C4D	-20.11	1.31	1.54
24	Y	608	CHL	C3D-C4D	-20.10	1.31	1.54
24	Y	606	CHL	C3D-C4D	-20.08	1.31	1.54
24	n	601	CHL	C3D-C4D	-20.07	1.31	1.54
24	n	609	CHL	C3D-C4D	-20.07	1.31	1.54
24	N	609	CHL	C3D-C4D	-20.06	1.31	1.54
24	N	601	CHL	C3D-C4D	-20.06	1.31	1.54
24	R	608	CHL	C3D-C4D	-20.03	1.31	1.54
24	r	608	CHL	C3D-C4D	-20.02	1.32	1.54
24	6	601	CHL	C3D-C4D	-19.98	1.32	1.54
24	2	601	CHL	C3D-C4D	-19.97	1.32	1.54
24	3	609	CHL	C3D-C4D	-19.93	1.32	1.54
24	7	609	CHL	C3D-C4D	-19.88	1.32	1.54
24	g	609	CHL	C3D-C4D	-19.84	1.32	1.54
24	G	609	CHL	C3D-C4D	-19.82	1.32	1.54
24	1	606	CHL	C3D-C4D	-19.81	1.32	1.54
24	G	608	CHL	C3D-C4D	-19.79	1.32	1.54
24	5	605	CHL	C3D-C4D	-19.78	1.32	1.54
24	5	606	CHL	C3D-C4D	-19.78	1.32	1.54
24	3	608	CHL	C3D-C4D	-19.76	1.32	1.54
24	2	607	CHL	C3D-C4D	-19.75	1.32	1.54
24	g	608	CHL	C3D-C4D	-19.75	1.32	1.54
24	7	608	CHL	C3D-C4D	-19.74	1.32	1.54
24	g	606	CHL	C3D-C4D	-19.73	1.32	1.54
24	6	607	CHL	C3D-C4D	-19.73	1.32	1.54
24	G	606	CHL	C3D-C4D	-19.72	1.32	1.54
24	2	609	CHL	C3D-C4D	-19.71	1.32	1.54
24	1	605	CHL	C3D-C4D	-19.71	1.32	1.54
24	6	609	CHL	C3D-C4D	-19.70	1.32	1.54
24	r	606	CHL	C3D-C4D	-19.70	1.32	1.54
24	y	607	CHL	C3D-C4D	-19.68	1.32	1.54
24	7	607	CHL	C3D-C4D	-19.67	1.32	1.54
24	1	607	CHL	C3D-C4D	-19.66	1.32	1.54
24	Y	607	CHL	C3D-C4D	-19.65	1.32	1.54
24	R	606	CHL	C3D-C4D	-19.63	1.32	1.54
24	8	609	CHL	C3D-C4D	-19.59	1.32	1.54
24	5	607	CHL	C3D-C4D	-19.59	1.32	1.54
24	3	607	CHL	C3D-C4D	-19.59	1.32	1.54
24	r	607	CHL	C3D-C4D	-19.58	1.32	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	607	CHL	C3D-C4D	-19.58	1.32	1.54
24	Y	605	CHL	C3D-C4D	-19.58	1.32	1.54
24	y	605	CHL	C3D-C4D	-19.55	1.32	1.54
24	4	609	CHL	C3D-C4D	-19.54	1.32	1.54
24	N	605	CHL	C3D-C4D	-19.50	1.32	1.54
24	n	605	CHL	C3D-C4D	-19.49	1.32	1.54
24	2	606	CHL	C3D-C4D	-19.48	1.32	1.54
24	6	606	CHL	C3D-C4D	-19.43	1.32	1.54
24	8	607	CHL	C3D-C4D	-19.43	1.32	1.54
24	4	606	CHL	C3D-C4D	-19.43	1.32	1.54
24	8	606	CHL	C3D-C4D	-19.43	1.32	1.54
24	4	607	CHL	C3D-C4D	-19.43	1.32	1.54
24	R	614	CHL	C3D-C4D	-19.38	1.32	1.54
24	7	605	CHL	C3D-C4D	-19.37	1.32	1.54
24	g	607	CHL	C3D-C4D	-19.37	1.32	1.54
24	6	608	CHL	C3D-C4D	-19.36	1.32	1.54
24	r	614	CHL	C3D-C4D	-19.36	1.32	1.54
24	2	608	CHL	C3D-C4D	-19.34	1.32	1.54
24	G	607	CHL	C3D-C4D	-19.31	1.32	1.54
24	3	605	CHL	C3D-C4D	-19.30	1.32	1.54
24	s	601	CHL	C3D-C4D	-19.30	1.32	1.54
24	S	601	CHL	C3D-C4D	-19.29	1.32	1.54
24	g	605	CHL	C3D-C4D	-19.20	1.32	1.54
24	G	605	CHL	C3D-C4D	-19.16	1.32	1.54
24	N	607	CHL	C3D-C4D	-19.12	1.33	1.54
24	6	605	CHL	C3D-C4D	-19.11	1.33	1.54
24	n	607	CHL	C3D-C4D	-19.10	1.33	1.54
24	2	605	CHL	C3D-C4D	-19.09	1.33	1.54
24	S	608	CHL	C3D-C4D	-18.97	1.33	1.54
24	s	608	CHL	C3D-C4D	-18.94	1.33	1.54
24	4	601	CHL	C3D-C4D	-18.82	1.33	1.54
24	8	601	CHL	C3D-C4D	-18.78	1.33	1.54
24	S	606	CHL	C3D-C4D	-18.63	1.33	1.54
24	s	606	CHL	C3D-C4D	-18.61	1.33	1.54
24	s	607	CHL	C3D-C4D	-18.42	1.33	1.54
24	S	607	CHL	C3D-C4D	-18.40	1.33	1.54
24	5	609	CHL	CHB-C4A	-8.80	1.31	1.52
24	1	609	CHL	CHB-C4A	-8.79	1.31	1.52
24	7	606	CHL	CHB-C4A	-8.77	1.31	1.52
24	3	606	CHL	CHB-C4A	-8.76	1.31	1.52
24	N	609	CHL	CHB-C4A	-8.75	1.31	1.52
24	n	609	CHL	CHB-C4A	-8.75	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	608	CHL	CHB-C4A	-8.68	1.31	1.52
24	G	609	CHL	CHB-C4A	-8.68	1.31	1.52
24	g	609	CHL	CHB-C4A	-8.66	1.31	1.52
24	1	608	CHL	CHB-C4A	-8.66	1.31	1.52
24	y	609	CHL	CHB-C4A	-8.66	1.32	1.52
24	1	607	CHL	CHB-C4A	-8.65	1.32	1.52
24	Y	609	CHL	CHB-C4A	-8.65	1.32	1.52
24	5	607	CHL	CHB-C4A	-8.64	1.32	1.52
24	g	601	CHL	CHB-C4A	-8.64	1.32	1.52
24	G	601	CHL	CHB-C4A	-8.64	1.32	1.52
24	7	601	CHL	CHB-C4A	-8.63	1.32	1.52
24	3	601	CHL	CHB-C4A	-8.62	1.32	1.52
24	r	606	CHL	CHB-C4A	-8.62	1.32	1.52
24	R	606	CHL	CHB-C4A	-8.61	1.32	1.52
24	8	606	CHL	CHB-C4A	-8.58	1.32	1.52
24	4	606	CHL	CHB-C4A	-8.58	1.32	1.52
24	G	607	CHL	CHB-C4A	-8.56	1.32	1.52
24	n	605	CHL	CHB-C4A	-8.56	1.32	1.52
24	Y	601	CHL	CHB-C4A	-8.56	1.32	1.52
24	N	605	CHL	CHB-C4A	-8.55	1.32	1.52
24	y	601	CHL	CHB-C4A	-8.55	1.32	1.52
24	g	607	CHL	CHB-C4A	-8.55	1.32	1.52
24	7	609	CHL	CHB-C4A	-8.54	1.32	1.52
24	y	607	CHL	CHB-C4A	-8.53	1.32	1.52
24	3	609	CHL	CHB-C4A	-8.53	1.32	1.52
24	6	606	CHL	CHB-C4A	-8.51	1.32	1.52
24	Y	607	CHL	CHB-C4A	-8.51	1.32	1.52
24	2	606	CHL	CHB-C4A	-8.51	1.32	1.52
24	n	606	CHL	CHB-C4A	-8.49	1.32	1.52
24	1	608	CHL	C3B-C2B	-8.48	1.45	1.55
24	6	609	CHL	CHB-C4A	-8.47	1.32	1.52
24	8	609	CHL	CHB-C4A	-8.47	1.32	1.52
24	N	606	CHL	CHB-C4A	-8.47	1.32	1.52
24	5	608	CHL	C3B-C2B	-8.47	1.45	1.55
24	s	601	CHL	CHB-C4A	-8.46	1.32	1.52
24	S	601	CHL	CHB-C4A	-8.46	1.32	1.52
24	g	606	CHL	CHB-C4A	-8.46	1.32	1.52
24	2	609	CHL	CHB-C4A	-8.46	1.32	1.52
24	Y	608	CHL	CHB-C4A	-8.46	1.32	1.52
24	4	609	CHL	CHB-C4A	-8.46	1.32	1.52
24	2	607	CHL	CHB-C4A	-8.46	1.32	1.52
24	G	606	CHL	CHB-C4A	-8.45	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	607	CHL	CHB-C4A	-8.45	1.32	1.52
24	N	608	CHL	CHB-C4A	-8.44	1.32	1.52
24	n	608	CHL	CHB-C4A	-8.44	1.32	1.52
24	y	608	CHL	CHB-C4A	-8.44	1.32	1.52
24	3	607	CHL	CHB-C4A	-8.43	1.32	1.52
24	7	607	CHL	CHB-C4A	-8.41	1.32	1.52
24	5	606	CHL	CHB-C4A	-8.40	1.32	1.52
24	R	607	CHL	CHB-C4A	-8.40	1.32	1.52
24	1	606	CHL	CHB-C4A	-8.40	1.32	1.52
24	3	608	CHL	CHB-C4A	-8.40	1.32	1.52
24	7	608	CHL	CHB-C4A	-8.40	1.32	1.52
24	r	608	CHL	CHB-C4A	-8.39	1.32	1.52
24	7	605	CHL	CHB-C4A	-8.39	1.32	1.52
24	3	605	CHL	CHB-C4A	-8.39	1.32	1.52
24	y	605	CHL	CHB-C4A	-8.39	1.32	1.52
24	Y	605	CHL	CHB-C4A	-8.38	1.32	1.52
24	R	608	CHL	CHB-C4A	-8.38	1.32	1.52
24	r	607	CHL	CHB-C4A	-8.37	1.32	1.52
24	4	607	CHL	CHB-C4A	-8.35	1.32	1.52
24	5	609	CHL	C1B-NB	-8.35	1.32	1.50
24	2	605	CHL	CHB-C4A	-8.35	1.32	1.52
24	1	605	CHL	CHB-C4A	-8.34	1.32	1.52
24	6	605	CHL	CHB-C4A	-8.34	1.32	1.52
24	8	607	CHL	CHB-C4A	-8.34	1.32	1.52
24	5	605	CHL	CHB-C4A	-8.32	1.32	1.52
24	n	607	CHL	CHB-C4A	-8.32	1.32	1.52
24	2	601	CHL	CHB-C4A	-8.32	1.32	1.52
24	1	609	CHL	C1B-NB	-8.32	1.32	1.50
24	4	608	CHL	CHB-C4A	-8.31	1.32	1.52
24	N	607	CHL	CHB-C4A	-8.31	1.32	1.52
24	6	601	CHL	CHB-C4A	-8.31	1.32	1.52
24	y	606	CHL	CHB-C4A	-8.29	1.32	1.52
24	Y	606	CHL	CHB-C4A	-8.29	1.32	1.52
24	2	608	CHL	CHB-C4A	-8.29	1.32	1.52
24	8	608	CHL	CHB-C4A	-8.29	1.32	1.52
24	n	601	CHL	CHB-C4A	-8.28	1.32	1.52
24	6	608	CHL	CHB-C4A	-8.28	1.32	1.52
24	N	601	CHL	CHB-C4A	-8.27	1.32	1.52
24	N	609	CHL	C3B-C2B	-8.27	1.45	1.55
24	1	601	CHL	CHB-C4A	-8.26	1.32	1.52
24	r	614	CHL	CHB-C4A	-8.26	1.32	1.52
24	5	607	CHL	C3B-C2B	-8.26	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	607	CHL	C3B-C2B	-8.24	1.45	1.55
24	R	614	CHL	CHB-C4A	-8.24	1.33	1.52
24	n	609	CHL	C3B-C2B	-8.24	1.45	1.55
24	5	601	CHL	CHB-C4A	-8.23	1.33	1.52
24	G	608	CHL	CHB-C4A	-8.23	1.33	1.52
24	g	608	CHL	CHB-C4A	-8.23	1.33	1.52
24	8	601	CHL	CHB-C4A	-8.20	1.33	1.52
24	4	601	CHL	CHB-C4A	-8.18	1.33	1.52
24	Y	606	CHL	C3B-C2B	-8.16	1.45	1.55
24	n	609	CHL	C1B-NB	-8.15	1.32	1.50
24	G	605	CHL	CHB-C4A	-8.14	1.33	1.52
24	g	605	CHL	CHB-C4A	-8.13	1.33	1.52
24	y	606	CHL	C3B-C2B	-8.13	1.45	1.55
24	Y	607	CHL	C3B-C2B	-8.12	1.45	1.55
24	N	609	CHL	C1B-NB	-8.11	1.32	1.50
24	y	607	CHL	C3B-C2B	-8.10	1.45	1.55
24	S	607	CHL	CHB-C4A	-8.08	1.33	1.52
24	N	606	CHL	C3B-C2B	-8.06	1.45	1.55
24	s	607	CHL	CHB-C4A	-8.06	1.33	1.52
24	y	609	CHL	C1B-NB	-8.05	1.33	1.50
24	Y	606	CHL	C1B-NB	-8.05	1.33	1.50
24	n	606	CHL	C3B-C2B	-8.03	1.45	1.55
24	G	609	CHL	C1B-NB	-8.03	1.33	1.50
24	g	609	CHL	C3B-C2B	-8.03	1.45	1.55
24	g	609	CHL	C1B-NB	-8.03	1.33	1.50
24	Y	609	CHL	C1B-NB	-8.02	1.33	1.50
24	n	608	CHL	C3B-C2B	-8.02	1.45	1.55
24	N	608	CHL	C3B-C2B	-8.02	1.45	1.55
24	S	606	CHL	CHB-C4A	-8.02	1.33	1.52
24	s	606	CHL	CHB-C4A	-8.02	1.33	1.52
24	y	606	CHL	C1B-NB	-8.01	1.33	1.50
24	N	606	CHL	C1B-NB	-8.00	1.33	1.50
24	8	609	CHL	C3B-C2B	-8.00	1.45	1.55
24	n	606	CHL	C1B-NB	-7.99	1.33	1.50
24	G	607	CHL	C3B-C2B	-7.99	1.45	1.55
24	G	609	CHL	C3B-C2B	-7.99	1.45	1.55
24	g	607	CHL	C3B-C2B	-7.98	1.45	1.55
24	y	609	CHL	C3B-C2B	-7.98	1.45	1.55
24	4	609	CHL	C3B-C2B	-7.98	1.45	1.55
24	Y	609	CHL	C3B-C2B	-7.96	1.45	1.55
24	y	607	CHL	C1B-NB	-7.96	1.33	1.50
24	1	606	CHL	C1B-NB	-7.95	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	609	CHL	C4B-NB	-7.95	1.33	1.50
24	y	601	CHL	C3B-C2B	-7.95	1.45	1.55
24	Y	601	CHL	C3B-C2B	-7.94	1.45	1.55
24	Y	607	CHL	C1B-NB	-7.94	1.33	1.50
24	5	606	CHL	C1B-NB	-7.94	1.33	1.50
24	2	606	CHL	C3B-C2B	-7.93	1.45	1.55
24	5	609	CHL	C4B-NB	-7.93	1.33	1.50
24	7	601	CHL	C1B-NB	-7.93	1.33	1.50
24	3	601	CHL	C1B-NB	-7.93	1.33	1.50
24	S	608	CHL	CHB-C4A	-7.92	1.33	1.52
24	5	609	CHL	C3B-C2B	-7.92	1.45	1.55
24	3	601	CHL	C3B-C2B	-7.92	1.45	1.55
24	y	608	CHL	C3B-C2B	-7.91	1.45	1.55
24	s	608	CHL	CHB-C4A	-7.90	1.33	1.52
24	n	607	CHL	C3B-C2B	-7.90	1.45	1.55
24	Y	608	CHL	C3B-C2B	-7.90	1.45	1.55
24	3	609	CHL	C1B-NB	-7.89	1.33	1.50
24	6	606	CHL	C3B-C2B	-7.88	1.45	1.55
24	1	609	CHL	C3B-C2B	-7.88	1.45	1.55
24	7	609	CHL	C1B-NB	-7.86	1.33	1.50
24	R	606	CHL	C3B-C2B	-7.86	1.45	1.55
24	7	601	CHL	C3B-C2B	-7.86	1.45	1.55
24	7	607	CHL	C1B-NB	-7.86	1.33	1.50
24	r	606	CHL	C3B-C2B	-7.86	1.45	1.55
24	y	601	CHL	C1B-NB	-7.84	1.33	1.50
24	1	606	CHL	C3B-C2B	-7.84	1.45	1.55
24	N	607	CHL	C3B-C2B	-7.84	1.45	1.55
24	3	607	CHL	C1B-NB	-7.83	1.33	1.50
24	6	607	CHL	C4B-NB	-7.82	1.33	1.50
24	2	607	CHL	C4B-NB	-7.82	1.33	1.50
24	Y	601	CHL	C1B-NB	-7.82	1.33	1.50
24	6	609	CHL	C1B-NB	-7.82	1.33	1.50
24	5	606	CHL	C3B-C2B	-7.82	1.45	1.55
24	3	608	CHL	C3B-C2B	-7.81	1.45	1.55
24	2	609	CHL	C1B-NB	-7.81	1.33	1.50
24	5	601	CHL	C4B-NB	-7.81	1.33	1.50
24	g	601	CHL	C3B-C2B	-7.80	1.45	1.55
24	S	601	CHL	C3B-C2B	-7.80	1.45	1.55
24	N	605	CHL	C3B-C2B	-7.80	1.45	1.55
24	G	601	CHL	C3B-C2B	-7.79	1.45	1.55
24	5	606	CHL	C4B-NB	-7.78	1.33	1.50
24	1	601	CHL	C4B-NB	-7.78	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	608	CHL	C1B-NB	-7.78	1.33	1.50
24	1	606	CHL	C4B-NB	-7.76	1.33	1.50
24	G	606	CHL	C1B-NB	-7.76	1.33	1.50
24	N	607	CHL	C4B-NB	-7.75	1.33	1.50
24	7	608	CHL	C3B-C2B	-7.75	1.45	1.55
24	s	601	CHL	C3B-C2B	-7.75	1.45	1.55
24	7	609	CHL	C4B-NB	-7.75	1.33	1.50
24	g	606	CHL	C1B-NB	-7.75	1.33	1.50
24	y	605	CHL	C3B-C2B	-7.75	1.45	1.55
24	n	607	CHL	C4B-NB	-7.75	1.33	1.50
24	y	607	CHL	C4B-NB	-7.75	1.33	1.50
24	1	608	CHL	C1B-NB	-7.75	1.33	1.50
24	R	608	CHL	C3B-C2B	-7.75	1.45	1.55
24	7	601	CHL	C4B-NB	-7.74	1.33	1.50
24	r	608	CHL	C3B-C2B	-7.74	1.45	1.55
24	n	605	CHL	C3B-C2B	-7.74	1.45	1.55
24	R	608	CHL	C1B-NB	-7.74	1.33	1.50
24	Y	605	CHL	C3B-C2B	-7.74	1.45	1.55
24	r	608	CHL	C1B-NB	-7.73	1.33	1.50
24	3	601	CHL	C4B-NB	-7.73	1.33	1.50
24	3	609	CHL	C4B-NB	-7.73	1.33	1.50
24	Y	607	CHL	C4B-NB	-7.73	1.33	1.50
24	7	606	CHL	C3B-C2B	-7.72	1.45	1.55
24	3	606	CHL	C3B-C2B	-7.72	1.45	1.55
24	G	601	CHL	C1B-NB	-7.71	1.33	1.50
24	N	606	CHL	C4B-NB	-7.71	1.33	1.50
24	2	607	CHL	C1B-NB	-7.71	1.33	1.50
24	n	606	CHL	C4B-NB	-7.70	1.33	1.50
24	g	601	CHL	C1B-NB	-7.70	1.33	1.50
24	y	608	CHL	C1B-NB	-7.69	1.33	1.50
24	g	606	CHL	C4B-NB	-7.69	1.33	1.50
24	6	607	CHL	C1B-NB	-7.69	1.33	1.50
24	g	607	CHL	C4B-NB	-7.69	1.33	1.50
24	7	607	CHL	C3B-C2B	-7.69	1.46	1.55
24	N	607	CHL	C1B-NB	-7.68	1.33	1.50
24	n	607	CHL	C1B-NB	-7.68	1.33	1.50
24	g	609	CHL	C4B-NB	-7.68	1.33	1.50
24	n	609	CHL	C4B-NB	-7.67	1.33	1.50
24	G	609	CHL	C4B-NB	-7.67	1.33	1.50
24	7	606	CHL	C1B-NB	-7.67	1.33	1.50
24	G	606	CHL	C4B-NB	-7.67	1.33	1.50
24	Y	608	CHL	C1B-NB	-7.67	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	607	CHL	C1B-NB	-7.66	1.33	1.50
24	1	607	CHL	C1B-NB	-7.66	1.33	1.50
24	G	607	CHL	C4B-NB	-7.66	1.33	1.50
24	G	607	CHL	C1B-NB	-7.66	1.33	1.50
24	g	607	CHL	C1B-NB	-7.66	1.33	1.50
24	3	607	CHL	C3B-C2B	-7.66	1.46	1.55
24	N	608	CHL	C1B-NB	-7.65	1.33	1.50
24	N	609	CHL	C4B-NB	-7.65	1.33	1.50
24	2	606	CHL	C1B-NB	-7.65	1.33	1.50
24	3	606	CHL	C1B-NB	-7.65	1.33	1.50
24	6	606	CHL	C1B-NB	-7.64	1.33	1.50
24	n	608	CHL	C1B-NB	-7.64	1.33	1.50
24	Y	605	CHL	C4B-NB	-7.64	1.33	1.50
24	y	605	CHL	C4B-NB	-7.64	1.33	1.50
24	8	601	CHL	C4B-NB	-7.64	1.33	1.50
24	6	608	CHL	C3B-C2B	-7.63	1.46	1.55
24	R	606	CHL	C1B-NB	-7.63	1.33	1.50
24	4	601	CHL	C4B-NB	-7.63	1.33	1.50
24	y	605	CHL	C1B-NB	-7.62	1.33	1.50
24	4	606	CHL	C1B-NB	-7.62	1.33	1.50
24	Y	605	CHL	C1B-NB	-7.62	1.33	1.50
24	g	606	CHL	C3B-C2B	-7.61	1.46	1.55
24	3	606	CHL	C4B-NB	-7.61	1.34	1.50
24	2	608	CHL	C3B-C2B	-7.61	1.46	1.55
24	r	606	CHL	C1B-NB	-7.61	1.34	1.50
24	1	605	CHL	C4B-NB	-7.61	1.34	1.50
24	2	606	CHL	C4B-NB	-7.61	1.34	1.50
24	8	606	CHL	C1B-NB	-7.60	1.34	1.50
24	Y	609	CHL	C4B-NB	-7.60	1.34	1.50
24	7	606	CHL	C4B-NB	-7.60	1.34	1.50
24	6	606	CHL	C4B-NB	-7.60	1.34	1.50
24	8	608	CHL	C3B-C2B	-7.59	1.46	1.55
24	y	609	CHL	C4B-NB	-7.59	1.34	1.50
24	4	608	CHL	C3B-C2B	-7.59	1.46	1.55
24	7	608	CHL	C1B-NB	-7.59	1.34	1.50
24	1	601	CHL	C3B-C2B	-7.59	1.46	1.55
24	5	605	CHL	C4B-NB	-7.58	1.34	1.50
24	2	609	CHL	C4B-NB	-7.58	1.34	1.50
24	y	606	CHL	C4B-NB	-7.58	1.34	1.50
24	3	608	CHL	C1B-NB	-7.58	1.34	1.50
24	4	609	CHL	C4B-NB	-7.57	1.34	1.50
24	8	609	CHL	C4B-NB	-7.57	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	606	CHL	C4B-NB	-7.57	1.34	1.50
24	G	606	CHL	C3B-C2B	-7.57	1.46	1.55
24	6	609	CHL	C4B-NB	-7.57	1.34	1.50
24	N	601	CHL	C1B-NB	-7.56	1.34	1.50
24	n	601	CHL	C1B-NB	-7.56	1.34	1.50
24	6	609	CHL	C3B-C2B	-7.56	1.46	1.55
24	7	605	CHL	C1B-NB	-7.55	1.34	1.50
24	3	605	CHL	C1B-NB	-7.55	1.34	1.50
24	3	608	CHL	C4B-NB	-7.54	1.34	1.50
24	2	601	CHL	C1B-NB	-7.54	1.34	1.50
24	R	607	CHL	C1B-NB	-7.53	1.34	1.50
24	5	601	CHL	C3B-C2B	-7.53	1.46	1.55
24	1	607	CHL	C4B-NB	-7.53	1.34	1.50
24	r	607	CHL	C1B-NB	-7.53	1.34	1.50
24	5	607	CHL	C4B-NB	-7.52	1.34	1.50
24	7	608	CHL	C4B-NB	-7.52	1.34	1.50
24	n	605	CHL	C1B-NB	-7.52	1.34	1.50
24	8	609	CHL	C1B-NB	-7.52	1.34	1.50
24	N	605	CHL	C1B-NB	-7.52	1.34	1.50
24	6	601	CHL	C1B-NB	-7.52	1.34	1.50
24	5	605	CHL	C1B-NB	-7.51	1.34	1.50
24	8	606	CHL	C3B-C2B	-7.51	1.46	1.55
24	7	605	CHL	C4B-NB	-7.51	1.34	1.50
24	R	614	CHL	C4B-NB	-7.51	1.34	1.50
24	r	614	CHL	C4B-NB	-7.51	1.34	1.50
24	3	605	CHL	C4B-NB	-7.50	1.34	1.50
24	4	609	CHL	C1B-NB	-7.49	1.34	1.50
24	2	609	CHL	C3B-C2B	-7.49	1.46	1.55
24	1	605	CHL	C1B-NB	-7.49	1.34	1.50
24	8	608	CHL	C1B-NB	-7.48	1.34	1.50
24	5	601	CHL	C1B-NB	-7.48	1.34	1.50
24	4	608	CHL	C1B-NB	-7.48	1.34	1.50
24	4	601	CHL	C1B-NB	-7.47	1.34	1.50
24	2	601	CHL	C4B-NB	-7.47	1.34	1.50
24	1	601	CHL	C1B-NB	-7.47	1.34	1.50
24	8	607	CHL	C1B-NB	-7.47	1.34	1.50
24	R	607	CHL	C3B-C2B	-7.47	1.46	1.55
24	8	601	CHL	C1B-NB	-7.46	1.34	1.50
24	4	607	CHL	C1B-NB	-7.46	1.34	1.50
24	4	607	CHL	C4B-NB	-7.46	1.34	1.50
24	6	601	CHL	C4B-NB	-7.46	1.34	1.50
24	6	608	CHL	C1B-NB	-7.46	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	606	CHL	C3B-C2B	-7.45	1.46	1.55
24	R	607	CHL	C4B-NB	-7.44	1.34	1.50
24	r	607	CHL	C3B-C2B	-7.44	1.46	1.55
24	8	607	CHL	C4B-NB	-7.43	1.34	1.50
24	S	608	CHL	C4B-NB	-7.43	1.34	1.50
24	y	601	CHL	C4B-NB	-7.43	1.34	1.50
24	r	607	CHL	C4B-NB	-7.42	1.34	1.50
24	G	608	CHL	C1B-NB	-7.42	1.34	1.50
24	5	608	CHL	C4B-NB	-7.42	1.34	1.50
24	g	608	CHL	C1B-NB	-7.42	1.34	1.50
24	2	608	CHL	C1B-NB	-7.41	1.34	1.50
24	R	608	CHL	C4B-NB	-7.41	1.34	1.50
24	s	608	CHL	C4B-NB	-7.41	1.34	1.50
24	r	608	CHL	C4B-NB	-7.40	1.34	1.50
24	r	606	CHL	C4B-NB	-7.40	1.34	1.50
24	1	608	CHL	C4B-NB	-7.39	1.34	1.50
24	Y	601	CHL	C4B-NB	-7.39	1.34	1.50
24	R	606	CHL	C4B-NB	-7.39	1.34	1.50
24	2	605	CHL	C4B-NB	-7.38	1.34	1.50
24	G	605	CHL	C1B-NB	-7.38	1.34	1.50
24	S	607	CHL	C1B-NB	-7.38	1.34	1.50
24	s	607	CHL	C1B-NB	-7.38	1.34	1.50
24	g	605	CHL	C1B-NB	-7.37	1.34	1.50
24	n	605	CHL	C4B-NB	-7.37	1.34	1.50
24	2	608	CHL	C4B-NB	-7.37	1.34	1.50
24	y	608	CHL	C4B-NB	-7.36	1.34	1.50
24	6	608	CHL	C4B-NB	-7.36	1.34	1.50
24	N	605	CHL	C4B-NB	-7.36	1.34	1.50
24	Y	608	CHL	C4B-NB	-7.35	1.34	1.50
24	n	601	CHL	C4B-NB	-7.35	1.34	1.50
24	2	605	CHL	C1B-NB	-7.34	1.34	1.50
24	3	607	CHL	C4B-NB	-7.34	1.34	1.50
24	6	605	CHL	C4B-NB	-7.33	1.34	1.50
24	N	601	CHL	C4B-NB	-7.33	1.34	1.50
24	3	605	CHL	C3B-C2B	-7.33	1.46	1.55
24	6	605	CHL	C1B-NB	-7.33	1.34	1.50
24	7	607	CHL	C4B-NB	-7.32	1.34	1.50
24	7	605	CHL	C3B-C2B	-7.32	1.46	1.55
24	8	608	CHL	C4B-NB	-7.30	1.34	1.50
24	s	606	CHL	C1B-NB	-7.30	1.34	1.50
24	8	607	CHL	C3B-C2B	-7.30	1.46	1.55
24	G	601	CHL	C4B-NB	-7.29	1.34	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	601	CHL	C1B-NB	-7.29	1.34	1.50
24	1	605	CHL	C3B-C2B	-7.28	1.46	1.55
24	S	606	CHL	C1B-NB	-7.28	1.34	1.50
24	6	601	CHL	C3B-C2B	-7.27	1.46	1.55
24	s	601	CHL	C1B-NB	-7.27	1.34	1.50
24	5	605	CHL	C3B-C2B	-7.26	1.46	1.55
24	g	601	CHL	C4B-NB	-7.26	1.34	1.50
24	4	608	CHL	C4B-NB	-7.26	1.34	1.50
24	g	605	CHL	C4B-NB	-7.26	1.34	1.50
24	n	608	CHL	C4B-NB	-7.26	1.34	1.50
24	2	601	CHL	C3B-C2B	-7.25	1.46	1.55
24	N	601	CHL	C3B-C2B	-7.25	1.46	1.55
24	N	608	CHL	C4B-NB	-7.24	1.34	1.50
24	4	607	CHL	C3B-C2B	-7.23	1.46	1.55
24	s	608	CHL	C1B-NB	-7.23	1.34	1.50
24	G	605	CHL	C4B-NB	-7.23	1.34	1.50
24	S	608	CHL	C1B-NB	-7.22	1.34	1.50
24	2	607	CHL	C3B-C2B	-7.22	1.46	1.55
24	Y	606	CHL	C1D-ND	-7.22	1.34	1.50
24	y	606	CHL	C1D-ND	-7.22	1.34	1.50
24	s	607	CHL	C4B-NB	-7.21	1.34	1.50
24	6	607	CHL	C3B-C2B	-7.19	1.46	1.55
24	g	608	CHL	C3B-C2B	-7.19	1.46	1.55
24	g	608	CHL	C4B-NB	-7.19	1.34	1.50
24	r	614	CHL	C1B-NB	-7.18	1.34	1.50
24	S	607	CHL	C4B-NB	-7.18	1.34	1.50
24	G	608	CHL	C3B-C2B	-7.18	1.46	1.55
24	n	601	CHL	C3B-C2B	-7.18	1.46	1.55
24	G	608	CHL	C4B-NB	-7.17	1.34	1.50
24	R	614	CHL	C1B-NB	-7.17	1.34	1.50
24	1	605	CHL	C1D-ND	-7.17	1.34	1.50
24	n	606	CHL	C1D-ND	-7.16	1.34	1.50
24	5	605	CHL	C1D-ND	-7.16	1.34	1.50
24	N	606	CHL	C1D-ND	-7.15	1.34	1.50
24	7	601	CHL	C1D-ND	-7.13	1.35	1.50
24	4	606	CHL	C4B-NB	-7.13	1.35	1.50
24	2	607	CHL	C1D-ND	-7.12	1.35	1.50
24	3	601	CHL	C1D-ND	-7.11	1.35	1.50
24	6	605	CHL	C3B-C2B	-7.11	1.46	1.55
24	3	608	CHL	C1D-ND	-7.11	1.35	1.50
24	8	606	CHL	C4B-NB	-7.11	1.35	1.50
24	6	607	CHL	C1D-ND	-7.11	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	608	CHL	C1D-ND	-7.10	1.35	1.50
24	7	609	CHL	C3B-C2B	-7.09	1.46	1.55
24	1	606	CHL	C1D-ND	-7.09	1.35	1.50
24	S	601	CHL	C4B-NB	-7.07	1.35	1.50
24	S	607	CHL	C3B-C2B	-7.07	1.46	1.55
24	g	605	CHL	C3B-C2B	-7.07	1.46	1.55
24	5	606	CHL	C1D-ND	-7.07	1.35	1.50
24	2	605	CHL	C3B-C2B	-7.07	1.46	1.55
24	r	614	CHL	C3B-C2B	-7.07	1.46	1.55
24	3	609	CHL	C3B-C2B	-7.07	1.46	1.55
24	G	605	CHL	C3B-C2B	-7.07	1.46	1.55
24	R	614	CHL	C3B-C2B	-7.06	1.46	1.55
24	s	601	CHL	C4B-NB	-7.05	1.35	1.50
24	s	607	CHL	C3B-C2B	-7.03	1.46	1.55
24	1	608	CHL	C1D-ND	-7.03	1.35	1.50
36	D	405	PL9	C3-C4	-7.02	1.37	1.49
36	d	405	PL9	C3-C4	-7.02	1.37	1.49
24	5	608	CHL	C1D-ND	-7.01	1.35	1.50
24	3	607	CHL	C1D-ND	-7.01	1.35	1.50
24	7	607	CHL	C1D-ND	-7.00	1.35	1.50
24	7	606	CHL	C1D-ND	-6.98	1.35	1.50
24	3	606	CHL	C1D-ND	-6.98	1.35	1.50
24	1	601	CHL	C1D-ND	-6.97	1.35	1.50
24	y	608	CHL	C1D-ND	-6.95	1.35	1.50
24	5	609	CHL	C1D-ND	-6.94	1.35	1.50
24	5	601	CHL	C1D-ND	-6.93	1.35	1.50
24	4	607	CHL	C1D-ND	-6.93	1.35	1.50
24	1	609	CHL	C1D-ND	-6.93	1.35	1.50
24	G	607	CHL	C1D-ND	-6.93	1.35	1.50
24	8	607	CHL	C1D-ND	-6.92	1.35	1.50
24	g	607	CHL	C1D-ND	-6.92	1.35	1.50
24	Y	608	CHL	C1D-ND	-6.92	1.35	1.50
24	Y	601	CHL	C1D-ND	-6.92	1.35	1.50
24	y	609	CHL	C1D-ND	-6.92	1.35	1.50
24	N	607	CHL	C1D-ND	-6.92	1.35	1.50
24	s	606	CHL	C3B-C2B	-6.91	1.46	1.55
24	6	609	CHL	C1D-ND	-6.90	1.35	1.50
24	y	601	CHL	C1D-ND	-6.90	1.35	1.50
24	y	607	CHL	C1D-ND	-6.90	1.35	1.50
24	n	601	CHL	C1D-ND	-6.90	1.35	1.50
24	2	606	CHL	C1D-ND	-6.90	1.35	1.50
24	6	606	CHL	C1D-ND	-6.90	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	609	CHL	C1D-ND	-6.89	1.35	1.50
24	S	606	CHL	C4B-NB	-6.89	1.35	1.50
24	n	607	CHL	C1D-ND	-6.89	1.35	1.50
24	N	608	CHL	C1D-ND	-6.89	1.35	1.50
24	N	601	CHL	C1D-ND	-6.89	1.35	1.50
24	n	608	CHL	C1D-ND	-6.88	1.35	1.50
24	g	601	CHL	C1D-ND	-6.88	1.35	1.50
24	3	605	CHL	C1D-ND	-6.88	1.35	1.50
24	s	606	CHL	C4B-NB	-6.87	1.35	1.50
24	8	606	CHL	C1D-ND	-6.87	1.35	1.50
24	S	606	CHL	C3B-C2B	-6.87	1.47	1.55
24	2	609	CHL	C1D-ND	-6.87	1.35	1.50
24	2	608	CHL	C1D-ND	-6.87	1.35	1.50
24	Y	607	CHL	C1D-ND	-6.86	1.35	1.50
24	6	608	CHL	C1D-ND	-6.86	1.35	1.50
24	r	606	CHL	C1D-ND	-6.86	1.35	1.50
24	7	605	CHL	C1D-ND	-6.85	1.35	1.50
24	7	609	CHL	C1D-ND	-6.85	1.35	1.50
24	4	606	CHL	C1D-ND	-6.85	1.35	1.50
24	G	601	CHL	C1D-ND	-6.85	1.35	1.50
24	R	606	CHL	C1D-ND	-6.84	1.35	1.50
24	R	608	CHL	C1D-ND	-6.83	1.35	1.50
24	y	605	CHL	C1D-ND	-6.83	1.35	1.50
24	g	609	CHL	C1D-ND	-6.82	1.35	1.50
24	g	606	CHL	C1D-ND	-6.82	1.35	1.50
24	G	606	CHL	C1D-ND	-6.82	1.35	1.50
24	r	608	CHL	C1D-ND	-6.80	1.35	1.50
24	G	609	CHL	C1D-ND	-6.80	1.35	1.50
24	3	609	CHL	C1D-ND	-6.80	1.35	1.50
24	r	614	CHL	C1D-ND	-6.80	1.35	1.50
24	Y	605	CHL	C1D-ND	-6.79	1.35	1.50
24	R	614	CHL	C1D-ND	-6.78	1.35	1.50
24	4	608	CHL	C1D-ND	-6.77	1.35	1.50
24	2	601	CHL	C1D-ND	-6.77	1.35	1.50
24	6	601	CHL	C1D-ND	-6.77	1.35	1.50
24	n	606	CHL	C3B-C4B	-6.76	1.46	1.54
24	1	608	CHL	C4D-ND	-6.75	1.35	1.50
24	5	608	CHL	C4D-ND	-6.75	1.35	1.50
24	R	608	CHL	C4D-ND	-6.74	1.35	1.50
24	8	608	CHL	C1D-ND	-6.74	1.35	1.50
24	2	605	CHL	C1D-ND	-6.73	1.35	1.50
24	r	608	CHL	C4D-ND	-6.73	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	608	CHL	C3B-C2B	-6.73	1.47	1.55
24	s	606	CHL	C1D-ND	-6.73	1.35	1.50
24	l	609	CHL	C4D-ND	-6.72	1.35	1.50
24	N	609	CHL	C1D-ND	-6.72	1.35	1.50
24	Y	608	CHL	C4D-ND	-6.72	1.35	1.50
24	r	607	CHL	C1D-ND	-6.72	1.35	1.50
24	N	606	CHL	C3B-C4B	-6.72	1.46	1.54
24	S	608	CHL	C3B-C2B	-6.72	1.47	1.55
24	y	608	CHL	C4D-ND	-6.72	1.35	1.50
24	R	607	CHL	C1D-ND	-6.72	1.35	1.50
24	6	605	CHL	C1D-ND	-6.71	1.35	1.50
24	l	601	CHL	C4D-ND	-6.70	1.35	1.50
24	5	609	CHL	C4D-ND	-6.70	1.35	1.50
24	N	605	CHL	C1D-ND	-6.70	1.35	1.50
24	n	605	CHL	C1D-ND	-6.70	1.35	1.50
24	S	606	CHL	C1D-ND	-6.70	1.35	1.50
24	5	601	CHL	C4D-ND	-6.69	1.35	1.50
24	n	609	CHL	C1D-ND	-6.69	1.35	1.50
24	g	608	CHL	C1D-ND	-6.69	1.35	1.50
24	4	608	CHL	C4D-ND	-6.68	1.35	1.50
24	8	608	CHL	C4D-ND	-6.68	1.36	1.50
24	s	601	CHL	C1D-ND	-6.68	1.36	1.50
24	G	608	CHL	C1D-ND	-6.67	1.36	1.50
24	S	601	CHL	C1D-ND	-6.67	1.36	1.50
24	4	601	CHL	C1D-ND	-6.66	1.36	1.50
24	3	608	CHL	C4D-ND	-6.66	1.36	1.50
24	n	606	CHL	C4D-ND	-6.66	1.36	1.50
24	N	606	CHL	C4D-ND	-6.65	1.36	1.50
24	5	607	CHL	C1D-ND	-6.65	1.36	1.50
24	l	605	CHL	C4D-ND	-6.65	1.36	1.50
24	8	601	CHL	C1D-ND	-6.64	1.36	1.50
24	l	607	CHL	C1D-ND	-6.64	1.36	1.50
24	5	605	CHL	C4D-ND	-6.64	1.36	1.50
24	7	608	CHL	C4D-ND	-6.64	1.36	1.50
24	Y	606	CHL	C4D-ND	-6.61	1.36	1.50
24	y	606	CHL	C3B-C4B	-6.60	1.46	1.54
24	Y	606	CHL	C3B-C4B	-6.59	1.46	1.54
24	y	606	CHL	C4D-ND	-6.58	1.36	1.50
24	y	601	CHL	C4D-ND	-6.57	1.36	1.50
24	g	605	CHL	C1D-ND	-6.57	1.36	1.50
24	G	605	CHL	C1D-ND	-6.57	1.36	1.50
24	Y	601	CHL	C4D-ND	-6.56	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	609	CHL	C4D-ND	-6.55	1.36	1.50
24	S	607	CHL	C1D-ND	-6.54	1.36	1.50
24	s	607	CHL	C1D-ND	-6.54	1.36	1.50
24	7	609	CHL	C4D-ND	-6.53	1.36	1.50
24	N	608	CHL	C4D-ND	-6.53	1.36	1.50
24	4	609	CHL	C1D-ND	-6.53	1.36	1.50
24	n	608	CHL	C4D-ND	-6.53	1.36	1.50
24	y	607	CHL	C4D-ND	-6.51	1.36	1.50
24	8	609	CHL	C1D-ND	-6.50	1.36	1.50
24	Y	607	CHL	C4D-ND	-6.50	1.36	1.50
24	6	609	CHL	C4D-ND	-6.49	1.36	1.50
36	D	405	PL9	C7-C3	-6.49	1.44	1.51
24	2	609	CHL	C4D-ND	-6.48	1.36	1.50
24	6	608	CHL	C4D-ND	-6.47	1.36	1.50
36	d	405	PL9	C7-C3	-6.47	1.44	1.51
24	4	601	CHL	C3B-C2B	-6.46	1.47	1.55
24	2	608	CHL	C4D-ND	-6.46	1.36	1.50
24	7	601	CHL	C4D-ND	-6.45	1.36	1.50
24	R	606	CHL	C4D-ND	-6.45	1.36	1.50
24	3	601	CHL	C4D-ND	-6.45	1.36	1.50
24	n	607	CHL	C4D-ND	-6.45	1.36	1.50
24	4	606	CHL	C4D-ND	-6.43	1.36	1.50
24	N	607	CHL	C4D-ND	-6.43	1.36	1.50
24	r	606	CHL	C4D-ND	-6.42	1.36	1.50
24	3	606	CHL	C4D-ND	-6.42	1.36	1.50
24	4	609	CHL	C4D-ND	-6.42	1.36	1.50
24	G	609	CHL	C4D-ND	-6.42	1.36	1.50
24	8	606	CHL	C4D-ND	-6.41	1.36	1.50
24	8	609	CHL	C4D-ND	-6.41	1.36	1.50
24	8	607	CHL	C4D-ND	-6.41	1.36	1.50
24	g	609	CHL	C4D-ND	-6.40	1.36	1.50
24	G	607	CHL	C4D-ND	-6.40	1.36	1.50
24	n	601	CHL	C4D-ND	-6.39	1.36	1.50
24	7	606	CHL	C4D-ND	-6.39	1.36	1.50
24	g	607	CHL	C4D-ND	-6.39	1.36	1.50
24	N	601	CHL	C4D-ND	-6.39	1.36	1.50
24	8	601	CHL	C3B-C2B	-6.38	1.47	1.55
24	n	609	CHL	C4D-ND	-6.38	1.36	1.50
24	2	607	CHL	C4D-ND	-6.37	1.36	1.50
24	2	601	CHL	C4D-ND	-6.37	1.36	1.50
24	4	607	CHL	C4D-ND	-6.37	1.36	1.50
24	5	607	CHL	C4D-ND	-6.37	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	608	CHL	C4D-ND	-6.37	1.36	1.50
24	G	601	CHL	C4D-ND	-6.36	1.36	1.50
24	6	607	CHL	C4D-ND	-6.36	1.36	1.50
24	1	606	CHL	C4D-ND	-6.36	1.36	1.50
24	g	608	CHL	C4D-ND	-6.36	1.36	1.50
24	Y	605	CHL	C4D-ND	-6.36	1.36	1.50
24	6	601	CHL	C4D-ND	-6.36	1.36	1.50
24	Y	609	CHL	C4D-ND	-6.36	1.36	1.50
24	1	607	CHL	C4D-ND	-6.35	1.36	1.50
24	y	605	CHL	C4D-ND	-6.35	1.36	1.50
24	g	601	CHL	C4D-ND	-6.35	1.36	1.50
24	y	609	CHL	C4D-ND	-6.35	1.36	1.50
24	N	609	CHL	C4D-ND	-6.35	1.36	1.50
24	3	607	CHL	C4D-ND	-6.33	1.36	1.50
24	s	608	CHL	C1D-ND	-6.33	1.36	1.50
24	5	606	CHL	C4D-ND	-6.33	1.36	1.50
24	2	606	CHL	C4D-ND	-6.33	1.36	1.50
24	6	606	CHL	C4D-ND	-6.32	1.36	1.50
24	g	606	CHL	C4D-ND	-6.32	1.36	1.50
24	S	608	CHL	C1D-ND	-6.32	1.36	1.50
24	G	606	CHL	C4D-ND	-6.31	1.36	1.50
24	5	606	CHL	C3B-C4B	-6.30	1.47	1.54
24	7	607	CHL	C4D-ND	-6.30	1.36	1.50
24	2	606	CHL	C3B-C4B	-6.28	1.47	1.54
24	2	605	CHL	C4D-ND	-6.28	1.36	1.50
24	5	609	CHL	C3B-C4B	-6.28	1.47	1.54
24	6	606	CHL	C3B-C4B	-6.27	1.47	1.54
24	1	606	CHL	C3B-C4B	-6.27	1.47	1.54
24	n	607	CHL	C3B-C4B	-6.27	1.47	1.54
24	R	614	CHL	C4D-ND	-6.27	1.36	1.50
24	6	605	CHL	C4D-ND	-6.27	1.36	1.50
24	r	614	CHL	C4D-ND	-6.27	1.36	1.50
24	1	609	CHL	C3B-C4B	-6.26	1.47	1.54
24	N	607	CHL	C3B-C4B	-6.24	1.47	1.54
24	4	601	CHL	C4D-ND	-6.24	1.36	1.50
24	8	601	CHL	C4D-ND	-6.24	1.36	1.50
24	R	607	CHL	C4D-ND	-6.22	1.36	1.50
24	3	605	CHL	C4D-ND	-6.21	1.37	1.50
24	7	605	CHL	C4D-ND	-6.20	1.37	1.50
24	r	607	CHL	C4D-ND	-6.19	1.37	1.50
24	7	601	CHL	C3B-C4B	-6.17	1.47	1.54
24	6	607	CHL	C3B-C4B	-6.16	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	605	CHL	C4D-ND	-6.15	1.37	1.50
24	2	609	CHL	C3B-C4B	-6.15	1.47	1.54
24	1	601	CHL	C3B-C4B	-6.15	1.47	1.54
24	4	609	CHL	C3B-C4B	-6.15	1.47	1.54
24	8	609	CHL	C3B-C4B	-6.14	1.47	1.54
24	g	606	CHL	C3B-C4B	-6.13	1.47	1.54
24	3	601	CHL	C3B-C4B	-6.12	1.47	1.54
24	n	605	CHL	C4D-ND	-6.12	1.37	1.50
24	2	607	CHL	C3B-C4B	-6.12	1.47	1.54
24	5	601	CHL	C3B-C4B	-6.12	1.47	1.54
24	S	608	CHL	C4D-ND	-6.11	1.37	1.50
24	s	608	CHL	C4D-ND	-6.11	1.37	1.50
24	2	608	CHL	C3B-C4B	-6.09	1.47	1.54
24	6	609	CHL	C3B-C4B	-6.08	1.47	1.54
24	G	606	CHL	C3B-C4B	-6.07	1.47	1.54
24	g	605	CHL	C4D-ND	-6.06	1.37	1.50
24	S	601	CHL	C4D-ND	-6.04	1.37	1.50
24	n	609	CHL	C3B-C4B	-6.03	1.47	1.54
24	G	605	CHL	C4D-ND	-6.03	1.37	1.50
24	Y	607	CHL	C3B-C4B	-6.03	1.47	1.54
24	N	609	CHL	C3B-C4B	-6.03	1.47	1.54
24	s	601	CHL	C4D-ND	-6.02	1.37	1.50
24	y	607	CHL	C3B-C4B	-6.01	1.47	1.54
24	6	608	CHL	C3B-C4B	-6.00	1.47	1.54
24	s	606	CHL	C4D-ND	-5.98	1.37	1.50
24	S	606	CHL	C4D-ND	-5.97	1.37	1.50
24	S	607	CHL	C4D-ND	-5.86	1.37	1.50
24	s	607	CHL	C4D-ND	-5.85	1.37	1.50
24	5	607	CHL	C4A-C3A	-5.85	1.46	1.53
24	1	607	CHL	C4A-C3A	-5.84	1.46	1.53
24	5	605	CHL	C3B-C4B	-5.83	1.47	1.54
24	3	608	CHL	C3B-C4B	-5.82	1.47	1.54
24	Y	605	CHL	C3B-C4B	-5.80	1.47	1.54
24	1	605	CHL	C3B-C4B	-5.80	1.47	1.54
24	7	608	CHL	C3B-C4B	-5.79	1.47	1.54
24	y	605	CHL	C3B-C4B	-5.77	1.47	1.54
24	G	609	CHL	C3B-C4B	-5.75	1.47	1.54
24	r	608	CHL	C3B-C4B	-5.74	1.47	1.54
24	R	608	CHL	CHD-C1D	-5.74	1.44	1.53
24	r	614	CHL	C3B-C4B	-5.73	1.47	1.54
24	R	608	CHL	C3B-C4B	-5.73	1.47	1.54
24	r	608	CHL	CHD-C1D	-5.73	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	609	CHL	C3B-C4B	-5.71	1.47	1.54
24	R	614	CHL	C3B-C4B	-5.66	1.47	1.54
24	g	605	CHL	C3B-C4B	-5.63	1.48	1.54
24	G	605	CHL	C3B-C4B	-5.59	1.48	1.54
24	7	608	CHL	CHD-C1D	-5.57	1.44	1.53
24	3	609	CHL	C3B-C4B	-5.56	1.48	1.54
24	3	605	CHL	C3B-C4B	-5.54	1.48	1.54
24	7	609	CHL	C3B-C4B	-5.53	1.48	1.54
24	3	601	CHL	C4A-C3A	-5.52	1.47	1.53
24	7	605	CHL	C3B-C4B	-5.52	1.48	1.54
24	2	605	CHL	C3B-C4B	-5.51	1.48	1.54
24	6	605	CHL	C3B-C4B	-5.50	1.48	1.54
24	3	608	CHL	CHD-C1D	-5.50	1.44	1.53
24	7	601	CHL	C4A-C3A	-5.48	1.47	1.53
24	Y	608	CHL	CHD-C1D	-5.47	1.44	1.53
24	y	608	CHL	CHD-C1D	-5.46	1.44	1.53
24	n	609	CHL	CHC-C4B	-5.45	1.44	1.53
24	Y	601	CHL	CHD-C1D	-5.44	1.44	1.53
24	G	607	CHL	C3B-C4B	-5.44	1.48	1.54
24	N	609	CHL	CHC-C4B	-5.43	1.44	1.53
24	y	601	CHL	CHD-C1D	-5.43	1.44	1.53
36	D	405	PL9	C6-C1	-5.39	1.39	1.48
24	8	607	CHL	C3B-C4B	-5.39	1.48	1.54
36	d	405	PL9	C6-C1	-5.39	1.39	1.48
24	y	606	CHL	CHD-C1D	-5.38	1.45	1.53
24	Y	606	CHL	CHD-C1D	-5.37	1.45	1.53
24	Y	609	CHL	C4A-C3A	-5.37	1.47	1.53
24	N	609	CHL	CHB-C1B	-5.37	1.45	1.53
24	n	609	CHL	CHB-C1B	-5.37	1.45	1.53
24	4	607	CHL	C3B-C4B	-5.37	1.48	1.54
24	g	607	CHL	C3B-C4B	-5.36	1.48	1.54
24	y	607	CHL	C4A-C3A	-5.34	1.47	1.53
24	y	609	CHL	C4A-C3A	-5.34	1.47	1.53
24	Y	607	CHL	C4A-C3A	-5.31	1.47	1.53
24	r	606	CHL	C3B-C4B	-5.30	1.48	1.54
24	Y	607	CHL	CHD-C1D	-5.30	1.45	1.53
24	Y	607	CHL	CHB-C1B	-5.29	1.45	1.53
24	R	606	CHL	C3B-C4B	-5.29	1.48	1.54
24	1	609	CHL	CHC-C4B	-5.28	1.45	1.53
24	Y	609	CHL	C3B-C4B	-5.28	1.48	1.54
24	4	608	CHL	CHD-C1D	-5.28	1.45	1.53
24	8	608	CHL	CHD-C1D	-5.26	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	607	CHL	CHD-C1D	-5.26	1.45	1.53
24	y	601	CHL	C4A-C3A	-5.26	1.47	1.53
24	y	607	CHL	CHB-C1B	-5.26	1.45	1.53
24	1	607	CHL	C3B-C4B	-5.25	1.48	1.54
24	N	607	CHL	CHD-C1D	-5.25	1.45	1.53
24	5	609	CHL	CHC-C4B	-5.25	1.45	1.53
24	N	609	CHL	C4A-C3A	-5.24	1.47	1.53
24	n	607	CHL	CHD-C1D	-5.23	1.45	1.53
24	g	609	CHL	CHC-C4B	-5.23	1.45	1.53
24	n	609	CHL	C4A-C3A	-5.23	1.47	1.53
24	7	601	CHL	CHD-C1D	-5.23	1.45	1.53
24	5	607	CHL	C3B-C4B	-5.22	1.48	1.54
24	N	605	CHL	C4A-C3A	-5.22	1.47	1.53
24	y	609	CHL	C3B-C4B	-5.22	1.48	1.54
24	n	605	CHL	C4A-C3A	-5.21	1.47	1.53
24	n	605	CHL	C3B-C4B	-5.21	1.48	1.54
24	3	601	CHL	CHD-C1D	-5.21	1.45	1.53
24	g	607	CHL	C4A-C3A	-5.20	1.47	1.53
24	s	607	CHL	C3B-C4B	-5.20	1.48	1.54
24	G	609	CHL	CHC-C4B	-5.19	1.45	1.53
24	N	608	CHL	CHD-C1D	-5.18	1.45	1.53
24	5	609	CHL	C4A-C3A	-5.17	1.47	1.53
24	5	608	CHL	CHD-C1D	-5.17	1.45	1.53
24	G	607	CHL	C4A-C3A	-5.17	1.47	1.53
24	n	608	CHL	CHD-C1D	-5.17	1.45	1.53
24	N	607	CHL	C4A-C3A	-5.16	1.47	1.53
24	Y	601	CHL	C4A-C3A	-5.15	1.47	1.53
24	n	607	CHL	C4A-C3A	-5.15	1.47	1.53
24	1	608	CHL	CHD-C1D	-5.15	1.45	1.53
24	N	605	CHL	C3B-C4B	-5.14	1.48	1.54
24	S	607	CHL	C3B-C4B	-5.13	1.48	1.54
24	1	609	CHL	C4A-C3A	-5.11	1.47	1.53
24	s	608	CHL	C3B-C4B	-5.10	1.48	1.54
24	G	601	CHL	C4A-C3A	-5.10	1.47	1.53
24	1	606	CHL	CHD-C1D	-5.10	1.45	1.53
24	g	601	CHL	C4A-C3A	-5.10	1.47	1.53
24	7	607	CHL	C4A-C3A	-5.07	1.47	1.53
24	3	601	CHL	CHB-C1B	-5.07	1.45	1.53
24	7	601	CHL	CHB-C1B	-5.07	1.45	1.53
24	3	607	CHL	C4A-C3A	-5.06	1.47	1.53
24	G	607	CHL	CHD-C1D	-5.06	1.45	1.53
24	8	608	CHL	C3B-C4B	-5.05	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	607	CHL	CHD-C1D	-5.05	1.45	1.53
24	n	607	CHL	CHB-C1B	-5.05	1.45	1.53
24	N	607	CHL	CHB-C1B	-5.05	1.45	1.53
24	5	606	CHL	CHD-C1D	-5.05	1.45	1.53
24	s	601	CHL	C3B-C4B	-5.04	1.48	1.54
24	y	601	CHL	C3B-C4B	-5.04	1.48	1.54
24	8	601	CHL	C3B-C4B	-5.04	1.48	1.54
24	4	608	CHL	C3B-C4B	-5.04	1.48	1.54
24	S	608	CHL	C3B-C4B	-5.03	1.48	1.54
24	Y	601	CHL	C3B-C4B	-5.01	1.48	1.54
24	4	601	CHL	C3B-C4B	-4.99	1.48	1.54
24	S	601	CHL	C3B-C4B	-4.99	1.48	1.54
24	4	606	CHL	C3B-C4B	-4.98	1.48	1.54
24	7	607	CHL	C3B-C4B	-4.98	1.48	1.54
24	3	607	CHL	C3B-C4B	-4.97	1.48	1.54
24	G	609	CHL	CHB-C1B	-4.97	1.45	1.53
24	g	609	CHL	CHB-C1B	-4.97	1.45	1.53
24	5	608	CHL	C3B-C4B	-4.97	1.48	1.54
24	8	606	CHL	C3B-C4B	-4.96	1.48	1.54
24	n	606	CHL	CHD-C1D	-4.96	1.45	1.53
24	1	607	CHL	CHB-C1B	-4.96	1.45	1.53
24	5	607	CHL	CHC-C4B	-4.95	1.45	1.53
24	2	601	CHL	C3B-C4B	-4.95	1.48	1.54
24	1	608	CHL	C3B-C4B	-4.95	1.48	1.54
24	6	601	CHL	C3B-C4B	-4.95	1.48	1.54
24	N	607	CHL	CHC-C4B	-4.94	1.45	1.53
24	n	607	CHL	CHC-C4B	-4.93	1.45	1.53
24	G	601	CHL	CHD-C1D	-4.93	1.45	1.53
24	N	606	CHL	CHD-C1D	-4.93	1.45	1.53
37	h	102	DGD	O2D-C2D	-4.93	1.31	1.43
24	6	608	CHL	CHD-C1D	-4.93	1.45	1.53
24	y	605	CHL	C4A-C3A	-4.93	1.47	1.53
24	N	601	CHL	CHD-C1D	-4.93	1.45	1.53
24	1	607	CHL	CHC-C4B	-4.92	1.45	1.53
24	5	607	CHL	CHB-C1B	-4.92	1.45	1.53
37	H	102	DGD	O2D-C2D	-4.92	1.31	1.43
24	G	608	CHL	CHD-C1D	-4.91	1.45	1.53
24	g	601	CHL	CHD-C1D	-4.91	1.45	1.53
24	n	601	CHL	CHD-C1D	-4.91	1.45	1.53
24	5	605	CHL	CHD-C1D	-4.91	1.45	1.53
24	8	609	CHL	CHD-C1D	-4.91	1.45	1.53
24	6	601	CHL	CHD-C1D	-4.91	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	608	CHL	CHD-C1D	-4.90	1.45	1.53
24	Y	605	CHL	C4A-C3A	-4.90	1.47	1.53
24	2	608	CHL	CHD-C1D	-4.90	1.45	1.53
24	Y	608	CHL	C3B-C4B	-4.90	1.48	1.54
24	g	607	CHL	CHB-C1B	-4.90	1.45	1.53
24	R	607	CHL	C3B-C4B	-4.88	1.48	1.54
24	y	608	CHL	C3B-C4B	-4.88	1.48	1.54
24	r	606	CHL	C4A-C3A	-4.88	1.48	1.53
24	2	606	CHL	C4A-C3A	-4.87	1.48	1.53
24	G	607	CHL	CHB-C1B	-4.87	1.45	1.53
24	2	601	CHL	CHD-C1D	-4.87	1.45	1.53
24	R	606	CHL	C4A-C3A	-4.87	1.48	1.53
24	3	605	CHL	CHD-C1D	-4.86	1.45	1.53
24	r	607	CHL	C3B-C4B	-4.86	1.48	1.54
24	1	605	CHL	CHD-C1D	-4.86	1.45	1.53
24	N	605	CHL	CHB-C1B	-4.85	1.45	1.53
24	G	601	CHL	CHB-C1B	-4.85	1.45	1.53
24	7	605	CHL	CHD-C1D	-4.85	1.45	1.53
24	4	609	CHL	CHD-C1D	-4.85	1.45	1.53
24	y	606	CHL	CHC-C4B	-4.85	1.45	1.53
24	6	606	CHL	C4A-C3A	-4.84	1.48	1.53
24	r	607	CHL	C4A-C3A	-4.84	1.48	1.53
24	R	606	CHL	CHB-C1B	-4.84	1.45	1.53
24	g	601	CHL	CHB-C1B	-4.84	1.45	1.53
24	5	601	CHL	CHD-C1D	-4.84	1.45	1.53
24	1	606	CHL	CHB-C1B	-4.83	1.45	1.53
24	1	601	CHL	CHD-C1D	-4.83	1.45	1.53
24	n	605	CHL	CHB-C1B	-4.83	1.45	1.53
24	g	606	CHL	CHB-C1B	-4.82	1.45	1.53
24	Y	606	CHL	CHC-C4B	-4.81	1.45	1.53
24	r	606	CHL	CHB-C1B	-4.81	1.45	1.53
24	Y	609	CHL	CHB-C1B	-4.80	1.45	1.53
24	G	606	CHL	CHB-C1B	-4.80	1.45	1.53
24	5	601	CHL	C4A-C3A	-4.79	1.48	1.53
24	5	606	CHL	CHB-C1B	-4.79	1.46	1.53
24	8	609	CHL	CHB-C1B	-4.78	1.46	1.53
24	r	606	CHL	CHD-C1D	-4.78	1.46	1.53
24	4	609	CHL	CHB-C1B	-4.78	1.46	1.53
24	6	605	CHL	CHD-C1D	-4.78	1.46	1.53
24	g	601	CHL	C3B-C4B	-4.77	1.48	1.54
24	7	607	CHL	CHD-C1D	-4.77	1.46	1.53
24	y	609	CHL	CHB-C1B	-4.77	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	605	CHL	CHC-C4B	-4.77	1.46	1.53
24	R	606	CHL	CHD-C1D	-4.76	1.46	1.53
24	2	605	CHL	CHD-C1D	-4.76	1.46	1.53
24	1	601	CHL	C4A-C3A	-4.76	1.48	1.53
24	3	607	CHL	CHD-C1D	-4.75	1.46	1.53
24	G	601	CHL	C3B-C4B	-4.75	1.48	1.54
24	R	607	CHL	C4A-C3A	-4.75	1.48	1.53
24	2	607	CHL	CHC-C4B	-4.75	1.46	1.53
24	7	606	CHL	C3B-C4B	-4.74	1.49	1.54
24	1	608	CHL	CHB-C1B	-4.74	1.46	1.53
24	Y	608	CHL	C4A-C3A	-4.73	1.48	1.53
24	5	608	CHL	CHB-C1B	-4.73	1.46	1.53
24	y	608	CHL	C4A-C3A	-4.72	1.48	1.53
24	N	601	CHL	C3B-C4B	-4.72	1.49	1.54
24	6	607	CHL	CHC-C4B	-4.72	1.46	1.53
24	6	609	CHL	CHD-C1D	-4.71	1.46	1.53
24	1	605	CHL	CHC-C4B	-4.71	1.46	1.53
24	3	601	CHL	CHC-C4B	-4.71	1.46	1.53
24	G	606	CHL	CHD-C1D	-4.71	1.46	1.53
24	3	606	CHL	CHB-C1B	-4.71	1.46	1.53
24	7	606	CHL	CHB-C1B	-4.70	1.46	1.53
24	S	601	CHL	CHB-C1B	-4.70	1.46	1.53
24	4	606	CHL	CHB-C1B	-4.70	1.46	1.53
24	8	606	CHL	CHD-C1D	-4.70	1.46	1.53
24	2	606	CHL	CHC-C4B	-4.70	1.46	1.53
24	g	606	CHL	CHD-C1D	-4.70	1.46	1.53
24	3	606	CHL	C3B-C4B	-4.70	1.49	1.54
24	8	607	CHL	C4A-C3A	-4.69	1.48	1.53
24	4	601	CHL	C4A-C3A	-4.69	1.48	1.53
24	n	601	CHL	C3B-C4B	-4.69	1.49	1.54
24	2	609	CHL	CHD-C1D	-4.69	1.46	1.53
24	7	601	CHL	CHC-C4B	-4.69	1.46	1.53
24	6	606	CHL	CHC-C4B	-4.69	1.46	1.53
24	N	606	CHL	CHC-C4B	-4.69	1.46	1.53
24	8	606	CHL	CHB-C1B	-4.69	1.46	1.53
24	Y	606	CHL	C4A-C3A	-4.68	1.48	1.53
24	s	601	CHL	CHB-C1B	-4.68	1.46	1.53
24	Y	609	CHL	CHC-C4B	-4.68	1.46	1.53
24	y	609	CHL	CHC-C4B	-4.68	1.46	1.53
24	8	601	CHL	C4A-C3A	-4.67	1.48	1.53
24	Y	605	CHL	CHB-C1B	-4.67	1.46	1.53
24	y	606	CHL	C4A-C3A	-4.67	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	605	CHL	CHB-C1B	-4.67	1.46	1.53
24	4	606	CHL	CHD-C1D	-4.66	1.46	1.53
24	n	606	CHL	CHC-C4B	-4.66	1.46	1.53
24	Y	601	CHL	CHB-C1B	-4.65	1.46	1.53
24	2	608	CHL	CHB-C1B	-4.65	1.46	1.53
24	n	608	CHL	CHB-C1B	-4.65	1.46	1.53
24	y	607	CHL	CHC-C4B	-4.65	1.46	1.53
24	G	607	CHL	CHC-C4B	-4.65	1.46	1.53
24	8	606	CHL	C4A-C3A	-4.65	1.48	1.53
24	g	607	CHL	CHC-C4B	-4.64	1.46	1.53
24	5	609	CHL	CHB-C1B	-4.64	1.46	1.53
24	s	607	CHL	C4A-C3A	-4.64	1.48	1.53
24	8	609	CHL	C4A-C3A	-4.64	1.48	1.53
24	N	609	CHL	CHC-C1C	-4.64	1.44	1.53
24	y	601	CHL	CHB-C1B	-4.64	1.46	1.53
24	Y	607	CHL	CHC-C4B	-4.64	1.46	1.53
24	6	608	CHL	CHB-C1B	-4.63	1.46	1.53
24	Y	605	CHL	CHD-C1D	-4.63	1.46	1.53
24	y	605	CHL	CHD-C1D	-4.63	1.46	1.53
24	5	601	CHL	CHC-C4B	-4.63	1.46	1.53
24	y	605	CHL	CHC-C4B	-4.63	1.46	1.53
24	5	607	CHL	CHD-C1D	-4.63	1.46	1.53
24	1	609	CHL	CHB-C1B	-4.62	1.46	1.53
24	n	609	CHL	CHC-C1C	-4.62	1.45	1.53
24	1	601	CHL	CHC-C4B	-4.62	1.46	1.53
24	n	606	CHL	CHB-C1B	-4.62	1.46	1.53
24	7	609	CHL	CHC-C4B	-4.62	1.46	1.53
24	4	607	CHL	C4A-C3A	-4.62	1.48	1.53
24	4	606	CHL	C4A-C3A	-4.61	1.48	1.53
24	6	607	CHL	C4A-C3A	-4.61	1.48	1.53
24	1	607	CHL	CHD-C1D	-4.61	1.46	1.53
24	R	607	CHL	CHD-C1D	-4.61	1.46	1.53
24	2	607	CHL	C4A-C3A	-4.61	1.48	1.53
24	4	608	CHL	CHC-C4B	-4.61	1.46	1.53
24	n	606	CHL	C4A-C3A	-4.61	1.48	1.53
24	N	606	CHL	CHB-C1B	-4.61	1.46	1.53
24	Y	605	CHL	CHC-C4B	-4.61	1.46	1.53
24	N	608	CHL	CHB-C1B	-4.61	1.46	1.53
24	r	607	CHL	CHB-C1B	-4.60	1.46	1.53
24	7	606	CHL	C4A-C3A	-4.60	1.48	1.53
24	3	609	CHL	CHC-C4B	-4.60	1.46	1.53
24	r	607	CHL	CHD-C1D	-4.60	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	609	CHL	C4A-C3A	-4.59	1.48	1.53
24	8	608	CHL	CHC-C4B	-4.59	1.46	1.53
24	Y	601	CHL	CHC-C4B	-4.59	1.46	1.53
24	S	607	CHL	C4A-C3A	-4.59	1.48	1.53
24	r	607	CHL	CHC-C4B	-4.59	1.46	1.53
24	r	608	CHL	CHB-C1B	-4.59	1.46	1.53
24	N	606	CHL	C4A-C3A	-4.59	1.48	1.53
24	s	607	CHL	CHD-C1D	-4.58	1.46	1.53
24	R	608	CHL	CHB-C1B	-4.58	1.46	1.53
24	y	601	CHL	CHC-C4B	-4.58	1.46	1.53
24	R	607	CHL	CHB-C1B	-4.57	1.46	1.53
24	g	609	CHL	C4A-C3A	-4.57	1.48	1.53
24	3	606	CHL	C4A-C3A	-4.57	1.48	1.53
24	6	609	CHL	CHC-C4B	-4.57	1.46	1.53
24	y	608	CHL	CHB-C1B	-4.57	1.46	1.53
24	S	607	CHL	CHD-C1D	-4.57	1.46	1.53
24	2	606	CHL	CHB-C1B	-4.56	1.46	1.53
24	n	608	CHL	C3B-C4B	-4.56	1.49	1.54
24	2	609	CHL	CHC-C4B	-4.55	1.46	1.53
24	6	606	CHL	CHB-C1B	-4.55	1.46	1.53
24	R	607	CHL	CHC-C4B	-4.55	1.46	1.53
24	Y	608	CHL	CHB-C1B	-4.55	1.46	1.53
24	G	609	CHL	C4A-C3A	-4.54	1.48	1.53
36	D	405	PL9	C7-C8	-4.52	1.43	1.50
24	7	607	CHL	CHB-C1B	-4.52	1.46	1.53
24	1	605	CHL	C4A-C3A	-4.52	1.48	1.53
24	N	608	CHL	C3B-C4B	-4.51	1.49	1.54
24	R	608	CHL	CHC-C4B	-4.51	1.46	1.53
24	4	607	CHL	CHD-C1D	-4.51	1.46	1.53
24	4	609	CHL	CHC-C4B	-4.51	1.46	1.53
24	3	607	CHL	CHB-C1B	-4.51	1.46	1.53
24	7	606	CHL	CHD-C1D	-4.50	1.46	1.53
24	8	609	CHL	CHC-C4B	-4.50	1.46	1.53
24	8	607	CHL	CHD-C1D	-4.50	1.46	1.53
24	2	606	CHL	CHD-C1D	-4.50	1.46	1.53
24	3	606	CHL	CHD-C1D	-4.49	1.46	1.53
24	6	606	CHL	CHD-C1D	-4.49	1.46	1.53
24	7	608	CHL	C4A-C3A	-4.49	1.48	1.53
24	8	608	CHL	C4A-C3A	-4.49	1.48	1.53
24	S	601	CHL	CHD-C1D	-4.48	1.46	1.53
24	r	608	CHL	CHC-C4B	-4.47	1.46	1.53
36	d	405	PL9	C7-C8	-4.47	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	607	CHL	CHB-C1B	-4.47	1.46	1.53
24	s	608	CHL	CHC-C4B	-4.47	1.46	1.53
24	2	607	CHL	CHB-C1B	-4.47	1.46	1.53
24	y	609	CHL	CHD-C1D	-4.46	1.46	1.53
24	Y	609	CHL	CHD-C1D	-4.46	1.46	1.53
24	n	609	CHL	CHD-C1D	-4.46	1.46	1.53
24	3	608	CHL	CHB-C1B	-4.46	1.46	1.53
24	7	605	CHL	CHB-C1B	-4.46	1.46	1.53
24	3	605	CHL	CHB-C1B	-4.45	1.46	1.53
24	S	608	CHL	CHC-C4B	-4.45	1.46	1.53
24	7	608	CHL	CHB-C1B	-4.45	1.46	1.53
24	5	605	CHL	C4A-C3A	-4.45	1.48	1.53
24	5	606	CHL	C4A-C3A	-4.45	1.48	1.53
24	s	601	CHL	CHD-C1D	-4.44	1.46	1.53
24	4	607	CHL	CHC-C4B	-4.44	1.46	1.53
24	G	608	CHL	CHB-C1B	-4.44	1.46	1.53
24	4	608	CHL	C4A-C3A	-4.44	1.48	1.53
24	G	608	CHL	C3B-C4B	-4.44	1.49	1.54
24	1	606	CHL	C4A-C3A	-4.43	1.48	1.53
24	r	606	CHL	CHC-C4B	-4.43	1.46	1.53
24	Y	606	CHL	CHB-C1B	-4.43	1.46	1.53
24	g	609	CHL	CHD-C1D	-4.43	1.46	1.53
24	y	606	CHL	CHB-C1B	-4.43	1.46	1.53
24	N	609	CHL	CHD-C1D	-4.43	1.46	1.53
24	2	608	CHL	CHC-C4B	-4.42	1.46	1.53
24	8	607	CHL	CHC-C4B	-4.42	1.46	1.53
24	g	608	CHL	CHB-C1B	-4.42	1.46	1.53
24	G	609	CHL	CHD-C1D	-4.42	1.46	1.53
24	s	601	CHL	C4A-C3A	-4.42	1.48	1.53
24	g	608	CHL	C3B-C4B	-4.42	1.49	1.54
24	s	606	CHL	CHD-C1D	-4.42	1.46	1.53
24	3	608	CHL	C4A-C3A	-4.42	1.48	1.53
24	6	608	CHL	CHC-C4B	-4.41	1.46	1.53
24	5	601	CHL	CHB-C1B	-4.41	1.46	1.53
24	S	606	CHL	CHD-C1D	-4.41	1.46	1.53
24	s	607	CHL	CHB-C1B	-4.41	1.46	1.53
24	G	605	CHL	C4A-C3A	-4.40	1.48	1.53
24	s	607	CHL	CHC-C4B	-4.40	1.46	1.53
24	G	605	CHL	CHB-C1B	-4.40	1.46	1.53
24	S	601	CHL	C4A-C3A	-4.40	1.48	1.53
24	3	605	CHL	CHC-C4B	-4.40	1.46	1.53
24	2	601	CHL	C4A-C3A	-4.40	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	608	CHL	CHC-C4B	-4.40	1.46	1.53
24	g	605	CHL	C4A-C3A	-4.40	1.48	1.53
24	g	606	CHL	CHC-C4B	-4.40	1.46	1.53
24	n	601	CHL	C4A-C3A	-4.40	1.48	1.53
24	S	607	CHL	CHC-C4B	-4.39	1.46	1.53
24	G	605	CHL	CHC-C4B	-4.39	1.46	1.53
24	6	609	CHL	CHB-C1B	-4.39	1.46	1.53
24	g	605	CHL	CHC-C4B	-4.39	1.46	1.53
24	R	606	CHL	CHC-C4B	-4.39	1.46	1.53
24	S	607	CHL	CHB-C1B	-4.39	1.46	1.53
24	G	601	CHL	CHC-C4B	-4.39	1.46	1.53
24	6	601	CHL	C4A-C3A	-4.39	1.48	1.53
24	Y	601	CHL	C3D-C2D	-4.39	1.43	1.55
24	6	601	CHL	CHC-C4B	-4.39	1.46	1.53
24	G	606	CHL	CHC-C4B	-4.39	1.46	1.53
24	2	605	CHL	CHB-C1B	-4.38	1.46	1.53
24	3	609	CHL	C4A-C3A	-4.38	1.48	1.53
24	6	605	CHL	CHB-C1B	-4.38	1.46	1.53
24	y	601	CHL	C3D-C2D	-4.38	1.43	1.55
24	7	605	CHL	CHC-C4B	-4.38	1.46	1.53
24	2	609	CHL	CHB-C1B	-4.38	1.46	1.53
24	s	608	CHL	CHD-C1D	-4.38	1.46	1.53
24	g	601	CHL	CHC-C4B	-4.38	1.46	1.53
24	1	601	CHL	CHB-C1B	-4.37	1.46	1.53
24	2	601	CHL	CHC-C4B	-4.37	1.46	1.53
24	N	601	CHL	C4A-C3A	-4.37	1.48	1.53
24	2	605	CHL	C4A-C3A	-4.37	1.48	1.53
24	y	608	CHL	CHC-C4B	-4.36	1.46	1.53
24	g	605	CHL	CHB-C1B	-4.36	1.46	1.53
24	r	614	CHL	CHD-C1D	-4.36	1.46	1.53
24	3	606	CHL	C1A-C2A	-4.36	1.48	1.53
24	7	609	CHL	CHB-C1B	-4.36	1.46	1.53
24	y	601	CHL	C1A-CHA	-4.35	1.46	1.53
24	g	605	CHL	CHD-C1D	-4.35	1.46	1.53
24	6	605	CHL	C4A-C3A	-4.35	1.48	1.53
24	7	606	CHL	C1A-C2A	-4.35	1.48	1.53
24	S	608	CHL	CHD-C1D	-4.35	1.46	1.53
24	G	605	CHL	CHD-C1D	-4.35	1.46	1.53
24	Y	601	CHL	C1A-CHA	-4.35	1.46	1.53
24	2	609	CHL	C4A-C3A	-4.35	1.48	1.53
24	7	609	CHL	C4A-C3A	-4.34	1.48	1.53
24	N	605	CHL	CHC-C4B	-4.33	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	601	CHL	C1A-C2A	-4.32	1.48	1.53
24	6	609	CHL	C4A-C3A	-4.32	1.48	1.53
24	3	609	CHL	CHB-C1B	-4.32	1.46	1.53
24	n	605	CHL	CHC-C4B	-4.32	1.46	1.53
24	Y	606	CHL	CHC-C1C	-4.32	1.45	1.53
24	R	614	CHL	CHD-C1D	-4.31	1.46	1.53
24	1	608	CHL	C4A-C3A	-4.31	1.48	1.53
24	n	601	CHL	CHB-C1B	-4.31	1.46	1.53
24	R	614	CHL	C4A-C3A	-4.31	1.48	1.53
24	3	607	CHL	CHC-C4B	-4.30	1.46	1.53
24	r	614	CHL	C4A-C3A	-4.30	1.48	1.53
24	8	607	CHL	CHB-C1B	-4.30	1.46	1.53
24	5	608	CHL	C4A-C3A	-4.30	1.48	1.53
24	n	608	CHL	CHC-C4B	-4.30	1.46	1.53
24	n	605	CHL	CHD-C1D	-4.30	1.46	1.53
24	N	605	CHL	CHD-C1D	-4.29	1.46	1.53
24	N	608	CHL	CHC-C4B	-4.29	1.46	1.53
24	y	601	CHL	C1A-C2A	-4.29	1.48	1.53
24	G	609	CHL	CHC-C1C	-4.28	1.45	1.53
24	7	607	CHL	CHC-C4B	-4.28	1.46	1.53
24	y	606	CHL	CHC-C1C	-4.28	1.45	1.53
24	5	605	CHL	CHB-C1B	-4.28	1.46	1.53
24	g	609	CHL	CHC-C1C	-4.28	1.45	1.53
24	5	601	CHL	C3D-C2D	-4.28	1.43	1.55
24	N	601	CHL	CHB-C1B	-4.27	1.46	1.53
24	4	607	CHL	CHB-C1B	-4.27	1.46	1.53
24	1	605	CHL	CHB-C1B	-4.27	1.46	1.53
24	6	601	CHL	CHB-C1B	-4.27	1.46	1.53
24	1	601	CHL	C3D-C2D	-4.27	1.43	1.55
24	2	601	CHL	CHB-C1B	-4.25	1.46	1.53
24	n	608	CHL	C4A-C3A	-4.25	1.48	1.53
24	N	608	CHL	C4A-C3A	-4.25	1.48	1.53
24	2	608	CHL	C4A-C3A	-4.25	1.48	1.53
24	G	606	CHL	C4A-C3A	-4.25	1.48	1.53
24	6	607	CHL	CHD-C1D	-4.23	1.46	1.53
24	g	606	CHL	C4A-C3A	-4.23	1.48	1.53
24	1	606	CHL	CHC-C4B	-4.23	1.46	1.53
24	2	607	CHL	CHD-C1D	-4.21	1.46	1.53
24	5	606	CHL	CHC-C4B	-4.21	1.46	1.53
24	7	609	CHL	CHD-C1D	-4.21	1.46	1.53
24	3	609	CHL	CHD-C1D	-4.21	1.46	1.53
24	7	605	CHL	C4A-C3A	-4.19	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	608	CHL	C4A-C3A	-4.19	1.48	1.53
24	3	605	CHL	C4A-C3A	-4.19	1.48	1.53
24	3	606	CHL	C1A-CHA	-4.17	1.47	1.53
24	8	606	CHL	CHC-C4B	-4.17	1.47	1.53
24	3	608	CHL	CHC-C4B	-4.16	1.47	1.53
24	4	606	CHL	CHC-C4B	-4.15	1.47	1.53
24	6	601	CHL	C3D-C2D	-4.15	1.44	1.55
24	7	608	CHL	CHC-C4B	-4.14	1.47	1.53
24	2	601	CHL	C3D-C2D	-4.13	1.44	1.55
24	7	606	CHL	C1A-CHA	-4.13	1.47	1.53
24	1	608	CHL	CHC-C4B	-4.12	1.47	1.53
24	R	614	CHL	CHB-C1B	-4.12	1.47	1.53
24	5	609	CHL	CHD-C1D	-4.12	1.47	1.53
24	s	608	CHL	CHB-C1B	-4.12	1.47	1.53
24	5	608	CHL	CHC-C4B	-4.12	1.47	1.53
24	r	614	CHL	CHB-C1B	-4.11	1.47	1.53
24	g	608	CHL	C4A-C3A	-4.11	1.48	1.53
24	8	601	CHL	CHB-C1B	-4.10	1.47	1.53
24	N	606	CHL	C3D-C2D	-4.10	1.44	1.55
24	r	608	CHL	C3D-C2D	-4.10	1.44	1.55
24	Y	607	CHL	C3D-C2D	-4.09	1.44	1.55
24	n	606	CHL	C3D-C2D	-4.09	1.44	1.55
24	y	609	CHL	CHC-C1C	-4.09	1.45	1.53
24	Y	609	CHL	CHC-C1C	-4.09	1.45	1.53
24	7	601	CHL	C3D-C2D	-4.09	1.44	1.55
24	1	609	CHL	CHD-C1D	-4.09	1.47	1.53
24	N	601	CHL	CHC-C4B	-4.09	1.47	1.53
24	R	608	CHL	C3D-C2D	-4.08	1.44	1.55
24	4	601	CHL	CHB-C1B	-4.08	1.47	1.53
24	7	608	CHL	C3D-C2D	-4.08	1.44	1.55
24	1	608	CHL	C3D-C2D	-4.08	1.44	1.55
24	Y	608	CHL	C3D-C2D	-4.08	1.44	1.55
24	S	608	CHL	CHB-C1B	-4.08	1.47	1.53
24	3	606	CHL	C3D-C2D	-4.08	1.44	1.55
24	5	608	CHL	C3D-C2D	-4.08	1.44	1.55
24	7	606	CHL	C3D-C2D	-4.07	1.44	1.55
24	3	601	CHL	C3D-C2D	-4.07	1.44	1.55
24	y	607	CHL	C3D-C2D	-4.07	1.44	1.55
24	3	608	CHL	C3D-C2D	-4.07	1.44	1.55
24	n	601	CHL	CHC-C4B	-4.07	1.47	1.53
24	y	608	CHL	C3D-C2D	-4.05	1.44	1.55
24	G	601	CHL	C1A-C2A	-4.05	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	604	CLA	CMB-C2B	-4.04	1.43	1.51
24	l	601	CHL	C1A-CHA	-4.04	1.47	1.53
24	G	608	CHL	CHC-C4B	-4.04	1.47	1.53
24	R	614	CHL	CHC-C4B	-4.03	1.47	1.53
25	Y	604	CLA	CMB-C2B	-4.02	1.43	1.51
24	r	614	CHL	CHC-C4B	-4.02	1.47	1.53
24	n	608	CHL	C3D-C2D	-4.02	1.44	1.55
24	G	608	CHL	C4A-C3A	-4.02	1.49	1.53
24	g	608	CHL	CHC-C4B	-4.02	1.47	1.53
24	5	607	CHL	C3D-C2D	-4.02	1.44	1.55
24	S	606	CHL	CHB-C1B	-4.01	1.47	1.53
24	N	608	CHL	C3D-C2D	-4.01	1.44	1.55
24	l	607	CHL	C3D-C2D	-4.01	1.44	1.55
24	r	608	CHL	CHD-C4C	-4.00	1.46	1.53
24	G	608	CHL	C3D-C2D	-4.00	1.44	1.55
24	2	605	CHL	CHC-C4B	-4.00	1.47	1.53
24	6	605	CHL	CHC-C4B	-3.99	1.47	1.53
24	g	601	CHL	C1A-C2A	-3.99	1.49	1.53
24	5	601	CHL	C1A-CHA	-3.99	1.47	1.53
24	8	608	CHL	CHB-C1B	-3.99	1.47	1.53
24	s	606	CHL	CHB-C1B	-3.98	1.47	1.53
24	g	608	CHL	C3D-C2D	-3.98	1.44	1.55
24	n	601	CHL	C1A-CHA	-3.98	1.47	1.53
24	N	601	CHL	C1A-CHA	-3.98	1.47	1.53
24	y	606	CHL	C3D-C2D	-3.97	1.44	1.55
24	R	608	CHL	CHD-C4C	-3.97	1.46	1.53
25	B	612	CLA	CMC-C2C	-3.97	1.42	1.50
25	b	612	CLA	CMC-C2C	-3.97	1.42	1.50
24	Y	606	CHL	C3D-C2D	-3.97	1.44	1.55
24	s	601	CHL	CHC-C4B	-3.96	1.47	1.53
24	5	606	CHL	C3D-C2D	-3.96	1.44	1.55
24	Y	606	CHL	CHD-C4C	-3.96	1.46	1.53
24	n	607	CHL	CHD-C4C	-3.96	1.46	1.53
24	4	608	CHL	CHB-C1B	-3.96	1.47	1.53
24	R	608	CHL	C4A-C3A	-3.95	1.49	1.53
24	y	606	CHL	CHD-C4C	-3.95	1.46	1.53
24	8	601	CHL	CHD-C1D	-3.94	1.47	1.53
24	l	606	CHL	C3D-C2D	-3.94	1.44	1.55
24	s	606	CHL	C3B-C4B	-3.94	1.49	1.54
24	N	607	CHL	C3D-C2D	-3.94	1.44	1.55
24	S	606	CHL	C3B-C4B	-3.93	1.49	1.54
24	S	601	CHL	CHC-C4B	-3.93	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	607	CHL	CHD-C4C	-3.93	1.46	1.53
24	3	601	CHL	C1A-CHA	-3.93	1.47	1.53
24	n	607	CHL	C3D-C2D	-3.92	1.44	1.55
25	r	613	CLA	C3B-C2B	-3.92	1.35	1.40
24	4	601	CHL	CHD-C1D	-3.91	1.47	1.53
24	3	606	CHL	CHC-C4B	-3.91	1.47	1.53
24	Y	607	CHL	CHD-C4C	-3.91	1.46	1.53
24	2	601	CHL	C1A-CHA	-3.90	1.47	1.53
24	6	601	CHL	C1A-CHA	-3.90	1.47	1.53
24	g	606	CHL	C3D-C2D	-3.90	1.44	1.55
24	r	608	CHL	C4A-C3A	-3.90	1.49	1.53
25	R	613	CLA	C3B-C2B	-3.90	1.35	1.40
24	G	601	CHL	C3D-C2D	-3.90	1.44	1.55
24	y	607	CHL	CHD-C4C	-3.89	1.46	1.53
24	5	606	CHL	CHD-C4C	-3.89	1.46	1.53
24	8	601	CHL	CHC-C4B	-3.89	1.47	1.53
24	7	601	CHL	C1A-CHA	-3.89	1.47	1.53
24	g	601	CHL	C1A-CHA	-3.88	1.47	1.53
24	G	601	CHL	C1A-CHA	-3.88	1.47	1.53
24	7	601	CHL	C1A-C2A	-3.88	1.49	1.53
24	G	606	CHL	C3D-C2D	-3.88	1.44	1.55
24	1	606	CHL	CHD-C4C	-3.88	1.46	1.53
24	s	608	CHL	C4A-C3A	-3.88	1.49	1.53
24	g	601	CHL	C3D-C2D	-3.88	1.45	1.55
24	y	609	CHL	C3D-C2D	-3.87	1.45	1.55
24	4	601	CHL	CHC-C4B	-3.87	1.47	1.53
25	N	604	CLA	CMB-C2B	-3.87	1.43	1.51
24	Y	609	CHL	C3D-C2D	-3.87	1.45	1.55
24	7	606	CHL	CHC-C4B	-3.87	1.47	1.53
24	y	608	CHL	CHD-C4C	-3.87	1.46	1.53
24	g	601	CHL	CHC-C1C	-3.87	1.46	1.53
24	Y	608	CHL	CHD-C4C	-3.87	1.46	1.53
24	G	601	CHL	CHC-C1C	-3.85	1.46	1.53
25	n	604	CLA	CMB-C2B	-3.85	1.43	1.51
24	2	601	CHL	CHC-C1C	-3.85	1.46	1.53
24	6	601	CHL	CHC-C1C	-3.85	1.46	1.53
24	5	608	CHL	C1A-CHA	-3.85	1.47	1.53
24	S	608	CHL	C4A-C3A	-3.85	1.49	1.53
24	s	606	CHL	C4A-C3A	-3.85	1.49	1.53
24	3	601	CHL	C1A-C2A	-3.85	1.49	1.53
24	5	605	CHL	C1A-C2A	-3.84	1.49	1.53
24	5	609	CHL	CHC-C1C	-3.83	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	606	CHL	CHC-C1C	-3.83	1.46	1.53
24	4	609	CHL	C3D-C2D	-3.83	1.45	1.55
24	1	609	CHL	CHC-C1C	-3.83	1.46	1.53
24	5	609	CHL	C3D-C2D	-3.82	1.45	1.55
24	4	608	CHL	C3D-C2D	-3.82	1.45	1.55
24	1	609	CHL	C3D-C2D	-3.82	1.45	1.55
24	N	606	CHL	CHC-C1C	-3.82	1.46	1.53
39	F	101	HEM	C3B-C2B	-3.82	1.35	1.40
24	1	608	CHL	C1A-CHA	-3.81	1.47	1.53
24	8	608	CHL	C3D-C2D	-3.81	1.45	1.55
24	G	609	CHL	C3D-C2D	-3.81	1.45	1.55
25	3	611	CLA	C3B-C2B	-3.81	1.35	1.40
24	S	606	CHL	C4A-C3A	-3.81	1.49	1.53
24	8	609	CHL	C3D-C2D	-3.81	1.45	1.55
25	7	611	CLA	CMB-C2B	-3.80	1.43	1.51
24	r	606	CHL	C3D-C2D	-3.80	1.45	1.55
24	5	601	CHL	C1A-C2A	-3.80	1.49	1.53
24	1	601	CHL	C1A-C2A	-3.80	1.49	1.53
24	6	606	CHL	CHC-C1C	-3.79	1.46	1.53
39	f	101	HEM	C3B-C2B	-3.79	1.35	1.40
24	1	605	CHL	C1A-C2A	-3.79	1.49	1.53
25	3	611	CLA	CMB-C2B	-3.79	1.43	1.51
24	g	609	CHL	C3D-C2D	-3.79	1.45	1.55
25	7	611	CLA	C3B-C2B	-3.79	1.35	1.40
24	n	601	CHL	C3D-C2D	-3.79	1.45	1.55
24	R	606	CHL	C3D-C2D	-3.79	1.45	1.55
24	2	606	CHL	CHC-C1C	-3.78	1.46	1.53
24	N	601	CHL	C3D-C2D	-3.78	1.45	1.55
24	1	605	CHL	C1A-CHA	-3.76	1.47	1.53
25	G	604	CLA	CMB-C2B	-3.76	1.44	1.51
24	2	606	CHL	C3D-C2D	-3.75	1.45	1.55
25	g	604	CLA	CMB-C2B	-3.75	1.44	1.51
24	7	605	CHL	CHC-C1C	-3.75	1.46	1.53
24	n	609	CHL	C1A-CHA	-3.75	1.47	1.53
24	N	601	CHL	C1A-C2A	-3.75	1.49	1.53
24	6	606	CHL	C3D-C2D	-3.75	1.45	1.55
24	3	605	CHL	CHC-C1C	-3.75	1.46	1.53
24	2	608	CHL	C3D-C2D	-3.74	1.45	1.55
24	n	609	CHL	C3D-C2D	-3.74	1.45	1.55
24	1	609	CHL	C1A-CHA	-3.74	1.47	1.53
24	4	609	CHL	CHC-C1C	-3.74	1.46	1.53
24	N	609	CHL	C1A-CHA	-3.74	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	609	CHL	C1A-CHA	-3.74	1.47	1.53
24	6	608	CHL	C3D-C2D	-3.74	1.45	1.55
24	3	607	CHL	CHD-C4C	-3.73	1.46	1.53
24	3	609	CHL	C1A-CHA	-3.73	1.47	1.53
24	G	606	CHL	C1A-C2A	-3.72	1.49	1.53
24	8	609	CHL	CHC-C1C	-3.72	1.46	1.53
24	1	608	CHL	CHD-C4C	-3.72	1.46	1.53
24	g	606	CHL	C1A-C2A	-3.72	1.49	1.53
24	n	601	CHL	C1A-C2A	-3.72	1.49	1.53
24	7	609	CHL	C3D-C2D	-3.71	1.45	1.55
24	8	608	CHL	C1A-CHA	-3.71	1.48	1.53
24	N	605	CHL	C3D-C2D	-3.71	1.45	1.55
24	g	607	CHL	CHD-C4C	-3.71	1.46	1.53
24	N	609	CHL	C3D-C2D	-3.71	1.45	1.55
24	7	609	CHL	C1A-CHA	-3.71	1.48	1.53
25	B	613	CLA	CMD-C2D	-3.71	1.43	1.51
24	5	608	CHL	CHD-C4C	-3.70	1.46	1.53
24	N	606	CHL	CHD-C4C	-3.70	1.46	1.53
24	5	605	CHL	C1A-CHA	-3.70	1.48	1.53
24	4	608	CHL	C1A-CHA	-3.69	1.48	1.53
24	3	609	CHL	C3D-C2D	-3.69	1.45	1.55
24	R	607	CHL	C3D-C2D	-3.69	1.45	1.55
24	g	607	CHL	C3D-C2D	-3.69	1.45	1.55
24	1	607	CHL	CHC-C1C	-3.69	1.46	1.53
24	G	607	CHL	CHD-C4C	-3.69	1.46	1.53
24	n	606	CHL	CHD-C4C	-3.69	1.46	1.53
24	1	601	CHL	CHC-C1C	-3.69	1.46	1.53
25	b	613	CLA	CMD-C2D	-3.68	1.43	1.51
24	n	605	CHL	C3D-C2D	-3.68	1.45	1.55
24	7	607	CHL	CHD-C4C	-3.68	1.46	1.53
24	G	607	CHL	C3D-C2D	-3.68	1.45	1.55
37	h	102	DGD	O5D-C6D	-3.68	1.37	1.43
24	8	608	CHL	CHD-C4C	-3.68	1.46	1.53
24	r	607	CHL	C3D-C2D	-3.67	1.45	1.55
25	b	604	CLA	CMB-C2B	-3.67	1.44	1.51
37	H	102	DGD	O5D-C6D	-3.67	1.37	1.43
24	3	607	CHL	C3D-C2D	-3.67	1.45	1.55
24	3	608	CHL	C1A-CHA	-3.67	1.48	1.53
24	5	607	CHL	CHC-C1C	-3.66	1.46	1.53
24	7	608	CHL	C1A-CHA	-3.66	1.48	1.53
25	B	604	CLA	CMB-C2B	-3.66	1.44	1.51
24	N	606	CHL	C1A-CHA	-3.66	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	609	CHL	C1A-CHA	-3.66	1.48	1.53
24	2	608	CHL	CHC-C1C	-3.66	1.46	1.53
39	F	101	HEM	C3C-C2C	-3.66	1.35	1.40
24	8	608	CHL	CHC-C1C	-3.66	1.46	1.53
24	7	607	CHL	C3D-C2D	-3.65	1.45	1.55
24	5	601	CHL	CHC-C1C	-3.65	1.46	1.53
24	6	608	CHL	CHC-C1C	-3.65	1.46	1.53
39	f	101	HEM	C3C-C2C	-3.65	1.35	1.40
24	s	601	CHL	C1A-CHA	-3.65	1.48	1.53
24	Y	609	CHL	C1A-CHA	-3.65	1.48	1.53
25	1	604	CLA	C3B-C2B	-3.64	1.35	1.40
24	4	608	CHL	CHC-C1C	-3.64	1.46	1.53
24	Y	605	CHL	C3D-C2D	-3.64	1.45	1.55
24	4	608	CHL	CHD-C4C	-3.63	1.46	1.53
25	Y	603	CLA	C3B-C2B	-3.63	1.35	1.40
24	8	606	CHL	C3D-C2D	-3.63	1.45	1.55
25	y	603	CLA	C3B-C2B	-3.63	1.35	1.40
24	n	601	CHL	CHC-C1C	-3.63	1.46	1.53
24	2	609	CHL	C3D-C2D	-3.63	1.45	1.55
24	n	606	CHL	C1A-CHA	-3.63	1.48	1.53
24	6	609	CHL	C3D-C2D	-3.63	1.45	1.55
24	4	606	CHL	C3D-C2D	-3.62	1.45	1.55
24	Y	601	CHL	CHC-C1C	-3.62	1.46	1.53
24	y	605	CHL	C3D-C2D	-3.62	1.45	1.55
24	S	601	CHL	C1A-CHA	-3.62	1.48	1.53
25	5	604	CLA	C3B-C2B	-3.61	1.35	1.40
24	N	601	CHL	CHC-C1C	-3.60	1.46	1.53
25	B	604	CLA	C3B-C2B	-3.60	1.35	1.40
25	1	604	CLA	CMB-C2B	-3.60	1.44	1.51
24	R	606	CHL	C1A-CHA	-3.60	1.48	1.53
25	5	604	CLA	CMB-C2B	-3.60	1.44	1.51
24	7	609	CHL	CHC-C1C	-3.60	1.46	1.53
24	g	606	CHL	C1A-CHA	-3.59	1.48	1.53
24	y	601	CHL	CHC-C1C	-3.59	1.46	1.53
24	3	609	CHL	CHC-C1C	-3.59	1.46	1.53
24	1	605	CHL	CHC-C1C	-3.59	1.46	1.53
24	G	606	CHL	C1A-CHA	-3.58	1.48	1.53
25	b	604	CLA	C3B-C2B	-3.58	1.35	1.40
24	8	607	CHL	C3D-C2D	-3.58	1.45	1.55
24	N	607	CHL	CHC-C1C	-3.57	1.46	1.53
24	r	614	CHL	C3D-C2D	-3.57	1.45	1.55
24	3	601	CHL	CHD-C4C	-3.57	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	605	CHL	CHC-C1C	-3.57	1.46	1.53
24	r	606	CHL	C1A-CHA	-3.57	1.48	1.53
24	s	601	CHL	C3D-C2D	-3.56	1.45	1.55
24	7	601	CHL	CHD-C4C	-3.56	1.46	1.53
24	S	601	CHL	C3D-C2D	-3.56	1.45	1.55
24	Y	605	CHL	CHC-C1C	-3.56	1.46	1.53
24	r	608	CHL	CHC-C1C	-3.56	1.46	1.53
24	n	607	CHL	CHC-C1C	-3.56	1.46	1.53
24	n	608	CHL	CHD-C4C	-3.55	1.46	1.53
24	4	607	CHL	C3D-C2D	-3.55	1.45	1.55
24	5	605	CHL	CHC-C1C	-3.55	1.46	1.53
24	4	606	CHL	C1A-CHA	-3.55	1.48	1.53
24	8	607	CHL	C1A-CHA	-3.55	1.48	1.53
24	S	606	CHL	CHC-C4B	-3.54	1.48	1.53
24	s	606	CHL	CHC-C4B	-3.54	1.48	1.53
24	R	614	CHL	C3D-C2D	-3.54	1.45	1.55
25	B	616	CLA	C3B-C2B	-3.54	1.35	1.40
24	6	609	CHL	C1A-CHA	-3.54	1.48	1.53
24	Y	607	CHL	CHC-C1C	-3.54	1.46	1.53
24	R	608	CHL	CHC-C1C	-3.53	1.46	1.53
24	r	608	CHL	CBD-CAD	-3.53	1.47	1.53
24	4	607	CHL	C1A-CHA	-3.53	1.48	1.53
24	N	608	CHL	CHD-C4C	-3.53	1.46	1.53
24	y	608	CHL	CHC-C1C	-3.53	1.46	1.53
24	Y	608	CHL	CHC-C1C	-3.52	1.46	1.53
24	2	607	CHL	C3D-C2D	-3.52	1.45	1.55
24	y	607	CHL	C3B-CAB	-3.52	1.47	1.50
25	b	616	CLA	C3B-C2B	-3.52	1.35	1.40
24	8	606	CHL	C1A-CHA	-3.52	1.48	1.53
24	Y	601	CHL	CBD-CAD	-3.51	1.47	1.53
24	G	605	CHL	C3D-C2D	-3.51	1.45	1.55
25	C	506	CLA	CMB-C2B	-3.51	1.44	1.51
24	6	607	CHL	C3D-C2D	-3.51	1.45	1.55
24	g	605	CHL	C3D-C2D	-3.51	1.45	1.55
24	y	607	CHL	CHC-C1C	-3.51	1.46	1.53
25	B	606	CLA	C3B-C2B	-3.51	1.35	1.40
25	c	506	CLA	CMB-C2B	-3.50	1.44	1.51
24	5	606	CHL	CHC-C1C	-3.50	1.46	1.53
24	Y	607	CHL	C3B-CAB	-3.50	1.47	1.50
24	6	609	CHL	CHC-C1C	-3.50	1.46	1.53
24	2	609	CHL	C1A-CHA	-3.49	1.48	1.53
24	1	606	CHL	CHC-C1C	-3.49	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	605	CHL	C1A-CHA	-3.49	1.48	1.53
24	Y	605	CHL	CHD-C4C	-3.49	1.46	1.53
24	3	605	CHL	C1A-CHA	-3.49	1.48	1.53
25	Y	612	CLA	C3B-C2B	-3.49	1.35	1.40
25	b	606	CLA	C3B-C2B	-3.48	1.35	1.40
25	y	612	CLA	C3B-C2B	-3.48	1.35	1.40
24	y	601	CHL	CBD-CAD	-3.48	1.47	1.53
24	1	605	CHL	C3D-C2D	-3.48	1.46	1.55
24	2	605	CHL	C3D-C2D	-3.48	1.46	1.55
24	g	606	CHL	CHC-C1C	-3.48	1.47	1.53
24	G	606	CHL	CHC-C1C	-3.47	1.47	1.53
24	R	608	CHL	CBD-CAD	-3.47	1.47	1.53
24	y	605	CHL	CHD-C4C	-3.47	1.47	1.53
24	7	605	CHL	C3D-C2D	-3.47	1.46	1.55
24	8	609	CHL	CHD-C4C	-3.47	1.47	1.53
24	5	605	CHL	C3D-C2D	-3.46	1.46	1.55
24	2	609	CHL	CHC-C1C	-3.46	1.47	1.53
24	r	606	CHL	CHD-C4C	-3.46	1.47	1.53
24	n	608	CHL	CHC-C1C	-3.45	1.47	1.53
24	Y	608	CHL	C1A-CHA	-3.45	1.48	1.53
24	6	605	CHL	C3D-C2D	-3.45	1.46	1.55
24	3	605	CHL	C3D-C2D	-3.45	1.46	1.55
25	B	612	CLA	CMB-C2B	-3.45	1.44	1.51
24	4	609	CHL	CHD-C4C	-3.45	1.47	1.53
25	b	612	CLA	CMB-C2B	-3.45	1.44	1.51
24	y	608	CHL	C1A-CHA	-3.44	1.48	1.53
24	R	606	CHL	CHD-C4C	-3.44	1.47	1.53
24	s	608	CHL	C3D-C2D	-3.44	1.46	1.55
28	1	1623	NEX	C7-C8	-3.44	1.26	1.32
24	S	607	CHL	CHC-C1C	-3.43	1.47	1.53
25	1	603	CLA	C3B-C2B	-3.43	1.35	1.40
24	N	608	CHL	CHC-C1C	-3.43	1.47	1.53
28	5	1623	NEX	C7-C8	-3.43	1.26	1.32
24	2	608	CHL	CHD-C4C	-3.43	1.47	1.53
24	4	607	CHL	CHC-C1C	-3.42	1.47	1.53
24	6	608	CHL	CHD-C4C	-3.42	1.47	1.53
24	6	606	CHL	CHD-C4C	-3.42	1.47	1.53
24	8	607	CHL	CHC-C1C	-3.42	1.47	1.53
24	S	608	CHL	C3D-C2D	-3.42	1.46	1.55
24	r	606	CHL	C1A-C2A	-3.41	1.49	1.53
24	2	606	CHL	CHD-C4C	-3.41	1.47	1.53
25	5	603	CLA	C3B-C2B	-3.41	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	601	CHL	C3B-CAB	-3.41	1.47	1.50
24	s	607	CHL	CHC-C1C	-3.41	1.47	1.53
24	8	606	CHL	CHD-C4C	-3.41	1.47	1.53
24	4	606	CHL	CHC-C1C	-3.41	1.47	1.53
25	B	605	CLA	CMD-C2D	-3.41	1.44	1.51
25	2	612	CLA	C3B-C2B	-3.40	1.35	1.40
25	b	605	CLA	CMD-C2D	-3.40	1.44	1.51
24	R	608	CHL	C3D-CAD	-3.40	1.45	1.51
24	8	606	CHL	CHC-C1C	-3.40	1.47	1.53
25	B	615	CLA	CMD-C2D	-3.40	1.44	1.51
24	Y	609	CHL	CHD-C4C	-3.40	1.47	1.53
24	1	609	CHL	C2B-C1B	-3.39	1.46	1.53
24	3	608	CHL	CHD-C4C	-3.39	1.47	1.53
24	R	607	CHL	CHC-C1C	-3.39	1.47	1.53
24	4	606	CHL	CHD-C4C	-3.39	1.47	1.53
24	G	605	CHL	CHC-C1C	-3.39	1.47	1.53
24	5	609	CHL	C2B-C1B	-3.39	1.46	1.53
24	G	608	CHL	CHD-C4C	-3.39	1.47	1.53
24	y	609	CHL	CHD-C4C	-3.39	1.47	1.53
24	7	601	CHL	C3B-CAB	-3.38	1.47	1.50
25	y	611	CLA	C3B-C2B	-3.38	1.35	1.40
24	r	614	CHL	C1A-C2A	-3.38	1.49	1.53
24	1	606	CHL	C1A-CHA	-3.38	1.48	1.53
24	R	606	CHL	C1A-C2A	-3.38	1.49	1.53
24	g	608	CHL	CHD-C4C	-3.38	1.47	1.53
25	b	605	CLA	CMB-C2B	-3.37	1.44	1.51
24	7	608	CHL	CHD-C4C	-3.37	1.47	1.53
25	6	612	CLA	C3B-C2B	-3.37	1.35	1.40
29	d	409	LHG	O7-C5	-3.37	1.37	1.46
36	D	405	PL9	C53-C6	-3.37	1.43	1.50
24	r	607	CHL	CHC-C1C	-3.37	1.47	1.53
24	6	607	CHL	C3B-CAB	-3.37	1.47	1.50
24	7	605	CHL	CHD-C4C	-3.37	1.47	1.53
25	G	603	CLA	C3B-C2B	-3.37	1.35	1.40
24	1	608	CHL	C2B-C1B	-3.36	1.46	1.53
24	r	608	CHL	C3D-CAD	-3.36	1.45	1.51
25	b	615	CLA	CMD-C2D	-3.36	1.44	1.51
24	R	614	CHL	C1A-C2A	-3.36	1.49	1.53
24	5	606	CHL	C1A-CHA	-3.36	1.48	1.53
24	2	606	CHL	C1A-CHA	-3.36	1.48	1.53
24	Y	601	CHL	C3D-CAD	-3.36	1.45	1.51
24	2	607	CHL	C3B-CAB	-3.36	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	605	CHL	CHD-C4C	-3.35	1.47	1.53
24	g	605	CHL	CHC-C1C	-3.35	1.47	1.53
24	3	605	CHL	CHD-C4C	-3.35	1.47	1.53
29	D	409	LHG	O7-C5	-3.35	1.37	1.46
24	y	601	CHL	C3D-CAD	-3.35	1.45	1.51
24	s	607	CHL	C3D-C2D	-3.35	1.46	1.55
25	B	605	CLA	CMB-C2B	-3.34	1.44	1.51
36	d	405	PL9	C53-C6	-3.34	1.43	1.50
28	s	1623	NEX	C7-C8	-3.34	1.26	1.32
24	5	605	CHL	CHD-C4C	-3.34	1.47	1.53
24	1	607	CHL	CHD-C4C	-3.34	1.47	1.53
24	8	609	CHL	C1A-CHA	-3.33	1.48	1.53
24	5	607	CHL	C1A-C2A	-3.33	1.49	1.53
25	Y	611	CLA	C3B-C2B	-3.33	1.36	1.40
24	S	607	CHL	C3D-C2D	-3.33	1.46	1.55
24	5	608	CHL	C2B-C1B	-3.33	1.46	1.53
24	N	607	CHL	C3B-CAB	-3.33	1.47	1.50
24	4	609	CHL	C1A-CHA	-3.33	1.48	1.53
24	6	606	CHL	C1A-CHA	-3.33	1.48	1.53
25	Y	610	CLA	C3B-C2B	-3.33	1.36	1.40
28	S	1623	NEX	C7-C8	-3.33	1.26	1.32
24	R	606	CHL	CHC-C1C	-3.33	1.47	1.53
25	g	603	CLA	C3B-C2B	-3.32	1.36	1.40
24	N	609	CHL	C2B-C1B	-3.32	1.46	1.53
24	5	607	CHL	CHD-C4C	-3.32	1.47	1.53
24	3	601	CHL	CHC-C1C	-3.31	1.47	1.53
25	y	610	CLA	C3B-C2B	-3.31	1.36	1.40
24	n	609	CHL	C2B-C1B	-3.31	1.46	1.53
24	3	606	CHL	CHD-C4C	-3.31	1.47	1.53
24	N	605	CHL	CHC-C1C	-3.30	1.47	1.53
24	3	606	CHL	CHC-C1C	-3.30	1.47	1.53
29	l	101	LHG	O7-C5	-3.30	1.38	1.46
29	L	101	LHG	O7-C5	-3.30	1.38	1.46
25	7	612	CLA	C3B-C2B	-3.30	1.36	1.40
25	3	612	CLA	C3B-C2B	-3.30	1.36	1.40
24	1	607	CHL	C1A-C2A	-3.30	1.49	1.53
24	6	605	CHL	C1A-CHA	-3.30	1.48	1.53
24	r	606	CHL	CHC-C1C	-3.30	1.47	1.53
24	7	606	CHL	CHC-C1C	-3.29	1.47	1.53
24	7	601	CHL	CHC-C1C	-3.29	1.47	1.53
24	2	605	CHL	C1A-CHA	-3.29	1.48	1.53
24	n	605	CHL	CHC-C1C	-3.29	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	609	CHL	CHD-C4C	-3.29	1.47	1.53
24	r	607	CHL	C1A-CHA	-3.28	1.48	1.53
24	g	606	CHL	CHD-C4C	-3.28	1.47	1.53
24	s	606	CHL	C3D-C2D	-3.27	1.46	1.55
24	R	607	CHL	C1A-CHA	-3.26	1.48	1.53
24	S	606	CHL	C3D-C2D	-3.26	1.46	1.55
24	S	601	CHL	C1A-C2A	-3.26	1.49	1.53
24	n	607	CHL	C3B-CAB	-3.26	1.47	1.50
24	G	609	CHL	CHD-C4C	-3.26	1.47	1.53
24	6	607	CHL	CHC-C1C	-3.26	1.47	1.53
24	n	609	CHL	CHD-C4C	-3.26	1.47	1.53
24	7	605	CHL	CBD-CAD	-3.26	1.48	1.53
25	7	610	CLA	C3B-C2B	-3.25	1.36	1.40
24	N	606	CHL	C3B-CAB	-3.25	1.47	1.50
24	G	608	CHL	C1A-CHA	-3.25	1.48	1.53
24	3	605	CHL	CBD-CAD	-3.25	1.48	1.53
24	7	606	CHL	CHD-C4C	-3.25	1.47	1.53
28	r	623	NEX	C7-C8	-3.25	1.26	1.32
24	1	608	CHL	CHC-C1C	-3.24	1.47	1.53
24	N	608	CHL	C1A-CHA	-3.24	1.48	1.53
24	g	605	CHL	C1A-CHA	-3.24	1.48	1.53
24	2	607	CHL	CHC-C1C	-3.24	1.47	1.53
25	3	610	CLA	C3B-C2B	-3.24	1.36	1.40
24	6	609	CHL	CHD-C4C	-3.24	1.47	1.53
25	7	613	CLA	C3B-C2B	-3.24	1.36	1.40
24	G	606	CHL	CHD-C4C	-3.23	1.47	1.53
24	s	607	CHL	CHD-C4C	-3.23	1.47	1.53
24	n	608	CHL	C1A-CHA	-3.23	1.48	1.53
24	2	609	CHL	CHD-C4C	-3.23	1.47	1.53
25	5	612	CLA	C3B-C2B	-3.23	1.36	1.40
28	2	1623	NEX	C7-C8	-3.23	1.26	1.32
24	3	601	CHL	CBD-CAD	-3.23	1.48	1.53
25	r	613	CLA	CMB-C2B	-3.23	1.45	1.51
24	g	609	CHL	CHD-C4C	-3.22	1.47	1.53
24	n	606	CHL	C3B-CAB	-3.22	1.47	1.50
24	7	601	CHL	CBD-CAD	-3.22	1.48	1.53
24	6	608	CHL	C1A-CHA	-3.22	1.48	1.53
28	R	623	NEX	C7-C8	-3.22	1.26	1.32
24	N	606	CHL	C2B-C1B	-3.22	1.46	1.53
24	G	605	CHL	C1A-CHA	-3.22	1.48	1.53
24	y	606	CHL	C1A-C2A	-3.22	1.49	1.53
24	S	608	CHL	CHC-C1C	-3.22	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	608	CHL	C1A-CHA	-3.22	1.48	1.53
24	s	601	CHL	C1A-C2A	-3.21	1.49	1.53
24	S	607	CHL	CHD-C4C	-3.21	1.47	1.53
24	g	608	CHL	C1A-CHA	-3.21	1.48	1.53
25	d	402	CLA	CMD-C2D	-3.21	1.44	1.51
24	2	601	CHL	CHD-C4C	-3.21	1.47	1.53
24	6	605	CHL	CHC-C1C	-3.21	1.47	1.53
25	R	613	CLA	CMB-C2B	-3.21	1.45	1.51
24	5	608	CHL	CHC-C1C	-3.21	1.47	1.53
24	6	601	CHL	CHD-C4C	-3.21	1.47	1.53
24	s	608	CHL	CHC-C1C	-3.20	1.47	1.53
25	3	613	CLA	C3B-C2B	-3.20	1.36	1.40
25	b	607	CLA	CMB-C2B	-3.20	1.45	1.51
25	1	612	CLA	C3B-C2B	-3.20	1.36	1.40
25	b	608	CLA	CMB-C2B	-3.20	1.45	1.51
24	Y	601	CHL	CHD-C4C	-3.20	1.47	1.53
28	6	1623	NEX	C7-C8	-3.20	1.26	1.32
25	B	614	CLA	CMB-C2B	-3.20	1.45	1.51
24	n	606	CHL	C2B-C1B	-3.19	1.47	1.53
24	2	605	CHL	CHC-C1C	-3.19	1.47	1.53
25	D	402	CLA	CMD-C2D	-3.19	1.44	1.51
24	g	606	CHL	C2B-C1B	-3.19	1.47	1.53
24	n	605	CHL	CHD-C4C	-3.19	1.47	1.53
24	G	606	CHL	C2B-C1B	-3.19	1.47	1.53
24	Y	606	CHL	CBD-CAD	-3.19	1.48	1.53
24	y	601	CHL	CHD-C4C	-3.18	1.47	1.53
25	B	607	CLA	CMB-C2B	-3.18	1.45	1.51
24	y	606	CHL	CBD-CAD	-3.18	1.48	1.53
24	G	605	CHL	CHD-C4C	-3.18	1.47	1.53
24	y	609	CHL	CBD-CAD	-3.18	1.48	1.53
24	6	606	CHL	C1A-C2A	-3.18	1.49	1.53
25	B	608	CLA	CMB-C2B	-3.17	1.45	1.51
24	4	601	CHL	C3D-C2D	-3.17	1.46	1.55
24	g	605	CHL	CHD-C4C	-3.17	1.47	1.53
24	G	609	CHL	C1A-CHA	-3.17	1.48	1.53
24	y	607	CHL	CBD-CAD	-3.17	1.48	1.53
24	N	605	CHL	CHD-C4C	-3.17	1.47	1.53
24	2	605	CHL	CHD-C4C	-3.17	1.47	1.53
25	n	603	CLA	C3B-C2B	-3.17	1.36	1.40
25	c	508	CLA	CMB-C2B	-3.16	1.45	1.51
24	Y	607	CHL	CBD-CAD	-3.16	1.48	1.53
24	Y	606	CHL	C1A-CHA	-3.16	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	CMB-C2B	-3.16	1.45	1.51
24	g	609	CHL	C1A-CHA	-3.16	1.48	1.53
24	Y	606	CHL	C1A-C2A	-3.16	1.49	1.53
24	6	605	CHL	CHD-C4C	-3.16	1.47	1.53
24	5	609	CHL	C1A-C2A	-3.16	1.49	1.53
24	s	606	CHL	CHC-C1C	-3.16	1.47	1.53
25	b	614	CLA	CMB-C2B	-3.16	1.45	1.51
24	8	601	CHL	C3D-C2D	-3.16	1.46	1.55
25	N	603	CLA	C3B-C2B	-3.16	1.36	1.40
24	5	608	CHL	CBD-CAD	-3.16	1.48	1.53
24	r	614	CHL	C1A-CHA	-3.15	1.48	1.53
24	Y	609	CHL	CBD-CAD	-3.15	1.48	1.53
24	y	608	CHL	C3D-CAD	-3.15	1.45	1.51
25	r	616	CLA	CMB-C2B	-3.15	1.45	1.51
24	5	601	CHL	CHD-C4C	-3.15	1.47	1.53
25	b	611	CLA	C3B-C2B	-3.15	1.36	1.40
24	2	606	CHL	C1A-C2A	-3.14	1.50	1.53
25	n	603	CLA	CMD-C2D	-3.14	1.44	1.51
24	6	607	CHL	C1A-CHA	-3.14	1.48	1.53
36	d	405	PL9	C52-C5	-3.14	1.44	1.50
25	3	611	CLA	CMD-C2D	-3.14	1.44	1.51
24	S	606	CHL	CHD-C4C	-3.14	1.47	1.53
24	1	607	CHL	C1A-CHA	-3.14	1.48	1.53
24	s	606	CHL	CHD-C4C	-3.14	1.47	1.53
24	1	608	CHL	CBD-CAD	-3.14	1.48	1.53
24	5	607	CHL	C1A-CHA	-3.14	1.48	1.53
36	D	405	PL9	C52-C5	-3.14	1.44	1.50
24	6	608	CHL	C3B-CAB	-3.13	1.47	1.50
24	y	606	CHL	C1A-CHA	-3.13	1.48	1.53
24	r	607	CHL	CHD-C4C	-3.13	1.47	1.53
24	2	607	CHL	C1A-CHA	-3.13	1.48	1.53
25	7	611	CLA	CMD-C2D	-3.13	1.44	1.51
24	1	601	CHL	CHD-C4C	-3.13	1.47	1.53
25	b	606	CLA	CMB-C2B	-3.13	1.45	1.51
24	Y	609	CHL	C1A-C2A	-3.12	1.50	1.53
24	7	608	CHL	C1A-C2A	-3.12	1.50	1.53
24	S	606	CHL	CHC-C1C	-3.12	1.47	1.53
24	1	609	CHL	C1A-C2A	-3.12	1.50	1.53
25	B	606	CLA	CMB-C2B	-3.12	1.45	1.51
25	R	616	CLA	CMB-C2B	-3.12	1.45	1.51
25	c	510	CLA	CMD-C2D	-3.11	1.44	1.51
24	Y	608	CHL	C3D-CAD	-3.11	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	604	CLA	C3B-C2B	-3.11	1.36	1.40
24	n	609	CHL	C2A-C3A	-3.11	1.48	1.55
25	8	604	CLA	C3B-C2B	-3.11	1.36	1.40
25	B	611	CLA	C3B-C2B	-3.11	1.36	1.40
25	N	603	CLA	CMD-C2D	-3.11	1.45	1.51
24	R	614	CHL	C1A-CHA	-3.11	1.48	1.53
25	1	603	CLA	CMB-C2B	-3.11	1.45	1.51
24	R	607	CHL	CHD-C4C	-3.10	1.47	1.53
25	N	604	CLA	C3B-C2B	-3.10	1.36	1.40
24	g	607	CHL	C3B-CAB	-3.10	1.47	1.50
24	y	605	CHL	C1A-CHA	-3.10	1.48	1.53
25	C	510	CLA	CMD-C2D	-3.10	1.45	1.51
24	3	607	CHL	CHC-C1C	-3.10	1.47	1.53
25	5	603	CLA	CMB-C2B	-3.09	1.45	1.51
24	g	607	CHL	CHC-C1C	-3.09	1.47	1.53
24	n	606	CHL	CBD-CAD	-3.09	1.48	1.53
24	G	608	CHL	CHC-C1C	-3.09	1.47	1.53
28	N	1623	NEX	C7-C8	-3.09	1.26	1.32
25	B	608	CLA	C3B-C2B	-3.09	1.36	1.40
24	N	609	CHL	C2A-C3A	-3.09	1.48	1.55
24	4	608	CHL	C1A-C2A	-3.09	1.50	1.53
24	7	607	CHL	CHC-C1C	-3.09	1.47	1.53
25	b	613	CLA	CMB-C2B	-3.08	1.45	1.51
29	G	2630	LHG	O7-C5	-3.08	1.38	1.46
24	r	606	CHL	CBD-CAD	-3.08	1.48	1.53
24	Y	605	CHL	C1A-CHA	-3.08	1.49	1.53
25	b	610	CLA	CMD-C2D	-3.08	1.45	1.51
37	h	102	DGD	O2G-C2G	-3.08	1.38	1.46
24	4	608	CHL	CBD-CAD	-3.08	1.48	1.53
29	g	2630	LHG	O7-C5	-3.08	1.38	1.46
25	2	610	CLA	C3B-C2B	-3.08	1.36	1.40
24	N	606	CHL	CBD-CAD	-3.08	1.48	1.53
24	y	609	CHL	C1A-C2A	-3.08	1.50	1.53
24	2	608	CHL	C3B-CAB	-3.08	1.47	1.50
25	4	610	CLA	CMD-C2D	-3.07	1.45	1.51
25	B	613	CLA	CMB-C2B	-3.07	1.45	1.51
28	n	1623	NEX	C7-C8	-3.07	1.26	1.32
25	8	610	CLA	CMD-C2D	-3.07	1.45	1.51
25	b	608	CLA	C3B-C2B	-3.07	1.36	1.40
25	4	604	CLA	C3B-C2B	-3.07	1.36	1.40
36	d	405	PL9	C36-C34	-3.07	1.44	1.51
24	G	607	CHL	C3B-CAB	-3.07	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	H	102	DGD	O2G-C2G	-3.07	1.38	1.46
24	1	606	CHL	CBD-CAD	-3.06	1.48	1.53
25	6	610	CLA	C3B-C2B	-3.06	1.36	1.40
25	3	612	CLA	CMD-C2D	-3.06	1.45	1.51
24	6	601	CHL	C1A-C2A	-3.06	1.50	1.53
24	G	607	CHL	CHC-C1C	-3.06	1.47	1.53
36	D	405	PL9	C36-C34	-3.06	1.44	1.51
24	3	608	CHL	C1A-C2A	-3.06	1.50	1.53
25	B	610	CLA	CMD-C2D	-3.05	1.45	1.51
24	R	606	CHL	CBD-CAD	-3.05	1.48	1.53
24	s	601	CHL	CHD-C4C	-3.05	1.47	1.53
24	g	608	CHL	CHC-C1C	-3.05	1.47	1.53
24	5	606	CHL	CBD-CAD	-3.05	1.48	1.53
24	y	609	CHL	C2B-C1B	-3.05	1.47	1.53
25	7	612	CLA	CMD-C2D	-3.05	1.45	1.51
25	y	604	CLA	C3B-C2B	-3.05	1.36	1.40
24	S	601	CHL	CHD-C4C	-3.05	1.47	1.53
24	8	608	CHL	C1A-C2A	-3.05	1.50	1.53
24	2	601	CHL	C2A-C3A	-3.04	1.49	1.55
25	7	604	CLA	C3B-C2B	-3.04	1.36	1.40
24	5	606	CHL	C2B-C1B	-3.04	1.47	1.53
24	G	605	CHL	C1A-C2A	-3.04	1.50	1.53
24	G	609	CHL	CBD-CAD	-3.04	1.48	1.53
25	r	609	CLA	C3B-C2B	-3.04	1.36	1.40
24	Y	609	CHL	C2B-C1B	-3.04	1.47	1.53
24	6	609	CHL	C2B-C1B	-3.04	1.47	1.53
24	G	601	CHL	CHD-C4C	-3.03	1.47	1.53
24	2	609	CHL	C2B-C1B	-3.03	1.47	1.53
25	7	604	CLA	CMB-C2B	-3.03	1.45	1.51
25	3	604	CLA	CMB-C2B	-3.03	1.45	1.51
25	3	604	CLA	C3B-C2B	-3.03	1.36	1.40
25	y	614	CLA	CMD-C2D	-3.03	1.45	1.51
25	Y	614	CLA	CMD-C2D	-3.03	1.45	1.51
25	Y	604	CLA	C3B-C2B	-3.03	1.36	1.40
24	8	608	CHL	CBD-CAD	-3.03	1.48	1.53
24	N	609	CHL	CBD-CAD	-3.03	1.48	1.53
24	2	601	CHL	C1A-C2A	-3.03	1.50	1.53
24	1	607	CHL	CBD-CAD	-3.03	1.48	1.53
25	Y	611	CLA	CMD-C2D	-3.03	1.45	1.51
25	B	617	CLA	CMC-C2C	-3.03	1.44	1.50
25	3	603	CLA	CMD-C2D	-3.03	1.45	1.51
24	7	608	CHL	C3B-CAB	-3.03	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	608	CHL	C1A-CHA	-3.02	1.49	1.53
24	g	605	CHL	C1A-C2A	-3.02	1.50	1.53
25	b	612	CLA	CMD-C2D	-3.02	1.45	1.51
25	y	611	CLA	CMD-C2D	-3.02	1.45	1.51
24	s	601	CHL	CHC-C1C	-3.02	1.47	1.53
25	B	602	CLA	CMD-C2D	-3.02	1.45	1.51
24	n	609	CHL	CBD-CAD	-3.02	1.48	1.53
25	b	617	CLA	CMC-C2C	-3.02	1.44	1.50
24	g	601	CHL	CHD-C4C	-3.02	1.47	1.53
25	R	609	CLA	C3B-C2B	-3.02	1.36	1.40
25	y	610	CLA	CMB-C2B	-3.02	1.45	1.51
24	g	609	CHL	CBD-CAD	-3.02	1.48	1.53
24	l	606	CHL	C2B-C1B	-3.02	1.47	1.53
24	S	601	CHL	CHC-C1C	-3.01	1.47	1.53
25	7	603	CLA	CMD-C2D	-3.01	1.45	1.51
24	N	608	CHL	C3D-CAD	-3.01	1.45	1.51
24	6	607	CHL	CHD-C4C	-3.01	1.47	1.53
25	r	604	CLA	CMB-C2B	-3.01	1.45	1.51
25	B	610	CLA	CMB-C2B	-3.01	1.45	1.51
25	6	603	CLA	C3B-C2B	-3.01	1.36	1.40
25	A	406	CLA	CMB-C2B	-3.01	1.45	1.51
24	5	607	CHL	CBD-CAD	-3.00	1.48	1.53
25	d	402	CLA	CMB-C2B	-3.00	1.45	1.51
24	3	608	CHL	C3B-CAB	-3.00	1.47	1.50
25	y	612	CLA	CMB-C2B	-3.00	1.45	1.51
25	4	604	CLA	CMB-C2B	-3.00	1.45	1.51
25	D	402	CLA	CMB-C2B	-3.00	1.45	1.51
24	6	601	CHL	C2A-C3A	-3.00	1.49	1.55
25	2	603	CLA	C3B-C2B	-3.00	1.36	1.40
24	G	607	CHL	C1A-CHA	-3.00	1.49	1.53
24	6	609	CHL	CBD-CAD	-3.00	1.48	1.53
24	2	609	CHL	CBD-CAD	-3.00	1.48	1.53
24	7	608	CHL	CHC-C1C	-3.00	1.47	1.53
24	1	609	CHL	C3B-CAB	-3.00	1.47	1.50
25	a	406	CLA	CMB-C2B	-3.00	1.45	1.51
25	Y	603	CLA	CMD-C2D	-3.00	1.45	1.51
24	5	609	CHL	C3B-CAB	-3.00	1.47	1.50
24	R	608	CHL	C1A-CHA	-3.00	1.49	1.53
25	b	610	CLA	CMB-C2B	-3.00	1.45	1.51
24	2	607	CHL	CHD-C4C	-3.00	1.47	1.53
25	3	603	CLA	C3B-C2B	-2.99	1.36	1.40
25	Y	610	CLA	CMB-C2B	-2.99	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	614	CLA	C3B-C2B	-2.99	1.36	1.40
24	1	607	CHL	C2A-C3A	-2.99	1.49	1.55
25	R	604	CLA	CMB-C2B	-2.99	1.45	1.51
26	y	1621	LUT	C22-C21	-2.99	1.51	1.54
25	b	602	CLA	CMD-C2D	-2.99	1.45	1.51
25	Y	602	CLA	CMB-C2B	-2.99	1.45	1.51
25	B	612	CLA	CMD-C2D	-2.99	1.45	1.51
25	b	617	CLA	CMB-C2B	-2.99	1.45	1.51
24	r	606	CHL	C2B-C1B	-2.98	1.47	1.53
24	n	607	CHL	CBD-CAD	-2.98	1.48	1.53
25	8	604	CLA	CMB-C2B	-2.98	1.45	1.51
24	R	606	CHL	C2B-C1B	-2.98	1.47	1.53
25	Y	611	CLA	CMB-C2B	-2.98	1.45	1.51
25	y	603	CLA	CMD-C2D	-2.97	1.45	1.51
25	7	603	CLA	C3B-C2B	-2.97	1.36	1.40
24	3	609	CHL	CHD-C4C	-2.97	1.47	1.53
24	8	607	CHL	CHD-C4C	-2.97	1.47	1.53
24	n	608	CHL	C3D-CAD	-2.97	1.45	1.51
28	y	1623	NEX	C7-C8	-2.97	1.27	1.32
24	1	608	CHL	C3D-CAD	-2.97	1.45	1.51
25	y	611	CLA	CMB-C2B	-2.97	1.45	1.51
24	N	607	CHL	CBD-CAD	-2.97	1.48	1.53
25	Y	612	CLA	CMB-C2B	-2.97	1.45	1.51
25	B	617	CLA	CMB-C2B	-2.96	1.45	1.51
24	S	608	CHL	CHD-C4C	-2.96	1.47	1.53
24	s	608	CHL	CHD-C4C	-2.96	1.47	1.53
25	y	602	CLA	CMB-C2B	-2.96	1.45	1.51
24	g	607	CHL	C1A-CHA	-2.96	1.49	1.53
24	5	608	CHL	C3D-CAD	-2.96	1.45	1.51
24	3	608	CHL	CHC-C1C	-2.96	1.47	1.53
25	b	606	CLA	CMD-C2D	-2.96	1.45	1.51
24	N	605	CHL	C1A-CHA	-2.95	1.49	1.53
25	b	611	CLA	CMB-C2B	-2.95	1.45	1.51
25	y	614	CLA	C3B-C2B	-2.95	1.36	1.40
24	Y	607	CHL	C2B-C1B	-2.95	1.47	1.53
25	1	610	CLA	C3B-C2B	-2.95	1.36	1.40
24	1	608	CHL	C1A-C2A	-2.95	1.50	1.53
24	5	607	CHL	C2A-C3A	-2.95	1.49	1.55
26	Y	1621	LUT	C22-C21	-2.95	1.51	1.54
24	n	605	CHL	C1A-C2A	-2.95	1.50	1.53
29	D	408	LHG	O7-C5	-2.94	1.38	1.46
24	4	607	CHL	CHD-C4C	-2.94	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	608	CHL	C2A-C3A	-2.94	1.49	1.55
25	B	611	CLA	CMB-C2B	-2.94	1.45	1.51
24	n	605	CHL	C1A-CHA	-2.94	1.49	1.53
25	a	407	CLA	CMB-C2B	-2.94	1.45	1.51
24	8	608	CHL	C2A-C3A	-2.94	1.49	1.55
24	y	607	CHL	C2B-C1B	-2.94	1.47	1.53
25	B	606	CLA	CMD-C2D	-2.94	1.45	1.51
28	Y	1623	NEX	C7-C8	-2.94	1.27	1.32
24	R	607	CHL	C1A-C2A	-2.94	1.50	1.53
24	n	606	CHL	C1A-C2A	-2.94	1.50	1.53
25	5	610	CLA	C3B-C2B	-2.93	1.36	1.40
24	N	606	CHL	C1A-C2A	-2.93	1.50	1.53
25	2	613	CLA	CMD-C2D	-2.93	1.45	1.51
24	5	606	CHL	C3B-CAB	-2.93	1.47	1.50
25	6	613	CLA	CMD-C2D	-2.93	1.45	1.51
24	7	609	CHL	CHD-C4C	-2.93	1.47	1.53
25	C	501	CLA	C3B-C2B	-2.93	1.36	1.40
25	r	604	CLA	CMD-C2D	-2.93	1.45	1.51
24	7	605	CHL	C1A-C2A	-2.93	1.50	1.53
25	R	604	CLA	CMD-C2D	-2.93	1.45	1.51
24	3	606	CHL	C2A-C3A	-2.93	1.49	1.55
25	c	501	CLA	C3B-C2B	-2.92	1.36	1.40
24	8	609	CHL	C3B-CAB	-2.92	1.47	1.50
25	G	604	CLA	C3B-C2B	-2.92	1.36	1.40
33	A	408	PHO	C1C-NC	-2.92	1.32	1.38
25	B	604	CLA	CMD-C2D	-2.92	1.45	1.51
33	a	408	PHO	C1C-NC	-2.92	1.32	1.38
29	d	408	LHG	O7-C5	-2.92	1.39	1.46
25	b	611	CLA	CMD-C2D	-2.92	1.45	1.51
24	R	614	CHL	CHD-C4C	-2.92	1.47	1.53
25	r	603	CLA	CMB-C2B	-2.92	1.45	1.51
37	h	102	DGD	O4D-C4D	-2.91	1.36	1.43
25	B	611	CLA	CMD-C2D	-2.91	1.45	1.51
24	7	606	CHL	C2A-C3A	-2.91	1.49	1.55
24	Y	608	CHL	CBD-CAD	-2.91	1.48	1.53
25	g	604	CLA	C3B-C2B	-2.91	1.36	1.40
25	a	405	CLA	CMD-C2D	-2.91	1.45	1.51
25	A	407	CLA	CMB-C2B	-2.91	1.45	1.51
25	b	604	CLA	CMD-C2D	-2.91	1.45	1.51
24	5	601	CHL	CBD-CAD	-2.91	1.48	1.53
25	7	610	CLA	CMB-C2B	-2.91	1.45	1.51
24	y	608	CHL	CBD-CAD	-2.91	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	H	102	DGD	O4D-C4D	-2.91	1.36	1.43
25	b	608	CLA	CMD-C2D	-2.90	1.45	1.51
24	7	607	CHL	C1A-CHA	-2.90	1.49	1.53
24	1	606	CHL	C3B-CAB	-2.90	1.47	1.50
24	4	609	CHL	C3B-CAB	-2.90	1.47	1.50
24	Y	606	CHL	C3B-CAB	-2.90	1.47	1.50
25	N	602	CLA	CMB-C2B	-2.90	1.45	1.51
25	Y	612	CLA	CMD-C2D	-2.90	1.45	1.51
24	5	608	CHL	C1A-C2A	-2.90	1.50	1.53
24	1	601	CHL	CBD-CAD	-2.90	1.48	1.53
25	8	603	CLA	CMD-C2D	-2.90	1.45	1.51
25	4	603	CLA	CMD-C2D	-2.90	1.45	1.51
25	R	603	CLA	CMB-C2B	-2.90	1.45	1.51
25	3	610	CLA	CMB-C2B	-2.90	1.45	1.51
25	c	505	CLA	CMD-C2D	-2.90	1.45	1.51
25	b	609	CLA	CMD-C2D	-2.89	1.45	1.51
24	3	607	CHL	C1A-CHA	-2.89	1.49	1.53
24	1	608	CHL	C2A-C3A	-2.89	1.49	1.55
24	8	608	CHL	C3D-CAD	-2.89	1.45	1.51
25	B	612	CLA	C3B-C2B	-2.89	1.36	1.40
24	r	607	CHL	C1A-C2A	-2.89	1.50	1.53
24	5	608	CHL	C2A-C3A	-2.89	1.49	1.55
25	B	609	CLA	CMD-C2D	-2.89	1.45	1.51
25	B	608	CLA	CMD-C2D	-2.89	1.45	1.51
25	a	405	CLA	CMC-C2C	-2.89	1.44	1.50
24	6	606	CHL	C2B-C1B	-2.88	1.47	1.53
25	D	403	CLA	CMD-C2D	-2.88	1.45	1.51
25	A	405	CLA	CMD-C2D	-2.88	1.45	1.51
25	b	612	CLA	C3B-C2B	-2.88	1.36	1.40
25	n	602	CLA	CMB-C2B	-2.88	1.45	1.51
24	g	606	CHL	C3B-CAB	-2.88	1.47	1.50
24	G	606	CHL	C3B-CAB	-2.88	1.47	1.50
24	6	607	CHL	C1A-C2A	-2.88	1.50	1.53
24	N	605	CHL	C1A-C2A	-2.88	1.50	1.53
25	G	602	CLA	CMB-C2B	-2.88	1.45	1.51
25	Y	603	CLA	CMB-C2B	-2.88	1.45	1.51
25	b	607	CLA	C3B-C2B	-2.88	1.36	1.40
25	7	602	CLA	CMD-C2D	-2.88	1.45	1.51
24	2	607	CHL	C1A-C2A	-2.88	1.50	1.53
24	2	606	CHL	C2B-C1B	-2.88	1.47	1.53
24	r	614	CHL	CHD-C4C	-2.88	1.48	1.53
24	N	601	CHL	CHD-C4C	-2.87	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	3	606	CHL	C2B-C1B	-2.87	1.47	1.53
25	A	405	CLA	CMC-C2C	-2.87	1.44	1.50
24	R	607	CHL	CBD-CAD	-2.87	1.48	1.53
25	C	509	CLA	CMD-C2D	-2.87	1.45	1.51
24	6	609	CHL	C2A-C3A	-2.87	1.49	1.55
25	3	602	CLA	CMD-C2D	-2.86	1.45	1.51
29	y	2630	LHG	O7-C5	-2.86	1.39	1.46
25	y	603	CLA	CMB-C2B	-2.86	1.45	1.51
24	4	607	CHL	C1A-C2A	-2.86	1.50	1.53
24	r	607	CHL	CBD-CAD	-2.86	1.48	1.53
24	4	608	CHL	C3D-CAD	-2.86	1.46	1.51
24	7	608	CHL	C3D-CAD	-2.86	1.46	1.51
24	1	609	CHL	CHD-C4C	-2.86	1.48	1.53
25	Y	602	CLA	CMD-C2D	-2.86	1.45	1.51
25	d	403	CLA	CMD-C2D	-2.86	1.45	1.51
25	y	612	CLA	CMD-C2D	-2.86	1.45	1.51
24	4	606	CHL	C2A-C3A	-2.86	1.49	1.55
24	Y	608	CHL	C1A-C2A	-2.86	1.50	1.53
24	y	606	CHL	C3B-CAB	-2.85	1.47	1.50
24	3	608	CHL	C3D-CAD	-2.85	1.46	1.51
25	C	505	CLA	CMD-C2D	-2.85	1.45	1.51
24	3	605	CHL	C1A-C2A	-2.85	1.50	1.53
24	7	606	CHL	CBD-CAD	-2.85	1.48	1.53
25	g	602	CLA	CMB-C2B	-2.85	1.45	1.51
24	5	609	CHL	CHD-C4C	-2.85	1.48	1.53
24	1	601	CHL	C3B-CAB	-2.85	1.47	1.50
25	G	603	CLA	CMB-C2B	-2.85	1.45	1.51
25	y	602	CLA	CMD-C2D	-2.85	1.45	1.51
26	N	1621	LUT	C22-C21	-2.85	1.51	1.54
25	b	607	CLA	CMD-C2D	-2.84	1.45	1.51
24	7	606	CHL	C2B-C1B	-2.84	1.47	1.53
24	y	608	CHL	C1A-C2A	-2.84	1.50	1.53
29	3	2630	LHG	O7-C5	-2.84	1.39	1.46
24	N	606	CHL	C3D-CAD	-2.84	1.46	1.51
24	7	608	CHL	C2B-C1B	-2.84	1.47	1.53
24	8	606	CHL	C2A-C3A	-2.84	1.49	1.55
25	3	613	CLA	CMB-C2B	-2.84	1.45	1.51
25	N	603	CLA	CMB-C2B	-2.84	1.45	1.51
25	g	603	CLA	CMB-C2B	-2.84	1.45	1.51
24	1	607	CHL	C2B-C1B	-2.84	1.47	1.53
25	A	410	CLA	CMD-C2D	-2.84	1.45	1.51
24	3	601	CHL	C3D-CAD	-2.84	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	607	CLA	CMD-C2D	-2.84	1.45	1.51
24	5	601	CHL	C3D-CAD	-2.84	1.46	1.51
24	1	607	CHL	C3B-CAB	-2.84	1.47	1.50
24	5	601	CHL	C3B-CAB	-2.84	1.47	1.50
25	B	607	CLA	C3B-C2B	-2.84	1.36	1.40
24	6	605	CHL	C1A-C2A	-2.84	1.50	1.53
26	n	1621	LUT	C22-C21	-2.84	1.51	1.54
25	6	610	CLA	CMB-C2B	-2.84	1.45	1.51
24	3	608	CHL	C2B-C1B	-2.84	1.47	1.53
24	n	601	CHL	CHD-C4C	-2.84	1.48	1.53
29	7	2630	LHG	O7-C5	-2.84	1.39	1.46
29	Y	2630	LHG	O7-C5	-2.83	1.39	1.46
29	n	2630	LHG	O7-C5	-2.83	1.39	1.46
24	R	606	CHL	C2A-C3A	-2.83	1.49	1.55
25	A	410	CLA	CMB-C2B	-2.83	1.45	1.51
24	2	605	CHL	C1A-C2A	-2.83	1.50	1.53
25	Y	610	CLA	CMD-C2D	-2.83	1.45	1.51
25	c	509	CLA	CMD-C2D	-2.83	1.45	1.51
24	3	606	CHL	CBD-CAD	-2.83	1.48	1.53
25	2	610	CLA	CMB-C2B	-2.83	1.45	1.51
24	2	609	CHL	C2A-C3A	-2.83	1.49	1.55
24	5	609	CHL	C2A-C3A	-2.83	1.49	1.55
24	6	606	CHL	C3B-CAB	-2.83	1.47	1.50
25	y	614	CLA	CMB-C2B	-2.83	1.45	1.51
24	g	601	CHL	C2B-C1B	-2.82	1.47	1.53
24	8	607	CHL	C1A-C2A	-2.82	1.50	1.53
26	y	1620	LUT	C22-C21	-2.82	1.51	1.54
25	a	410	CLA	CMD-C2D	-2.82	1.45	1.51
25	r	610	CLA	CMB-C2B	-2.82	1.45	1.51
24	n	606	CHL	C3D-CAD	-2.82	1.46	1.51
24	2	606	CHL	C3B-CAB	-2.82	1.47	1.50
29	N	2630	LHG	O7-C5	-2.82	1.39	1.46
24	1	609	CHL	C2A-C3A	-2.82	1.49	1.55
25	n	603	CLA	CMB-C2B	-2.82	1.45	1.51
25	7	612	CLA	CMB-C2B	-2.82	1.45	1.51
25	N	604	CLA	CMD-C2D	-2.82	1.45	1.51
25	b	615	CLA	CMB-C2B	-2.82	1.45	1.51
25	B	615	CLA	CMB-C2B	-2.82	1.45	1.51
24	n	608	CHL	CBD-CAD	-2.82	1.48	1.53
25	R	610	CLA	CMB-C2B	-2.82	1.45	1.51
25	G	612	CLA	CMD-C2D	-2.82	1.45	1.51
25	3	610	CLA	C3B-CAB	-2.82	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	607	CHL	C2B-C1B	-2.82	1.47	1.53
25	y	610	CLA	CMD-C2D	-2.82	1.45	1.51
24	1	601	CHL	C3D-CAD	-2.82	1.46	1.51
25	Y	614	CLA	CMB-C2B	-2.82	1.45	1.51
25	5	614	CLA	CMD-C2D	-2.82	1.45	1.51
26	8	620	LUT	C22-C21	-2.81	1.51	1.54
25	1	613	CLA	CMB-C2B	-2.81	1.45	1.51
25	r	610	CLA	C3B-C2B	-2.81	1.36	1.40
24	8	601	CHL	CHC-C1C	-2.81	1.48	1.53
25	D	403	CLA	CMB-C2B	-2.81	1.45	1.51
25	5	611	CLA	CMB-C2B	-2.81	1.45	1.51
24	4	601	CHL	CHC-C1C	-2.81	1.48	1.53
24	G	601	CHL	CBD-CAD	-2.81	1.48	1.53
25	2	612	CLA	CMB-C2B	-2.81	1.45	1.51
25	R	610	CLA	C3B-C2B	-2.81	1.36	1.40
25	B	617	CLA	CMD-C2D	-2.81	1.45	1.51
25	7	613	CLA	CMB-C2B	-2.81	1.46	1.51
25	a	410	CLA	CMB-C2B	-2.81	1.46	1.51
25	g	612	CLA	CMD-C2D	-2.80	1.45	1.51
24	G	609	CHL	C2B-C1B	-2.80	1.47	1.53
25	5	613	CLA	CMB-C2B	-2.80	1.46	1.51
25	3	612	CLA	CMB-C2B	-2.80	1.46	1.51
25	1	610	CLA	C3B-CAB	-2.80	1.42	1.47
25	6	612	CLA	CMB-C2B	-2.80	1.46	1.51
25	5	610	CLA	C3B-CAB	-2.80	1.42	1.47
24	r	606	CHL	C2A-C3A	-2.80	1.49	1.55
25	g	610	CLA	CMB-C2B	-2.80	1.46	1.51
25	R	610	CLA	CMD-C2D	-2.80	1.45	1.51
25	7	610	CLA	C3B-CAB	-2.80	1.42	1.47
25	7	613	CLA	CMD-C2D	-2.80	1.45	1.51
25	b	617	CLA	CMD-C2D	-2.80	1.45	1.51
26	4	620	LUT	C22-C21	-2.80	1.51	1.54
27	7	1622	XAT	C10-C9	-2.80	1.32	1.35
25	c	509	CLA	CMB-C2B	-2.80	1.46	1.51
24	G	601	CHL	C2B-C1B	-2.80	1.47	1.53
28	7	1623	NEX	C7-C8	-2.80	1.27	1.32
24	5	607	CHL	C3B-CAB	-2.80	1.47	1.50
26	Y	1620	LUT	C22-C21	-2.80	1.51	1.54
25	d	403	CLA	CMB-C2B	-2.80	1.46	1.51
24	3	607	CHL	CBD-CAD	-2.80	1.48	1.53
25	G	610	CLA	CMB-C2B	-2.80	1.46	1.51
25	b	615	CLA	C3B-C2B	-2.80	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	601	CHL	C3D-CAD	-2.80	1.46	1.51
33	A	409	PHO	C1C-NC	-2.79	1.32	1.38
28	3	1623	NEX	C7-C8	-2.79	1.27	1.32
24	S	606	CHL	C1A-CHA	-2.79	1.49	1.53
36	d	405	PL9	C26-C24	-2.79	1.45	1.51
25	6	602	CLA	CMD-C2D	-2.79	1.45	1.51
25	A	407	CLA	CMD-C2D	-2.79	1.45	1.51
33	a	409	PHO	C1C-NC	-2.79	1.32	1.38
24	Y	606	CHL	C3D-CAD	-2.79	1.46	1.51
25	R	612	CLA	CMB-C2B	-2.79	1.46	1.51
25	n	604	CLA	CMD-C2D	-2.79	1.45	1.51
25	5	604	CLA	CMD-C2D	-2.79	1.45	1.51
24	7	607	CHL	CBD-CAD	-2.79	1.48	1.53
24	n	606	CHL	C2A-C3A	-2.79	1.49	1.55
25	C	501	CLA	CMB-C2B	-2.79	1.46	1.51
25	B	615	CLA	C3B-C2B	-2.79	1.36	1.40
24	2	608	CHL	CBD-CAD	-2.79	1.48	1.53
25	1	611	CLA	C3B-C2B	-2.78	1.36	1.40
25	2	602	CLA	CMD-C2D	-2.78	1.45	1.51
25	g	611	CLA	CMB-C2B	-2.78	1.46	1.51
25	R	609	CLA	CMB-C2B	-2.78	1.46	1.51
25	6	604	CLA	CMB-C2B	-2.78	1.46	1.51
25	2	604	CLA	CMB-C2B	-2.78	1.46	1.51
24	g	609	CHL	C2B-C1B	-2.78	1.47	1.53
25	g	602	CLA	CMC-C2C	-2.78	1.44	1.50
25	1	614	CLA	CMD-C2D	-2.78	1.45	1.51
24	g	609	CHL	C2A-C3A	-2.78	1.49	1.55
26	G	1621	LUT	C22-C21	-2.78	1.51	1.54
24	8	606	CHL	C2B-C1B	-2.78	1.47	1.53
24	s	606	CHL	C1A-CHA	-2.78	1.49	1.53
25	c	501	CLA	CMB-C2B	-2.78	1.46	1.51
25	C	509	CLA	CMB-C2B	-2.78	1.46	1.51
24	Y	608	CHL	C2B-C1B	-2.78	1.47	1.53
25	1	612	CLA	CMB-C2B	-2.78	1.46	1.51
25	3	613	CLA	CMD-C2D	-2.78	1.45	1.51
36	d	405	PL9	C16-C14	-2.78	1.45	1.51
25	1	611	CLA	CMB-C2B	-2.78	1.46	1.51
25	B	616	CLA	CMB-C2B	-2.78	1.46	1.51
24	g	601	CHL	CBD-CAD	-2.78	1.48	1.53
36	D	405	PL9	C26-C24	-2.78	1.45	1.51
25	5	602	CLA	CMD-C2D	-2.78	1.45	1.51
26	g	1621	LUT	C22-C21	-2.78	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	616	CLA	CMD-C2D	-2.78	1.45	1.51
24	y	608	CHL	C2B-C1B	-2.77	1.47	1.53
24	G	606	CHL	CBD-CAD	-2.77	1.48	1.53
25	C	504	CLA	CMB-C2B	-2.77	1.46	1.51
24	y	609	CHL	C2A-C3A	-2.77	1.49	1.55
25	a	407	CLA	CMD-C2D	-2.77	1.45	1.51
25	G	611	CLA	CMB-C2B	-2.77	1.46	1.51
25	6	603	CLA	CMD-C2D	-2.77	1.45	1.51
24	G	609	CHL	C2A-C3A	-2.77	1.49	1.55
24	N	608	CHL	CBD-CAD	-2.77	1.48	1.53
24	Y	607	CHL	C2A-C3A	-2.77	1.49	1.55
24	g	606	CHL	CBD-CAD	-2.77	1.48	1.53
25	s	613	CLA	CMB-C2B	-2.77	1.46	1.51
25	r	610	CLA	CMD-C2D	-2.77	1.45	1.51
24	R	614	CHL	CHC-C1C	-2.77	1.48	1.53
25	r	612	CLA	CMB-C2B	-2.77	1.46	1.51
25	1	602	CLA	CMD-C2D	-2.77	1.45	1.51
24	y	606	CHL	C3D-CAD	-2.77	1.46	1.51
24	Y	609	CHL	C2A-C3A	-2.77	1.49	1.55
25	r	609	CLA	CMB-C2B	-2.77	1.46	1.51
25	5	602	CLA	CMB-C2B	-2.77	1.46	1.51
25	4	612	CLA	CMD-C2D	-2.76	1.45	1.51
25	1	602	CLA	CMB-C2B	-2.76	1.46	1.51
25	b	616	CLA	CMB-C2B	-2.76	1.46	1.51
25	A	406	CLA	CMD-C2D	-2.76	1.45	1.51
25	7	603	CLA	CMB-C2B	-2.76	1.46	1.51
24	S	601	CHL	C3B-CAB	-2.76	1.48	1.50
25	2	603	CLA	CMD-C2D	-2.76	1.45	1.51
24	3	608	CHL	CBD-CAD	-2.76	1.48	1.53
24	N	606	CHL	C2A-C3A	-2.76	1.49	1.55
24	4	606	CHL	C2B-C1B	-2.76	1.47	1.53
25	b	616	CLA	CMD-C2D	-2.76	1.45	1.51
24	G	607	CHL	CBD-CAD	-2.76	1.48	1.53
24	5	609	CHL	CBD-CAD	-2.76	1.48	1.53
24	r	614	CHL	CHC-C1C	-2.76	1.48	1.53
24	s	601	CHL	C3B-CAB	-2.76	1.48	1.50
25	C	502	CLA	CMB-C2B	-2.76	1.46	1.51
25	8	612	CLA	CMD-C2D	-2.76	1.45	1.51
25	c	504	CLA	CMB-C2B	-2.76	1.46	1.51
24	g	607	CHL	CBD-CAD	-2.76	1.48	1.53
25	B	614	CLA	CMD-C2D	-2.75	1.45	1.51
24	6	608	CHL	CBD-CAD	-2.75	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	606	CHL	CBD-CAD	-2.75	1.48	1.53
24	y	607	CHL	C2A-C3A	-2.75	1.49	1.55
25	1	604	CLA	CMD-C2D	-2.75	1.45	1.51
36	D	405	PL9	C16-C14	-2.75	1.45	1.51
25	r	616	CLA	C3B-C2B	-2.75	1.36	1.40
24	r	614	CHL	C3B-CAB	-2.75	1.48	1.50
24	y	606	CHL	C2A-C3A	-2.75	1.49	1.55
25	5	613	CLA	C3B-C2B	-2.75	1.36	1.40
35	b	622	LMG	O8-C9	-2.75	1.39	1.45
25	3	614	CLA	CMB-C2B	-2.75	1.46	1.51
25	n	610	CLA	CMB-C2B	-2.75	1.46	1.51
24	N	608	CHL	C2A-C3A	-2.75	1.49	1.55
25	6	614	CLA	CMD-C2D	-2.75	1.45	1.51
24	6	606	CHL	CBD-CAD	-2.75	1.48	1.53
24	7	609	CHL	C1A-C2A	-2.74	1.50	1.53
25	a	406	CLA	CMD-C2D	-2.74	1.45	1.51
25	d	402	CLA	CMC-C2C	-2.74	1.44	1.50
24	Y	606	CHL	C2A-C3A	-2.74	1.49	1.55
24	2	609	CHL	C3B-CAB	-2.74	1.48	1.50
24	1	605	CHL	C3B-CAB	-2.74	1.48	1.50
27	3	1622	XAT	C10-C9	-2.74	1.32	1.35
25	G	611	CLA	C3B-C2B	-2.74	1.36	1.40
25	b	614	CLA	CMD-C2D	-2.74	1.45	1.51
25	N	612	CLA	CMD-C2D	-2.74	1.45	1.51
25	g	614	CLA	CMD-C2D	-2.74	1.45	1.51
25	B	603	CLA	CMB-C2B	-2.74	1.46	1.51
25	b	605	CLA	C3B-C2B	-2.74	1.36	1.40
24	R	614	CHL	C3B-CAB	-2.74	1.48	1.50
25	G	614	CLA	CMD-C2D	-2.74	1.45	1.51
25	b	603	CLA	CMB-C2B	-2.74	1.46	1.51
25	r	603	CLA	CMD-C2D	-2.74	1.45	1.51
25	G	602	CLA	CMC-C2C	-2.74	1.44	1.50
25	5	611	CLA	C3B-C2B	-2.74	1.36	1.40
24	1	609	CHL	CBD-CAD	-2.74	1.49	1.53
24	7	608	CHL	CBD-CAD	-2.74	1.49	1.53
25	a	410	CLA	C3B-C2B	-2.74	1.36	1.40
25	r	602	CLA	CMD-C2D	-2.74	1.45	1.51
25	r	609	CLA	CMD-C2D	-2.74	1.45	1.51
25	N	610	CLA	CMB-C2B	-2.74	1.46	1.51
25	R	603	CLA	CMD-C2D	-2.73	1.45	1.51
24	6	606	CHL	C2A-C3A	-2.73	1.49	1.55
36	d	405	PL9	C11-C9	-2.73	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	609	CLA	CMD-C2D	-2.73	1.45	1.51
25	N	611	CLA	CMB-C2B	-2.73	1.46	1.51
25	B	602	CLA	CMB-C2B	-2.73	1.46	1.51
25	D	402	CLA	CMC-C2C	-2.73	1.44	1.50
35	B	622	LMG	O8-C9	-2.73	1.39	1.45
24	7	607	CHL	C1A-C2A	-2.73	1.50	1.53
25	R	602	CLA	CMD-C2D	-2.73	1.45	1.51
24	y	607	CHL	C3D-CAD	-2.73	1.46	1.51
25	S	613	CLA	CMB-C2B	-2.73	1.46	1.51
24	n	608	CHL	C2A-C3A	-2.73	1.49	1.55
25	R	616	CLA	C3B-C2B	-2.73	1.36	1.40
25	4	602	CLA	CMB-C2B	-2.73	1.46	1.51
25	g	602	CLA	CMD-C2D	-2.73	1.45	1.51
25	y	613	CLA	CMB-C2B	-2.73	1.46	1.51
25	G	602	CLA	CMD-C2D	-2.73	1.45	1.51
25	5	612	CLA	CMB-C2B	-2.73	1.46	1.51
25	c	502	CLA	CMB-C2B	-2.72	1.46	1.51
25	2	614	CLA	CMD-C2D	-2.72	1.45	1.51
25	3	603	CLA	CMB-C2B	-2.72	1.46	1.51
25	b	602	CLA	CMB-C2B	-2.72	1.46	1.51
25	B	603	CLA	CMD-C2D	-2.72	1.45	1.51
25	1	603	CLA	CMD-C2D	-2.72	1.45	1.51
24	5	605	CHL	C3B-CAB	-2.72	1.48	1.50
25	1	613	CLA	C3B-C2B	-2.72	1.36	1.40
26	3	1620	LUT	C22-C21	-2.72	1.51	1.54
25	8	602	CLA	CMB-C2B	-2.72	1.46	1.51
25	Y	613	CLA	CMB-C2B	-2.72	1.46	1.51
24	7	609	CHL	C2B-C1B	-2.72	1.47	1.53
24	Y	607	CHL	C3D-CAD	-2.72	1.46	1.51
25	g	604	CLA	CMD-C2D	-2.72	1.45	1.51
30	b	618	BCR	C21-C22	-2.71	1.32	1.35
25	b	614	CLA	C3B-C2B	-2.71	1.36	1.40
36	d	405	PL9	C41-C39	-2.71	1.45	1.51
25	5	603	CLA	CMD-C2D	-2.71	1.45	1.51
24	4	609	CHL	C2A-C3A	-2.71	1.49	1.55
25	N	612	CLA	CMB-C2B	-2.71	1.46	1.51
24	6	609	CHL	C3B-CAB	-2.71	1.48	1.50
24	6	608	CHL	C2A-C3A	-2.71	1.49	1.55
25	n	614	CLA	CMB-C2B	-2.71	1.46	1.51
25	8	610	CLA	CMC-C2C	-2.71	1.44	1.50
24	3	607	CHL	C1A-C2A	-2.71	1.50	1.53
25	G	604	CLA	CMD-C2D	-2.71	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	612	CLA	CMD-C2D	-2.71	1.45	1.51
25	B	602	CLA	C3B-C2B	-2.71	1.36	1.40
25	B	605	CLA	C3B-C2B	-2.71	1.36	1.40
25	5	613	CLA	CMD-C2D	-2.71	1.45	1.51
25	6	614	CLA	CMB-C2B	-2.71	1.46	1.51
24	Y	607	CHL	C1A-CHA	-2.70	1.49	1.53
24	2	608	CHL	C2A-C3A	-2.70	1.49	1.55
25	b	602	CLA	C3B-C2B	-2.70	1.36	1.40
36	D	405	PL9	C41-C39	-2.70	1.45	1.51
24	g	601	CHL	C3D-CAD	-2.70	1.46	1.51
25	g	611	CLA	C3B-C2B	-2.70	1.36	1.40
25	y	610	CLA	CMC-C2C	-2.70	1.44	1.50
25	7	614	CLA	CMB-C2B	-2.70	1.46	1.51
24	2	606	CHL	C2A-C3A	-2.70	1.49	1.55
25	1	613	CLA	CMD-C2D	-2.70	1.45	1.51
25	Y	602	CLA	CMC-C2C	-2.70	1.44	1.50
25	2	614	CLA	CMB-C2B	-2.70	1.46	1.51
36	D	405	PL9	C11-C9	-2.70	1.45	1.51
25	n	612	CLA	CMB-C2B	-2.70	1.46	1.51
25	5	614	CLA	CMB-C2B	-2.70	1.46	1.51
24	3	609	CHL	C2B-C1B	-2.70	1.47	1.53
26	7	1620	LUT	C22-C21	-2.70	1.51	1.54
25	n	611	CLA	CMB-C2B	-2.70	1.46	1.51
24	G	601	CHL	C3D-CAD	-2.70	1.46	1.51
25	4	610	CLA	CMC-C2C	-2.70	1.44	1.50
25	7	602	CLA	CMB-C2B	-2.69	1.46	1.51
25	2	613	CLA	CMB-C2B	-2.69	1.46	1.51
24	8	609	CHL	C2A-C3A	-2.69	1.49	1.55
25	b	603	CLA	CMD-C2D	-2.69	1.45	1.51
25	1	614	CLA	CMB-C2B	-2.69	1.46	1.51
25	r	612	CLA	CMD-C2D	-2.69	1.45	1.51
24	3	609	CHL	C1A-C2A	-2.69	1.50	1.53
24	Y	609	CHL	C3D-CAD	-2.69	1.46	1.51
25	8	603	CLA	CMB-C2B	-2.69	1.46	1.51
25	4	603	CLA	CMB-C2B	-2.69	1.46	1.51
25	R	611	CLA	CMB-C2B	-2.69	1.46	1.51
30	B	618	BCR	C21-C22	-2.69	1.32	1.35
25	y	602	CLA	CMC-C2C	-2.68	1.45	1.50
25	R	612	CLA	CMD-C2D	-2.68	1.45	1.51
24	1	607	CHL	C3D-CAD	-2.68	1.46	1.51
24	g	608	CHL	C3D-CAD	-2.68	1.46	1.51
24	y	606	CHL	C2B-C1B	-2.68	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	607	CHL	C1A-CHA	-2.68	1.49	1.53
25	N	614	CLA	CMB-C2B	-2.68	1.46	1.51
24	n	607	CHL	C3D-CAD	-2.68	1.46	1.51
25	r	611	CLA	CMB-C2B	-2.68	1.46	1.51
25	A	410	CLA	C3B-C2B	-2.68	1.36	1.40
24	G	608	CHL	C3D-CAD	-2.68	1.46	1.51
24	N	607	CHL	C3D-CAD	-2.68	1.46	1.51
25	3	602	CLA	CMB-C2B	-2.68	1.46	1.51
25	6	613	CLA	CMB-C2B	-2.67	1.46	1.51
24	r	608	CHL	C2B-C1B	-2.67	1.48	1.53
25	g	611	CLA	CMD-C2D	-2.67	1.45	1.51
24	n	605	CHL	C3B-CAB	-2.67	1.48	1.50
24	R	608	CHL	C2B-C1B	-2.67	1.48	1.53
24	4	609	CHL	CBD-CAD	-2.67	1.49	1.53
24	g	606	CHL	C2A-C3A	-2.67	1.49	1.55
24	N	608	CHL	C2B-C1B	-2.67	1.48	1.53
24	Y	606	CHL	C2B-C1B	-2.67	1.48	1.53
24	R	608	CHL	C2A-C3A	-2.67	1.49	1.55
24	3	607	CHL	C3B-CAB	-2.67	1.48	1.50
25	b	613	CLA	CMC-C2C	-2.67	1.45	1.50
25	Y	604	CLA	CMD-C2D	-2.67	1.45	1.51
24	n	607	CHL	C2A-C3A	-2.67	1.49	1.55
25	r	612	CLA	C3B-C2B	-2.67	1.36	1.40
24	N	605	CHL	C3B-CAB	-2.67	1.48	1.50
24	3	608	CHL	C2A-C3A	-2.67	1.49	1.55
25	1	610	CLA	CMB-C2B	-2.67	1.46	1.51
24	5	607	CHL	C3D-CAD	-2.67	1.46	1.51
24	N	607	CHL	C2A-C3A	-2.67	1.49	1.55
29	R	2630	LHG	O7-C5	-2.66	1.39	1.46
25	y	604	CLA	CMD-C2D	-2.66	1.45	1.51
29	r	2630	LHG	O7-C5	-2.66	1.39	1.46
25	Y	610	CLA	CMC-C2C	-2.66	1.45	1.50
25	1	602	CLA	C3B-C2B	-2.66	1.36	1.40
24	y	607	CHL	CBD-CGD	-2.66	1.47	1.52
29	c	522	LHG	O7-C5	-2.66	1.39	1.46
25	C	501	CLA	CMD-C2D	-2.66	1.45	1.51
24	7	607	CHL	C3B-CAB	-2.66	1.48	1.50
24	y	609	CHL	C3D-CAD	-2.66	1.46	1.51
25	C	512	CLA	CMD-C2D	-2.66	1.45	1.51
37	c	519	DGD	O1G-C1G	-2.66	1.39	1.45
24	r	608	CHL	C2A-C3A	-2.66	1.49	1.55
25	5	610	CLA	CMB-C2B	-2.66	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	522	LHG	O7-C5	-2.66	1.39	1.46
25	B	613	CLA	CMC-C2C	-2.66	1.45	1.50
24	n	608	CHL	C2B-C1B	-2.65	1.48	1.53
37	C	519	DGD	O1G-C1G	-2.65	1.39	1.45
24	G	606	CHL	C2A-C3A	-2.65	1.49	1.55
25	B	603	CLA	C3B-C2B	-2.65	1.36	1.40
24	7	608	CHL	C2A-C3A	-2.65	1.49	1.55
25	7	602	CLA	CMC-C2C	-2.65	1.45	1.50
24	g	607	CHL	C2A-C3A	-2.65	1.49	1.55
24	Y	607	CHL	CBD-CGD	-2.65	1.47	1.52
24	y	601	CHL	C2A-C3A	-2.65	1.49	1.55
25	6	611	CLA	CMD-C2D	-2.65	1.45	1.51
27	7	1622	XAT	C14-C13	-2.64	1.32	1.35
24	Y	601	CHL	C2A-C3A	-2.64	1.49	1.55
25	2	611	CLA	CMD-C2D	-2.64	1.46	1.51
25	G	614	CLA	CMB-C2B	-2.64	1.46	1.51
25	2	611	CLA	CMB-C2B	-2.64	1.46	1.51
25	1	612	CLA	CMD-C2D	-2.64	1.46	1.51
25	R	612	CLA	C3B-C2B	-2.64	1.36	1.40
24	r	608	CHL	C3B-CAB	-2.64	1.48	1.50
24	G	607	CHL	C2A-C3A	-2.64	1.49	1.55
24	8	609	CHL	CBD-CAD	-2.64	1.49	1.53
25	B	614	CLA	C3B-C2B	-2.64	1.36	1.40
25	5	602	CLA	C3B-C2B	-2.64	1.36	1.40
24	6	605	CHL	CBD-CAD	-2.64	1.49	1.53
25	c	512	CLA	CMD-C2D	-2.64	1.46	1.51
25	g	614	CLA	CMB-C2B	-2.64	1.46	1.51
24	3	605	CHL	C2A-C3A	-2.63	1.49	1.55
25	6	603	CLA	CMB-C2B	-2.63	1.46	1.51
25	2	603	CLA	CMB-C2B	-2.63	1.46	1.51
25	y	614	CLA	C3B-CAB	-2.63	1.42	1.47
37	c	520	DGD	O5D-C6D	-2.63	1.39	1.43
25	B	611	CLA	C3B-CAB	-2.63	1.42	1.47
37	c	518	DGD	O1G-C1G	-2.63	1.39	1.45
25	Y	614	CLA	C3B-CAB	-2.63	1.42	1.47
29	s	2630	LHG	O7-C5	-2.63	1.39	1.46
24	7	605	CHL	C2A-C3A	-2.63	1.49	1.55
24	Y	608	CHL	C2A-C3A	-2.63	1.49	1.55
25	4	611	CLA	CMD-C2D	-2.63	1.46	1.51
25	3	602	CLA	CMC-C2C	-2.63	1.45	1.50
25	B	608	CLA	CMC-C2C	-2.63	1.45	1.50
24	7	606	CHL	C3B-CAB	-2.63	1.48	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	2630	LHG	O7-C5	-2.62	1.39	1.46
25	6	611	CLA	CMB-C2B	-2.62	1.46	1.51
25	G	611	CLA	CMD-C2D	-2.62	1.46	1.51
25	c	501	CLA	CMD-C2D	-2.62	1.46	1.51
24	y	608	CHL	C2A-C3A	-2.62	1.49	1.55
25	A	407	CLA	C3B-C2B	-2.62	1.36	1.40
25	7	610	CLA	CMD-C2D	-2.62	1.46	1.51
37	C	518	DGD	O1G-C1G	-2.62	1.39	1.45
25	3	610	CLA	CMD-C2D	-2.62	1.46	1.51
27	3	1622	XAT	C34-C33	-2.62	1.32	1.35
25	N	602	CLA	CMD-C2D	-2.62	1.46	1.51
25	n	602	CLA	CMD-C2D	-2.62	1.46	1.51
24	2	605	CHL	CBD-CAD	-2.62	1.49	1.53
25	a	407	CLA	C3B-C2B	-2.62	1.36	1.40
24	8	601	CHL	CHD-C4C	-2.62	1.48	1.53
26	5	1621	LUT	C10-C9	-2.62	1.32	1.35
37	C	520	DGD	O5D-C6D	-2.62	1.39	1.43
25	6	602	CLA	CMB-C2B	-2.62	1.46	1.51
25	g	610	CLA	CMD-C2D	-2.61	1.46	1.51
24	g	609	CHL	C3D-CAD	-2.61	1.46	1.51
25	s	610	CLA	CMB-C2B	-2.61	1.46	1.51
25	B	607	CLA	CMC-C2C	-2.61	1.45	1.50
27	3	1622	XAT	C14-C13	-2.61	1.32	1.35
25	b	608	CLA	CMC-C2C	-2.61	1.45	1.50
25	S	614	CLA	CMD-C2D	-2.61	1.46	1.51
25	2	602	CLA	CMC-C2C	-2.61	1.45	1.50
25	2	610	CLA	CMD-C2D	-2.61	1.46	1.51
25	8	611	CLA	CMD-C2D	-2.61	1.46	1.51
25	b	609	CLA	CMB-C2B	-2.61	1.46	1.51
25	r	601	CLA	CMB-C2B	-2.61	1.46	1.51
24	r	607	CHL	C2B-C1B	-2.61	1.48	1.53
25	5	612	CLA	CMD-C2D	-2.61	1.46	1.51
24	4	601	CHL	CHD-C4C	-2.60	1.48	1.53
24	g	608	CHL	C1A-C2A	-2.60	1.50	1.53
25	R	601	CLA	CMB-C2B	-2.60	1.46	1.51
24	5	608	CHL	CBD-CGD	-2.60	1.47	1.52
25	s	614	CLA	CMD-C2D	-2.60	1.46	1.51
24	R	608	CHL	C3B-CAB	-2.60	1.48	1.50
26	1	1621	LUT	C10-C9	-2.60	1.32	1.35
24	3	601	CHL	C2B-C1B	-2.60	1.48	1.53
24	1	606	CHL	C2A-C3A	-2.60	1.49	1.55
25	B	613	CLA	CMA-C3A	-2.60	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	611	CLA	C3B-CAB	-2.60	1.42	1.47
25	r	604	CLA	C3B-C2B	-2.60	1.36	1.40
24	s	608	CHL	C1A-CHA	-2.60	1.49	1.53
25	6	610	CLA	CMD-C2D	-2.60	1.46	1.51
25	6	602	CLA	CMC-C2C	-2.60	1.45	1.50
25	s	611	CLA	CMB-C2B	-2.60	1.46	1.51
24	7	601	CHL	C2B-C1B	-2.59	1.48	1.53
25	B	609	CLA	CMB-C2B	-2.59	1.46	1.51
25	C	505	CLA	CMB-C2B	-2.59	1.46	1.51
25	8	604	CLA	CMD-C2D	-2.59	1.46	1.51
24	G	608	CHL	C1A-C2A	-2.59	1.50	1.53
25	4	611	CLA	CMB-C2B	-2.59	1.46	1.51
25	b	607	CLA	CMC-C2C	-2.59	1.45	1.50
24	2	607	CHL	C2A-C3A	-2.59	1.49	1.55
27	7	1622	XAT	C34-C33	-2.59	1.32	1.35
24	1	601	CHL	C2A-C3A	-2.59	1.49	1.55
25	4	604	CLA	CMD-C2D	-2.59	1.46	1.51
25	C	511	CLA	CMB-C2B	-2.59	1.46	1.51
25	8	611	CLA	CMB-C2B	-2.59	1.46	1.51
25	S	610	CLA	CMB-C2B	-2.59	1.46	1.51
25	8	610	CLA	CMB-C2B	-2.59	1.46	1.51
25	r	611	CLA	C3B-C2B	-2.59	1.36	1.40
24	1	608	CHL	CBD-CGD	-2.58	1.47	1.52
24	3	601	CHL	C2A-C3A	-2.58	1.49	1.55
25	2	602	CLA	CMB-C2B	-2.58	1.46	1.51
26	5	1621	LUT	C1-C6	-2.58	1.50	1.53
24	g	608	CHL	CBD-CAD	-2.58	1.49	1.53
25	4	610	CLA	CMB-C2B	-2.58	1.46	1.51
25	R	604	CLA	C3B-C2B	-2.58	1.36	1.40
24	8	606	CHL	CBD-CAD	-2.58	1.49	1.53
25	b	613	CLA	CMA-C3A	-2.58	1.47	1.53
24	4	607	CHL	C2A-C3A	-2.58	1.49	1.55
25	b	603	CLA	C3B-C2B	-2.58	1.36	1.40
25	s	602	CLA	CMB-C2B	-2.58	1.46	1.51
25	2	604	CLA	CMD-C2D	-2.58	1.46	1.51
25	S	604	CLA	CMB-C2B	-2.58	1.46	1.51
25	G	610	CLA	CMD-C2D	-2.58	1.46	1.51
24	6	605	CHL	C2A-C3A	-2.58	1.49	1.55
25	5	604	CLA	C3B-CAB	-2.58	1.42	1.47
25	c	505	CLA	CMB-C2B	-2.57	1.46	1.51
28	g	1623	NEX	C7-C8	-2.57	1.27	1.32
24	4	607	CHL	CBD-CAD	-2.57	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	606	CHL	C2A-C3A	-2.57	1.49	1.55
25	g	613	CLA	CMD-C2D	-2.57	1.46	1.51
24	6	607	CHL	C2A-C3A	-2.57	1.49	1.55
26	3	1621	LUT	C22-C21	-2.57	1.51	1.54
25	r	616	CLA	CMD-C2D	-2.57	1.46	1.51
24	y	605	CHL	CBD-CAD	-2.57	1.49	1.53
24	7	601	CHL	C2A-C3A	-2.57	1.49	1.55
25	c	511	CLA	CMB-C2B	-2.57	1.46	1.51
26	7	1621	LUT	C22-C21	-2.57	1.51	1.54
24	y	605	CHL	C2B-C1B	-2.57	1.48	1.53
25	R	611	CLA	C3B-C2B	-2.57	1.37	1.40
25	n	612	CLA	C3B-C2B	-2.57	1.37	1.40
25	n	610	CLA	CMD-C2D	-2.57	1.46	1.51
24	G	609	CHL	C3D-CAD	-2.56	1.46	1.51
24	3	606	CHL	C3B-CAB	-2.56	1.48	1.50
24	Y	606	CHL	C2D-C1D	-2.56	1.48	1.53
24	4	606	CHL	CBD-CAD	-2.56	1.49	1.53
24	y	606	CHL	C2D-C1D	-2.56	1.48	1.53
24	2	605	CHL	C2A-C3A	-2.56	1.49	1.55
25	G	613	CLA	CMD-C2D	-2.56	1.46	1.51
25	N	612	CLA	C3B-C2B	-2.56	1.37	1.40
25	R	602	CLA	CMB-C2B	-2.56	1.46	1.51
24	5	601	CHL	C2A-C3A	-2.56	1.50	1.55
25	G	603	CLA	CMD-C2D	-2.56	1.46	1.51
25	S	611	CLA	CMB-C2B	-2.56	1.46	1.51
24	S	608	CHL	C1A-CHA	-2.56	1.49	1.53
25	N	613	CLA	CMB-C2B	-2.56	1.46	1.51
24	R	607	CHL	C2B-C1B	-2.56	1.48	1.53
25	s	612	CLA	CMD-C2D	-2.56	1.46	1.51
25	g	603	CLA	CMD-C2D	-2.56	1.46	1.51
24	s	606	CHL	C1A-C2A	-2.56	1.50	1.53
24	G	608	CHL	C2A-C3A	-2.56	1.50	1.55
25	r	602	CLA	CMB-C2B	-2.56	1.46	1.51
25	l	604	CLA	C3B-CAB	-2.56	1.42	1.47
25	b	604	CLA	C3B-CAB	-2.56	1.42	1.47
25	N	610	CLA	CMD-C2D	-2.55	1.46	1.51
25	S	612	CLA	CMD-C2D	-2.55	1.46	1.51
24	8	607	CHL	C2A-C3A	-2.55	1.50	1.55
25	s	604	CLA	CMB-C2B	-2.55	1.46	1.51
25	S	602	CLA	CMB-C2B	-2.55	1.46	1.51
24	n	601	CHL	CBD-CAD	-2.55	1.49	1.53
24	n	601	CHL	C2B-C1B	-2.55	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	601	CHL	C2B-C1B	-2.55	1.48	1.53
24	6	609	CHL	C1A-C2A	-2.55	1.50	1.53
25	2	613	CLA	C3B-C2B	-2.55	1.37	1.40
24	4	609	CHL	C2B-C1B	-2.55	1.48	1.53
24	Y	605	CHL	CBD-CAD	-2.55	1.49	1.53
24	S	606	CHL	C1A-C2A	-2.55	1.50	1.53
24	4	606	CHL	C1A-C2A	-2.55	1.50	1.53
24	4	607	CHL	C2B-C1B	-2.55	1.48	1.53
24	7	609	CHL	CBD-CAD	-2.55	1.49	1.53
28	G	1623	NEX	C7-C8	-2.55	1.27	1.32
24	5	606	CHL	C3D-CAD	-2.54	1.46	1.51
25	N	614	CLA	CMD-C2D	-2.54	1.46	1.51
25	n	613	CLA	CMB-C2B	-2.54	1.46	1.51
24	8	607	CHL	C2B-C1B	-2.54	1.48	1.53
25	5	611	CLA	CMD-C2D	-2.54	1.46	1.51
24	6	605	CHL	C3B-CAB	-2.54	1.48	1.50
24	8	607	CHL	CBD-CAD	-2.54	1.49	1.53
25	6	604	CLA	CMD-C2D	-2.54	1.46	1.51
24	N	605	CHL	C2B-C1B	-2.54	1.48	1.53
25	d	402	CLA	C3B-C2B	-2.54	1.37	1.40
25	N	611	CLA	CMD-C2D	-2.54	1.46	1.51
24	n	601	CHL	C2A-C3A	-2.54	1.50	1.55
24	Y	605	CHL	C2B-C1B	-2.54	1.48	1.53
25	c	507	CLA	CMB-C2B	-2.54	1.46	1.51
25	C	503	CLA	CMB-C2B	-2.54	1.46	1.51
24	R	606	CHL	C3B-CAB	-2.54	1.48	1.50
24	G	608	CHL	CBD-CAD	-2.54	1.49	1.53
24	r	606	CHL	C3B-CAB	-2.53	1.48	1.50
24	g	608	CHL	C2A-C3A	-2.53	1.50	1.55
25	c	503	CLA	CMB-C2B	-2.53	1.46	1.51
25	R	616	CLA	CMD-C2D	-2.53	1.46	1.51
24	N	608	CHL	C1A-C2A	-2.53	1.50	1.53
25	B	604	CLA	C3B-CAB	-2.53	1.42	1.47
25	A	405	CLA	CMB-C2B	-2.53	1.46	1.51
24	N	601	CHL	C2A-C3A	-2.53	1.50	1.55
24	Y	601	CHL	C2B-C1B	-2.53	1.48	1.53
24	g	608	CHL	C2B-C1B	-2.53	1.48	1.53
25	6	612	CLA	CMD-C2D	-2.53	1.46	1.51
24	3	609	CHL	CBD-CAD	-2.53	1.49	1.53
25	n	614	CLA	CMD-C2D	-2.53	1.46	1.51
24	y	601	CHL	C2B-C1B	-2.53	1.48	1.53
36	d	405	PL9	C35-C34	-2.53	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	CMD-C2D	-2.53	1.46	1.51
24	8	609	CHL	C2B-C1B	-2.52	1.48	1.53
27	Y	1622	XAT	C10-C9	-2.52	1.32	1.35
24	2	609	CHL	C1A-C2A	-2.52	1.50	1.53
25	c	506	CLA	CMD-C2D	-2.52	1.46	1.51
24	N	607	CHL	C2B-C1B	-2.52	1.48	1.53
24	n	605	CHL	C2B-C1B	-2.52	1.48	1.53
25	G	612	CLA	CMB-C2B	-2.52	1.46	1.51
25	6	613	CLA	C3B-C2B	-2.52	1.37	1.40
25	b	616	CLA	CMC-C2C	-2.52	1.45	1.50
25	B	616	CLA	CMC-C2C	-2.52	1.45	1.50
24	8	609	CHL	C1A-C2A	-2.52	1.50	1.53
24	G	601	CHL	C2A-C3A	-2.52	1.50	1.55
37	H	102	DGD	O3E-C3E	-2.52	1.37	1.43
25	g	612	CLA	CMB-C2B	-2.52	1.46	1.51
26	y	1620	LUT	C14-C13	-2.52	1.32	1.35
24	8	606	CHL	C1A-C2A	-2.52	1.50	1.53
25	5	602	CLA	C3B-CAB	-2.52	1.42	1.47
24	n	607	CHL	C2B-C1B	-2.52	1.48	1.53
24	N	609	CHL	C3D-CAD	-2.52	1.46	1.51
25	N	602	CLA	CMC-C2C	-2.52	1.45	1.50
25	n	602	CLA	CMC-C2C	-2.52	1.45	1.50
25	1	610	CLA	CMD-C2D	-2.52	1.46	1.51
24	y	607	CHL	C1A-C2A	-2.52	1.50	1.53
25	B	614	CLA	CMC-C2C	-2.52	1.45	1.50
36	D	405	PL9	C35-C34	-2.52	1.44	1.50
36	d	405	PL9	C2-C1	-2.52	1.37	1.44
26	1	1621	LUT	C1-C6	-2.51	1.50	1.53
25	C	507	CLA	CMB-C2B	-2.51	1.46	1.51
25	a	405	CLA	CMB-C2B	-2.51	1.46	1.51
24	g	601	CHL	C2A-C3A	-2.51	1.50	1.55
25	B	606	CLA	CMC-C2C	-2.51	1.45	1.50
25	n	611	CLA	CMD-C2D	-2.51	1.46	1.51
25	5	610	CLA	CMD-C2D	-2.51	1.46	1.51
37	h	102	DGD	O3E-C3E	-2.51	1.37	1.43
25	b	613	CLA	C3B-CAB	-2.51	1.42	1.47
24	s	601	CHL	C2B-C1B	-2.51	1.48	1.53
25	1	611	CLA	CMD-C2D	-2.51	1.46	1.51
25	D	402	CLA	C3B-C2B	-2.51	1.37	1.40
24	N	601	CHL	CBD-CAD	-2.51	1.49	1.53
25	b	615	CLA	CMC-C2C	-2.51	1.45	1.50
25	r	611	CLA	CMD-C2D	-2.51	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	605	CHL	C3B-CAB	-2.51	1.48	1.50
25	2	612	CLA	CMD-C2D	-2.51	1.46	1.51
25	G	613	CLA	CMB-C2B	-2.51	1.46	1.51
25	S	602	CLA	CMD-C2D	-2.51	1.46	1.51
30	b	620	BCR	C1-C6	-2.51	1.50	1.53
25	s	602	CLA	CMD-C2D	-2.51	1.46	1.51
24	g	607	CHL	C2B-C1B	-2.50	1.48	1.53
26	N	1620	LUT	C22-C21	-2.50	1.51	1.54
25	7	604	CLA	CMD-C2D	-2.50	1.46	1.51
25	3	604	CLA	CMD-C2D	-2.50	1.46	1.51
24	S	601	CHL	C2B-C1B	-2.50	1.48	1.53
30	B	620	BCR	C1-C6	-2.50	1.50	1.53
25	1	602	CLA	C3B-CAB	-2.50	1.42	1.47
25	Y	610	CLA	C3B-CAB	-2.50	1.42	1.47
25	b	614	CLA	CMC-C2C	-2.50	1.45	1.50
24	4	609	CHL	C1A-C2A	-2.50	1.50	1.53
25	C	511	CLA	CMD-C2D	-2.50	1.46	1.51
36	D	405	PL9	C2-C1	-2.49	1.37	1.44
24	G	607	CHL	C2B-C1B	-2.49	1.48	1.53
24	G	606	CHL	C3D-CAD	-2.49	1.46	1.51
25	B	613	CLA	C3B-CAB	-2.49	1.42	1.47
25	R	611	CLA	CMD-C2D	-2.49	1.46	1.51
24	n	608	CHL	C1A-C2A	-2.49	1.50	1.53
24	1	606	CHL	C3D-CAD	-2.49	1.46	1.51
27	y	1622	XAT	C10-C9	-2.49	1.32	1.35
24	6	607	CHL	CBD-CAD	-2.49	1.49	1.53
24	3	606	CHL	C3D-CAD	-2.49	1.46	1.51
25	b	606	CLA	CMC-C2C	-2.49	1.45	1.50
24	2	607	CHL	CBD-CAD	-2.49	1.49	1.53
24	7	606	CHL	C3D-CAD	-2.49	1.46	1.51
24	5	606	CHL	C1A-C2A	-2.49	1.50	1.53
24	3	609	CHL	C2A-C3A	-2.49	1.50	1.55
25	s	609	CLA	CMB-C2B	-2.49	1.46	1.51
26	Y	1620	LUT	C14-C13	-2.49	1.32	1.35
25	8	612	CLA	CMB-C2B	-2.49	1.46	1.51
25	c	507	CLA	CMD-C2D	-2.49	1.46	1.51
25	4	612	CLA	CMB-C2B	-2.49	1.46	1.51
24	G	608	CHL	C2B-C1B	-2.49	1.48	1.53
25	y	610	CLA	C3B-CAB	-2.48	1.42	1.47
26	1	1621	LUT	C22-C21	-2.48	1.51	1.54
25	c	511	CLA	CMD-C2D	-2.48	1.46	1.51
25	r	613	CLA	C3B-CAB	-2.48	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	613	CLA	CMD-C2D	-2.48	1.46	1.51
24	n	609	CHL	C3D-CAD	-2.48	1.46	1.51
25	g	613	CLA	CMB-C2B	-2.48	1.46	1.51
24	3	607	CHL	C2B-C1B	-2.48	1.48	1.53
24	1	601	CHL	CBD-CGD	-2.48	1.48	1.52
24	2	601	CHL	C3D-CAD	-2.48	1.46	1.51
25	G	610	CLA	C3B-C2B	-2.48	1.37	1.40
25	b	612	CLA	C3B-CAB	-2.48	1.43	1.47
24	2	601	CHL	CBD-CAD	-2.48	1.49	1.53
24	6	601	CHL	CBD-CAD	-2.48	1.49	1.53
24	s	601	CHL	C2A-C3A	-2.47	1.50	1.55
24	5	601	CHL	CBD-CGD	-2.47	1.48	1.52
25	S	611	CLA	CMD-C2D	-2.47	1.46	1.51
24	7	609	CHL	C2A-C3A	-2.47	1.50	1.55
25	S	609	CLA	CMB-C2B	-2.47	1.46	1.51
25	g	610	CLA	C3B-C2B	-2.47	1.37	1.40
25	B	615	CLA	CMC-C2C	-2.47	1.45	1.50
25	7	614	CLA	CMD-C2D	-2.47	1.46	1.51
24	2	601	CHL	C2B-C1B	-2.47	1.48	1.53
25	R	613	CLA	C3B-CAB	-2.47	1.43	1.47
24	1	609	CHL	C3D-CAD	-2.47	1.46	1.51
36	D	405	PL9	C46-C44	-2.47	1.45	1.51
36	d	405	PL9	C46-C44	-2.47	1.45	1.51
25	S	610	CLA	C3B-CAB	-2.47	1.43	1.47
37	C	520	DGD	O1G-C1G	-2.47	1.39	1.45
25	B	612	CLA	C3B-CAB	-2.47	1.43	1.47
25	C	507	CLA	CMD-C2D	-2.47	1.46	1.51
24	G	607	CHL	C1A-C2A	-2.47	1.50	1.53
24	Y	607	CHL	C1A-C2A	-2.47	1.50	1.53
25	2	610	CLA	C3B-CAB	-2.47	1.43	1.47
24	g	607	CHL	C1A-C2A	-2.46	1.50	1.53
25	s	610	CLA	C3B-CAB	-2.46	1.43	1.47
25	Y	602	CLA	C3B-C2B	-2.46	1.37	1.40
24	S	601	CHL	C2A-C3A	-2.46	1.50	1.55
25	6	604	CLA	C3B-C2B	-2.46	1.37	1.40
36	D	405	PL9	C21-C19	-2.46	1.45	1.51
25	S	613	CLA	CMD-C2D	-2.46	1.46	1.51
24	2	608	CHL	C3D-CAD	-2.46	1.46	1.51
24	6	601	CHL	C3D-CAD	-2.46	1.46	1.51
25	s	611	CLA	CMD-C2D	-2.46	1.46	1.51
24	7	607	CHL	C2B-C1B	-2.46	1.48	1.53
25	2	604	CLA	C3B-C2B	-2.46	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	602	CLA	C3B-C2B	-2.46	1.37	1.40
37	c	520	DGD	O1G-C1G	-2.46	1.39	1.45
36	d	405	PL9	C21-C19	-2.46	1.45	1.51
24	6	608	CHL	C3D-CAD	-2.46	1.46	1.51
24	1	606	CHL	C1A-C2A	-2.45	1.50	1.53
25	3	604	CLA	C3B-CAB	-2.45	1.43	1.47
24	N	609	CHL	C3B-CAB	-2.45	1.48	1.50
25	7	604	CLA	C3B-CAB	-2.45	1.43	1.47
24	g	606	CHL	C3D-CAD	-2.45	1.46	1.51
25	C	512	CLA	CMB-C2B	-2.45	1.46	1.51
25	A	410	CLA	C3B-CAB	-2.45	1.43	1.47
25	6	610	CLA	C3B-CAB	-2.45	1.43	1.47
24	y	601	CHL	CBD-CGD	-2.45	1.48	1.52
25	C	503	CLA	CMD-C2D	-2.45	1.46	1.51
25	3	614	CLA	CMD-C2D	-2.45	1.46	1.51
25	7	612	CLA	C3B-CAB	-2.45	1.43	1.47
24	5	609	CHL	C3D-CAD	-2.45	1.46	1.51
24	1	608	CHL	C3B-CAB	-2.45	1.48	1.50
24	7	607	CHL	C2A-C3A	-2.44	1.50	1.55
26	n	1620	LUT	C22-C21	-2.44	1.51	1.54
24	3	607	CHL	C2A-C3A	-2.44	1.50	1.55
25	s	603	CLA	CMB-C2B	-2.44	1.46	1.51
26	G	1621	LUT	C1-C6	-2.44	1.50	1.53
25	R	601	CLA	CMD-C2D	-2.44	1.46	1.51
25	C	508	CLA	CMD-C2D	-2.44	1.46	1.51
24	6	601	CHL	C2B-C1B	-2.44	1.48	1.53
29	c	2630	LHG	O7-C5	-2.44	1.40	1.46
24	2	608	CHL	C1A-C2A	-2.44	1.50	1.53
25	3	612	CLA	C3B-CAB	-2.44	1.43	1.47
25	c	503	CLA	CMD-C2D	-2.43	1.46	1.51
25	C	513	CLA	CMD-C2D	-2.43	1.46	1.51
25	S	603	CLA	CMB-C2B	-2.43	1.46	1.51
26	R	620	LUT	C22-C21	-2.43	1.51	1.54
29	C	2630	LHG	O7-C5	-2.43	1.40	1.46
24	Y	601	CHL	CBD-CGD	-2.43	1.48	1.52
25	r	601	CLA	CMD-C2D	-2.43	1.46	1.51
26	g	1621	LUT	C1-C6	-2.43	1.50	1.53
24	1	607	CHL	CBD-CGD	-2.43	1.48	1.52
26	R	620	LUT	C1-C6	-2.43	1.50	1.53
25	s	603	CLA	CMD-C2D	-2.43	1.46	1.51
25	S	603	CLA	CMD-C2D	-2.43	1.46	1.51
25	c	508	CLA	CMD-C2D	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	609	CHL	C3B-CAB	-2.43	1.48	1.50
35	B	622	LMG	O7-C8	-2.43	1.40	1.46
26	5	1621	LUT	C22-C21	-2.42	1.51	1.54
25	1	602	CLA	CMC-C2C	-2.42	1.45	1.50
25	S	614	CLA	CMB-C2B	-2.42	1.46	1.51
25	a	410	CLA	C3B-CAB	-2.42	1.43	1.47
25	s	614	CLA	CMB-C2B	-2.42	1.46	1.51
24	Y	605	CHL	C2A-C3A	-2.42	1.50	1.55
24	5	607	CHL	CBD-CGD	-2.42	1.48	1.52
35	b	622	LMG	O7-C8	-2.42	1.40	1.46
25	c	513	CLA	CMD-C2D	-2.41	1.46	1.51
25	C	504	CLA	CMD-C2D	-2.41	1.46	1.51
26	y	1620	LUT	C10-C9	-2.41	1.32	1.35
24	n	605	CHL	C2A-C3A	-2.41	1.50	1.55
25	r	602	CLA	CMC-C2C	-2.41	1.45	1.50
25	y	613	CLA	C3B-C2B	-2.41	1.37	1.40
24	1	609	CHL	CBD-CGD	-2.41	1.48	1.52
25	c	512	CLA	CMB-C2B	-2.41	1.46	1.51
24	N	605	CHL	C2A-C3A	-2.41	1.50	1.55
24	5	609	CHL	CBD-CGD	-2.41	1.48	1.52
25	c	508	CLA	CMC-C2C	-2.41	1.45	1.50
25	c	504	CLA	CMD-C2D	-2.40	1.46	1.51
25	Y	602	CLA	C3B-CAB	-2.40	1.43	1.47
25	5	602	CLA	CMC-C2C	-2.40	1.45	1.50
25	Y	613	CLA	CMD-C2D	-2.40	1.46	1.51
25	4	604	CLA	C3B-CAB	-2.40	1.43	1.47
25	y	602	CLA	C3B-CAB	-2.40	1.43	1.47
25	b	603	CLA	C3B-CAB	-2.40	1.43	1.47
25	4	602	CLA	CMD-C2D	-2.39	1.46	1.51
25	C	508	CLA	CMC-C2C	-2.39	1.45	1.50
24	8	609	CHL	C3D-CAD	-2.39	1.46	1.51
25	r	610	CLA	C3B-CAB	-2.39	1.43	1.47
24	8	607	CHL	C3B-CAB	-2.39	1.48	1.50
25	y	604	CLA	CMC-C2C	-2.39	1.45	1.50
24	6	608	CHL	C1A-C2A	-2.39	1.50	1.53
25	B	617	CLA	C3B-C2B	-2.39	1.37	1.40
25	y	613	CLA	CMD-C2D	-2.39	1.46	1.51
25	N	610	CLA	C3B-CAB	-2.39	1.43	1.47
24	y	605	CHL	C2A-C3A	-2.38	1.50	1.55
25	g	614	CLA	C3B-C2B	-2.38	1.37	1.40
24	3	601	CHL	CBD-CGD	-2.38	1.48	1.52
24	g	607	CHL	C3D-CAD	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	617	CLA	C3B-C2B	-2.38	1.37	1.40
25	n	610	CLA	C3B-CAB	-2.38	1.43	1.47
26	r	620	LUT	C1-C6	-2.38	1.50	1.53
25	D	402	CLA	C3B-CAB	-2.38	1.43	1.47
25	8	602	CLA	CMD-C2D	-2.38	1.46	1.51
25	R	602	CLA	CMC-C2C	-2.38	1.45	1.50
25	B	615	CLA	C3B-CAB	-2.38	1.43	1.47
25	8	604	CLA	C3B-CAB	-2.38	1.43	1.47
24	4	609	CHL	C3D-CAD	-2.37	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.37	1.46	1.51
25	B	609	CLA	CMC-C2C	-2.37	1.45	1.50
26	Y	1620	LUT	C10-C9	-2.37	1.32	1.35
25	R	610	CLA	C3B-CAB	-2.37	1.43	1.47
25	Y	613	CLA	C3B-C2B	-2.37	1.37	1.40
25	G	612	CLA	C3B-C2B	-2.37	1.37	1.40
25	G	614	CLA	C3B-C2B	-2.37	1.37	1.40
25	d	402	CLA	C3B-CAB	-2.36	1.43	1.47
24	5	608	CHL	C3B-CAB	-2.36	1.48	1.50
25	B	605	CLA	C3B-CAB	-2.36	1.43	1.47
25	Y	604	CLA	CMC-C2C	-2.36	1.45	1.50
25	b	605	CLA	C3B-CAB	-2.36	1.43	1.47
25	c	513	CLA	CMB-C2B	-2.36	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.36	1.46	1.51
26	r	620	LUT	C22-C21	-2.36	1.51	1.54
24	5	601	CHL	C2B-C1B	-2.36	1.48	1.53
25	b	609	CLA	CMC-C2C	-2.36	1.45	1.50
25	4	610	CLA	C3B-C2B	-2.36	1.37	1.40
25	B	603	CLA	C3B-CAB	-2.36	1.43	1.47
25	g	612	CLA	C3B-C2B	-2.36	1.37	1.40
34	A	412	SQD	O2-C2	-2.36	1.37	1.43
25	b	615	CLA	C3B-CAB	-2.36	1.43	1.47
25	B	616	CLA	C3B-CAB	-2.36	1.43	1.47
25	s	612	CLA	CMB-C2B	-2.36	1.46	1.51
25	S	612	CLA	CMB-C2B	-2.36	1.46	1.51
24	5	605	CHL	C2A-C3A	-2.36	1.50	1.55
25	c	510	CLA	CMB-C2B	-2.36	1.46	1.51
24	1	601	CHL	C2B-C1B	-2.36	1.48	1.53
24	4	607	CHL	C3B-CAB	-2.35	1.48	1.50
24	7	607	CHL	C3D-CAD	-2.35	1.47	1.51
34	a	412	SQD	O2-C2	-2.35	1.37	1.43
24	r	606	CHL	C3D-CAD	-2.35	1.47	1.51
25	b	616	CLA	C3B-CAB	-2.35	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	607	CHL	C3D-CAD	-2.35	1.47	1.51
28	R	623	NEX	C30-C29	-2.35	1.32	1.35
25	c	506	CLA	C3B-C2B	-2.35	1.37	1.40
25	N	613	CLA	CMD-C2D	-2.35	1.46	1.51
25	B	606	CLA	C3B-CAB	-2.35	1.43	1.47
25	n	613	CLA	CMD-C2D	-2.35	1.46	1.51
29	5	2630	LHG	O7-C5	-2.35	1.40	1.46
25	N	611	CLA	C3B-C2B	-2.35	1.37	1.40
25	s	610	CLA	C3B-C2B	-2.35	1.37	1.40
24	3	607	CHL	C3D-CAD	-2.34	1.47	1.51
25	b	606	CLA	C3B-CAB	-2.34	1.43	1.47
28	r	623	NEX	C30-C29	-2.34	1.32	1.35
24	7	605	CHL	C2B-C1B	-2.34	1.48	1.53
25	Y	612	CLA	CMC-C2C	-2.34	1.45	1.50
25	C	506	CLA	C3B-C2B	-2.34	1.37	1.40
24	s	606	CHL	C2B-C1B	-2.34	1.48	1.53
24	3	605	CHL	C2B-C1B	-2.34	1.48	1.53
25	s	610	CLA	CMD-C2D	-2.34	1.46	1.51
29	1	2630	LHG	O7-C5	-2.34	1.40	1.46
25	S	604	CLA	CMD-C2D	-2.34	1.46	1.51
25	7	612	CLA	CMC-C2C	-2.34	1.45	1.50
24	1	605	CHL	C2A-C3A	-2.34	1.50	1.55
29	B	2630	LHG	O7-C5	-2.34	1.40	1.46
25	g	613	CLA	C3B-C2B	-2.34	1.37	1.40
25	5	603	CLA	C3B-CAB	-2.34	1.43	1.47
24	7	601	CHL	CBD-CGD	-2.33	1.48	1.52
37	H	102	DGD	O2E-C2E	-2.33	1.37	1.43
37	h	102	DGD	O2E-C2E	-2.33	1.37	1.43
24	S	606	CHL	C2B-C1B	-2.33	1.48	1.53
25	A	406	CLA	C3B-C2B	-2.33	1.37	1.40
24	R	606	CHL	C3D-CAD	-2.33	1.47	1.51
25	8	610	CLA	C3B-C2B	-2.33	1.37	1.40
25	n	610	CLA	C3B-C2B	-2.33	1.37	1.40
25	r	603	CLA	C3B-C2B	-2.33	1.37	1.40
37	C	518	DGD	O5D-C6D	-2.33	1.39	1.43
25	N	610	CLA	C3B-C2B	-2.33	1.37	1.40
25	S	610	CLA	C3B-C2B	-2.32	1.37	1.40
25	1	603	CLA	C3B-CAB	-2.32	1.43	1.47
27	Y	1622	XAT	C34-C33	-2.32	1.32	1.35
25	y	612	CLA	CMC-C2C	-2.32	1.45	1.50
27	y	1622	XAT	C34-C33	-2.32	1.32	1.35
25	R	603	CLA	C3B-C2B	-2.32	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	d	405	PL9	C31-C29	-2.32	1.46	1.51
29	b	2630	LHG	O7-C5	-2.32	1.40	1.46
25	S	610	CLA	CMD-C2D	-2.32	1.46	1.51
25	n	611	CLA	C3B-C2B	-2.32	1.37	1.40
24	8	608	CHL	CBD-CGD	-2.32	1.48	1.52
35	D	411	LMG	O7-C8	-2.32	1.40	1.46
25	g	610	CLA	CMC-C2C	-2.31	1.45	1.50
25	n	610	CLA	CMC-C2C	-2.31	1.45	1.50
24	4	608	CHL	C2B-C1B	-2.31	1.48	1.53
36	D	405	PL9	C31-C29	-2.31	1.46	1.51
24	4	608	CHL	CBD-CGD	-2.31	1.48	1.52
25	N	610	CLA	CMC-C2C	-2.31	1.45	1.50
24	r	607	CHL	C2A-C3A	-2.31	1.50	1.55
37	c	518	DGD	O5D-C6D	-2.31	1.39	1.43
25	a	406	CLA	C3B-C2B	-2.30	1.37	1.40
37	C	518	DGD	O3E-C3E	-2.30	1.37	1.43
25	G	610	CLA	CMC-C2C	-2.30	1.45	1.50
25	3	612	CLA	CMC-C2C	-2.30	1.45	1.50
24	r	608	CHL	CBD-CGD	-2.30	1.48	1.52
24	6	606	CHL	C3D-CAD	-2.30	1.47	1.51
37	c	518	DGD	O3E-C3E	-2.30	1.37	1.43
24	R	607	CHL	C2A-C3A	-2.30	1.50	1.55
24	8	608	CHL	C2B-C1B	-2.29	1.48	1.53
25	s	604	CLA	CMD-C2D	-2.29	1.46	1.51
25	G	613	CLA	C3B-C2B	-2.29	1.37	1.40
24	S	601	CHL	CBD-CAD	-2.29	1.49	1.53
24	g	605	CHL	C2A-C3A	-2.29	1.50	1.55
34	B	623	SQD	O3-C3	-2.29	1.37	1.43
25	r	603	CLA	CMC-C2C	-2.29	1.45	1.50
25	8	603	CLA	C3B-C2B	-2.29	1.37	1.40
25	C	502	CLA	CMD-C2D	-2.29	1.46	1.51
34	b	623	SQD	O3-C3	-2.29	1.37	1.43
35	d	411	LMG	O7-C8	-2.29	1.40	1.46
24	N	607	CHL	C1A-CHA	-2.28	1.50	1.53
25	2	614	CLA	C3B-C2B	-2.28	1.37	1.40
25	1	612	CLA	CMC-C2C	-2.28	1.45	1.50
25	R	603	CLA	CMC-C2C	-2.28	1.45	1.50
25	N	604	CLA	CMC-C2C	-2.28	1.45	1.50
24	s	601	CHL	CBD-CAD	-2.28	1.49	1.53
30	b	618	BCR	C17-C18	-2.28	1.32	1.35
25	B	611	CLA	CMC-C2C	-2.28	1.45	1.50
25	6	614	CLA	C3B-C2B	-2.28	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	608	CHL	CBD-CGD	-2.28	1.48	1.52
24	4	606	CHL	C3D-CAD	-2.27	1.47	1.51
25	c	502	CLA	CMD-C2D	-2.27	1.46	1.51
34	b	623	SQD	O2-C2	-2.27	1.37	1.43
25	5	612	CLA	CMC-C2C	-2.27	1.45	1.50
24	5	605	CHL	C2B-C1B	-2.27	1.48	1.53
25	a	407	CLA	C3B-CAB	-2.27	1.43	1.47
25	A	407	CLA	C3B-CAB	-2.27	1.43	1.47
25	5	603	CLA	CMC-C2C	-2.27	1.45	1.50
25	G	610	CLA	C3B-CAB	-2.27	1.43	1.47
24	R	608	CHL	C2D-C1D	-2.27	1.48	1.53
25	2	610	CLA	CMC-C2C	-2.27	1.45	1.50
24	6	609	CHL	CBD-CGD	-2.27	1.48	1.52
25	6	603	CLA	CMC-C2C	-2.27	1.45	1.50
24	S	607	CHL	C1A-CHA	-2.27	1.50	1.53
24	Y	605	CHL	C3B-CAB	-2.27	1.48	1.50
25	2	603	CLA	CMC-C2C	-2.27	1.45	1.50
24	n	609	CHL	CMB-C2B	-2.27	1.48	1.53
34	B	623	SQD	O2-C2	-2.26	1.37	1.43
24	G	605	CHL	C2A-C3A	-2.26	1.50	1.55
24	6	609	CHL	C3D-CAD	-2.26	1.47	1.51
26	G	1621	LUT	C30-C29	-2.26	1.32	1.35
25	3	611	CLA	C3B-CAB	-2.26	1.43	1.47
24	n	607	CHL	C1A-CHA	-2.26	1.50	1.53
24	2	609	CHL	C3D-CAD	-2.26	1.47	1.51
25	8	602	CLA	C3B-C2B	-2.26	1.37	1.40
25	n	604	CLA	CMC-C2C	-2.26	1.45	1.50
26	g	1621	LUT	C30-C29	-2.26	1.32	1.35
25	1	603	CLA	CMC-C2C	-2.26	1.45	1.50
25	g	611	CLA	C3B-CAB	-2.26	1.43	1.47
24	1	605	CHL	C2B-C1B	-2.26	1.48	1.53
24	2	609	CHL	CBD-CGD	-2.26	1.48	1.52
24	3	607	CHL	CBD-CGD	-2.26	1.48	1.52
34	B	623	SQD	O4-C4	-2.26	1.37	1.43
24	y	605	CHL	C3B-CAB	-2.25	1.48	1.50
25	g	610	CLA	C3B-CAB	-2.25	1.43	1.47
25	4	611	CLA	C3B-C2B	-2.25	1.37	1.40
24	8	606	CHL	C3D-CAD	-2.25	1.47	1.51
25	4	602	CLA	C3B-C2B	-2.25	1.37	1.40
25	7	614	CLA	C3B-C2B	-2.25	1.37	1.40
34	b	623	SQD	O4-C4	-2.25	1.37	1.43
25	s	609	CLA	CMD-C2D	-2.25	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	609	CLA	CMD-C2D	-2.25	1.46	1.51
25	6	610	CLA	CMC-C2C	-2.25	1.45	1.50
25	4	603	CLA	C3B-C2B	-2.25	1.37	1.40
24	2	606	CHL	C3D-CAD	-2.25	1.47	1.51
25	Y	613	CLA	C4B-CHC	-2.25	1.34	1.40
24	6	607	CHL	C2B-C1B	-2.25	1.48	1.53
30	B	618	BCR	C17-C18	-2.25	1.32	1.35
25	Y	611	CLA	CMC-C2C	-2.25	1.45	1.50
24	y	608	CHL	CBD-CGD	-2.25	1.48	1.52
26	y	1621	LUT	C1-C6	-2.25	1.50	1.53
25	r	603	CLA	C3B-CAB	-2.24	1.43	1.47
24	r	608	CHL	C2D-C1D	-2.24	1.48	1.53
25	b	611	CLA	CMC-C2C	-2.24	1.45	1.50
25	b	604	CLA	CMC-C2C	-2.24	1.45	1.50
24	7	607	CHL	CBD-CGD	-2.24	1.48	1.52
25	B	610	CLA	C3B-C2B	-2.24	1.37	1.40
25	G	611	CLA	C3B-CAB	-2.24	1.43	1.47
25	y	613	CLA	C4B-CHC	-2.24	1.34	1.40
24	Y	606	CHL	CBD-CGD	-2.24	1.48	1.52
24	1	605	CHL	CBD-CAD	-2.24	1.49	1.53
25	B	604	CLA	CMC-C2C	-2.24	1.45	1.50
34	A	418	SQD	O2-C2	-2.24	1.37	1.43
25	R	610	CLA	CMC-C2C	-2.24	1.45	1.50
33	A	409	PHO	CMD-C2D	-2.24	1.45	1.50
27	7	1622	XAT	O4-C5	-2.24	1.42	1.46
25	7	611	CLA	C3B-CAB	-2.24	1.43	1.47
25	y	611	CLA	CMC-C2C	-2.23	1.45	1.50
25	3	613	CLA	C3B-CAB	-2.23	1.43	1.47
24	N	609	CHL	CMB-C2B	-2.23	1.48	1.53
34	a	418	SQD	O2-C2	-2.23	1.37	1.43
24	8	606	CHL	CBD-CGD	-2.23	1.48	1.52
33	A	409	PHO	CMC-C2C	-2.23	1.46	1.50
24	4	606	CHL	CBD-CGD	-2.23	1.48	1.52
25	D	402	CLA	CAA-C2A	-2.23	1.49	1.54
25	R	603	CLA	C3B-CAB	-2.23	1.43	1.47
25	3	610	CLA	CMC-C2C	-2.23	1.46	1.50
24	2	607	CHL	C2B-C1B	-2.23	1.48	1.53
24	3	609	CHL	C3D-CAD	-2.23	1.47	1.51
24	s	607	CHL	C1A-CHA	-2.23	1.50	1.53
27	3	1622	XAT	O4-C5	-2.23	1.42	1.46
25	B	605	CLA	CMC-C2C	-2.23	1.46	1.50
24	y	606	CHL	CBD-CGD	-2.23	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	a	409	PHO	CMC-C2C	-2.22	1.46	1.50
24	N	601	CHL	C3D-CAD	-2.22	1.47	1.51
25	3	611	CLA	C4B-CHC	-2.22	1.34	1.40
25	8	611	CLA	C3B-CAB	-2.22	1.43	1.47
24	R	614	CHL	C2B-C1B	-2.22	1.48	1.53
24	y	609	CHL	CBD-CGD	-2.22	1.48	1.52
24	n	601	CHL	C3D-CAD	-2.22	1.47	1.51
25	1	603	CLA	CAC-C3C	-2.22	1.45	1.51
25	5	603	CLA	CAC-C3C	-2.22	1.45	1.51
25	6	604	CLA	CMC-C2C	-2.22	1.46	1.50
25	5	610	CLA	CMC-C2C	-2.22	1.46	1.50
25	r	610	CLA	CMC-C2C	-2.22	1.46	1.50
24	7	609	CHL	C3D-CAD	-2.22	1.47	1.51
25	g	604	CLA	CMC-C2C	-2.22	1.46	1.50
24	6	608	CHL	C2B-C1B	-2.22	1.48	1.53
24	2	608	CHL	C2B-C1B	-2.22	1.48	1.53
25	b	610	CLA	C3B-C2B	-2.22	1.37	1.40
24	5	606	CHL	CBD-CGD	-2.21	1.48	1.52
25	7	611	CLA	C4B-CHC	-2.21	1.34	1.40
33	a	409	PHO	CMD-C2D	-2.21	1.46	1.50
27	r	622	XAT	C2-C1	-2.21	1.51	1.54
24	6	605	CHL	C2B-C1B	-2.21	1.48	1.53
26	Y	1621	LUT	C10-C9	-2.21	1.32	1.35
26	y	1621	LUT	C10-C9	-2.21	1.32	1.35
25	G	614	CLA	C3B-CAB	-2.21	1.43	1.47
24	Y	608	CHL	CBD-CGD	-2.21	1.48	1.52
27	r	622	XAT	O4-C5	-2.21	1.42	1.46
25	a	406	CLA	CAC-C3C	-2.21	1.45	1.51
25	A	406	CLA	CAC-C3C	-2.21	1.45	1.51
25	r	609	CLA	CMC-C2C	-2.21	1.46	1.50
25	G	604	CLA	CMC-C2C	-2.21	1.46	1.50
25	8	611	CLA	C3B-C2B	-2.21	1.37	1.40
26	y	1620	LUT	C30-C29	-2.21	1.32	1.35
25	7	603	CLA	C3B-CAB	-2.21	1.43	1.47
25	b	605	CLA	CMC-C2C	-2.21	1.46	1.50
25	1	611	CLA	C3B-CAB	-2.21	1.43	1.47
25	5	612	CLA	C3B-CAB	-2.21	1.43	1.47
25	5	612	CLA	C4B-CHC	-2.21	1.34	1.40
25	n	612	CLA	CMC-C2C	-2.21	1.46	1.50
25	g	614	CLA	C3B-CAB	-2.21	1.43	1.47
24	1	606	CHL	CBD-CGD	-2.21	1.48	1.52
24	Y	605	CHL	C3D-CAD	-2.21	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	605	CHL	C3D-CAD	-2.21	1.47	1.51
25	b	610	CLA	CMC-C2C	-2.21	1.46	1.50
27	R	622	XAT	C2-C1	-2.20	1.51	1.54
26	Y	1621	LUT	C1-C6	-2.20	1.50	1.53
25	d	402	CLA	CAA-C2A	-2.20	1.49	1.54
25	4	611	CLA	C3B-CAB	-2.20	1.43	1.47
25	7	613	CLA	C3B-CAB	-2.20	1.43	1.47
24	8	601	CHL	C1A-CHA	-2.20	1.50	1.53
24	n	609	CHL	C1A-C2A	-2.20	1.51	1.53
25	1	610	CLA	CMC-C2C	-2.20	1.46	1.50
25	B	614	CLA	C3B-CAB	-2.20	1.43	1.47
25	5	603	CLA	C4B-CHC	-2.20	1.34	1.40
25	7	603	CLA	CMC-C2C	-2.20	1.46	1.50
25	B	607	CLA	C3B-CAB	-2.20	1.43	1.47
27	R	622	XAT	O4-C5	-2.20	1.42	1.46
25	N	612	CLA	CMC-C2C	-2.20	1.46	1.50
25	7	610	CLA	CMC-C2C	-2.20	1.46	1.50
25	3	603	CLA	CMC-C2C	-2.20	1.46	1.50
24	5	605	CHL	CBD-CAD	-2.20	1.49	1.53
25	2	604	CLA	CMC-C2C	-2.20	1.46	1.50
25	r	613	CLA	CMD-C2D	-2.20	1.46	1.51
25	R	613	CLA	CMD-C2D	-2.20	1.46	1.51
25	5	611	CLA	C3B-CAB	-2.20	1.43	1.47
24	2	605	CHL	C2B-C1B	-2.20	1.48	1.53
25	3	614	CLA	C3B-C2B	-2.20	1.37	1.40
24	Y	609	CHL	CBD-CGD	-2.20	1.48	1.52
25	1	603	CLA	C4B-CHC	-2.19	1.34	1.40
25	7	613	CLA	CMC-C2C	-2.19	1.46	1.50
25	n	603	CLA	CMC-C2C	-2.19	1.46	1.50
24	y	605	CHL	C1A-C2A	-2.19	1.51	1.53
25	1	612	CLA	C4B-CHC	-2.19	1.34	1.40
25	R	609	CLA	CMC-C2C	-2.19	1.46	1.50
25	1	612	CLA	C3B-CAB	-2.19	1.43	1.47
25	b	614	CLA	C3B-CAB	-2.19	1.43	1.47
24	r	614	CHL	C2B-C1B	-2.19	1.48	1.53
28	1	1623	NEX	O24-C25	-2.19	1.42	1.46
33	A	408	PHO	CMC-C2C	-2.19	1.46	1.50
25	B	617	CLA	C4B-CHC	-2.19	1.34	1.40
25	3	613	CLA	CMC-C2C	-2.19	1.46	1.50
25	3	603	CLA	C3B-CAB	-2.19	1.43	1.47
25	B	610	CLA	CMC-C2C	-2.19	1.46	1.50
24	4	601	CHL	C2B-C1B	-2.19	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	408	PHO	CMD-C2D	-2.18	1.46	1.50
25	3	613	CLA	C4B-CHC	-2.18	1.34	1.40
25	s	602	CLA	CMC-C2C	-2.18	1.46	1.50
24	r	607	CHL	C3B-CAB	-2.18	1.48	1.50
25	7	613	CLA	C4B-CHC	-2.18	1.34	1.40
25	d	403	CLA	CMC-C2C	-2.18	1.46	1.50
25	b	617	CLA	C4B-CHC	-2.18	1.34	1.40
25	N	603	CLA	CMC-C2C	-2.18	1.46	1.50
25	b	607	CLA	C3B-CAB	-2.18	1.43	1.47
24	3	608	CHL	CBD-CGD	-2.18	1.48	1.52
24	n	605	CHL	C3D-CAD	-2.18	1.47	1.51
28	5	1623	NEX	O24-C25	-2.18	1.42	1.46
29	B	2631	LHG	O7-C5	-2.18	1.40	1.46
24	S	608	CHL	C3D-CAD	-2.18	1.47	1.51
33	a	408	PHO	CMD-C2D	-2.18	1.46	1.50
25	8	612	CLA	CMC-C2C	-2.18	1.46	1.50
25	b	613	CLA	C3B-C2B	-2.17	1.37	1.40
25	S	602	CLA	CMC-C2C	-2.17	1.46	1.50
25	5	614	CLA	C3B-C2B	-2.17	1.37	1.40
24	8	601	CHL	C2B-C1B	-2.17	1.48	1.53
34	A	412	SQD	O4-C4	-2.17	1.38	1.43
34	a	412	SQD	O4-C4	-2.17	1.38	1.43
29	b	2631	LHG	O7-C5	-2.17	1.40	1.46
25	B	613	CLA	C3B-C2B	-2.17	1.37	1.40
25	1	614	CLA	C3B-C2B	-2.17	1.37	1.40
33	a	408	PHO	CMC-C2C	-2.17	1.46	1.50
24	Y	605	CHL	C1A-C2A	-2.17	1.51	1.53
34	B	621	SQD	O2-C2	-2.17	1.38	1.43
25	4	612	CLA	CMC-C2C	-2.17	1.46	1.50
24	s	608	CHL	C3D-CAD	-2.17	1.47	1.51
25	5	611	CLA	CMC-C2C	-2.17	1.46	1.50
24	2	608	CHL	CBD-CGD	-2.17	1.48	1.52
26	5	1620	LUT	C10-C9	-2.16	1.32	1.35
25	1	611	CLA	CMC-C2C	-2.16	1.46	1.50
24	G	605	CHL	C2B-C1B	-2.16	1.48	1.53
25	y	603	CLA	CAC-C3C	-2.16	1.45	1.51
25	8	602	CLA	CMC-C2C	-2.16	1.46	1.50
25	g	613	CLA	C4B-CHC	-2.16	1.34	1.40
25	G	603	CLA	CAC-C3C	-2.16	1.45	1.51
25	y	614	CLA	CMC-C2C	-2.16	1.46	1.50
25	B	605	CLA	C4B-CHC	-2.16	1.34	1.40
26	y	1620	LUT	C34-C33	-2.16	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	606	CHL	C2A-C3A	-2.16	1.50	1.55
25	b	605	CLA	C4B-CHC	-2.16	1.34	1.40
24	4	601	CHL	C1A-CHA	-2.16	1.50	1.53
25	Y	614	CLA	CMC-C2C	-2.16	1.46	1.50
25	g	603	CLA	CAC-C3C	-2.16	1.45	1.51
24	7	608	CHL	CBD-CGD	-2.16	1.48	1.52
24	7	609	CHL	CBD-CGD	-2.16	1.48	1.52
25	G	613	CLA	C4B-CHC	-2.16	1.34	1.40
25	Y	603	CLA	CMC-C2C	-2.16	1.46	1.50
24	g	605	CHL	C2B-C1B	-2.16	1.48	1.53
25	r	601	CLA	C3B-C2B	-2.16	1.37	1.40
34	A	412	SQD	O3-C3	-2.16	1.38	1.43
25	G	613	CLA	C3B-CAB	-2.16	1.43	1.47
25	g	612	CLA	CMC-C2C	-2.16	1.46	1.50
28	R	623	NEX	O24-C25	-2.16	1.42	1.46
30	b	618	BCR	C30-C25	-2.15	1.50	1.53
30	B	618	BCR	C30-C25	-2.15	1.50	1.53
25	D	403	CLA	CMC-C2C	-2.15	1.46	1.50
25	g	613	CLA	C3B-CAB	-2.15	1.43	1.47
25	4	602	CLA	CMC-C2C	-2.15	1.46	1.50
34	b	621	SQD	O2-C2	-2.15	1.38	1.43
25	3	603	CLA	CAC-C3C	-2.15	1.45	1.51
24	3	609	CHL	C3B-CAB	-2.15	1.48	1.50
24	N	605	CHL	C3D-CAD	-2.15	1.47	1.51
24	G	609	CHL	C1A-C2A	-2.15	1.51	1.53
33	A	408	PHO	CMB-C2B	-2.15	1.46	1.50
24	N	609	CHL	C1A-C2A	-2.15	1.51	1.53
33	a	408	PHO	CMB-C2B	-2.15	1.46	1.50
29	6	2630	LHG	O7-C5	-2.15	1.41	1.46
24	3	605	CHL	CBD-CGD	-2.15	1.48	1.52
28	Y	1623	NEX	O24-C25	-2.15	1.42	1.46
24	s	607	CHL	CBD-CAD	-2.15	1.49	1.53
24	S	607	CHL	CBD-CAD	-2.15	1.49	1.53
25	2	613	CLA	C3B-CAB	-2.15	1.43	1.47
25	G	614	CLA	CMC-C2C	-2.15	1.46	1.50
25	1	604	CLA	CMC-C2C	-2.15	1.46	1.50
25	7	603	CLA	CAC-C3C	-2.15	1.45	1.51
25	R	604	CLA	CMC-C2C	-2.14	1.46	1.50
26	3	1620	LUT	C14-C13	-2.14	1.32	1.35
24	6	608	CHL	CBD-CGD	-2.14	1.48	1.52
24	3	609	CHL	CBD-CGD	-2.14	1.48	1.52
29	2	2630	LHG	O7-C5	-2.14	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	1620	LUT	C30-C29	-2.14	1.32	1.35
26	6	1621	LUT	C22-C21	-2.14	1.52	1.54
25	Y	603	CLA	CAC-C3C	-2.14	1.45	1.51
25	G	612	CLA	CMC-C2C	-2.14	1.46	1.50
34	a	412	SQD	O3-C3	-2.14	1.38	1.43
25	b	602	CLA	C3B-CAB	-2.14	1.43	1.47
25	4	603	CLA	CMC-C2C	-2.14	1.46	1.50
27	g	1622	XAT	O4-C5	-2.14	1.42	1.46
24	s	606	CHL	C2A-C3A	-2.14	1.50	1.55
26	7	1620	LUT	C14-C13	-2.14	1.32	1.35
25	n	603	CLA	CAC-C3C	-2.14	1.45	1.51
25	6	613	CLA	C3B-CAB	-2.14	1.43	1.47
25	B	602	CLA	C3B-CAB	-2.14	1.43	1.47
25	5	604	CLA	CMC-C2C	-2.14	1.46	1.50
25	g	614	CLA	CMC-C2C	-2.14	1.46	1.50
25	8	603	CLA	CMC-C2C	-2.14	1.46	1.50
25	N	603	CLA	CAC-C3C	-2.13	1.45	1.51
25	R	616	CLA	CMC-C2C	-2.13	1.46	1.50
25	G	603	CLA	CMC-C2C	-2.13	1.46	1.50
29	c	523	LHG	O7-C5	-2.13	1.41	1.46
26	G	1621	LUT	C10-C9	-2.13	1.33	1.35
25	R	601	CLA	C3B-C2B	-2.13	1.37	1.40
24	7	605	CHL	CBD-CGD	-2.13	1.48	1.52
26	Y	1621	LUT	C30-C29	-2.13	1.33	1.35
25	g	604	CLA	C3B-CAB	-2.13	1.43	1.47
24	y	607	CHL	C2D-C1D	-2.13	1.49	1.53
26	4	620	LUT	C1-C6	-2.13	1.50	1.53
29	y	2630	LHG	O8-C6	-2.13	1.40	1.45
26	1	1620	LUT	C10-C9	-2.13	1.33	1.35
26	Y	1620	LUT	C34-C33	-2.13	1.33	1.35
25	6	604	CLA	C4B-CHC	-2.13	1.34	1.40
25	2	604	CLA	C4B-CHC	-2.13	1.34	1.40
25	y	603	CLA	CMC-C2C	-2.13	1.46	1.50
25	a	410	CLA	CMC-C2C	-2.13	1.46	1.50
35	d	411	LMG	O4-C4	-2.13	1.38	1.43
25	A	410	CLA	CMC-C2C	-2.13	1.46	1.50
25	Y	612	CLA	C3B-CAB	-2.13	1.43	1.47
24	3	605	CHL	C3B-CAB	-2.13	1.48	1.50
25	n	602	CLA	C3B-CAB	-2.13	1.43	1.47
26	N	1621	LUT	C10-C9	-2.13	1.33	1.35
25	r	604	CLA	CMC-C2C	-2.12	1.46	1.50
24	y	608	CHL	C2D-C1D	-2.12	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	1621	LUT	C30-C29	-2.12	1.33	1.35
25	y	612	CLA	C3B-CAB	-2.12	1.43	1.47
24	g	609	CHL	C1A-C2A	-2.12	1.51	1.53
26	G	1620	LUT	C30-C29	-2.12	1.33	1.35
24	R	607	CHL	C3B-CAB	-2.12	1.48	1.50
25	2	603	CLA	C3B-CAB	-2.12	1.43	1.47
25	r	616	CLA	CMC-C2C	-2.12	1.46	1.50
28	y	1623	NEX	O24-C25	-2.12	1.43	1.46
25	r	609	CLA	C3B-CAB	-2.12	1.43	1.47
27	G	1622	XAT	O4-C5	-2.12	1.43	1.46
25	n	612	CLA	C4B-CHC	-2.12	1.34	1.40
25	N	612	CLA	C4B-CHC	-2.12	1.34	1.40
25	b	602	CLA	CMC-C2C	-2.12	1.46	1.50
28	5	1623	NEX	C22-C21	-2.12	1.51	1.54
25	b	606	CLA	CAC-C3C	-2.12	1.45	1.51
26	2	1621	LUT	C22-C21	-2.11	1.52	1.54
25	B	606	CLA	CAC-C3C	-2.11	1.45	1.51
25	7	602	CLA	C3B-C2B	-2.11	1.37	1.40
25	S	603	CLA	C3B-C2B	-2.11	1.37	1.40
25	N	602	CLA	C3B-CAB	-2.11	1.43	1.47
25	r	601	CLA	C3B-CAB	-2.11	1.43	1.47
25	G	604	CLA	C3B-CAB	-2.11	1.43	1.47
25	B	614	CLA	CAA-C2A	-2.11	1.50	1.54
25	5	613	CLA	C3B-CAB	-2.11	1.43	1.47
24	G	605	CHL	CBD-CAD	-2.11	1.49	1.53
25	7	604	CLA	CMC-C2C	-2.11	1.46	1.50
25	B	606	CLA	C4B-CHC	-2.11	1.34	1.40
29	Y	2630	LHG	O8-C6	-2.11	1.40	1.45
35	D	411	LMG	O4-C4	-2.11	1.38	1.43
25	b	606	CLA	C4B-CHC	-2.11	1.34	1.40
37	C	519	DGD	O2G-C2G	-2.11	1.41	1.46
25	r	613	CLA	C4B-CHC	-2.11	1.34	1.40
24	8	607	CHL	C3D-CAD	-2.11	1.47	1.51
26	g	1621	LUT	C10-C9	-2.11	1.33	1.35
25	1	613	CLA	CMC-C2C	-2.11	1.46	1.50
28	1	1623	NEX	C22-C21	-2.11	1.51	1.54
25	8	604	CLA	CMC-C2C	-2.11	1.46	1.50
25	s	603	CLA	C3B-C2B	-2.11	1.37	1.40
37	C	518	DGD	O2G-C2G	-2.11	1.41	1.46
25	1	613	CLA	C4B-CHC	-2.11	1.34	1.40
24	R	607	CHL	C3D-CAD	-2.11	1.47	1.51
29	C	523	LHG	O7-C5	-2.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	606	CHL	CBD-CAD	-2.11	1.49	1.53
24	g	605	CHL	CBD-CAD	-2.11	1.49	1.53
25	b	614	CLA	CAA-C2A	-2.10	1.50	1.54
25	n	602	CLA	C3B-C2B	-2.10	1.37	1.40
28	r	623	NEX	O24-C25	-2.10	1.43	1.46
25	3	604	CLA	CMC-C2C	-2.10	1.46	1.50
25	g	603	CLA	CMC-C2C	-2.10	1.46	1.50
25	1	613	CLA	C3B-CAB	-2.10	1.43	1.47
25	b	603	CLA	CMC-C2C	-2.10	1.46	1.50
24	7	605	CHL	C3B-CAB	-2.10	1.48	1.50
25	B	603	CLA	CMC-C2C	-2.10	1.46	1.50
25	4	604	CLA	CMC-C2C	-2.10	1.46	1.50
37	c	519	DGD	O2G-C2G	-2.10	1.41	1.46
25	R	609	CLA	C3B-CAB	-2.10	1.43	1.47
25	B	602	CLA	CMC-C2C	-2.10	1.46	1.50
24	Y	607	CHL	C2D-C1D	-2.10	1.49	1.53
25	S	611	CLA	C3B-C2B	-2.10	1.37	1.40
25	g	602	CLA	C3B-C2B	-2.10	1.37	1.40
25	8	610	CLA	C3B-CAB	-2.10	1.43	1.47
26	1	1620	LUT	C30-C29	-2.10	1.33	1.35
36	D	405	PL9	C10-C9	-2.10	1.45	1.50
24	r	607	CHL	C3D-CAD	-2.10	1.47	1.51
25	N	602	CLA	C3B-C2B	-2.09	1.37	1.40
27	4	622	XAT	O4-C5	-2.09	1.43	1.46
25	R	613	CLA	C4B-CHC	-2.09	1.34	1.40
36	d	405	PL9	C10-C9	-2.09	1.45	1.50
27	8	622	XAT	O4-C5	-2.09	1.43	1.46
25	5	613	CLA	CMC-C2C	-2.09	1.46	1.50
25	R	601	CLA	C3B-CAB	-2.09	1.43	1.47
37	c	518	DGD	O2G-C2G	-2.09	1.41	1.46
24	4	607	CHL	C3D-CAD	-2.09	1.47	1.51
27	y	1622	XAT	O4-C5	-2.09	1.43	1.46
25	N	614	CLA	CMC-C2C	-2.09	1.46	1.50
25	4	610	CLA	C3B-CAB	-2.09	1.43	1.47
26	n	1621	LUT	C10-C9	-2.09	1.33	1.35
24	Y	608	CHL	C2D-C1D	-2.09	1.49	1.53
24	s	606	CHL	CBD-CAD	-2.09	1.49	1.53
25	2	611	CLA	C3B-C2B	-2.09	1.37	1.40
24	n	607	CHL	CBD-CGD	-2.09	1.48	1.52
26	8	620	LUT	C1-C6	-2.08	1.50	1.53
25	6	603	CLA	C3B-CAB	-2.08	1.43	1.47
34	b	621	SQD	O4-C4	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	1622	XAT	O4-C5	-2.08	1.43	1.46
24	6	607	CHL	C3D-CAD	-2.08	1.47	1.51
25	7	612	CLA	C4B-CHC	-2.08	1.34	1.40
25	G	602	CLA	C3B-C2B	-2.08	1.37	1.40
25	6	611	CLA	C3B-C2B	-2.08	1.37	1.40
30	T	101	BCR	C1-C6	-2.08	1.50	1.53
26	r	620	LUT	C34-C33	-2.08	1.33	1.35
25	g	613	CLA	CMC-C2C	-2.08	1.46	1.50
25	3	603	CLA	C4B-CHC	-2.08	1.34	1.40
27	Y	1622	XAT	O4-C5	-2.08	1.43	1.46
30	t	101	BCR	C1-C6	-2.08	1.50	1.53
25	3	612	CLA	C4B-CHC	-2.08	1.34	1.40
24	7	609	CHL	C3B-CAB	-2.08	1.48	1.50
35	b	2633	LMG	O2-C2	-2.08	1.38	1.43
34	a	412	SQD	O47-C45	-2.08	1.41	1.46
34	B	621	SQD	O4-C4	-2.07	1.38	1.43
25	5	613	CLA	C4B-CHC	-2.07	1.34	1.40
25	b	616	CLA	C4B-CHC	-2.07	1.34	1.40
25	7	603	CLA	C4B-CHC	-2.07	1.34	1.40
25	B	616	CLA	C4B-CHC	-2.07	1.34	1.40
27	n	1622	XAT	O4-C5	-2.07	1.43	1.46
25	r	602	CLA	C3B-CAB	-2.07	1.43	1.47
25	n	614	CLA	CMC-C2C	-2.07	1.46	1.50
34	A	418	SQD	O4-C4	-2.07	1.38	1.43
24	Y	606	CHL	CMD-C2D	-2.07	1.48	1.53
25	B	610	CLA	C4B-CHC	-2.07	1.34	1.40
24	4	606	CHL	C3B-CAB	-2.07	1.48	1.50
27	Y	1622	XAT	C14-C13	-2.07	1.33	1.35
25	3	602	CLA	C3B-C2B	-2.07	1.37	1.40
34	a	418	SQD	O4-C4	-2.07	1.38	1.43
25	S	609	CLA	C3B-C2B	-2.07	1.37	1.40
25	n	611	CLA	CMC-C2C	-2.07	1.46	1.50
25	G	613	CLA	CMC-C2C	-2.07	1.46	1.50
27	1	1622	XAT	O4-C5	-2.07	1.43	1.46
24	1	609	CHL	CMB-C2B	-2.07	1.48	1.53
24	R	607	CHL	CBD-CGD	-2.07	1.48	1.52
28	n	1623	NEX	C10-C9	-2.07	1.33	1.35
25	R	602	CLA	C3B-CAB	-2.06	1.43	1.47
24	8	606	CHL	C3B-CAB	-2.06	1.48	1.50
25	s	609	CLA	C3B-C2B	-2.06	1.37	1.40
25	C	506	CLA	CMC-C2C	-2.06	1.46	1.50
25	r	612	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	613	CLA	CMC-C2C	-2.06	1.46	1.50
24	n	606	CHL	CMB-C2B	-2.06	1.48	1.53
34	A	412	SQD	O47-C45	-2.06	1.41	1.46
26	R	620	LUT	C34-C33	-2.06	1.33	1.35
25	2	611	CLA	CMC-C2C	-2.06	1.46	1.50
25	R	612	CLA	CMC-C2C	-2.06	1.46	1.50
26	7	1620	LUT	C30-C29	-2.06	1.33	1.35
25	6	613	CLA	CMC-C2C	-2.06	1.46	1.50
24	r	607	CHL	CBD-CGD	-2.06	1.48	1.52
37	b	626	DGD	O2G-C2G	-2.06	1.41	1.46
25	c	506	CLA	CMC-C2C	-2.06	1.46	1.50
25	C	513	CLA	CMC-C2C	-2.06	1.46	1.50
25	5	604	CLA	C4B-CHC	-2.05	1.34	1.40
26	5	1620	LUT	C30-C29	-2.05	1.33	1.35
28	N	1623	NEX	C10-C9	-2.05	1.33	1.35
25	6	611	CLA	CMC-C2C	-2.05	1.46	1.50
35	B	2633	LMG	O2-C2	-2.05	1.38	1.43
24	y	606	CHL	CMD-C2D	-2.05	1.48	1.53
25	R	616	CLA	C4B-CHC	-2.05	1.34	1.40
25	b	610	CLA	C4B-CHC	-2.05	1.34	1.40
26	g	1620	LUT	C30-C29	-2.05	1.33	1.35
25	C	501	CLA	CMC-C2C	-2.05	1.46	1.50
25	r	616	CLA	C4B-CHC	-2.05	1.34	1.40
24	2	607	CHL	C3D-CAD	-2.05	1.47	1.51
27	7	1622	XAT	O24-C25	-2.05	1.43	1.46
25	B	605	CLA	CAC-C3C	-2.05	1.45	1.51
26	3	1620	LUT	C30-C29	-2.05	1.33	1.35
25	s	611	CLA	C3B-C2B	-2.05	1.37	1.40
24	r	606	CHL	CBD-CGD	-2.05	1.48	1.52
37	h	102	DGD	O3D-C3D	-2.04	1.38	1.43
37	C	519	DGD	O5D-C6D	-2.04	1.40	1.43
37	B	626	DGD	O2G-C2G	-2.04	1.41	1.46
25	c	513	CLA	CMC-C2C	-2.04	1.46	1.50
24	R	606	CHL	CBD-CGD	-2.04	1.48	1.52
24	5	606	CHL	C2D-C1D	-2.04	1.49	1.53
24	g	605	CHL	C3D-CAD	-2.04	1.47	1.51
35	a	413	LMG	O7-C8	-2.04	1.41	1.46
24	N	607	CHL	CBD-CGD	-2.04	1.48	1.52
37	c	519	DGD	O5D-C6D	-2.04	1.40	1.43
25	1	604	CLA	C4B-CHC	-2.04	1.34	1.40
25	B	608	CLA	C4B-CHC	-2.04	1.34	1.40
25	b	605	CLA	CAC-C3C	-2.04	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	608	CHL	C2A-C3A	-2.04	1.51	1.55
25	1	614	CLA	CMC-C2C	-2.04	1.46	1.50
25	c	504	CLA	CMC-C2C	-2.04	1.46	1.50
26	R	620	LUT	C30-C29	-2.04	1.33	1.35
24	5	609	CHL	CMB-C2B	-2.04	1.48	1.53
28	7	1623	NEX	O24-C25	-2.04	1.43	1.46
25	d	403	CLA	C3B-CAB	-2.03	1.43	1.47
30	b	619	BCR	C14-C13	-2.03	1.33	1.35
25	G	611	CLA	CMC-C2C	-2.03	1.46	1.50
25	5	614	CLA	CMC-C2C	-2.03	1.46	1.50
26	G	1620	LUT	C22-C21	-2.03	1.52	1.54
24	g	601	CHL	CBD-CGD	-2.03	1.48	1.52
35	A	413	LMG	O7-C8	-2.03	1.41	1.46
25	6	614	CLA	CMC-C2C	-2.03	1.46	1.50
30	B	619	BCR	C14-C13	-2.03	1.33	1.35
25	r	611	CLA	C3B-CAB	-2.03	1.43	1.47
25	C	505	CLA	CMC-C2C	-2.03	1.46	1.50
24	s	608	CHL	C2A-C3A	-2.03	1.51	1.55
28	1	1623	NEX	C30-C29	-2.03	1.33	1.35
28	n	1623	NEX	O24-C25	-2.03	1.43	1.46
25	b	608	CLA	C4B-CHC	-2.03	1.34	1.40
28	3	1623	NEX	O24-C25	-2.03	1.43	1.46
24	y	606	CHL	CMB-C2B	-2.03	1.49	1.53
25	g	611	CLA	CMC-C2C	-2.03	1.46	1.50
25	D	403	CLA	C3B-CAB	-2.03	1.43	1.47
24	N	606	CHL	CMB-C2B	-2.03	1.49	1.53
24	S	601	CHL	C3D-CAD	-2.03	1.47	1.51
24	G	605	CHL	C3D-CAD	-2.03	1.47	1.51
25	N	611	CLA	CMC-C2C	-2.03	1.46	1.50
34	A	418	SQD	O3-C3	-2.02	1.38	1.43
25	b	608	CLA	C3B-CAB	-2.02	1.43	1.47
25	c	505	CLA	CMC-C2C	-2.02	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.02	1.46	1.50
26	n	1620	LUT	C14-C13	-2.02	1.33	1.35
25	C	504	CLA	CMC-C2C	-2.02	1.46	1.50
24	S	608	CHL	CBD-CAD	-2.02	1.50	1.53
24	8	607	CHL	CBD-CGD	-2.02	1.48	1.52
28	N	1623	NEX	O24-C25	-2.02	1.43	1.46
27	y	1622	XAT	C14-C13	-2.02	1.33	1.35
25	B	608	CLA	C3B-CAB	-2.02	1.43	1.47
24	1	606	CHL	C2D-C1D	-2.02	1.49	1.53
25	6	604	CLA	C3B-CAB	-2.02	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	611	CLA	C3B-CAB	-2.02	1.43	1.47
35	z	101	LMG	O4-C4	-2.02	1.38	1.43
24	8	601	CHL	C3D-CAD	-2.02	1.47	1.51
24	s	608	CHL	CBD-CAD	-2.02	1.50	1.53
34	a	418	SQD	O3-C3	-2.02	1.38	1.43
30	b	619	BCR	C21-C22	-2.02	1.33	1.35
30	H	101	BCR	C30-C25	-2.02	1.51	1.53
25	B	604	CLA	C4B-CHC	-2.02	1.34	1.40
24	s	608	CHL	C2B-C1B	-2.02	1.49	1.53
35	Z	101	LMG	O4-C4	-2.02	1.38	1.43
25	r	602	CLA	CAC-C3C	-2.02	1.45	1.51
25	7	611	CLA	CMC-C2C	-2.02	1.46	1.50
34	B	621	SQD	O3-C3	-2.02	1.38	1.43
25	y	613	CLA	CMC-C2C	-2.02	1.46	1.50
25	n	613	CLA	C4B-CHC	-2.02	1.34	1.40
27	N	1622	XAT	O4-C5	-2.02	1.43	1.46
25	A	407	CLA	CMC-C2C	-2.01	1.46	1.50
26	r	620	LUT	C30-C29	-2.01	1.33	1.35
25	R	616	CLA	CAC-C3C	-2.01	1.45	1.51
25	b	609	CLA	C3B-C2B	-2.01	1.37	1.40
25	a	407	CLA	CMC-C2C	-2.01	1.46	1.50
26	N	1620	LUT	C14-C13	-2.01	1.33	1.35
24	S	608	CHL	C2B-C1B	-2.01	1.49	1.53
25	2	614	CLA	CMC-C2C	-2.01	1.46	1.50
24	4	601	CHL	C3D-CAD	-2.01	1.47	1.51
25	r	616	CLA	CAC-C3C	-2.01	1.45	1.51
25	D	403	CLA	C3B-C2B	-2.01	1.37	1.40
24	G	601	CHL	CBD-CGD	-2.01	1.48	1.52
25	N	611	CLA	C3B-CAB	-2.01	1.43	1.47
25	b	604	CLA	C4B-CHC	-2.01	1.34	1.40
25	R	602	CLA	CAC-C3C	-2.01	1.45	1.51
24	s	608	CHL	C1A-C2A	-2.01	1.51	1.53
25	c	505	CLA	C3B-C2B	-2.01	1.37	1.40
25	S	612	CLA	CMC-C2C	-2.01	1.46	1.50
25	2	604	CLA	C3B-CAB	-2.01	1.43	1.47
24	y	609	CHL	C3B-CAB	-2.01	1.48	1.50
25	R	611	CLA	C3B-CAB	-2.00	1.43	1.47
37	H	102	DGD	O3D-C3D	-2.00	1.38	1.43
25	Y	613	CLA	CMC-C2C	-2.00	1.46	1.50
24	Y	606	CHL	CMB-C2B	-2.00	1.49	1.53
24	n	607	CHL	C1A-C2A	-2.00	1.51	1.53
25	3	611	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	605	CHL	C3D-CAD	-2.00	1.47	1.51
25	d	403	CLA	C3B-C2B	-2.00	1.37	1.40
28	y	1623	NEX	C22-C21	-2.00	1.51	1.54
29	d	410	LHG	O7-C5	-2.00	1.41	1.46
25	1	614	CLA	C3B-CAB	-2.00	1.43	1.47
25	2	604	CLA	CHC-C1C	2.00	1.41	1.35
33	a	409	PHO	CHD-C1D	2.00	1.42	1.38
29	b	2630	LHG	P-O6	2.00	1.67	1.59
35	B	2633	LMG	C3-C2	2.01	1.57	1.52
24	1	601	CHL	CMC-C2C	2.01	1.48	1.45
25	b	617	CLA	CHC-C1C	2.01	1.41	1.35
35	b	2633	LMG	C3-C2	2.01	1.57	1.52
29	B	2630	LHG	P-O6	2.02	1.67	1.59
25	5	610	CLA	CHB-C4A	2.02	1.36	1.33
25	6	604	CLA	CHC-C1C	2.02	1.41	1.35
25	2	612	CLA	CHC-C1C	2.02	1.41	1.35
25	B	617	CLA	CHC-C1C	2.02	1.41	1.35
24	5	601	CHL	CMC-C2C	2.03	1.48	1.45
25	Y	612	CLA	CHC-C1C	2.03	1.41	1.35
25	A	406	CLA	CHC-C1C	2.03	1.41	1.35
25	y	603	CLA	CHC-C1C	2.03	1.41	1.35
33	a	408	PHO	C4C-C3C	2.04	1.49	1.45
25	5	613	CLA	CHC-C1C	2.04	1.41	1.35
24	g	601	CHL	CMC-C2C	2.04	1.48	1.45
25	y	612	CLA	CHC-C1C	2.04	1.41	1.35
25	1	613	CLA	CHC-C1C	2.05	1.41	1.35
25	6	612	CLA	CHC-C1C	2.05	1.41	1.35
25	a	406	CLA	CHC-C1C	2.05	1.41	1.35
25	7	612	CLA	CHC-C1C	2.05	1.41	1.35
25	Y	603	CLA	CHC-C1C	2.05	1.41	1.35
25	B	602	CLA	CHC-C1C	2.05	1.41	1.35
25	3	612	CLA	CHC-C1C	2.05	1.41	1.35
33	A	408	PHO	C4C-C3C	2.05	1.49	1.45
24	G	601	CHL	CMC-C2C	2.05	1.48	1.45
24	n	609	CHL	CMC-C2C	2.06	1.48	1.45
25	7	603	CLA	CHC-C1C	2.06	1.41	1.35
25	1	604	CLA	CHC-C1C	2.06	1.41	1.35
25	b	602	CLA	CHC-C1C	2.06	1.41	1.35
25	5	604	CLA	CHC-C1C	2.07	1.41	1.35
25	B	610	CLA	CHC-C1C	2.07	1.41	1.35
25	y	610	CLA	CHB-C4A	2.07	1.36	1.33
24	N	609	CHL	CMC-C2C	2.07	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	408	PHO	C1A-NA	2.07	1.41	1.37
25	d	403	CLA	CHC-C1C	2.07	1.41	1.35
25	b	610	CLA	CHC-C1C	2.08	1.41	1.35
33	a	408	PHO	C1A-NA	2.08	1.41	1.37
25	D	403	CLA	CHC-C1C	2.08	1.41	1.35
25	3	603	CLA	CHC-C1C	2.09	1.41	1.35
25	1	611	CLA	CHC-C1C	2.09	1.41	1.35
25	5	611	CLA	CHC-C1C	2.09	1.41	1.35
25	D	402	CLA	CHC-C1C	2.10	1.41	1.35
24	s	608	CHL	CMC-C2C	2.10	1.48	1.45
25	3	604	CLA	CHC-C1C	2.10	1.41	1.35
24	1	608	CHL	CMC-C2C	2.10	1.48	1.45
25	B	613	CLA	CHC-C1C	2.10	1.41	1.35
25	R	611	CLA	CHC-C1C	2.11	1.41	1.35
25	b	604	CLA	CHC-C1C	2.11	1.41	1.35
25	b	616	CLA	CHC-C1C	2.11	1.41	1.35
25	d	402	CLA	CHC-C1C	2.11	1.41	1.35
25	b	608	CLA	CHC-C1C	2.11	1.41	1.35
24	N	601	CHL	CMC-C2C	2.11	1.48	1.45
25	Y	610	CLA	CHB-C4A	2.11	1.36	1.33
25	g	613	CLA	CHC-C1C	2.11	1.41	1.35
25	b	613	CLA	CHC-C1C	2.11	1.41	1.35
25	G	613	CLA	CHC-C1C	2.11	1.41	1.35
25	r	611	CLA	CHC-C1C	2.12	1.41	1.35
25	B	616	CLA	CHC-C1C	2.12	1.41	1.35
25	7	604	CLA	CHC-C1C	2.12	1.41	1.35
24	S	608	CHL	CMC-C2C	2.12	1.48	1.45
24	n	601	CHL	CMC-C2C	2.12	1.48	1.45
24	4	601	CHL	CMC-C2C	2.12	1.48	1.45
24	5	608	CHL	CMC-C2C	2.12	1.48	1.45
25	b	615	CLA	CHC-C1C	2.12	1.41	1.35
25	B	604	CLA	CHC-C1C	2.13	1.41	1.35
25	B	608	CLA	CHC-C1C	2.13	1.41	1.35
25	B	615	CLA	CHC-C1C	2.13	1.41	1.35
25	N	614	CLA	CHC-C1C	2.13	1.41	1.35
25	g	604	CLA	CHC-C1C	2.13	1.41	1.35
25	y	604	CLA	CHB-C4A	2.14	1.36	1.33
25	G	604	CLA	CHC-C1C	2.15	1.41	1.35
25	2	603	CLA	CHC-C1C	2.15	1.41	1.35
24	8	601	CHL	CMC-C2C	2.15	1.49	1.45
37	C	519	DGD	C4E-C3E	2.15	1.57	1.52
24	6	608	CHL	CMC-C2C	2.15	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	610	CLA	CHC-C1C	2.15	1.41	1.35
37	c	519	DGD	C4E-C3E	2.16	1.57	1.52
25	Y	611	CLA	CHB-C4A	2.16	1.36	1.33
25	n	614	CLA	CHC-C1C	2.16	1.41	1.35
25	6	603	CLA	CHC-C1C	2.16	1.41	1.35
25	C	506	CLA	CHC-C1C	2.16	1.41	1.35
25	g	610	CLA	CHC-C1C	2.17	1.41	1.35
25	y	611	CLA	CHB-C4A	2.17	1.36	1.33
25	5	610	CLA	CHC-C1C	2.17	1.41	1.35
25	n	604	CLA	CHC-C1C	2.17	1.41	1.35
25	1	610	CLA	CHC-C1C	2.17	1.41	1.35
25	Y	604	CLA	CHB-C4A	2.17	1.36	1.33
25	4	603	CLA	CHC-C1C	2.18	1.41	1.35
25	C	507	CLA	CHC-C1C	2.18	1.41	1.35
25	C	505	CLA	CHC-C1C	2.18	1.41	1.35
25	B	611	CLA	CHC-C1C	2.18	1.41	1.35
25	8	603	CLA	CHC-C1C	2.18	1.41	1.35
25	N	604	CLA	CHC-C1C	2.18	1.41	1.35
25	B	609	CLA	CHC-C1C	2.18	1.41	1.35
33	a	409	PHO	C4C-NC	2.18	1.41	1.36
25	b	609	CLA	CHC-C1C	2.18	1.41	1.35
25	c	506	CLA	CHC-C1C	2.19	1.41	1.35
25	C	508	CLA	CHC-C1C	2.19	1.41	1.35
24	2	608	CHL	CMC-C2C	2.19	1.49	1.45
25	r	612	CLA	CHC-C1C	2.19	1.41	1.35
25	c	508	CLA	CHC-C1C	2.19	1.41	1.35
25	c	507	CLA	CHC-C1C	2.20	1.41	1.35
25	r	613	CLA	CHC-C1C	2.20	1.41	1.35
25	b	611	CLA	CHC-C1C	2.20	1.41	1.35
25	a	407	CLA	CHC-C1C	2.20	1.41	1.35
25	c	502	CLA	CHC-C1C	2.20	1.41	1.35
25	y	614	CLA	CHC-C1C	2.20	1.41	1.35
25	R	612	CLA	CHC-C1C	2.20	1.41	1.35
25	7	602	CLA	CHC-C1C	2.20	1.41	1.35
25	C	502	CLA	CHC-C1C	2.20	1.41	1.35
25	R	613	CLA	CHC-C1C	2.20	1.41	1.35
25	A	407	CLA	CHC-C1C	2.20	1.41	1.35
25	Y	614	CLA	CHC-C1C	2.20	1.41	1.35
25	c	505	CLA	CHC-C1C	2.20	1.41	1.35
25	3	602	CLA	CHC-C1C	2.21	1.41	1.35
35	z	101	LMG	C4-C3	2.21	1.58	1.52
25	4	604	CLA	CHC-C1C	2.21	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	613	CLA	CHC-C1C	2.21	1.41	1.35
25	8	604	CLA	CHC-C1C	2.21	1.41	1.35
35	z	101	LMG	C4-C5	2.21	1.57	1.53
25	r	610	CLA	CHC-C1C	2.22	1.41	1.35
25	Y	604	CLA	CHC-C1C	2.22	1.41	1.35
35	Z	101	LMG	C4-C3	2.22	1.58	1.52
33	A	409	PHO	C4C-NC	2.23	1.41	1.36
25	R	610	CLA	CHC-C1C	2.23	1.41	1.35
25	B	615	CLA	CHB-C4A	2.23	1.36	1.33
25	y	604	CLA	CHC-C1C	2.23	1.41	1.35
35	Z	101	LMG	C4-C5	2.23	1.57	1.53
25	Y	602	CLA	CHC-C1C	2.23	1.41	1.35
25	n	613	CLA	CHC-C1C	2.23	1.41	1.35
25	6	613	CLA	CHC-C1C	2.23	1.41	1.35
25	7	610	CLA	CHB-C4A	2.23	1.36	1.33
25	y	602	CLA	CHC-C1C	2.23	1.41	1.35
25	a	405	CLA	CHC-C1C	2.24	1.41	1.35
25	A	405	CLA	CHC-C1C	2.24	1.41	1.35
25	2	613	CLA	CHC-C1C	2.24	1.41	1.35
25	a	410	CLA	CHC-C1C	2.24	1.41	1.35
25	N	603	CLA	CHC-C1C	2.24	1.41	1.35
25	n	611	CLA	CHC-C1C	2.25	1.41	1.35
25	n	603	CLA	CHC-C1C	2.25	1.41	1.35
25	R	603	CLA	CHC-C1C	2.25	1.41	1.35
25	G	612	CLA	CHC-C1C	2.25	1.41	1.35
25	g	612	CLA	CHC-C1C	2.25	1.41	1.35
25	A	410	CLA	CHC-C1C	2.26	1.41	1.35
25	b	615	CLA	CHB-C4A	2.26	1.36	1.33
25	G	602	CLA	CHC-C1C	2.26	1.41	1.35
25	N	611	CLA	CHC-C1C	2.26	1.41	1.35
33	A	408	PHO	C4C-NC	2.26	1.42	1.36
25	r	603	CLA	CHC-C1C	2.27	1.41	1.35
33	a	408	PHO	C4C-NC	2.27	1.42	1.36
25	C	504	CLA	CHC-C1C	2.27	1.41	1.35
25	g	602	CLA	CHC-C1C	2.27	1.41	1.35
25	r	602	CLA	CHC-C1C	2.27	1.41	1.35
24	g	609	CHL	CMC-C2C	2.27	1.49	1.45
25	3	610	CLA	CHB-C4A	2.27	1.36	1.33
25	c	504	CLA	CHC-C1C	2.28	1.41	1.35
24	G	609	CHL	CMC-C2C	2.29	1.49	1.45
25	R	602	CLA	CHC-C1C	2.29	1.41	1.35
25	R	604	CLA	CHC-C1C	2.29	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	611	CLA	CHC-C1C	2.29	1.41	1.35
25	8	611	CLA	CHC-C1C	2.30	1.42	1.35
25	6	610	CLA	CHC-C1C	2.30	1.42	1.35
24	2	601	CHL	CMC-C2C	2.30	1.49	1.45
33	A	409	PHO	C1A-NA	2.30	1.42	1.37
24	7	608	CHL	CMC-C2C	2.31	1.49	1.45
25	6	611	CLA	CHC-C1C	2.31	1.42	1.35
25	r	604	CLA	CHC-C1C	2.31	1.42	1.35
33	a	409	PHO	C1A-NA	2.31	1.42	1.37
24	6	601	CHL	CMC-C2C	2.32	1.49	1.45
25	y	610	CLA	CHC-C1C	2.32	1.42	1.35
25	7	610	CLA	CHC-C1C	2.32	1.42	1.35
25	3	610	CLA	CHC-C1C	2.32	1.42	1.35
25	n	602	CLA	CHC-C1C	2.32	1.42	1.35
25	2	610	CLA	CHC-C1C	2.32	1.42	1.35
25	2	611	CLA	CHC-C1C	2.32	1.42	1.35
24	3	608	CHL	CMC-C2C	2.32	1.49	1.45
25	G	603	CLA	CHB-C4A	2.33	1.36	1.33
25	N	602	CLA	CHC-C1C	2.33	1.42	1.35
25	C	512	CLA	CHC-C1C	2.33	1.42	1.35
25	g	603	CLA	CHC-C1C	2.33	1.42	1.35
25	G	603	CLA	CHC-C1C	2.33	1.42	1.35
25	Y	611	CLA	CHC-C1C	2.33	1.42	1.35
25	b	603	CLA	CHC-C1C	2.33	1.42	1.35
25	5	602	CLA	CHC-C1C	2.34	1.42	1.35
25	y	611	CLA	CHC-C1C	2.34	1.42	1.35
25	c	512	CLA	CHC-C1C	2.34	1.42	1.35
25	Y	610	CLA	CHC-C1C	2.34	1.42	1.35
25	N	603	CLA	CHB-C4A	2.34	1.36	1.33
25	S	613	CLA	CHC-C1C	2.35	1.42	1.35
25	s	613	CLA	CHC-C1C	2.35	1.42	1.35
25	b	604	CLA	CHB-C4A	2.35	1.36	1.33
25	g	603	CLA	CHB-C4A	2.35	1.36	1.33
25	B	603	CLA	CHC-C1C	2.35	1.42	1.35
25	c	509	CLA	CHC-C1C	2.36	1.42	1.35
25	Y	603	CLA	CHB-C4A	2.36	1.36	1.33
25	B	604	CLA	CHB-C4A	2.36	1.36	1.33
25	1	602	CLA	CHC-C1C	2.37	1.42	1.35
25	1	604	CLA	CHB-C4A	2.38	1.36	1.33
25	C	509	CLA	CHC-C1C	2.39	1.42	1.35
25	g	614	CLA	CHC-C1C	2.39	1.42	1.35
25	n	603	CLA	CHB-C4A	2.39	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	602	CLA	CHB-C4A	2.39	1.36	1.33
25	y	603	CLA	CHB-C4A	2.39	1.36	1.33
25	S	612	CLA	CHC-C1C	2.40	1.42	1.35
25	4	602	CLA	CHB-C4A	2.40	1.36	1.33
25	5	604	CLA	CHB-C4A	2.40	1.36	1.33
25	S	611	CLA	CHC-C1C	2.40	1.42	1.35
25	3	614	CLA	CHC-C1C	2.40	1.42	1.35
25	G	614	CLA	CHC-C1C	2.40	1.42	1.35
25	s	603	CLA	CHC-C1C	2.40	1.42	1.35
25	4	610	CLA	CHC-C1C	2.40	1.42	1.35
25	8	610	CLA	CHC-C1C	2.41	1.42	1.35
25	S	603	CLA	CHC-C1C	2.41	1.42	1.35
25	5	614	CLA	CHC-C1C	2.41	1.42	1.35
25	s	612	CLA	CHC-C1C	2.41	1.42	1.35
25	4	612	CLA	CHC-C1C	2.41	1.42	1.35
25	8	612	CLA	CHC-C1C	2.42	1.42	1.35
25	s	614	CLA	CHC-C1C	2.42	1.42	1.35
25	s	611	CLA	CHC-C1C	2.42	1.42	1.35
25	N	604	CLA	CHB-C4A	2.42	1.36	1.33
25	7	614	CLA	CHC-C1C	2.42	1.42	1.35
25	n	604	CLA	CHB-C4A	2.42	1.36	1.33
25	6	602	CLA	CHC-C1C	2.42	1.42	1.35
25	b	614	CLA	CHC-C1C	2.43	1.42	1.35
25	S	614	CLA	CHC-C1C	2.43	1.42	1.35
25	s	609	CLA	CHC-C1C	2.43	1.42	1.35
25	6	614	CLA	CHC-C1C	2.43	1.42	1.35
25	4	602	CLA	CHC-C1C	2.43	1.42	1.35
25	8	602	CLA	CHC-C1C	2.43	1.42	1.35
25	2	602	CLA	CHC-C1C	2.43	1.42	1.35
25	1	614	CLA	CHC-C1C	2.43	1.42	1.35
25	C	513	CLA	CHC-C1C	2.44	1.42	1.35
25	S	609	CLA	CHC-C1C	2.44	1.42	1.35
25	r	609	CLA	CHB-C4A	2.44	1.36	1.33
25	6	603	CLA	CHB-C4A	2.44	1.36	1.33
25	R	609	CLA	CHB-C4A	2.44	1.36	1.33
25	B	614	CLA	CHC-C1C	2.45	1.42	1.35
25	2	614	CLA	CHC-C1C	2.45	1.42	1.35
25	c	513	CLA	CHC-C1C	2.45	1.42	1.35
25	s	604	CLA	CHC-C1C	2.48	1.42	1.35
25	C	503	CLA	CHC-C1C	2.48	1.42	1.35
25	S	604	CLA	CHC-C1C	2.48	1.42	1.35
25	C	501	CLA	CHC-C1C	2.48	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	503	CLA	CHC-C1C	2.48	1.42	1.35
25	2	603	CLA	CHB-C4A	2.48	1.36	1.33
25	c	501	CLA	CHC-C1C	2.49	1.42	1.35
25	C	511	CLA	CHC-C1C	2.51	1.42	1.35
25	g	611	CLA	CHC-C1C	2.51	1.42	1.35
25	G	611	CLA	CHC-C1C	2.51	1.42	1.35
25	7	603	CLA	CHB-C4A	2.51	1.36	1.33
25	1	602	CLA	CHB-C4A	2.52	1.36	1.33
25	B	609	CLA	CHB-C4A	2.53	1.36	1.33
25	c	511	CLA	CHC-C1C	2.53	1.42	1.35
25	B	611	CLA	CHB-C4A	2.54	1.36	1.33
25	S	602	CLA	CHC-C1C	2.54	1.42	1.35
25	3	603	CLA	CHB-C4A	2.54	1.36	1.33
25	S	610	CLA	CHC-C1C	2.54	1.42	1.35
25	s	602	CLA	CHC-C1C	2.54	1.42	1.35
25	8	610	CLA	CHB-C4A	2.54	1.36	1.33
25	s	610	CLA	CHC-C1C	2.54	1.42	1.35
25	b	609	CLA	CHB-C4A	2.54	1.36	1.33
25	b	611	CLA	CHB-C4A	2.54	1.36	1.33
25	c	510	CLA	CHC-C1C	2.55	1.42	1.35
25	C	510	CLA	CHC-C1C	2.55	1.42	1.35
25	1	613	CLA	CHB-C4A	2.56	1.36	1.33
25	b	608	CLA	CHB-C4A	2.56	1.36	1.33
25	5	602	CLA	CHB-C4A	2.57	1.36	1.33
25	B	606	CLA	CHB-C4A	2.57	1.36	1.33
25	b	606	CLA	CHB-C4A	2.57	1.36	1.33
25	2	604	CLA	CHB-C4A	2.57	1.36	1.33
25	4	612	CLA	CHB-C4A	2.57	1.36	1.33
25	5	612	CLA	CHB-C4A	2.58	1.36	1.33
25	3	613	CLA	CHB-C4A	2.58	1.36	1.33
25	2	614	CLA	CHB-C4A	2.58	1.36	1.33
35	z	101	LMG	C7-C8	2.59	1.58	1.50
25	B	608	CLA	CHB-C4A	2.60	1.36	1.33
25	6	604	CLA	CHB-C4A	2.60	1.36	1.33
25	7	613	CLA	CHB-C4A	2.60	1.36	1.33
25	8	612	CLA	CHB-C4A	2.60	1.36	1.33
25	g	613	CLA	CHB-C4A	2.61	1.36	1.33
25	4	610	CLA	CHB-C4A	2.61	1.36	1.33
35	Z	101	LMG	C7-C8	2.61	1.58	1.50
25	1	612	CLA	CHB-C4A	2.62	1.36	1.33
25	6	614	CLA	CHB-C4A	2.62	1.36	1.33
25	G	613	CLA	CHB-C4A	2.63	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	412	SQD	O47-C7	2.63	1.41	1.34
25	6	613	CLA	CHB-C4A	2.64	1.36	1.33
34	A	412	SQD	O47-C7	2.64	1.41	1.34
25	5	613	CLA	CHB-C4A	2.64	1.36	1.33
25	5	614	CLA	CHB-C4A	2.65	1.36	1.33
25	b	616	CLA	CHB-C4A	2.66	1.36	1.33
25	B	616	CLA	CHB-C4A	2.66	1.36	1.33
25	2	613	CLA	CHB-C4A	2.67	1.37	1.33
25	R	604	CLA	CHB-C4A	2.68	1.37	1.33
25	r	601	CLA	CHC-C1C	2.69	1.43	1.35
25	y	612	CLA	CHB-C4A	2.69	1.37	1.33
25	1	614	CLA	CHB-C4A	2.69	1.37	1.33
25	4	604	CLA	CHB-C4A	2.70	1.37	1.33
25	R	601	CLA	CHC-C1C	2.71	1.43	1.35
25	C	501	CLA	CHB-C4A	2.72	1.37	1.33
25	Y	612	CLA	CHB-C4A	2.73	1.37	1.33
25	G	610	CLA	CHB-C4A	2.73	1.37	1.33
25	r	604	CLA	CHB-C4A	2.73	1.37	1.33
25	8	604	CLA	CHB-C4A	2.74	1.37	1.33
25	g	610	CLA	CHB-C4A	2.74	1.37	1.33
25	3	612	CLA	CHB-C4A	2.75	1.37	1.33
25	G	604	CLA	CHB-C4A	2.75	1.37	1.33
25	c	501	CLA	CHB-C4A	2.76	1.37	1.33
25	B	602	CLA	CHB-C4A	2.76	1.37	1.33
25	b	614	CLA	CHB-C4A	2.77	1.37	1.33
25	g	604	CLA	CHB-C4A	2.77	1.37	1.33
25	b	602	CLA	CHB-C4A	2.77	1.37	1.33
25	B	614	CLA	CHB-C4A	2.78	1.37	1.33
25	s	610	CLA	CHB-C4A	2.78	1.37	1.33
25	y	614	CLA	CHB-C4A	2.78	1.37	1.33
25	7	612	CLA	CHB-C4A	2.78	1.37	1.33
25	B	612	CLA	CHB-C4A	2.79	1.37	1.33
25	6	610	CLA	CHB-C4A	2.79	1.37	1.33
33	A	409	PHO	CHC-C1C	2.80	1.44	1.38
25	6	612	CLA	CHB-C4A	2.80	1.37	1.33
33	a	409	PHO	CHC-C1C	2.80	1.44	1.38
25	S	610	CLA	CHB-C4A	2.80	1.37	1.33
25	2	612	CLA	CHB-C4A	2.81	1.37	1.33
25	b	612	CLA	CHB-C4A	2.82	1.37	1.33
34	A	418	SQD	O48-C23	2.82	1.41	1.33
33	A	408	PHO	CHC-C1C	2.82	1.44	1.38
25	Y	614	CLA	CHB-C4A	2.82	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	602	CLA	CHB-C4A	2.83	1.37	1.33
25	2	610	CLA	CHB-C4A	2.83	1.37	1.33
34	a	418	SQD	O48-C23	2.84	1.41	1.33
25	7	604	CLA	CHB-C4A	2.84	1.37	1.33
25	3	604	CLA	CHB-C4A	2.84	1.37	1.33
25	D	403	CLA	CHB-C4A	2.84	1.37	1.33
34	b	621	SQD	O47-C7	2.84	1.42	1.34
34	A	412	SQD	O48-C23	2.84	1.41	1.33
34	A	418	SQD	O47-C7	2.84	1.42	1.34
34	a	412	SQD	O48-C23	2.84	1.41	1.33
25	d	403	CLA	CHB-C4A	2.84	1.37	1.33
25	B	607	CLA	CHB-C4A	2.85	1.37	1.33
25	6	602	CLA	CHB-C4A	2.85	1.37	1.33
33	a	408	PHO	CHC-C1C	2.85	1.44	1.38
25	n	610	CLA	CHB-C4A	2.86	1.37	1.33
34	B	621	SQD	O47-C7	2.86	1.42	1.34
25	N	610	CLA	CHB-C4A	2.86	1.37	1.33
34	a	418	SQD	O47-C7	2.87	1.42	1.34
25	r	610	CLA	CHB-C4A	2.87	1.37	1.33
25	g	612	CLA	CHB-C4A	2.87	1.37	1.33
34	B	621	SQD	O48-C23	2.87	1.41	1.33
25	G	612	CLA	CHB-C4A	2.87	1.37	1.33
34	b	621	SQD	O48-C23	2.88	1.41	1.33
25	R	601	CLA	CHB-C4A	2.90	1.37	1.33
25	b	607	CLA	CHB-C4A	2.90	1.37	1.33
25	l	611	CLA	CHB-C4A	2.91	1.37	1.33
25	R	610	CLA	CHB-C4A	2.91	1.37	1.33
34	B	623	SQD	O47-C7	2.94	1.42	1.34
25	R	602	CLA	CHB-C4A	2.94	1.37	1.33
34	b	623	SQD	O47-C7	2.94	1.42	1.34
33	a	408	PHO	C3B-C4B	2.95	1.49	1.43
25	5	611	CLA	CHB-C4A	2.95	1.37	1.33
25	r	601	CLA	CHB-C4A	2.95	1.37	1.33
25	r	603	CLA	CHB-C4A	2.95	1.37	1.33
25	r	602	CLA	CHB-C4A	2.95	1.37	1.33
25	d	402	CLA	CHB-C4A	2.95	1.37	1.33
25	A	407	CLA	CHB-C4A	2.96	1.37	1.33
25	D	402	CLA	CHB-C4A	2.96	1.37	1.33
25	a	407	CLA	CHB-C4A	2.96	1.37	1.33
33	A	408	PHO	C3B-C4B	2.96	1.49	1.43
25	g	611	CLA	CHB-C4A	2.97	1.37	1.33
25	b	603	CLA	CHB-C4A	2.97	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	603	CLA	CHB-C4A	2.97	1.37	1.33
25	R	603	CLA	CHB-C4A	2.98	1.37	1.33
25	G	611	CLA	CHB-C4A	2.98	1.37	1.33
25	6	611	CLA	CHB-C4A	2.98	1.37	1.33
24	R	608	CHL	OBD-CAD	2.99	1.26	1.21
24	r	608	CHL	OBD-CAD	2.99	1.26	1.21
25	B	603	CLA	CHB-C4A	2.99	1.37	1.33
25	3	602	CLA	CHB-C4A	3.00	1.37	1.33
33	A	409	PHO	C3B-C4B	3.01	1.49	1.43
33	a	409	PHO	C3B-C4B	3.01	1.49	1.43
25	4	603	CLA	CHB-C4A	3.03	1.37	1.33
25	7	602	CLA	CHB-C4A	3.03	1.37	1.33
25	r	611	CLA	CHB-C4A	3.03	1.37	1.33
34	B	623	SQD	O48-C23	3.03	1.42	1.33
34	b	623	SQD	O48-C23	3.04	1.42	1.33
25	1	603	CLA	CHB-C4A	3.04	1.37	1.33
25	2	611	CLA	CHB-C4A	3.04	1.37	1.33
25	a	406	CLA	CHB-C4A	3.05	1.37	1.33
25	5	603	CLA	CHB-C4A	3.05	1.37	1.33
25	B	613	CLA	CHB-C4A	3.05	1.37	1.33
25	y	613	CLA	CHB-C4A	3.05	1.37	1.33
25	g	614	CLA	CHB-C4A	3.05	1.37	1.33
25	A	406	CLA	CHB-C4A	3.05	1.37	1.33
25	b	613	CLA	CHB-C4A	3.06	1.37	1.33
25	C	508	CLA	CHB-C4A	3.06	1.37	1.33
25	s	614	CLA	CHB-C4A	3.06	1.37	1.33
25	Y	613	CLA	CHB-C4A	3.07	1.37	1.33
25	c	504	CLA	CHB-C4A	3.08	1.37	1.33
25	G	614	CLA	CHB-C4A	3.09	1.37	1.33
25	S	614	CLA	CHB-C4A	3.10	1.37	1.33
25	C	504	CLA	CHB-C4A	3.10	1.37	1.33
25	R	611	CLA	CHB-C4A	3.10	1.37	1.33
25	c	508	CLA	CHB-C4A	3.10	1.37	1.33
25	B	617	CLA	CHB-C4A	3.12	1.37	1.33
25	C	512	CLA	CHB-C4A	3.13	1.37	1.33
25	b	617	CLA	CHB-C4A	3.13	1.37	1.33
25	A	410	CLA	CHB-C4A	3.13	1.37	1.33
24	y	601	CHL	OBD-CAD	3.15	1.26	1.21
24	4	608	CHL	OBD-CAD	3.15	1.26	1.21
25	B	610	CLA	CHB-C4A	3.15	1.37	1.33
24	8	608	CHL	OBD-CAD	3.16	1.26	1.21
25	3	611	CLA	CHB-C4A	3.16	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	512	CLA	CHB-C4A	3.16	1.37	1.33
25	a	410	CLA	CHB-C4A	3.17	1.37	1.33
25	y	602	CLA	CHB-C4A	3.17	1.37	1.33
24	Y	601	CHL	OBD-CAD	3.17	1.27	1.21
25	b	610	CLA	CHB-C4A	3.18	1.37	1.33
25	7	611	CLA	CHB-C4A	3.19	1.37	1.33
25	Y	602	CLA	CHB-C4A	3.20	1.37	1.33
25	A	405	CLA	CHB-C4A	3.22	1.37	1.33
24	G	601	CHL	OBD-CAD	3.23	1.27	1.21
24	g	601	CHL	OBD-CAD	3.24	1.27	1.21
25	3	614	CLA	CHB-C4A	3.24	1.37	1.33
25	c	510	CLA	CHB-C4A	3.25	1.37	1.33
25	7	614	CLA	CHB-C4A	3.26	1.37	1.33
25	B	605	CLA	CHB-C4A	3.27	1.37	1.33
25	a	405	CLA	CHB-C4A	3.27	1.37	1.33
25	c	511	CLA	CHB-C4A	3.28	1.37	1.33
25	C	510	CLA	CHB-C4A	3.29	1.37	1.33
25	r	612	CLA	CHB-C4A	3.29	1.37	1.33
25	R	612	CLA	CHB-C4A	3.30	1.37	1.33
25	b	605	CLA	CHB-C4A	3.30	1.37	1.33
24	N	608	CHL	OBD-CAD	3.30	1.27	1.21
24	n	608	CHL	OBD-CAD	3.31	1.27	1.21
25	N	602	CLA	CHB-C4A	3.33	1.37	1.33
24	Y	608	CHL	OBD-CAD	3.33	1.27	1.21
25	C	511	CLA	CHB-C4A	3.34	1.37	1.33
25	n	602	CLA	CHB-C4A	3.34	1.37	1.33
25	N	612	CLA	CHB-C4A	3.34	1.37	1.33
25	c	503	CLA	CHB-C4A	3.35	1.37	1.33
25	C	506	CLA	CHB-C4A	3.36	1.37	1.33
24	y	608	CHL	OBD-CAD	3.36	1.27	1.21
25	g	602	CLA	CHB-C4A	3.38	1.37	1.33
25	c	506	CLA	CHB-C4A	3.38	1.37	1.33
25	n	612	CLA	CHB-C4A	3.38	1.37	1.33
25	C	503	CLA	CHB-C4A	3.39	1.37	1.33
24	n	606	CHL	OBD-CAD	3.40	1.27	1.21
24	5	608	CHL	OBD-CAD	3.41	1.27	1.21
25	G	602	CLA	CHB-C4A	3.42	1.37	1.33
25	C	505	CLA	CHB-C4A	3.42	1.37	1.33
24	1	608	CHL	OBD-CAD	3.42	1.27	1.21
25	C	513	CLA	CHB-C4A	3.43	1.37	1.33
24	N	606	CHL	OBD-CAD	3.44	1.27	1.21
24	y	606	CHL	OBD-CAD	3.45	1.27	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	606	CHL	OBD-CAD	3.45	1.27	1.21
25	s	602	CLA	CHB-C4A	3.46	1.38	1.33
25	S	603	CLA	CHB-C4A	3.46	1.38	1.33
24	y	609	CHL	OBD-CAD	3.47	1.27	1.21
25	s	603	CLA	CHB-C4A	3.47	1.38	1.33
24	n	609	CHL	OBD-CAD	3.47	1.27	1.21
25	c	513	CLA	CHB-C4A	3.47	1.38	1.33
25	n	614	CLA	CHB-C4A	3.47	1.38	1.33
25	s	609	CLA	CHB-C4A	3.47	1.38	1.33
25	N	614	CLA	CHB-C4A	3.47	1.38	1.33
25	c	505	CLA	CHB-C4A	3.48	1.38	1.33
24	N	609	CHL	OBD-CAD	3.48	1.27	1.21
24	3	608	CHL	OBD-CAD	3.50	1.27	1.21
25	S	613	CLA	CHB-C4A	3.50	1.38	1.33
25	s	611	CLA	CHB-C4A	3.50	1.38	1.33
24	7	608	CHL	OBD-CAD	3.50	1.27	1.21
24	Y	609	CHL	OBD-CAD	3.51	1.27	1.21
25	s	613	CLA	CHB-C4A	3.51	1.38	1.33
25	S	611	CLA	CHB-C4A	3.52	1.38	1.33
25	S	609	CLA	CHB-C4A	3.53	1.38	1.33
25	S	602	CLA	CHB-C4A	3.54	1.38	1.33
25	R	613	CLA	CHB-C4A	3.54	1.38	1.33
24	7	601	CHL	OBD-CAD	3.55	1.27	1.21
25	r	613	CLA	CHB-C4A	3.56	1.38	1.33
25	C	509	CLA	CHB-C4A	3.57	1.38	1.33
24	3	601	CHL	OBD-CAD	3.57	1.27	1.21
25	S	612	CLA	CHB-C4A	3.57	1.38	1.33
25	s	612	CLA	CHB-C4A	3.57	1.38	1.33
24	G	609	CHL	OBD-CAD	3.57	1.27	1.21
24	g	609	CHL	OBD-CAD	3.58	1.27	1.21
24	N	601	CHL	OBD-CAD	3.58	1.27	1.21
25	S	604	CLA	CHB-C4A	3.59	1.38	1.33
25	c	509	CLA	CHB-C4A	3.59	1.38	1.33
24	n	601	CHL	OBD-CAD	3.59	1.27	1.21
25	s	604	CLA	CHB-C4A	3.61	1.38	1.33
25	N	611	CLA	CHB-C4A	3.63	1.38	1.33
25	n	611	CLA	CHB-C4A	3.64	1.38	1.33
25	N	613	CLA	CHB-C4A	3.69	1.38	1.33
25	4	611	CLA	CHB-C4A	3.69	1.38	1.33
25	n	613	CLA	CHB-C4A	3.71	1.38	1.33
24	5	601	CHL	OBD-CAD	3.72	1.27	1.21
24	6	608	CHL	OBD-CAD	3.72	1.27	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	611	CLA	CHB-C4A	3.72	1.38	1.33
24	1	601	CHL	OBD-CAD	3.73	1.27	1.21
24	2	608	CHL	OBD-CAD	3.74	1.27	1.21
24	G	608	CHL	OBD-CAD	3.80	1.28	1.21
24	g	608	CHL	OBD-CAD	3.80	1.28	1.21
24	5	609	CHL	OBD-CAD	3.81	1.28	1.21
24	1	609	CHL	OBD-CAD	3.83	1.28	1.21
24	S	608	CHL	OBD-CAD	3.84	1.28	1.21
24	s	608	CHL	OBD-CAD	3.84	1.28	1.21
24	2	601	CHL	OBD-CAD	3.85	1.28	1.21
24	n	607	CHL	OBD-CAD	3.86	1.28	1.21
24	6	601	CHL	OBD-CAD	3.86	1.28	1.21
24	Y	607	CHL	OBD-CAD	3.87	1.28	1.21
24	5	607	CHL	OBD-CAD	3.87	1.28	1.21
24	1	606	CHL	OBD-CAD	3.87	1.28	1.21
24	5	606	CHL	OBD-CAD	3.88	1.28	1.21
24	7	607	CHL	OBD-CAD	3.88	1.28	1.21
24	G	606	CHL	OBD-CAD	3.88	1.28	1.21
24	Y	605	CHL	OBD-CAD	3.88	1.28	1.21
24	R	606	CHL	OBD-CAD	3.89	1.28	1.21
24	y	605	CHL	OBD-CAD	3.89	1.28	1.21
25	C	502	CLA	CHB-C4A	3.89	1.38	1.33
24	N	607	CHL	OBD-CAD	3.90	1.28	1.21
24	3	606	CHL	OBD-CAD	3.90	1.28	1.21
24	g	606	CHL	OBD-CAD	3.90	1.28	1.21
24	1	607	CHL	OBD-CAD	3.91	1.28	1.21
24	r	606	CHL	OBD-CAD	3.91	1.28	1.21
24	3	607	CHL	OBD-CAD	3.91	1.28	1.21
25	c	502	CLA	CHB-C4A	3.91	1.38	1.33
24	y	607	CHL	OBD-CAD	3.92	1.28	1.21
24	s	601	CHL	OBD-CAD	3.92	1.28	1.21
24	S	601	CHL	OBD-CAD	3.92	1.28	1.21
24	2	609	CHL	OBD-CAD	3.92	1.28	1.21
24	3	609	CHL	OBD-CAD	3.93	1.28	1.21
24	2	606	CHL	OBD-CAD	3.93	1.28	1.21
24	6	609	CHL	OBD-CAD	3.93	1.28	1.21
24	2	607	CHL	OBD-CAD	3.93	1.28	1.21
24	7	606	CHL	OBD-CAD	3.93	1.28	1.21
24	6	606	CHL	OBD-CAD	3.93	1.28	1.21
24	y	607	CHL	O2A-CGA	3.95	1.45	1.33
24	7	609	CHL	OBD-CAD	3.95	1.28	1.21
24	y	601	CHL	O2A-CGA	3.95	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	606	CHL	OBD-CAD	3.96	1.28	1.21
39	F	101	HEM	C3B-CAB	3.96	1.55	1.47
24	Y	601	CHL	O2A-CGA	3.96	1.45	1.33
24	Y	607	CHL	O2A-CGA	3.97	1.45	1.33
39	f	101	HEM	C3B-CAB	3.97	1.55	1.47
24	6	607	CHL	OBD-CAD	3.97	1.28	1.21
24	8	606	CHL	OBD-CAD	3.97	1.28	1.21
25	R	616	CLA	CHB-C4A	3.98	1.38	1.33
24	5	605	CHL	OBD-CAD	3.99	1.28	1.21
24	1	605	CHL	OBD-CAD	3.99	1.28	1.21
24	4	609	CHL	OBD-CAD	3.99	1.28	1.21
24	3	605	CHL	OBD-CAD	4.00	1.28	1.21
24	7	605	CHL	OBD-CAD	4.00	1.28	1.21
25	C	507	CLA	CHB-C4A	4.00	1.38	1.33
24	4	607	CHL	OBD-CAD	4.01	1.28	1.21
24	8	609	CHL	OBD-CAD	4.01	1.28	1.21
24	g	607	CHL	O2A-CGA	4.01	1.45	1.33
24	n	608	CHL	O2A-CGA	4.01	1.45	1.33
24	8	607	CHL	OBD-CAD	4.01	1.28	1.21
24	G	601	CHL	O2A-CGA	4.03	1.45	1.33
24	G	607	CHL	O2A-CGA	4.03	1.45	1.33
24	N	608	CHL	O2A-CGA	4.03	1.45	1.33
24	Y	608	CHL	O2A-CGA	4.03	1.45	1.33
24	y	608	CHL	O2A-CGA	4.04	1.45	1.33
25	c	507	CLA	CHB-C4A	4.06	1.38	1.33
24	g	601	CHL	O2A-CGA	4.06	1.45	1.33
25	r	616	CLA	CHB-C4A	4.06	1.38	1.33
24	g	607	CHL	OBD-CAD	4.06	1.28	1.21
24	2	607	CHL	O2A-CGA	4.07	1.45	1.33
24	G	607	CHL	OBD-CAD	4.07	1.28	1.21
24	6	607	CHL	O2A-CGA	4.08	1.45	1.33
24	R	607	CHL	O2A-CGA	4.10	1.45	1.33
24	r	607	CHL	O2A-CGA	4.10	1.45	1.33
24	s	606	CHL	OBD-CAD	4.11	1.28	1.21
39	f	101	HEM	C3C-CAC	4.11	1.55	1.47
24	S	606	CHL	OBD-CAD	4.11	1.28	1.21
39	F	101	HEM	C3C-CAC	4.11	1.55	1.47
24	7	601	CHL	O2A-CGA	4.13	1.45	1.33
24	y	605	CHL	O2A-CGA	4.13	1.45	1.33
24	G	606	CHL	O2A-CGA	4.14	1.45	1.33
24	2	605	CHL	OBD-CAD	4.14	1.28	1.21
24	g	605	CHL	OBD-CAD	4.14	1.28	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	605	CHL	O2A-CGA	4.14	1.45	1.33
24	8	601	CHL	OBD-CAD	4.14	1.28	1.21
24	g	606	CHL	O2A-CGA	4.14	1.45	1.33
24	G	605	CHL	OBD-CAD	4.15	1.28	1.21
24	3	601	CHL	O2A-CGA	4.15	1.45	1.33
24	G	609	CHL	O2A-CGA	4.17	1.45	1.33
24	6	605	CHL	OBD-CAD	4.17	1.28	1.21
24	2	609	CHL	O2A-CGA	4.18	1.45	1.33
24	5	607	CHL	O2A-CGA	4.18	1.45	1.33
24	G	608	CHL	O2A-CGA	4.18	1.45	1.33
24	g	609	CHL	O2A-CGA	4.18	1.45	1.33
24	g	608	CHL	O2A-CGA	4.19	1.45	1.33
24	4	601	CHL	OBD-CAD	4.19	1.28	1.21
24	6	609	CHL	O2A-CGA	4.19	1.45	1.33
24	Y	609	CHL	O2A-CGA	4.19	1.45	1.33
24	1	609	CHL	O2A-CGA	4.20	1.45	1.33
24	n	605	CHL	O2A-CGA	4.20	1.45	1.33
24	r	607	CHL	OBD-CAD	4.20	1.28	1.21
24	y	609	CHL	O2A-CGA	4.20	1.45	1.33
24	N	605	CHL	O2A-CGA	4.20	1.45	1.33
24	r	606	CHL	O2A-CGA	4.20	1.45	1.33
24	R	606	CHL	O2A-CGA	4.21	1.45	1.33
24	5	609	CHL	O2A-CGA	4.21	1.45	1.33
24	1	607	CHL	O2A-CGA	4.21	1.45	1.33
24	R	607	CHL	OBD-CAD	4.21	1.28	1.21
24	R	608	CHL	O2A-CGA	4.21	1.45	1.33
24	n	607	CHL	O2A-CGA	4.24	1.45	1.33
24	r	608	CHL	O2A-CGA	4.25	1.45	1.33
24	N	607	CHL	O2A-CGA	4.25	1.45	1.33
24	y	606	CHL	O2A-CGA	4.26	1.45	1.33
24	Y	606	CHL	O2A-CGA	4.26	1.45	1.33
24	3	607	CHL	O2A-CGA	4.28	1.45	1.33
24	n	601	CHL	O2A-CGA	4.28	1.45	1.33
24	N	601	CHL	O2A-CGA	4.28	1.45	1.33
24	7	607	CHL	O2A-CGA	4.29	1.46	1.33
24	n	609	CHL	O2A-CGA	4.32	1.46	1.33
24	N	609	CHL	O2A-CGA	4.33	1.46	1.33
24	N	605	CHL	OBD-CAD	4.34	1.28	1.21
24	S	607	CHL	OBD-CAD	4.34	1.28	1.21
24	R	614	CHL	OBD-CAD	4.34	1.28	1.21
24	n	605	CHL	OBD-CAD	4.35	1.29	1.21
24	s	607	CHL	OBD-CAD	4.36	1.29	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	607	CHL	O2A-CGA	4.37	1.46	1.33
24	s	607	CHL	O2A-CGA	4.37	1.46	1.33
24	r	614	CHL	OBD-CAD	4.37	1.29	1.21
24	Y	608	CHL	O2D-CGD	4.38	1.44	1.33
24	y	608	CHL	O2D-CGD	4.38	1.44	1.33
24	7	609	CHL	O2A-CGA	4.39	1.46	1.33
24	3	609	CHL	O2A-CGA	4.40	1.46	1.33
24	r	608	CHL	O2D-CGD	4.42	1.44	1.33
24	5	609	CHL	O2D-CGD	4.42	1.44	1.33
24	R	608	CHL	O2D-CGD	4.44	1.44	1.33
24	n	606	CHL	O2A-CGA	4.44	1.46	1.33
24	N	606	CHL	O2A-CGA	4.45	1.46	1.33
24	1	609	CHL	O2D-CGD	4.45	1.44	1.33
24	Y	607	CHL	O2D-CGD	4.45	1.44	1.33
24	y	607	CHL	O2D-CGD	4.45	1.44	1.33
24	Y	609	CHL	O2D-CGD	4.50	1.44	1.33
24	Y	601	CHL	O2D-CGD	4.51	1.44	1.33
24	3	607	CHL	O2D-CGD	4.51	1.44	1.33
24	5	601	CHL	O2D-CGD	4.51	1.44	1.33
24	1	608	CHL	O2D-CGD	4.51	1.44	1.33
24	y	609	CHL	O2D-CGD	4.52	1.44	1.33
24	7	607	CHL	O2D-CGD	4.52	1.44	1.33
24	5	607	CHL	O2D-CGD	4.52	1.44	1.33
24	y	601	CHL	O2D-CGD	4.52	1.44	1.33
24	1	607	CHL	O2D-CGD	4.53	1.44	1.33
24	3	609	CHL	O2D-CGD	4.54	1.44	1.33
24	n	609	CHL	O2D-CGD	4.54	1.44	1.33
24	1	601	CHL	O2D-CGD	4.54	1.44	1.33
24	N	605	CHL	O2D-CGD	4.55	1.44	1.33
24	N	609	CHL	O2D-CGD	4.55	1.44	1.33
24	5	608	CHL	O2D-CGD	4.55	1.44	1.33
24	G	609	CHL	O2D-CGD	4.58	1.44	1.33
24	n	605	CHL	O2D-CGD	4.58	1.44	1.33
24	7	609	CHL	O2D-CGD	4.58	1.44	1.33
24	7	608	CHL	O2D-CGD	4.59	1.44	1.33
24	N	608	CHL	O2D-CGD	4.60	1.44	1.33
24	n	608	CHL	O2D-CGD	4.60	1.44	1.33
24	y	605	CHL	O2D-CGD	4.60	1.44	1.33
24	y	606	CHL	O2D-CGD	4.60	1.44	1.33
24	g	609	CHL	O2D-CGD	4.60	1.44	1.33
24	3	608	CHL	O2D-CGD	4.61	1.44	1.33
24	R	614	CHL	O2D-CGD	4.62	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	r	614	CHL	O2D-CGD	4.62	1.44	1.33
24	Y	606	CHL	O2D-CGD	4.62	1.44	1.33
24	Y	605	CHL	O2D-CGD	4.64	1.45	1.33
24	3	601	CHL	O2D-CGD	4.65	1.45	1.33
24	8	607	CHL	O2D-CGD	4.65	1.45	1.33
24	4	607	CHL	O2D-CGD	4.65	1.45	1.33
24	7	601	CHL	O2D-CGD	4.65	1.45	1.33
24	R	606	CHL	O2D-CGD	4.66	1.45	1.33
24	6	608	CHL	O2D-CGD	4.66	1.45	1.33
24	N	606	CHL	O2D-CGD	4.67	1.45	1.33
24	1	606	CHL	O2D-CGD	4.67	1.45	1.33
24	r	606	CHL	O2D-CGD	4.67	1.45	1.33
24	2	608	CHL	O2D-CGD	4.68	1.45	1.33
24	5	606	CHL	O2D-CGD	4.68	1.45	1.33
24	n	607	CHL	O2D-CGD	4.69	1.45	1.33
24	N	607	CHL	O2D-CGD	4.69	1.45	1.33
24	4	606	CHL	O2D-CGD	4.69	1.45	1.33
24	n	606	CHL	O2D-CGD	4.70	1.45	1.33
24	g	606	CHL	O2D-CGD	4.70	1.45	1.33
24	G	606	CHL	O2D-CGD	4.70	1.45	1.33
24	8	606	CHL	O2D-CGD	4.70	1.45	1.33
24	1	605	CHL	O2D-CGD	4.70	1.45	1.33
24	5	605	CHL	O2D-CGD	4.72	1.45	1.33
24	G	607	CHL	O2D-CGD	4.73	1.45	1.33
24	g	607	CHL	O2D-CGD	4.73	1.45	1.33
24	8	608	CHL	O2D-CGD	4.75	1.45	1.33
24	G	601	CHL	O2D-CGD	4.75	1.45	1.33
24	g	601	CHL	O2D-CGD	4.75	1.45	1.33
24	6	609	CHL	O2D-CGD	4.75	1.45	1.33
24	2	606	CHL	O2D-CGD	4.77	1.45	1.33
24	4	608	CHL	O2D-CGD	4.77	1.45	1.33
24	7	605	CHL	O2D-CGD	4.77	1.45	1.33
24	3	606	CHL	O2D-CGD	4.77	1.45	1.33
24	2	609	CHL	O2D-CGD	4.77	1.45	1.33
24	7	606	CHL	O2D-CGD	4.78	1.45	1.33
24	3	605	CHL	O2D-CGD	4.78	1.45	1.33
24	6	606	CHL	O2D-CGD	4.78	1.45	1.33
24	S	606	CHL	O2D-CGD	4.79	1.45	1.33
24	s	608	CHL	O2D-CGD	4.79	1.45	1.33
24	G	608	CHL	O2D-CGD	4.79	1.45	1.33
24	S	608	CHL	O2D-CGD	4.80	1.45	1.33
24	g	608	CHL	O2D-CGD	4.80	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	s	606	CHL	O2D-CGD	4.81	1.45	1.33
24	G	605	CHL	O2D-CGD	4.81	1.45	1.33
24	6	601	CHL	O2D-CGD	4.81	1.45	1.33
24	2	605	CHL	O2D-CGD	4.82	1.45	1.33
24	N	601	CHL	O2D-CGD	4.82	1.45	1.33
24	n	601	CHL	O2D-CGD	4.82	1.45	1.33
24	2	601	CHL	O2D-CGD	4.82	1.45	1.33
24	r	607	CHL	O2D-CGD	4.82	1.45	1.33
24	g	605	CHL	O2D-CGD	4.82	1.45	1.33
24	6	605	CHL	O2D-CGD	4.83	1.45	1.33
24	R	607	CHL	O2D-CGD	4.83	1.45	1.33
24	s	601	CHL	O2D-CGD	4.87	1.45	1.33
24	S	601	CHL	O2D-CGD	4.89	1.45	1.33
24	4	609	CHL	O2D-CGD	4.92	1.45	1.33
24	2	607	CHL	O2D-CGD	4.93	1.45	1.33
24	8	609	CHL	O2D-CGD	4.93	1.45	1.33
24	6	607	CHL	O2D-CGD	4.93	1.45	1.33
24	s	607	CHL	O2D-CGD	5.00	1.45	1.33
24	S	607	CHL	O2D-CGD	5.01	1.45	1.33
24	y	601	CHL	C3C-C2C	8.13	1.44	1.34
24	Y	601	CHL	C3C-C2C	8.13	1.44	1.34
24	R	608	CHL	C3C-C2C	8.17	1.44	1.34
24	r	608	CHL	C3C-C2C	8.19	1.44	1.34
24	n	606	CHL	C3C-C2C	8.22	1.44	1.34
24	N	606	CHL	C3C-C2C	8.23	1.44	1.34
24	Y	606	CHL	C3C-C2C	8.25	1.44	1.34
24	y	606	CHL	C3C-C2C	8.26	1.44	1.34
24	G	601	CHL	C3C-C2C	8.33	1.44	1.34
24	g	601	CHL	C3C-C2C	8.34	1.44	1.34
24	3	601	CHL	C3C-C2C	8.38	1.44	1.34
24	7	601	CHL	C3C-C2C	8.42	1.44	1.34
24	8	608	CHL	C3C-C2C	8.43	1.44	1.34
24	4	608	CHL	C3C-C2C	8.49	1.45	1.34
24	y	609	CHL	C3C-C2C	8.68	1.45	1.34
24	G	607	CHL	C3C-C2C	8.68	1.45	1.34
24	3	607	CHL	C3C-C2C	8.69	1.45	1.34
24	7	607	CHL	C3C-C2C	8.70	1.45	1.34
24	Y	609	CHL	C3C-C2C	8.71	1.45	1.34
24	g	607	CHL	C3C-C2C	8.72	1.45	1.34
24	6	609	CHL	C3C-C2C	8.75	1.45	1.34
24	2	609	CHL	C3C-C2C	8.76	1.45	1.34
24	N	608	CHL	C3C-C2C	8.79	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	608	CHL	C3C-C2C	8.80	1.45	1.34
24	Y	608	CHL	C3C-C2C	8.82	1.45	1.34
24	y	608	CHL	C3C-C2C	8.83	1.45	1.34
24	N	609	CHL	C3C-C2C	8.83	1.45	1.34
24	n	609	CHL	C3C-C2C	8.84	1.45	1.34
24	y	605	CHL	C3C-C2C	8.85	1.45	1.34
24	5	601	CHL	C3C-C2C	8.86	1.45	1.34
24	Y	605	CHL	C3C-C2C	8.87	1.45	1.34
24	1	601	CHL	C3C-C2C	8.88	1.45	1.34
24	n	601	CHL	C3C-C2C	8.90	1.45	1.34
24	y	607	CHL	C3C-C2C	8.90	1.45	1.34
24	N	607	CHL	C3C-C2C	8.92	1.45	1.34
24	Y	607	CHL	C3C-C2C	8.92	1.45	1.34
24	8	609	CHL	C3C-C2C	8.93	1.45	1.34
24	N	601	CHL	C3C-C2C	8.95	1.45	1.34
24	n	607	CHL	C3C-C2C	8.96	1.45	1.34
24	4	609	CHL	C3C-C2C	8.98	1.45	1.34
24	g	606	CHL	C3C-C2C	8.99	1.45	1.34
24	G	606	CHL	C3C-C2C	9.01	1.45	1.34
24	3	606	CHL	C3C-C2C	9.06	1.45	1.34
24	N	605	CHL	C3C-C2C	9.07	1.45	1.34
24	n	605	CHL	C3C-C2C	9.07	1.45	1.34
24	8	607	CHL	C3C-C2C	9.08	1.45	1.34
24	7	606	CHL	C3C-C2C	9.09	1.45	1.34
24	1	607	CHL	C3C-C2C	9.10	1.45	1.34
24	5	607	CHL	C3C-C2C	9.10	1.45	1.34
24	4	607	CHL	C3C-C2C	9.11	1.45	1.34
24	r	607	CHL	C3C-C2C	9.12	1.45	1.34
24	R	607	CHL	C3C-C2C	9.12	1.45	1.34
24	s	601	CHL	C3C-C2C	9.12	1.45	1.34
24	6	601	CHL	C3C-C2C	9.12	1.45	1.34
24	S	601	CHL	C3C-C2C	9.14	1.45	1.34
24	1	608	CHL	C3C-C2C	9.16	1.45	1.34
24	5	608	CHL	C3C-C2C	9.17	1.45	1.34
24	2	601	CHL	C3C-C2C	9.18	1.45	1.34
24	S	607	CHL	C3C-C2C	9.18	1.45	1.34
24	G	608	CHL	C3C-C2C	9.19	1.45	1.34
24	s	607	CHL	C3C-C2C	9.19	1.45	1.34
24	g	608	CHL	C3C-C2C	9.21	1.45	1.34
24	G	609	CHL	C3C-C2C	9.21	1.45	1.34
24	g	609	CHL	C3C-C2C	9.23	1.45	1.34
24	5	606	CHL	C3C-C2C	9.24	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	605	CHL	C3C-C2C	9.28	1.46	1.34
24	G	605	CHL	C3C-C2C	9.30	1.46	1.34
24	R	614	CHL	C3C-C2C	9.31	1.46	1.34
24	5	605	CHL	C3C-C2C	9.31	1.46	1.34
24	r	614	CHL	C3C-C2C	9.31	1.46	1.34
24	1	606	CHL	C3C-C2C	9.32	1.46	1.34
24	1	609	CHL	C3C-C2C	9.34	1.46	1.34
24	1	605	CHL	C3C-C2C	9.34	1.46	1.34
24	5	609	CHL	C3C-C2C	9.34	1.46	1.34
24	3	605	CHL	C3C-C2C	9.38	1.46	1.34
24	7	605	CHL	C3C-C2C	9.42	1.46	1.34
24	R	606	CHL	C3C-C2C	9.46	1.46	1.34
24	6	606	CHL	C3C-C2C	9.50	1.46	1.34
24	2	607	CHL	C3C-C2C	9.50	1.46	1.34
24	S	606	CHL	C3C-C2C	9.51	1.46	1.34
24	r	606	CHL	C3C-C2C	9.52	1.46	1.34
24	6	607	CHL	C3C-C2C	9.52	1.46	1.34
24	s	606	CHL	C3C-C2C	9.53	1.46	1.34
24	2	606	CHL	C3C-C2C	9.53	1.46	1.34
24	8	606	CHL	C3C-C2C	9.54	1.46	1.34
24	4	606	CHL	C3C-C2C	9.56	1.46	1.34
24	7	609	CHL	C3C-C2C	9.57	1.46	1.34
24	3	609	CHL	C3C-C2C	9.58	1.46	1.34
24	7	608	CHL	C3C-C2C	9.62	1.46	1.34
24	2	608	CHL	C3C-C2C	9.63	1.46	1.34
24	6	608	CHL	C3C-C2C	9.65	1.46	1.34
24	3	608	CHL	C3C-C2C	9.65	1.46	1.34
24	6	605	CHL	C3C-C2C	9.77	1.46	1.34
24	2	605	CHL	C3C-C2C	9.79	1.46	1.34
24	8	601	CHL	C3C-C2C	9.96	1.46	1.34
24	s	608	CHL	C3C-C2C	9.97	1.46	1.34
24	S	608	CHL	C3C-C2C	9.98	1.46	1.34
24	4	601	CHL	C3C-C2C	9.99	1.46	1.34

All (5416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	623	BCR	C24-C23-C22	-7.66	114.70	126.21
30	4	623	BCR	C24-C23-C22	-7.64	114.73	126.21
24	g	609	CHL	C1C-C2C-C3C	-7.64	103.91	111.52
24	G	609	CHL	C1C-C2C-C3C	-7.64	103.91	111.52
27	N	1622	XAT	C15-C14-C13	-7.55	116.54	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	n	1622	XAT	C15-C14-C13	-7.52	116.58	127.31
24	N	609	CHL	C1C-C2C-C3C	-7.52	104.03	111.52
24	n	609	CHL	C1C-C2C-C3C	-7.51	104.03	111.52
24	7	601	CHL	C1C-C2C-C3C	-7.33	104.22	111.52
24	6	601	CHL	C1C-C2C-C3C	-7.30	104.24	111.52
24	3	601	CHL	C1C-C2C-C3C	-7.30	104.25	111.52
24	2	601	CHL	C1C-C2C-C3C	-7.29	104.25	111.52
24	y	601	CHL	C1C-C2C-C3C	-7.20	104.35	111.52
24	g	601	CHL	C1C-C2C-C3C	-7.19	104.35	111.52
24	Y	601	CHL	C1C-C2C-C3C	-7.18	104.36	111.52
24	G	601	CHL	C1C-C2C-C3C	-7.17	104.37	111.52
24	N	601	CHL	C1C-C2C-C3C	-7.07	104.47	111.52
30	t	101	BCR	C24-C23-C22	-7.06	115.60	126.21
30	T	101	BCR	C24-C23-C22	-7.06	115.60	126.21
24	n	601	CHL	C1C-C2C-C3C	-7.06	104.48	111.52
24	1	601	CHL	C1C-C2C-C3C	-7.05	104.50	111.52
26	4	620	LUT	C23-C24-C25	-7.04	118.62	125.22
24	5	601	CHL	C1C-C2C-C3C	-7.03	104.51	111.52
24	y	609	CHL	C1C-C2C-C3C	-7.03	104.52	111.52
27	y	1622	XAT	C15-C14-C13	-7.03	117.28	127.31
27	Y	1622	XAT	C15-C14-C13	-7.03	117.28	127.31
26	8	620	LUT	C23-C24-C25	-7.02	118.64	125.22
24	Y	609	CHL	C1C-C2C-C3C	-7.02	104.53	111.52
24	6	607	CHL	CBA-CAA-C2A	-7.00	106.11	115.76
24	2	607	CHL	CBA-CAA-C2A	-6.97	106.14	115.76
24	3	609	CHL	C1C-C2C-C3C	-6.93	104.61	111.52
24	7	609	CHL	C1C-C2C-C3C	-6.92	104.62	111.52
24	1	609	CHL	C1C-C2C-C3C	-6.87	104.67	111.52
24	5	609	CHL	C1C-C2C-C3C	-6.84	104.70	111.52
24	6	608	CHL	C1C-C2C-C3C	-6.80	104.74	111.52
24	2	608	CHL	C1C-C2C-C3C	-6.77	104.78	111.52
24	1	608	CHL	C1C-C2C-C3C	-6.74	104.80	111.52
24	5	608	CHL	C1C-C2C-C3C	-6.73	104.82	111.52
24	2	609	CHL	C1C-C2C-C3C	-6.72	104.82	111.52
24	S	607	CHL	C1C-C2C-C3C	-6.70	104.84	111.52
24	6	609	CHL	C1C-C2C-C3C	-6.70	104.84	111.52
24	s	607	CHL	C1C-C2C-C3C	-6.66	104.89	111.52
24	n	608	CHL	C1C-C2C-C3C	-6.60	104.94	111.52
24	N	608	CHL	C1C-C2C-C3C	-6.59	104.95	111.52
24	7	606	CHL	C1C-C2C-C3C	-6.58	104.97	111.52
25	Y	604	CLA	CMB-C2B-C1B	-6.57	118.37	128.46
24	4	608	CHL	C1C-C2C-C3C	-6.56	104.98	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	604	CLA	CMB-C2B-C1B	-6.55	118.39	128.46
24	7	605	CHL	C1C-C2C-C3C	-6.55	104.99	111.52
24	y	605	CHL	C1C-C2C-C3C	-6.54	105.00	111.52
24	g	605	CHL	C1C-C2C-C3C	-6.54	105.00	111.52
24	6	605	CHL	C1C-C2C-C3C	-6.54	105.00	111.52
24	3	605	CHL	C1C-C2C-C3C	-6.54	105.00	111.52
24	G	605	CHL	C1C-C2C-C3C	-6.53	105.01	111.52
24	3	606	CHL	C1C-C2C-C3C	-6.53	105.02	111.52
24	Y	605	CHL	C1C-C2C-C3C	-6.52	105.02	111.52
30	t	101	BCR	C16-C17-C18	-6.52	118.00	127.31
30	T	101	BCR	C16-C17-C18	-6.52	118.01	127.31
24	r	606	CHL	C1C-C2C-C3C	-6.51	105.03	111.52
24	2	605	CHL	C1C-C2C-C3C	-6.51	105.03	111.52
24	8	608	CHL	C1C-C2C-C3C	-6.50	105.04	111.52
24	s	608	CHL	C1C-C2C-C3C	-6.46	105.08	111.52
24	2	606	CHL	C1C-C2C-C3C	-6.46	105.08	111.52
24	R	606	CHL	C1C-C2C-C3C	-6.46	105.08	111.52
30	T	101	BCR	C20-C21-C22	-6.43	118.13	127.31
30	t	101	BCR	C20-C21-C22	-6.43	118.14	127.31
24	6	606	CHL	C1C-C2C-C3C	-6.42	105.12	111.52
27	n	1622	XAT	C31-C30-C29	-6.42	118.15	127.31
24	r	614	CHL	C1C-C2C-C3C	-6.42	105.12	111.52
24	S	608	CHL	C1C-C2C-C3C	-6.42	105.12	111.52
27	N	1622	XAT	C31-C30-C29	-6.41	118.16	127.31
27	G	1622	XAT	C15-C14-C13	-6.38	118.20	127.31
27	g	1622	XAT	C15-C14-C13	-6.38	118.21	127.31
24	4	606	CHL	C1C-C2C-C3C	-6.38	105.16	111.52
24	R	614	CHL	C1C-C2C-C3C	-6.37	105.17	111.52
24	8	606	CHL	C1C-C2C-C3C	-6.36	105.18	111.52
24	4	609	CHL	C1C-C2C-C3C	-6.36	105.18	111.52
24	8	609	CHL	C1C-C2C-C3C	-6.36	105.18	111.52
24	4	607	CHL	C1C-C2C-C3C	-6.29	105.25	111.52
24	3	608	CHL	C1C-C2C-C3C	-6.27	105.27	111.52
24	8	607	CHL	C1C-C2C-C3C	-6.27	105.27	111.52
24	7	608	CHL	C1C-C2C-C3C	-6.26	105.28	111.52
24	1	606	CHL	C1C-C2C-C3C	-6.24	105.30	111.52
24	4	601	CHL	C1C-C2C-C3C	-6.24	105.30	111.52
24	8	601	CHL	C1C-C2C-C3C	-6.23	105.31	111.52
24	5	606	CHL	C1C-C2C-C3C	-6.21	105.33	111.52
24	N	605	CHL	C1C-C2C-C3C	-6.19	105.35	111.52
24	r	608	CHL	C1C-C2C-C3C	-6.17	105.37	111.52
24	n	605	CHL	C1C-C2C-C3C	-6.16	105.38	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	608	CHL	C1C-C2C-C3C	-6.16	105.38	111.52
24	g	608	CHL	C1C-C2C-C3C	-6.14	105.40	111.52
24	r	607	CHL	C1C-C2C-C3C	-6.13	105.41	111.52
24	G	608	CHL	C1C-C2C-C3C	-6.13	105.41	111.52
26	3	1620	LUT	C7-C8-C9	-6.12	117.02	126.21
26	7	1620	LUT	C7-C8-C9	-6.12	117.02	126.21
24	S	601	CHL	C1C-C2C-C3C	-6.11	105.43	111.52
24	R	607	CHL	C1C-C2C-C3C	-6.11	105.43	111.52
24	s	601	CHL	C1C-C2C-C3C	-6.10	105.44	111.52
26	5	1620	LUT	C23-C24-C25	-6.08	119.52	125.22
24	Y	606	CHL	C1C-C2C-C3C	-6.08	105.46	111.52
30	d	404	BCR	C7-C8-C9	-6.07	117.10	126.21
24	y	606	CHL	C1C-C2C-C3C	-6.05	105.48	111.52
24	Y	608	CHL	C1C-C2C-C3C	-6.05	105.48	111.52
34	B	623	SQD	C5-C6-S	-6.04	105.92	114.34
30	D	404	BCR	C7-C8-C9	-6.04	117.14	126.21
24	y	608	CHL	C1C-C2C-C3C	-6.04	105.50	111.52
24	s	606	CHL	C1C-C2C-C3C	-6.04	105.50	111.52
26	1	1620	LUT	C23-C24-C25	-6.03	119.57	125.22
24	S	606	CHL	C1C-C2C-C3C	-6.03	105.51	111.52
30	C	516	BCR	C24-C23-C22	-6.02	117.17	126.21
30	c	516	BCR	C24-C23-C22	-6.01	117.18	126.21
34	b	623	SQD	C5-C6-S	-6.01	105.96	114.34
24	5	607	CHL	CBA-CAA-C2A	-5.97	107.52	115.76
24	1	607	CHL	CBA-CAA-C2A	-5.96	107.54	115.76
25	N	604	CLA	CMB-C2B-C1B	-5.95	119.31	128.46
25	n	604	CLA	CMB-C2B-C1B	-5.95	119.32	128.46
28	y	1623	NEX	C17-C1-C6	-5.91	105.18	110.47
28	Y	1623	NEX	C17-C1-C6	-5.91	105.19	110.47
27	y	1622	XAT	C31-C30-C29	-5.89	118.90	127.31
27	Y	1622	XAT	C6-C7-C8	-5.89	113.53	125.99
27	Y	1622	XAT	C31-C30-C29	-5.88	118.92	127.31
27	y	1622	XAT	C6-C7-C8	-5.87	113.58	125.99
25	b	609	CLA	CMB-C2B-C1B	-5.86	119.46	128.46
27	8	622	XAT	C6-C7-C8	-5.85	113.62	125.99
25	B	609	CLA	CMB-C2B-C1B	-5.85	119.47	128.46
27	4	622	XAT	C6-C7-C8	-5.84	113.65	125.99
27	7	1622	XAT	C31-C30-C29	-5.84	118.98	127.31
24	6	607	CHL	C1C-C2C-C3C	-5.83	105.71	111.52
30	4	623	BCR	C28-C27-C26	-5.81	103.78	113.78
30	8	623	BCR	C28-C27-C26	-5.80	103.80	113.78
27	3	1622	XAT	C31-C30-C29	-5.80	119.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	607	CHL	C1C-C2C-C3C	-5.79	105.75	111.52
30	c	517	BCR	C7-C8-C9	-5.76	117.55	126.21
24	7	601	CHL	CBC-CAC-C3C	-5.76	104.20	112.95
24	N	606	CHL	C1C-C2C-C3C	-5.76	105.78	111.52
24	5	605	CHL	C1C-C2C-C3C	-5.76	105.78	111.52
24	1	605	CHL	C1C-C2C-C3C	-5.76	105.78	111.52
25	B	605	CLA	CAA-C2A-C3A	-5.75	97.03	112.81
24	n	606	CHL	C1C-C2C-C3C	-5.75	105.78	111.52
25	b	605	CLA	CAA-C2A-C3A	-5.75	97.04	112.81
30	C	517	BCR	C7-C8-C9	-5.75	117.57	126.21
27	G	1622	XAT	C6-C7-C8	-5.74	113.85	125.99
27	g	1622	XAT	C6-C7-C8	-5.74	113.86	125.99
24	3	601	CHL	CBC-CAC-C3C	-5.74	104.24	112.95
27	3	1622	XAT	C27-C28-C29	-5.73	116.64	125.53
27	7	1622	XAT	C27-C28-C29	-5.72	116.66	125.53
25	C	508	CLA	CMB-C2B-C1B	-5.70	119.70	128.46
25	c	508	CLA	CMB-C2B-C1B	-5.70	119.70	128.46
24	G	606	CHL	C1C-C2C-C3C	-5.65	105.89	111.52
27	7	1622	XAT	C6-C7-C8	-5.64	114.07	125.99
28	1	1623	NEX	C27-C28-C29	-5.64	116.78	125.53
25	B	612	CLA	CMB-C2B-C1B	-5.63	119.81	128.46
25	b	612	CLA	CMB-C2B-C1B	-5.63	119.81	128.46
27	r	622	XAT	C6-C7-C8	-5.62	114.12	125.99
27	3	1622	XAT	C6-C7-C8	-5.61	114.13	125.99
27	R	622	XAT	C26-C27-C28	-5.61	114.13	125.99
28	5	1623	NEX	C27-C28-C29	-5.61	116.83	125.53
27	r	622	XAT	C26-C27-C28	-5.61	114.13	125.99
24	g	606	CHL	C1C-C2C-C3C	-5.61	105.93	111.52
27	R	622	XAT	C6-C7-C8	-5.60	114.15	125.99
30	H	101	BCR	C11-C10-C9	-5.60	119.32	127.31
30	h	101	BCR	C11-C10-C9	-5.59	119.33	127.31
27	8	622	XAT	C38-C25-C26	-5.57	112.88	122.31
27	7	1622	XAT	C15-C14-C13	-5.56	119.37	127.31
27	4	622	XAT	C38-C25-C26	-5.55	112.91	122.31
28	6	1623	NEX	C27-C28-C29	-5.55	116.92	125.53
27	3	1622	XAT	C15-C14-C13	-5.54	119.40	127.31
28	3	1623	NEX	C15-C14-C13	-5.54	119.41	127.31
28	2	1623	NEX	C27-C28-C29	-5.53	116.94	125.53
28	7	1623	NEX	C15-C14-C13	-5.53	119.42	127.31
24	G	607	CHL	C1C-C2C-C3C	-5.50	106.04	111.52
27	R	622	XAT	C38-C25-C26	-5.50	113.01	122.31
30	B	620	BCR	C7-C8-C9	-5.49	117.96	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	607	CHL	C1C-C2C-C3C	-5.49	106.05	111.52
30	b	620	BCR	C7-C8-C9	-5.49	117.97	126.21
27	r	622	XAT	C38-C25-C26	-5.48	113.04	122.31
24	S	607	CHL	CBC-CAC-C3C	-5.46	104.66	112.95
24	s	607	CHL	CBC-CAC-C3C	-5.46	104.66	112.95
24	g	607	CHL	C1C-C2C-C3C	-5.45	106.08	111.52
24	N	607	CHL	C1C-C2C-C3C	-5.45	106.09	111.52
28	Y	1623	NEX	C35-C34-C33	-5.42	119.58	127.31
30	C	517	BCR	C11-C10-C9	-5.39	119.62	127.31
28	y	1623	NEX	C35-C34-C33	-5.39	119.62	127.31
30	c	517	BCR	C11-C10-C9	-5.38	119.63	127.31
30	D	404	BCR	C24-C23-C22	-5.34	118.19	126.21
27	n	1622	XAT	C38-C25-C26	-5.34	113.28	122.31
30	d	404	BCR	C24-C23-C22	-5.34	118.19	126.21
28	y	1623	NEX	C11-C10-C9	-5.33	119.70	127.31
27	N	1622	XAT	C38-C25-C26	-5.33	113.30	122.31
25	A	405	CLA	CMB-C2B-C1B	-5.32	120.29	128.46
28	Y	1623	NEX	C11-C10-C9	-5.31	119.73	127.31
25	a	405	CLA	CMB-C2B-C1B	-5.30	120.32	128.46
28	Y	1623	NEX	C38-C25-C26	-5.30	113.35	122.31
28	y	1623	NEX	C38-C25-C26	-5.29	113.36	122.31
24	Y	606	CHL	CBA-CAA-C2A	-5.28	108.48	115.76
24	n	606	CHL	CBA-CAA-C2A	-5.27	108.49	115.76
28	G	1623	NEX	C27-C28-C29	-5.27	117.35	125.53
24	y	606	CHL	CBA-CAA-C2A	-5.27	108.49	115.76
28	g	1623	NEX	C27-C28-C29	-5.27	117.36	125.53
24	N	606	CHL	CBA-CAA-C2A	-5.26	108.50	115.76
27	8	622	XAT	C18-C5-C6	-5.26	113.42	122.31
25	R	602	CLA	CMB-C2B-C1B	-5.24	120.40	128.46
27	4	622	XAT	C18-C5-C6	-5.24	113.44	122.31
25	r	602	CLA	CMB-C2B-C1B	-5.23	120.43	128.46
27	r	622	XAT	C18-C5-C6	-5.22	113.48	122.31
27	R	622	XAT	C18-C5-C6	-5.21	113.50	122.31
26	6	1620	LUT	C23-C24-C25	-5.20	120.34	125.22
28	G	1623	NEX	C35-C34-C33	-5.18	119.91	127.31
28	G	1623	NEX	C11-C10-C9	-5.18	119.92	127.31
28	R	623	NEX	C15-C14-C13	-5.17	119.93	127.31
26	2	1620	LUT	C23-C24-C25	-5.17	120.38	125.22
25	C	513	CLA	CMB-C2B-C1B	-5.17	120.53	128.46
27	4	622	XAT	C26-C27-C28	-5.16	115.08	125.99
28	g	1623	NEX	C35-C34-C33	-5.15	119.95	127.31
28	r	623	NEX	C15-C14-C13	-5.15	119.96	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	622	XAT	C26-C27-C28	-5.15	115.11	125.99
28	g	1623	NEX	C11-C10-C9	-5.14	119.97	127.31
25	c	513	CLA	CMB-C2B-C1B	-5.14	120.56	128.46
25	g	602	CLA	CMB-C2B-C1B	-5.14	120.57	128.46
25	G	604	CLA	CMB-C2B-C1B	-5.13	120.57	128.46
24	Y	607	CHL	C1C-C2C-C3C	-5.13	106.41	111.52
25	G	602	CLA	CMB-C2B-C1B	-5.12	120.59	128.46
27	Y	1622	XAT	C38-C25-C26	-5.12	113.66	122.31
24	g	606	CHL	CBA-CAA-C2A	-5.12	108.70	115.76
25	g	604	CLA	CMB-C2B-C1B	-5.11	120.61	128.46
27	y	1622	XAT	C38-C25-C26	-5.11	113.66	122.31
24	y	607	CHL	C1C-C2C-C3C	-5.11	106.43	111.52
27	N	1622	XAT	C6-C7-C8	-5.09	115.22	125.99
27	n	1622	XAT	C6-C7-C8	-5.09	115.23	125.99
28	r	623	NEX	C38-C25-C26	-5.09	113.70	122.31
28	R	623	NEX	C38-C25-C26	-5.08	113.71	122.31
26	N	1621	LUT	C23-C24-C25	-5.08	120.46	125.22
24	G	606	CHL	CBA-CAA-C2A	-5.08	108.75	115.76
25	c	506	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
25	b	613	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
25	b	608	CLA	CMB-C2B-C1B	-5.08	120.66	128.46
25	C	506	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
30	c	517	BCR	C24-C23-C22	-5.07	118.59	126.21
25	B	608	CLA	CMB-C2B-C1B	-5.07	120.68	128.46
25	S	614	CLA	CMB-C2B-C1B	-5.07	120.68	128.46
26	n	1621	LUT	C23-C24-C25	-5.06	120.48	125.22
25	B	613	CLA	CMB-C2B-C1B	-5.05	120.70	128.46
30	C	517	BCR	C24-C23-C22	-5.04	118.64	126.21
25	s	614	CLA	CMB-C2B-C1B	-5.04	120.72	128.46
30	C	516	BCR	C16-C17-C18	-5.04	120.12	127.31
37	c	518	DGD	O3G-C3G-C2G	-5.04	99.00	110.99
37	C	518	DGD	O3G-C3G-C2G	-5.03	99.02	110.99
26	G	1620	LUT	C35-C34-C33	-5.03	120.13	127.31
26	g	1620	LUT	C35-C34-C33	-5.03	120.13	127.31
30	c	516	BCR	C16-C17-C18	-5.02	120.15	127.31
25	b	614	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
25	C	504	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
25	c	504	CLA	CMB-C2B-C1B	-4.99	120.79	128.46
30	T	101	BCR	C7-C8-C9	-4.99	118.72	126.21
28	3	1623	NEX	C38-C25-C26	-4.98	113.88	122.31
30	4	623	BCR	C11-C10-C9	-4.98	120.20	127.31
30	t	101	BCR	C7-C8-C9	-4.98	118.73	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	8	623	BCR	C11-C10-C9	-4.97	120.21	127.31
25	B	614	CLA	CMB-C2B-C1B	-4.97	120.83	128.46
28	r	623	NEX	C11-C10-C9	-4.97	120.22	127.31
28	7	1623	NEX	C38-C25-C26	-4.96	113.91	122.31
30	4	623	BCR	C15-C14-C13	-4.96	120.24	127.31
28	R	623	NEX	C11-C10-C9	-4.95	120.24	127.31
25	d	403	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
25	7	602	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
24	1	607	CHL	C1C-C2C-C3C	-4.94	106.59	111.52
24	5	607	CHL	C1C-C2C-C3C	-4.94	106.59	111.52
27	N	1622	XAT	C27-C28-C29	-4.94	117.86	125.53
28	r	623	NEX	C27-C28-C29	-4.94	117.86	125.53
27	n	1622	XAT	C27-C28-C29	-4.94	117.86	125.53
27	6	1622	XAT	C38-C25-C26	-4.94	113.95	122.31
25	3	602	CLA	CMB-C2B-C1B	-4.94	120.88	128.46
27	7	1622	XAT	C38-C25-C26	-4.94	113.96	122.31
27	3	1622	XAT	C38-C25-C26	-4.94	113.96	122.31
30	8	623	BCR	C15-C14-C13	-4.93	120.27	127.31
27	2	1622	XAT	C38-C25-C26	-4.93	113.97	122.31
28	R	623	NEX	C27-C28-C29	-4.93	117.89	125.53
25	D	403	CLA	CMB-C2B-C1B	-4.92	120.89	128.46
27	g	1622	XAT	C31-C30-C29	-4.90	120.31	127.31
27	G	1622	XAT	C31-C30-C29	-4.90	120.32	127.31
30	c	517	BCR	C15-C14-C13	-4.88	120.34	127.31
30	C	517	BCR	C15-C14-C13	-4.88	120.35	127.31
25	n	613	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
25	N	613	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
26	5	1620	LUT	C35-C34-C33	-4.86	120.37	127.31
25	C	510	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
24	7	607	CHL	C1C-C2C-C3C	-4.85	106.69	111.52
26	1	1620	LUT	C35-C34-C33	-4.85	120.39	127.31
25	c	510	CLA	CMB-C2B-C1B	-4.84	121.03	128.46
27	2	1622	XAT	C31-C30-C29	-4.82	120.42	127.31
27	5	1622	XAT	C15-C14-C13	-4.82	120.43	127.31
27	7	1622	XAT	C11-C10-C9	-4.82	120.43	127.31
27	6	1622	XAT	C31-C30-C29	-4.82	120.43	127.31
27	3	1622	XAT	C11-C10-C9	-4.82	120.43	127.31
27	1	1622	XAT	C15-C14-C13	-4.82	120.44	127.31
26	4	620	LUT	C35-C34-C33	-4.81	120.44	127.31
30	b	618	BCR	C15-C14-C13	-4.81	120.44	127.31
24	3	607	CHL	C1C-C2C-C3C	-4.81	106.72	111.52
28	N	1623	NEX	C15-C14-C13	-4.81	120.45	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	515	BCR	C15-C14-C13	-4.81	120.45	127.31
30	B	618	BCR	C15-C14-C13	-4.79	120.47	127.31
30	C	515	BCR	C15-C14-C13	-4.79	120.47	127.31
28	n	1623	NEX	C15-C14-C13	-4.79	120.47	127.31
25	n	602	CLA	CMB-C2B-C1B	-4.79	121.10	128.46
26	8	620	LUT	C35-C34-C33	-4.79	120.48	127.31
30	C	514	BCR	C15-C14-C13	-4.78	120.48	127.31
30	T	101	BCR	C11-C10-C9	-4.78	120.48	127.31
25	b	610	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
30	t	101	BCR	C11-C10-C9	-4.77	120.50	127.31
25	B	610	CLA	CMB-C2B-C1B	-4.77	121.13	128.46
30	c	514	BCR	C15-C14-C13	-4.76	120.51	127.31
25	N	602	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
28	N	1623	NEX	C38-C25-C26	-4.76	114.27	122.31
28	n	1623	NEX	C38-C25-C26	-4.75	114.27	122.31
28	6	1623	NEX	C15-C14-C13	-4.75	120.54	127.31
27	y	1622	XAT	C18-C5-C6	-4.74	114.28	122.31
28	y	1623	NEX	C27-C28-C29	-4.74	118.17	125.53
28	s	1623	NEX	C27-C28-C29	-4.74	118.17	125.53
27	1	1622	XAT	C27-C28-C29	-4.74	118.18	125.53
28	2	1623	NEX	C15-C14-C13	-4.73	120.56	127.31
25	s	612	CLA	CMB-C2B-C1B	-4.73	121.20	128.46
27	2	1622	XAT	C27-C28-C29	-4.73	118.20	125.53
28	S	1623	NEX	C27-C28-C29	-4.73	118.20	125.53
30	b	619	BCR	C15-C14-C13	-4.72	120.57	127.31
25	S	612	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
26	8	620	LUT	C7-C8-C9	-4.72	119.12	126.21
27	6	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
27	Y	1622	XAT	C18-C5-C6	-4.72	114.33	122.31
27	2	1622	XAT	C15-C35-C34	-4.72	113.39	123.46
27	5	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
27	6	1622	XAT	C15-C35-C34	-4.71	113.40	123.46
26	4	620	LUT	C7-C8-C9	-4.71	119.13	126.21
30	B	619	BCR	C15-C14-C13	-4.71	120.59	127.31
27	y	1622	XAT	C11-C10-C9	-4.71	120.59	127.31
26	N	1621	LUT	C15-C14-C13	-4.71	120.59	127.31
25	2	602	CLA	CMB-C2B-C1B	-4.70	121.23	128.46
26	n	1621	LUT	C15-C14-C13	-4.70	120.60	127.31
27	2	1622	XAT	C7-C8-C9	-4.70	118.24	125.53
25	6	602	CLA	CMB-C2B-C1B	-4.70	121.25	128.46
28	Y	1623	NEX	C27-C28-C29	-4.69	118.25	125.53
25	B	604	CLA	CMB-C2B-C1B	-4.69	121.25	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	602	CLA	CMB-C2B-C1B	-4.69	121.26	128.46
30	H	101	BCR	C16-C17-C18	-4.68	120.62	127.31
26	4	620	LUT	C15-C14-C13	-4.68	120.63	127.31
25	D	402	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
27	y	1622	XAT	C15-C35-C34	-4.68	113.48	123.46
27	6	1622	XAT	C7-C8-C9	-4.68	118.27	125.53
25	8	612	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
25	b	604	CLA	CMB-C2B-C1B	-4.68	121.28	128.46
26	8	620	LUT	C15-C14-C13	-4.67	120.64	127.31
25	s	602	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
27	Y	1622	XAT	C11-C10-C9	-4.67	120.65	127.31
27	Y	1622	XAT	C15-C35-C34	-4.67	113.50	123.46
24	3	607	CHL	CBA-CAA-C2A	-4.67	109.32	115.76
25	d	402	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
28	S	1623	NEX	C15-C14-C13	-4.66	120.66	127.31
24	5	605	CHL	OMC-CMC-C2C	-4.66	118.34	124.29
24	6	601	CHL	CBA-CAA-C2A	-4.66	108.95	115.66
25	s	604	CLA	CMB-C2B-C1B	-4.66	121.30	128.46
24	2	601	CHL	CBA-CAA-C2A	-4.66	108.95	115.66
30	h	101	BCR	C16-C17-C18	-4.66	120.67	127.31
24	7	607	CHL	CBA-CAA-C2A	-4.66	109.34	115.76
25	r	604	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
37	C	520	DGD	O3G-C3G-C2G	-4.65	99.93	110.99
28	N	1623	NEX	C35-C34-C33	-4.65	120.68	127.31
25	4	612	CLA	CMB-C2B-C1B	-4.65	121.32	128.46
37	c	520	DGD	O3G-C3G-C2G	-4.65	99.94	110.99
27	g	1622	XAT	C38-C25-C26	-4.64	114.45	122.31
25	R	604	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
25	B	615	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
28	6	1623	NEX	C38-C25-C26	-4.63	114.47	122.31
28	s	1623	NEX	C15-C14-C13	-4.63	120.70	127.31
27	G	1622	XAT	C38-C25-C26	-4.63	114.48	122.31
25	b	615	CLA	CMB-C2B-C1B	-4.63	121.35	128.46
28	n	1623	NEX	C35-C34-C33	-4.63	120.71	127.31
24	1	605	CHL	OMC-CMC-C2C	-4.62	118.39	124.29
25	S	604	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
28	S	1623	NEX	C38-C25-C26	-4.62	114.49	122.31
28	2	1623	NEX	C38-C25-C26	-4.61	114.50	122.31
25	8	602	CLA	CMB-C2B-C1B	-4.60	121.39	128.46
28	s	1623	NEX	C38-C25-C26	-4.60	114.53	122.31
28	G	1623	NEX	C15-C14-C13	-4.60	120.75	127.31
28	1	1623	NEX	C35-C34-C33	-4.58	120.77	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	602	CLA	CMB-C2B-C1B	-4.58	121.43	128.46
28	5	1623	NEX	C35-C34-C33	-4.57	120.78	127.31
28	g	1623	NEX	C15-C14-C13	-4.57	120.78	127.31
25	s	613	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
26	S	1620	LUT	C35-C34-C33	-4.56	120.80	127.31
25	S	613	CLA	CMB-C2B-C1B	-4.56	121.45	128.46
26	s	1620	LUT	C35-C34-C33	-4.56	120.80	127.31
30	A	411	BCR	C7-C8-C9	-4.56	119.37	126.21
25	C	509	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
28	y	1623	NEX	C15-C14-C13	-4.55	120.82	127.31
30	a	411	BCR	C7-C8-C9	-4.55	119.38	126.21
24	1	607	CHL	OMC-CMC-C2C	-4.55	118.49	124.29
25	c	509	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
28	Y	1623	NEX	C15-C14-C13	-4.53	120.84	127.31
30	h	101	BCR	C15-C14-C13	-4.52	120.86	127.31
24	5	607	CHL	OMC-CMC-C2C	-4.52	118.52	124.29
30	H	101	BCR	C15-C14-C13	-4.51	120.87	127.31
30	4	623	BCR	C16-C17-C18	-4.50	120.89	127.31
24	5	606	CHL	CBA-CAA-C2A	-4.50	109.18	115.66
26	y	1621	LUT	C23-C24-C25	-4.50	121.01	125.22
30	8	623	BCR	C16-C17-C18	-4.50	120.89	127.31
26	S	1621	LUT	C35-C34-C33	-4.49	120.90	127.31
26	Y	1621	LUT	C23-C24-C25	-4.49	121.01	125.22
24	1	606	CHL	CBA-CAA-C2A	-4.49	109.20	115.66
26	s	1621	LUT	C35-C34-C33	-4.48	120.91	127.31
30	H	101	BCR	C24-C23-C22	-4.48	119.48	126.21
30	h	101	BCR	C24-C23-C22	-4.48	119.48	126.21
27	n	1622	XAT	C18-C5-C6	-4.48	114.73	122.31
26	G	1621	LUT	C15-C14-C13	-4.48	120.92	127.31
27	N	1622	XAT	C18-C5-C6	-4.48	114.73	122.31
27	g	1622	XAT	C18-C5-C6	-4.48	114.73	122.31
26	g	1621	LUT	C15-C14-C13	-4.48	120.92	127.31
24	2	609	CHL	CHA-CBD-CGD	-4.47	104.62	115.00
27	G	1622	XAT	C18-C5-C6	-4.47	114.75	122.31
24	6	609	CHL	CHA-CBD-CGD	-4.47	104.64	115.00
26	1	1621	LUT	C15-C14-C13	-4.46	120.94	127.31
28	G	1623	NEX	C38-C25-C26	-4.46	114.76	122.31
28	g	1623	NEX	C38-C25-C26	-4.46	114.77	122.31
24	g	609	CHL	CBC-CAC-C3C	-4.45	106.20	112.95
25	6	604	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
26	5	1621	LUT	C15-C14-C13	-4.44	120.97	127.31
30	H	101	BCR	C7-C8-C9	-4.44	119.54	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	406	CLA	CMB-C2B-C1B	-4.44	121.64	128.46
36	a	414	PL9	C7-C3-C2	-4.44	116.92	123.23
27	4	622	XAT	C35-C34-C33	-4.43	120.98	127.31
27	2	1622	XAT	C15-C14-C13	-4.43	120.98	127.31
25	N	610	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
25	b	605	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
28	5	1623	NEX	C38-C25-C26	-4.43	114.82	122.31
25	a	406	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
25	2	604	CLA	CMB-C2B-C1B	-4.43	121.66	128.46
25	R	603	CLA	CMB-C2B-C1B	-4.42	121.66	128.46
25	n	610	CLA	CMB-C2B-C1B	-4.42	121.66	128.46
27	1	1622	XAT	C31-C30-C29	-4.42	121.00	127.31
25	B	605	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
25	r	603	CLA	CMB-C2B-C1B	-4.42	121.67	128.46
30	h	101	BCR	C7-C8-C9	-4.42	119.57	126.21
24	G	609	CHL	CBC-CAC-C3C	-4.42	106.24	112.95
27	6	1622	XAT	C15-C14-C13	-4.42	121.00	127.31
30	c	515	BCR	C21-C20-C19	-4.41	109.71	123.23
28	1	1623	NEX	C38-C25-C26	-4.41	114.85	122.31
26	N	1620	LUT	C35-C34-C33	-4.40	121.03	127.31
30	C	515	BCR	C21-C20-C19	-4.40	109.72	123.23
36	A	414	PL9	C7-C3-C2	-4.40	116.97	123.23
27	5	1622	XAT	C31-C30-C29	-4.40	121.03	127.31
26	n	1620	LUT	C35-C34-C33	-4.40	121.03	127.31
27	8	622	XAT	C35-C34-C33	-4.39	121.04	127.31
25	1	614	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
25	R	610	CLA	C1B-CHB-C4A	-4.38	121.45	130.12
25	5	614	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
24	r	606	CHL	CBA-CAA-C2A	-4.37	109.73	115.76
25	r	610	CLA	C1B-CHB-C4A	-4.37	121.46	130.12
24	R	606	CHL	CBA-CAA-C2A	-4.37	109.74	115.76
24	N	609	CHL	CBC-CAC-C3C	-4.36	106.33	112.95
30	D	404	BCR	C11-C10-C9	-4.36	121.09	127.31
27	5	1622	XAT	C38-C25-C26	-4.35	114.94	122.31
24	n	609	CHL	CBC-CAC-C3C	-4.35	106.34	112.95
25	4	602	CLA	O2D-CGD-O1D	-4.35	115.06	123.82
30	c	515	BCR	C7-C8-C9	-4.35	119.67	126.21
27	1	1622	XAT	C38-C25-C26	-4.35	114.96	122.31
26	Y	1621	LUT	C35-C34-C33	-4.34	121.12	127.31
25	c	502	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
30	C	515	BCR	C7-C8-C9	-4.34	119.70	126.21
26	y	1621	LUT	C35-C34-C33	-4.34	121.12	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	609	CHL	OMC-CMC-C2C	-4.33	118.76	124.29
30	d	404	BCR	C11-C10-C9	-4.33	121.13	127.31
25	Y	602	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
25	C	505	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
25	8	602	CLA	O2D-CGD-O1D	-4.32	115.12	123.82
25	c	505	CLA	CMB-C2B-C1B	-4.32	121.82	128.46
24	8	609	CHL	OMC-CMC-C2C	-4.32	118.77	124.29
25	N	614	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
25	y	602	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
25	C	502	CLA	CMB-C2B-C1B	-4.31	121.84	128.46
25	n	614	CLA	CMB-C2B-C1B	-4.31	121.85	128.46
26	Y	1621	LUT	C15-C14-C13	-4.30	121.18	127.31
26	y	1621	LUT	C15-C14-C13	-4.29	121.19	127.31
30	t	101	BCR	C20-C19-C18	-4.29	114.36	126.42
30	T	101	BCR	C20-C19-C18	-4.28	114.38	126.42
24	2	606	CHL	CBA-CAA-C2A	-4.27	109.52	115.66
24	6	606	CHL	CBA-CAA-C2A	-4.26	109.53	115.66
37	c	519	DGD	O3G-C3G-C2G	-4.26	100.86	110.99
25	4	610	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
37	C	519	DGD	O3G-C3G-C2G	-4.24	100.89	110.99
27	1	1622	XAT	C11-C10-C9	-4.23	121.27	127.31
27	1	1622	XAT	C18-C5-C6	-4.23	115.16	122.31
30	b	618	BCR	C16-C17-C18	-4.22	121.29	127.31
25	y	603	CLA	OBD-CAD-CBD	-4.22	119.57	125.94
25	8	610	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
27	5	1622	XAT	C11-C10-C9	-4.21	121.30	127.31
27	n	1622	XAT	C11-C10-C9	-4.21	121.30	127.31
27	5	1622	XAT	C18-C5-C6	-4.21	115.19	122.31
27	4	622	XAT	C15-C14-C13	-4.20	121.31	127.31
25	B	617	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
25	Y	603	CLA	OBD-CAD-CBD	-4.20	119.60	125.94
27	8	622	XAT	C15-C14-C13	-4.20	121.32	127.31
27	N	1622	XAT	C11-C10-C9	-4.20	121.32	127.31
25	b	617	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
25	C	511	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
30	B	618	BCR	C16-C17-C18	-4.18	121.34	127.31
28	1	1623	NEX	C17-C1-C6	-4.18	106.73	110.47
27	G	1622	XAT	C27-C28-C29	-4.18	119.04	125.53
27	g	1622	XAT	C27-C28-C29	-4.18	119.04	125.53
25	4	603	CLA	CMB-C2B-C1B	-4.18	122.05	128.46
24	8	608	CHL	CBC-CAC-C3C	-4.17	106.61	112.95
25	5	613	CLA	CMB-C2B-C1B	-4.17	122.05	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	603	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
25	1	613	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
25	b	607	CLA	CMB-C2B-C1B	-4.17	122.06	128.46
26	n	1621	LUT	C22-C23-C24	-4.16	107.02	111.73
30	c	516	BCR	C28-C27-C26	-4.16	106.62	113.78
28	5	1623	NEX	C17-C1-C6	-4.16	106.75	110.47
30	C	516	BCR	C28-C27-C26	-4.16	106.62	113.78
25	g	610	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
25	c	511	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
24	4	608	CHL	CBC-CAC-C3C	-4.15	106.65	112.95
26	N	1621	LUT	C22-C23-C24	-4.15	107.04	111.73
25	B	607	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
25	G	610	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
25	C	507	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
26	g	1621	LUT	C35-C34-C33	-4.13	121.41	127.31
30	c	514	BCR	C16-C17-C18	-4.13	121.42	127.31
25	c	507	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
26	3	1621	LUT	C10-C11-C12	-4.12	110.59	123.23
30	A	411	BCR	C11-C10-C9	-4.12	121.43	127.31
25	3	614	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
26	G	1621	LUT	C35-C34-C33	-4.12	121.43	127.31
26	6	1621	LUT	C22-C23-C24	-4.12	107.08	111.73
30	a	411	BCR	C11-C10-C9	-4.11	121.44	127.31
25	7	614	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
26	7	1621	LUT	C10-C11-C12	-4.11	110.63	123.23
24	y	606	CHL	OMC-CMC-C2C	-4.10	119.05	124.29
30	C	514	BCR	C16-C17-C18	-4.10	121.45	127.31
25	r	604	CLA	CAA-C2A-C3A	-4.10	101.57	112.81
25	R	604	CLA	CAA-C2A-C3A	-4.10	101.57	112.81
30	C	517	BCR	C20-C21-C22	-4.10	121.46	127.31
26	2	1621	LUT	C22-C23-C24	-4.10	107.09	111.73
24	Y	606	CHL	OMC-CMC-C2C	-4.10	119.06	124.29
25	Y	610	CLA	CMB-C2B-C1B	-4.10	122.17	128.46
25	5	610	CLA	C1B-CHB-C4A	-4.09	122.01	130.12
25	s	610	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
30	c	517	BCR	C20-C21-C22	-4.09	121.47	127.31
25	S	610	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
26	2	1621	LUT	C35-C34-C33	-4.09	121.47	127.31
25	B	611	CLA	CAA-C2A-C3A	-4.09	101.60	112.81
26	N	1621	LUT	C35-C34-C33	-4.09	121.48	127.31
25	b	611	CLA	CAA-C2A-C3A	-4.08	101.63	112.81
26	n	1621	LUT	C35-C34-C33	-4.08	121.49	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	613	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
25	Y	613	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
27	r	622	XAT	C35-C34-C33	-4.08	121.49	127.31
25	1	610	CLA	C1B-CHB-C4A	-4.07	122.05	130.12
25	y	610	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
27	2	1622	XAT	C18-C5-C6	-4.06	115.44	122.31
26	6	1621	LUT	C35-C34-C33	-4.06	121.51	127.31
37	H	102	DGD	C1D-C2D-C3D	-4.06	102.44	109.98
27	R	622	XAT	C35-C34-C33	-4.06	121.52	127.31
28	N	1623	NEX	C27-C28-C29	-4.05	119.24	125.53
27	6	1622	XAT	C18-C5-C6	-4.05	115.45	122.31
25	G	612	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
37	h	102	DGD	C1D-C2D-C3D	-4.05	102.44	109.98
26	g	1621	LUT	C23-C24-C25	-4.04	121.43	125.22
26	6	1620	LUT	C15-C14-C13	-4.04	121.54	127.31
26	G	1621	LUT	C23-C24-C25	-4.04	121.44	125.22
25	g	612	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
25	C	503	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
26	2	1620	LUT	C15-C14-C13	-4.03	121.55	127.31
28	n	1623	NEX	C27-C28-C29	-4.03	119.28	125.53
25	5	610	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
24	6	605	CHL	C4A-C3A-C2A	-4.03	97.70	103.86
24	2	605	CHL	C4A-C3A-C2A	-4.03	97.70	103.86
25	1	610	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
30	B	620	BCR	C16-C17-C18	-4.02	121.57	127.31
25	6	614	CLA	CMB-C2B-C1B	-4.02	122.29	128.46
30	B	620	BCR	C28-C27-C26	-4.02	106.87	113.78
28	R	623	NEX	C31-C30-C29	-4.01	121.58	127.31
24	n	605	CHL	O2D-CGD-O1D	-4.01	115.75	123.82
30	b	620	BCR	C28-C27-C26	-4.01	106.89	113.78
25	c	503	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
30	b	620	BCR	C16-C17-C18	-4.00	121.60	127.31
24	N	605	CHL	O2D-CGD-O1D	-4.00	115.78	123.82
24	s	601	CHL	OMC-CMC-C2C	-4.00	119.19	124.29
30	T	101	BCR	C28-C27-C26	-3.99	106.91	113.78
30	C	517	BCR	C33-C5-C6	-3.99	120.04	124.51
30	t	101	BCR	C28-C27-C26	-3.99	106.92	113.78
28	3	1623	NEX	C11-C10-C9	-3.99	121.61	127.31
28	7	1623	NEX	C11-C10-C9	-3.99	121.61	127.31
25	2	614	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
27	g	1622	XAT	C4-C3-C2	-3.99	102.56	110.68
25	r	610	CLA	CMB-C2B-C1B	-3.99	122.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	517	BCR	C33-C5-C6	-3.98	120.05	124.51
25	r	609	CLA	C1B-CHB-C4A	-3.98	122.23	130.12
27	3	1622	XAT	C18-C5-C6	-3.98	115.58	122.31
24	2	609	CHL	CBC-CAC-C3C	-3.98	106.91	112.95
25	b	611	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
27	Y	1622	XAT	C27-C28-C29	-3.98	119.36	125.53
24	6	609	CHL	CBC-CAC-C3C	-3.98	106.92	112.95
28	r	623	NEX	C31-C30-C29	-3.97	121.64	127.31
26	r	620	LUT	C35-C34-C33	-3.97	121.64	127.31
25	R	609	CLA	C1B-CHB-C4A	-3.97	122.26	130.12
26	R	620	LUT	C35-C34-C33	-3.97	121.65	127.31
24	y	609	CHL	CBC-CAC-C3C	-3.97	106.93	112.95
27	G	1622	XAT	C4-C3-C2	-3.97	102.60	110.68
25	B	603	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
25	B	611	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
25	R	610	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
28	7	1623	NEX	C27-C28-C29	-3.96	119.38	125.53
27	7	1622	XAT	C18-C5-C6	-3.96	115.62	122.31
24	Y	609	CHL	CBC-CAC-C3C	-3.96	106.94	112.95
24	7	606	CHL	CBA-CAA-C2A	-3.96	109.96	115.66
30	c	517	BCR	C16-C17-C18	-3.95	121.67	127.31
24	3	606	CHL	CBA-CAA-C2A	-3.95	109.97	115.66
26	1	1621	LUT	C35-C34-C33	-3.95	121.68	127.31
24	S	601	CHL	OMC-CMC-C2C	-3.95	119.25	124.29
27	y	1622	XAT	C27-C28-C29	-3.94	119.41	125.53
28	3	1623	NEX	C27-C28-C29	-3.94	119.42	125.53
25	5	602	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
25	b	603	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
30	C	517	BCR	C16-C17-C18	-3.93	121.70	127.31
26	5	1621	LUT	C35-C34-C33	-3.93	121.70	127.31
30	b	619	BCR	C11-C10-C9	-3.93	121.70	127.31
25	6	611	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
27	y	1622	XAT	C10-C11-C12	-3.92	111.20	123.23
25	1	602	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
25	2	611	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
26	2	1621	LUT	C23-C24-C25	-3.92	121.55	125.22
25	B	605	CLA	CAA-CBA-CGA	-3.92	101.55	113.35
25	b	605	CLA	CAA-CBA-CGA	-3.91	101.56	113.35
30	B	619	BCR	C11-C10-C9	-3.91	121.73	127.31
27	Y	1622	XAT	C10-C11-C12	-3.91	111.25	123.23
27	Y	1622	XAT	C4-C3-C2	-3.90	102.73	110.68
30	b	619	BCR	C16-C17-C18	-3.90	121.75	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	618	BCR	C21-C20-C19	-3.90	111.27	123.23
26	6	1621	LUT	C23-C24-C25	-3.90	121.57	125.22
25	r	601	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
30	b	618	BCR	C24-C23-C22	-3.90	120.36	126.21
26	R	620	LUT	C10-C11-C12	-3.89	111.29	123.23
26	r	620	LUT	C10-C11-C12	-3.89	111.29	123.23
25	R	601	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
30	B	618	BCR	C21-C20-C19	-3.89	111.31	123.23
27	y	1622	XAT	C4-C3-C2	-3.89	102.76	110.68
37	c	520	DGD	O6D-C1D-O3G	-3.88	100.81	110.02
30	B	619	BCR	C16-C17-C18	-3.88	121.77	127.31
27	7	1622	XAT	C4-C3-C2	-3.88	102.77	110.68
28	r	623	NEX	C26-C27-C28	-3.88	117.79	125.99
30	B	618	BCR	C24-C23-C22	-3.88	120.38	126.21
26	r	620	LUT	C15-C14-C13	-3.87	121.78	127.31
27	3	1622	XAT	C4-C3-C2	-3.87	102.79	110.68
30	h	101	BCR	C20-C21-C22	-3.87	121.79	127.31
26	R	620	LUT	C15-C14-C13	-3.87	121.79	127.31
28	R	623	NEX	C26-C27-C28	-3.87	117.81	125.99
25	8	604	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
37	C	520	DGD	O6D-C1D-O3G	-3.86	100.85	110.02
30	C	516	BCR	C20-C21-C22	-3.86	121.80	127.31
25	4	604	CLA	CMB-C2B-C1B	-3.86	122.54	128.46
30	C	515	BCR	C11-C10-C9	-3.85	121.81	127.31
30	c	516	BCR	C20-C21-C22	-3.85	121.81	127.31
30	c	515	BCR	C11-C10-C9	-3.85	121.81	127.31
24	R	608	CHL	CBC-CAC-C3C	-3.85	107.11	112.95
24	r	608	CHL	CBC-CAC-C3C	-3.85	107.11	112.95
25	1	604	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
30	H	101	BCR	C20-C21-C22	-3.84	121.83	127.31
25	5	604	CLA	CMB-C2B-C1B	-3.84	122.57	128.46
37	H	102	DGD	C3D-C4D-C5D	-3.83	103.46	110.22
24	g	605	CHL	C4A-C3A-C2A	-3.83	98.01	103.86
37	h	102	DGD	C3D-C4D-C5D	-3.83	103.47	110.22
24	G	605	CHL	C4A-C3A-C2A	-3.82	98.01	103.86
24	7	609	CHL	CHA-CBD-CGD	-3.82	106.14	115.00
27	n	1622	XAT	C15-C35-C34	-3.82	115.31	123.46
30	T	101	BCR	C4-C5-C6	-3.82	117.14	122.74
24	N	606	CHL	OMC-CMC-C2C	-3.81	119.42	124.29
30	A	411	BCR	C15-C14-C13	-3.81	121.87	127.31
24	5	609	CHL	CHA-CBD-CGD	-3.81	106.16	115.00
24	n	606	CHL	OMC-CMC-C2C	-3.81	119.43	124.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	1622	XAT	C15-C35-C34	-3.81	115.33	123.46
24	1	609	CHL	CHA-CBD-CGD	-3.81	106.16	115.00
28	N	1623	NEX	C11-C10-C9	-3.81	121.88	127.31
34	a	412	SQD	O9-S-O7	-3.80	100.67	113.86
30	a	411	BCR	C15-C14-C13	-3.80	121.88	127.31
26	Y	1620	LUT	C35-C34-C33	-3.80	121.88	127.31
26	R	620	LUT	C23-C24-C25	-3.80	121.66	125.22
30	a	411	BCR	C24-C23-C22	-3.80	120.50	126.21
34	A	412	SQD	O9-S-O7	-3.80	100.69	113.86
30	c	516	BCR	C33-C5-C6	-3.80	120.25	124.51
30	C	516	BCR	C33-C5-C6	-3.80	120.25	124.51
25	Y	610	CLA	C1B-CHB-C4A	-3.80	122.59	130.12
30	A	411	BCR	C24-C23-C22	-3.80	120.51	126.21
26	y	1620	LUT	C35-C34-C33	-3.80	121.89	127.31
24	3	609	CHL	CHA-CBD-CGD	-3.80	106.19	115.00
30	t	101	BCR	C4-C5-C6	-3.80	117.17	122.74
25	2	613	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
30	A	411	BCR	C20-C21-C22	-3.79	121.90	127.31
25	c	512	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	y	610	CLA	C1B-CHB-C4A	-3.79	122.62	130.12
25	g	613	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
25	6	613	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
30	d	404	BCR	C38-C26-C25	-3.78	120.28	124.51
30	H	101	BCR	C31-C1-C6	-3.78	104.18	110.31
30	D	404	BCR	C38-C26-C25	-3.78	120.28	124.51
25	C	512	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
30	h	101	BCR	C31-C1-C6	-3.78	104.18	110.31
34	b	623	SQD	O9-S-O7	-3.78	100.77	113.86
30	a	411	BCR	C20-C21-C22	-3.77	121.93	127.31
28	n	1623	NEX	C11-C10-C9	-3.77	121.93	127.31
26	r	620	LUT	C23-C24-C25	-3.77	121.69	125.22
34	B	623	SQD	O9-S-O7	-3.76	100.81	113.86
26	s	1621	LUT	C23-C24-C25	-3.76	121.70	125.22
26	1	1620	LUT	C10-C11-C12	-3.76	111.70	123.23
25	G	613	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
27	7	1622	XAT	C15-C35-C34	-3.75	115.45	123.46
26	5	1620	LUT	C10-C11-C12	-3.75	111.73	123.23
26	S	1621	LUT	C23-C24-C25	-3.75	121.71	125.22
27	3	1622	XAT	C15-C35-C34	-3.73	115.49	123.46
27	4	622	XAT	C4-C3-C2	-3.73	103.08	110.68
33	a	409	PHO	CMB-C2B-C1B	-3.73	119.23	125.04
27	7	1622	XAT	C35-C34-C33	-3.72	122.00	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	622	XAT	C4-C3-C2	-3.72	103.09	110.68
26	7	1620	LUT	C35-C34-C33	-3.72	122.00	127.31
33	A	409	PHO	CMB-C2B-C1B	-3.72	119.25	125.04
26	3	1620	LUT	C35-C34-C33	-3.72	122.00	127.31
28	s	1623	NEX	C11-C10-C9	-3.72	122.00	127.31
25	r	613	CLA	O2D-CGD-O1D	-3.72	116.34	123.82
26	y	1620	LUT	C10-C11-C12	-3.70	111.88	123.23
27	1	1622	XAT	C6-C7-C8	-3.70	118.17	125.99
26	Y	1620	LUT	C10-C11-C12	-3.70	111.88	123.23
24	3	601	CHL	CBA-CAA-C2A	-3.70	110.66	115.76
24	7	601	CHL	CBA-CAA-C2A	-3.70	110.66	115.76
30	b	620	BCR	C11-C10-C9	-3.70	122.03	127.31
25	6	604	CLA	C1B-CHB-C4A	-3.70	122.80	130.12
25	2	604	CLA	C1B-CHB-C4A	-3.70	122.80	130.12
27	5	1622	XAT	C6-C7-C8	-3.70	118.18	125.99
25	G	614	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
25	2	613	CLA	C1B-CHB-C4A	-3.69	122.81	130.12
25	g	614	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
27	3	1622	XAT	C35-C34-C33	-3.69	122.04	127.31
30	B	620	BCR	C24-C23-C22	-3.69	120.67	126.21
30	b	620	BCR	C24-C23-C22	-3.69	120.67	126.21
25	R	613	CLA	O2D-CGD-O1D	-3.69	116.41	123.82
28	S	1623	NEX	C11-C10-C9	-3.68	122.05	127.31
25	1	604	CLA	C1B-CHB-C4A	-3.68	122.83	130.12
25	C	501	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
25	c	501	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
27	2	1622	XAT	C11-C10-C9	-3.68	122.06	127.31
28	s	1623	NEX	C35-C34-C33	-3.68	122.06	127.31
25	6	613	CLA	C1B-CHB-C4A	-3.67	122.84	130.12
35	d	411	LMG	C1-C2-C3	-3.67	103.15	109.98
35	D	411	LMG	C1-C2-C3	-3.67	103.15	109.98
25	A	407	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
30	B	620	BCR	C11-C10-C9	-3.67	122.08	127.31
26	1	1620	LUT	C15-C14-C13	-3.67	122.08	127.31
26	5	1620	LUT	C15-C14-C13	-3.66	122.08	127.31
34	A	418	SQD	O9-S-O7	-3.66	101.16	113.86
25	5	604	CLA	C1B-CHB-C4A	-3.66	122.86	130.12
27	6	1622	XAT	C11-C10-C9	-3.66	122.09	127.31
25	a	407	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
37	b	626	DGD	C3G-C2G-C1G	-3.66	103.61	111.86
34	a	418	SQD	O9-S-O7	-3.66	101.19	113.86
28	3	1623	NEX	C19-C9-C10	-3.66	117.80	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	1622	XAT	C4-C3-C2	-3.65	103.24	110.68
37	h	102	DGD	O2D-C2D-C3D	-3.65	102.41	110.36
37	H	102	DGD	O2D-C2D-C3D	-3.65	102.42	110.36
28	7	1623	NEX	C19-C9-C10	-3.65	117.81	122.92
37	c	518	DGD	O6D-C1D-O3G	-3.64	101.37	110.02
27	n	1622	XAT	C4-C3-C2	-3.64	103.25	110.68
24	s	606	CHL	OMC-CMC-C2C	-3.64	119.64	124.29
26	g	1620	LUT	C30-C31-C32	-3.64	112.06	123.23
24	S	606	CHL	OMC-CMC-C2C	-3.64	119.64	124.29
26	G	1620	LUT	C30-C31-C32	-3.64	112.07	123.23
37	B	626	DGD	C3G-C2G-C1G	-3.64	103.65	111.86
25	2	614	CLA	C1B-CHB-C4A	-3.64	122.92	130.12
37	C	518	DGD	O6D-C1D-O3G	-3.63	101.39	110.02
28	S	1623	NEX	C35-C34-C33	-3.63	122.12	127.31
25	S	610	CLA	C1B-CHB-C4A	-3.63	122.93	130.12
25	5	613	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
30	A	411	BCR	C16-C17-C18	-3.62	122.14	127.31
25	1	613	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
25	6	614	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
25	s	610	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
24	Y	605	CHL	CBC-CAC-C3C	-3.62	107.46	112.95
24	n	605	CHL	C4A-C3A-C2A	-3.62	98.33	103.86
24	y	605	CHL	CBC-CAC-C3C	-3.62	107.46	112.95
30	a	411	BCR	C16-C17-C18	-3.61	122.15	127.31
27	r	622	XAT	C15-C14-C13	-3.61	122.16	127.31
30	C	516	BCR	C16-C15-C14	-3.61	115.76	123.46
26	7	1620	LUT	C16-C1-C6	-3.61	104.46	110.31
30	c	516	BCR	C16-C15-C14	-3.61	115.77	123.46
24	N	605	CHL	C4A-C3A-C2A	-3.60	98.36	103.86
27	Y	1622	XAT	C26-C27-C28	-3.60	118.39	125.99
26	3	1620	LUT	C16-C1-C6	-3.60	104.48	110.31
25	1	611	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
25	c	505	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
30	b	619	BCR	C20-C21-C22	-3.59	122.19	127.31
26	8	620	LUT	C31-C30-C29	-3.59	122.19	127.31
30	B	618	BCR	C7-C8-C9	-3.59	120.82	126.21
25	5	611	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
27	R	622	XAT	C15-C14-C13	-3.58	122.20	127.31
30	B	619	BCR	C20-C21-C22	-3.58	122.20	127.31
26	4	620	LUT	C31-C30-C29	-3.58	122.20	127.31
25	y	611	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
25	2	614	CLA	O2D-CGD-O1D	-3.58	116.63	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	505	CLA	C1B-CHB-C4A	-3.57	123.04	130.12
27	y	1622	XAT	C26-C27-C28	-3.57	118.44	125.99
25	6	614	CLA	O2D-CGD-O1D	-3.57	116.64	123.82
25	n	603	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
24	R	606	CHL	CBC-CAC-C3C	-3.57	107.54	112.95
25	G	603	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
26	l	1620	LUT	C35-C15-C14	-3.56	115.86	123.46
25	Y	611	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
30	b	620	BCR	C15-C14-C13	-3.56	122.23	127.31
26	5	1620	LUT	C35-C15-C14	-3.56	115.87	123.46
24	S	606	CHL	CBA-CAA-C2A	-3.55	110.55	115.66
25	r	609	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
25	r	613	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
28	s	1623	NEX	C24-C23-C22	-3.55	103.45	110.68
30	b	618	BCR	C7-C8-C9	-3.55	120.88	126.21
25	g	603	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
27	G	1622	XAT	C10-C11-C12	-3.55	112.35	123.23
25	R	609	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
24	3	607	CHL	OMC-CMC-C2C	-3.54	119.77	124.29
27	g	1622	XAT	C10-C11-C12	-3.54	112.36	123.23
26	s	1621	LUT	C10-C11-C12	-3.54	112.36	123.23
26	S	1621	LUT	C10-C11-C12	-3.54	112.37	123.23
25	b	602	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
25	4	610	CLA	C1B-CHB-C4A	-3.53	123.12	130.12
25	8	610	CLA	C1B-CHB-C4A	-3.53	123.12	130.12
24	r	606	CHL	CBC-CAC-C3C	-3.53	107.59	112.95
25	N	603	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	R	613	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
28	S	1623	NEX	C24-C23-C22	-3.52	103.50	110.68
26	Y	1620	LUT	C15-C14-C13	-3.52	122.28	127.31
30	B	620	BCR	C15-C14-C13	-3.52	122.29	127.31
24	s	606	CHL	CBA-CAA-C2A	-3.52	110.59	115.66
25	n	610	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
28	R	623	NEX	C15-C35-C34	-3.51	115.96	123.46
26	y	1620	LUT	C15-C14-C13	-3.51	122.30	127.31
30	B	619	BCR	C39-C30-C25	-3.51	104.61	110.31
30	C	514	BCR	C10-C11-C12	-3.51	112.47	123.23
25	Y	613	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
25	B	602	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
30	b	619	BCR	C39-C30-C25	-3.51	104.62	110.31
25	N	612	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
34	B	621	SQD	O9-S-O7	-3.51	101.71	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	607	CHL	OMC-CMC-C2C	-3.50	119.82	124.29
25	N	610	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
28	s	1623	NEX	C31-C30-C29	-3.50	122.31	127.31
30	c	514	BCR	C10-C11-C12	-3.50	112.49	123.23
25	3	610	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
25	n	612	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
24	8	608	CHL	OMC-CMC-C2C	-3.50	119.83	124.29
34	a	418	SQD	C5-C6-S	-3.50	109.47	114.34
34	b	621	SQD	O9-S-O7	-3.50	101.74	113.86
28	S	1623	NEX	C31-C30-C29	-3.50	122.32	127.31
26	Y	1620	LUT	C23-C24-C25	-3.50	121.94	125.22
25	B	608	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
25	3	612	CLA	OBD-CAD-CBD	-3.49	120.66	125.94
28	r	623	NEX	C15-C35-C34	-3.49	116.01	123.46
26	G	1620	LUT	C15-C14-C13	-3.49	122.33	127.31
25	g	603	CLA	CBC-CAC-C3C	-3.49	102.51	112.41
25	y	613	CLA	C1B-CHB-C4A	-3.49	123.21	130.12
24	4	608	CHL	OMC-CMC-C2C	-3.49	119.84	124.29
25	G	603	CLA	CBC-CAC-C3C	-3.48	102.52	112.41
25	2	610	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
25	G	613	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
28	N	1623	NEX	C39-C29-C30	-3.48	118.05	122.92
34	A	418	SQD	C5-C6-S	-3.48	109.49	114.34
25	b	612	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
25	7	612	CLA	OBD-CAD-CBD	-3.48	120.69	125.94
26	N	1621	LUT	C10-C11-C12	-3.48	112.57	123.23
26	y	1620	LUT	C23-C24-C25	-3.48	121.96	125.22
25	B	612	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
26	G	1621	LUT	C10-C11-C12	-3.47	112.58	123.23
30	T	101	BCR	C33-C5-C6	-3.47	120.62	124.51
26	g	1620	LUT	C15-C14-C13	-3.47	122.35	127.31
25	7	610	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
25	6	610	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	g	613	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	C	513	CLA	O2D-CGD-O1D	-3.47	116.84	123.82
28	n	1623	NEX	C39-C29-C30	-3.47	118.06	122.92
35	B	2633	LMG	O2-C2-C1	-3.47	102.77	110.03
25	b	608	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	a	410	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
26	g	1621	LUT	C10-C11-C12	-3.46	112.61	123.23
30	t	101	BCR	C33-C5-C6	-3.46	120.63	124.51
25	c	513	CLA	O2D-CGD-O1D	-3.46	116.86	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	1621	LUT	C10-C11-C12	-3.46	112.62	123.23
25	s	611	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
25	S	611	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
35	b	2633	LMG	O2-C2-C1	-3.45	102.81	110.03
28	2	1623	NEX	C11-C10-C9	-3.45	122.39	127.31
25	2	612	CLA	C1B-CHB-C4A	-3.45	123.29	130.12
25	6	612	CLA	C1B-CHB-C4A	-3.44	123.30	130.12
24	G	608	CHL	CBC-CAC-C3C	-3.44	107.73	112.95
25	8	602	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
25	4	602	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
24	R	607	CHL	CBA-CAA-C2A	-3.43	111.02	115.76
26	Y	1620	LUT	C35-C15-C14	-3.43	116.14	123.46
24	r	607	CHL	CBA-CAA-C2A	-3.43	111.03	115.76
28	6	1623	NEX	C11-C10-C9	-3.43	122.42	127.31
24	g	608	CHL	CBC-CAC-C3C	-3.43	107.75	112.95
26	S	1620	LUT	C15-C14-C13	-3.43	122.42	127.31
25	G	603	CLA	OBD-CAD-CBD	-3.43	120.76	125.94
24	Y	608	CHL	CBC-CAC-C3C	-3.43	107.75	112.95
25	A	410	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
28	5	1623	NEX	C39-C29-C30	-3.42	118.13	122.92
25	7	610	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
28	5	1623	NEX	C15-C35-C34	-3.42	116.16	123.46
28	1	1623	NEX	C15-C35-C34	-3.42	116.16	123.46
26	y	1620	LUT	C35-C15-C14	-3.42	116.16	123.46
28	G	1623	NEX	C39-C29-C30	-3.42	118.14	122.92
26	6	1620	LUT	C35-C34-C33	-3.42	122.43	127.31
26	2	1620	LUT	C35-C34-C33	-3.41	122.44	127.31
25	4	604	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
25	r	612	CLA	CAA-C2A-C3A	-3.41	103.46	112.81
25	8	604	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
25	3	610	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
24	y	608	CHL	CBC-CAC-C3C	-3.41	107.78	112.95
25	c	507	CLA	CAA-C2A-C3A	-3.41	103.47	112.81
25	7	604	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
25	3	613	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
28	1	1623	NEX	C39-C29-C30	-3.40	118.16	122.92
26	s	1620	LUT	C15-C14-C13	-3.40	122.45	127.31
25	c	508	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
25	3	604	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
25	C	507	CLA	CAA-C2A-C3A	-3.40	103.49	112.81
25	R	612	CLA	CAA-C2A-C3A	-3.40	103.49	112.81
26	7	1621	LUT	C23-C24-C25	-3.40	122.03	125.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	612	CLA	O2D-CGD-O1D	-3.40	116.98	123.82
30	d	404	BCR	C21-C20-C19	-3.40	112.81	123.23
26	n	1621	LUT	C7-C8-C9	-3.39	121.11	126.21
26	N	1621	LUT	C7-C8-C9	-3.39	121.11	126.21
25	C	508	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
28	g	1623	NEX	C39-C29-C30	-3.39	118.17	122.92
25	3	612	CLA	O2D-CGD-O1D	-3.39	117.00	123.82
25	5	612	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
25	7	613	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
26	G	1620	LUT	C35-C15-C14	-3.39	116.23	123.46
26	5	1620	LUT	C30-C31-C32	-3.39	112.84	123.23
26	3	1620	LUT	C11-C10-C9	-3.39	122.48	127.31
26	1	1621	LUT	C18-C5-C6	-3.39	120.72	124.51
26	1	1620	LUT	C30-C31-C32	-3.39	112.85	123.23
30	D	404	BCR	C21-C20-C19	-3.38	112.86	123.23
26	g	1620	LUT	C16-C1-C6	-3.38	104.82	110.31
25	g	603	CLA	OBD-CAD-CBD	-3.38	120.84	125.94
26	3	1621	LUT	C7-C8-C9	-3.38	121.13	126.21
27	N	1622	XAT	C10-C11-C12	-3.38	112.87	123.23
24	7	606	CHL	CHA-CBD-CGD	-3.38	107.17	115.00
26	r	620	LUT	C30-C31-C32	-3.38	112.87	123.23
26	R	620	LUT	C30-C31-C32	-3.38	112.88	123.23
25	B	602	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
30	B	618	BCR	C11-C10-C9	-3.37	122.50	127.31
26	7	1621	LUT	C7-C8-C9	-3.37	121.15	126.21
27	n	1622	XAT	C10-C11-C12	-3.37	112.89	123.23
25	C	501	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
26	3	1621	LUT	C23-C24-C25	-3.37	122.06	125.22
24	3	606	CHL	CHA-CBD-CGD	-3.37	107.19	115.00
26	G	1620	LUT	C16-C1-C6	-3.37	104.85	110.31
26	y	1621	LUT	C10-C11-C12	-3.37	112.90	123.23
25	1	612	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
28	5	1623	NEX	C11-C10-C9	-3.37	122.51	127.31
26	5	1621	LUT	C18-C5-C6	-3.37	120.74	124.51
25	S	609	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
26	g	1620	LUT	C35-C15-C14	-3.36	116.28	123.46
25	S	609	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
26	Y	1621	LUT	C10-C11-C12	-3.36	112.91	123.23
26	7	1620	LUT	C11-C10-C9	-3.36	122.51	127.31
28	7	1623	NEX	C39-C29-C30	-3.36	118.21	122.92
25	b	602	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
28	2	1623	NEX	C39-C29-C30	-3.35	118.22	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	H	102	DGD	O3E-C3E-C2E	-3.35	103.06	110.36
25	c	501	CLA	C1B-CHB-C4A	-3.35	123.47	130.12
28	1	1623	NEX	C11-C10-C9	-3.35	122.53	127.31
25	s	609	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
27	8	622	XAT	C24-C23-C22	-3.35	103.86	110.68
25	s	609	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
28	3	1623	NEX	C39-C29-C30	-3.34	118.24	122.92
37	h	102	DGD	O3E-C3E-C2E	-3.34	103.08	110.36
30	b	618	BCR	C11-C10-C9	-3.34	122.54	127.31
37	c	519	DGD	O6D-C1D-O3G	-3.34	102.09	110.02
25	5	602	CLA	OBD-CAD-CBD	-3.34	120.90	125.94
24	1	601	CHL	CBA-CAA-C2A	-3.34	110.85	115.66
25	B	604	CLA	C1B-CHB-C4A	-3.34	123.50	130.12
25	G	603	CLA	CAA-C2A-C3A	-3.34	103.66	112.81
25	G	604	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
24	2	605	CHL	CBA-CAA-C2A	-3.34	110.85	115.66
30	4	623	BCR	C11-C12-C13	-3.34	117.05	126.42
25	g	603	CLA	CAA-C2A-C3A	-3.34	103.67	112.81
25	b	607	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
37	C	519	DGD	O6D-C1D-O3G	-3.33	102.10	110.02
25	b	604	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
27	1	1622	XAT	C4-C3-C2	-3.33	103.89	110.68
27	5	1622	XAT	C4-C3-C2	-3.33	103.89	110.68
27	7	1622	XAT	C35-C15-C14	-3.33	116.35	123.46
28	6	1623	NEX	C39-C29-C30	-3.33	118.26	122.92
24	5	601	CHL	CBA-CAA-C2A	-3.33	110.86	115.66
24	6	605	CHL	CBA-CAA-C2A	-3.33	110.87	115.66
27	4	622	XAT	C24-C23-C22	-3.33	103.90	110.68
30	8	623	BCR	C11-C12-C13	-3.33	117.07	126.42
25	g	604	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
25	y	604	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
25	B	607	CLA	C1B-CHB-C4A	-3.33	123.53	130.12
30	t	101	BCR	C15-C14-C13	-3.33	122.56	127.31
30	T	101	BCR	C15-C14-C13	-3.32	122.56	127.31
25	g	610	CLA	C1B-CHB-C4A	-3.32	123.53	130.12
25	b	606	CLA	C1B-CHB-C4A	-3.32	123.53	130.12
26	N	1620	LUT	C15-C14-C13	-3.32	122.57	127.31
25	1	602	CLA	OBD-CAD-CBD	-3.32	120.92	125.94
26	N	1620	LUT	C35-C15-C14	-3.32	116.37	123.46
27	3	1622	XAT	C35-C15-C14	-3.32	116.38	123.46
26	3	1621	LUT	C35-C34-C33	-3.32	122.57	127.31
25	Y	611	CLA	C1B-CHB-C4A	-3.32	123.54	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	604	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
25	G	610	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
30	c	515	BCR	C16-C17-C18	-3.31	122.58	127.31
26	n	1620	LUT	C35-C15-C14	-3.31	116.39	123.46
25	B	617	CLA	CAA-C2A-C3A	-3.31	103.74	112.81
26	n	1620	LUT	C15-C14-C13	-3.31	122.59	127.31
25	y	611	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
25	n	604	CLA	C1B-CHB-C4A	-3.31	123.57	130.12
30	C	515	BCR	C16-C17-C18	-3.31	122.59	127.31
25	R	612	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
25	b	617	CLA	CAA-C2A-C3A	-3.30	103.75	112.81
25	r	612	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	B	606	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	b	615	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	n	603	CLA	CAA-C2A-C3A	-3.30	103.76	112.81
25	N	604	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	C	507	CLA	O2D-CGD-O1D	-3.30	117.18	123.82
33	a	409	PHO	CBD-CHA-C4D	-3.30	104.83	108.54
25	N	603	CLA	CAA-C2A-C3A	-3.29	103.78	112.81
33	A	409	PHO	CBD-CHA-C4D	-3.29	104.83	108.54
30	B	618	BCR	C28-C27-C26	-3.29	108.12	113.78
25	c	507	CLA	O2D-CGD-O1D	-3.29	117.20	123.82
25	2	612	CLA	CAA-C2A-C3A	-3.29	103.79	112.81
30	b	618	BCR	C28-C27-C26	-3.29	108.13	113.78
26	7	1621	LUT	C35-C34-C33	-3.28	122.62	127.31
25	B	615	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
25	6	612	CLA	CAA-C2A-C3A	-3.28	103.81	112.81
24	2	605	CHL	OMC-CMC-C2C	-3.28	120.10	124.29
26	n	1620	LUT	C10-C11-C12	-3.28	113.18	123.23
24	N	601	CHL	CBC-CAC-C3C	-3.28	107.98	112.95
26	8	620	LUT	C11-C10-C9	-3.28	122.64	127.31
26	N	1620	LUT	C10-C11-C12	-3.27	113.19	123.23
24	n	601	CHL	CBC-CAC-C3C	-3.27	107.99	112.95
30	t	101	BCR	C1-C6-C5	-3.27	118.00	122.59
30	T	101	BCR	C1-C6-C5	-3.26	118.00	122.59
27	7	1622	XAT	C30-C31-C32	-3.26	113.23	123.23
26	4	620	LUT	C11-C10-C9	-3.26	122.66	127.31
25	r	602	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
25	2	603	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
27	g	1622	XAT	C15-C35-C34	-3.25	116.52	123.46
25	1	614	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
25	A	410	CLA	C1B-CHB-C4A	-3.25	123.67	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	1620	LUT	C15-C14-C13	-3.25	122.67	127.31
26	1	1621	LUT	C10-C11-C12	-3.25	113.25	123.23
25	R	602	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
26	5	1621	LUT	C10-C11-C12	-3.25	113.26	123.23
26	7	1620	LUT	C15-C14-C13	-3.25	122.67	127.31
25	5	614	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
30	b	619	BCR	C24-C23-C22	-3.25	121.33	126.21
27	G	1622	XAT	C15-C35-C34	-3.25	116.53	123.46
25	C	506	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
25	6	603	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
25	b	609	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
24	6	605	CHL	OMC-CMC-C2C	-3.24	120.15	124.29
27	3	1622	XAT	C30-C31-C32	-3.24	113.29	123.23
24	R	614	CHL	CBC-CAC-C3C	-3.24	108.03	112.95
25	c	506	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
25	a	410	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
25	S	603	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
25	a	406	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
24	g	601	CHL	CBA-CAA-C2A	-3.23	111.30	115.76
25	G	611	CLA	CMB-C2B-C1B	-3.23	123.49	128.46
25	4	612	CLA	CAA-C2A-C3A	-3.23	103.95	112.81
25	B	609	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
25	r	601	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
24	G	601	CHL	CBA-CAA-C2A	-3.23	111.31	115.76
26	N	1620	LUT	C16-C1-C6	-3.23	105.08	110.31
26	n	1620	LUT	C16-C1-C6	-3.22	105.08	110.31
25	r	613	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
25	8	612	CLA	CAA-C2A-C3A	-3.22	103.98	112.81
25	R	601	CLA	C1B-CHB-C4A	-3.22	123.74	130.12
25	g	611	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
26	7	1620	LUT	C30-C31-C32	-3.22	113.36	123.23
30	B	618	BCR	C29-C28-C27	-3.22	103.68	111.34
30	B	619	BCR	C24-C23-C22	-3.22	121.38	126.21
25	1	603	CLA	OBD-CAD-CBD	-3.21	121.09	125.94
25	A	406	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
30	b	618	BCR	C29-C28-C27	-3.21	103.69	111.34
25	R	613	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
24	r	614	CHL	CBC-CAC-C3C	-3.21	108.08	112.95
25	s	603	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
25	3	603	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
26	y	1621	LUT	C7-C8-C9	-3.20	121.40	126.21
26	1	1620	LUT	C31-C30-C29	-3.20	122.74	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	1620	LUT	C30-C31-C32	-3.20	113.41	123.23
30	A	411	BCR	C33-C5-C6	-3.20	120.92	124.51
30	b	619	BCR	C8-C7-C6	-3.20	118.29	127.25
25	5	603	CLA	OBD-CAD-CBD	-3.20	121.11	125.94
30	B	619	BCR	C8-C7-C6	-3.20	118.30	127.25
25	c	504	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
26	5	1620	LUT	C31-C30-C29	-3.20	122.75	127.31
25	r	611	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
25	7	603	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
25	R	611	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
27	4	622	XAT	C10-C11-C12	-3.19	113.43	123.23
27	Y	1622	XAT	C35-C34-C33	-3.19	122.75	127.31
25	G	614	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
37	b	626	DGD	O3G-C3G-C2G	-3.19	103.40	110.99
25	r	611	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
27	8	622	XAT	C10-C11-C12	-3.19	113.45	123.23
30	a	411	BCR	C33-C5-C6	-3.19	120.94	124.51
26	Y	1621	LUT	C7-C8-C9	-3.19	121.43	126.21
25	3	611	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
25	R	611	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
26	Y	1620	LUT	C30-C31-C32	-3.18	113.48	123.23
27	y	1622	XAT	C35-C34-C33	-3.18	122.78	127.31
25	4	611	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
25	7	611	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
25	C	504	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
24	s	608	CHL	C4A-C3A-C2A	-3.17	99.01	103.86
37	b	626	DGD	O6D-C1D-O3G	-3.17	102.49	110.02
37	B	626	DGD	O6D-C1D-O3G	-3.17	102.49	110.02
28	5	1623	NEX	C15-C14-C13	-3.17	122.79	127.31
26	y	1620	LUT	C30-C31-C32	-3.17	113.51	123.23
30	c	515	BCR	C15-C16-C17	-3.17	116.70	123.46
37	h	102	DGD	O3G-C3G-C2G	-3.17	103.45	110.99
37	B	626	DGD	O3G-C3G-C2G	-3.17	103.45	110.99
37	H	102	DGD	O3G-C3G-C2G	-3.17	103.45	110.99
25	7	614	CLA	O2D-CGD-O1D	-3.17	117.45	123.82
25	Y	612	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
24	S	608	CHL	C4A-C3A-C2A	-3.16	99.02	103.86
26	3	1620	LUT	C35-C15-C14	-3.16	116.71	123.46
30	b	618	BCR	C15-C16-C17	-3.16	116.71	123.46
26	n	1620	LUT	C30-C31-C32	-3.16	113.53	123.23
26	7	1620	LUT	C35-C15-C14	-3.16	116.71	123.46
24	Y	601	CHL	CBC-CAC-C3C	-3.16	108.15	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	611	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
26	N	1620	LUT	C30-C31-C32	-3.16	113.54	123.23
28	N	1623	NEX	C26-C27-C28	-3.16	119.31	125.99
36	d	405	PL9	C7-C3-C2	-3.16	118.74	123.23
28	l	1623	NEX	C15-C14-C13	-3.16	122.81	127.31
24	y	601	CHL	CBC-CAC-C3C	-3.16	108.16	112.95
30	b	618	BCR	C20-C21-C22	-3.15	122.81	127.31
28	n	1623	NEX	C26-C27-C28	-3.15	119.33	125.99
30	C	515	BCR	C15-C16-C17	-3.15	116.73	123.46
25	y	603	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
25	g	614	CLA	C1B-CHB-C4A	-3.15	123.88	130.12
30	B	618	BCR	C15-C16-C17	-3.15	116.74	123.46
36	D	405	PL9	C7-C3-C2	-3.15	118.75	123.23
25	D	403	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
25	3	603	CLA	CBC-CAC-C3C	-3.14	103.48	112.41
25	3	614	CLA	O2D-CGD-O1D	-3.14	117.49	123.82
25	7	603	CLA	CBC-CAC-C3C	-3.14	103.49	112.41
25	d	403	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
25	y	612	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	r	604	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
25	B	611	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
25	6	611	CLA	O2D-CGD-O1D	-3.14	117.51	123.82
25	2	611	CLA	O2D-CGD-O1D	-3.14	117.51	123.82
30	C	514	BCR	C21-C20-C19	-3.14	113.61	123.23
30	c	514	BCR	C21-C20-C19	-3.14	113.61	123.23
25	Y	603	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
36	a	414	PL9	O2-C1-C2	-3.13	116.74	121.39
25	b	611	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
30	B	618	BCR	C20-C21-C22	-3.13	122.84	127.31
25	R	604	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
25	y	613	CLA	C1C-NC-C4C	-3.12	105.26	107.06
25	A	407	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	2	611	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	a	407	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	B	603	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	C	501	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
25	c	501	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
26	l	1621	LUT	C15-C35-C34	-3.12	116.81	123.46
26	S	1620	LUT	C11-C10-C9	-3.12	122.86	127.31
30	b	619	BCR	C15-C16-C17	-3.11	116.82	123.46
30	B	619	BCR	C15-C16-C17	-3.11	116.82	123.46
28	6	1623	NEX	C35-C34-C33	-3.11	122.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	604	CLA	O2D-CGD-O1D	-3.11	117.56	123.82
25	6	603	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
25	b	603	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
25	2	603	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
26	5	1621	LUT	C15-C35-C34	-3.11	116.83	123.46
25	Y	604	CLA	O2D-CGD-O1D	-3.11	117.57	123.82
25	s	602	CLA	O2D-CGD-O1D	-3.11	117.57	123.82
25	6	611	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
24	7	608	CHL	C3B-CAB-CBB	-3.10	118.23	125.20
25	S	602	CLA	O2D-CGD-O1D	-3.10	117.58	123.82
25	Y	613	CLA	C1C-NC-C4C	-3.10	105.27	107.06
36	A	414	PL9	O2-C1-C2	-3.10	116.79	121.39
25	G	603	CLA	C1B-CHB-C4A	-3.10	123.98	130.12
26	s	1620	LUT	C11-C10-C9	-3.10	122.89	127.31
30	D	404	BCR	C16-C17-C18	-3.09	122.89	127.31
27	Y	1622	XAT	C24-C23-C22	-3.09	104.38	110.68
24	3	608	CHL	C3B-CAB-CBB	-3.09	118.25	125.20
25	5	610	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
30	B	618	BCR	C3-C4-C5	-3.09	108.46	113.78
25	g	603	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
25	B	605	CLA	C6-C5-C3	-3.09	105.65	112.66
25	l	610	CLA	OBD-CAD-CBD	-3.09	121.27	125.94
25	b	605	CLA	C6-C5-C3	-3.09	105.65	112.66
26	r	620	LUT	C18-C5-C6	-3.09	121.05	124.51
25	y	612	CLA	CAA-C2A-C3A	-3.09	104.34	112.81
30	c	517	BCR	C15-C16-C17	-3.09	116.87	123.46
30	b	618	BCR	C3-C4-C5	-3.09	108.47	113.78
25	Y	614	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
30	d	404	BCR	C16-C17-C18	-3.09	122.90	127.31
28	2	1623	NEX	C35-C34-C33	-3.09	122.91	127.31
27	y	1622	XAT	C24-C23-C22	-3.09	104.39	110.68
30	C	517	BCR	C15-C16-C17	-3.09	116.88	123.46
24	8	608	CHL	CMA-C3A-C2A	-3.09	105.58	115.84
24	2	607	CHL	C3B-CAB-CBB	-3.08	118.28	125.20
24	4	608	CHL	CMA-C3A-C2A	-3.08	105.59	115.84
25	Y	612	CLA	CAA-C2A-C3A	-3.08	104.36	112.81
27	1	1622	XAT	C35-C34-C33	-3.08	122.92	127.31
25	C	508	CLA	O2D-CGD-O1D	-3.08	117.63	123.82
25	N	614	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
24	6	607	CHL	C3B-CAB-CBB	-3.08	118.29	125.20
25	n	614	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	y	614	CLA	C1B-CHB-C4A	-3.07	124.03	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	604	CLA	OBD-CAD-CBD	-3.07	121.31	125.94
33	a	408	PHO	CBD-CHA-C4D	-3.07	105.08	108.54
25	y	612	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
27	5	1622	XAT	C7-C8-C9	-3.07	120.77	125.53
28	y	1623	NEX	C39-C29-C30	-3.07	118.63	122.92
25	Y	612	CLA	C1B-CHB-C4A	-3.07	124.05	130.12
27	G	1622	XAT	C11-C10-C9	-3.06	122.94	127.31
28	6	1623	NEX	C24-C23-C22	-3.06	104.44	110.68
25	S	614	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
24	7	608	CHL	C4A-C3A-C2A	-3.06	99.18	103.86
26	6	1621	LUT	C10-C11-C12	-3.06	113.84	123.23
27	g	1622	XAT	C11-C10-C9	-3.06	122.94	127.31
25	R	610	CLA	O2D-CGD-O1D	-3.06	117.67	123.82
25	3	612	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
24	3	608	CHL	C4A-C3A-C2A	-3.05	99.19	103.86
25	b	604	CLA	OBD-CAD-CBD	-3.05	121.33	125.94
26	2	1621	LUT	C10-C11-C12	-3.05	113.87	123.23
25	c	508	CLA	O2D-CGD-O1D	-3.05	117.68	123.82
25	n	603	CLA	CBC-CAC-C3C	-3.05	103.75	112.41
28	3	1623	NEX	C11-C12-C13	-3.05	117.85	126.42
28	2	1623	NEX	C24-C23-C22	-3.05	104.47	110.68
25	7	612	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
30	C	514	BCR	C15-C16-C17	-3.05	116.95	123.46
25	s	614	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
30	c	514	BCR	C15-C16-C17	-3.05	116.96	123.46
33	A	408	PHO	CBD-CHA-C4D	-3.05	105.11	108.54
25	1	612	CLA	CAA-C2A-C3A	-3.05	104.46	112.81
30	B	620	BCR	C1-C6-C5	-3.05	118.31	122.59
28	y	1623	NEX	C26-C27-C28	-3.05	119.55	125.99
37	C	520	DGD	O5D-C6D-C5D	-3.04	103.85	108.94
25	7	604	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
25	5	612	CLA	CAA-C2A-C3A	-3.04	104.46	112.81
27	1	1622	XAT	C7-C8-C9	-3.04	120.81	125.53
26	g	1621	LUT	C7-C8-C9	-3.04	121.64	126.21
27	5	1622	XAT	C35-C34-C33	-3.04	122.97	127.31
25	3	612	CLA	CAA-C2A-C3A	-3.04	104.47	112.81
24	7	605	CHL	C4A-C3A-C2A	-3.04	99.21	103.86
25	7	612	CLA	CAA-C2A-C3A	-3.04	104.47	112.81
26	S	1620	LUT	C35-C15-C14	-3.04	116.97	123.46
28	7	1623	NEX	C11-C12-C13	-3.04	117.87	126.42
25	c	505	CLA	O2D-CGD-O1D	-3.04	117.70	123.82
30	b	620	BCR	C1-C6-C5	-3.04	118.32	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	610	CLA	O2D-CGD-O1D	-3.04	117.70	123.82
25	N	603	CLA	CBC-CAC-C3C	-3.04	103.78	112.41
24	r	614	CHL	O2D-CGD-O1D	-3.04	117.70	123.82
28	1	1623	NEX	C24-C23-C22	-3.04	104.49	110.68
25	1	603	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
27	3	1622	XAT	C7-C8-C9	-3.04	120.81	125.53
26	2	1621	LUT	C30-C31-C32	-3.04	113.91	123.23
28	5	1623	NEX	C24-C23-C22	-3.04	104.49	110.68
28	Y	1623	NEX	C39-C29-C30	-3.04	118.67	122.92
25	5	603	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
24	3	605	CHL	C4A-C3A-C2A	-3.04	99.22	103.86
26	S	1621	LUT	C30-C31-C32	-3.03	113.93	123.23
25	C	505	CLA	O2D-CGD-O1D	-3.03	117.72	123.82
26	s	1621	LUT	C30-C31-C32	-3.03	113.94	123.23
26	R	620	LUT	C18-C5-C6	-3.03	121.12	124.51
24	R	614	CHL	O2D-CGD-O1D	-3.03	117.72	123.82
27	7	1622	XAT	C7-C8-C9	-3.03	120.83	125.53
26	6	1621	LUT	C30-C31-C32	-3.03	113.94	123.23
28	S	1623	NEX	C39-C29-C30	-3.03	118.68	122.92
28	s	1623	NEX	C39-C29-C30	-3.03	118.68	122.92
26	s	1620	LUT	C35-C15-C14	-3.03	117.00	123.46
24	s	601	CHL	CBA-CAA-C2A	-3.02	111.30	115.66
25	2	603	CLA	CAA-C2A-C3A	-3.02	104.53	112.81
25	6	603	CLA	CAA-C2A-C3A	-3.02	104.53	112.81
24	S	601	CHL	CBA-CAA-C2A	-3.02	111.31	115.66
35	A	413	LMG	O6-C1-O1	-3.02	102.86	110.02
24	Y	607	CHL	C3B-CAB-CBB	-3.02	118.42	125.20
35	a	413	LMG	O6-C1-O1	-3.02	102.86	110.02
28	Y	1623	NEX	C26-C27-C28	-3.02	119.62	125.99
25	3	604	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
26	G	1621	LUT	C7-C8-C9	-3.02	121.68	126.21
25	3	603	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
30	c	515	BCR	C23-C22-C21	-3.01	114.32	118.94
25	7	603	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
37	c	520	DGD	O5D-C6D-C5D	-3.01	103.91	108.94
25	S	609	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
25	s	609	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
25	C	512	CLA	CAA-C2A-C3A	-3.01	104.57	112.81
24	7	605	CHL	CHA-CBD-CGD	-3.00	108.03	115.00
24	y	607	CHL	C3B-CAB-CBB	-3.00	118.46	125.20
26	4	620	LUT	C30-C31-C32	-3.00	114.02	123.23
25	c	512	CLA	CAA-C2A-C3A	-3.00	104.58	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	520	DGD	C3G-C2G-C1G	-3.00	105.09	111.86
26	8	620	LUT	C18-C5-C6	-3.00	121.15	124.51
26	Y	1621	LUT	C30-C31-C32	-3.00	114.03	123.23
25	B	607	CLA	CAA-CBA-CGA	-3.00	104.31	113.35
26	8	620	LUT	C30-C31-C32	-3.00	114.03	123.23
27	g	1622	XAT	C24-C23-C22	-3.00	104.58	110.68
25	G	611	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
25	b	607	CLA	CAA-CBA-CGA	-2.99	104.33	113.35
26	4	620	LUT	C18-C5-C6	-2.99	121.16	124.51
28	N	1623	NEX	C24-C23-C22	-2.99	104.59	110.68
37	C	520	DGD	C3G-C2G-C1G	-2.99	105.11	111.86
28	S	1623	NEX	C19-C9-C10	-2.99	118.73	122.92
25	g	611	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
26	y	1621	LUT	C30-C31-C32	-2.99	114.07	123.23
30	C	515	BCR	C23-C22-C21	-2.99	114.36	118.94
25	N	603	CLA	OBD-CAD-CBD	-2.99	121.43	125.94
25	B	616	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
28	n	1623	NEX	C24-C23-C22	-2.98	104.60	110.68
26	2	1621	LUT	C15-C14-C13	-2.98	123.05	127.31
24	3	605	CHL	CHA-CBD-CGD	-2.98	108.08	115.00
25	n	603	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	b	616	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
26	1	1621	LUT	C23-C24-C25	-2.98	122.43	125.22
24	7	609	CHL	CBC-CAC-C3C	-2.98	108.43	112.95
24	3	609	CHL	CBC-CAC-C3C	-2.98	108.43	112.95
28	r	623	NEX	C11-C12-C13	-2.98	118.05	126.42
28	y	1623	NEX	C11-C12-C13	-2.97	118.06	126.42
26	6	1621	LUT	C15-C14-C13	-2.97	123.07	127.31
28	R	623	NEX	C11-C12-C13	-2.97	118.06	126.42
30	C	514	BCR	C20-C21-C22	-2.97	123.07	127.31
37	H	102	DGD	CDB-CCB-CBB	-2.97	99.14	114.45
37	h	102	DGD	CDB-CCB-CBB	-2.97	99.14	114.45
27	G	1622	XAT	C24-C23-C22	-2.97	104.63	110.68
25	N	614	CLA	O2D-CGD-O1D	-2.97	117.84	123.82
28	Y	1623	NEX	C11-C12-C13	-2.97	118.08	126.42
26	y	1621	LUT	C22-C23-C24	-2.97	108.37	111.73
25	1	602	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
25	3	610	CLA	OBD-CAD-CBD	-2.97	121.46	125.94
25	N	603	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	n	603	CLA	OBD-CAD-CBD	-2.96	121.47	125.94
26	S	1620	LUT	C10-C11-C12	-2.96	114.14	123.23
25	S	602	CLA	C1B-CHB-C4A	-2.96	124.25	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	1620	LUT	C31-C30-C29	-2.96	123.08	127.31
25	n	612	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
28	s	1623	NEX	C19-C9-C10	-2.96	118.78	122.92
25	C	513	CLA	CAA-C2A-C3A	-2.96	104.70	112.81
26	g	1620	LUT	C10-C11-C12	-2.96	114.16	123.23
30	b	620	BCR	C4-C5-C6	-2.96	118.40	122.74
25	N	612	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
25	y	614	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
26	5	1621	LUT	C23-C24-C25	-2.95	122.45	125.22
26	s	1620	LUT	C10-C11-C12	-2.95	114.17	123.23
25	R	611	CLA	OBD-CAD-CBD	-2.95	121.48	125.94
26	Y	1621	LUT	C22-C23-C24	-2.95	108.39	111.73
28	Y	1623	NEX	C24-C23-C22	-2.95	104.67	110.68
25	s	602	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	5	602	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
25	1	604	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
25	7	610	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
30	c	514	BCR	C20-C21-C22	-2.95	123.10	127.31
25	r	603	CLA	CAA-C2A-C3A	-2.95	104.72	112.81
28	y	1623	NEX	C24-C23-C22	-2.95	104.68	110.68
26	2	1620	LUT	C31-C30-C29	-2.95	123.11	127.31
26	G	1620	LUT	C10-C11-C12	-2.95	114.20	123.23
26	r	620	LUT	C15-C35-C34	-2.95	117.17	123.46
25	c	513	CLA	CAA-C2A-C3A	-2.95	104.73	112.81
25	n	614	CLA	O2D-CGD-O1D	-2.94	117.89	123.82
26	R	620	LUT	C15-C35-C34	-2.94	117.18	123.46
25	R	603	CLA	CAA-C2A-C3A	-2.94	104.74	112.81
27	N	1622	XAT	C24-C23-C22	-2.94	104.69	110.68
25	5	611	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
36	d	405	PL9	C7-C8-C9	-2.94	121.79	126.71
25	b	616	CLA	O2D-CGD-O1D	-2.94	117.90	123.82
25	R	616	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
25	d	402	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
25	5	604	CLA	O2D-CGD-O1D	-2.94	117.91	123.82
27	n	1622	XAT	C24-C23-C22	-2.94	104.70	110.68
25	4	611	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
27	8	622	XAT	C31-C30-C29	-2.94	123.12	127.31
26	3	1620	LUT	C10-C11-C12	-2.94	114.23	123.23
25	B	616	CLA	O2D-CGD-O1D	-2.94	117.91	123.82
25	7	611	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
37	c	519	DGD	O5D-C6D-C5D	-2.93	104.03	108.94
30	B	620	BCR	C4-C5-C6	-2.93	118.43	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	611	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
25	N	611	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
36	D	405	PL9	C7-C8-C9	-2.93	121.81	126.71
25	Y	614	CLA	O2D-CGD-O1D	-2.93	117.92	123.82
30	4	623	BCR	C20-C21-C22	-2.93	123.12	127.31
25	r	616	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
27	4	622	XAT	C31-C30-C29	-2.93	123.13	127.31
30	8	623	BCR	C20-C21-C22	-2.93	123.13	127.31
25	6	602	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
25	3	611	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
25	2	602	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
26	7	1620	LUT	C10-C11-C12	-2.92	114.27	123.23
25	Y	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
25	r	611	CLA	OBD-CAD-CBD	-2.92	121.53	125.94
25	A	405	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
28	R	623	NEX	C17-C1-C6	-2.92	107.86	110.47
25	c	513	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
25	C	513	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
28	1	1623	NEX	C26-C27-C28	-2.92	119.82	125.99
25	G	612	CLA	CAA-C2A-C3A	-2.92	104.81	112.81
25	8	611	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	3	1621	LUT	C15-C14-C13	-2.92	123.15	127.31
25	D	402	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	1	611	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
27	r	622	XAT	C10-C11-C12	-2.91	114.29	123.23
25	5	603	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
24	g	607	CHL	CHA-CBD-CGD	-2.91	108.24	115.00
29	3	2630	LHG	O8-C6-C5	-2.91	101.34	108.66
26	G	1621	LUT	C28-C29-C30	-2.91	114.47	118.94
25	a	405	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
29	7	2630	LHG	O8-C6-C5	-2.91	101.35	108.66
27	R	622	XAT	C10-C11-C12	-2.91	114.31	123.23
37	C	519	DGD	O5D-C6D-C5D	-2.91	104.08	108.94
26	7	1621	LUT	C15-C14-C13	-2.91	123.16	127.31
27	1	1622	XAT	C15-C35-C34	-2.90	117.26	123.46
25	c	507	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	y	602	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	g	612	CLA	CAA-C2A-C3A	-2.90	104.85	112.81
25	4	612	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
24	G	607	CHL	CHA-CBD-CGD	-2.90	108.27	115.00
25	6	604	CLA	O2D-CGD-O1D	-2.90	117.98	123.82
26	g	1620	LUT	C23-C24-C25	-2.90	122.50	125.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1620	LUT	C8-C9-C10	-2.90	114.49	118.94
28	r	623	NEX	C17-C1-C6	-2.90	107.88	110.47
25	S	614	CLA	O2D-CGD-O1D	-2.90	117.99	123.82
25	8	612	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
28	5	1623	NEX	C26-C27-C28	-2.90	119.87	125.99
25	g	602	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
25	B	609	CLA	O2D-CGD-O1D	-2.89	118.00	123.82
25	s	614	CLA	O2D-CGD-O1D	-2.89	118.00	123.82
25	1	603	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
24	8	601	CHL	OMC-CMC-C2C	-2.89	120.60	124.29
24	4	601	CHL	OMC-CMC-C2C	-2.89	120.60	124.29
25	C	507	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
25	s	611	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
30	h	101	BCR	C38-C26-C25	-2.88	121.28	124.51
26	5	1620	LUT	C8-C9-C10	-2.88	114.52	118.94
26	g	1621	LUT	C28-C29-C30	-2.88	114.52	118.94
25	3	602	CLA	O2D-CGD-O1D	-2.88	118.03	123.82
25	b	611	CLA	CAA-CBA-CGA	-2.88	104.67	113.35
25	S	611	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	Y	603	CLA	CBC-CAC-C3C	-2.88	104.25	112.41
24	n	605	CHL	OMC-CMC-C2C	-2.88	120.62	124.29
25	g	612	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
26	6	1620	LUT	C30-C31-C32	-2.88	114.41	123.23
24	G	606	CHL	C3B-CAB-CBB	-2.87	118.75	125.20
25	G	602	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
25	B	611	CLA	CAA-CBA-CGA	-2.87	104.69	113.35
35	a	415	LMG	O6-C1-O1	-2.87	103.20	110.02
26	2	1620	LUT	C30-C31-C32	-2.87	114.42	123.23
26	G	1620	LUT	C23-C24-C25	-2.87	122.53	125.22
27	5	1622	XAT	C15-C35-C34	-2.87	117.34	123.46
25	b	609	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
24	g	606	CHL	C3B-CAB-CBB	-2.87	118.76	125.20
24	y	607	CHL	CBA-CAA-C2A	-2.87	111.81	115.76
24	N	605	CHL	OMC-CMC-C2C	-2.87	120.63	124.29
25	R	601	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
24	g	605	CHL	O2D-CGD-O1D	-2.87	118.05	123.82
25	2	604	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
28	r	623	NEX	C24-C23-C22	-2.87	104.84	110.68
37	h	102	DGD	O2D-C2D-C1D	-2.86	104.04	110.03
26	y	1620	LUT	C38-C25-C24	-2.86	117.52	123.68
37	H	102	DGD	O2D-C2D-C1D	-2.86	104.04	110.03
35	A	415	LMG	O6-C1-O1	-2.86	103.22	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
28	R	623	NEX	C24-C23-C22	-2.86	104.85	110.68
25	7	613	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
25	r	601	CLA	O2D-CGD-O1D	-2.86	118.06	123.82
24	Y	607	CHL	CBA-CAA-C2A	-2.86	111.81	115.76
25	G	612	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
26	4	620	LUT	C15-C35-C34	-2.86	117.36	123.46
26	S	1621	LUT	C15-C14-C13	-2.86	123.23	127.31
25	n	612	CLA	CAA-C2A-C3A	-2.86	104.98	112.81
26	g	1620	LUT	C38-C25-C24	-2.86	117.53	123.68
24	s	607	CHL	OMC-CMC-C2C	-2.86	120.64	124.29
25	y	603	CLA	CBC-CAC-C3C	-2.85	104.31	112.41
25	C	511	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
25	7	602	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
25	S	610	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
25	3	613	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
26	Y	1620	LUT	C38-C25-C24	-2.85	117.54	123.68
24	G	605	CHL	O2D-CGD-O1D	-2.85	118.08	123.82
30	H	101	BCR	C38-C26-C25	-2.85	121.32	124.51
25	B	616	CLA	CAA-C2A-C3A	-2.85	105.01	112.81
25	b	616	CLA	CAA-C2A-C3A	-2.85	105.01	112.81
25	B	606	CLA	C6-C5-C3	-2.85	106.21	112.66
25	C	502	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
30	c	515	BCR	C33-C5-C6	-2.85	121.32	124.51
25	A	410	CLA	O2D-CGD-O1D	-2.84	118.10	123.82
25	N	612	CLA	CAA-C2A-C3A	-2.84	105.01	112.81
25	R	602	CLA	OBD-CAD-CBD	-2.84	121.65	125.94
25	s	610	CLA	O2D-CGD-O1D	-2.84	118.10	123.82
24	3	605	CHL	OMC-CMC-C2C	-2.84	120.66	124.29
28	R	623	NEX	C35-C34-C33	-2.84	123.26	127.31
25	c	511	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
30	t	101	BCR	C16-C15-C14	-2.84	117.40	123.46
26	s	1621	LUT	C15-C14-C13	-2.84	123.26	127.31
25	b	606	CLA	C6-C5-C3	-2.84	106.22	112.66
25	c	502	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
24	S	607	CHL	OMC-CMC-C2C	-2.84	120.67	124.29
25	g	602	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
24	g	606	CHL	OMC-CMC-C2C	-2.84	120.67	124.29
26	8	620	LUT	C15-C35-C34	-2.84	117.41	123.46
30	C	515	BCR	C33-C5-C6	-2.83	121.33	124.51
26	s	1620	LUT	C30-C31-C32	-2.83	114.54	123.23
28	R	623	NEX	C39-C29-C30	-2.83	118.95	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	605	CHL	OMC-CMC-C2C	-2.83	120.67	124.29
24	y	608	CHL	C4A-C3A-C2A	-2.83	99.53	103.86
24	G	606	CHL	OMC-CMC-C2C	-2.83	120.68	124.29
28	R	623	NEX	C30-C31-C32	-2.83	114.55	123.23
25	C	503	CLA	O2D-CGD-O1D	-2.83	118.12	123.82
24	G	606	CHL	C4A-C3A-C2A	-2.83	99.53	103.86
26	S	1620	LUT	C30-C31-C32	-2.83	114.55	123.23
30	D	404	BCR	C16-C15-C14	-2.83	117.43	123.46
25	r	602	CLA	OBD-CAD-CBD	-2.83	121.67	125.94
26	G	1620	LUT	C38-C25-C24	-2.83	117.59	123.68
25	2	610	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
24	n	607	CHL	CBA-CAA-C2A	-2.82	111.86	115.76
30	T	101	BCR	C16-C15-C14	-2.82	117.44	123.46
29	d	409	LHG	C11-C10-C9	-2.82	99.91	114.45
25	n	613	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
29	D	409	LHG	C11-C10-C9	-2.82	99.91	114.45
24	4	607	CHL	OMC-CMC-C2C	-2.82	120.69	124.29
25	G	602	CLA	O2D-CGD-O1D	-2.82	118.14	123.82
25	6	610	CLA	CMB-C2B-C1B	-2.82	124.13	128.46
26	N	1620	LUT	C38-C25-C24	-2.82	117.61	123.68
24	3	605	CHL	CBA-CAA-C2A	-2.82	111.60	115.66
28	r	623	NEX	C30-C31-C32	-2.82	114.59	123.23
24	8	607	CHL	OMC-CMC-C2C	-2.82	120.69	124.29
30	d	404	BCR	C16-C15-C14	-2.82	117.45	123.46
25	c	503	CLA	O2D-CGD-O1D	-2.82	118.15	123.82
24	N	607	CHL	CBA-CAA-C2A	-2.82	111.88	115.76
28	5	1623	NEX	C31-C30-C29	-2.82	123.29	127.31
24	Y	608	CHL	C4A-C3A-C2A	-2.82	99.56	103.86
25	N	613	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
26	n	1620	LUT	C38-C25-C24	-2.81	117.62	123.68
28	r	623	NEX	C35-C34-C33	-2.81	123.29	127.31
28	r	623	NEX	C39-C29-C30	-2.81	118.98	122.92
28	1	1623	NEX	C31-C30-C29	-2.81	123.30	127.31
24	R	614	CHL	CAA-C2A-C3A	-2.81	109.67	115.37
24	g	606	CHL	C4A-C3A-C2A	-2.80	99.57	103.86
27	7	1622	XAT	C24-C23-C22	-2.80	104.97	110.68
24	G	601	CHL	CBC-CAC-C3C	-2.80	108.69	112.95
35	A	413	LMG	O3-C3-C2	-2.80	104.26	110.36
24	G	606	CHL	CBC-CAC-C3C	-2.80	108.70	112.95
28	g	1623	NEX	C24-C23-C22	-2.80	104.97	110.68
27	2	1622	XAT	C35-C34-C33	-2.80	123.31	127.31
25	G	611	CLA	O2D-CGD-O1D	-2.80	118.19	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	1620	LUT	C10-C11-C12	-2.80	114.64	123.23
24	8	601	CHL	C4A-C3A-C2A	-2.80	99.58	103.86
25	R	601	CLA	CAC-C3C-C2C	-2.80	122.64	127.49
24	7	605	CHL	CBA-CAA-C2A	-2.80	111.63	115.66
25	c	510	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
27	6	1622	XAT	C35-C34-C33	-2.80	123.32	127.31
25	N	604	CLA	C1-C2-C3	-2.80	122.26	126.68
25	C	510	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
25	y	612	CLA	OBD-CAD-CBD	-2.80	121.72	125.94
35	a	413	LMG	O3-C3-C2	-2.80	104.28	110.36
28	G	1623	NEX	C24-C23-C22	-2.79	104.99	110.68
24	r	614	CHL	CAA-C2A-C3A	-2.79	109.70	115.37
24	4	601	CHL	C4A-C3A-C2A	-2.79	99.59	103.86
25	b	606	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
25	B	606	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
26	2	1620	LUT	C10-C11-C12	-2.79	114.69	123.23
25	n	604	CLA	C1-C2-C3	-2.78	122.28	126.68
25	g	611	CLA	O2D-CGD-O1D	-2.78	118.22	123.82
24	g	606	CHL	CBC-CAC-C3C	-2.78	108.72	112.95
24	g	609	CHL	CBA-CAA-C2A	-2.78	111.92	115.76
24	r	606	CHL	C4A-C3A-C2A	-2.78	99.61	103.86
28	5	1623	NEX	C30-C31-C32	-2.78	114.70	123.23
25	r	601	CLA	CAC-C3C-C2C	-2.78	122.67	127.49
25	3	614	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
37	c	518	DGD	CDB-CCB-CBB	-2.78	100.13	114.45
27	3	1622	XAT	C24-C23-C22	-2.78	105.02	110.68
25	c	503	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
24	G	609	CHL	CBA-CAA-C2A	-2.78	111.93	115.76
37	C	518	DGD	CDB-CCB-CBB	-2.78	100.14	114.45
25	C	503	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
28	1	1623	NEX	C30-C31-C32	-2.78	114.71	123.23
24	R	606	CHL	C4A-C3A-C2A	-2.78	99.61	103.86
25	Y	612	CLA	OBD-CAD-CBD	-2.78	121.75	125.94
24	g	601	CHL	CBC-CAC-C3C	-2.77	108.74	112.95
25	B	614	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
25	7	614	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
28	1	1623	NEX	C11-C12-C13	-2.77	118.64	126.42
25	7	612	CLA	C1B-CHB-C4A	-2.77	124.64	130.12
28	5	1623	NEX	C11-C12-C13	-2.77	118.64	126.42
24	G	601	CHL	C1-C2-C3	-2.76	120.86	125.96
25	8	603	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
24	3	606	CHL	C4A-C3A-C2A	-2.76	99.63	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
25	A	410	CLA	CAA-CBA-CGA	-2.76	105.03	113.35
25	N	611	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	a	410	CLA	CAA-CBA-CGA	-2.76	105.03	113.35
25	R	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	r	603	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
25	G	610	CLA	OBD-CAD-CBD	-2.76	121.77	125.94
25	b	614	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
37	B	626	DGD	CDB-CCB-CBB	-2.76	100.24	114.45
24	s	606	CHL	O2D-CGD-O1D	-2.76	118.27	123.82
24	Y	606	CHL	CBC-CAC-C3C	-2.76	108.77	112.95
26	Y	1620	LUT	C11-C10-C9	-2.76	123.38	127.31
37	b	626	DGD	CDB-CCB-CBB	-2.76	100.25	114.45
25	n	611	CLA	C1B-CHB-C4A	-2.75	124.66	130.12
24	y	606	CHL	CBC-CAC-C3C	-2.75	108.77	112.95
25	3	612	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
25	B	615	CLA	O2D-CGD-O1D	-2.75	118.28	123.82
25	4	603	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
25	b	616	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
25	y	611	CLA	O2A-CGA-O1A	-2.75	116.72	123.55
25	B	605	CLA	C1-C2-C3	-2.75	120.89	125.96
25	g	610	CLA	OBD-CAD-CBD	-2.75	121.79	125.94
25	Y	614	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
24	n	609	CHL	CBA-CAA-C2A	-2.75	111.97	115.76
25	b	615	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
26	y	1620	LUT	C11-C10-C9	-2.75	123.39	127.31
25	b	605	CLA	C1-C2-C3	-2.75	120.90	125.96
24	g	601	CHL	C1-C2-C3	-2.74	120.90	125.96
24	N	609	CHL	CBA-CAA-C2A	-2.74	111.97	115.76
29	n	2630	LHG	C11-C10-C9	-2.74	100.31	114.45
28	3	1623	NEX	C35-C34-C33	-2.74	123.39	127.31
24	S	606	CHL	O2D-CGD-O1D	-2.74	118.30	123.82
25	y	611	CLA	O2D-CGD-O1D	-2.74	118.30	123.82
24	Y	605	CHL	C4A-C3A-C2A	-2.74	99.67	103.86
29	N	2630	LHG	C11-C10-C9	-2.74	100.32	114.45
24	7	606	CHL	C4A-C3A-C2A	-2.74	99.67	103.86
27	r	622	XAT	C35-C15-C14	-2.74	117.61	123.46
26	5	1621	LUT	C31-C30-C29	-2.74	123.40	127.31
25	S	613	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
24	y	605	CHL	C4A-C3A-C2A	-2.74	99.67	103.86
25	Y	611	CLA	O2A-CGA-O1A	-2.74	116.76	123.55
25	6	612	CLA	CMB-C2B-C1B	-2.73	124.26	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	609	CHL	O1D-CGD-CBD	-2.73	118.89	124.53
27	R	622	XAT	C35-C15-C14	-2.73	117.63	123.46
24	8	606	CHL	CBC-CAC-C3C	-2.73	108.80	112.95
30	b	618	BCR	C10-C11-C12	-2.73	114.86	123.23
25	2	613	CLA	O2D-CGD-O1D	-2.73	118.33	123.82
24	4	606	CHL	CBC-CAC-C3C	-2.73	108.81	112.95
29	d	408	LHG	C11-C10-C9	-2.73	100.40	114.45
26	S	1621	LUT	C35-C15-C14	-2.73	117.64	123.46
25	y	611	CLA	OBD-CAD-CBD	-2.73	121.82	125.94
29	D	408	LHG	C11-C10-C9	-2.73	100.41	114.45
30	B	618	BCR	C10-C11-C12	-2.73	114.87	123.23
25	C	504	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
27	7	1622	XAT	C10-C11-C12	-2.72	114.88	123.23
26	R	620	LUT	C28-C29-C30	-2.72	114.76	118.94
25	y	614	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
27	3	1622	XAT	C10-C11-C12	-2.72	114.88	123.23
25	7	602	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	c	504	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
26	r	620	LUT	C28-C29-C30	-2.72	114.77	118.94
25	Y	611	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
25	2	612	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
25	s	613	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
25	Y	611	CLA	OBD-CAD-CBD	-2.72	121.84	125.94
35	z	101	LMG	C1-O6-C5	-2.72	108.60	113.72
25	6	613	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
30	b	620	BCR	C20-C21-C22	-2.71	123.44	127.31
26	g	1621	LUT	C11-C10-C9	-2.71	123.44	127.31
35	Z	101	LMG	C1-O6-C5	-2.71	108.60	113.72
28	7	1623	NEX	C35-C34-C33	-2.71	123.44	127.31
25	5	612	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
26	s	1621	LUT	C35-C15-C14	-2.71	117.67	123.46
25	Y	610	CLA	OBD-CAD-CBD	-2.71	121.84	125.94
26	1	1621	LUT	C31-C30-C29	-2.71	123.44	127.31
30	A	411	BCR	C21-C20-C19	-2.71	114.92	123.23
25	3	602	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
26	G	1621	LUT	C11-C10-C9	-2.71	123.44	127.31
24	7	605	CHL	CBC-CAC-C3C	-2.71	108.84	112.95
25	y	610	CLA	OBD-CAD-CBD	-2.71	121.85	125.94
28	G	1623	NEX	C31-C30-C29	-2.71	123.45	127.31
25	s	611	CLA	O2D-CGD-O1D	-2.71	118.37	123.82
35	D	411	LMG	O6-C1-O1	-2.71	103.60	110.02
25	r	604	CLA	O2D-CGD-O1D	-2.71	118.38	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	403	CLA	O2D-CGD-O1D	-2.71	118.38	123.82
24	2	609	CHL	O1D-CGD-CBD	-2.70	118.95	124.53
26	6	1620	LUT	C15-C35-C34	-2.70	117.69	123.46
25	S	611	CLA	O2D-CGD-O1D	-2.70	118.38	123.82
25	d	403	CLA	O2D-CGD-O1D	-2.70	118.38	123.82
25	R	604	CLA	O2D-CGD-O1D	-2.70	118.39	123.82
30	C	516	BCR	C7-C8-C9	-2.70	122.15	126.21
30	a	411	BCR	C21-C20-C19	-2.70	114.95	123.23
26	g	1621	LUT	C30-C31-C32	-2.70	114.95	123.23
25	g	603	CLA	O2D-CGD-O1D	-2.70	118.39	123.82
35	d	411	LMG	O6-C1-O1	-2.70	103.62	110.02
25	D	402	CLA	CBA-CAA-C2A	-2.69	105.73	113.80
30	C	516	BCR	C10-C11-C12	-2.69	114.97	123.23
25	b	610	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
25	y	603	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
25	d	402	CLA	CBA-CAA-C2A	-2.69	105.74	113.80
24	7	601	CHL	C3B-CAB-CBB	-2.69	119.16	125.20
25	G	603	CLA	O2D-CGD-O1D	-2.69	118.41	123.82
24	3	601	CHL	C3B-CAB-CBB	-2.69	119.17	125.20
25	B	602	CLA	O2D-CGD-O1D	-2.69	118.41	123.82
25	B	610	CLA	C1B-CHB-C4A	-2.69	124.80	130.12
24	5	605	CHL	O2D-CGD-O1D	-2.69	118.42	123.82
25	b	602	CLA	O2D-CGD-O1D	-2.69	118.42	123.82
27	N	1622	XAT	C35-C34-C33	-2.69	123.48	127.31
25	c	510	CLA	O2D-CGD-O1D	-2.68	118.42	123.82
28	g	1623	NEX	C31-C30-C29	-2.68	123.48	127.31
25	S	603	CLA	O2D-CGD-O1D	-2.68	118.42	123.82
24	G	608	CHL	C4A-C3A-C2A	-2.68	99.76	103.86
25	s	603	CLA	O2D-CGD-O1D	-2.68	118.42	123.82
30	B	620	BCR	C20-C21-C22	-2.68	123.48	127.31
24	3	605	CHL	CBC-CAC-C3C	-2.68	108.88	112.95
25	1	612	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
25	Y	603	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
26	2	1620	LUT	C15-C35-C34	-2.68	117.74	123.46
24	8	606	CHL	OMC-CMC-C2C	-2.68	120.87	124.29
30	c	516	BCR	C7-C8-C9	-2.68	122.19	126.21
25	B	608	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
24	6	606	CHL	CBC-CAC-C3C	-2.68	108.89	112.95
26	G	1621	LUT	C30-C31-C32	-2.67	115.03	123.23
27	n	1622	XAT	C35-C34-C33	-2.67	123.49	127.31
26	r	620	LUT	C37-C21-C22	-2.67	104.31	109.42
35	b	622	LMG	O6-C1-O1	-2.67	103.67	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	606	CHL	CBC-CAC-C3C	-2.67	108.89	112.95
25	C	510	CLA	CAA-C2A-C3A	-2.67	105.48	112.81
25	c	510	CLA	CAA-C2A-C3A	-2.67	105.49	112.81
25	b	613	CLA	O2D-CGD-O1D	-2.67	118.45	123.82
25	C	509	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
30	c	516	BCR	C10-C11-C12	-2.67	115.05	123.23
24	g	608	CHL	C4A-C3A-C2A	-2.67	99.78	103.86
27	y	1622	XAT	C31-C32-C33	-2.67	118.92	126.42
24	1	605	CHL	O2D-CGD-O1D	-2.67	118.45	123.82
24	2	606	CHL	C4A-C3A-C2A	-2.67	99.78	103.86
25	4	603	CLA	CAA-C2A-C3A	-2.66	105.50	112.81
25	c	509	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
24	3	609	CHL	OMC-CMC-C2C	-2.66	120.89	124.29
24	6	606	CHL	C4A-C3A-C2A	-2.66	99.79	103.86
25	b	608	CLA	O2D-CGD-O1D	-2.66	118.46	123.82
25	C	510	CLA	O2D-CGD-O1D	-2.66	118.46	123.82
24	4	606	CHL	OMC-CMC-C2C	-2.66	120.89	124.29
24	r	607	CHL	CBC-CAC-C3C	-2.66	108.91	112.95
37	c	519	DGD	CDB-CCB-CBB	-2.66	100.75	114.45
25	8	603	CLA	CAA-C2A-C3A	-2.66	105.52	112.81
24	7	609	CHL	OMC-CMC-C2C	-2.66	120.89	124.29
27	Y	1622	XAT	C31-C32-C33	-2.66	118.94	126.42
30	b	620	BCR	C33-C5-C6	-2.66	121.53	124.51
25	n	602	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
37	C	519	DGD	CDB-CCB-CBB	-2.66	100.75	114.45
35	B	622	LMG	O6-C1-O1	-2.66	103.71	110.02
26	R	620	LUT	C37-C21-C22	-2.66	104.35	109.42
30	A	411	BCR	C16-C15-C14	-2.66	117.79	123.46
25	B	613	CLA	O2D-CGD-O1D	-2.66	118.48	123.82
30	A	411	BCR	C38-C26-C25	-2.65	121.54	124.51
26	N	1621	LUT	C31-C30-C29	-2.65	123.52	127.31
26	n	1621	LUT	C31-C30-C29	-2.65	123.52	127.31
25	5	603	CLA	CBC-CAC-C3C	-2.65	104.88	112.41
27	R	622	XAT	C24-C23-C22	-2.65	105.28	110.68
25	1	603	CLA	CBC-CAC-C3C	-2.65	104.88	112.41
25	N	602	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
30	B	620	BCR	C33-C5-C6	-2.65	121.54	124.51
27	r	622	XAT	C24-C23-C22	-2.65	105.28	110.68
24	n	601	CHL	C1-C2-C3	-2.65	121.08	125.96
28	3	1623	NEX	C15-C35-C34	-2.65	117.81	123.46
25	g	610	CLA	O2D-CGD-O1D	-2.65	118.50	123.82
24	N	601	CHL	C1-C2-C3	-2.64	121.09	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	610	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
25	s	612	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
30	C	517	BCR	C21-C20-C19	-2.64	115.13	123.23
30	c	517	BCR	C21-C20-C19	-2.64	115.13	123.23
30	a	411	BCR	C16-C15-C14	-2.64	117.83	123.46
24	R	607	CHL	CBC-CAC-C3C	-2.64	108.94	112.95
26	7	1621	LUT	C30-C31-C32	-2.64	115.14	123.23
24	y	608	CHL	C1-C2-C3	-2.64	121.09	125.96
25	S	603	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
26	R	620	LUT	C38-C25-C24	-2.63	118.01	123.68
25	s	604	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
25	A	407	CLA	O2D-CGD-O1D	-2.63	118.52	123.82
25	B	605	CLA	O2D-CGD-O1D	-2.63	118.52	123.82
24	g	605	CHL	OMC-CMC-C2C	-2.63	120.93	124.29
37	c	518	DGD	O3E-C3E-C2E	-2.63	104.63	110.36
28	s	1623	NEX	C11-C12-C13	-2.63	119.03	126.42
25	s	603	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
25	S	604	CLA	C1B-CHB-C4A	-2.63	124.91	130.12
24	Y	609	CHL	CBA-CAA-C2A	-2.63	112.14	115.76
30	a	411	BCR	C38-C26-C25	-2.63	121.57	124.51
25	2	610	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
25	6	610	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
25	c	509	CLA	O2D-CGD-O1D	-2.63	118.54	123.82
24	n	607	CHL	C3B-CAB-CBB	-2.63	119.30	125.20
25	B	613	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
26	3	1621	LUT	C30-C31-C32	-2.62	115.18	123.23
30	4	623	BCR	C1-C6-C5	-2.62	118.90	122.59
25	S	612	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
35	b	622	LMG	C38-C37-C36	-2.62	100.94	114.45
35	B	622	LMG	C38-C37-C36	-2.62	100.94	114.45
37	C	518	DGD	O3E-C3E-C2E	-2.62	104.65	110.36
28	g	1623	NEX	C11-C12-C13	-2.62	119.05	126.42
28	7	1623	NEX	C15-C35-C34	-2.62	117.87	123.46
25	C	509	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
28	G	1623	NEX	C11-C12-C13	-2.62	119.06	126.42
25	b	605	CLA	O2D-CGD-O1D	-2.62	118.55	123.82
24	4	607	CHL	CHA-CBD-CGD	-2.62	108.93	115.00
24	G	605	CHL	OMC-CMC-C2C	-2.62	120.95	124.29
24	N	608	CHL	C1-C2-C3	-2.62	121.14	125.96
26	y	1621	LUT	C8-C9-C10	-2.62	114.93	118.94
24	N	607	CHL	C3B-CAB-CBB	-2.61	119.33	125.20
26	r	620	LUT	C38-C25-C24	-2.61	118.05	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	601	CHL	CBC-CAC-C3C	-2.61	108.98	112.95
26	1	1621	LUT	C8-C7-C6	-2.61	119.94	127.25
25	a	407	CLA	O2D-CGD-O1D	-2.61	118.56	123.82
24	8	607	CHL	CHA-CBD-CGD	-2.61	108.94	115.00
24	Y	608	CHL	C1-C2-C3	-2.61	121.15	125.96
26	n	1621	LUT	C30-C31-C32	-2.61	115.23	123.23
30	4	623	BCR	C7-C8-C9	-2.61	122.29	126.21
24	n	608	CHL	C1-C2-C3	-2.61	121.15	125.96
28	S	1623	NEX	C11-C12-C13	-2.61	119.09	126.42
26	5	1621	LUT	C8-C7-C6	-2.61	119.95	127.25
25	C	512	CLA	O2D-CGD-O1D	-2.61	118.57	123.82
30	8	623	BCR	C7-C8-C9	-2.61	122.30	126.21
26	N	1621	LUT	C30-C31-C32	-2.61	115.24	123.23
25	c	506	CLA	O2D-CGD-O1D	-2.61	118.58	123.82
25	D	402	CLA	O2D-CGD-O1D	-2.60	118.58	123.82
24	y	609	CHL	CBA-CAA-C2A	-2.60	112.17	115.76
29	c	522	LHG	C11-C10-C9	-2.60	101.05	114.45
25	C	506	CLA	O2D-CGD-O1D	-2.60	118.58	123.82
25	c	512	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
30	8	623	BCR	C1-C6-C5	-2.60	118.94	122.59
25	d	402	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
25	b	613	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
29	C	522	LHG	C11-C10-C9	-2.60	101.06	114.45
26	s	1620	LUT	C38-C25-C24	-2.60	118.09	123.68
24	8	601	CHL	CBC-CAC-C3C	-2.60	109.01	112.95
25	c	511	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
24	1	606	CHL	CBC-CAC-C3C	-2.59	109.01	112.95
27	2	1622	XAT	C6-C7-C8	-2.59	120.51	125.99
26	Y	1621	LUT	C8-C9-C10	-2.59	114.96	118.94
37	C	518	DGD	C3G-C2G-C1G	-2.59	106.01	111.86
28	R	623	NEX	C4-C3-C2	-2.59	105.40	110.68
26	4	620	LUT	C35-C15-C14	-2.59	117.94	123.46
25	3	603	CLA	CAA-C2A-C3A	-2.59	105.72	112.81
37	c	518	DGD	C3G-C2G-C1G	-2.59	106.02	111.86
27	6	1622	XAT	C6-C7-C8	-2.59	120.52	125.99
26	S	1620	LUT	C38-C25-C24	-2.59	118.11	123.68
28	r	623	NEX	C4-C3-C2	-2.59	105.41	110.68
25	1	612	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
25	5	612	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
29	g	2630	LHG	C20-C19-C18	-2.58	101.16	114.45
25	6	603	CLA	O2D-CGD-O1D	-2.58	118.63	123.82
25	5	602	CLA	O2D-CGD-O1D	-2.58	118.63	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	606	CHL	CBC-CAC-C3C	-2.58	109.03	112.95
24	4	609	CHL	CHA-CBD-CGD	-2.58	109.02	115.00
25	R	603	CLA	OBD-CAD-CBD	-2.58	122.05	125.94
26	g	1621	LUT	C31-C30-C29	-2.58	123.63	127.31
25	7	603	CLA	CAA-C2A-C3A	-2.58	105.74	112.81
24	8	609	CHL	CHA-CBD-CGD	-2.58	109.02	115.00
25	1	602	CLA	O2D-CGD-O1D	-2.58	118.64	123.82
26	8	620	LUT	C35-C15-C14	-2.58	117.96	123.46
25	8	610	CLA	O2D-CGD-O1D	-2.57	118.64	123.82
25	C	511	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
29	G	2630	LHG	C20-C19-C18	-2.57	101.21	114.45
25	4	604	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
26	G	1621	LUT	C31-C30-C29	-2.57	123.64	127.31
26	5	1621	LUT	C30-C31-C32	-2.57	115.35	123.23
25	6	602	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
25	6	612	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
35	B	622	LMG	C40-C39-C38	-2.57	101.23	114.45
26	y	1621	LUT	C28-C29-C30	-2.57	115.00	118.94
25	1	603	CLA	CAA-C2A-C3A	-2.57	105.78	112.81
26	1	1621	LUT	C30-C31-C32	-2.56	115.36	123.23
35	b	622	LMG	C40-C39-C38	-2.56	101.24	114.45
26	7	1621	LUT	C38-C25-C24	-2.56	118.16	123.68
35	d	411	LMG	C6-C5-C4	-2.56	107.00	113.00
29	l	101	LHG	C11-C10-C9	-2.56	101.25	114.45
25	B	607	CLA	O2D-CGD-O1D	-2.56	118.66	123.82
36	d	405	PL9	O1-C4-C3	-2.56	117.80	120.71
26	2	1620	LUT	C8-C7-C6	-2.56	120.08	127.25
26	4	620	LUT	C8-C7-C6	-2.56	120.08	127.25
27	4	622	XAT	C15-C35-C34	-2.56	118.00	123.46
35	D	411	LMG	C6-C5-C4	-2.56	107.01	113.00
25	5	603	CLA	CAA-C2A-C3A	-2.56	105.79	112.81
24	y	609	CHL	O1D-CGD-CBD	-2.56	119.25	124.53
25	2	603	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
24	1	608	CHL	CBC-CAC-C3C	-2.56	109.06	112.95
24	Y	609	CHL	O1D-CGD-CBD	-2.56	119.25	124.53
25	4	610	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
29	L	101	LHG	C11-C10-C9	-2.56	101.27	114.45
27	y	1622	XAT	C7-C8-C9	-2.56	121.56	125.53
27	Y	1622	XAT	C7-C8-C9	-2.56	121.56	125.53
25	2	602	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
26	Y	1621	LUT	C28-C29-C30	-2.56	115.02	118.94
26	6	1620	LUT	C8-C7-C6	-2.56	120.10	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	608	CHL	CBC-CAC-C3C	-2.56	109.07	112.95
24	3	609	CHL	O1D-CGD-CBD	-2.55	119.26	124.53
25	8	604	CLA	O2D-CGD-O1D	-2.55	118.68	123.82
26	8	620	LUT	C8-C7-C6	-2.55	120.11	127.25
25	r	603	CLA	OBD-CAD-CBD	-2.55	122.09	125.94
33	a	408	PHO	C2B-C1B-NB	-2.55	106.04	109.82
24	N	608	CHL	CBC-CAC-C3C	-2.55	109.08	112.95
30	b	618	BCR	C16-C15-C14	-2.55	118.02	123.46
24	5	608	CHL	CBC-CAC-C3C	-2.55	109.08	112.95
24	Y	601	CHL	C1-C2-C3	-2.55	121.26	125.96
24	5	601	CHL	C3B-CAB-CBB	-2.55	119.48	125.20
29	g	2630	LHG	C11-C10-C9	-2.55	101.32	114.45
25	B	604	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
26	3	1621	LUT	C38-C25-C24	-2.55	118.19	123.68
35	C	521	LMG	O6-C1-O1	-2.55	103.98	110.02
24	1	601	CHL	C3B-CAB-CBB	-2.55	119.48	125.20
25	2	612	CLA	O2D-CGD-O1D	-2.54	118.70	123.82
26	S	1620	LUT	C31-C30-C29	-2.54	123.68	127.31
35	c	521	LMG	O6-C1-O1	-2.54	103.98	110.02
25	N	613	CLA	O2D-CGD-O1D	-2.54	118.70	123.82
26	7	1620	LUT	C31-C30-C29	-2.54	123.68	127.31
25	b	607	CLA	O2D-CGD-O1D	-2.54	118.71	123.82
25	a	406	CLA	O2D-CGD-O1D	-2.54	118.71	123.82
29	C	2630	LHG	C11-C10-C9	-2.54	101.36	114.45
30	C	516	BCR	C11-C10-C9	-2.54	123.68	127.31
29	G	2630	LHG	C11-C10-C9	-2.54	101.37	114.45
33	A	408	PHO	C2B-C1B-NB	-2.54	106.06	109.82
29	d	410	LHG	C11-C10-C9	-2.54	101.37	114.45
26	3	1620	LUT	C31-C30-C29	-2.54	123.69	127.31
36	D	405	PL9	O1-C4-C3	-2.54	117.83	120.71
29	c	2630	LHG	C11-C10-C9	-2.54	101.38	114.45
29	D	410	LHG	C11-C10-C9	-2.54	101.38	114.45
25	b	604	CLA	O2D-CGD-O1D	-2.54	118.72	123.82
30	B	618	BCR	C16-C15-C14	-2.54	118.05	123.46
25	r	602	CLA	O2D-CGD-O1D	-2.54	118.72	123.82
24	y	601	CHL	C1-C2-C3	-2.54	121.29	125.96
25	C	502	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
26	s	1620	LUT	C16-C1-C6	-2.53	106.20	110.31
25	S	613	CLA	O2D-CGD-O1D	-2.53	118.72	123.82
25	n	610	CLA	O2D-CGD-O1D	-2.53	118.72	123.82
25	c	502	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
27	8	622	XAT	C15-C35-C34	-2.53	118.06	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	609	CHL	O1D-CGD-CBD	-2.53	119.31	124.53
24	2	608	CHL	C3B-CAB-CBB	-2.53	119.52	125.20
30	B	619	BCR	C28-C27-C26	-2.53	109.43	113.78
25	N	604	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
25	3	611	CLA	O2D-CGD-O1D	-2.53	118.74	123.82
30	C	517	BCR	C38-C26-C25	-2.52	121.68	124.51
25	A	406	CLA	O2D-CGD-O1D	-2.52	118.74	123.82
24	G	608	CHL	C1-C2-C3	-2.52	121.31	125.96
25	n	613	CLA	O2D-CGD-O1D	-2.52	118.74	123.82
24	6	608	CHL	C3B-CAB-CBB	-2.52	119.53	125.20
28	n	1623	NEX	C19-C9-C10	-2.52	119.39	122.92
26	s	1621	LUT	C38-C25-C24	-2.52	118.25	123.68
26	s	1620	LUT	C31-C30-C29	-2.52	123.71	127.31
25	R	602	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
28	y	1623	NEX	C35-C15-C14	-2.52	118.08	123.46
25	7	611	CLA	O2D-CGD-O1D	-2.52	118.75	123.82
26	S	1620	LUT	C16-C1-C6	-2.52	106.22	110.31
26	3	1620	LUT	C23-C24-C25	-2.52	122.86	125.22
26	7	1620	LUT	C38-C25-C24	-2.52	118.26	123.68
24	g	609	CHL	O2D-CGD-O1D	-2.52	118.75	123.82
24	g	608	CHL	C1-C2-C3	-2.52	121.32	125.96
28	y	1623	NEX	C31-C30-C29	-2.52	123.72	127.31
30	b	619	BCR	C28-C27-C26	-2.52	109.46	113.78
29	3	2630	LHG	C11-C10-C9	-2.51	101.50	114.45
25	y	602	CLA	CAA-CBA-CGA	-2.51	105.77	113.35
26	7	1620	LUT	C37-C21-C22	-2.51	104.62	109.42
35	Z	101	LMG	O8-C28-O10	-2.51	117.31	123.55
35	D	411	LMG	O1-C7-C8	-2.51	105.01	110.99
30	c	517	BCR	C38-C26-C25	-2.51	121.70	124.51
25	g	603	CLA	C3C-C4C-NC	-2.51	107.67	110.21
25	Y	602	CLA	O2D-CGD-O1D	-2.51	118.77	123.82
28	Y	1623	NEX	C35-C15-C14	-2.51	118.11	123.46
25	Y	602	CLA	CAA-CBA-CGA	-2.51	105.79	113.35
25	N	610	CLA	O2D-CGD-O1D	-2.51	118.77	123.82
25	n	604	CLA	O2D-CGD-O1D	-2.51	118.77	123.82
29	7	2630	LHG	C11-C10-C9	-2.51	101.53	114.45
25	s	613	CLA	O2D-CGD-O1D	-2.51	118.77	123.82
28	Y	1623	NEX	C31-C30-C29	-2.51	123.73	127.31
26	7	1620	LUT	C23-C24-C25	-2.51	122.87	125.22
26	G	1621	LUT	C22-C23-C24	-2.51	108.89	111.73
24	G	609	CHL	O2D-CGD-O1D	-2.51	118.78	123.82
26	S	1621	LUT	C38-C25-C24	-2.51	118.29	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	603	CLA	O2D-CGD-O1D	-2.50	118.78	123.82
26	3	1620	LUT	C37-C21-C22	-2.50	104.64	109.42
34	b	623	SQD	O6-C44-C45	-2.50	105.03	110.99
26	3	1620	LUT	C38-C25-C24	-2.50	118.29	123.68
25	G	603	CLA	C3C-C4C-NC	-2.50	107.68	110.21
35	d	411	LMG	O1-C7-C8	-2.50	105.04	110.99
29	D	409	LHG	C20-C19-C18	-2.50	101.57	114.45
26	Y	1620	LUT	C8-C9-C10	-2.50	115.11	118.94
25	6	602	CLA	OBD-CAD-CBD	-2.50	122.17	125.94
28	s	1623	NEX	C15-C35-C34	-2.50	118.13	123.46
29	c	2630	LHG	C20-C19-C18	-2.50	101.58	114.45
29	C	2630	LHG	C20-C19-C18	-2.50	101.58	114.45
35	z	101	LMG	O8-C28-O10	-2.50	117.35	123.55
28	3	1623	NEX	C24-C23-C22	-2.50	105.59	110.68
27	1	1622	XAT	C5-C4-C3	-2.50	107.85	112.64
24	y	609	CHL	O2D-CGD-O1D	-2.50	118.80	123.82
29	d	409	LHG	C20-C19-C18	-2.49	101.60	114.45
25	r	610	CLA	O2A-CGA-O1A	-2.49	117.36	123.55
24	Y	609	CHL	O2D-CGD-O1D	-2.49	118.80	123.82
28	N	1623	NEX	C19-C9-C10	-2.49	119.43	122.92
26	g	1621	LUT	C22-C23-C24	-2.49	108.91	111.73
24	3	601	CHL	O1D-CGD-CBD	-2.49	119.39	124.53
25	y	602	CLA	O2D-CGD-O1D	-2.49	118.81	123.82
28	7	1623	NEX	C24-C23-C22	-2.49	105.61	110.68
24	7	601	CHL	O1D-CGD-CBD	-2.49	119.39	124.53
25	R	610	CLA	O2A-CGA-O1A	-2.49	117.37	123.55
24	2	605	CHL	O1D-CGD-CBD	-2.49	119.39	124.53
35	D	411	LMG	O3-C3-C2	-2.49	104.95	110.36
25	r	602	CLA	CAA-CBA-CGA	-2.49	105.86	113.35
25	4	611	CLA	O2D-CGD-O1D	-2.49	118.82	123.82
25	Y	603	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
29	D	409	LHG	O8-C6-C5	-2.48	102.41	108.66
24	2	607	CHL	C4A-C3A-C2A	-2.48	100.06	103.86
35	d	411	LMG	O3-C3-C2	-2.48	104.95	110.36
28	S	1623	NEX	C15-C35-C34	-2.48	118.16	123.46
27	n	1622	XAT	C39-C29-C30	-2.48	119.44	122.92
26	y	1620	LUT	C8-C9-C10	-2.48	115.13	118.94
29	d	409	LHG	O8-C6-C5	-2.48	102.42	108.66
28	Y	1623	NEX	C30-C31-C32	-2.48	115.61	123.23
24	6	607	CHL	C4A-C3A-C2A	-2.48	100.06	103.86
34	B	623	SQD	O6-C44-C45	-2.48	105.08	110.99
24	r	606	CHL	CHA-CBD-CGD	-2.48	109.24	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	516	BCR	C11-C10-C9	-2.48	123.77	127.31
30	b	619	BCR	C21-C20-C19	-2.48	115.62	123.23
35	c	521	LMG	C1-C2-C3	-2.48	105.37	109.98
27	N	1622	XAT	C39-C29-C30	-2.48	119.45	122.92
29	d	409	LHG	C18-C17-C16	-2.48	101.68	114.45
29	D	409	LHG	C18-C17-C16	-2.48	101.68	114.45
25	3	604	CLA	O2D-CGD-O1D	-2.48	118.83	123.82
26	Y	1621	LUT	C15-C35-C34	-2.48	118.17	123.46
27	R	622	XAT	C8-C9-C10	-2.48	115.14	118.94
25	2	602	CLA	OBD-CAD-CBD	-2.48	122.20	125.94
25	R	602	CLA	CAA-CBA-CGA	-2.48	105.88	113.35
25	S	604	CLA	C1-C2-C3	-2.48	122.77	126.68
27	5	1622	XAT	C5-C4-C3	-2.48	107.89	112.64
35	a	413	LMG	C40-C39-C38	-2.48	101.70	114.45
25	R	612	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
35	C	521	LMG	C1-C2-C3	-2.48	105.38	109.98
30	B	619	BCR	C21-C20-C19	-2.48	115.64	123.23
27	r	622	XAT	C8-C9-C10	-2.48	115.14	118.94
24	6	605	CHL	O1D-CGD-CBD	-2.48	119.42	124.53
28	y	1623	NEX	C30-C31-C32	-2.48	115.64	123.23
28	g	1623	NEX	O4-C5-C18	-2.47	105.18	109.51
24	y	601	CHL	CBA-CAA-C2A	-2.47	112.35	115.76
30	h	101	BCR	C3-C4-C5	-2.47	109.53	113.78
25	s	604	CLA	C1-C2-C3	-2.47	122.77	126.68
25	g	602	CLA	C6-C7-C8	-2.47	107.62	115.73
26	6	1621	LUT	C8-C7-C6	-2.47	120.33	127.25
35	A	413	LMG	C40-C39-C38	-2.47	101.72	114.45
24	R	606	CHL	CHA-CBD-CGD	-2.47	109.27	115.00
25	r	612	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
26	r	620	LUT	C12-C13-C14	-2.47	115.15	118.94
25	7	604	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
26	1	1621	LUT	O3-C3-C2	-2.47	104.85	109.86
27	G	1622	XAT	C5-C4-C3	-2.47	107.91	112.64
25	8	611	CLA	O2D-CGD-O1D	-2.47	118.86	123.82
25	R	611	CLA	O2A-CGA-O1A	-2.47	117.42	123.55
24	n	605	CHL	CBC-CAC-C3C	-2.47	109.21	112.95
27	R	622	XAT	C4-C3-C2	-2.47	105.66	110.68
26	R	620	LUT	C12-C13-C14	-2.46	115.16	118.94
28	G	1623	NEX	O4-C5-C18	-2.46	105.19	109.51
37	C	519	DGD	C3G-C2G-C1G	-2.46	106.30	111.86
27	g	1622	XAT	C5-C4-C3	-2.46	107.91	112.64
36	D	405	PL9	C22-C23-C24	-2.46	121.49	127.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	2630	LHG	C11-C10-C9	-2.46	101.77	114.45
30	B	619	BCR	C10-C11-C12	-2.46	115.68	123.23
33	a	408	PHO	O2A-CGA-O1A	-2.46	117.44	123.55
30	H	101	BCR	C3-C4-C5	-2.46	109.55	113.78
35	B	622	LMG	O2-C2-C1	-2.46	104.89	110.03
24	Y	601	CHL	CBA-CAA-C2A	-2.46	112.37	115.76
24	y	609	CHL	CHA-CBD-CGD	-2.46	109.30	115.00
29	R	2630	LHG	C11-C10-C9	-2.46	101.79	114.45
26	2	1621	LUT	C8-C7-C6	-2.46	120.37	127.25
26	y	1621	LUT	C15-C35-C34	-2.46	118.22	123.46
25	G	602	CLA	C6-C7-C8	-2.46	107.66	115.73
35	A	415	LMG	O2-C2-C1	-2.46	104.89	110.03
35	b	622	LMG	O2-C2-C1	-2.46	104.89	110.03
27	2	1622	XAT	C10-C11-C12	-2.46	115.69	123.23
26	5	1621	LUT	O3-C3-C2	-2.46	104.87	109.86
30	b	619	BCR	C10-C11-C12	-2.46	115.70	123.23
26	Y	1620	LUT	C15-C35-C34	-2.45	118.22	123.46
27	6	1622	XAT	C10-C11-C12	-2.45	115.70	123.23
30	C	517	BCR	C11-C12-C13	-2.45	119.52	126.42
25	r	611	CLA	O2A-CGA-O1A	-2.45	117.46	123.55
25	G	612	CLA	O2D-CGD-O1D	-2.45	118.88	123.82
30	B	620	BCR	C16-C15-C14	-2.45	118.23	123.46
25	R	609	CLA	OBD-CAD-CBD	-2.45	122.24	125.94
24	l	601	CHL	CBC-CAC-C3C	-2.45	109.23	112.95
25	g	612	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
29	D	408	LHG	O8-C23-O10	-2.45	117.46	123.55
30	b	620	BCR	C16-C15-C14	-2.45	118.23	123.46
25	4	603	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
25	b	614	CLA	CAA-C2A-C3A	-2.45	106.09	112.81
37	c	519	DGD	C3G-C2G-C1G	-2.45	106.33	111.86
36	d	405	PL9	C22-C23-C24	-2.45	121.53	127.68
24	N	605	CHL	CBC-CAC-C3C	-2.45	109.24	112.95
24	Y	609	CHL	CHA-CBD-CGD	-2.45	109.33	115.00
27	r	622	XAT	C4-C3-C2	-2.45	105.70	110.68
24	l	609	CHL	O1D-CGD-CBD	-2.45	119.48	124.53
36	D	405	PL9	C50-C49-C48	-2.45	115.27	122.65
24	5	608	CHL	CHA-CBD-CGD	-2.45	109.33	115.00
25	B	614	CLA	CAA-C2A-C3A	-2.44	106.11	112.81
25	y	603	CLA	CAA-C2A-C3A	-2.44	106.11	112.81
33	A	408	PHO	O2A-CGA-O1A	-2.44	117.48	123.55
26	y	1620	LUT	C15-C35-C34	-2.44	118.25	123.46
25	Y	603	CLA	CAA-C2A-C3A	-2.44	106.11	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	1621	LUT	C8-C9-C10	-2.44	115.19	118.94
35	a	415	LMG	O2-C2-C1	-2.44	104.92	110.03
29	d	408	LHG	O8-C23-O10	-2.44	117.49	123.55
30	c	517	BCR	C11-C12-C13	-2.44	119.56	126.42
25	B	613	CLA	CAA-CBA-CGA	-2.44	105.99	113.35
24	S	601	CHL	C4A-C3A-C2A	-2.44	100.13	103.86
36	d	405	PL9	C50-C49-C48	-2.44	115.28	122.65
25	4	612	CLA	O2D-CGD-O1D	-2.44	118.91	123.82
24	6	605	CHL	CHA-CBD-CGD	-2.44	109.34	115.00
27	6	1622	XAT	C39-C29-C30	-2.44	119.51	122.92
35	b	2633	LMG	C40-C39-C38	-2.44	101.89	114.45
25	r	609	CLA	OBD-CAD-CBD	-2.44	122.26	125.94
27	3	1622	XAT	C39-C29-C30	-2.44	119.51	122.92
25	1	604	CLA	OBD-CAD-CBD	-2.44	122.26	125.94
24	5	609	CHL	O1D-CGD-CBD	-2.44	119.50	124.53
35	B	2633	LMG	C40-C39-C38	-2.44	101.90	114.45
28	3	1623	NEX	C20-C13-C14	-2.44	119.51	122.92
24	N	606	CHL	CBC-CAC-C3C	-2.44	109.25	112.95
24	5	601	CHL	CBC-CAC-C3C	-2.44	109.25	112.95
25	8	603	CLA	O2D-CGD-O1D	-2.44	118.92	123.82
25	b	613	CLA	CAA-CBA-CGA	-2.44	106.01	113.35
28	1	1623	NEX	C19-C9-C10	-2.43	119.51	122.92
25	S	612	CLA	O2D-CGD-O1D	-2.43	118.92	123.82
24	2	605	CHL	CHA-CBD-CGD	-2.43	109.36	115.00
27	7	1622	XAT	C25-C24-C23	-2.43	107.97	112.64
24	s	601	CHL	C4A-C3A-C2A	-2.43	100.14	103.86
26	r	620	LUT	C35-C15-C14	-2.43	118.27	123.46
29	N	2630	LHG	C20-C19-C18	-2.43	101.92	114.45
24	n	606	CHL	CBC-CAC-C3C	-2.43	109.26	112.95
30	b	620	BCR	C10-C11-C12	-2.43	115.77	123.23
29	n	2630	LHG	C20-C19-C18	-2.43	101.93	114.45
27	3	1622	XAT	C25-C24-C23	-2.43	107.98	112.64
26	R	620	LUT	C35-C15-C14	-2.43	118.28	123.46
30	8	623	BCR	C27-C26-C25	-2.43	119.17	122.74
24	1	608	CHL	CHA-CBD-CGD	-2.43	109.37	115.00
26	N	1621	LUT	C8-C9-C10	-2.43	115.22	118.94
25	R	612	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
26	Y	1621	LUT	C16-C1-C6	-2.43	106.37	110.31
25	B	610	CLA	C7-C6-C5	-2.43	106.37	113.11
28	5	1623	NEX	C19-C9-C10	-2.43	119.53	122.92
35	b	622	LMG	O1-C7-C8	-2.43	105.22	110.99
25	Y	602	CLA	OBD-CAD-CBD	-2.43	122.28	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	604	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
26	S	1620	LUT	C7-C8-C9	-2.42	122.57	126.21
29	1	2630	LHG	C18-C17-C16	-2.42	101.96	114.45
25	s	604	CLA	O2D-CGD-O1D	-2.42	118.94	123.82
25	n	602	CLA	CAA-CBA-CGA	-2.42	106.05	113.35
25	d	402	CLA	CAA-CBA-CGA	-2.42	106.05	113.35
29	5	2630	LHG	C18-C17-C16	-2.42	101.97	114.45
27	7	1622	XAT	C39-C29-C30	-2.42	119.53	122.92
25	N	612	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
27	2	1622	XAT	C39-C29-C30	-2.42	119.53	122.92
25	N	602	CLA	CAA-CBA-CGA	-2.42	106.05	113.35
25	N	611	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
28	7	1623	NEX	C20-C13-C14	-2.42	119.53	122.92
26	g	1620	LUT	C28-C29-C30	-2.42	115.23	118.94
24	3	609	CHL	O2D-CGD-O1D	-2.42	118.95	123.82
33	A	409	PHO	O2D-CGD-O1D	-2.42	118.95	123.82
24	7	609	CHL	O2D-CGD-O1D	-2.42	118.95	123.82
25	s	612	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
25	n	612	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
25	D	402	CLA	CAA-CBA-CGA	-2.42	106.07	113.35
30	B	620	BCR	C10-C11-C12	-2.42	115.82	123.23
25	N	610	CLA	O2A-CGA-O1A	-2.42	117.55	123.55
25	5	604	CLA	OBD-CAD-CBD	-2.42	122.29	125.94
26	2	1621	LUT	C31-C30-C29	-2.42	123.86	127.31
35	B	622	LMG	O1-C7-C8	-2.42	105.24	110.99
27	5	1622	XAT	C31-C32-C33	-2.41	119.63	126.42
25	n	610	CLA	O2A-CGA-O1A	-2.41	117.56	123.55
25	b	610	CLA	C7-C6-C5	-2.41	106.40	113.11
25	y	602	CLA	OBD-CAD-CBD	-2.41	122.30	125.94
27	1	1622	XAT	C31-C32-C33	-2.41	119.64	126.42
25	r	612	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
24	R	614	CHL	C3B-CAB-CBB	-2.41	119.78	125.20
25	1	604	CLA	C1-C2-C3	-2.41	122.87	126.68
25	G	604	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
25	8	612	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
25	S	604	CLA	O2D-CGD-O1D	-2.41	118.98	123.82
25	y	604	CLA	C1-C2-C3	-2.41	122.88	126.68
26	y	1621	LUT	C16-C1-C6	-2.40	106.41	110.31
26	G	1620	LUT	C28-C29-C30	-2.40	115.25	118.94
26	8	620	LUT	C1-C6-C5	-2.40	119.21	122.59
26	s	1620	LUT	C7-C8-C9	-2.40	122.60	126.21
25	r	609	CLA	O2D-CGD-O1D	-2.40	118.99	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	614	CHL	C3B-CAB-CBB	-2.40	119.81	125.20
29	L	101	LHG	C20-C19-C18	-2.40	102.08	114.45
25	C	509	CLA	CAA-C2A-C3A	-2.40	106.23	112.81
25	c	509	CLA	CAA-C2A-C3A	-2.40	106.23	112.81
29	y	2630	LHG	C20-C19-C18	-2.40	102.09	114.45
25	n	611	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
35	A	415	LMG	O3-C3-C2	-2.40	105.14	110.36
30	4	623	BCR	C27-C26-C25	-2.40	119.22	122.74
29	Y	2630	LHG	C20-C19-C18	-2.40	102.09	114.45
25	1	613	CLA	O2D-CGD-O1D	-2.40	119.00	123.82
26	4	620	LUT	C1-C6-C5	-2.40	119.22	122.59
33	a	409	PHO	O2D-CGD-O1D	-2.39	119.00	123.82
26	n	1621	LUT	C16-C1-C6	-2.39	106.43	110.31
24	3	606	CHL	O1D-CGD-CBD	-2.39	119.59	124.53
25	5	613	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
29	l	101	LHG	C20-C19-C18	-2.39	102.13	114.45
36	d	405	PL9	C46-C47-C48	-2.39	103.76	111.97
24	7	606	CHL	O2D-CGD-O1D	-2.39	119.01	123.82
26	Y	1620	LUT	C8-C7-C6	-2.39	120.56	127.25
24	3	606	CHL	O2D-CGD-O1D	-2.39	119.01	123.82
24	4	608	CHL	C4A-C3A-C2A	-2.39	100.21	103.86
25	R	609	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
24	8	608	CHL	C4A-C3A-C2A	-2.39	100.21	103.86
25	5	604	CLA	C1-C2-C3	-2.39	122.91	126.68
28	Y	1623	NEX	O4-C5-C18	-2.39	105.33	109.51
25	B	612	CLA	OBD-CAD-CBD	-2.39	122.33	125.94
26	6	1621	LUT	C31-C30-C29	-2.39	123.90	127.31
25	y	610	CLA	O2A-CGA-O1A	-2.39	117.62	123.55
24	5	605	CHL	C3B-CAB-CBB	-2.39	119.84	125.20
24	r	607	CHL	O1D-CGD-CBD	-2.39	119.60	124.53
29	n	2630	LHG	C27-C26-C25	-2.39	102.16	114.45
24	7	606	CHL	O1D-CGD-CBD	-2.39	119.61	124.53
25	1	611	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
36	D	405	PL9	C46-C47-C48	-2.39	103.78	111.97
25	R	616	CLA	O2D-CGD-O1D	-2.38	119.02	123.82
26	N	1621	LUT	C16-C1-C6	-2.38	106.44	110.31
30	t	101	BCR	C39-C30-C25	-2.38	106.44	110.31
24	1	605	CHL	C3B-CAB-CBB	-2.38	119.85	125.20
35	a	415	LMG	O3-C3-C2	-2.38	105.17	110.36
26	n	1620	LUT	C28-C29-C30	-2.38	115.28	118.94
29	B	2631	LHG	C11-C10-C9	-2.38	102.18	114.45
29	N	2630	LHG	C27-C26-C25	-2.38	102.18	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	610	CLA	O2A-CGA-O1A	-2.38	117.64	123.55
26	y	1620	LUT	C8-C7-C6	-2.38	120.58	127.25
25	Y	604	CLA	C1-C2-C3	-2.38	122.92	126.68
29	n	2630	LHG	C18-C17-C16	-2.38	102.19	114.45
29	N	2630	LHG	C18-C17-C16	-2.38	102.20	114.45
25	R	616	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	r	616	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
25	g	604	CLA	C1-C2-C3	-2.38	122.92	126.68
36	D	405	PL9	C27-C28-C29	-2.38	121.71	127.68
26	y	1620	LUT	C37-C21-C22	-2.38	104.88	109.42
26	6	1621	LUT	C7-C8-C9	-2.37	122.64	126.21
27	7	1622	XAT	C32-C33-C34	-2.37	115.30	118.94
37	c	520	DGD	O2D-C2D-C1D	-2.37	105.06	110.03
29	5	2630	LHG	C20-C19-C18	-2.37	102.22	114.45
25	G	604	CLA	C1-C2-C3	-2.37	122.93	126.68
36	d	405	PL9	C27-C28-C29	-2.37	121.72	127.68
25	n	603	CLA	C3C-C4C-NC	-2.37	107.81	110.21
25	r	616	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
25	7	603	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
26	Y	1620	LUT	C37-C21-C22	-2.37	104.89	109.42
25	5	611	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
25	b	612	CLA	OBD-CAD-CBD	-2.37	122.36	125.94
30	c	516	BCR	C15-C14-C13	-2.37	123.93	127.31
29	b	2631	LHG	C11-C10-C9	-2.37	102.24	114.45
29	s	2630	LHG	C11-C10-C9	-2.37	102.24	114.45
29	S	2630	LHG	C11-C10-C9	-2.37	102.24	114.45
25	b	611	CLA	O2D-CGD-O1D	-2.37	119.05	123.82
25	2	602	CLA	CAA-CBA-CGA	-2.37	106.21	113.35
30	T	101	BCR	C39-C30-C25	-2.37	106.47	110.31
24	4	609	CHL	C4A-C3A-C2A	-2.37	100.24	103.86
29	1	2630	LHG	C20-C19-C18	-2.37	102.25	114.45
28	y	1623	NEX	O4-C5-C18	-2.37	105.36	109.51
25	y	611	CLA	CAA-CBA-CGA	-2.37	106.22	113.35
26	5	1621	LUT	C8-C9-C10	-2.37	115.31	118.94
24	4	609	CHL	O1D-CGD-CBD	-2.37	119.65	124.53
26	1	1621	LUT	C8-C9-C10	-2.37	115.31	118.94
25	n	602	CLA	O2D-CGD-O1D	-2.37	119.06	123.82
26	2	1621	LUT	C35-C15-C14	-2.36	118.41	123.46
24	8	609	CHL	C4A-C3A-C2A	-2.36	100.24	103.86
24	R	607	CHL	O1D-CGD-CBD	-2.36	119.65	124.53
24	1	606	CHL	O1D-CGD-CBD	-2.36	119.65	124.53
37	h	102	DGD	O6D-C1D-O3G	-2.36	104.41	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	605	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
25	B	605	CLA	C1-O2A-CGA	-2.36	111.10	116.77
25	N	602	CLA	O2D-CGD-O1D	-2.36	119.07	123.82
25	3	603	CLA	O2D-CGD-O1D	-2.36	119.07	123.82
28	n	1623	NEX	C11-C12-C13	-2.36	119.78	126.42
25	b	605	CLA	C1-O2A-CGA	-2.36	111.11	116.77
28	N	1623	NEX	C11-C12-C13	-2.36	119.78	126.42
26	N	1620	LUT	C28-C29-C30	-2.36	115.32	118.94
26	S	1621	LUT	C8-C9-C10	-2.36	115.32	118.94
24	5	605	CHL	CHA-CBD-CGD	-2.36	109.53	115.00
29	c	2630	LHG	C18-C17-C16	-2.36	102.30	114.45
29	C	2630	LHG	C18-C17-C16	-2.36	102.30	114.45
26	6	1621	LUT	C35-C15-C14	-2.36	118.43	123.46
24	N	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.53
25	1	604	CLA	O2A-CGA-O1A	-2.36	117.70	123.55
24	8	609	CHL	O1D-CGD-CBD	-2.36	119.66	124.53
25	5	604	CLA	O2A-CGA-O1A	-2.36	117.70	123.55
25	S	604	CLA	OBD-CAD-CBD	-2.36	122.38	125.94
24	n	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.53
25	B	606	CLA	C1-C2-C3	-2.36	121.61	125.96
25	b	605	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
25	6	602	CLA	CAA-CBA-CGA	-2.36	106.25	113.35
25	N	603	CLA	C3C-C4C-NC	-2.36	107.83	110.21
29	G	2630	LHG	O8-C6-C5	-2.35	102.74	108.66
37	B	626	DGD	C1D-C2D-C3D	-2.35	105.60	109.98
37	C	520	DGD	O2D-C2D-C1D	-2.35	105.10	110.03
30	C	516	BCR	C15-C14-C13	-2.35	123.95	127.31
26	5	1621	LUT	C7-C8-C9	-2.35	122.68	126.21
25	b	605	CLA	O2A-CGA-O1A	-2.35	117.71	123.55
26	6	1620	LUT	C35-C15-C14	-2.35	118.44	123.46
24	1	605	CHL	CHA-CBD-CGD	-2.35	109.54	115.00
25	Y	611	CLA	CAA-CBA-CGA	-2.35	106.26	113.35
27	3	1622	XAT	C32-C33-C34	-2.35	115.33	118.94
25	R	601	CLA	CAA-C2A-C3A	-2.35	106.36	112.81
24	5	606	CHL	O1D-CGD-CBD	-2.35	119.68	124.53
25	N	603	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
26	2	1621	LUT	C7-C8-C9	-2.35	122.68	126.21
26	s	1621	LUT	C8-C9-C10	-2.35	115.34	118.94
25	B	611	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
26	1	1621	LUT	C7-C8-C9	-2.35	122.69	126.21
25	1	610	CLA	O2D-CGD-O1D	-2.35	119.10	123.82
37	b	626	DGD	C1D-C2D-C3D	-2.35	105.62	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	617	CLA	O2D-CGD-O1D	-2.35	119.10	123.82
37	H	102	DGD	O6D-C1D-O3G	-2.35	104.45	110.02
28	n	1623	NEX	C30-C31-C32	-2.35	116.04	123.23
25	b	606	CLA	C1-C2-C3	-2.34	121.64	125.96
26	N	1621	LUT	C15-C35-C34	-2.34	118.46	123.46
25	Y	610	CLA	O2D-CGD-O1D	-2.34	119.10	123.82
29	6	2630	LHG	C11-C10-C9	-2.34	102.38	114.45
26	Y	1620	LUT	C28-C29-C30	-2.34	115.35	118.94
25	r	601	CLA	CAA-C2A-C3A	-2.34	106.39	112.81
28	N	1623	NEX	C30-C31-C32	-2.34	116.05	123.23
25	N	610	CLA	OBD-CAD-CBD	-2.34	122.41	125.94
26	2	1620	LUT	C35-C15-C14	-2.34	118.47	123.46
25	R	603	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
25	N	602	CLA	OBD-CAD-CBD	-2.34	122.41	125.94
26	7	1620	LUT	C18-C5-C6	-2.34	121.89	124.51
25	n	603	CLA	O2D-CGD-O1D	-2.34	119.12	123.82
29	g	2630	LHG	O8-C6-C5	-2.34	102.78	108.66
25	B	605	CLA	O2A-CGA-O1A	-2.34	117.75	123.55
25	7	610	CLA	O2D-CGD-O1D	-2.34	119.12	123.82
26	S	1621	LUT	C7-C8-C9	-2.34	122.70	126.21
37	C	520	DGD	C3D-C4D-C5D	-2.34	106.10	110.22
25	B	617	CLA	O2D-CGD-O1D	-2.34	119.12	123.82
26	n	1621	LUT	C15-C35-C34	-2.33	118.48	123.46
29	2	2630	LHG	C11-C10-C9	-2.33	102.43	114.45
25	S	612	CLA	CAA-C2A-C3A	-2.33	106.41	112.81
24	S	601	CHL	CBC-CAC-C3C	-2.33	109.41	112.95
25	n	610	CLA	OBD-CAD-CBD	-2.33	122.42	125.94
25	y	610	CLA	O2D-CGD-O1D	-2.33	119.13	123.82
29	c	523	LHG	C20-C19-C18	-2.33	102.45	114.45
25	N	602	CLA	C1-C2-C3	-2.33	121.67	125.96
26	3	1621	LUT	C15-C35-C34	-2.33	118.49	123.46
25	5	610	CLA	O2D-CGD-O1D	-2.33	119.13	123.82
37	c	520	DGD	C3D-C4D-C5D	-2.33	106.12	110.22
25	B	610	CLA	C1-C2-C3	-2.33	121.67	125.96
25	g	614	CLA	O2D-CGD-O1D	-2.33	119.14	123.82
29	C	523	LHG	C20-C19-C18	-2.32	102.48	114.45
35	B	2633	LMG	C6-C5-C4	-2.32	107.56	113.00
29	d	408	LHG	C27-C26-C25	-2.32	102.48	114.45
25	n	602	CLA	C1-C2-C3	-2.32	121.67	125.96
35	b	2633	LMG	C6-C5-C4	-2.32	107.56	113.00
26	3	1621	LUT	C18-C5-C6	-2.32	121.91	124.51
25	b	610	CLA	C1-C2-C3	-2.32	121.68	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	604	CLA	OBD-CAD-CBD	-2.32	122.43	125.94
25	s	612	CLA	CAA-C2A-C3A	-2.32	106.44	112.81
25	r	603	CLA	O2D-CGD-O1D	-2.32	119.15	123.82
26	7	1621	LUT	C18-C5-C6	-2.32	121.91	124.51
26	G	1621	LUT	C18-C5-C6	-2.32	121.91	124.51
25	A	407	CLA	C1-C2-C3	-2.32	123.01	126.68
26	7	1621	LUT	C15-C35-C34	-2.32	118.51	123.46
26	s	1621	LUT	C7-C8-C9	-2.32	122.73	126.21
25	1	610	CLA	O2A-CGA-O1A	-2.32	117.79	123.55
29	D	408	LHG	C27-C26-C25	-2.32	102.50	114.45
26	3	1620	LUT	C18-C5-C6	-2.32	121.91	124.51
30	C	515	BCR	C23-C24-C25	-2.32	120.76	127.25
24	6	605	CHL	C3B-CAB-CBB	-2.32	119.99	125.20
27	n	1622	XAT	C26-C27-C28	-2.32	121.09	125.99
25	a	407	CLA	C1-C2-C3	-2.31	123.02	126.68
24	s	601	CHL	CBC-CAC-C3C	-2.31	109.44	112.95
25	G	614	CLA	O2D-CGD-O1D	-2.31	119.16	123.82
26	y	1620	LUT	C28-C29-C30	-2.31	115.39	118.94
25	n	602	CLA	OBD-CAD-CBD	-2.31	122.45	125.94
25	3	610	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
35	c	521	LMG	C40-C39-C38	-2.31	102.57	114.45
35	C	521	LMG	C40-C39-C38	-2.31	102.57	114.45
25	N	604	CLA	OBD-CAD-CBD	-2.31	122.46	125.94
27	3	1622	XAT	C26-C27-C28	-2.30	121.12	125.99
27	N	1622	XAT	C26-C27-C28	-2.30	121.12	125.99
24	2	605	CHL	C3B-CAB-CBB	-2.30	120.03	125.20
26	y	1620	LUT	C16-C1-C6	-2.30	106.57	110.31
29	R	2630	LHG	C20-C19-C18	-2.30	102.59	114.45
30	c	515	BCR	C23-C24-C25	-2.30	120.80	127.25
25	5	610	CLA	O2A-CGA-O1A	-2.30	117.83	123.55
24	3	609	CHL	CBA-CAA-C2A	-2.30	112.58	115.76
36	D	405	PL9	C41-C39-C38	-2.30	116.39	121.10
24	n	606	CHL	C3B-CAB-CBB	-2.30	120.03	125.20
29	1	2630	LHG	C11-C10-C9	-2.30	102.60	114.45
25	2	602	CLA	C1-C2-C3	-2.30	121.72	125.96
28	s	1623	NEX	C26-C27-C28	-2.30	121.13	125.99
25	6	602	CLA	C1-C2-C3	-2.30	121.72	125.96
36	d	405	PL9	C41-C39-C38	-2.30	116.40	121.10
26	R	620	LUT	C7-C8-C9	-2.30	122.76	126.21
28	S	1623	NEX	C26-C27-C28	-2.30	121.14	125.99
30	t	101	BCR	C11-C12-C13	-2.30	119.96	126.42
35	A	415	LMG	C40-C39-C38	-2.30	102.62	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	2630	LHG	C20-C19-C18	-2.30	102.63	114.45
29	5	2630	LHG	C11-C10-C9	-2.30	102.63	114.45
27	7	1622	XAT	C26-C27-C28	-2.29	121.14	125.99
30	T	101	BCR	C11-C12-C13	-2.29	119.97	126.42
24	N	606	CHL	C3B-CAB-CBB	-2.29	120.05	125.20
35	b	2633	LMG	C38-C37-C36	-2.29	102.65	114.45
35	a	415	LMG	C40-C39-C38	-2.29	102.65	114.45
26	g	1621	LUT	C18-C5-C6	-2.29	121.94	124.51
35	B	2633	LMG	C38-C37-C36	-2.29	102.65	114.45
37	c	519	DGD	O2D-C2D-C1D	-2.29	105.24	110.03
24	N	608	CHL	C4A-C3A-C2A	-2.29	100.36	103.86
29	C	523	LHG	C11-C10-C9	-2.29	102.67	114.45
24	7	609	CHL	CBA-CAA-C2A	-2.29	112.61	115.76
29	c	523	LHG	C11-C10-C9	-2.29	102.67	114.45
26	Y	1621	LUT	C38-C25-C24	-2.28	118.76	123.68
24	G	607	CHL	CBA-CAA-C2A	-2.28	112.61	115.76
25	n	604	CLA	OBD-CAD-CBD	-2.28	122.49	125.94
26	Y	1620	LUT	C16-C1-C6	-2.28	106.61	110.31
35	c	521	LMG	O1-C7-C8	-2.28	105.56	110.99
24	5	601	CHL	O1D-CGD-CBD	-2.28	119.82	124.53
26	r	620	LUT	C7-C8-C9	-2.28	122.78	126.21
24	n	608	CHL	C4A-C3A-C2A	-2.28	100.37	103.86
30	c	515	BCR	C8-C7-C6	-2.28	120.87	127.25
26	2	1621	LUT	C38-C25-C24	-2.28	118.77	123.68
35	z	101	LMG	O2-C2-C1	-2.28	105.26	110.03
35	Z	101	LMG	O2-C2-C1	-2.28	105.26	110.03
35	C	521	LMG	O1-C7-C8	-2.28	105.57	110.99
25	N	611	CLA	O2A-CGA-O1A	-2.28	117.90	123.55
30	C	516	BCR	C8-C7-C6	-2.28	120.88	127.25
35	A	413	LMG	C38-C37-C36	-2.28	102.73	114.45
25	n	611	CLA	O2A-CGA-O1A	-2.28	117.90	123.55
29	b	2631	LHG	C27-C26-C25	-2.28	102.73	114.45
27	5	1622	XAT	C39-C29-C30	-2.28	119.73	122.92
35	a	413	LMG	C38-C37-C36	-2.28	102.73	114.45
26	N	1621	LUT	C28-C29-C30	-2.27	115.45	118.94
26	y	1621	LUT	C38-C25-C24	-2.27	118.78	123.68
29	B	2631	LHG	C27-C26-C25	-2.27	102.73	114.45
37	C	519	DGD	O2D-C2D-C1D	-2.27	105.27	110.03
26	n	1621	LUT	C28-C29-C30	-2.27	115.45	118.94
26	6	1621	LUT	C38-C25-C24	-2.27	118.78	123.68
26	1	1620	LUT	C8-C7-C6	-2.27	120.89	127.25
30	C	515	BCR	C8-C7-C6	-2.27	120.89	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	607	CHL	CBA-CAA-C2A	-2.27	112.63	115.76
25	B	610	CLA	O2A-CGA-O1A	-2.27	117.91	123.55
30	c	516	BCR	C8-C7-C6	-2.27	120.90	127.25
25	B	613	CLA	C16-C15-C13	-2.27	108.28	115.73
25	b	613	CLA	C16-C15-C13	-2.27	108.28	115.73
25	g	602	CLA	C1-C2-C3	-2.27	121.78	125.96
29	r	2630	LHG	C18-C17-C16	-2.27	102.77	114.45
35	c	521	LMG	O3-C3-C2	-2.27	105.42	110.36
27	1	1622	XAT	C39-C29-C30	-2.27	119.75	122.92
24	1	601	CHL	O1D-CGD-CBD	-2.27	119.85	124.53
25	b	610	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
25	G	602	CLA	C1-C2-C3	-2.27	121.78	125.96
26	5	1620	LUT	C8-C7-C6	-2.27	120.91	127.25
25	B	609	CLA	OBD-CAD-CBD	-2.26	122.52	125.94
27	8	622	XAT	C8-C9-C10	-2.26	115.47	118.94
27	g	1622	XAT	C39-C29-C30	-2.26	119.75	122.92
26	8	620	LUT	C10-C11-C12	-2.26	116.29	123.23
29	R	2630	LHG	C18-C17-C16	-2.26	102.81	114.45
29	B	2630	LHG	C20-C19-C18	-2.26	102.81	114.45
27	4	622	XAT	C8-C9-C10	-2.26	115.47	118.94
26	G	1620	LUT	C8-C9-C10	-2.26	115.47	118.94
26	4	620	LUT	C10-C11-C12	-2.26	116.31	123.23
35	C	521	LMG	O3-C3-C2	-2.26	105.45	110.36
37	c	519	DGD	CBB-CAB-C9B	-2.26	102.83	114.45
25	7	610	CLA	O2A-CGA-O1A	-2.25	117.95	123.55
24	Y	606	CHL	O2A-CGA-O1A	-2.25	117.95	123.55
29	y	2630	LHG	C27-C26-C25	-2.25	102.84	114.45
29	b	2630	LHG	C20-C19-C18	-2.25	102.84	114.45
27	g	1622	XAT	C26-C27-C28	-2.25	121.24	125.99
24	1	608	CHL	O1D-CGD-CBD	-2.25	119.89	124.53
26	g	1621	LUT	C38-C25-C24	-2.25	118.84	123.68
24	Y	605	CHL	O2D-CGD-O1D	-2.25	119.29	123.82
37	C	519	DGD	CBB-CAB-C9B	-2.25	102.87	114.45
29	g	2630	LHG	C27-C26-C25	-2.25	102.88	114.45
26	g	1620	LUT	C8-C9-C10	-2.25	115.50	118.94
29	Y	2630	LHG	C27-C26-C25	-2.25	102.88	114.45
28	2	1623	NEX	C20-C13-C14	-2.25	119.78	122.92
26	G	1621	LUT	C38-C25-C24	-2.24	118.85	123.68
29	L	101	LHG	C18-C17-C16	-2.24	102.89	114.45
27	G	1622	XAT	C26-C27-C28	-2.24	121.25	125.99
24	7	606	CHL	CBC-CAC-C3C	-2.24	109.55	112.95
29	l	101	LHG	C18-C17-C16	-2.24	102.90	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	607	CHL	C6-C7-C8	-2.24	108.37	115.73
25	3	613	CLA	O2D-CGD-O1D	-2.24	119.31	123.82
26	5	1620	LUT	C38-C25-C24	-2.24	118.86	123.68
35	Z	101	LMG	C38-C37-C36	-2.24	102.92	114.45
25	G	604	CLA	OBD-CAD-CBD	-2.24	122.56	125.94
26	1	1620	LUT	C38-C25-C24	-2.24	118.86	123.68
24	N	608	CHL	O2D-CGD-O1D	-2.24	119.32	123.82
30	t	101	BCR	C31-C1-C6	-2.24	106.68	110.31
24	1	608	CHL	C4A-C3A-C2A	-2.24	100.44	103.86
29	G	2630	LHG	C27-C26-C25	-2.24	102.93	114.45
27	5	1622	XAT	C24-C23-C22	-2.24	106.13	110.68
24	2	609	CHL	OMC-CMC-C2C	-2.24	121.44	124.29
25	7	613	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
24	3	606	CHL	CBC-CAC-C3C	-2.23	109.56	112.95
24	n	608	CHL	O2D-CGD-O1D	-2.23	119.32	123.82
35	z	101	LMG	C38-C37-C36	-2.23	102.94	114.45
27	G	1622	XAT	C39-C29-C30	-2.23	119.80	122.92
27	1	1622	XAT	C24-C23-C22	-2.23	106.13	110.68
25	R	611	CLA	O2D-CGD-O1D	-2.23	119.33	123.82
30	T	101	BCR	C31-C1-C6	-2.23	106.69	110.31
25	S	610	CLA	O2A-CGA-O1A	-2.23	118.01	123.55
30	B	620	BCR	C21-C20-C19	-2.23	116.39	123.23
24	y	605	CHL	O2D-CGD-O1D	-2.23	119.33	123.82
35	b	2633	LMG	C42-C41-C40	-2.23	102.96	114.45
24	G	607	CHL	C6-C7-C8	-2.23	108.41	115.73
24	n	608	CHL	O1D-CGD-CBD	-2.23	119.93	124.53
24	5	608	CHL	C4A-C3A-C2A	-2.23	100.45	103.86
24	n	601	CHL	CHA-CBD-CGD	-2.23	109.83	115.00
25	b	609	CLA	OBD-CAD-CBD	-2.23	122.57	125.94
35	B	2633	LMG	C42-C41-C40	-2.23	102.97	114.45
25	3	610	CLA	O2A-CGA-O1A	-2.23	118.02	123.55
30	b	620	BCR	C21-C20-C19	-2.23	116.39	123.23
29	s	2630	LHG	C5-O7-C7	-2.23	112.61	117.88
24	g	606	CHL	O2A-CGA-O1A	-2.23	118.02	123.55
30	B	619	BCR	C33-C5-C6	-2.23	122.02	124.51
26	6	1620	LUT	C38-C25-C24	-2.23	118.89	123.68
24	N	608	CHL	O1D-CGD-CBD	-2.23	119.94	124.53
36	D	405	PL9	C36-C37-C38	-2.23	104.33	111.97
36	d	405	PL9	C36-C37-C38	-2.23	104.33	111.97
25	y	612	CLA	O2D-CGD-O1D	-2.22	119.34	123.82
24	5	608	CHL	O1D-CGD-CBD	-2.22	119.94	124.53
37	c	520	DGD	O3G-C1D-C2D	-2.22	104.61	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	602	CLA	C6-C7-C8	-2.22	108.44	115.73
29	S	2630	LHG	C5-O7-C7	-2.22	112.63	117.88
25	6	612	CLA	C1C-NC-C4C	-2.22	105.78	107.06
37	C	520	DGD	O3G-C1D-C2D	-2.22	104.61	108.23
24	N	601	CHL	CHA-CBD-CGD	-2.22	109.85	115.00
24	y	606	CHL	O2A-CGA-O1A	-2.22	118.03	123.55
25	g	604	CLA	OBD-CAD-CBD	-2.22	122.58	125.94
25	r	611	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
28	6	1623	NEX	C20-C13-C14	-2.22	119.81	122.92
24	6	609	CHL	OMC-CMC-C2C	-2.22	121.46	124.29
24	2	609	CHL	C1-C2-C3	-2.22	121.87	125.96
29	d	409	LHG	C27-C26-C25	-2.22	103.04	114.45
25	N	602	CLA	C6-C7-C8	-2.21	108.46	115.73
25	b	616	CLA	O2A-CGA-O1A	-2.21	118.05	123.55
25	Y	612	CLA	O2D-CGD-O1D	-2.21	119.37	123.82
30	b	619	BCR	C33-C5-C6	-2.21	122.03	124.51
25	1	614	CLA	O2D-CGD-O1D	-2.21	119.37	123.82
26	2	1620	LUT	C38-C25-C24	-2.21	118.92	123.68
37	B	626	DGD	C3D-C4D-C5D	-2.21	106.32	110.22
24	n	601	CHL	O2D-CGD-O1D	-2.21	119.37	123.82
24	8	608	CHL	O1D-CGD-CBD	-2.21	119.97	124.53
29	D	409	LHG	C27-C26-C25	-2.21	103.07	114.45
25	s	610	CLA	O2A-CGA-O1A	-2.21	118.07	123.55
24	y	601	CHL	O2D-CGD-O1D	-2.21	119.38	123.82
29	d	410	LHG	C27-C26-C25	-2.21	103.08	114.45
30	c	515	BCR	C4-C5-C6	-2.21	119.50	122.74
24	4	608	CHL	O1D-CGD-CBD	-2.21	119.97	124.53
25	c	505	CLA	OBD-CAD-CBD	-2.21	122.61	125.94
29	D	410	LHG	C27-C26-C25	-2.20	103.09	114.45
37	c	519	DGD	O3E-C3E-C2E	-2.20	105.56	110.36
29	y	2630	LHG	C18-C17-C16	-2.20	103.10	114.45
29	Y	2630	LHG	C18-C17-C16	-2.20	103.10	114.45
24	G	606	CHL	O2A-CGA-O1A	-2.20	118.08	123.55
30	A	411	BCR	C10-C11-C12	-2.20	116.47	123.23
35	B	622	LMG	O3-C3-C2	-2.20	105.57	110.36
25	B	616	CLA	O2A-CGA-O1A	-2.20	118.09	123.55
30	t	101	BCR	C7-C6-C5	-2.20	116.29	121.54
25	c	513	CLA	O2A-CGA-O1A	-2.20	118.09	123.55
37	b	626	DGD	C3D-C4D-C5D	-2.20	106.34	110.22
35	Z	101	LMG	O3-C3-C2	-2.20	105.57	110.36
25	5	614	CLA	O2D-CGD-O1D	-2.20	119.39	123.82
30	D	404	BCR	C33-C5-C6	-2.20	122.05	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	411	BCR	C10-C11-C12	-2.20	116.48	123.23
35	C	521	LMG	C38-C37-C36	-2.20	103.12	114.45
29	R	2630	LHG	O8-C6-C5	-2.20	103.13	108.66
30	T	101	BCR	C7-C6-C5	-2.20	116.30	121.54
35	z	101	LMG	O3-C3-C2	-2.20	105.57	110.36
35	c	521	LMG	C38-C37-C36	-2.20	103.13	114.45
35	C	521	LMG	O2-C2-C1	-2.20	105.43	110.03
25	b	612	CLA	CGD-CBD-CAD	-2.20	103.35	110.71
39	f	101	HEM	CBD-CAD-C3D	-2.20	108.28	112.47
30	C	515	BCR	C4-C5-C6	-2.20	119.52	122.74
26	6	1620	LUT	C8-C9-C10	-2.20	115.57	118.94
29	r	2630	LHG	O8-C6-C5	-2.20	103.14	108.66
26	n	1621	LUT	C37-C21-C22	-2.20	105.23	109.42
24	R	606	CHL	O1D-CGD-CBD	-2.19	120.00	124.53
30	C	515	BCR	C1-C6-C5	-2.19	119.51	122.59
24	6	609	CHL	C1-C2-C3	-2.19	121.92	125.96
35	b	622	LMG	O3-C3-C2	-2.19	105.58	110.36
24	4	607	CHL	CBC-CAC-C3C	-2.19	109.62	112.95
39	F	101	HEM	CBD-CAD-C3D	-2.19	108.28	112.47
25	N	611	CLA	CAA-CBA-CGA	-2.19	106.75	113.35
24	1	609	CHL	CBC-CAC-C3C	-2.19	109.62	112.95
25	B	612	CLA	CGD-CBD-CAD	-2.19	103.37	110.71
30	H	101	BCR	C2-C3-C4	-2.19	106.12	111.34
25	C	505	CLA	OBD-CAD-CBD	-2.19	122.63	125.94
25	1	612	CLA	CHA-C1A-NA	-2.19	121.09	126.18
26	R	620	LUT	C31-C30-C29	-2.19	124.19	127.31
35	c	521	LMG	O2-C2-C1	-2.19	105.45	110.03
37	C	519	DGD	O3E-C3E-C2E	-2.19	105.59	110.36
24	N	601	CHL	O2D-CGD-O1D	-2.19	119.42	123.82
30	D	404	BCR	C3-C4-C5	-2.19	110.02	113.78
26	r	620	LUT	C31-C30-C29	-2.19	124.19	127.31
37	c	520	DGD	CAB-C9B-C8B	-2.19	103.18	114.45
25	n	611	CLA	CAA-CBA-CGA	-2.19	106.76	113.35
35	d	411	LMG	O2-C2-C1	-2.19	105.46	110.03
25	c	501	CLA	O2A-CGA-O1A	-2.19	118.12	123.55
25	7	611	CLA	CAA-C2A-C3A	-2.19	106.82	112.81
37	C	520	DGD	CAB-C9B-C8B	-2.18	103.20	114.45
30	c	515	BCR	C1-C6-C5	-2.18	119.52	122.59
25	C	513	CLA	O2A-CGA-O1A	-2.18	118.14	123.55
29	G	2630	LHG	C18-C17-C16	-2.18	103.22	114.45
25	n	614	CLA	O2A-CGA-O1A	-2.18	118.14	123.55
26	2	1621	LUT	C16-C1-C6	-2.18	106.77	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	D	411	LMG	O2-C2-C1	-2.18	105.47	110.03
24	r	606	CHL	O1D-CGD-CBD	-2.18	120.03	124.53
24	Y	601	CHL	O2D-CGD-O1D	-2.18	119.43	123.82
24	5	609	CHL	CBC-CAC-C3C	-2.18	109.64	112.95
30	h	101	BCR	C2-C3-C4	-2.18	106.15	111.34
25	5	612	CLA	CHA-C1A-NA	-2.18	121.12	126.18
29	C	522	LHG	C27-C26-C25	-2.18	103.23	114.45
25	C	501	CLA	O2A-CGA-O1A	-2.18	118.15	123.55
29	g	2630	LHG	C18-C17-C16	-2.18	103.25	114.45
26	Y	1620	LUT	C31-C30-C29	-2.17	124.21	127.31
24	6	609	CHL	C6-C5-C3	-2.17	107.73	112.66
37	C	518	DGD	CBB-CAB-C9B	-2.17	103.25	114.45
25	3	611	CLA	CAA-C2A-C3A	-2.17	106.85	112.81
26	2	1620	LUT	C8-C9-C10	-2.17	115.61	118.94
25	N	614	CLA	O2A-CGA-O1A	-2.17	118.15	123.55
29	c	522	LHG	C27-C26-C25	-2.17	103.25	114.45
29	Y	2630	LHG	C11-C10-C9	-2.17	103.26	114.45
29	y	2630	LHG	C11-C10-C9	-2.17	103.26	114.45
24	2	609	CHL	C6-C5-C3	-2.17	107.73	112.66
37	c	518	DGD	CBB-CAB-C9B	-2.17	103.26	114.45
30	c	514	BCR	C3-C4-C5	-2.17	110.05	113.78
24	8	607	CHL	CBC-CAC-C3C	-2.17	109.66	112.95
29	7	2630	LHG	C18-C17-C16	-2.17	103.28	114.45
24	6	607	CHL	C1-C2-C3	-2.17	121.96	125.96
30	C	514	BCR	C3-C4-C5	-2.17	110.05	113.78
25	3	611	CLA	C1C-NC-C4C	-2.17	105.81	107.06
29	3	2630	LHG	C18-C17-C16	-2.17	103.29	114.45
29	c	523	LHG	C18-C17-C16	-2.17	103.29	114.45
25	Y	612	CLA	C1-C2-C3	-2.16	121.97	125.96
24	2	607	CHL	C1-C2-C3	-2.16	121.97	125.96
26	6	1621	LUT	C16-C1-C6	-2.16	106.80	110.31
30	d	404	BCR	C3-C4-C5	-2.16	110.06	113.78
30	d	404	BCR	C33-C5-C6	-2.16	122.09	124.51
25	y	612	CLA	C1-C2-C3	-2.16	121.97	125.96
26	N	1621	LUT	C37-C21-C22	-2.16	105.29	109.42
26	G	1621	LUT	C37-C21-C22	-2.16	105.29	109.42
29	C	523	LHG	C18-C17-C16	-2.16	103.32	114.45
25	b	606	CLA	OBD-CAD-CBD	-2.16	122.68	125.94
24	N	606	CHL	C4A-C3A-C2A	-2.16	100.56	103.86
36	D	405	PL9	C11-C12-C13	-2.16	104.56	111.97
29	C	2630	LHG	O8-C6-C5	-2.16	103.23	108.66
24	Y	609	CHL	CMA-C3A-C2A	-2.16	108.66	115.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	602	CLA	CAA-CBA-CGA	-2.16	106.85	113.35
35	a	415	LMG	O1-C7-C8	-2.16	105.86	110.99
24	y	609	CHL	CMA-C3A-C2A	-2.15	108.67	115.84
35	B	2633	LMG	O6-C1-O1	-2.15	104.91	110.02
29	c	2630	LHG	O8-C6-C5	-2.15	103.25	108.66
24	s	608	CHL	CBC-CAC-C3C	-2.15	109.68	112.95
29	D	408	LHG	O8-C6-C5	-2.15	103.25	108.66
37	c	518	DGD	O6D-C5D-C6D	-2.15	102.34	106.64
24	N	609	CHL	O2D-CGD-O1D	-2.15	119.49	123.82
36	d	405	PL9	C11-C12-C13	-2.15	104.58	111.97
37	H	102	DGD	O1G-C1A-O1A	-2.15	118.21	123.55
29	l	101	LHG	C27-C26-C25	-2.15	103.38	114.45
25	c	507	CLA	O2A-CGA-O1A	-2.15	118.22	123.55
35	A	415	LMG	O1-C7-C8	-2.15	105.88	110.99
29	S	2630	LHG	C18-C17-C16	-2.15	103.39	114.45
30	8	623	BCR	C21-C20-C19	-2.15	116.64	123.23
26	y	1620	LUT	C31-C30-C29	-2.15	124.25	127.31
28	7	1623	NEX	C30-C31-C32	-2.15	116.65	123.23
29	L	101	LHG	C27-C26-C25	-2.15	103.40	114.45
25	y	603	CLA	C1-C2-C3	-2.15	122.00	125.96
25	G	602	CLA	CAA-CBA-CGA	-2.14	106.89	113.35
26	g	1621	LUT	C37-C21-C22	-2.14	105.33	109.42
25	b	609	CLA	O2A-CGA-O1A	-2.14	118.23	123.55
26	y	1621	LUT	C31-C30-C29	-2.14	124.25	127.31
24	4	606	CHL	O1D-CGD-CBD	-2.14	120.11	124.53
27	2	1622	XAT	C16-C1-C2	-2.14	105.18	108.97
35	b	2633	LMG	O6-C1-O1	-2.14	104.94	110.02
29	s	2630	LHG	C18-C17-C16	-2.14	103.42	114.45
24	R	607	CHL	C1-C2-C3	-2.14	122.01	125.96
30	4	623	BCR	C21-C20-C19	-2.14	116.66	123.23
37	C	518	DGD	O6D-C5D-C6D	-2.14	102.36	106.64
29	d	408	LHG	O8-C6-C5	-2.14	103.28	108.66
24	n	609	CHL	O1D-CGD-CBD	-2.14	120.12	124.53
26	Y	1621	LUT	C31-C30-C29	-2.14	124.26	127.31
24	n	606	CHL	O2D-CGD-O1D	-2.14	119.52	123.82
37	h	102	DGD	O1G-C1A-O1A	-2.14	118.25	123.55
25	2	612	CLA	C1C-NC-C4C	-2.14	105.83	107.06
25	B	609	CLA	O2A-CGA-O1A	-2.14	118.25	123.55
35	a	415	LMG	C38-C37-C36	-2.14	103.45	114.45
24	r	606	CHL	C1-C2-C3	-2.14	122.02	125.96
25	Y	613	CLA	O2D-CGD-O1D	-2.13	119.52	123.82
35	A	415	LMG	C38-C37-C36	-2.13	103.46	114.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	603	CLA	C1-C2-C3	-2.13	122.02	125.96
28	3	1623	NEX	C30-C31-C32	-2.13	116.68	123.23
24	R	607	CHL	CAA-CBA-CGA	-2.13	106.92	113.35
25	c	512	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
27	2	1622	XAT	C4-C3-C2	-2.13	106.33	110.68
25	B	606	CLA	OBD-CAD-CBD	-2.13	122.72	125.94
24	n	609	CHL	O2D-CGD-O1D	-2.13	119.53	123.82
25	C	507	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
28	6	1623	NEX	C30-C31-C32	-2.13	116.69	123.23
26	6	1621	LUT	C11-C10-C9	-2.13	124.27	127.31
24	n	606	CHL	C4A-C3A-C2A	-2.13	100.60	103.86
25	2	603	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
24	N	606	CHL	O2D-CGD-O1D	-2.13	119.53	123.82
29	2	2630	LHG	C27-C26-C25	-2.13	103.48	114.45
29	C	2630	LHG	C27-C26-C25	-2.13	103.48	114.45
36	D	405	PL9	O2-C1-C2	-2.13	116.79	121.77
25	c	502	CLA	CBC-CAC-C3C	-2.13	106.37	112.41
24	8	606	CHL	O1D-CGD-CBD	-2.13	120.14	124.53
25	r	611	CLA	CHA-C1A-NA	-2.13	121.23	126.18
28	2	1623	NEX	C30-C31-C32	-2.13	116.70	123.23
25	b	612	CLA	C11-C12-C13	-2.13	108.75	115.73
24	s	607	CHL	CBA-CAA-C2A	-2.13	112.83	115.76
30	A	411	BCR	C15-C16-C17	-2.13	118.92	123.46
29	6	2630	LHG	C27-C26-C25	-2.13	103.50	114.45
24	r	607	CHL	CAA-CBA-CGA	-2.13	106.94	113.35
24	7	607	CHL	CHA-CBD-CGD	-2.13	110.07	115.00
24	3	607	CHL	CHA-CBD-CGD	-2.13	110.07	115.00
29	c	2630	LHG	C27-C26-C25	-2.12	103.51	114.45
27	6	1622	XAT	C16-C1-C2	-2.12	105.21	108.97
25	R	611	CLA	CHA-C1A-NA	-2.12	121.25	126.18
27	6	1622	XAT	C4-C3-C2	-2.12	106.36	110.68
24	G	607	CHL	O1D-CGD-CBD	-2.12	120.15	124.53
24	S	608	CHL	CBC-CAC-C3C	-2.12	109.73	112.95
25	y	613	CLA	O2D-CGD-O1D	-2.12	119.55	123.82
28	y	1623	NEX	C40-C33-C34	-2.12	119.95	122.92
30	C	515	BCR	C10-C11-C12	-2.12	116.72	123.23
30	c	515	BCR	C10-C11-C12	-2.12	116.72	123.23
25	6	603	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
24	N	609	CHL	O1D-CGD-CBD	-2.12	120.15	124.53
27	R	622	XAT	O24-C25-C26	-2.12	57.16	58.94
25	B	612	CLA	C11-C12-C13	-2.12	108.77	115.73
24	r	607	CHL	C1-C2-C3	-2.12	122.05	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	604	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
30	c	514	BCR	C7-C8-C9	-2.12	123.03	126.21
25	Y	612	CLA	O2A-CGA-O1A	-2.12	118.28	123.55
24	R	606	CHL	C1-C2-C3	-2.12	122.05	125.96
29	B	2630	LHG	C27-C26-C25	-2.12	103.53	114.45
29	5	2630	LHG	C27-C26-C25	-2.12	103.53	114.45
26	2	1621	LUT	C11-C10-C9	-2.12	124.28	127.31
29	b	2630	LHG	C27-C26-C25	-2.12	103.53	114.45
25	n	604	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
25	B	604	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
25	C	502	CLA	CBC-CAC-C3C	-2.12	106.40	112.41
27	r	622	XAT	O24-C25-C26	-2.12	57.16	58.94
37	C	518	DGD	CAB-C9B-C8B	-2.12	103.55	114.45
27	g	1622	XAT	C35-C34-C33	-2.12	124.29	127.31
28	g	1623	NEX	C19-C9-C10	-2.12	119.96	122.92
30	C	514	BCR	C7-C8-C9	-2.12	123.03	126.21
26	5	1621	LUT	C22-C23-C24	-2.11	109.34	111.73
30	D	404	BCR	C10-C11-C12	-2.11	116.75	123.23
29	1	2630	LHG	C27-C26-C25	-2.11	103.57	114.45
26	n	1620	LUT	C8-C9-C10	-2.11	115.70	118.94
30	a	411	BCR	C15-C16-C17	-2.11	118.95	123.46
36	d	405	PL9	O2-C1-C2	-2.11	116.83	121.77
37	c	520	DGD	CBB-CAB-C9B	-2.11	103.58	114.45
37	c	518	DGD	CAB-C9B-C8B	-2.11	103.58	114.45
24	g	607	CHL	O1D-CGD-CBD	-2.11	120.17	124.53
29	c	522	LHG	C18-C17-C16	-2.11	103.58	114.45
29	b	2630	LHG	C11-C10-C9	-2.11	103.58	114.45
27	G	1622	XAT	C35-C34-C33	-2.11	124.30	127.31
26	1	1621	LUT	C31-C32-C33	-2.11	120.49	126.42
29	B	2630	LHG	C11-C10-C9	-2.11	103.59	114.45
25	b	607	CLA	C6-C7-C8	-2.11	108.81	115.73
35	Z	101	LMG	O5-C6-C5	-2.11	104.25	111.34
37	C	520	DGD	CBB-CAB-C9B	-2.11	103.59	114.45
25	B	607	CLA	C6-C7-C8	-2.11	108.81	115.73
25	b	610	CLA	OBD-CAD-CBD	-2.11	122.76	125.94
26	1	1621	LUT	C38-C25-C24	-2.11	119.14	123.68
30	d	404	BCR	C10-C11-C12	-2.11	116.77	123.23
26	5	1621	LUT	C38-C25-C24	-2.11	119.15	123.68
26	1	1621	LUT	C22-C23-C24	-2.10	109.35	111.73
24	4	606	CHL	C4A-C3A-C2A	-2.10	100.64	103.86
25	d	403	CLA	OBD-CAD-CBD	-2.10	122.76	125.94
28	G	1623	NEX	C35-C15-C14	-2.10	118.97	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	612	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
37	c	519	DGD	CAB-C9B-C8B	-2.10	103.62	114.45
29	C	522	LHG	C18-C17-C16	-2.10	103.62	114.45
25	1	603	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
24	S	607	CHL	CBA-CAA-C2A	-2.10	112.86	115.76
28	Y	1623	NEX	C40-C33-C34	-2.10	119.98	122.92
25	N	604	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
28	g	1623	NEX	C35-C15-C14	-2.10	118.97	123.46
26	5	1621	LUT	C31-C32-C33	-2.10	120.51	126.42
25	C	512	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
25	C	512	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
35	z	101	LMG	O5-C6-C5	-2.10	104.27	111.34
25	y	614	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
25	B	617	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
27	7	1622	XAT	C11-C12-C13	-2.10	120.52	126.42
30	H	101	BCR	C16-C15-C14	-2.10	118.98	123.46
25	Y	614	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
24	8	606	CHL	C4A-C3A-C2A	-2.10	100.66	103.86
29	S	2630	LHG	C27-C26-C25	-2.10	103.65	114.45
24	5	605	CHL	C4A-C3A-C2A	-2.10	100.66	103.86
26	N	1620	LUT	C8-C9-C10	-2.10	115.73	118.94
29	B	2631	LHG	C20-C19-C18	-2.10	103.66	114.45
37	h	102	DGD	CBB-CAB-C9B	-2.09	103.66	114.45
25	B	610	CLA	OBD-CAD-CBD	-2.09	122.78	125.94
37	H	102	DGD	CBB-CAB-C9B	-2.09	103.67	114.45
29	b	2631	LHG	C5-O7-C7	-2.09	112.93	117.88
25	7	611	CLA	C1C-NC-C4C	-2.09	105.85	107.06
25	c	512	CLA	O2A-CGA-O1A	-2.09	118.35	123.55
26	N	1621	LUT	C38-C25-C24	-2.09	119.17	123.68
29	r	2630	LHG	C27-C26-C25	-2.09	103.67	114.45
37	C	519	DGD	CAB-C9B-C8B	-2.09	103.67	114.45
29	L	101	LHG	O8-C6-C5	-2.09	103.40	108.66
25	D	403	CLA	OBD-CAD-CBD	-2.09	122.78	125.94
28	G	1623	NEX	C19-C9-C10	-2.09	119.99	122.92
29	s	2630	LHG	C27-C26-C25	-2.09	103.68	114.45
29	R	2630	LHG	C27-C26-C25	-2.09	103.68	114.45
25	B	613	CLA	C9-C8-C10	-2.09	103.74	111.36
25	G	613	CLA	OBD-CAD-CBD	-2.09	122.78	125.94
24	y	609	CHL	C11-C12-C13	-2.09	108.87	115.73
24	g	601	CHL	O1D-CGD-CBD	-2.09	120.22	124.53
26	y	1621	LUT	C37-C21-C22	-2.09	105.43	109.42
30	h	101	BCR	C16-C15-C14	-2.09	119.00	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	603	CLA	O2D-CGD-O1D	-2.09	119.62	123.82
25	C	508	CLA	CMC-C2C-C1C	-2.09	121.86	125.02
27	3	1622	XAT	C11-C12-C13	-2.09	120.55	126.42
24	N	605	CHL	O2A-CGA-O1A	-2.09	118.37	123.55
29	b	2631	LHG	C20-C19-C18	-2.09	103.70	114.45
25	B	603	CLA	O2D-CGD-O1D	-2.09	119.62	123.82
26	n	1621	LUT	C38-C25-C24	-2.09	119.19	123.68
30	4	623	BCR	C3-C4-C5	-2.09	110.19	113.78
30	8	623	BCR	C3-C4-C5	-2.09	110.19	113.78
24	n	605	CHL	O2A-CGA-O1A	-2.08	118.38	123.55
25	g	613	CLA	OBD-CAD-CBD	-2.08	122.80	125.94
29	l	101	LHG	O8-C6-C5	-2.08	103.42	108.66
25	b	613	CLA	C9-C8-C10	-2.08	103.77	111.36
24	G	608	CHL	O2D-CGD-O1D	-2.08	119.63	123.82
24	G	601	CHL	O1D-CGD-CBD	-2.08	120.24	124.53
25	b	617	CLA	OBD-CAD-CBD	-2.08	122.80	125.94
26	S	1621	LUT	C16-C1-C6	-2.08	106.94	110.31
25	D	403	CLA	O2A-CGA-O1A	-2.08	118.39	123.55
25	5	603	CLA	O2D-CGD-O1D	-2.08	119.64	123.82
30	H	101	BCR	C15-C16-C17	-2.08	119.03	123.46
24	Y	609	CHL	C11-C12-C13	-2.08	108.92	115.73
26	Y	1621	LUT	C37-C21-C22	-2.08	105.46	109.42
25	d	403	CLA	O2A-CGA-O1A	-2.07	118.40	123.55
29	C	522	LHG	C20-C19-C18	-2.07	103.76	114.45
35	Z	101	LMG	C9-C8-C7	-2.07	107.18	111.86
26	s	1621	LUT	C16-C1-C6	-2.07	106.95	110.31
35	z	101	LMG	C9-C8-C7	-2.07	107.18	111.86
27	g	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
24	n	607	CHL	CAA-CBA-CGA	-2.07	107.11	113.35
29	B	2631	LHG	C5-O7-C7	-2.07	112.98	117.88
24	g	608	CHL	O2D-CGD-O1D	-2.07	119.65	123.82
25	r	613	CLA	C1-C2-C3	-2.07	122.14	125.96
24	N	607	CHL	CAA-CBA-CGA	-2.07	107.11	113.35
37	C	519	DGD	C5B-C4B-C3B	-2.07	103.79	114.45
29	c	522	LHG	C20-C19-C18	-2.07	103.79	114.45
27	N	1622	XAT	C7-C8-C9	-2.07	122.32	125.53
25	b	615	CLA	O2A-CGA-O1A	-2.07	118.41	123.55
36	d	405	PL9	C31-C32-C33	-2.07	104.86	111.97
24	l	605	CHL	C4A-C3A-C2A	-2.07	100.70	103.86
26	y	1620	LUT	O3-C3-C4	-2.07	105.08	109.63
37	c	519	DGD	C5B-C4B-C3B	-2.07	103.80	114.45
36	D	405	PL9	C31-C32-C33	-2.07	104.88	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	615	CLA	O2A-CGA-O1A	-2.07	118.42	123.55
26	N	1620	LUT	C23-C24-C25	-2.07	123.28	125.22
37	c	518	DGD	O5D-C6D-C5D	-2.06	105.49	108.94
25	R	613	CLA	C1-C2-C3	-2.06	122.15	125.96
25	a	405	CLA	C16-C15-C13	-2.06	108.96	115.73
25	B	611	CLA	CAA-C2A-C1A	-2.06	105.21	111.97
25	c	508	CLA	CMC-C2C-C1C	-2.06	121.89	125.02
24	y	606	CHL	C4A-C3A-C2A	-2.06	100.71	103.86
27	n	1622	XAT	C7-C8-C9	-2.06	122.33	125.53
24	3	608	CHL	CMA-C3A-C2A	-2.06	108.98	115.84
26	7	1621	LUT	C31-C30-C29	-2.06	124.37	127.31
25	3	610	CLA	C1-C2-C3	-2.06	122.16	125.96
29	S	2630	LHG	C20-C19-C18	-2.06	103.83	114.45
26	g	1621	LUT	C8-C9-C10	-2.06	115.78	118.94
24	r	606	CHL	O2D-CGD-O1D	-2.06	119.67	123.82
24	7	608	CHL	CMA-C3A-C2A	-2.06	108.98	115.84
27	6	1622	XAT	C24-C23-C22	-2.06	106.48	110.68
25	A	405	CLA	C16-C15-C13	-2.06	108.97	115.73
26	7	1620	LUT	C15-C35-C34	-2.06	119.06	123.46
27	G	1622	XAT	C7-C8-C9	-2.06	122.33	125.53
37	B	626	DGD	O3E-C3E-C2E	-2.06	105.87	110.36
25	S	602	CLA	O2A-CGA-O1A	-2.06	118.44	123.55
33	a	409	PHO	C2B-C1B-NB	-2.06	106.77	109.82
25	s	602	CLA	O2A-CGA-O1A	-2.06	118.44	123.55
24	R	607	CHL	O2A-CGA-O1A	-2.06	118.44	123.55
24	2	609	CHL	CMA-C3A-C2A	-2.06	108.99	115.84
27	2	1622	XAT	C24-C23-C22	-2.06	106.49	110.68
30	C	514	BCR	C24-C23-C22	-2.06	123.12	126.21
26	Y	1620	LUT	O3-C3-C4	-2.06	105.10	109.63
27	G	1622	XAT	O24-C25-C26	-2.06	57.21	58.94
26	3	1620	LUT	C15-C35-C34	-2.06	119.07	123.46
29	s	2630	LHG	C20-C19-C18	-2.06	103.86	114.45
30	t	101	BCR	C34-C9-C10	-2.06	120.04	122.92
24	Y	605	CHL	OMC-CMC-C2C	-2.06	121.67	124.29
25	R	603	CLA	O2A-CGA-O1A	-2.06	118.45	123.55
28	N	1623	NEX	C40-C33-C34	-2.06	120.04	122.92
25	7	610	CLA	C1-C2-C3	-2.06	122.17	125.96
37	C	518	DGD	C5B-C4B-C3B	-2.06	103.86	114.45
24	8	607	CHL	O2D-CGD-O1D	-2.06	119.68	123.82
25	b	605	CLA	CHA-C1A-NA	-2.06	121.41	126.18
25	B	602	CLA	O2A-CGA-O1A	-2.06	118.45	123.55
37	c	520	DGD	O6E-C1E-O5D	-2.06	105.14	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	611	CLA	CAA-C2A-C1A	-2.05	105.24	111.97
30	h	101	BCR	C15-C16-C17	-2.05	119.08	123.46
33	A	409	PHO	C2B-C1B-NB	-2.05	106.78	109.82
27	l	1622	XAT	C10-C11-C12	-2.05	116.93	123.23
24	r	607	CHL	O2A-CGA-O1A	-2.05	118.45	123.55
26	Y	1621	LUT	C35-C15-C14	-2.05	119.08	123.46
30	c	514	BCR	C24-C23-C22	-2.05	123.13	126.21
24	Y	606	CHL	C4A-C3A-C2A	-2.05	100.72	103.86
27	g	1622	XAT	O24-C25-C26	-2.05	57.22	58.94
24	R	608	CHL	O2D-CGD-O1D	-2.05	119.69	123.82
24	g	606	CHL	O2D-CGD-O1D	-2.05	119.69	123.82
25	b	610	CLA	CAA-CBA-CGA	-2.05	107.17	113.35
25	B	605	CLA	CHA-C1A-NA	-2.05	121.42	126.18
28	n	1623	NEX	C40-C33-C34	-2.05	120.05	122.92
25	b	602	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
24	6	609	CHL	CMA-C3A-C2A	-2.05	109.02	115.84
24	R	606	CHL	O2D-CGD-O1D	-2.05	119.69	123.82
30	C	515	BCR	C3-C4-C5	-2.05	110.26	113.78
24	r	608	CHL	O2D-CGD-O1D	-2.05	119.70	123.82
37	c	518	DGD	C5B-C4B-C3B	-2.05	103.90	114.45
37	b	626	DGD	O3E-C3E-C2E	-2.05	105.90	110.36
30	c	515	BCR	C3-C4-C5	-2.05	110.26	113.78
25	r	603	CLA	O2A-CGA-O1A	-2.05	118.47	123.55
25	B	610	CLA	CAA-CBA-CGA	-2.05	107.18	113.35
27	5	1622	XAT	C10-C11-C12	-2.05	116.96	123.23
29	C	523	LHG	C27-C26-C25	-2.05	103.92	114.45
37	C	518	DGD	O5D-C6D-C5D	-2.05	105.52	108.94
30	T	101	BCR	C34-C9-C10	-2.05	120.06	122.92
24	Y	601	CHL	O1D-CGD-CBD	-2.05	120.31	124.53
25	B	617	CLA	O2A-CGA-O1A	-2.04	118.47	123.55
25	b	612	CLA	CAA-CBA-CGA	-2.04	107.19	113.35
37	C	520	DGD	O6E-C1E-O5D	-2.04	105.17	110.02
27	8	622	XAT	C30-C31-C32	-2.04	116.97	123.23
29	c	523	LHG	C27-C26-C25	-2.04	103.93	114.45
24	G	606	CHL	O2D-CGD-O1D	-2.04	119.71	123.82
26	n	1620	LUT	C11-C10-C9	-2.04	124.40	127.31
30	D	404	BCR	C15-C14-C13	-2.04	124.40	127.31
30	d	404	BCR	C15-C14-C13	-2.04	124.40	127.31
25	B	612	CLA	CAA-CBA-CGA	-2.04	107.20	113.35
28	G	1623	NEX	C30-C31-C32	-2.04	116.98	123.23
27	4	622	XAT	C30-C31-C32	-2.04	116.98	123.23
25	b	617	CLA	O2A-CGA-O1A	-2.04	118.49	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	410	CLA	C1-C2-C3	-2.04	122.20	125.96
25	G	602	CLA	OBD-CAD-CBD	-2.04	122.86	125.94
24	5	607	CHL	C4A-C3A-C2A	-2.04	100.75	103.86
25	s	604	CLA	O2A-CGA-O1A	-2.03	118.50	123.55
25	S	604	CLA	O2A-CGA-O1A	-2.03	118.50	123.55
26	6	1620	LUT	C11-C10-C9	-2.03	124.41	127.31
29	C	522	LHG	O8-C6-C5	-2.03	103.55	108.66
25	a	410	CLA	C1-C2-C3	-2.03	122.21	125.96
25	Y	603	CLA	C11-C10-C8	-2.03	109.06	115.73
28	g	1623	NEX	C30-C31-C32	-2.03	116.99	123.23
24	4	607	CHL	O2D-CGD-O1D	-2.03	119.73	123.82
26	y	1621	LUT	C35-C15-C14	-2.03	119.12	123.46
30	T	101	BCR	C38-C26-C25	-2.03	122.23	124.51
25	1	602	CLA	CHA-C1A-NA	-2.03	121.46	126.18
25	3	611	CLA	O2A-CGA-O1A	-2.03	118.51	123.55
24	y	605	CHL	OMC-CMC-C2C	-2.03	121.70	124.29
26	G	1621	LUT	C8-C9-C10	-2.03	115.82	118.94
26	n	1620	LUT	C23-C24-C25	-2.03	123.32	125.22
30	d	404	BCR	C20-C21-C22	-2.03	124.41	127.31
30	8	623	BCR	C4-C5-C6	-2.03	119.76	122.74
25	g	602	CLA	OBD-CAD-CBD	-2.03	122.88	125.94
24	S	608	CHL	O2D-CGD-O1D	-2.03	119.74	123.82
26	N	1620	LUT	C11-C10-C9	-2.03	124.42	127.31
25	5	602	CLA	CHA-C1A-NA	-2.03	121.47	126.18
25	s	614	CLA	O2A-CGA-O1A	-2.03	118.52	123.55
25	y	603	CLA	C11-C10-C8	-2.03	109.08	115.73
29	N	2630	LHG	C29-C28-C27	-2.03	104.01	114.45
30	t	101	BCR	C38-C26-C25	-2.03	122.24	124.51
25	r	602	CLA	O2A-CGA-O1A	-2.03	118.52	123.55
25	S	614	CLA	O2A-CGA-O1A	-2.02	118.52	123.55
25	B	614	CLA	O2D-CGD-O1D	-2.02	119.75	123.82
25	7	611	CLA	O2A-CGA-O1A	-2.02	118.53	123.55
29	n	2630	LHG	C29-C28-C27	-2.02	104.03	114.45
25	R	602	CLA	O2A-CGA-O1A	-2.02	118.53	123.55
25	5	602	CLA	C1-C2-C3	-2.02	122.23	125.96
29	2	2630	LHG	O8-C6-C5	-2.02	103.58	108.66
29	c	522	LHG	O8-C6-C5	-2.02	103.58	108.66
25	D	402	CLA	CAC-C3C-C2C	-2.02	123.99	127.49
25	7	603	CLA	CHA-C1A-NA	-2.02	121.49	126.18
25	3	603	CLA	CHA-C1A-NA	-2.02	121.49	126.18
24	3	601	CHL	O2D-CGD-O1D	-2.02	119.75	123.82
26	3	1621	LUT	C31-C30-C29	-2.02	124.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	615	CLA	OBD-CAD-CBD	-2.02	122.89	125.94
25	d	402	CLA	C3C-C4C-NC	-2.02	108.17	110.21
27	6	1622	XAT	C31-C32-C33	-2.02	120.75	126.42
24	y	601	CHL	O1D-CGD-CBD	-2.01	120.37	124.53
25	1	602	CLA	C1-C2-C3	-2.01	122.25	125.96
27	6	1622	XAT	C19-C9-C10	-2.01	120.10	122.92
29	B	2630	LHG	O8-C6-C5	-2.01	103.60	108.66
24	1	607	CHL	C4A-C3A-C2A	-2.01	100.79	103.86
25	S	611	CLA	O2A-CGA-O1A	-2.01	118.56	123.55
24	s	608	CHL	O2D-CGD-O1D	-2.01	119.78	123.82
30	4	623	BCR	C4-C5-C6	-2.01	119.79	122.74
29	6	2630	LHG	O8-C6-C5	-2.01	103.61	108.66
37	c	520	DGD	O3E-C3E-C2E	-2.01	105.99	110.36
25	d	402	CLA	CAC-C3C-C2C	-2.01	124.01	127.49
37	c	518	DGD	O2D-C2D-C1D	-2.01	105.83	110.03
27	2	1622	XAT	C31-C32-C33	-2.01	120.78	126.42
28	r	623	NEX	O24-C25-C26	-2.01	57.26	58.94
24	1	607	CHL	CAA-CBA-CGA	-2.00	107.31	113.35
26	2	1620	LUT	C11-C10-C9	-2.00	124.45	127.31
24	G	605	CHL	CBC-CAC-C3C	-2.00	109.91	112.95
37	C	518	DGD	O2D-C2D-C1D	-2.00	105.84	110.03
26	g	1621	LUT	C15-C35-C34	-2.00	119.19	123.46
24	8	601	CHL	C3B-CAB-CBB	-2.00	120.70	125.20
37	C	520	DGD	O3E-C3E-C2E	-2.00	106.00	110.36
25	c	510	CLA	O2A-CGA-O1A	-2.00	118.58	123.55
25	D	402	CLA	C3C-C4C-NC	-2.00	108.18	110.21
24	5	607	CHL	CAA-CBA-CGA	-2.00	107.32	113.35
25	b	614	CLA	O2D-CGD-O1D	-2.00	119.79	123.82
24	g	605	CHL	CBC-CAC-C3C	-2.00	109.91	112.95
25	B	605	CLA	CAA-C2A-C1A	2.00	118.53	111.97
24	Y	608	CHL	C7-C6-C5	2.00	118.68	113.11
25	c	507	CLA	O2D-CGD-CBD	2.00	114.88	111.30
24	n	609	CHL	C1-O2A-CGA	2.00	121.58	116.77
25	a	406	CLA	CMD-C2D-C3D	2.01	128.61	124.89
28	g	1623	NEX	C28-C29-C30	2.01	122.02	118.94
25	c	512	CLA	C4A-NA-C1A	2.01	108.94	106.45
25	B	616	CLA	C2A-C1A-CHA	2.01	127.47	123.92
25	C	512	CLA	C4A-NA-C1A	2.01	108.94	106.45
33	a	408	PHO	CBD-CHA-C1A	2.01	131.09	126.36
25	b	605	CLA	CAA-C2A-C1A	2.01	118.55	111.97
33	A	408	PHO	CBD-CHA-C1A	2.01	131.09	126.36
26	S	1621	LUT	C20-C13-C12	2.01	121.30	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	614	CLA	C4A-NA-C1A	2.01	108.94	106.45
37	b	626	DGD	C1E-O6E-C5E	2.01	117.50	113.72
28	y	1623	NEX	C5-C6-C1	2.01	121.69	119.70
25	C	507	CLA	O2D-CGD-CBD	2.01	114.89	111.30
30	C	514	BCR	C37-C22-C23	2.01	121.31	118.10
30	B	619	BCR	C34-C9-C8	2.01	121.31	118.10
25	y	614	CLA	CMD-C2D-C3D	2.01	128.63	124.89
25	6	603	CLA	C2A-C1A-CHA	2.01	127.49	123.92
24	n	608	CHL	C7-C6-C5	2.02	118.72	113.11
26	N	1620	LUT	C20-C13-C12	2.02	121.31	118.10
26	n	1620	LUT	C20-C13-C12	2.02	121.31	118.10
24	y	608	CHL	C7-C6-C5	2.02	118.72	113.11
28	Y	1623	NEX	C5-C6-C1	2.02	121.70	119.70
25	b	614	CLA	C3A-C2A-C1A	2.02	104.36	101.34
24	y	608	CHL	CHB-C1B-C2B	2.02	122.58	116.99
25	r	611	CLA	O1D-CGD-CBD	2.02	128.23	124.60
26	8	620	LUT	C20-C13-C12	2.02	121.32	118.10
25	4	612	CLA	O1D-CGD-CBD	2.02	128.23	124.60
25	c	511	CLA	CMD-C2D-C3D	2.02	128.64	124.89
24	Y	608	CHL	CHB-C1B-C2B	2.02	122.59	116.99
36	d	405	PL9	O2-C1-C6	2.02	124.21	120.57
25	C	511	CLA	CMD-C2D-C3D	2.02	128.65	124.89
24	7	609	CHL	C4D-C3D-CAD	2.02	109.41	104.71
24	R	606	CHL	C4-C3-C5	2.02	118.80	115.29
25	N	612	CLA	C2A-C1A-CHA	2.03	127.51	123.92
25	n	612	CLA	C2A-C1A-CHA	2.03	127.51	123.92
30	H	101	BCR	C2-C1-C6	2.03	113.64	110.48
25	G	604	CLA	O1D-CGD-CBD	2.03	128.24	124.60
25	C	511	CLA	CAA-C2A-C1A	2.03	118.61	111.97
30	C	517	BCR	C36-C18-C19	2.03	121.33	118.10
26	4	620	LUT	C20-C13-C12	2.03	121.33	118.10
30	c	514	BCR	C37-C22-C23	2.03	121.33	118.10
28	S	1623	NEX	C16-C1-C6	2.03	112.29	110.47
25	B	605	CLA	CMD-C2D-C3D	2.03	128.65	124.89
25	c	511	CLA	CAA-C2A-C1A	2.03	118.62	111.97
30	c	517	BCR	C36-C18-C19	2.03	121.33	118.10
24	1	607	CHL	C4-C3-C5	2.03	118.81	115.29
24	r	606	CHL	C4-C3-C5	2.03	118.81	115.29
25	s	610	CLA	O2D-CGD-CBD	2.03	114.93	111.30
25	R	611	CLA	O1D-CGD-CBD	2.03	128.25	124.60
25	2	602	CLA	O1D-CGD-CBD	2.03	128.25	124.60
28	G	1623	NEX	C28-C29-C30	2.03	122.06	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	614	CLA	CMD-C2D-C3D	2.03	128.67	124.89
25	s	613	CLA	C4A-NA-C1A	2.04	108.98	106.45
30	h	101	BCR	C2-C1-C6	2.04	113.66	110.48
25	S	610	CLA	O2D-CGD-CBD	2.04	114.94	111.30
36	D	405	PL9	O2-C1-C6	2.04	124.24	120.57
30	b	619	BCR	C34-C9-C8	2.04	121.35	118.10
25	y	614	CLA	C4A-NA-C1A	2.04	108.98	106.45
25	c	503	CLA	CMD-C2D-C3D	2.04	128.68	124.89
25	6	602	CLA	O1D-CGD-CBD	2.04	128.27	124.60
33	a	408	PHO	CHD-C4C-C3C	2.04	128.70	124.59
30	a	411	BCR	C33-C5-C4	2.04	117.33	113.45
25	b	612	CLA	CHC-C1C-NC	2.04	127.93	124.08
25	G	602	CLA	C4A-NA-C1A	2.04	108.99	106.45
25	S	613	CLA	C4A-NA-C1A	2.04	108.99	106.45
33	A	408	PHO	CHD-C4C-C3C	2.05	128.71	124.59
25	g	602	CLA	C4A-NA-C1A	2.05	108.99	106.45
25	C	503	CLA	CMD-C2D-C3D	2.05	128.69	124.89
25	b	605	CLA	CMD-C2D-C3D	2.05	128.69	124.89
26	7	1621	LUT	C39-C29-C28	2.05	121.36	118.10
25	c	508	CLA	C4A-NA-C1A	2.05	109.00	106.45
25	g	604	CLA	O1D-CGD-CBD	2.05	128.29	124.60
25	C	508	CLA	C4A-NA-C1A	2.05	109.00	106.45
26	3	1621	LUT	C39-C29-C28	2.05	121.37	118.10
30	d	404	BCR	C36-C18-C19	2.05	121.37	118.10
30	A	411	BCR	C33-C5-C4	2.05	117.35	113.45
30	B	619	BCR	C37-C22-C23	2.05	121.37	118.10
25	n	614	CLA	C4A-NA-C1A	2.05	109.00	106.45
24	3	609	CHL	C4D-C3D-CAD	2.05	109.48	104.71
34	a	418	SQD	C3-C4-C5	2.06	113.84	110.22
25	Y	604	CLA	CHB-C4A-NA	2.06	127.36	124.51
34	a	418	SQD	C44-O6-C1	2.06	117.98	113.76
24	R	608	CHL	CHB-C1B-C2B	2.06	122.69	116.99
25	B	614	CLA	C3A-C2A-C1A	2.06	104.42	101.34
25	2	603	CLA	C4A-NA-C1A	2.06	109.01	106.45
24	r	608	CHL	CHB-C1B-C2B	2.07	122.71	116.99
26	Y	1620	LUT	C36-C21-C26	2.07	112.79	109.59
24	4	608	CHL	C4D-C3D-CAD	2.07	109.51	104.71
30	D	404	BCR	C36-C18-C19	2.07	121.39	118.10
28	R	623	NEX	C40-C33-C32	2.07	121.39	118.10
34	A	418	SQD	C44-O6-C1	2.07	118.00	113.76
26	5	1620	LUT	C1-C2-C3	2.07	117.88	113.40
25	y	604	CLA	CHB-C4A-NA	2.07	127.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	610	CLA	C2A-C1A-CHA	2.07	127.59	123.92
30	b	619	BCR	C37-C22-C23	2.07	121.40	118.10
26	6	1620	LUT	C1-C2-C3	2.07	117.88	113.40
25	Y	612	CLA	O1D-CGD-CBD	2.07	128.33	124.60
24	8	608	CHL	C4D-C3D-CAD	2.08	109.53	104.71
25	3	613	CLA	C4A-NA-C1A	2.08	109.03	106.45
30	C	515	BCR	C36-C18-C19	2.08	121.41	118.10
24	5	606	CHL	CHB-C1B-C2B	2.08	122.74	116.99
25	N	614	CLA	C4A-NA-C1A	2.08	109.03	106.45
34	A	418	SQD	C3-C4-C5	2.08	113.88	110.22
26	y	1620	LUT	C36-C21-C26	2.08	112.81	109.59
25	B	612	CLA	CHC-C1C-NC	2.08	128.00	124.08
24	s	608	CHL	C4D-C3D-CAD	2.08	109.54	104.71
25	7	610	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	1	606	CHL	CHB-C1B-C2B	2.08	122.75	116.99
25	6	610	CLA	O1D-CGD-CBD	2.08	128.34	124.60
24	G	609	CHL	C1-O2A-CGA	2.08	121.77	116.77
25	g	610	CLA	C2A-C1A-CHA	2.08	127.61	123.92
28	r	623	NEX	C40-C33-C32	2.08	121.42	118.10
25	C	506	CLA	C4A-NA-C1A	2.08	109.04	106.45
24	g	609	CHL	C1-O2A-CGA	2.09	121.78	116.77
25	5	613	CLA	C4A-NA-C1A	2.09	109.04	106.45
34	b	621	SQD	C3-C4-C5	2.09	113.89	110.22
26	2	1620	LUT	C1-C2-C3	2.09	117.91	113.40
24	2	606	CHL	CED-O2D-CGD	2.09	120.86	115.97
25	7	604	CLA	C4A-NA-C1A	2.09	109.04	106.45
25	6	603	CLA	C4A-NA-C1A	2.09	109.04	106.45
26	1	1620	LUT	C1-C2-C3	2.09	117.91	113.40
24	s	606	CHL	C4D-C3D-CAD	2.09	109.56	104.71
24	S	606	CHL	C4D-C3D-CAD	2.09	109.56	104.71
25	c	506	CLA	C4A-NA-C1A	2.09	109.05	106.45
25	2	610	CLA	O1D-CGD-CBD	2.09	128.36	124.60
25	7	611	CLA	CAA-CBA-CGA	2.09	119.65	113.35
30	c	515	BCR	C36-C18-C19	2.09	121.43	118.10
24	6	606	CHL	CED-O2D-CGD	2.09	120.88	115.97
24	3	601	CHL	C1-O2A-CGA	2.09	121.80	116.77
25	s	613	CLA	CHB-C4A-NA	2.10	127.41	124.51
25	G	610	CLA	CAA-C2A-C1A	2.10	118.85	111.97
25	C	511	CLA	C4A-NA-C1A	2.10	109.06	106.45
25	3	604	CLA	C4A-NA-C1A	2.10	109.06	106.45
26	2	1621	LUT	C1-C2-C3	2.10	117.94	113.40
25	7	613	CLA	C4A-NA-C1A	2.10	109.06	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	601	CHL	C1-O2A-CGA	2.10	121.81	116.77
24	S	608	CHL	C4D-C3D-CAD	2.10	109.59	104.71
25	y	612	CLA	O1D-CGD-CBD	2.10	128.38	124.60
30	c	516	BCR	C35-C13-C12	2.10	121.45	118.10
25	7	612	CLA	O1D-CGD-CBD	2.10	128.38	124.60
25	c	513	CLA	O2D-CGD-CBD	2.10	115.05	111.30
25	g	610	CLA	CAA-C2A-C1A	2.10	118.86	111.97
30	C	516	BCR	C35-C13-C12	2.10	121.45	118.10
25	N	610	CLA	C2A-C1A-CHA	2.10	127.65	123.92
25	3	611	CLA	CAA-CBA-CGA	2.10	119.68	113.35
26	1	1620	LUT	C20-C13-C12	2.10	121.45	118.10
25	3	610	CLA	CHB-C4A-NA	2.10	127.42	124.51
24	n	601	CHL	C4D-C3D-CAD	2.10	109.60	104.71
26	6	1621	LUT	C1-C2-C3	2.11	117.95	113.40
26	5	1620	LUT	C20-C13-C12	2.11	121.45	118.10
25	C	507	CLA	C2A-C1A-CHA	2.11	127.65	123.92
25	C	513	CLA	O2D-CGD-CBD	2.11	115.06	111.30
25	c	507	CLA	C2A-C1A-CHA	2.11	127.66	123.92
24	N	601	CHL	C4D-C3D-CAD	2.11	109.61	104.71
33	a	408	PHO	CHB-C1B-NB	2.11	128.78	124.64
26	7	1620	LUT	C17-C1-C6	2.11	113.73	110.31
25	3	612	CLA	O1D-CGD-CBD	2.11	128.40	124.60
25	c	501	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	S	613	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	B	616	CLA	C4A-NA-C1A	2.12	109.08	106.45
26	n	1620	LUT	C36-C21-C26	2.12	112.86	109.59
25	R	610	CLA	O1D-CGD-CBD	2.12	128.41	124.60
25	A	405	CLA	CMD-C2D-C3D	2.12	128.82	124.89
33	A	408	PHO	CHB-C1B-NB	2.12	128.79	124.64
25	r	610	CLA	O1D-CGD-CBD	2.12	128.41	124.60
25	C	501	CLA	CHB-C4A-NA	2.12	127.44	124.51
25	6	611	CLA	C4A-NA-C1A	2.12	109.08	106.45
25	1	613	CLA	C4A-NA-C1A	2.12	109.08	106.45
34	B	621	SQD	C3-C4-C5	2.12	113.95	110.22
26	6	1620	LUT	C2-C3-C4	2.12	113.25	110.32
26	3	1620	LUT	C17-C1-C6	2.12	113.75	110.31
25	r	616	CLA	CMD-C2D-C3D	2.12	128.83	124.89
25	n	610	CLA	C2A-C1A-CHA	2.12	127.68	123.92
25	R	616	CLA	CMD-C2D-C3D	2.12	128.83	124.89
25	b	616	CLA	O2D-CGD-CBD	2.13	115.09	111.30
25	c	511	CLA	C4A-NA-C1A	2.13	109.09	106.45
25	C	506	CLA	O1D-CGD-CBD	2.13	128.42	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	601	CHL	CED-O2D-CGD	2.13	120.96	115.97
26	N	1620	LUT	C36-C21-C26	2.13	112.89	109.59
34	B	623	SQD	O5-C5-C4	2.13	113.58	109.66
25	8	603	CLA	CMD-C2D-C3D	2.13	128.85	124.89
34	b	623	SQD	O5-C5-C4	2.13	113.59	109.66
25	c	506	CLA	O1D-CGD-CBD	2.13	128.43	124.60
24	n	605	CHL	CHB-C1B-C2B	2.13	122.90	116.99
24	5	609	CHL	C4D-C3D-CAD	2.13	109.67	104.71
25	R	602	CLA	O2D-CGD-CBD	2.14	115.11	111.30
24	2	609	CHL	C4D-C3D-CAD	2.14	109.67	104.71
26	2	1620	LUT	C2-C3-C4	2.14	113.27	110.32
24	1	609	CHL	C4D-C3D-CAD	2.14	109.68	104.71
25	5	602	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	N	605	CHL	CHB-C1B-C2B	2.14	122.92	116.99
24	6	608	CHL	CHC-C4B-C3B	2.14	123.30	118.23
25	B	616	CLA	O2D-CGD-CBD	2.14	115.12	111.30
24	7	609	CHL	C4-C3-C5	2.14	119.00	115.29
30	b	619	BCR	C40-C30-C25	2.14	113.78	110.31
25	c	506	CLA	CHB-C4A-NA	2.14	127.47	124.51
24	R	607	CHL	CED-O2D-CGD	2.14	120.99	115.97
24	G	601	CHL	CHB-C1B-C2B	2.14	122.92	116.99
30	B	619	BCR	C40-C30-C25	2.14	113.78	110.31
25	2	611	CLA	C4A-NA-C1A	2.14	109.11	106.45
25	b	610	CLA	O1D-CGD-CBD	2.14	128.45	124.60
25	4	603	CLA	CMD-C2D-C3D	2.14	128.87	124.89
24	r	607	CHL	CED-O2D-CGD	2.14	120.99	115.97
24	2	608	CHL	CHC-C4B-C3B	2.14	123.31	118.23
25	S	602	CLA	CHB-C4A-NA	2.14	127.48	124.51
24	7	605	CHL	CHB-C1B-C2B	2.14	122.93	116.99
25	b	616	CLA	C4A-NA-C1A	2.14	109.11	106.45
24	3	609	CHL	C4-C3-C5	2.14	119.01	115.29
24	2	601	CHL	CED-O2D-CGD	2.15	121.00	115.97
25	a	405	CLA	CHB-C4A-NA	2.15	127.48	124.51
24	G	601	CHL	C4D-C3D-CAD	2.15	109.69	104.71
25	y	613	CLA	C2C-C1C-NC	2.15	111.70	110.22
33	A	408	PHO	C4A-NA-C1A	2.15	109.90	108.16
25	n	603	CLA	O1D-CGD-CBD	2.15	128.46	124.60
24	g	609	CHL	CHB-C1B-C2B	2.15	122.94	116.99
25	B	610	CLA	O1D-CGD-CBD	2.15	128.46	124.60
24	g	601	CHL	C4D-C3D-CAD	2.15	109.70	104.71
25	1	602	CLA	CHB-C4A-NA	2.15	127.48	124.51
25	C	506	CLA	CHB-C4A-NA	2.15	127.48	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	607	CHL	C4D-C3D-CAD	2.15	109.71	104.71
25	N	602	CLA	CHB-C4A-NA	2.15	127.49	124.51
24	3	605	CHL	CHB-C1B-C2B	2.15	122.95	116.99
24	G	609	CHL	CHB-C1B-C2B	2.15	122.95	116.99
25	s	602	CLA	CHB-C4A-NA	2.15	127.49	124.51
25	a	405	CLA	CMD-C2D-C3D	2.15	128.89	124.89
24	g	601	CHL	CHB-C1B-C2B	2.16	122.96	116.99
33	a	408	PHO	C4A-NA-C1A	2.16	109.91	108.16
24	6	609	CHL	C4D-C3D-CAD	2.16	109.72	104.71
24	n	609	CHL	C4-C3-C5	2.16	119.03	115.29
24	N	609	CHL	C4-C3-C5	2.16	119.03	115.29
25	y	603	CLA	CMB-C2B-C3B	2.16	128.90	124.89
33	A	409	PHO	CBD-CHA-C1A	2.16	131.45	126.36
24	8	607	CHL	C4D-C3D-CAD	2.16	109.73	104.71
25	r	602	CLA	O2D-CGD-CBD	2.16	115.16	111.30
25	8	611	CLA	CMD-C2D-C3D	2.17	128.91	124.89
25	D	402	CLA	O2D-CGD-CBD	2.17	115.17	111.30
25	d	402	CLA	O2D-CGD-CBD	2.17	115.17	111.30
25	N	603	CLA	O1D-CGD-CBD	2.17	128.49	124.60
25	Y	603	CLA	CMB-C2B-C3B	2.17	128.91	124.89
24	N	607	CHL	CHB-C1B-C2B	2.17	122.99	116.99
25	4	611	CLA	CMD-C2D-C3D	2.17	128.92	124.89
24	n	607	CHL	CHB-C1B-C2B	2.17	123.00	116.99
36	d	405	PL9	C20-C19-C21	2.17	119.06	115.29
25	n	602	CLA	CHB-C4A-NA	2.17	127.52	124.51
24	8	609	CHL	CHB-C1B-C2B	2.17	123.01	116.99
24	4	609	CHL	CHB-C1B-C2B	2.17	123.01	116.99
33	a	409	PHO	CBD-CHA-C1A	2.17	131.48	126.36
24	6	608	CHL	CHB-C1B-C2B	2.17	123.01	116.99
36	D	405	PL9	C20-C19-C21	2.17	119.06	115.29
24	s	607	CHL	CED-O2D-CGD	2.18	121.07	115.97
25	R	603	CLA	C4A-NA-C1A	2.18	109.15	106.45
26	6	1621	LUT	C36-C21-C26	2.18	112.96	109.59
26	s	1621	LUT	C2-C3-C4	2.18	113.33	110.32
30	C	516	BCR	C33-C5-C4	2.18	117.59	113.45
25	1	612	CLA	O2D-CGD-CBD	2.18	115.20	111.30
30	c	516	BCR	C33-C5-C4	2.18	117.59	113.45
25	r	603	CLA	C4A-NA-C1A	2.18	109.16	106.45
25	5	612	CLA	O2D-CGD-CBD	2.18	115.20	111.30
25	g	604	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	A	410	CLA	O2D-CGD-CBD	2.19	115.21	111.30
28	G	1623	NEX	C16-C1-C6	2.19	112.43	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	607	CHL	C4-C3-C5	2.19	119.09	115.29
25	B	610	CLA	C4A-NA-C1A	2.19	109.17	106.45
25	B	612	CLA	OBD-CAD-C3D	2.19	132.06	128.03
25	1	603	CLA	C2A-C1A-CHA	2.19	127.80	123.92
24	S	607	CHL	CED-O2D-CGD	2.19	121.11	115.97
24	G	607	CHL	CHB-C1B-C2B	2.19	123.06	116.99
25	A	405	CLA	CHB-C4A-NA	2.19	127.54	124.51
25	3	613	CLA	CMD-C2D-C3D	2.19	128.96	124.89
25	2	614	CLA	O1D-CGD-CBD	2.19	128.54	124.60
25	g	614	CLA	CHB-C4A-NA	2.19	127.55	124.51
24	2	608	CHL	CHB-C1B-C2B	2.19	123.06	116.99
25	Y	613	CLA	C2C-C1C-NC	2.19	111.73	110.22
25	6	614	CLA	O1D-CGD-CBD	2.19	128.54	124.60
25	B	611	CLA	C4A-NA-C1A	2.19	109.18	106.45
25	5	603	CLA	C2A-C1A-CHA	2.19	127.81	123.92
26	2	1621	LUT	C36-C21-C26	2.20	112.99	109.59
25	b	612	CLA	OBD-CAD-C3D	2.20	132.07	128.03
25	n	604	CLA	CHB-C4A-NA	2.20	127.55	124.51
24	g	607	CHL	CHB-C1B-C2B	2.20	123.08	116.99
25	N	603	CLA	C1C-NC-C4C	2.20	108.32	107.06
24	4	608	CHL	CHB-C1B-C2B	2.20	123.09	116.99
24	S	601	CHL	C4D-C3D-CAD	2.20	109.83	104.71
28	R	623	NEX	C2-C1-C6	2.20	111.35	109.21
25	N	604	CLA	CHB-C4A-NA	2.20	127.56	124.51
24	7	605	CHL	C4D-C3D-CAD	2.20	109.83	104.71
24	2	607	CHL	C4D-C3D-CAD	2.20	109.83	104.71
24	s	601	CHL	C4D-C3D-CAD	2.20	109.83	104.71
24	6	607	CHL	C4-C3-C5	2.20	119.11	115.29
26	S	1621	LUT	C2-C3-C4	2.20	113.36	110.32
25	b	611	CLA	C4A-NA-C1A	2.20	109.19	106.45
25	b	610	CLA	C4A-NA-C1A	2.20	109.19	106.45
24	8	608	CHL	CHB-C1B-C2B	2.20	123.09	116.99
25	4	603	CLA	C4A-NA-C1A	2.21	109.19	106.45
25	b	611	CLA	C2A-C1A-CHA	2.21	127.83	123.92
24	6	607	CHL	C4D-C3D-CAD	2.21	109.84	104.71
25	7	613	CLA	CMD-C2D-C3D	2.21	128.99	124.89
25	g	602	CLA	CMD-C2D-C3D	2.21	128.99	124.89
25	G	604	CLA	CHB-C4A-NA	2.21	127.56	124.51
24	Y	606	CHL	C4D-C3D-CAD	2.21	109.84	104.71
24	7	601	CHL	C4-C3-C5	2.21	119.12	115.29
24	y	606	CHL	C4D-C3D-CAD	2.21	109.84	104.71
25	8	603	CLA	C4A-NA-C1A	2.21	109.20	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	609	CHL	C4D-C3D-CAD	2.21	109.85	104.71
25	G	602	CLA	CMD-C2D-C3D	2.21	129.00	124.89
25	s	609	CLA	CMD-C2D-C3D	2.21	129.00	124.89
24	N	609	CHL	C4D-C3D-CAD	2.21	109.85	104.71
25	N	613	CLA	CAC-C3C-C4C	2.21	127.95	124.83
24	3	605	CHL	C4D-C3D-CAD	2.21	109.85	104.71
25	B	608	CLA	C4A-NA-C1A	2.21	109.20	106.45
25	S	609	CLA	CMD-C2D-C3D	2.21	129.00	124.89
24	n	601	CHL	C1-O2A-CGA	2.21	122.08	116.77
25	4	604	CLA	CMD-C2D-C3D	2.21	129.00	124.89
25	7	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	N	601	CHL	C1-O2A-CGA	2.22	122.09	116.77
24	r	608	CHL	C4D-C3D-CAD	2.22	109.86	104.71
28	g	1623	NEX	C16-C1-C6	2.22	112.46	110.47
30	c	516	BCR	C29-C30-C25	2.22	113.94	110.48
24	Y	608	CHL	C4D-C3D-CAD	2.22	109.86	104.71
24	3	601	CHL	C4-C3-C5	2.22	119.14	115.29
25	n	613	CLA	CAC-C3C-C4C	2.22	127.96	124.83
27	r	622	XAT	C20-C13-C12	2.22	121.63	118.10
25	a	410	CLA	O2D-CGD-CBD	2.22	115.26	111.30
30	C	516	BCR	C29-C30-C25	2.22	113.95	110.48
25	7	602	CLA	O1D-CGD-CBD	2.22	128.59	124.60
25	r	613	CLA	CMD-C2D-C3D	2.22	129.01	124.89
25	3	614	CLA	C4A-NA-C1A	2.22	109.21	106.45
24	4	609	CHL	C4D-C3D-CAD	2.22	109.87	104.71
25	B	611	CLA	C2A-C1A-CHA	2.22	127.86	123.92
27	n	1622	XAT	C38-C25-C24	2.22	116.82	114.28
25	7	614	CLA	C4A-NA-C1A	2.22	109.21	106.45
28	r	623	NEX	C2-C1-C6	2.22	111.37	109.21
25	S	609	CLA	O2D-CGD-CBD	2.22	115.27	111.30
25	n	603	CLA	C1C-NC-C4C	2.22	108.33	107.06
25	s	609	CLA	CHB-C4A-NA	2.22	127.59	124.51
25	R	613	CLA	CMD-C2D-C3D	2.22	129.02	124.89
24	R	608	CHL	C4D-C3D-CAD	2.23	109.88	104.71
24	G	607	CHL	C4D-C3D-CAD	2.23	109.88	104.71
25	S	609	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	8	611	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	b	608	CLA	C4A-NA-C1A	2.23	109.22	106.45
24	y	608	CHL	C4D-C3D-CAD	2.23	109.89	104.71
25	3	602	CLA	CHB-C4A-NA	2.23	127.59	124.51
27	R	622	XAT	C20-C13-C12	2.23	121.65	118.10
27	n	1622	XAT	C40-C33-C32	2.23	121.65	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	609	CLA	O2D-CGD-CBD	2.23	115.28	111.30
25	G	614	CLA	CHB-C4A-NA	2.23	127.60	124.51
25	C	509	CLA	C4A-NA-C1A	2.23	109.22	106.45
24	7	608	CHL	C4D-C3D-CAD	2.23	109.89	104.71
26	Y	1621	LUT	C19-C9-C8	2.23	121.66	118.10
25	R	611	CLA	CHB-C4A-NA	2.23	127.60	124.51
25	2	612	CLA	CMB-C2B-C3B	2.23	129.04	124.89
24	R	608	CHL	C4-C3-C5	2.23	119.16	115.29
24	8	609	CHL	C4D-C3D-CAD	2.23	109.90	104.71
24	g	607	CHL	C4D-C3D-CAD	2.23	109.90	104.71
25	8	604	CLA	CMD-C2D-C3D	2.24	129.04	124.89
24	3	601	CHL	CMD-C2D-C3D	2.24	119.93	114.27
25	6	612	CLA	CMB-C2B-C3B	2.24	129.04	124.89
25	3	602	CLA	O1D-CGD-CBD	2.24	128.62	124.60
27	N	1622	XAT	C38-C25-C24	2.24	116.84	114.28
25	s	603	CLA	C4A-NA-C1A	2.24	109.23	106.45
26	y	1621	LUT	C19-C9-C8	2.24	121.67	118.10
24	6	605	CHL	C4D-C3D-CAD	2.24	109.92	104.71
25	n	612	CLA	C4A-NA-C1A	2.24	109.24	106.45
24	2	605	CHL	C4D-C3D-CAD	2.24	109.92	104.71
25	N	612	CLA	C4A-NA-C1A	2.24	109.24	106.45
25	B	611	CLA	O1D-CGD-CBD	2.25	128.64	124.60
24	3	608	CHL	C4D-C3D-CAD	2.25	109.94	104.71
26	5	1620	LUT	C40-C33-C32	2.25	121.68	118.10
25	S	603	CLA	C4A-NA-C1A	2.25	109.25	106.45
27	N	1622	XAT	C28-C29-C30	2.25	122.39	118.94
27	N	1622	XAT	C40-C33-C32	2.25	121.69	118.10
26	s	1620	LUT	C20-C13-C12	2.25	121.69	118.10
24	R	607	CHL	CHB-C1B-C2B	2.25	123.23	116.99
26	s	1621	LUT	C39-C29-C28	2.25	121.69	118.10
24	r	608	CHL	C4-C3-C5	2.25	119.20	115.29
24	7	601	CHL	CMD-C2D-C3D	2.26	119.98	114.27
25	4	611	CLA	CHB-C4A-NA	2.26	127.63	124.51
25	Y	604	CLA	O1D-CGD-CBD	2.26	128.66	124.60
25	n	611	CLA	CMD-C2D-C3D	2.26	129.08	124.89
25	8	612	CLA	CMD-C2D-C3D	2.26	129.08	124.89
25	c	509	CLA	C4A-NA-C1A	2.26	109.25	106.45
26	S	1621	LUT	C39-C29-C28	2.26	121.70	118.10
26	2	1620	LUT	C39-C29-C28	2.26	121.70	118.10
25	C	502	CLA	O1D-CGD-CBD	2.26	128.66	124.60
25	B	605	CLA	C2A-C1A-CHA	2.26	127.93	123.92
25	b	605	CLA	C2A-C1A-CHA	2.26	127.93	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	604	CLA	O1D-CGD-CBD	2.26	128.66	124.60
24	r	607	CHL	CHB-C1B-C2B	2.26	123.25	116.99
26	S	1620	LUT	C20-C13-C12	2.26	121.70	118.10
25	n	611	CLA	CMB-C2B-C3B	2.26	129.09	124.89
37	c	518	DGD	O6E-C5E-C4E	2.26	113.83	109.66
25	6	612	CLA	C2A-C1A-CHA	2.26	127.93	123.92
24	5	608	CHL	C4D-C3D-CAD	2.27	109.97	104.71
26	1	1620	LUT	C40-C33-C32	2.27	121.71	118.10
27	4	622	XAT	C38-C25-C24	2.27	116.88	114.28
25	6	613	CLA	O1D-CGD-CBD	2.27	128.68	124.60
25	4	612	CLA	CMD-C2D-C3D	2.27	129.10	124.89
24	y	608	CHL	C6-C5-C3	2.27	117.80	112.66
25	b	615	CLA	O1D-CGD-CBD	2.27	128.68	124.60
25	r	611	CLA	CHB-C4A-NA	2.27	127.65	124.51
24	y	605	CHL	C4D-C3D-CAD	2.27	109.98	104.71
25	2	612	CLA	C2C-C1C-NC	2.27	111.78	110.22
24	Y	605	CHL	C4D-C3D-CAD	2.27	109.98	104.71
25	b	611	CLA	O1D-CGD-CBD	2.27	128.68	124.60
25	2	613	CLA	O1D-CGD-CBD	2.27	128.68	124.60
24	s	607	CHL	CHC-C4B-C3B	2.27	123.61	118.23
25	b	616	CLA	C3A-C2A-C1A	2.27	104.74	101.34
24	1	608	CHL	C4D-C3D-CAD	2.27	109.98	104.71
27	n	1622	XAT	C28-C29-C30	2.27	122.43	118.94
26	6	1620	LUT	C39-C29-C28	2.27	121.72	118.10
24	S	607	CHL	CHC-C4B-C3B	2.27	123.62	118.23
30	8	623	BCR	C29-C30-C25	2.28	114.03	110.48
25	y	611	CLA	CMB-C2B-C3B	2.28	129.12	124.89
25	2	612	CLA	C2A-C1A-CHA	2.28	127.95	123.92
24	y	605	CHL	CHB-C1B-C2B	2.28	123.30	116.99
24	Y	605	CHL	CHB-C1B-C2B	2.28	123.30	116.99
24	5	607	CHL	CMD-C2D-C3D	2.28	120.03	114.27
24	g	601	CHL	C1-O2A-CGA	2.28	122.24	116.77
25	c	502	CLA	O1D-CGD-CBD	2.28	128.69	124.60
25	B	615	CLA	O1D-CGD-CBD	2.28	128.70	124.60
25	N	611	CLA	CMD-C2D-C3D	2.28	129.12	124.89
37	C	518	DGD	O6E-C5E-C4E	2.28	113.86	109.66
34	b	623	SQD	C44-O6-C1	2.28	118.43	113.76
27	8	622	XAT	C38-C25-C24	2.28	116.89	114.28
24	8	606	CHL	C4D-C3D-CAD	2.28	110.01	104.71
24	1	607	CHL	CMD-C2D-C3D	2.28	120.05	114.27
24	Y	608	CHL	C6-C5-C3	2.28	117.83	112.66
25	N	611	CLA	CMB-C2B-C3B	2.28	129.13	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	601	CHL	C1-O2A-CGA	2.28	122.25	116.77
25	7	611	CLA	C4A-NA-C1A	2.28	109.29	106.45
25	3	611	CLA	C4A-NA-C1A	2.28	109.29	106.45
24	3	601	CHL	O2A-CGA-CBA	2.29	118.55	111.90
25	Y	603	CLA	OBD-CAD-C3D	2.29	132.24	128.03
25	Y	611	CLA	CMB-C2B-C3B	2.29	129.14	124.89
26	G	1621	LUT	C1-C2-C3	2.29	118.35	113.40
25	s	604	CLA	CMD-C2D-C3D	2.29	129.14	124.89
30	4	623	BCR	C29-C30-C25	2.29	114.06	110.48
25	s	603	CLA	C2A-C1A-CHA	2.29	127.98	123.92
30	c	514	BCR	C34-C9-C8	2.29	121.75	118.10
25	S	603	CLA	C2A-C1A-CHA	2.29	127.98	123.92
30	C	514	BCR	C34-C9-C8	2.29	121.75	118.10
24	N	607	CHL	CHC-C4B-C3B	2.30	123.67	118.23
25	b	609	CLA	C4A-NA-C1A	2.30	109.30	106.45
25	y	603	CLA	OBD-CAD-C3D	2.30	132.25	128.03
24	4	606	CHL	C4D-C3D-CAD	2.30	110.05	104.71
30	t	101	BCR	C29-C30-C25	2.30	114.07	110.48
24	G	606	CHL	CHC-C4B-C3B	2.30	123.67	118.23
26	g	1621	LUT	C1-C2-C3	2.30	118.37	113.40
28	R	623	NEX	C38-C25-C24	2.30	116.91	114.28
34	B	623	SQD	C44-O6-C1	2.30	118.47	113.76
24	7	601	CHL	O2A-CGA-CBA	2.30	118.59	111.90
25	b	614	CLA	CHB-C4A-NA	2.30	127.69	124.51
27	4	622	XAT	C19-C9-C8	2.30	121.77	118.10
25	B	616	CLA	C3A-C2A-C1A	2.30	104.79	101.34
26	3	1620	LUT	C39-C29-C28	2.30	121.77	118.10
24	s	607	CHL	C4D-C3D-CAD	2.31	110.06	104.71
25	c	509	CLA	CMD-C2D-C3D	2.31	129.17	124.89
24	s	607	CHL	CHB-C1B-C2B	2.31	123.38	116.99
24	g	606	CHL	CHC-C4B-C3B	2.31	123.69	118.23
24	6	606	CHL	CHC-C4B-C3B	2.31	123.70	118.23
25	B	614	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	c	501	CLA	CMD-C2D-C3D	2.31	129.18	124.89
24	2	608	CHL	C4D-C3D-CAD	2.31	110.07	104.71
25	B	604	CLA	O2D-CGD-CBD	2.31	115.42	111.30
25	7	603	CLA	C2A-C1A-CHA	2.31	128.01	123.92
26	7	1620	LUT	C39-C29-C28	2.31	121.78	118.10
25	C	509	CLA	CMD-C2D-C3D	2.31	129.18	124.89
25	b	616	CLA	CMB-C2B-C3B	2.31	129.18	124.89
24	n	607	CHL	CHC-C4B-C3B	2.31	123.71	118.23
33	a	409	PHO	O1D-CGD-CBD	2.31	128.76	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	622	XAT	C19-C9-C8	2.31	121.79	118.10
25	B	609	CLA	C4A-NA-C1A	2.31	109.33	106.45
25	R	604	CLA	CBA-CAA-C2A	2.32	120.73	113.80
24	8	601	CHL	CHB-C4A-C3A	2.32	123.39	117.08
25	S	604	CLA	CMD-C2D-C3D	2.32	129.19	124.89
29	N	2630	LHG	O8-C23-C24	2.32	118.65	111.90
34	a	418	SQD	O48-C23-C24	2.32	118.65	111.90
25	8	610	CLA	CHB-C4A-NA	2.32	127.72	124.51
25	y	613	CLA	CAC-C3C-C4C	2.32	128.10	124.83
27	1	1622	XAT	C18-C5-C4	2.32	116.94	114.28
25	r	616	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	2	601	CHL	CHB-C1B-C2B	2.32	123.42	116.99
30	T	101	BCR	C29-C30-C25	2.32	114.11	110.48
25	b	604	CLA	O2D-CGD-CBD	2.32	115.45	111.30
24	S	607	CHL	CHB-C1B-C2B	2.32	123.42	116.99
25	7	612	CLA	OBD-CAD-C3D	2.32	132.31	128.03
24	4	601	CHL	CHB-C4A-C3A	2.32	123.40	117.08
25	R	612	CLA	CMB-C2B-C3B	2.32	129.20	124.89
24	6	608	CHL	C4D-C3D-CAD	2.32	110.11	104.71
29	n	2630	LHG	O8-C23-C24	2.32	118.66	111.90
24	S	607	CHL	C4D-C3D-CAD	2.32	110.11	104.71
24	2	606	CHL	CHC-C4B-C3B	2.32	123.73	118.23
24	4	609	CHL	CMD-C2D-C3D	2.32	120.15	114.27
25	4	610	CLA	CHB-C4A-NA	2.32	127.73	124.51
26	y	1620	LUT	C39-C29-C28	2.33	121.80	118.10
33	A	409	PHO	O1D-CGD-CBD	2.33	128.78	124.60
24	S	606	CHL	CHB-C1B-C2B	2.33	123.43	116.99
27	5	1622	XAT	C18-C5-C4	2.33	116.94	114.28
25	r	604	CLA	CBA-CAA-C2A	2.33	120.76	113.80
24	2	609	CHL	CHB-C1B-C2B	2.33	123.44	116.99
24	s	606	CHL	CHB-C1B-C2B	2.33	123.44	116.99
24	R	607	CHL	C4D-C3D-CAD	2.33	110.12	104.71
25	R	616	CLA	CHB-C4A-NA	2.33	127.73	124.51
24	y	609	CHL	CHB-C1B-C2B	2.33	123.44	116.99
24	6	601	CHL	CHB-C1B-C2B	2.33	123.44	116.99
34	A	418	SQD	O48-C23-C24	2.33	118.68	111.90
24	Y	609	CHL	CHB-C1B-C2B	2.33	123.44	116.99
25	Y	612	CLA	CMB-C2B-C3B	2.33	129.22	124.89
26	3	1620	LUT	C20-C13-C12	2.33	121.81	118.10
25	C	501	CLA	CMD-C2D-C3D	2.33	129.22	124.89
24	y	609	CHL	C4D-C3D-CAD	2.33	110.13	104.71
25	y	612	CLA	CMB-C2B-C3B	2.33	129.22	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	612	CLA	CMB-C2B-C3B	2.33	129.22	124.89
28	n	1623	NEX	C28-C29-C30	2.33	122.52	118.94
25	6	612	CLA	C2C-C1C-NC	2.33	111.83	110.22
25	3	603	CLA	C2A-C1A-CHA	2.33	128.06	123.92
25	B	616	CLA	CMB-C2B-C3B	2.33	129.22	124.89
25	r	611	CLA	CMB-C2B-C3B	2.34	129.23	124.89
24	Y	609	CHL	C4D-C3D-CAD	2.34	110.14	104.71
24	8	609	CHL	CMD-C2D-C3D	2.34	120.19	114.27
24	3	607	CHL	C4D-C3D-CAD	2.34	110.14	104.71
26	Y	1620	LUT	C39-C29-C28	2.34	121.83	118.10
25	B	611	CLA	C3A-C2A-C1A	2.34	104.85	101.34
24	r	607	CHL	C4D-C3D-CAD	2.34	110.15	104.71
24	2	606	CHL	C4D-C3D-CAD	2.34	110.15	104.71
28	N	1623	NEX	C28-C29-C30	2.34	122.54	118.94
25	b	611	CLA	C3A-C2A-C1A	2.34	104.85	101.34
28	r	623	NEX	C38-C25-C24	2.34	116.96	114.28
25	3	612	CLA	OBD-CAD-C3D	2.34	132.35	128.03
24	r	614	CHL	C4D-C3D-CAD	2.34	110.16	104.71
24	n	609	CHL	CHC-C4B-C3B	2.34	123.78	118.23
25	7	603	CLA	C4A-NA-C1A	2.35	109.36	106.45
24	6	609	CHL	CHB-C1B-C2B	2.35	123.49	116.99
26	7	1620	LUT	C20-C13-C12	2.35	121.84	118.10
25	R	611	CLA	CMB-C2B-C3B	2.35	129.25	124.89
24	N	609	CHL	O2A-CGA-CBA	2.35	118.73	111.90
25	g	603	CLA	CMD-C2D-C3D	2.35	129.25	124.89
24	6	606	CHL	C4D-C3D-CAD	2.35	110.17	104.71
25	N	602	CLA	CAC-C3C-C4C	2.35	128.14	124.83
25	2	610	CLA	CMD-C2D-C3D	2.35	129.25	124.89
26	n	1620	LUT	C19-C9-C8	2.35	121.84	118.10
24	g	601	CHL	CMD-C2D-C3D	2.35	120.22	114.27
25	6	610	CLA	CMD-C2D-C3D	2.35	129.26	124.89
24	G	601	CHL	CMD-C2D-C3D	2.35	120.22	114.27
25	2	611	CLA	CHB-C4A-NA	2.35	127.77	124.51
25	Y	613	CLA	CAC-C3C-C4C	2.35	128.15	124.83
24	N	609	CHL	CHC-C4B-C3B	2.36	123.81	118.23
25	6	611	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	y	614	CLA	CMB-C2B-C3B	2.36	129.27	124.89
24	n	609	CHL	O2A-CGA-CBA	2.36	118.77	111.90
25	G	603	CLA	CMD-C2D-C3D	2.36	129.28	124.89
26	N	1620	LUT	C19-C9-C8	2.36	121.86	118.10
24	7	607	CHL	C4D-C3D-CAD	2.36	110.20	104.71
26	s	1620	LUT	C19-C9-C8	2.36	121.87	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	606	CHL	C4D-C3D-CAD	2.37	110.20	104.71
24	R	614	CHL	C4D-C3D-CAD	2.37	110.20	104.71
25	3	603	CLA	C4A-NA-C1A	2.37	109.39	106.45
24	5	609	CHL	CHB-C1B-C2B	2.37	123.55	116.99
25	2	604	CLA	CMD-C2D-C3D	2.37	129.29	124.89
25	Y	614	CLA	CMB-C2B-C3B	2.37	129.30	124.89
24	1	609	CHL	CHB-C1B-C2B	2.37	123.56	116.99
26	S	1620	LUT	C19-C9-C8	2.37	121.88	118.10
25	a	406	CLA	C4A-NA-C1A	2.37	109.40	106.45
24	n	608	CHL	C4D-C3D-CAD	2.37	110.23	104.71
25	6	604	CLA	CMD-C2D-C3D	2.38	129.30	124.89
24	y	601	CHL	C4D-C3D-CAD	2.38	110.23	104.71
24	Y	601	CHL	C4D-C3D-CAD	2.38	110.23	104.71
24	n	606	CHL	C4D-C3D-CAD	2.38	110.23	104.71
24	G	609	CHL	C4D-C3D-CAD	2.38	110.23	104.71
26	R	620	LUT	C19-C9-C8	2.38	121.89	118.10
25	1	613	CLA	CMD-C2D-C3D	2.38	129.31	124.89
25	6	602	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	Y	606	CHL	CHB-C1B-C2B	2.38	123.59	116.99
25	2	602	CLA	CHB-C4A-NA	2.38	127.81	124.51
24	8	609	CHL	CHC-C4B-C3B	2.38	123.87	118.23
24	g	605	CHL	CHB-C1B-C2B	2.38	123.59	116.99
24	y	606	CHL	CHB-C1B-C2B	2.38	123.59	116.99
24	n	601	CHL	O2A-CGA-CBA	2.38	118.83	111.90
26	s	1621	LUT	C19-C9-C8	2.38	121.90	118.10
24	Y	605	CHL	O2A-CGA-CBA	2.39	118.84	111.90
25	Y	602	CLA	CMD-C2D-C3D	2.39	129.32	124.89
24	g	609	CHL	C4D-C3D-CAD	2.39	110.25	104.71
33	A	409	PHO	C1B-NB-C4B	2.39	111.25	106.52
24	R	614	CHL	CMD-C2D-C3D	2.39	120.31	114.27
24	G	605	CHL	CHB-C1B-C2B	2.39	123.60	116.99
25	5	613	CLA	CMD-C2D-C3D	2.39	129.32	124.89
25	y	602	CLA	CMD-C2D-C3D	2.39	129.32	124.89
34	A	418	SQD	O47-C45-C44	2.39	117.12	108.44
24	r	606	CHL	C4D-C3D-CAD	2.39	110.26	104.71
24	4	609	CHL	CHC-C4B-C3B	2.39	123.89	118.23
24	N	608	CHL	C4D-C3D-CAD	2.39	110.26	104.71
24	y	605	CHL	O2A-CGA-CBA	2.39	118.86	111.90
25	B	606	CLA	CMB-C2B-C3B	2.39	129.33	124.89
24	R	606	CHL	C4D-C3D-CAD	2.39	110.27	104.71
25	g	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	Y	607	CHL	O2A-CGA-CBA	2.39	118.87	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	607	CHL	C4D-C3D-CAD	2.40	110.27	104.71
26	r	620	LUT	C19-C9-C8	2.40	121.92	118.10
33	a	409	PHO	C1B-NB-C4B	2.40	111.27	106.52
24	G	609	CHL	CHC-C4B-C3B	2.40	123.91	118.23
24	N	601	CHL	O2A-CGA-CBA	2.40	118.88	111.90
25	G	613	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	n	602	CLA	CAC-C3C-C4C	2.40	128.21	124.83
24	g	609	CHL	CHC-C4B-C3B	2.40	123.91	118.23
24	y	607	CHL	C4D-C3D-CAD	2.40	110.28	104.71
25	b	611	CLA	CMD-C2D-C3D	2.40	129.34	124.89
24	y	607	CHL	O2A-CGA-CBA	2.40	118.88	111.90
34	a	418	SQD	O47-C45-C44	2.40	117.16	108.44
26	N	1621	LUT	C19-C9-C8	2.40	121.92	118.10
28	5	1623	NEX	C2-C1-C6	2.40	111.54	109.21
24	r	614	CHL	CMD-C2D-C3D	2.40	120.34	114.27
25	B	611	CLA	CMD-C2D-C3D	2.40	129.35	124.89
24	g	606	CHL	C4D-C3D-CAD	2.40	110.29	104.71
26	G	1621	LUT	C19-C9-C8	2.40	121.93	118.10
26	S	1621	LUT	C19-C9-C8	2.41	121.93	118.10
24	g	605	CHL	CHC-C4B-C3B	2.41	123.93	118.23
25	b	606	CLA	CMB-C2B-C3B	2.41	129.36	124.89
25	R	613	CLA	C4A-NA-C1A	2.41	109.45	106.45
25	C	512	CLA	CHB-C4A-NA	2.41	127.85	124.51
24	G	606	CHL	C4D-C3D-CAD	2.41	110.32	104.71
26	N	1620	LUT	C39-C29-C28	2.42	121.95	118.10
26	n	1621	LUT	C19-C9-C8	2.42	121.95	118.10
25	y	611	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	S	610	CLA	CMD-C2D-C3D	2.42	129.38	124.89
28	1	1623	NEX	C2-C1-C6	2.42	111.56	109.21
25	A	406	CLA	C4A-NA-C1A	2.42	109.46	106.45
25	N	604	CLA	O1D-CGD-CBD	2.42	128.95	124.60
24	G	605	CHL	CHC-C4B-C3B	2.42	123.97	118.23
25	n	604	CLA	O1D-CGD-CBD	2.42	128.96	124.60
25	r	613	CLA	C4A-NA-C1A	2.42	109.46	106.45
25	R	613	CLA	CMB-C2B-C3B	2.42	129.39	124.89
25	c	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	1	1620	LUT	C39-C29-C28	2.43	121.97	118.10
24	R	607	CHL	CMD-C2D-C3D	2.43	120.41	114.27
25	c	512	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	A	406	CLA	O2D-CGD-CBD	2.43	115.64	111.30
24	r	607	CHL	CMD-C2D-C3D	2.43	120.41	114.27
25	C	510	CLA	CHB-C4A-NA	2.43	127.87	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	613	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	g	1621	LUT	C19-C9-C8	2.43	121.97	118.10
29	r	2630	LHG	O8-C23-C24	2.43	118.97	111.90
25	N	613	CLA	CHB-C4A-NA	2.43	127.88	124.51
25	n	602	CLA	CMD-C2D-C3D	2.43	129.41	124.89
26	n	1620	LUT	C39-C29-C28	2.44	121.98	118.10
30	b	619	BCR	C29-C30-C25	2.44	114.29	110.48
26	s	1620	LUT	C39-C29-C28	2.44	121.98	118.10
29	R	2630	LHG	O8-C23-C24	2.44	118.99	111.90
25	R	616	CLA	C4A-NA-C1A	2.44	109.48	106.45
25	r	616	CLA	C4A-NA-C1A	2.44	109.48	106.45
25	a	406	CLA	O2D-CGD-CBD	2.44	115.66	111.30
25	R	612	CLA	C4A-NA-C1A	2.44	109.48	106.45
25	r	612	CLA	C4A-NA-C1A	2.44	109.48	106.45
25	Y	611	CLA	CHB-C4A-NA	2.44	127.89	124.51
30	B	619	BCR	C29-C30-C25	2.44	114.29	110.48
25	r	613	CLA	CMB-C2B-C3B	2.44	129.42	124.89
25	N	602	CLA	CMD-C2D-C3D	2.44	129.42	124.89
28	6	1623	NEX	C28-C29-C30	2.44	122.69	118.94
25	C	507	CLA	CMD-C2D-C3D	2.44	129.43	124.89
24	S	607	CHL	C4-C3-C5	2.44	119.53	115.29
25	N	610	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	s	607	CHL	C4-C3-C5	2.45	119.53	115.29
25	s	604	CLA	C4A-NA-C1A	2.45	109.49	106.45
26	5	1620	LUT	C39-C29-C28	2.45	122.00	118.10
25	s	610	CLA	CMD-C2D-C3D	2.45	129.43	124.89
25	S	604	CLA	C4A-NA-C1A	2.45	109.49	106.45
26	2	1620	LUT	C19-C9-C8	2.45	122.00	118.10
25	G	611	CLA	C4A-NA-C1A	2.45	109.49	106.45
25	a	410	CLA	C4A-NA-C1A	2.45	109.49	106.45
26	S	1620	LUT	C39-C29-C28	2.45	122.00	118.10
25	y	610	CLA	CHB-C4A-NA	2.45	127.90	124.51
26	6	1620	LUT	C19-C9-C8	2.45	122.01	118.10
24	y	601	CHL	CHB-C1B-C2B	2.45	123.79	116.99
25	7	614	CLA	CMD-C2D-C3D	2.46	129.45	124.89
25	A	410	CLA	C4A-NA-C1A	2.46	109.50	106.45
24	5	606	CHL	CHC-C4B-C3B	2.46	124.05	118.23
25	1	610	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	G	603	CLA	CMB-C2B-C3B	2.46	129.46	124.89
25	C	504	CLA	CMD-C2D-C3D	2.46	129.46	124.89
25	c	507	CLA	CMD-C2D-C3D	2.46	129.46	124.89
25	1	603	CLA	C4A-NA-C1A	2.46	109.51	106.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	609	CHL	O2A-CGA-CBA	2.46	119.06	111.90
25	g	611	CLA	C4A-NA-C1A	2.46	109.51	106.45
25	5	603	CLA	C4A-NA-C1A	2.46	109.51	106.45
24	1	606	CHL	CHC-C4B-C3B	2.46	124.06	118.23
26	g	1620	LUT	C19-C9-C8	2.46	122.02	118.10
24	Y	605	CHL	CHC-C4B-C3B	2.46	124.06	118.23
25	n	610	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	7	613	CLA	CMB-C2B-C3B	2.46	129.47	124.89
25	g	603	CLA	CMB-C2B-C3B	2.46	129.47	124.89
25	b	603	CLA	CMD-C2D-C3D	2.46	129.47	124.89
24	Y	601	CHL	CHB-C1B-C2B	2.47	123.82	116.99
24	7	601	CHL	CHB-C1B-C2B	2.47	123.82	116.99
25	3	614	CLA	CMD-C2D-C3D	2.47	129.47	124.89
25	c	504	CLA	CMD-C2D-C3D	2.47	129.47	124.89
25	C	506	CLA	CMD-C2D-C3D	2.47	129.47	124.89
25	5	610	CLA	CHB-C4A-NA	2.47	127.92	124.51
26	G	1620	LUT	C19-C9-C8	2.47	122.03	118.10
25	c	505	CLA	C4A-NA-C1A	2.47	109.52	106.45
24	5	606	CHL	C4D-C3D-CAD	2.47	110.44	104.71
24	Y	609	CHL	O2A-CGA-CBA	2.47	119.08	111.90
24	1	606	CHL	C4D-C3D-CAD	2.47	110.45	104.71
25	c	506	CLA	CMD-C2D-C3D	2.47	129.48	124.89
24	G	605	CHL	C4D-C3D-CAD	2.47	110.45	104.71
24	3	601	CHL	CHB-C1B-C2B	2.47	123.84	116.99
25	S	611	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	C	505	CLA	C4A-NA-C1A	2.47	109.52	106.45
24	y	605	CHL	CHC-C4B-C3B	2.47	124.09	118.23
28	2	1623	NEX	C28-C29-C30	2.47	122.74	118.94
25	5	602	CLA	CMD-C2D-C3D	2.47	129.48	124.89
25	6	610	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	y	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	Y	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	B	603	CLA	CMD-C2D-C3D	2.48	129.49	124.89
25	Y	610	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	3	613	CLA	CMB-C2B-C3B	2.48	129.49	124.89
26	y	1620	LUT	C1-C2-C3	2.48	118.76	113.40
26	3	1621	LUT	C1-C2-C3	2.48	118.76	113.40
25	1	602	CLA	CMD-C2D-C3D	2.48	129.50	124.89
26	Y	1621	LUT	C39-C29-C28	2.48	122.05	118.10
28	3	1623	NEX	C12-C13-C14	2.48	122.75	118.94
25	s	611	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	C	503	CLA	CHB-C4A-NA	2.48	127.94	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	1621	LUT	C39-C29-C28	2.48	122.06	118.10
25	B	611	CLA	CHB-C4A-NA	2.48	127.95	124.51
25	c	503	CLA	CHB-C4A-NA	2.49	127.95	124.51
27	7	1622	XAT	C19-C9-C8	2.49	122.06	118.10
26	Y	1620	LUT	C1-C2-C3	2.49	118.78	113.40
24	7	605	CHL	CHC-C4B-C3B	2.49	124.12	118.23
25	C	505	CLA	CMD-C2D-C3D	2.49	129.51	124.89
24	G	609	CHL	C4-C3-C5	2.49	119.61	115.29
24	y	609	CHL	CMD-C2D-C3D	2.49	120.57	114.27
25	2	610	CLA	CHB-C4A-NA	2.49	127.95	124.51
25	c	505	CLA	CMD-C2D-C3D	2.49	129.51	124.89
24	7	609	CHL	CMD-C2D-C3D	2.49	120.57	114.27
24	R	606	CHL	CMD-C2D-C3D	2.49	120.57	114.27
25	b	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	Y	609	CHL	CMD-C2D-C3D	2.49	120.58	114.27
25	G	603	CLA	C1C-NC-C4C	2.49	108.49	107.06
24	g	605	CHL	C4D-C3D-CAD	2.49	110.50	104.71
24	3	605	CHL	CHC-C4B-C3B	2.49	124.14	118.23
25	n	610	CLA	CMD-C2D-C3D	2.49	129.52	124.89
24	5	607	CHL	C4D-C3D-CAD	2.50	110.51	104.71
25	r	602	CLA	CHB-C4A-NA	2.50	127.96	124.51
26	7	1621	LUT	C1-C2-C3	2.50	118.80	113.40
24	3	609	CHL	CMD-C2D-C3D	2.50	120.59	114.27
24	1	607	CHL	C4D-C3D-CAD	2.50	110.51	104.71
24	n	601	CHL	CHB-C1B-C2B	2.50	123.90	116.99
24	2	607	CHL	CED-O2D-CGD	2.50	121.83	115.97
25	N	610	CLA	CMD-C2D-C3D	2.50	129.53	124.89
25	s	602	CLA	O1D-CGD-CBD	2.50	129.09	124.60
28	7	1623	NEX	C12-C13-C14	2.50	122.78	118.94
24	g	609	CHL	C4-C3-C5	2.50	119.62	115.29
25	3	603	CLA	CMD-C2D-C3D	2.50	129.53	124.89
25	2	611	CLA	O2D-CGD-CBD	2.50	115.77	111.30
24	N	609	CHL	CMD-C2D-C3D	2.50	120.60	114.27
24	n	609	CHL	CMD-C2D-C3D	2.50	120.60	114.27
26	r	620	LUT	C1-C2-C3	2.50	118.81	113.40
24	N	601	CHL	CHB-C1B-C2B	2.50	123.92	116.99
25	R	602	CLA	CHB-C4A-NA	2.50	127.97	124.51
24	6	607	CHL	CED-O2D-CGD	2.50	121.84	115.97
27	R	622	XAT	C38-C25-C24	2.50	117.15	114.28
25	7	603	CLA	CMD-C2D-C3D	2.51	129.54	124.89
26	R	620	LUT	C1-C2-C3	2.51	118.82	113.40
24	r	606	CHL	CMD-C2D-C3D	2.51	120.61	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	CMD-C2D-C3D	2.51	129.54	124.89
27	3	1622	XAT	C19-C9-C8	2.51	122.10	118.10
25	G	610	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	1	603	CLA	CMB-C2B-C3B	2.51	129.56	124.89
24	N	601	CHL	CMD-C2D-C3D	2.51	120.63	114.27
24	7	601	CHL	C4D-C3D-CAD	2.51	110.55	104.71
25	g	603	CLA	C1C-NC-C4C	2.51	108.50	107.06
25	S	602	CLA	O1D-CGD-CBD	2.52	129.12	124.60
24	3	601	CHL	C4D-C3D-CAD	2.52	110.56	104.71
25	g	610	CLA	CHB-C4A-NA	2.52	127.99	124.51
25	C	513	CLA	CMD-C2D-C3D	2.52	129.56	124.89
24	n	601	CHL	CMD-C2D-C3D	2.52	120.64	114.27
36	D	405	PL9	C40-C39-C41	2.52	119.66	115.29
27	r	622	XAT	C38-C25-C24	2.52	117.17	114.28
25	2	610	CLA	CMB-C2B-C3B	2.52	129.57	124.89
24	G	608	CHL	C4D-C3D-CAD	2.52	110.56	104.71
25	5	603	CLA	CMB-C2B-C3B	2.52	129.57	124.89
25	B	606	CLA	C4A-NA-C1A	2.52	109.58	106.45
24	g	601	CHL	C4-C3-C5	2.52	119.66	115.29
24	g	608	CHL	C4D-C3D-CAD	2.52	110.57	104.71
24	N	607	CHL	C4D-C3D-CAD	2.52	110.57	104.71
25	b	615	CLA	CHB-C4A-NA	2.53	128.00	124.51
24	7	607	CHL	C4-C3-C5	2.53	119.67	115.29
24	3	607	CHL	C4-C3-C5	2.53	119.67	115.29
25	6	611	CLA	O2D-CGD-CBD	2.53	115.82	111.30
25	6	610	CLA	CMB-C2B-C3B	2.53	129.59	124.89
25	B	615	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	1	611	CLA	C4A-NA-C1A	2.53	109.59	106.45
25	R	609	CLA	C2C-C1C-NC	2.53	111.97	110.22
24	G	601	CHL	C4-C3-C5	2.53	119.68	115.29
24	5	605	CHL	CHB-C1B-C2B	2.54	124.01	116.99
24	6	609	CHL	C4-C3-C5	2.54	119.69	115.29
25	n	613	CLA	CMD-C2D-C3D	2.54	129.60	124.89
24	1	605	CHL	CHB-C1B-C2B	2.54	124.02	116.99
25	2	602	CLA	CMD-C2D-C3D	2.54	129.60	124.89
24	n	607	CHL	C4D-C3D-CAD	2.54	110.60	104.71
36	d	405	PL9	C40-C39-C41	2.54	119.69	115.29
25	R	613	CLA	O1D-CGD-CBD	2.54	129.16	124.60
25	s	603	CLA	CMD-C2D-C3D	2.54	129.60	124.89
25	r	609	CLA	C2C-C1C-NC	2.54	111.97	110.22
25	8	602	CLA	CMD-C2D-C3D	2.54	129.61	124.89
25	s	611	CLA	CMD-C2D-C3D	2.55	129.62	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	603	CLA	CMD-C2D-C3D	2.55	129.62	124.89
34	b	621	SQD	O48-C23-C24	2.55	119.31	111.90
26	y	1620	LUT	C19-C9-C8	2.55	122.16	118.10
25	b	604	CLA	CMD-C2D-C3D	2.55	129.62	124.89
25	R	612	CLA	CMD-C2D-C3D	2.55	129.62	124.89
25	r	613	CLA	O1D-CGD-CBD	2.55	129.18	124.60
25	N	613	CLA	CMD-C2D-C3D	2.55	129.62	124.89
25	r	612	CLA	CMD-C2D-C3D	2.55	129.62	124.89
37	C	518	DGD	C1E-O6E-C5E	2.55	118.52	113.72
24	G	608	CHL	CMD-C2D-C3D	2.55	120.73	114.27
25	b	606	CLA	C4A-NA-C1A	2.55	109.62	106.45
25	5	611	CLA	C4A-NA-C1A	2.55	109.62	106.45
25	d	402	CLA	CAC-C3C-C4C	2.55	128.43	124.83
24	3	606	CHL	C4D-C3D-CAD	2.55	110.64	104.71
24	g	608	CHL	CMD-C2D-C3D	2.55	120.73	114.27
25	6	602	CLA	CMD-C2D-C3D	2.55	129.63	124.89
37	c	518	DGD	C1E-O6E-C5E	2.55	118.53	113.72
25	B	604	CLA	CMD-C2D-C3D	2.55	129.63	124.89
34	B	621	SQD	O48-C23-C24	2.56	119.33	111.90
25	4	602	CLA	CMD-C2D-C3D	2.56	129.63	124.89
34	a	418	SQD	O5-C5-C4	2.56	114.37	109.66
24	7	606	CHL	C4D-C3D-CAD	2.56	110.65	104.71
24	2	609	CHL	C4-C3-C5	2.56	119.72	115.29
25	S	611	CLA	CMD-C2D-C3D	2.56	129.64	124.89
26	G	1620	LUT	C39-C29-C28	2.56	122.17	118.10
25	C	513	CLA	CBA-CAA-C2A	2.56	121.45	113.80
25	r	603	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	r	607	CHL	C4-C3-C5	2.56	119.73	115.29
26	Y	1620	LUT	C19-C9-C8	2.56	122.18	118.10
25	8	612	CLA	CHB-C4A-NA	2.56	128.06	124.51
25	5	604	CLA	CHB-C4A-NA	2.57	128.06	124.51
24	Y	609	CHL	C4-C3-C5	2.57	119.74	115.29
25	C	501	CLA	CMB-C2B-C3B	2.57	129.66	124.89
25	4	612	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	R	603	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	y	613	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	c	501	CLA	CMB-C2B-C3B	2.57	129.66	124.89
25	3	604	CLA	CHB-C4A-NA	2.57	128.07	124.51
24	R	607	CHL	C4-C3-C5	2.57	119.75	115.29
24	g	607	CHL	O2A-CGA-CBA	2.57	119.38	111.90
24	G	607	CHL	O2A-CGA-CBA	2.57	119.39	111.90
25	d	402	CLA	CMD-C2D-C3D	2.57	129.67	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	613	CLA	CHB-C4A-NA	2.57	128.07	124.51
24	2	605	CHL	CHB-C1B-C2B	2.58	124.12	116.99
25	c	513	CLA	CBA-CAA-C2A	2.58	121.51	113.80
24	5	601	CHL	C4D-C3D-CAD	2.58	110.69	104.71
25	3	614	CLA	CHB-C4A-NA	2.58	128.07	124.51
34	A	418	SQD	O5-C5-C4	2.58	114.41	109.66
25	D	402	CLA	CAC-C3C-C4C	2.58	128.47	124.83
24	y	609	CHL	C4-C3-C5	2.58	119.76	115.29
25	5	612	CLA	C2A-C1A-CHA	2.58	128.49	123.92
25	B	617	CLA	C4A-NA-C1A	2.58	109.65	106.45
24	s	607	CHL	O2A-CGA-CBA	2.58	119.41	111.90
25	g	611	CLA	CMB-C2B-C3B	2.58	129.68	124.89
24	1	601	CHL	C4D-C3D-CAD	2.58	110.71	104.71
25	7	614	CLA	CHB-C4A-NA	2.58	128.09	124.51
25	3	604	CLA	CMB-C2B-C3B	2.59	129.69	124.89
25	1	604	CLA	CHB-C4A-NA	2.59	128.09	124.51
24	G	606	CHL	CMD-C2D-C3D	2.59	120.82	114.27
24	6	605	CHL	CHB-C1B-C2B	2.59	124.17	116.99
25	D	402	CLA	CMD-C2D-C3D	2.59	129.70	124.89
24	5	601	CHL	CHC-C4B-C3B	2.59	124.37	118.23
34	B	623	SQD	O48-C23-C24	2.59	119.44	111.90
25	7	611	CLA	CHB-C4A-NA	2.59	128.10	124.51
25	1	612	CLA	C2A-C1A-CHA	2.59	128.52	123.92
25	G	602	CLA	CHB-C4A-NA	2.59	128.10	124.51
26	g	1620	LUT	C39-C29-C28	2.60	122.23	118.10
24	S	607	CHL	O2A-CGA-CBA	2.60	119.45	111.90
25	G	611	CLA	CMB-C2B-C3B	2.60	129.71	124.89
24	5	609	CHL	CMD-C2D-C3D	2.60	120.84	114.27
24	N	605	CHL	C4D-C3D-CAD	2.60	110.75	104.71
25	b	612	CLA	C4A-NA-C1A	2.60	109.68	106.45
25	5	612	CLA	CMD-C2D-C3D	2.60	129.72	124.89
24	y	601	CHL	O2A-CGA-CBA	2.60	119.47	111.90
25	7	604	CLA	CHB-C4A-NA	2.60	128.11	124.51
24	g	606	CHL	CMD-C2D-C3D	2.60	120.85	114.27
25	b	617	CLA	C4A-NA-C1A	2.60	109.68	106.45
33	a	408	PHO	C1B-NB-C4B	2.60	111.67	106.52
24	n	605	CHL	C4D-C3D-CAD	2.60	110.76	104.71
25	3	611	CLA	CHB-C4A-NA	2.60	128.11	124.51
25	S	602	CLA	CMD-C2D-C3D	2.61	129.73	124.89
34	b	623	SQD	O48-C23-C24	2.61	119.48	111.90
24	1	609	CHL	CMD-C2D-C3D	2.61	120.87	114.27
24	1	601	CHL	CHC-C4B-C3B	2.61	124.41	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	601	CLA	CMD-C2D-C3D	2.61	129.73	124.89
25	1	612	CLA	CMD-C2D-C3D	2.61	129.73	124.89
33	A	408	PHO	C1B-NB-C4B	2.61	111.68	106.52
24	Y	601	CHL	O2A-CGA-CBA	2.61	119.49	111.90
25	7	604	CLA	CMB-C2B-C3B	2.61	129.73	124.89
25	y	613	CLA	CMD-C2D-C3D	2.61	129.73	124.89
25	B	612	CLA	C4A-NA-C1A	2.61	109.69	106.45
24	5	601	CHL	CHB-C1B-C2B	2.61	124.22	116.99
28	5	1623	NEX	C16-C1-C6	2.61	112.81	110.47
25	2	613	CLA	CHB-C4A-NA	2.61	128.12	124.51
24	r	608	CHL	CHC-C4B-C3B	2.61	124.42	118.23
24	g	609	CHL	CMD-C2D-C3D	2.61	120.88	114.27
24	1	601	CHL	CHB-C1B-C2B	2.62	124.23	116.99
25	6	613	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	s	602	CLA	CMD-C2D-C3D	2.62	129.75	124.89
25	A	407	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	b	612	CLA	CAC-C3C-C4C	2.62	128.53	124.83
25	s	610	CLA	CHB-C4A-NA	2.62	128.13	124.51
25	R	601	CLA	CMD-C2D-C3D	2.62	129.75	124.89
25	a	407	CLA	CHB-C4A-NA	2.62	128.14	124.51
25	g	602	CLA	CHB-C4A-NA	2.62	128.14	124.51
28	6	1623	NEX	C16-C1-C6	2.62	112.82	110.47
25	Y	613	CLA	CMD-C2D-C3D	2.63	129.76	124.89
24	R	608	CHL	CHC-C4B-C3B	2.63	124.45	118.23
24	G	609	CHL	CMD-C2D-C3D	2.63	120.92	114.27
25	S	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
36	d	405	PL9	C8-C7-C3	2.63	119.50	111.73
25	s	614	CLA	CHB-C4A-NA	2.63	128.15	124.51
25	c	507	CLA	C4A-NA-C1A	2.63	109.71	106.45
29	s	2630	LHG	O8-C23-C24	2.63	119.55	111.90
25	B	612	CLA	CAC-C3C-C4C	2.63	128.54	124.83
25	b	610	CLA	CHB-C4A-NA	2.63	128.15	124.51
29	S	2630	LHG	O8-C23-C24	2.63	119.56	111.90
25	6	612	CLA	CMD-C2D-C3D	2.64	129.78	124.89
36	D	405	PL9	C8-C7-C3	2.64	119.52	111.73
25	C	507	CLA	C4A-NA-C1A	2.64	109.72	106.45
25	G	602	CLA	CAC-C3C-C4C	2.64	128.55	124.83
25	B	610	CLA	CHB-C4A-NA	2.64	128.16	124.51
36	a	414	PL9	C8-C7-C3	2.64	119.54	111.73
25	g	603	CLA	CHB-C4A-NA	2.64	128.16	124.51
28	2	1623	NEX	C16-C1-C6	2.64	112.84	110.47
25	g	602	CLA	CAC-C3C-C4C	2.65	128.56	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	605	CLA	C4A-NA-C1A	2.65	109.74	106.45
25	c	513	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	B	614	CLA	C4A-NA-C1A	2.65	109.74	106.45
33	A	409	PHO	C4A-NA-C1A	2.65	110.30	108.16
25	y	603	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	Y	603	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	7	611	CLA	C2C-C1C-NC	2.65	112.05	110.22
25	b	614	CLA	C4A-NA-C1A	2.65	109.74	106.45
25	C	513	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	7	608	CHL	CHC-C4B-C3B	2.65	124.52	118.23
25	S	614	CLA	CHB-C4A-NA	2.65	128.18	124.51
36	A	414	PL9	C8-C7-C3	2.65	119.58	111.73
28	1	1623	NEX	C16-C1-C6	2.65	112.85	110.47
24	3	608	CHL	CHC-C4B-C3B	2.66	124.52	118.23
24	6	601	CHL	C4D-C3D-CAD	2.66	110.88	104.71
30	T	101	BCR	C8-C9-C10	2.66	123.02	118.94
25	1	603	CLA	CMD-C2D-C3D	2.66	129.83	124.89
25	r	601	CLA	CHB-C4A-NA	2.66	128.19	124.51
25	G	603	CLA	CHB-C4A-NA	2.66	128.19	124.51
30	B	620	BCR	C29-C30-C25	2.66	114.64	110.48
24	2	601	CHL	C4D-C3D-CAD	2.66	110.90	104.71
24	y	608	CHL	O2A-CGA-CBA	2.66	119.65	111.90
25	2	612	CLA	CMD-C2D-C3D	2.66	129.84	124.89
25	B	605	CLA	C4A-NA-C1A	2.67	109.76	106.45
25	b	605	CLA	CHB-C4A-NA	2.67	128.20	124.51
29	5	2630	LHG	O8-C23-C24	2.67	119.66	111.90
30	t	101	BCR	C8-C9-C10	2.67	123.03	118.94
25	b	617	CLA	CHB-C4A-NA	2.67	128.20	124.51
24	2	609	CHL	CHC-C4B-C3B	2.67	124.55	118.23
26	5	1620	LUT	C19-C9-C8	2.67	122.35	118.10
26	6	1621	LUT	C39-C29-C28	2.67	122.35	118.10
25	5	603	CLA	CMD-C2D-C3D	2.67	129.85	124.89
25	3	611	CLA	C2C-C1C-NC	2.67	112.06	110.22
25	5	604	CLA	CMB-C2B-C3B	2.67	129.85	124.89
25	B	617	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	N	604	CLA	CMD-C2D-C3D	2.67	129.85	124.89
25	3	604	CLA	CMD-C2D-C3D	2.67	129.85	124.89
25	b	616	CLA	CMD-C2D-C3D	2.67	129.85	124.89
24	n	606	CHL	CMD-C2D-C3D	2.67	121.04	114.27
24	4	607	CHL	CHB-C1B-C2B	2.68	124.40	116.99
26	2	1621	LUT	C39-C29-C28	2.68	122.36	118.10
29	1	2630	LHG	O8-C23-C24	2.68	119.69	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	b	620	BCR	C29-C30-C25	2.68	114.66	110.48
24	6	609	CHL	CHC-C4B-C3B	2.68	124.57	118.23
25	D	403	CLA	CMD-C2D-C3D	2.68	129.86	124.89
24	N	606	CHL	CMD-C2D-C3D	2.68	121.05	114.27
25	n	604	CLA	CMD-C2D-C3D	2.68	129.86	124.89
25	1	604	CLA	CMB-C2B-C3B	2.68	129.86	124.89
25	Y	614	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	Y	608	CHL	O2A-CGA-CBA	2.68	119.70	111.90
25	7	604	CLA	CMD-C2D-C3D	2.68	129.87	124.89
27	n	1622	XAT	C18-C5-C4	2.68	117.35	114.28
25	R	601	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	G	610	CLA	CMD-C2D-C3D	2.68	129.87	124.89
25	g	610	CLA	CMD-C2D-C3D	2.68	129.87	124.89
26	1	1620	LUT	C19-C9-C8	2.68	122.37	118.10
25	S	604	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	g	601	CHL	O2A-CGA-CBA	2.68	119.71	111.90
24	1	606	CHL	CMD-C2D-C3D	2.69	121.07	114.27
24	8	607	CHL	CHB-C1B-C2B	2.69	124.43	116.99
24	G	601	CHL	O2A-CGA-CBA	2.69	119.72	111.90
34	B	621	SQD	C44-O6-C1	2.69	119.27	113.76
24	1	609	CHL	C4-C3-C5	2.69	119.95	115.29
25	d	403	CLA	CMD-C2D-C3D	2.69	129.88	124.89
24	n	605	CHL	CMD-C2D-C3D	2.69	121.08	114.27
24	5	606	CHL	CMD-C2D-C3D	2.69	121.08	114.27
25	s	604	CLA	CHB-C4A-NA	2.69	128.23	124.51
34	b	621	SQD	C44-O6-C1	2.69	119.28	113.76
25	B	605	CLA	CHB-C4A-NA	2.69	128.24	124.51
25	5	604	CLA	CMD-C2D-C3D	2.69	129.89	124.89
27	N	1622	XAT	C18-C5-C4	2.70	117.37	114.28
25	B	616	CLA	CMD-C2D-C3D	2.70	129.89	124.89
25	y	614	CLA	CHB-C4A-NA	2.70	128.24	124.51
24	y	607	CHL	CHC-C4B-C3B	2.70	124.62	118.23
24	5	609	CHL	C4-C3-C5	2.70	119.97	115.29
24	1	605	CHL	CHC-C4B-C3B	2.70	124.62	118.23
25	n	614	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	3	612	CLA	CHB-C4A-NA	2.70	128.25	124.51
33	a	409	PHO	C4A-NA-C1A	2.70	110.35	108.16
26	R	620	LUT	C20-C13-C12	2.71	122.41	118.10
25	1	604	CLA	CMD-C2D-C3D	2.71	129.91	124.89
25	C	504	CLA	CHB-C4A-NA	2.71	128.25	124.51
25	g	604	CLA	CMD-C2D-C3D	2.71	129.91	124.89
25	N	614	CLA	CHB-C4A-NA	2.71	128.26	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	622	XAT	C19-C9-C8	2.71	122.41	118.10
24	N	605	CHL	CMD-C2D-C3D	2.71	121.12	114.27
24	5	605	CHL	CHC-C4B-C3B	2.71	124.64	118.23
25	C	511	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	R	608	CHL	CHD-C1D-C2D	2.71	124.50	116.99
25	a	410	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	G	604	CLA	CMD-C2D-C3D	2.71	129.93	124.89
24	Y	607	CHL	CHC-C4B-C3B	2.71	124.66	118.23
27	r	622	XAT	C19-C9-C8	2.71	122.42	118.10
25	R	609	CLA	CMB-C2B-C3B	2.72	129.93	124.89
25	7	612	CLA	CHB-C4A-NA	2.72	128.27	124.51
24	r	608	CHL	CHD-C1D-C2D	2.72	124.52	116.99
25	r	612	CLA	CHB-C4A-NA	2.72	128.27	124.51
25	c	504	CLA	CHB-C4A-NA	2.72	128.28	124.51
25	b	610	CLA	CMD-C2D-C3D	2.72	129.95	124.89
26	r	620	LUT	C20-C13-C12	2.72	122.44	118.10
25	1	611	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	B	610	CLA	CMD-C2D-C3D	2.73	129.96	124.89
25	5	613	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	7	611	CLA	CMD-C2D-C3D	2.73	129.96	124.89
24	2	605	CHL	CHC-C4B-C3B	2.73	124.70	118.23
25	r	609	CLA	CMB-C2B-C3B	2.73	129.96	124.89
24	6	607	CHL	O2A-CGA-CBA	2.74	119.86	111.90
25	R	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	c	511	CLA	CHB-C4A-NA	2.74	128.30	124.51
24	g	605	CHL	CMD-C2D-C3D	2.74	121.20	114.27
25	A	410	CLA	CHB-C4A-NA	2.74	128.30	124.51
24	7	607	CHL	CHB-C1B-C2B	2.74	124.58	116.99
29	2	2630	LHG	O8-C23-C24	2.74	119.87	111.90
24	S	608	CHL	CHB-C1B-C2B	2.74	124.58	116.99
30	T	101	BCR	C35-C13-C12	2.74	122.47	118.10
25	5	611	CLA	CHB-C4A-NA	2.74	128.31	124.51
24	G	605	CHL	CMD-C2D-C3D	2.74	121.21	114.27
24	R	614	CHL	CHC-C4B-C3B	2.74	124.73	118.23
29	6	2630	LHG	O8-C23-C24	2.74	119.89	111.90
27	4	622	XAT	C18-C5-C4	2.75	117.42	114.28
24	s	608	CHL	CHB-C1B-C2B	2.75	124.60	116.99
24	6	605	CHL	CHC-C4B-C3B	2.75	124.74	118.23
30	t	101	BCR	C35-C13-C12	2.75	122.48	118.10
25	7	612	CLA	CMB-C2B-C3B	2.75	130.00	124.89
24	2	607	CHL	O2A-CGA-CBA	2.75	119.90	111.90
24	3	607	CHL	CHB-C1B-C2B	2.75	124.61	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	614	CHL	CHC-C4B-C3B	2.75	124.75	118.23
25	b	602	CLA	CHB-C4A-NA	2.75	128.32	124.51
27	7	1622	XAT	C38-C25-C24	2.75	117.43	114.28
25	N	603	CLA	CHB-C4A-NA	2.75	128.32	124.51
25	2	603	CLA	CMB-C2B-C3B	2.76	130.01	124.89
25	N	603	CLA	CMB-C2B-C3B	2.76	130.01	124.89
25	3	611	CLA	CMD-C2D-C3D	2.76	130.01	124.89
25	3	612	CLA	CMB-C2B-C3B	2.76	130.01	124.89
30	D	404	BCR	C38-C26-C27	2.76	118.69	113.45
34	b	621	SQD	O8-S-C6	2.76	109.38	106.01
25	1	611	CLA	CMB-C2B-C3B	2.76	130.02	124.89
25	G	613	CLA	CMD-C2D-C3D	2.76	130.02	124.89
25	S	609	CLA	CMB-C2B-C3B	2.76	130.02	124.89
25	8	611	CLA	CMB-C2B-C3B	2.76	130.02	124.89
25	1	613	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	s	609	CLA	CMB-C2B-C3B	2.76	130.02	124.89
24	3	607	CHL	O2A-CGA-CBA	2.76	119.94	111.90
25	g	613	CLA	CMD-C2D-C3D	2.77	130.03	124.89
27	8	622	XAT	C18-C5-C4	2.77	117.45	114.28
30	d	404	BCR	C38-C26-C27	2.77	118.71	113.45
25	n	603	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	6	603	CLA	CMB-C2B-C3B	2.77	130.04	124.89
25	n	611	CLA	CHB-C4A-NA	2.77	128.35	124.51
25	7	614	CLA	CMB-C2B-C3B	2.78	130.04	124.89
25	d	402	CLA	C1D-CHD-C4C	2.78	126.28	122.48
25	s	611	CLA	CMB-C2B-C3B	2.78	130.04	124.89
25	4	611	CLA	CMB-C2B-C3B	2.78	130.04	124.89
25	C	508	CLA	CHB-C4A-NA	2.78	128.35	124.51
25	n	603	CLA	CMB-C2B-C3B	2.78	130.05	124.89
25	B	602	CLA	CHB-C4A-NA	2.78	128.35	124.51
24	7	607	CHL	O2A-CGA-CBA	2.78	119.98	111.90
25	5	611	CLA	CMB-C2B-C3B	2.78	130.05	124.89
29	D	409	LHG	O8-C23-C24	2.78	119.99	111.90
25	N	611	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	S	611	CLA	CMB-C2B-C3B	2.78	130.05	124.89
25	c	508	CLA	CHB-C4A-NA	2.78	128.36	124.51
27	3	1622	XAT	C38-C25-C24	2.78	117.47	114.28
25	D	402	CLA	C1D-CHD-C4C	2.78	126.29	122.48
29	d	409	LHG	O8-C23-C24	2.79	120.00	111.90
34	B	621	SQD	O8-S-C6	2.79	109.41	106.01
25	1	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	C	505	CLA	CHB-C4A-NA	2.79	128.38	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	612	CLA	CMD-C2D-C3D	2.79	130.08	124.89
25	S	612	CLA	CMD-C2D-C3D	2.79	130.08	124.89
25	1	611	CLA	CMD-C2D-C3D	2.80	130.08	124.89
25	b	617	CLA	CMD-C2D-C3D	2.80	130.08	124.89
25	s	603	CLA	CMB-C2B-C3B	2.80	130.09	124.89
25	S	603	CLA	CMB-C2B-C3B	2.80	130.09	124.89
25	2	603	CLA	CMD-C2D-C3D	2.80	130.09	124.89
24	6	607	CHL	CMD-C2D-C3D	2.80	121.36	114.27
25	r	604	CLA	CMD-C2D-C3D	2.80	130.09	124.89
24	2	607	CHL	CMD-C2D-C3D	2.80	121.36	114.27
25	3	614	CLA	CMB-C2B-C3B	2.80	130.09	124.89
25	B	617	CLA	CMD-C2D-C3D	2.80	130.10	124.89
25	c	505	CLA	CHB-C4A-NA	2.81	128.39	124.51
25	y	612	CLA	CMD-C2D-C3D	2.81	130.10	124.89
25	G	612	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	s	612	CLA	CMD-C2D-C3D	2.81	130.10	124.89
25	R	604	CLA	CMD-C2D-C3D	2.81	130.10	124.89
24	n	605	CHL	CHC-C4B-C3B	2.81	124.88	118.23
25	b	613	CLA	C4A-NA-C1A	2.81	109.94	106.45
25	D	403	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	R	609	CLA	CMD-C2D-C3D	2.81	130.11	124.89
25	B	613	CLA	C4A-NA-C1A	2.81	109.94	106.45
25	5	612	CLA	CHB-C4A-NA	2.81	128.40	124.51
25	d	403	CLA	CHB-C4A-NA	2.81	128.40	124.51
26	n	1620	LUT	C17-C1-C6	2.82	114.87	110.31
25	R	601	CLA	C1D-CHD-C4C	2.82	126.33	122.48
29	l	101	LHG	O8-C23-C24	2.82	120.09	111.90
29	L	101	LHG	O8-C23-C24	2.82	120.10	111.90
25	a	406	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	5	611	CLA	CMD-C2D-C3D	2.82	130.12	124.89
24	y	607	CHL	CMD-C2D-C3D	2.82	121.41	114.27
24	r	606	CHL	O2A-CGA-CBA	2.82	120.11	111.90
25	N	611	CLA	C4A-NA-C1A	2.82	109.95	106.45
25	R	611	CLA	CMD-C2D-C3D	2.82	130.13	124.89
24	3	609	CHL	CHB-C1B-C2B	2.82	124.80	116.99
25	n	611	CLA	C4A-NA-C1A	2.82	109.95	106.45
25	r	601	CLA	C1D-CHD-C4C	2.82	126.34	122.48
25	g	612	CLA	CHB-C4A-NA	2.82	128.41	124.51
25	C	508	CLA	CMD-C2D-C3D	2.82	130.13	124.89
24	Y	607	CHL	CMD-C2D-C3D	2.82	121.42	114.27
25	A	406	CLA	CHB-C4A-NA	2.82	128.42	124.51
25	c	502	CLA	CHB-C4A-NA	2.83	128.42	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	612	CLA	CHB-C4A-NA	2.83	128.42	124.51
24	1	607	CHL	O2A-CGA-CBA	2.83	120.13	111.90
24	s	601	CHL	CMD-C2D-C3D	2.83	121.43	114.27
24	S	601	CHL	CMD-C2D-C3D	2.83	121.43	114.27
25	b	614	CLA	CMD-C2D-C3D	2.83	130.14	124.89
25	c	508	CLA	CMD-C2D-C3D	2.83	130.15	124.89
24	S	608	CHL	CHC-C4B-C3B	2.83	124.94	118.23
24	N	605	CHL	CHC-C4B-C3B	2.83	124.94	118.23
25	r	611	CLA	CMD-C2D-C3D	2.83	130.15	124.89
24	7	609	CHL	CHB-C1B-C2B	2.83	124.83	116.99
24	7	607	CHL	CMD-C2D-C3D	2.83	121.44	114.27
25	b	608	CLA	CHB-C4A-NA	2.84	128.43	124.51
25	6	603	CLA	CMD-C2D-C3D	2.84	130.15	124.89
25	R	602	CLA	CMD-C2D-C3D	2.84	130.15	124.89
24	7	609	CHL	O2A-CGA-CBA	2.84	120.15	111.90
24	3	609	CHL	O2A-CGA-CBA	2.84	120.15	111.90
24	s	608	CHL	CHC-C4B-C3B	2.84	124.95	118.23
24	R	606	CHL	O2A-CGA-CBA	2.84	120.16	111.90
24	4	606	CHL	CHC-C4B-C3B	2.84	124.95	118.23
25	r	609	CLA	CMD-C2D-C3D	2.84	130.16	124.89
25	C	502	CLA	CHB-C4A-NA	2.84	128.44	124.51
29	C	522	LHG	O8-C23-C24	2.84	120.16	111.90
26	N	1620	LUT	C17-C1-C6	2.84	114.91	110.31
25	r	602	CLA	CMD-C2D-C3D	2.84	130.16	124.89
24	5	607	CHL	O2A-CGA-CBA	2.84	120.17	111.90
25	B	614	CLA	C4-C3-C5	2.84	120.22	115.29
24	3	607	CHL	CMD-C2D-C3D	2.84	121.46	114.27
24	8	608	CHL	CHC-C4B-C3B	2.84	124.96	118.23
24	G	606	CHL	O2D-CGD-CBD	2.84	118.14	111.20
24	N	607	CHL	CHD-C1D-C2D	2.85	124.88	116.99
24	1	609	CHL	CHC-C4B-C3B	2.85	124.98	118.23
25	G	613	CLA	C4A-NA-C1A	2.85	109.99	106.45
24	n	607	CHL	CHD-C1D-C2D	2.85	124.88	116.99
25	g	613	CLA	C4A-NA-C1A	2.85	109.99	106.45
25	b	607	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	r	604	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	b	612	CLA	CHB-C4A-NA	2.85	128.46	124.51
25	B	608	CLA	CHB-C4A-NA	2.85	128.46	124.51
24	5	609	CHL	CHC-C4B-C3B	2.85	124.99	118.23
25	B	612	CLA	CHB-C4A-NA	2.85	128.46	124.51
24	8	606	CHL	CHC-C4B-C3B	2.85	124.99	118.23
25	B	607	CLA	CHB-C4A-NA	2.85	128.46	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	522	LHG	O8-C23-C24	2.85	120.21	111.90
24	g	606	CHL	O2D-CGD-CBD	2.85	118.17	111.20
24	y	608	CHL	CHD-C1D-C2D	2.86	124.90	116.99
24	4	608	CHL	CHC-C4B-C3B	2.86	124.99	118.23
25	B	614	CLA	CMD-C2D-C3D	2.86	130.19	124.89
24	Y	608	CHL	CHD-C1D-C2D	2.86	124.90	116.99
25	s	612	CLA	CHB-C4A-NA	2.86	128.46	124.51
24	N	608	CHL	CMD-C2D-C3D	2.86	121.50	114.27
25	6	604	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	5	610	CLA	CMD-C2D-C3D	2.86	130.19	124.89
24	n	608	CHL	CMD-C2D-C3D	2.86	121.50	114.27
27	2	1622	XAT	C40-C33-C32	2.86	122.65	118.10
25	b	614	CLA	C4-C3-C5	2.86	120.25	115.29
24	S	601	CHL	CHC-C4B-C3B	2.86	125.01	118.23
25	R	604	CLA	CHB-C4A-NA	2.86	128.47	124.51
24	8	607	CHL	CMD-C2D-C3D	2.86	121.52	114.27
24	4	607	CHL	CMD-C2D-C3D	2.86	121.52	114.27
25	4	603	CLA	CHB-C4A-NA	2.87	128.48	124.51
24	y	606	CHL	CHD-C1D-C2D	2.87	124.93	116.99
25	c	505	CLA	O2D-CGD-CBD	2.87	116.42	111.30
25	B	602	CLA	CMB-C2B-C3B	2.87	130.22	124.89
24	8	607	CHL	CHC-C4B-C3B	2.87	125.03	118.23
24	s	601	CHL	CHC-C4B-C3B	2.87	125.03	118.23
24	4	607	CHL	CHC-C4B-C3B	2.87	125.03	118.23
25	1	610	CLA	CMD-C2D-C3D	2.87	130.22	124.89
29	g	2630	LHG	O8-C23-C24	2.87	120.26	111.90
25	C	505	CLA	O2D-CGD-CBD	2.87	116.43	111.30
24	Y	606	CHL	CHD-C1D-C2D	2.87	124.95	116.99
27	6	1622	XAT	C40-C33-C32	2.88	122.68	118.10
24	6	606	CHL	CMD-C2D-C3D	2.88	121.55	114.27
25	b	602	CLA	CMB-C2B-C3B	2.88	130.23	124.89
24	5	608	CHL	CMD-C2D-C3D	2.88	121.56	114.27
25	2	604	CLA	CHB-C4A-NA	2.88	128.50	124.51
24	1	608	CHL	CMD-C2D-C3D	2.88	121.56	114.27
29	G	2630	LHG	O8-C23-C24	2.88	120.28	111.90
24	R	614	CHL	CHB-C1B-C2B	2.89	124.98	116.99
25	s	603	CLA	CHB-C4A-NA	2.89	128.50	124.51
25	6	614	CLA	CHB-C4A-NA	2.89	128.50	124.51
24	r	606	CHL	CHC-C4B-C3B	2.89	125.07	118.23
29	C	523	LHG	O8-C23-C24	2.89	120.31	111.90
28	g	1623	NEX	O24-C25-C38	2.89	118.64	115.02
24	r	614	CHL	CHB-C1B-C2B	2.89	124.99	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	612	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	2	606	CHL	CMD-C2D-C3D	2.89	121.59	114.27
25	Y	612	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	R	606	CHL	CHC-C4B-C3B	2.89	125.09	118.23
29	c	523	LHG	O8-C23-C24	2.90	120.33	111.90
25	Y	603	CLA	CMD-C2D-C3D	2.90	130.27	124.89
24	N	607	CHL	O2A-CGA-CBA	2.90	120.33	111.90
24	y	608	CHL	O2D-CGD-CBD	2.90	118.27	111.20
25	y	603	CLA	CMD-C2D-C3D	2.90	130.27	124.89
25	n	612	CLA	CMB-C2B-C3B	2.90	130.27	124.89
25	8	603	CLA	CHB-C4A-NA	2.90	128.52	124.51
24	n	607	CHL	O2A-CGA-CBA	2.90	120.35	111.90
25	G	612	CLA	CMD-C2D-C3D	2.90	130.28	124.89
24	Y	608	CHL	O2D-CGD-CBD	2.91	118.29	111.20
25	g	612	CLA	CMD-C2D-C3D	2.91	130.28	124.89
28	7	1623	NEX	C28-C29-C30	2.91	123.40	118.94
24	g	608	CHL	O2A-CGA-CBA	2.91	120.37	111.90
25	6	612	CLA	CHB-C4A-NA	2.92	128.54	124.51
25	2	612	CLA	CHB-C4A-NA	2.92	128.54	124.51
29	y	2630	LHG	O8-C23-C24	2.92	120.38	111.90
28	G	1623	NEX	O24-C25-C38	2.92	118.67	115.02
29	Y	2630	LHG	O8-C23-C24	2.92	120.39	111.90
24	G	608	CHL	O2A-CGA-CBA	2.92	120.39	111.90
25	S	603	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	2	614	CLA	CHB-C4A-NA	2.92	128.55	124.51
25	a	407	CLA	CMB-C2B-C3B	2.92	130.31	124.89
28	3	1623	NEX	C28-C29-C30	2.92	123.43	118.94
25	A	407	CLA	CMB-C2B-C3B	2.92	130.32	124.89
24	2	609	CHL	CMD-C2D-C3D	2.93	121.67	114.27
24	y	609	CHL	CHC-C4B-C3B	2.93	125.16	118.23
25	N	612	CLA	CMB-C2B-C3B	2.93	130.32	124.89
25	r	609	CLA	CHB-C4A-NA	2.93	128.56	124.51
24	6	609	CHL	CMD-C2D-C3D	2.93	121.68	114.27
25	y	604	CLA	CMD-C2D-C3D	2.93	130.33	124.89
24	Y	609	CHL	CHC-C4B-C3B	2.93	125.18	118.23
24	7	601	CHL	CHC-C4B-C3B	2.94	125.18	118.23
25	r	604	CLA	O2D-CGD-CBD	2.94	116.55	111.30
29	C	2630	LHG	O8-C23-C24	2.94	120.45	111.90
25	R	609	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	Y	611	CLA	CMD-C2D-C3D	2.94	130.35	124.89
25	y	611	CLA	CMD-C2D-C3D	2.94	130.35	124.89
24	y	607	CHL	CHD-C1D-C2D	2.94	125.14	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	2630	LHG	O8-C23-C24	2.94	120.46	111.90
24	n	606	CHL	O2A-CGA-CBA	2.94	120.46	111.90
25	Y	604	CLA	CMD-C2D-C3D	2.94	130.35	124.89
25	7	613	CLA	CHB-C4A-NA	2.94	128.58	124.51
24	2	601	CHL	O2D-CGD-CBD	2.95	118.39	111.20
34	B	621	SQD	C4-C3-C2	2.95	116.03	110.84
25	g	613	CLA	CMB-C2B-C3B	2.95	130.36	124.89
25	4	602	CLA	CHB-C4A-NA	2.95	128.59	124.51
27	3	1622	XAT	C40-C33-C32	2.95	122.80	118.10
25	R	604	CLA	O2D-CGD-CBD	2.95	116.57	111.30
24	N	606	CHL	O2A-CGA-CBA	2.95	120.49	111.90
24	6	601	CHL	O2D-CGD-CBD	2.95	118.41	111.20
24	Y	607	CHL	CHD-C1D-C2D	2.96	125.17	116.99
25	G	613	CLA	CMB-C2B-C3B	2.96	130.38	124.89
34	A	418	SQD	O47-C7-C8	2.96	117.69	111.55
25	3	602	CLA	CMD-C2D-C3D	2.96	130.38	124.89
24	3	601	CHL	CHC-C4B-C3B	2.96	125.24	118.23
25	3	613	CLA	CHB-C4A-NA	2.96	128.60	124.51
30	c	517	BCR	C33-C5-C4	2.96	119.07	113.45
25	7	602	CLA	CMD-C2D-C3D	2.96	130.38	124.89
24	s	608	CHL	CMD-C2D-C3D	2.96	121.76	114.27
27	7	1622	XAT	C40-C33-C32	2.96	122.82	118.10
34	a	418	SQD	O47-C7-C8	2.96	117.70	111.55
25	8	602	CLA	CHB-C4A-NA	2.96	128.61	124.51
34	b	621	SQD	C4-C3-C2	2.96	116.06	110.84
25	3	603	CLA	CMB-C2B-C3B	2.96	130.39	124.89
25	B	607	CLA	CMB-C2B-C3B	2.97	130.40	124.89
30	C	517	BCR	C33-C5-C4	2.97	119.08	113.45
24	S	608	CHL	CMD-C2D-C3D	2.97	121.78	114.27
25	B	609	CLA	CHB-C4A-NA	2.97	128.62	124.51
25	g	611	CLA	CMD-C2D-C3D	2.97	130.41	124.89
24	4	608	CHL	O2D-CGD-CBD	2.97	118.46	111.20
25	1	614	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	G	611	CLA	CMD-C2D-C3D	2.98	130.41	124.89
25	3	610	CLA	CMB-C2B-C3B	2.98	130.41	124.89
24	7	608	CHL	CMD-C2D-C3D	2.98	121.81	114.27
24	3	608	CHL	CMD-C2D-C3D	2.98	121.81	114.27
24	6	608	CHL	O2D-CGD-CBD	2.98	118.47	111.20
24	8	608	CHL	O2D-CGD-CBD	2.98	118.47	111.20
25	7	603	CLA	CMB-C2B-C3B	2.98	130.42	124.89
25	b	609	CLA	CHB-C4A-NA	2.98	128.64	124.51
24	2	608	CHL	O2D-CGD-CBD	2.99	118.49	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	609	CHL	O2A-CGA-CBA	2.99	120.59	111.90
24	2	608	CHL	CMD-C2D-C3D	2.99	121.83	114.27
25	5	614	CLA	CHB-C4A-NA	2.99	128.64	124.51
29	B	2630	LHG	O8-C23-C24	2.99	120.60	111.90
29	b	2630	LHG	O8-C23-C24	2.99	120.60	111.90
24	r	608	CHL	O2A-CGA-CBA	2.99	120.60	111.90
25	y	610	CLA	CMD-C2D-C3D	2.99	130.44	124.89
24	R	608	CHL	O2A-CGA-CBA	2.99	120.60	111.90
25	b	607	CLA	CMB-C2B-C3B	2.99	130.44	124.89
26	8	620	LUT	C18-C5-C4	2.99	119.79	114.33
25	7	610	CLA	CMB-C2B-C3B	2.99	130.44	124.89
25	Y	610	CLA	CMD-C2D-C3D	2.99	130.44	124.89
24	6	609	CHL	O2A-CGA-CBA	2.99	120.61	111.90
33	A	408	PHO	O1D-CGD-CBD	2.99	129.98	124.60
30	C	515	BCR	C33-C5-C4	2.99	119.13	113.45
25	c	507	CLA	CHB-C4A-NA	2.99	128.65	124.51
25	G	611	CLA	CHB-C4A-NA	3.00	128.66	124.51
34	A	412	SQD	O48-C23-C24	3.00	120.62	111.90
24	y	607	CHL	O2D-CGD-CBD	3.00	118.52	111.20
26	4	620	LUT	C18-C5-C4	3.00	119.81	114.33
24	Y	607	CHL	O2D-CGD-CBD	3.00	118.53	111.20
25	g	611	CLA	CHB-C4A-NA	3.00	128.66	124.51
25	C	507	CLA	CHB-C4A-NA	3.00	128.66	124.51
24	8	606	CHL	O2D-CGD-CBD	3.00	118.53	111.20
24	6	608	CHL	CMD-C2D-C3D	3.00	121.87	114.27
34	a	412	SQD	O48-C23-C24	3.01	120.65	111.90
33	a	408	PHO	O1D-CGD-CBD	3.01	130.00	124.60
24	N	607	CHL	O2D-CGD-CBD	3.01	118.54	111.20
30	c	515	BCR	C33-C5-C4	3.01	119.16	113.45
24	N	607	CHL	CMD-C2D-C3D	3.01	121.89	114.27
24	2	607	CHL	O2D-CGD-CBD	3.01	118.56	111.20
24	n	607	CHL	CMD-C2D-C3D	3.02	121.90	114.27
24	6	607	CHL	O2D-CGD-CBD	3.02	118.56	111.20
34	A	418	SQD	C4-C3-C2	3.02	116.16	110.84
24	4	606	CHL	O2D-CGD-CBD	3.02	118.56	111.20
25	B	612	CLA	CMD-C2D-C3D	3.02	130.49	124.89
24	7	605	CHL	CMD-C2D-C3D	3.02	121.91	114.27
24	4	608	CHL	CHD-C1D-C2D	3.02	125.36	116.99
25	B	616	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	2	607	CHL	CHB-C1B-C2B	3.02	125.36	116.99
24	n	608	CHL	O2A-CGA-CBA	3.02	120.69	111.90
24	5	609	CHL	O2A-CGA-CBA	3.02	120.70	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	613	CLA	CHB-C4A-NA	3.02	128.69	124.51
24	3	605	CHL	CMD-C2D-C3D	3.03	121.93	114.27
24	N	608	CHL	O2A-CGA-CBA	3.03	120.70	111.90
24	g	607	CHL	CHC-C4B-C3B	3.03	125.40	118.23
25	1	603	CLA	CHB-C4A-NA	3.03	128.70	124.51
27	G	1622	XAT	C18-C5-C4	3.03	117.75	114.28
24	n	607	CHL	O2D-CGD-CBD	3.03	118.59	111.20
24	6	607	CHL	CHB-C1B-C2B	3.03	125.38	116.99
27	g	1622	XAT	C18-C5-C4	3.03	117.75	114.28
24	y	601	CHL	C4-C3-C5	3.03	120.54	115.29
24	Y	601	CHL	C4-C3-C5	3.03	120.55	115.29
25	b	616	CLA	CHB-C4A-NA	3.03	128.71	124.51
24	7	608	CHL	O2D-CGD-CBD	3.03	118.60	111.20
24	1	609	CHL	O2A-CGA-CBA	3.03	120.72	111.90
25	8	604	CLA	CMB-C2B-C3B	3.03	130.52	124.89
24	8	608	CHL	CHD-C1D-C2D	3.04	125.40	116.99
24	2	607	CHL	CHC-C4B-C3B	3.04	125.42	118.23
24	5	608	CHL	CHD-C1D-C2D	3.04	125.40	116.99
34	a	418	SQD	C4-C3-C2	3.04	116.19	110.84
24	G	606	CHL	O2A-CGA-CBA	3.04	120.74	111.90
24	G	607	CHL	CHC-C4B-C3B	3.04	125.42	118.23
24	5	605	CHL	CMD-C2D-C3D	3.04	121.96	114.27
24	1	606	CHL	CHD-C1D-C2D	3.04	125.41	116.99
24	1	608	CHL	CHD-C1D-C2D	3.04	125.41	116.99
24	6	607	CHL	CHC-C4B-C3B	3.04	125.43	118.23
25	4	604	CLA	CMB-C2B-C3B	3.04	130.54	124.89
25	5	603	CLA	CHB-C4A-NA	3.04	128.72	124.51
29	B	2631	LHG	O8-C23-C24	3.05	120.77	111.90
25	r	613	CLA	CHB-C4A-NA	3.05	128.73	124.51
29	b	2631	LHG	O8-C23-C24	3.05	120.77	111.90
24	2	605	CHL	CMD-C2D-C3D	3.05	121.99	114.27
24	3	608	CHL	O2D-CGD-CBD	3.05	118.65	111.20
25	b	612	CLA	CMD-C2D-C3D	3.05	130.56	124.89
24	n	608	CHL	CHD-C1D-C2D	3.05	125.45	116.99
24	1	605	CHL	CMD-C2D-C3D	3.05	122.00	114.27
25	5	612	CLA	CMB-C2B-C3B	3.05	130.56	124.89
24	N	608	CHL	CHD-C1D-C2D	3.05	125.45	116.99
24	g	606	CHL	O2A-CGA-CBA	3.05	120.79	111.90
24	5	606	CHL	CHD-C1D-C2D	3.05	125.45	116.99
26	g	1621	LUT	C39-C29-C28	3.05	122.97	118.10
24	y	605	CHL	CMD-C2D-C3D	3.05	122.00	114.27
24	6	605	CHL	CMD-C2D-C3D	3.06	122.00	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	608	CHL	CHD-C1D-C2D	3.06	125.46	116.99
30	C	515	BCR	C37-C22-C23	3.06	122.98	118.10
24	7	608	CHL	CHD-C1D-C2D	3.06	125.48	116.99
25	1	612	CLA	CMB-C2B-C3B	3.07	130.58	124.89
24	2	608	CHL	CHD-C1D-C2D	3.07	125.49	116.99
25	8	604	CLA	CHB-C4A-NA	3.07	128.76	124.51
26	S	1621	LUT	C17-C1-C6	3.07	115.28	110.31
24	6	608	CHL	CHD-C1D-C2D	3.07	125.49	116.99
34	a	418	SQD	O6-C1-C2	3.07	113.24	108.23
24	4	606	CHL	CMD-C2D-C3D	3.07	122.04	114.27
24	Y	605	CHL	CMD-C2D-C3D	3.07	122.05	114.27
26	G	1621	LUT	C39-C29-C28	3.07	123.00	118.10
30	c	515	BCR	C37-C22-C23	3.07	123.00	118.10
24	1	607	CHL	O2D-CGD-CBD	3.07	118.70	111.20
24	S	607	CHL	CHD-C1D-C2D	3.08	125.52	116.99
25	4	604	CLA	CHB-C4A-NA	3.08	128.77	124.51
29	d	410	LHG	O8-C23-C24	3.08	120.87	111.90
24	8	606	CHL	CMD-C2D-C3D	3.08	122.08	114.27
29	D	410	LHG	O8-C23-C24	3.09	120.88	111.90
24	5	607	CHL	O2D-CGD-CBD	3.09	118.74	111.20
26	s	1621	LUT	C17-C1-C6	3.09	115.32	110.31
24	s	606	CHL	CMD-C2D-C3D	3.09	122.09	114.27
24	8	608	CHL	CMD-C2D-C3D	3.09	122.09	114.27
25	C	502	CLA	C4A-NA-C1A	3.09	110.29	106.45
24	8	601	CHL	CMD-C2D-C3D	3.09	122.09	114.27
24	3	609	CHL	CHC-C4B-C3B	3.09	125.55	118.23
24	s	607	CHL	CHD-C1D-C2D	3.09	125.55	116.99
24	g	608	CHL	CHC-C4B-C3B	3.09	125.56	118.23
34	A	418	SQD	O6-C1-C2	3.09	113.28	108.23
26	R	620	LUT	C39-C29-C28	3.09	123.03	118.10
25	A	410	CLA	CMB-C2B-C3B	3.09	130.63	124.89
24	7	609	CHL	CHC-C4B-C3B	3.09	125.56	118.23
24	S	606	CHL	CMD-C2D-C3D	3.10	122.10	114.27
25	c	509	CLA	CHB-C4A-NA	3.10	128.79	124.51
25	n	612	CLA	CHB-C4A-NA	3.10	128.79	124.51
24	4	608	CHL	CMD-C2D-C3D	3.10	122.11	114.27
25	c	502	CLA	C4A-NA-C1A	3.10	110.30	106.45
26	r	620	LUT	C39-C29-C28	3.10	123.04	118.10
24	4	601	CHL	CMD-C2D-C3D	3.10	122.12	114.27
25	C	509	CLA	CHB-C4A-NA	3.10	128.80	124.51
24	G	608	CHL	CHC-C4B-C3B	3.10	125.58	118.23
25	6	613	CLA	CMB-C2B-C3B	3.11	130.65	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	5	1622	XAT	O24-C25-C38	3.11	118.91	115.02
25	N	612	CLA	CHB-C4A-NA	3.11	128.81	124.51
25	2	613	CLA	CMB-C2B-C3B	3.11	130.67	124.89
27	1	1622	XAT	O24-C25-C38	3.12	118.92	115.02
24	G	607	CHL	CMD-C2D-C3D	3.12	122.16	114.27
34	B	623	SQD	O5-C1-C2	3.12	116.31	110.30
25	a	410	CLA	CMB-C2B-C3B	3.12	130.68	124.89
25	g	614	CLA	CMB-C2B-C3B	3.12	130.69	124.89
34	b	623	SQD	O5-C1-C2	3.12	116.32	110.30
28	N	1623	NEX	C16-C1-C6	3.13	113.27	110.47
25	y	613	CLA	CMB-C2B-C3B	3.13	130.70	124.89
24	g	607	CHL	CMD-C2D-C3D	3.13	122.19	114.27
24	2	605	CHL	CHD-C1D-C2D	3.13	125.66	116.99
26	7	1620	LUT	C22-C23-C24	3.13	115.27	111.73
25	G	614	CLA	CMB-C2B-C3B	3.13	130.71	124.89
25	Y	613	CLA	CMB-C2B-C3B	3.13	130.71	124.89
24	6	605	CHL	CHD-C1D-C2D	3.14	125.68	116.99
28	n	1623	NEX	C16-C1-C6	3.14	113.28	110.47
26	3	1620	LUT	C22-C23-C24	3.15	115.28	111.73
25	S	613	CLA	CMD-C2D-C3D	3.16	130.75	124.89
24	1	607	CHL	CHC-C4B-C3B	3.16	125.72	118.23
24	5	607	CHL	CHC-C4B-C3B	3.16	125.72	118.23
24	G	608	CHL	CHD-C1D-C2D	3.16	125.75	116.99
24	g	608	CHL	CHD-C1D-C2D	3.17	125.76	116.99
34	B	623	SQD	O8-S-C6	3.17	109.88	106.01
25	B	611	CLA	CMB-C2B-C3B	3.17	130.78	124.89
25	b	611	CLA	CMB-C2B-C3B	3.17	130.78	124.89
24	s	608	CHL	O2D-CGD-CBD	3.17	118.94	111.20
34	b	623	SQD	O8-S-C6	3.18	109.89	106.01
25	s	613	CLA	CMD-C2D-C3D	3.18	130.79	124.89
24	n	608	CHL	CHC-C4B-C3B	3.18	125.76	118.23
24	N	608	CHL	CHC-C4B-C3B	3.18	125.77	118.23
24	G	601	CHL	CHC-C4B-C3B	3.19	125.78	118.23
25	6	603	CLA	CHB-C4A-NA	3.19	128.93	124.51
24	y	605	CHL	CHD-C1D-C2D	3.19	125.83	116.99
24	S	608	CHL	O2D-CGD-CBD	3.20	119.00	111.20
24	g	601	CHL	CHC-C4B-C3B	3.20	125.81	118.23
25	2	603	CLA	CHB-C4A-NA	3.20	128.94	124.51
25	n	612	CLA	CMD-C2D-C3D	3.20	130.83	124.89
24	R	607	CHL	CHC-C4B-C3B	3.21	125.83	118.23
25	N	612	CLA	CMD-C2D-C3D	3.21	130.85	124.89
24	5	608	CHL	O2D-CGD-CBD	3.21	119.04	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	605	CHL	CHD-C1D-C2D	3.21	125.89	116.99
24	g	607	CHL	CHD-C1D-C2D	3.22	125.90	116.99
24	G	607	CHL	CHD-C1D-C2D	3.22	125.90	116.99
27	2	1622	XAT	O4-C5-C18	3.22	119.05	115.02
24	1	608	CHL	O2D-CGD-CBD	3.22	119.06	111.20
27	6	1622	XAT	O4-C5-C18	3.22	119.05	115.02
24	r	607	CHL	CHC-C4B-C3B	3.22	125.86	118.23
24	n	605	CHL	O2A-CGA-CBA	3.22	121.28	111.90
24	2	606	CHL	CHD-C1D-C2D	3.23	125.92	116.99
25	2	611	CLA	CMB-C2B-C3B	3.23	130.88	124.89
24	y	608	CHL	CMD-C2D-C3D	3.23	122.44	114.27
25	6	611	CLA	CMB-C2B-C3B	3.23	130.88	124.89
39	f	101	HEM	CMB-C2B-C3B	3.23	130.88	124.89
24	N	605	CHL	O2A-CGA-CBA	3.23	121.30	111.90
24	s	607	CHL	O2D-CGD-CBD	3.23	119.09	111.20
24	6	606	CHL	CHD-C1D-C2D	3.24	125.95	116.99
39	F	101	HEM	CMB-C2B-C3B	3.24	130.90	124.89
24	Y	608	CHL	CMD-C2D-C3D	3.24	122.46	114.27
27	1	1622	XAT	O4-C5-C18	3.24	119.07	115.02
24	R	608	CHL	CMD-C2D-C3D	3.24	122.48	114.27
24	g	608	CHL	O2D-CGD-CBD	3.25	119.13	111.20
24	y	606	CHL	O2A-CGA-CBA	3.25	121.35	111.90
24	3	605	CHL	CHD-C1D-C2D	3.25	125.99	116.99
24	S	607	CHL	O2D-CGD-CBD	3.25	119.13	111.20
24	Y	606	CHL	O2D-CGD-CBD	3.25	119.14	111.20
24	2	601	CHL	CHC-C4B-C3B	3.26	125.94	118.23
24	7	605	CHL	CHD-C1D-C2D	3.26	126.01	116.99
24	G	608	CHL	O2D-CGD-CBD	3.26	119.16	111.20
24	r	608	CHL	CMD-C2D-C3D	3.26	122.52	114.27
25	c	503	CLA	CMB-C2B-C3B	3.26	130.94	124.89
25	B	617	CLA	CMB-C2B-C3B	3.26	130.94	124.89
25	c	512	CLA	CMB-C2B-C3B	3.26	130.94	124.89
24	Y	606	CHL	O2A-CGA-CBA	3.26	121.39	111.90
27	5	1622	XAT	O4-C5-C18	3.26	119.10	115.02
25	C	512	CLA	CMB-C2B-C3B	3.26	130.95	124.89
24	5	601	CHL	O2D-CGD-CBD	3.26	119.17	111.20
24	6	601	CHL	CHC-C4B-C3B	3.27	125.96	118.23
25	b	617	CLA	CMB-C2B-C3B	3.27	130.95	124.89
24	y	606	CHL	O2D-CGD-CBD	3.27	119.17	111.20
24	1	601	CHL	O2D-CGD-CBD	3.27	119.17	111.20
24	n	605	CHL	CHD-C1D-C2D	3.27	126.04	116.99
24	N	605	CHL	CHD-C1D-C2D	3.27	126.05	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	503	CLA	CMB-C2B-C3B	3.28	130.98	124.89
25	b	604	CLA	CMB-C2B-C3B	3.28	130.99	124.89
27	3	1622	XAT	O4-C5-C18	3.29	119.13	115.02
25	b	603	CLA	CMB-C2B-C3B	3.29	130.99	124.89
25	2	614	CLA	CMB-C2B-C3B	3.29	130.99	124.89
25	b	609	CLA	CMD-C2D-C3D	3.29	131.00	124.89
27	7	1622	XAT	O4-C5-C18	3.30	119.14	115.02
25	B	604	CLA	CMB-C2B-C3B	3.30	131.01	124.89
25	B	603	CLA	CMB-C2B-C3B	3.30	131.01	124.89
25	B	609	CLA	CMD-C2D-C3D	3.30	131.02	124.89
25	6	614	CLA	CMB-C2B-C3B	3.30	131.02	124.89
24	6	606	CHL	O2D-CGD-CBD	3.30	119.26	111.20
24	4	606	CHL	CHD-C1D-C2D	3.31	126.15	116.99
24	2	606	CHL	O2D-CGD-CBD	3.31	119.28	111.20
25	C	502	CLA	CMD-C2D-C3D	3.31	131.03	124.89
24	8	606	CHL	CHD-C1D-C2D	3.31	126.16	116.99
24	Y	606	CHL	CMD-C2D-C3D	3.31	122.65	114.27
25	c	502	CLA	CMD-C2D-C3D	3.31	131.04	124.89
34	b	621	SQD	O5-C5-C4	3.31	115.77	109.66
25	B	606	CLA	CHB-C4A-NA	3.32	129.10	124.51
24	y	606	CHL	CMD-C2D-C3D	3.32	122.67	114.27
24	S	607	CHL	CMD-C2D-C3D	3.32	122.67	114.27
34	B	621	SQD	O5-C5-C4	3.32	115.78	109.66
24	7	607	CHL	O2D-CGD-CBD	3.32	119.30	111.20
25	R	610	CLA	CMB-C2B-C3B	3.32	131.06	124.89
25	r	610	CLA	CMB-C2B-C3B	3.33	131.07	124.89
24	s	607	CHL	CMD-C2D-C3D	3.33	122.70	114.27
24	N	606	CHL	CHD-C1D-C2D	3.33	126.22	116.99
24	3	607	CHL	O2D-CGD-CBD	3.33	119.33	111.20
24	n	606	CHL	CHD-C1D-C2D	3.33	126.22	116.99
25	8	603	CLA	CMB-C2B-C3B	3.34	131.08	124.89
24	y	601	CHL	CHC-C4B-C3B	3.34	126.14	118.23
25	N	613	CLA	C4A-NA-C1A	3.34	110.60	106.45
24	g	605	CHL	CHD-C1D-C2D	3.34	126.25	116.99
25	b	606	CLA	CHB-C4A-NA	3.34	129.13	124.51
29	d	408	LHG	O8-C23-C24	3.34	121.63	111.90
24	y	608	CHL	CHC-C4B-C3B	3.35	126.16	118.23
24	Y	608	CHL	CHC-C4B-C3B	3.35	126.16	118.23
24	G	605	CHL	CHD-C1D-C2D	3.35	126.27	116.99
25	c	512	CLA	CMD-C2D-C3D	3.35	131.11	124.89
24	5	605	CHL	O2D-CGD-CBD	3.35	119.38	111.20
25	C	512	CLA	CMD-C2D-C3D	3.35	131.11	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	605	CHL	O2D-CGD-CBD	3.36	119.39	111.20
25	4	603	CLA	CMB-C2B-C3B	3.36	131.12	124.89
24	Y	601	CHL	CHC-C4B-C3B	3.36	126.18	118.23
29	D	408	LHG	O8-C23-C24	3.36	121.68	111.90
25	n	613	CLA	C4A-NA-C1A	3.36	110.63	106.45
24	y	605	CHL	O2D-CGD-CBD	3.36	119.41	111.20
24	Y	605	CHL	O2D-CGD-CBD	3.37	119.42	111.20
25	1	613	CLA	CMB-C2B-C3B	3.37	131.15	124.89
25	5	613	CLA	CMB-C2B-C3B	3.37	131.15	124.89
24	r	607	CHL	O2A-CGA-CBA	3.38	121.73	111.90
25	g	604	CLA	CMB-C2B-C3B	3.38	131.16	124.89
24	R	607	CHL	O2A-CGA-CBA	3.38	121.74	111.90
25	c	506	CLA	CMB-C2B-C3B	3.38	131.17	124.89
25	C	506	CLA	CMB-C2B-C3B	3.39	131.18	124.89
25	A	410	CLA	CMD-C2D-C3D	3.39	131.18	124.89
24	5	608	CHL	CHC-C4B-C3B	3.40	126.28	118.23
25	G	612	CLA	CMB-C2B-C3B	3.40	131.20	124.89
25	g	612	CLA	CMB-C2B-C3B	3.41	131.22	124.89
25	a	410	CLA	CMD-C2D-C3D	3.41	131.22	124.89
24	7	605	CHL	O2D-CGD-CBD	3.41	119.52	111.20
25	G	604	CLA	CMB-C2B-C3B	3.41	131.22	124.89
24	s	601	CHL	CHD-C1D-C2D	3.41	126.44	116.99
24	S	601	CHL	CHD-C1D-C2D	3.41	126.44	116.99
24	R	614	CHL	O2D-CGD-CBD	3.41	119.53	111.20
24	1	608	CHL	CHC-C4B-C3B	3.42	126.32	118.23
24	r	614	CHL	O2D-CGD-CBD	3.42	119.53	111.20
25	C	502	CLA	CMB-C2B-C3B	3.42	131.24	124.89
24	S	608	CHL	CHD-C1D-C2D	3.42	126.47	116.99
30	B	620	BCR	C33-C5-C4	3.42	119.95	113.45
24	s	608	CHL	CHD-C1D-C2D	3.43	126.48	116.99
24	3	605	CHL	O2D-CGD-CBD	3.43	119.56	111.20
24	g	609	CHL	CHD-C1D-C2D	3.43	126.49	116.99
26	1	1621	LUT	C19-C9-C8	3.43	123.57	118.10
25	7	603	CLA	CHB-C4A-NA	3.43	129.26	124.51
25	3	603	CLA	CHB-C4A-NA	3.44	129.26	124.51
24	G	606	CHL	CHD-C1D-C2D	3.44	126.51	116.99
26	5	1621	LUT	C19-C9-C8	3.44	123.58	118.10
24	G	609	CHL	CHD-C1D-C2D	3.44	126.53	116.99
30	b	620	BCR	C33-C5-C4	3.44	119.99	113.45
24	g	607	CHL	O2D-CGD-CBD	3.45	119.61	111.20
25	c	502	CLA	CMB-C2B-C3B	3.45	131.29	124.89
24	n	601	CHL	CHC-C4B-C3B	3.45	126.40	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	601	CHL	CHD-C1D-C2D	3.45	126.54	116.99
24	R	606	CHL	CHD-C1D-C2D	3.45	126.55	116.99
24	S	601	CHL	O2D-CGD-CBD	3.45	119.63	111.20
24	g	606	CHL	CHD-C1D-C2D	3.45	126.56	116.99
25	b	613	CLA	CHB-C4A-NA	3.46	129.29	124.51
24	G	607	CHL	O2D-CGD-CBD	3.46	119.64	111.20
24	r	606	CHL	CHD-C1D-C2D	3.46	126.57	116.99
24	6	609	CHL	CHD-C1D-C2D	3.46	126.57	116.99
34	a	418	SQD	C45-O47-C7	3.46	126.05	117.88
24	2	609	CHL	CHD-C1D-C2D	3.46	126.58	116.99
24	s	601	CHL	O2D-CGD-CBD	3.46	119.65	111.20
27	8	622	XAT	O4-C5-C18	3.46	119.35	115.02
24	N	601	CHL	CHC-C4B-C3B	3.46	126.43	118.23
27	n	1622	XAT	O4-C5-C18	3.47	119.36	115.02
25	c	511	CLA	CMB-C2B-C3B	3.47	131.33	124.89
25	B	613	CLA	CHB-C4A-NA	3.47	129.31	124.51
25	r	603	CLA	CMB-C2B-C3B	3.47	131.33	124.89
24	G	601	CHL	CHD-C1D-C2D	3.47	126.60	116.99
27	N	1622	XAT	O4-C5-C18	3.47	119.36	115.02
34	A	418	SQD	C45-O47-C7	3.47	126.07	117.88
24	s	606	CHL	CHD-C1D-C2D	3.47	126.61	116.99
24	S	606	CHL	CHC-C4B-C3B	3.47	126.46	118.23
25	R	603	CLA	CMB-C2B-C3B	3.47	131.34	124.89
28	5	1623	NEX	O24-C25-C38	3.48	119.37	115.02
25	4	602	CLA	O2D-CGD-CBD	3.48	117.52	111.30
24	S	606	CHL	CHD-C1D-C2D	3.48	126.63	116.99
25	8	602	CLA	O2D-CGD-CBD	3.48	117.52	111.30
27	4	622	XAT	O4-C5-C18	3.48	119.38	115.02
24	s	606	CHL	CHC-C4B-C3B	3.49	126.49	118.23
25	C	511	CLA	CMB-C2B-C3B	3.49	131.37	124.89
25	S	613	CLA	CMB-C2B-C3B	3.49	131.37	124.89
24	R	608	CHL	O2D-CGD-CBD	3.50	119.74	111.20
24	n	601	CHL	CHD-C1D-C2D	3.50	126.68	116.99
24	r	608	CHL	O2D-CGD-CBD	3.50	119.74	111.20
25	6	611	CLA	CMD-C2D-C3D	3.50	131.39	124.89
25	c	507	CLA	CMB-C2B-C3B	3.50	131.39	124.89
25	2	611	CLA	CMD-C2D-C3D	3.51	131.40	124.89
24	8	609	CHL	O2D-CGD-CBD	3.51	119.76	111.20
24	4	607	CHL	O2D-CGD-CBD	3.51	119.76	111.20
24	8	607	CHL	O2D-CGD-CBD	3.51	119.76	111.20
24	N	601	CHL	CHD-C1D-C2D	3.51	126.71	116.99
28	1	1623	NEX	O24-C25-C38	3.51	119.42	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	613	CLA	CMB-C2B-C3B	3.51	131.41	124.89
25	C	507	CLA	CMB-C2B-C3B	3.51	131.41	124.89
25	Y	610	CLA	CMB-C2B-C3B	3.52	131.42	124.89
25	a	406	CLA	CMB-C2B-C3B	3.52	131.42	124.89
24	4	601	CHL	CHB-C1B-C2B	3.52	126.73	116.99
24	8	601	CHL	CHB-C1B-C2B	3.52	126.73	116.99
25	R	610	CLA	CHB-C4A-NA	3.52	129.38	124.51
25	B	605	CLA	CMB-C2B-C3B	3.52	131.42	124.89
25	r	610	CLA	CHB-C4A-NA	3.52	129.38	124.51
24	Y	601	CHL	CHD-C1D-C2D	3.52	126.75	116.99
34	B	621	SQD	C1-O5-C5	3.52	120.35	113.72
25	y	610	CLA	CMB-C2B-C3B	3.52	131.43	124.89
24	4	609	CHL	O2D-CGD-CBD	3.53	119.80	111.20
24	y	601	CHL	CHD-C1D-C2D	3.53	126.76	116.99
28	6	1623	NEX	O24-C25-C38	3.53	119.43	115.02
30	T	101	BCR	C1-C6-C7	3.53	125.65	115.73
25	A	406	CLA	CMB-C2B-C3B	3.53	131.44	124.89
24	5	607	CHL	CHD-C1D-C2D	3.53	126.77	116.99
34	b	621	SQD	C1-O5-C5	3.53	120.37	113.72
30	t	101	BCR	C1-C6-C7	3.53	125.66	115.73
25	b	605	CLA	CMB-C2B-C3B	3.54	131.45	124.89
24	8	601	CHL	CHC-C4B-C3B	3.54	126.62	118.23
27	N	1622	XAT	O24-C25-C38	3.54	119.45	115.02
25	N	614	CLA	CMB-C2B-C3B	3.54	131.47	124.89
24	1	607	CHL	CHD-C1D-C2D	3.55	126.81	116.99
24	4	601	CHL	CHC-C4B-C3B	3.55	126.63	118.23
24	4	609	CHL	CHD-C1D-C2D	3.55	126.82	116.99
28	2	1623	NEX	O24-C25-C38	3.55	119.46	115.02
27	n	1622	XAT	O24-C25-C38	3.55	119.47	115.02
25	n	614	CLA	CMB-C2B-C3B	3.55	131.48	124.89
24	2	601	CHL	CHD-C1D-C2D	3.55	126.84	116.99
25	5	602	CLA	CMB-C2B-C3B	3.56	131.49	124.89
24	8	609	CHL	CHD-C1D-C2D	3.56	126.84	116.99
24	6	601	CHL	CHD-C1D-C2D	3.56	126.84	116.99
25	1	602	CLA	CMB-C2B-C3B	3.56	131.50	124.89
24	G	605	CHL	O2D-CGD-CBD	3.56	119.89	111.20
24	R	607	CHL	O2D-CGD-CBD	3.57	119.91	111.20
24	g	605	CHL	O2D-CGD-CBD	3.57	119.91	111.20
25	y	613	CLA	C4A-NA-C1A	3.57	110.89	106.45
24	G	601	CHL	O2D-CGD-CBD	3.57	119.92	111.20
24	N	606	CHL	O2D-CGD-CBD	3.58	119.93	111.20
24	n	606	CHL	O2D-CGD-CBD	3.58	119.93	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	606	CHL	O2D-CGD-CBD	3.58	119.93	111.20
34	a	412	SQD	O47-C7-C8	3.58	118.98	111.55
34	A	412	SQD	O47-C7-C8	3.58	118.98	111.55
24	g	601	CHL	O2D-CGD-CBD	3.58	119.94	111.20
24	l	606	CHL	O2D-CGD-CBD	3.58	119.94	111.20
24	r	607	CHL	O2D-CGD-CBD	3.58	119.94	111.20
25	Y	613	CLA	C4A-NA-C1A	3.58	110.90	106.45
25	6	604	CLA	CMB-C2B-C3B	3.58	131.54	124.89
28	n	1623	NEX	O24-C25-C38	3.59	119.51	115.02
25	2	604	CLA	CMB-C2B-C3B	3.59	131.56	124.89
25	R	604	CLA	CMB-C2B-C3B	3.59	131.56	124.89
28	N	1623	NEX	O24-C25-C38	3.59	119.52	115.02
24	l	601	CHL	CHD-C1D-C2D	3.59	126.94	116.99
25	G	610	CLA	CMB-C2B-C3B	3.60	131.58	124.89
25	8	610	CLA	CMB-C2B-C3B	3.60	131.58	124.89
25	r	601	CLA	CMB-C2B-C3B	3.61	131.58	124.89
25	r	604	CLA	CMB-C2B-C3B	3.61	131.59	124.89
24	N	609	CHL	CHD-C1D-C2D	3.61	127.00	116.99
25	R	601	CLA	CMB-C2B-C3B	3.61	131.60	124.89
24	5	601	CHL	CHD-C1D-C2D	3.62	127.01	116.99
39	F	101	HEM	CMC-C2C-C3C	3.62	131.60	124.89
25	4	610	CLA	CMB-C2B-C3B	3.62	131.60	124.89
25	g	610	CLA	CMB-C2B-C3B	3.62	131.61	124.89
24	3	607	CHL	CHD-C1D-C2D	3.62	127.01	116.99
25	y	602	CLA	CMB-C2B-C3B	3.62	131.61	124.89
24	g	609	CHL	O2D-CGD-CBD	3.62	120.04	111.20
39	f	101	HEM	CMC-C2C-C3C	3.62	131.62	124.89
24	7	607	CHL	CHD-C1D-C2D	3.63	127.04	116.99
24	n	609	CHL	CHD-C1D-C2D	3.63	127.04	116.99
24	G	609	CHL	O2D-CGD-CBD	3.63	120.06	111.20
25	c	509	CLA	CMB-C2B-C3B	3.63	131.63	124.89
25	Y	602	CLA	CMB-C2B-C3B	3.63	131.63	124.89
25	l	614	CLA	CMB-C2B-C3B	3.64	131.64	124.89
24	6	605	CHL	O2D-CGD-CBD	3.64	120.07	111.20
24	y	609	CHL	CHD-C1D-C2D	3.64	127.07	116.99
25	C	509	CLA	CMB-C2B-C3B	3.64	131.64	124.89
28	3	1623	NEX	O24-C25-C38	3.64	119.58	115.02
25	5	614	CLA	CMB-C2B-C3B	3.64	131.66	124.89
28	7	1623	NEX	O24-C25-C38	3.65	119.58	115.02
24	s	606	CHL	O2D-CGD-CBD	3.65	120.10	111.20
24	S	606	CHL	O2D-CGD-CBD	3.65	120.11	111.20
24	2	605	CHL	O2D-CGD-CBD	3.66	120.12	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	601	CHL	CHD-C1D-C2D	3.66	127.12	116.99
24	3	601	CHL	CHD-C1D-C2D	3.66	127.12	116.99
24	Y	609	CHL	CHD-C1D-C2D	3.66	127.12	116.99
25	b	608	CLA	CMB-C2B-C3B	3.66	131.69	124.89
28	r	623	NEX	O24-C25-C38	3.67	119.61	115.02
28	R	623	NEX	O24-C25-C38	3.67	119.61	115.02
25	B	608	CLA	CMB-C2B-C3B	3.67	131.71	124.89
24	R	607	CHL	CHD-C1D-C2D	3.68	127.17	116.99
34	a	412	SQD	O5-C5-C4	3.68	116.43	109.66
24	r	607	CHL	CHD-C1D-C2D	3.68	127.19	116.99
28	S	1623	NEX	O24-C25-C38	3.68	119.63	115.02
24	y	601	CHL	O2D-CGD-CBD	3.69	120.20	111.20
24	Y	601	CHL	O2D-CGD-CBD	3.69	120.21	111.20
27	R	622	XAT	O24-C25-C38	3.70	119.65	115.02
34	A	412	SQD	O5-C5-C4	3.70	116.47	109.66
27	r	622	XAT	O24-C25-C38	3.71	119.66	115.02
25	R	601	CLA	CBC-CAC-C3C	3.71	122.94	112.41
25	d	402	CLA	CMB-C2B-C3B	3.71	131.77	124.89
25	r	601	CLA	CBC-CAC-C3C	3.71	122.96	112.41
24	3	607	CHL	CHC-C4B-C3B	3.72	127.03	118.23
24	7	607	CHL	CHC-C4B-C3B	3.72	127.03	118.23
25	c	505	CLA	CMB-C2B-C3B	3.72	131.80	124.89
28	s	1623	NEX	O24-C25-C38	3.72	119.68	115.02
25	N	613	CLA	CMB-C2B-C3B	3.73	131.80	124.89
24	r	606	CHL	O2D-CGD-CBD	3.73	120.30	111.20
25	S	610	CLA	CMB-C2B-C3B	3.73	131.81	124.89
24	R	606	CHL	O2D-CGD-CBD	3.73	120.30	111.20
25	n	613	CLA	CMB-C2B-C3B	3.73	131.82	124.89
25	D	402	CLA	CMB-C2B-C3B	3.73	131.82	124.89
25	s	602	CLA	CMB-C2B-C3B	3.74	131.84	124.89
25	C	505	CLA	CMB-C2B-C3B	3.75	131.84	124.89
25	S	602	CLA	CMB-C2B-C3B	3.75	131.85	124.89
25	s	610	CLA	CMB-C2B-C3B	3.75	131.85	124.89
24	n	609	CHL	O2D-CGD-CBD	3.75	120.35	111.20
24	N	609	CHL	O2D-CGD-CBD	3.75	120.36	111.20
24	3	606	CHL	CHC-C4B-C3B	3.76	127.14	118.23
34	A	412	SQD	C1-O5-C5	3.77	120.82	113.72
24	1	605	CHL	CHD-C1D-C2D	3.77	127.44	116.99
36	A	414	PL9	C7-C3-C4	3.77	123.64	118.29
24	7	606	CHL	CHC-C4B-C3B	3.78	127.17	118.23
36	a	414	PL9	C7-C3-C4	3.78	123.65	118.29
25	N	602	CLA	CMB-C2B-C3B	3.78	131.90	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	605	CHL	CHD-C1D-C2D	3.78	127.46	116.99
25	n	602	CLA	CMB-C2B-C3B	3.78	131.91	124.89
25	1	610	CLA	CMB-C2B-C3B	3.79	131.92	124.89
34	B	621	SQD	O47-C7-C8	3.79	119.42	111.55
34	a	412	SQD	C1-O5-C5	3.79	120.86	113.72
34	b	621	SQD	O47-C7-C8	3.79	119.43	111.55
25	r	603	CLA	CMD-C2D-C3D	3.80	131.95	124.89
25	5	610	CLA	CMB-C2B-C3B	3.81	131.96	124.89
24	7	606	CHL	CHD-C1D-C2D	3.81	127.56	116.99
24	2	607	CHL	CHD-C1D-C2D	3.82	127.56	116.99
27	g	1622	XAT	O24-C25-C38	3.82	119.80	115.02
25	S	604	CLA	CMB-C2B-C3B	3.82	131.99	124.89
24	3	606	CHL	CHD-C1D-C2D	3.82	127.58	116.99
25	s	604	CLA	CMB-C2B-C3B	3.82	131.99	124.89
25	R	603	CLA	CMD-C2D-C3D	3.83	131.99	124.89
25	n	604	CLA	CMB-C2B-C3B	3.83	131.99	124.89
24	4	607	CHL	CHD-C1D-C2D	3.83	127.59	116.99
29	3	2630	LHG	O4-P-O5	3.83	132.09	112.28
24	6	607	CHL	CHD-C1D-C2D	3.83	127.60	116.99
29	7	2630	LHG	O4-P-O5	3.83	132.12	112.28
28	y	1623	NEX	C2-C1-C6	3.84	112.94	109.21
24	8	607	CHL	CHD-C1D-C2D	3.84	127.62	116.99
25	N	604	CLA	CMB-C2B-C3B	3.84	132.02	124.89
34	a	418	SQD	O8-S-C6	3.84	110.70	106.01
24	1	609	CHL	O2D-CGD-CBD	3.84	120.58	111.20
34	A	418	SQD	O8-S-C6	3.85	110.70	106.01
24	5	609	CHL	O2D-CGD-CBD	3.85	120.59	111.20
28	Y	1623	NEX	C2-C1-C6	3.85	112.95	109.21
25	B	610	CLA	CMB-C2B-C3B	3.85	132.04	124.89
27	G	1622	XAT	O24-C25-C38	3.86	119.85	115.02
25	b	610	CLA	CMB-C2B-C3B	3.86	132.06	124.89
29	g	2630	LHG	O4-P-O5	3.86	132.27	112.28
29	G	2630	LHG	O4-P-O5	3.86	132.27	112.28
24	7	609	CHL	CHD-C1D-C2D	3.87	127.72	116.99
24	n	605	CHL	O2D-CGD-CBD	3.88	120.66	111.20
25	B	615	CLA	CMB-C2B-C3B	3.89	132.10	124.89
24	N	605	CHL	O2D-CGD-CBD	3.89	120.69	111.20
24	3	609	CHL	CHD-C1D-C2D	3.89	127.78	116.99
24	N	608	CHL	O2D-CGD-CBD	3.90	120.71	111.20
24	n	608	CHL	O2D-CGD-CBD	3.90	120.72	111.20
25	b	615	CLA	CMB-C2B-C3B	3.90	132.13	124.89
25	c	504	CLA	CMB-C2B-C3B	3.91	132.15	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	2631	LHG	O4-P-O5	3.92	132.55	112.28
29	B	2631	LHG	O4-P-O5	3.92	132.56	112.28
25	C	504	CLA	CMB-C2B-C3B	3.92	132.17	124.89
24	7	601	CHL	O2D-CGD-CBD	3.92	120.78	111.20
25	6	602	CLA	CMB-C2B-C3B	3.94	132.21	124.89
29	b	2630	LHG	O4-P-O5	3.95	132.72	112.28
25	2	602	CLA	CMB-C2B-C3B	3.95	132.22	124.89
29	B	2630	LHG	O4-P-O5	3.95	132.74	112.28
24	3	601	CHL	O2D-CGD-CBD	3.95	120.85	111.20
25	b	614	CLA	CMB-C2B-C3B	3.96	132.24	124.89
29	5	2630	LHG	O4-P-O5	3.96	132.80	112.28
25	B	614	CLA	CMB-C2B-C3B	3.96	132.25	124.89
29	C	2630	LHG	O4-P-O5	3.96	132.80	112.28
29	1	2630	LHG	O4-P-O5	3.96	132.80	112.28
26	g	1621	LUT	C2-C3-C4	3.97	115.80	110.32
24	5	609	CHL	CHD-C1D-C2D	3.97	127.99	116.99
29	c	2630	LHG	O4-P-O5	3.97	132.84	112.28
25	4	612	CLA	CMB-C2B-C3B	3.97	132.27	124.89
24	1	609	CHL	CHD-C1D-C2D	3.98	128.00	116.99
25	S	612	CLA	CMB-C2B-C3B	3.98	132.28	124.89
25	4	602	CLA	CMB-C2B-C3B	3.98	132.28	124.89
24	N	601	CHL	O2D-CGD-CBD	3.98	120.92	111.20
26	G	1621	LUT	C2-C3-C4	3.99	115.83	110.32
25	8	602	CLA	CMB-C2B-C3B	3.99	132.29	124.89
25	N	610	CLA	CMB-C2B-C3B	3.99	132.29	124.89
25	s	612	CLA	CMB-C2B-C3B	3.99	132.30	124.89
25	8	612	CLA	CMB-C2B-C3B	4.00	132.31	124.89
24	n	601	CHL	O2D-CGD-CBD	4.00	120.96	111.20
27	2	1622	XAT	O24-C25-C38	4.00	120.03	115.02
25	n	610	CLA	CMB-C2B-C3B	4.01	132.32	124.89
29	2	2630	LHG	O4-P-O5	4.01	133.02	112.28
29	c	522	LHG	O4-P-O5	4.01	133.03	112.28
27	6	1622	XAT	O24-C25-C38	4.01	120.04	115.02
29	6	2630	LHG	O4-P-O5	4.01	133.04	112.28
29	C	522	LHG	O4-P-O5	4.01	133.04	112.28
34	B	623	SQD	C1-O5-C5	4.02	121.28	113.72
29	S	2630	LHG	O4-P-O5	4.02	133.07	112.28
29	N	2630	LHG	O4-P-O5	4.02	133.08	112.28
25	3	602	CLA	CMB-C2B-C3B	4.02	132.35	124.89
29	n	2630	LHG	O4-P-O5	4.02	133.09	112.28
29	s	2630	LHG	O4-P-O5	4.02	133.10	112.28
24	R	614	CHL	CHD-C1D-C2D	4.02	128.13	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	614	CHL	CHD-C1D-C2D	4.03	128.14	116.99
29	D	409	LHG	O4-P-O5	4.03	133.12	112.28
29	d	409	LHG	O4-P-O5	4.03	133.12	112.28
34	b	623	SQD	C1-O5-C5	4.03	121.30	113.72
25	7	602	CLA	CMB-C2B-C3B	4.04	132.39	124.89
34	B	623	SQD	O47-C7-C8	4.04	119.95	111.55
24	2	609	CHL	O2D-CGD-CBD	4.05	121.09	111.20
29	r	2630	LHG	O4-P-O5	4.05	133.26	112.28
29	D	410	LHG	O4-P-O5	4.05	133.26	112.28
34	b	623	SQD	O47-C7-C8	4.05	119.97	111.55
29	d	410	LHG	O4-P-O5	4.06	133.28	112.28
29	R	2630	LHG	O4-P-O5	4.06	133.28	112.28
29	C	523	LHG	O4-P-O5	4.06	133.31	112.28
24	6	609	CHL	O2D-CGD-CBD	4.07	121.12	111.20
29	c	523	LHG	O4-P-O5	4.07	133.34	112.28
34	A	418	SQD	O9-S-C6	4.08	110.31	106.83
29	y	2630	LHG	O4-P-O5	4.09	133.45	112.28
29	Y	2630	LHG	O4-P-O5	4.09	133.45	112.28
29	8	2630	LHG	O4-P-O5	4.11	133.55	112.28
29	4	2630	LHG	O4-P-O5	4.11	133.57	112.28
34	a	418	SQD	O9-S-C6	4.12	110.34	106.83
29	L	101	LHG	O4-P-O5	4.12	133.60	112.28
29	l	101	LHG	O4-P-O5	4.13	133.64	112.28
26	5	1621	LUT	C2-C3-C4	4.14	116.04	110.32
25	d	403	CLA	CMB-C2B-C3B	4.16	132.61	124.89
24	4	601	CHL	CHD-C1D-C2D	4.16	128.52	116.99
24	8	601	CHL	CHD-C1D-C2D	4.16	128.52	116.99
26	1	1621	LUT	C2-C3-C4	4.16	116.07	110.32
25	D	403	CLA	CMB-C2B-C3B	4.17	132.63	124.89
24	7	606	CHL	O2D-CGD-CBD	4.17	121.38	111.20
24	3	606	CHL	O2D-CGD-CBD	4.18	121.39	111.20
25	7	612	CLA	CMD-C2D-C3D	4.19	132.67	124.89
25	G	602	CLA	CMB-C2B-C3B	4.22	132.72	124.89
25	3	612	CLA	CMD-C2D-C3D	4.22	132.73	124.89
25	g	602	CLA	CMB-C2B-C3B	4.23	132.75	124.89
29	d	408	LHG	O4-P-O5	4.25	134.26	112.28
29	D	408	LHG	O4-P-O5	4.25	134.28	112.28
25	c	510	CLA	CMB-C2B-C3B	4.25	132.78	124.89
25	C	510	CLA	CMB-C2B-C3B	4.27	132.81	124.89
27	4	622	XAT	O24-C25-C38	4.27	120.36	115.02
25	s	614	CLA	CMB-C2B-C3B	4.27	132.82	124.89
27	8	622	XAT	O24-C25-C38	4.28	120.38	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	508	CLA	CMB-C2B-C3B	4.28	132.84	124.89
25	S	614	CLA	CMB-C2B-C3B	4.30	132.87	124.89
25	c	508	CLA	CMB-C2B-C3B	4.30	132.88	124.89
24	7	609	CHL	O2D-CGD-CBD	4.32	121.74	111.20
24	3	609	CHL	O2D-CGD-CBD	4.34	121.79	111.20
25	y	604	CLA	CMB-C2B-C3B	4.35	132.97	124.89
27	3	1622	XAT	O24-C25-C38	4.36	120.47	115.02
25	Y	604	CLA	CMB-C2B-C3B	4.36	132.98	124.89
25	a	405	CLA	CMB-C2B-C3B	4.37	133.00	124.89
27	7	1622	XAT	O24-C25-C38	4.37	120.49	115.02
24	4	608	CHL	C1D-CHD-C4C	4.39	121.72	112.37
25	B	613	CLA	CMB-C2B-C3B	4.39	133.04	124.89
25	A	405	CLA	CMB-C2B-C3B	4.39	133.04	124.89
24	8	608	CHL	C1D-CHD-C4C	4.40	121.74	112.37
24	Y	609	CHL	O2D-CGD-CBD	4.41	121.95	111.20
24	y	609	CHL	O2D-CGD-CBD	4.41	121.95	111.20
25	b	613	CLA	CMB-C2B-C3B	4.41	133.07	124.89
25	r	602	CLA	CMB-C2B-C3B	4.42	133.09	124.89
25	R	602	CLA	CMB-C2B-C3B	4.43	133.11	124.89
25	c	513	CLA	CMB-C2B-C3B	4.44	133.12	124.89
24	4	609	CHL	C1D-CHD-C4C	4.44	121.83	112.37
25	C	513	CLA	CMB-C2B-C3B	4.46	133.16	124.89
24	8	609	CHL	C1D-CHD-C4C	4.46	121.88	112.37
25	b	612	CLA	CMB-C2B-C3B	4.46	133.18	124.89
24	7	609	CHL	C1D-CHD-C4C	4.47	121.89	112.37
25	B	612	CLA	CMB-C2B-C3B	4.48	133.20	124.89
24	3	609	CHL	C1D-CHD-C4C	4.49	121.93	112.37
27	G	1622	XAT	O4-C5-C18	4.50	120.65	115.02
27	g	1622	XAT	O4-C5-C18	4.54	120.70	115.02
34	b	623	SQD	O7-S-C6	4.59	110.75	106.83
34	B	623	SQD	O7-S-C6	4.60	110.76	106.83
30	t	101	BCR	C33-C5-C4	4.60	122.19	113.45
30	T	101	BCR	C33-C5-C4	4.63	122.23	113.45
24	y	607	CHL	C1D-CHD-C4C	4.64	122.27	112.37
24	Y	607	CHL	C1D-CHD-C4C	4.64	122.27	112.37
24	r	614	CHL	C1D-CHD-C4C	4.66	122.30	112.37
34	a	412	SQD	O8-S-C6	4.67	111.70	106.01
24	R	614	CHL	C1D-CHD-C4C	4.67	122.32	112.37
24	r	608	CHL	C1D-CHD-C4C	4.67	122.33	112.37
36	D	405	PL9	C7-C3-C4	4.68	120.68	116.88
24	R	608	CHL	C1D-CHD-C4C	4.69	122.36	112.37
34	A	412	SQD	O8-S-C6	4.69	111.73	106.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	d	405	PL9	C7-C3-C4	4.69	120.69	116.88
24	g	607	CHL	C1D-CHD-C4C	4.71	122.40	112.37
25	r	601	CLA	CAC-C3C-C4C	4.72	131.49	124.83
27	Y	1622	XAT	O4-C5-C4	4.73	116.76	113.33
24	G	607	CHL	C1D-CHD-C4C	4.73	122.45	112.37
24	6	609	CHL	C1D-CHD-C4C	4.73	122.46	112.37
24	2	609	CHL	C1D-CHD-C4C	4.74	122.47	112.37
25	R	601	CLA	CAC-C3C-C4C	4.75	131.53	124.83
25	b	613	CLA	CMD-C2D-C3D	4.75	133.71	124.89
24	3	607	CHL	C1D-CHD-C4C	4.76	122.51	112.37
24	8	601	CHL	C1D-CHD-C4C	4.76	122.51	112.37
24	4	601	CHL	C1D-CHD-C4C	4.76	122.52	112.37
24	7	607	CHL	C1D-CHD-C4C	4.77	122.53	112.37
25	B	613	CLA	CMD-C2D-C3D	4.77	133.74	124.89
24	Y	606	CHL	C1D-CHD-C4C	4.77	122.55	112.37
24	7	606	CHL	C1D-CHD-C4C	4.78	122.56	112.37
24	y	606	CHL	C1D-CHD-C4C	4.79	122.57	112.37
27	y	1622	XAT	O4-C5-C4	4.79	116.81	113.33
24	Y	608	CHL	C1D-CHD-C4C	4.79	122.58	112.37
27	Y	1622	XAT	O24-C25-C38	4.79	121.02	115.02
24	3	606	CHL	C1D-CHD-C4C	4.80	122.61	112.37
27	y	1622	XAT	O24-C25-C38	4.81	121.04	115.02
24	R	607	CHL	C1D-CHD-C4C	4.82	122.63	112.37
24	y	608	CHL	C1D-CHD-C4C	4.82	122.63	112.37
24	r	607	CHL	C1D-CHD-C4C	4.84	122.67	112.37
24	2	607	CHL	C1D-CHD-C4C	4.84	122.69	112.37
24	6	607	CHL	C1D-CHD-C4C	4.86	122.73	112.37
25	B	609	CLA	CMB-C2B-C3B	4.87	133.94	124.89
25	b	609	CLA	CMB-C2B-C3B	4.90	133.97	124.89
24	N	607	CHL	C1D-CHD-C4C	4.91	122.83	112.37
24	n	607	CHL	C1D-CHD-C4C	4.92	122.84	112.37
24	2	605	CHL	C1D-CHD-C4C	4.94	122.91	112.37
24	6	605	CHL	C1D-CHD-C4C	4.96	122.93	112.37
24	5	607	CHL	C1D-CHD-C4C	4.97	122.95	112.37
24	y	609	CHL	C1D-CHD-C4C	4.98	122.99	112.37
24	1	606	CHL	C1D-CHD-C4C	4.99	123.00	112.37
24	4	607	CHL	C1D-CHD-C4C	4.99	123.00	112.37
24	1	607	CHL	C1D-CHD-C4C	4.99	123.01	112.37
24	N	608	CHL	C1D-CHD-C4C	4.99	123.01	112.37
24	5	606	CHL	C1D-CHD-C4C	4.99	123.01	112.37
34	A	412	SQD	O7-S-C6	4.99	111.09	106.83
24	n	608	CHL	C1D-CHD-C4C	4.99	123.01	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	609	CHL	C1D-CHD-C4C	4.99	123.02	112.37
24	8	607	CHL	C1D-CHD-C4C	5.00	123.03	112.37
24	G	608	CHL	C1D-CHD-C4C	5.01	123.04	112.37
24	1	605	CHL	C1D-CHD-C4C	5.02	123.06	112.37
28	Y	1623	NEX	O24-C25-C38	5.02	121.30	115.02
24	5	605	CHL	C1D-CHD-C4C	5.02	123.07	112.37
34	a	412	SQD	O7-S-C6	5.02	111.12	106.83
24	g	608	CHL	C1D-CHD-C4C	5.02	123.08	112.37
24	y	605	CHL	C1D-CHD-C4C	5.03	123.09	112.37
28	y	1623	NEX	O24-C25-C38	5.03	121.32	115.02
24	Y	605	CHL	C1D-CHD-C4C	5.04	123.11	112.37
34	A	412	SQD	O9-S-C6	5.05	111.14	106.83
24	2	606	CHL	C1D-CHD-C4C	5.06	123.14	112.37
34	a	412	SQD	O9-S-C6	5.06	111.15	106.83
24	6	606	CHL	C1D-CHD-C4C	5.06	123.15	112.37
24	5	609	CHL	C1D-CHD-C4C	5.06	123.16	112.37
24	1	609	CHL	C1D-CHD-C4C	5.08	123.19	112.37
24	G	605	CHL	C1D-CHD-C4C	5.08	123.19	112.37
24	g	605	CHL	C1D-CHD-C4C	5.08	123.20	112.37
24	s	608	CHL	C1D-CHD-C4C	5.08	123.20	112.37
24	S	608	CHL	C1D-CHD-C4C	5.09	123.21	112.37
24	5	608	CHL	C1D-CHD-C4C	5.09	123.22	112.37
24	1	608	CHL	C1D-CHD-C4C	5.09	123.23	112.37
24	N	605	CHL	C1D-CHD-C4C	5.10	123.24	112.37
24	n	605	CHL	C1D-CHD-C4C	5.12	123.27	112.37
24	g	609	CHL	C1D-CHD-C4C	5.12	123.28	112.37
34	B	621	SQD	O7-S-C6	5.13	111.21	106.83
24	G	609	CHL	C1D-CHD-C4C	5.13	123.30	112.37
24	S	607	CHL	C1D-CHD-C4C	5.14	123.32	112.37
24	r	606	CHL	C1D-CHD-C4C	5.14	123.33	112.37
24	n	606	CHL	C1D-CHD-C4C	5.15	123.34	112.37
24	N	606	CHL	C1D-CHD-C4C	5.15	123.34	112.37
24	R	606	CHL	C1D-CHD-C4C	5.15	123.34	112.37
24	2	608	CHL	C1D-CHD-C4C	5.15	123.35	112.37
24	s	607	CHL	C1D-CHD-C4C	5.15	123.35	112.37
24	6	608	CHL	C1D-CHD-C4C	5.16	123.37	112.37
24	1	608	CHL	C3B-C4B-NB	5.17	112.57	103.55
34	b	621	SQD	O7-S-C6	5.17	111.25	106.83
24	5	608	CHL	C3B-C4B-NB	5.18	112.58	103.55
24	4	601	CHL	C3B-C4B-NB	5.22	112.65	103.55
24	8	601	CHL	C3B-C4B-NB	5.24	112.68	103.55
24	7	605	CHL	C1D-CHD-C4C	5.24	123.53	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	609	CHL	C1D-CHD-C4C	5.25	123.55	112.37
24	3	605	CHL	C1D-CHD-C4C	5.25	123.56	112.37
24	n	609	CHL	C1D-CHD-C4C	5.25	123.56	112.37
24	G	606	CHL	C1D-CHD-C4C	5.25	123.56	112.37
24	S	606	CHL	C1D-CHD-C4C	5.27	123.59	112.37
24	g	606	CHL	C1D-CHD-C4C	5.27	123.59	112.37
24	s	606	CHL	C1D-CHD-C4C	5.27	123.60	112.37
24	S	601	CHL	C1D-CHD-C4C	5.27	123.61	112.37
24	s	601	CHL	C1D-CHD-C4C	5.28	123.61	112.37
24	6	601	CHL	C1D-CHD-C4C	5.32	123.70	112.37
24	7	606	CHL	C3B-C4B-NB	5.32	112.82	103.55
24	2	601	CHL	C1D-CHD-C4C	5.32	123.71	112.37
24	3	606	CHL	C3B-C4B-NB	5.32	112.83	103.55
24	4	606	CHL	C1D-CHD-C4C	5.33	123.73	112.37
27	g	1622	XAT	O4-C5-C4	5.33	117.20	113.33
24	8	606	CHL	C1D-CHD-C4C	5.34	123.75	112.37
24	7	608	CHL	C1D-CHD-C4C	5.34	123.75	112.37
24	3	608	CHL	C1D-CHD-C4C	5.34	123.76	112.37
27	r	622	XAT	O4-C5-C18	5.35	121.72	115.02
27	R	622	XAT	O4-C5-C18	5.35	121.72	115.02
24	1	601	CHL	C1D-CHD-C4C	5.35	123.78	112.37
27	G	1622	XAT	O4-C5-C4	5.35	117.22	113.33
24	r	614	CHL	C3B-C4B-NB	5.36	112.90	103.55
24	3	601	CHL	C1D-CHD-C4C	5.36	123.80	112.37
24	s	606	CHL	C3B-C4B-NB	5.36	112.90	103.55
24	7	601	CHL	C1D-CHD-C4C	5.36	123.80	112.37
24	7	607	CHL	C3B-C4B-NB	5.37	112.91	103.55
24	R	614	CHL	C3B-C4B-NB	5.37	112.92	103.55
24	S	606	CHL	C3B-C4B-NB	5.37	112.92	103.55
24	5	601	CHL	C1D-CHD-C4C	5.38	123.83	112.37
24	3	607	CHL	C3B-C4B-NB	5.38	112.93	103.55
24	7	608	CHL	C3B-C4B-NB	5.43	113.01	103.55
24	S	601	CHL	C3B-C4B-NB	5.43	113.01	103.55
24	8	606	CHL	C3B-C4B-NB	5.43	113.02	103.55
24	s	601	CHL	C3B-C4B-NB	5.43	113.02	103.55
24	3	608	CHL	C3B-C4B-NB	5.43	113.02	103.55
24	4	606	CHL	C3B-C4B-NB	5.45	113.05	103.55
24	N	601	CHL	C3B-C4B-NB	5.46	113.08	103.55
34	b	623	SQD	O9-S-C6	5.47	111.50	106.83
34	B	623	SQD	O9-S-C6	5.47	111.50	106.83
24	n	601	CHL	C3B-C4B-NB	5.49	113.13	103.55
24	R	606	CHL	C3B-C4B-NB	5.50	113.14	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	606	CHL	C3B-C4B-NB	5.51	113.16	103.55
24	1	606	CHL	C3B-C4B-NB	5.52	113.17	103.55
24	y	601	CHL	C1D-CHD-C4C	5.52	124.13	112.37
24	Y	601	CHL	C1D-CHD-C4C	5.52	124.14	112.37
24	4	607	CHL	C3B-C4B-NB	5.53	113.19	103.55
24	8	607	CHL	C3B-C4B-NB	5.54	113.21	103.55
24	5	606	CHL	C3B-C4B-NB	5.54	113.21	103.55
24	6	605	CHL	C3B-C4B-NB	5.56	113.24	103.55
24	2	605	CHL	C3B-C4B-NB	5.56	113.24	103.55
24	n	601	CHL	C1D-CHD-C4C	5.58	124.27	112.37
24	G	606	CHL	C3B-C4B-NB	5.58	113.29	103.55
24	5	605	CHL	C3B-C4B-NB	5.59	113.30	103.55
24	g	606	CHL	C3B-C4B-NB	5.59	113.30	103.55
24	2	607	CHL	C3B-C4B-NB	5.59	113.30	103.55
24	N	601	CHL	C1D-CHD-C4C	5.60	124.30	112.37
24	6	601	CHL	C3B-C4B-NB	5.61	113.32	103.55
24	2	601	CHL	C3B-C4B-NB	5.61	113.32	103.55
24	6	607	CHL	C3B-C4B-NB	5.61	113.33	103.55
24	5	601	CHL	C3B-C4B-NB	5.61	113.33	103.55
24	1	605	CHL	C3B-C4B-NB	5.62	113.34	103.55
24	1	601	CHL	C3B-C4B-NB	5.62	113.35	103.55
24	g	601	CHL	C1D-CHD-C4C	5.62	124.35	112.37
24	y	608	CHL	C3B-C4B-NB	5.63	113.37	103.55
24	g	607	CHL	C3B-C4B-NB	5.63	113.37	103.55
24	N	606	CHL	C3B-C4B-NB	5.63	113.37	103.55
24	6	608	CHL	C3B-C4B-NB	5.64	113.37	103.55
24	G	601	CHL	C1D-CHD-C4C	5.64	124.38	112.37
24	Y	608	CHL	C3B-C4B-NB	5.64	113.39	103.55
24	n	606	CHL	C3B-C4B-NB	5.65	113.39	103.55
24	3	601	CHL	C3B-C4B-NB	5.65	113.41	103.55
24	6	609	CHL	C3B-C4B-NB	5.65	113.41	103.55
24	G	607	CHL	C3B-C4B-NB	5.66	113.41	103.55
24	2	608	CHL	C3B-C4B-NB	5.66	113.42	103.55
24	n	608	CHL	C3B-C4B-NB	5.66	113.42	103.55
24	R	608	CHL	C3B-C4B-NB	5.66	113.42	103.55
24	r	608	CHL	C3B-C4B-NB	5.68	113.44	103.55
24	N	608	CHL	C3B-C4B-NB	5.68	113.45	103.55
24	7	601	CHL	C3B-C4B-NB	5.68	113.46	103.55
24	2	609	CHL	C3B-C4B-NB	5.69	113.47	103.55
24	r	607	CHL	C3B-C4B-NB	5.71	113.50	103.55
27	y	1622	XAT	O4-C5-C18	5.73	122.19	115.02
24	R	607	CHL	C3B-C4B-NB	5.73	113.53	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	1622	XAT	O4-C5-C18	5.73	122.19	115.02
24	g	601	CHL	C3B-C4B-NB	5.73	113.55	103.55
24	7	609	CHL	C3B-C4B-NB	5.73	113.55	103.55
24	G	601	CHL	C3B-C4B-NB	5.74	113.56	103.55
24	N	605	CHL	C3B-C4B-NB	5.74	113.56	103.55
24	2	606	CHL	C3B-C4B-NB	5.75	113.58	103.55
24	G	608	CHL	C3B-C4B-NB	5.75	113.58	103.55
24	6	606	CHL	C3B-C4B-NB	5.77	113.60	103.55
24	g	608	CHL	C3B-C4B-NB	5.77	113.60	103.55
24	3	609	CHL	C3B-C4B-NB	5.77	113.61	103.55
24	n	605	CHL	C3B-C4B-NB	5.78	113.62	103.55
24	Y	601	CHL	C3B-C4B-NB	5.78	113.63	103.55
24	y	601	CHL	C3B-C4B-NB	5.80	113.66	103.55
24	5	607	CHL	C3B-C4B-NB	5.81	113.67	103.55
24	1	607	CHL	C3B-C4B-NB	5.82	113.70	103.55
24	8	609	CHL	C3B-C4B-NB	5.84	113.73	103.55
24	4	609	CHL	C3B-C4B-NB	5.84	113.73	103.55
24	3	605	CHL	C3B-C4B-NB	5.85	113.75	103.55
24	7	605	CHL	C3B-C4B-NB	5.86	113.77	103.55
24	4	608	CHL	C3B-C4B-NB	5.87	113.79	103.55
27	3	1622	XAT	O24-C25-C24	5.88	117.60	113.33
24	8	608	CHL	C3B-C4B-NB	5.89	113.81	103.55
24	7	601	CHL	C4B-CHC-C1C	5.89	124.92	112.37
24	Y	607	CHL	C3B-C4B-NB	5.90	113.83	103.55
24	3	601	CHL	C4B-CHC-C1C	5.90	124.94	112.37
24	y	607	CHL	C3B-C4B-NB	5.91	113.85	103.55
27	7	1622	XAT	O24-C25-C24	5.91	117.62	113.33
24	y	609	CHL	C3B-C4B-NB	5.94	113.91	103.55
24	Y	609	CHL	C3B-C4B-NB	5.95	113.93	103.55
24	N	606	CHL	C4B-CHC-C1C	5.96	125.07	112.37
24	n	606	CHL	C4B-CHC-C1C	5.96	125.07	112.37
24	1	609	CHL	C3B-C4B-NB	5.98	113.98	103.55
24	5	609	CHL	C3B-C4B-NB	5.99	113.99	103.55
24	G	605	CHL	C3B-C4B-NB	6.01	114.03	103.55
24	g	605	CHL	C3B-C4B-NB	6.05	114.09	103.55
24	n	607	CHL	C3B-C4B-NB	6.05	114.10	103.55
24	y	605	CHL	C3B-C4B-NB	6.06	114.12	103.55
24	N	607	CHL	C3B-C4B-NB	6.07	114.13	103.55
24	Y	605	CHL	C3B-C4B-NB	6.08	114.16	103.55
24	s	608	CHL	C3B-C4B-NB	6.12	114.23	103.55
24	S	608	CHL	C3B-C4B-NB	6.12	114.23	103.55
24	4	608	CHL	CMB-C2B-C3B	6.14	127.98	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	608	CHL	CMB-C2B-C3B	6.15	127.98	113.69
24	S	607	CHL	C3B-C4B-NB	6.16	114.30	103.55
24	s	607	CHL	C3B-C4B-NB	6.18	114.32	103.55
24	Y	601	CHL	CMB-C2B-C3B	6.20	128.10	113.69
24	y	601	CHL	CMB-C2B-C3B	6.20	128.11	113.69
24	Y	606	CHL	C3B-C4B-NB	6.21	114.37	103.55
24	y	606	CHL	C3B-C4B-NB	6.21	114.38	103.55
24	g	609	CHL	C3B-C4B-NB	6.23	114.41	103.55
24	G	606	CHL	C4B-CHC-C1C	6.24	125.66	112.37
24	7	607	CHL	C4B-CHC-C1C	6.24	125.66	112.37
24	4	601	CHL	C4B-CHC-C1C	6.24	125.67	112.37
24	G	609	CHL	C3B-C4B-NB	6.25	114.44	103.55
24	3	607	CHL	C4B-CHC-C1C	6.25	125.68	112.37
24	8	601	CHL	C4B-CHC-C1C	6.25	125.69	112.37
24	g	606	CHL	C4B-CHC-C1C	6.26	125.70	112.37
24	N	608	CHL	CMB-C2B-C3B	6.31	128.38	113.69
24	5	601	CHL	C4B-CHC-C1C	6.32	125.84	112.37
24	1	606	CHL	C4B-CHC-C1C	6.33	125.86	112.37
24	n	608	CHL	CMB-C2B-C3B	6.33	128.42	113.69
24	5	606	CHL	C4B-CHC-C1C	6.33	125.87	112.37
24	1	601	CHL	C4B-CHC-C1C	6.34	125.87	112.37
24	n	609	CHL	C3B-C4B-NB	6.35	114.63	103.55
24	N	609	CHL	C3B-C4B-NB	6.36	114.65	103.55
24	1	605	CHL	C4B-CHC-C1C	6.37	125.94	112.37
24	2	607	CHL	C4B-CHC-C1C	6.38	125.96	112.37
24	6	607	CHL	C4B-CHC-C1C	6.38	125.96	112.37
24	5	605	CHL	C4B-CHC-C1C	6.38	125.97	112.37
24	Y	606	CHL	C4B-CHC-C1C	6.47	126.16	112.37
24	g	601	CHL	CMB-C2B-C3B	6.47	128.75	113.69
24	Y	608	CHL	CMB-C2B-C3B	6.47	128.75	113.69
24	y	608	CHL	CMB-C2B-C3B	6.48	128.75	113.69
24	G	601	CHL	CMB-C2B-C3B	6.48	128.76	113.69
24	y	606	CHL	C4B-CHC-C1C	6.48	126.19	112.37
24	6	606	CHL	C4B-CHC-C1C	6.49	126.19	112.37
24	2	606	CHL	C4B-CHC-C1C	6.51	126.23	112.37
24	S	601	CHL	C4B-CHC-C1C	6.52	126.26	112.37
24	5	601	CHL	CMB-C2B-C3B	6.53	128.87	113.69
24	s	601	CHL	C4B-CHC-C1C	6.54	126.30	112.37
24	1	601	CHL	CMB-C2B-C3B	6.54	128.90	113.69
24	g	607	CHL	CMB-C2B-C3B	6.54	128.90	113.69
24	G	607	CHL	CMB-C2B-C3B	6.55	128.92	113.69
24	Y	606	CHL	CMB-C2B-C3B	6.56	128.95	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	601	CHL	CMB-C2B-C3B	6.56	128.96	113.69
24	y	606	CHL	CMB-C2B-C3B	6.57	128.97	113.69
24	N	601	CHL	CMB-C2B-C3B	6.57	128.98	113.69
24	2	601	CHL	CMB-C2B-C3B	6.58	128.99	113.69
24	6	601	CHL	CMB-C2B-C3B	6.59	129.02	113.69
24	1	608	CHL	CMB-C2B-C3B	6.60	129.04	113.69
24	3	607	CHL	CMB-C2B-C3B	6.60	129.04	113.69
24	7	607	CHL	CMB-C2B-C3B	6.61	129.06	113.69
24	7	605	CHL	C4B-CHC-C1C	6.61	126.45	112.37
24	5	608	CHL	CMB-C2B-C3B	6.61	129.07	113.69
24	3	605	CHL	C4B-CHC-C1C	6.61	126.46	112.37
27	4	622	XAT	O24-C25-C24	6.62	118.13	113.33
27	8	622	XAT	O24-C25-C24	6.63	118.14	113.33
24	R	614	CHL	CMB-C2B-C3B	6.63	129.11	113.69
24	4	609	CHL	CMB-C2B-C3B	6.63	129.12	113.69
24	6	608	CHL	CMB-C2B-C3B	6.64	129.14	113.69
24	8	607	CHL	C4B-CHC-C1C	6.64	126.52	112.37
24	4	607	CHL	C4B-CHC-C1C	6.65	126.54	112.37
24	8	609	CHL	CMB-C2B-C3B	6.65	129.16	113.69
24	r	614	CHL	CMB-C2B-C3B	6.65	129.17	113.69
24	2	608	CHL	CMB-C2B-C3B	6.66	129.18	113.69
24	s	606	CHL	CMB-C2B-C3B	6.66	129.19	113.69
24	S	606	CHL	CMB-C2B-C3B	6.67	129.19	113.69
24	s	607	CHL	C4B-CHC-C1C	6.67	126.58	112.37
24	2	605	CHL	C4B-CHC-C1C	6.67	126.58	112.37
24	S	607	CHL	C4B-CHC-C1C	6.67	126.59	112.37
24	2	605	CHL	CMB-C2B-C3B	6.68	129.22	113.69
24	6	605	CHL	C4B-CHC-C1C	6.68	126.60	112.37
24	y	609	CHL	CMB-C2B-C3B	6.68	129.24	113.69
24	6	605	CHL	CMB-C2B-C3B	6.69	129.25	113.69
24	3	601	CHL	CMB-C2B-C3B	6.69	129.25	113.69
24	3	605	CHL	CMB-C2B-C3B	6.69	129.26	113.69
24	Y	609	CHL	CMB-C2B-C3B	6.69	129.26	113.69
24	N	605	CHL	CMB-C2B-C3B	6.69	129.26	113.69
24	1	609	CHL	C4B-CHC-C1C	6.69	126.63	112.37
24	7	605	CHL	CMB-C2B-C3B	6.70	129.26	113.69
24	4	606	CHL	C4B-CHC-C1C	6.70	126.64	112.37
24	5	609	CHL	C4B-CHC-C1C	6.70	126.66	112.37
24	7	601	CHL	CMB-C2B-C3B	6.70	129.28	113.69
24	8	606	CHL	C4B-CHC-C1C	6.71	126.67	112.37
24	n	605	CHL	CMB-C2B-C3B	6.71	129.31	113.69
24	S	607	CHL	CMB-C2B-C3B	6.72	129.32	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	s	607	CHL	CMB-C2B-C3B	6.72	129.33	113.69
24	G	605	CHL	CMB-C2B-C3B	6.72	129.33	113.69
28	y	1623	NEX	O24-C25-C24	6.73	118.21	113.33
24	g	605	CHL	CMB-C2B-C3B	6.73	129.34	113.69
24	G	609	CHL	CMB-C2B-C3B	6.73	129.35	113.69
24	n	607	CHL	C4B-CHC-C1C	6.74	126.73	112.37
24	g	609	CHL	CMB-C2B-C3B	6.75	129.39	113.69
24	6	609	CHL	C4B-CHC-C1C	6.75	126.76	112.37
24	2	609	CHL	C4B-CHC-C1C	6.76	126.77	112.37
24	N	607	CHL	C4B-CHC-C1C	6.76	126.77	112.37
24	y	605	CHL	CMB-C2B-C3B	6.76	129.42	113.69
24	Y	605	CHL	CMB-C2B-C3B	6.77	129.44	113.69
28	Y	1623	NEX	O24-C25-C24	6.78	118.25	113.33
24	r	607	CHL	CMB-C2B-C3B	6.78	129.46	113.69
24	R	608	CHL	CMB-C2B-C3B	6.78	129.46	113.69
24	5	606	CHL	CMB-C2B-C3B	6.79	129.48	113.69
24	8	601	CHL	CMB-C2B-C3B	6.79	129.48	113.69
24	r	608	CHL	CMB-C2B-C3B	6.79	129.49	113.69
24	1	606	CHL	CMB-C2B-C3B	6.79	129.49	113.69
24	4	601	CHL	CMB-C2B-C3B	6.79	129.49	113.69
24	R	607	CHL	CMB-C2B-C3B	6.80	129.51	113.69
24	r	606	CHL	C4B-CHC-C1C	6.81	126.88	112.37
24	S	608	CHL	CMB-C2B-C3B	6.81	129.53	113.69
24	R	606	CHL	C4B-CHC-C1C	6.81	126.89	112.37
24	s	608	CHL	CMB-C2B-C3B	6.81	129.54	113.69
27	4	622	XAT	O4-C5-C4	6.82	118.28	113.33
24	6	607	CHL	CMB-C2B-C3B	6.82	129.55	113.69
24	6	608	CHL	C4B-CHC-C1C	6.82	126.91	112.37
24	R	606	CHL	CMB-C2B-C3B	6.83	129.57	113.69
24	S	601	CHL	CMB-C2B-C3B	6.83	129.57	113.69
24	2	607	CHL	CMB-C2B-C3B	6.83	129.58	113.69
27	8	622	XAT	O4-C5-C4	6.83	118.29	113.33
24	4	607	CHL	CMB-C2B-C3B	6.83	129.59	113.69
24	1	607	CHL	CMB-C2B-C3B	6.83	129.59	113.69
24	s	601	CHL	CMB-C2B-C3B	6.84	129.59	113.69
24	8	607	CHL	CMB-C2B-C3B	6.84	129.60	113.69
24	1	605	CHL	CMB-C2B-C3B	6.84	129.60	113.69
24	5	605	CHL	CMB-C2B-C3B	6.84	129.60	113.69
24	2	608	CHL	C4B-CHC-C1C	6.84	126.95	112.37
24	g	608	CHL	CMB-C2B-C3B	6.85	129.62	113.69
24	g	605	CHL	C4B-CHC-C1C	6.85	126.96	112.37
24	r	606	CHL	CMB-C2B-C3B	6.85	129.63	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	607	CHL	CMB-C2B-C3B	6.85	129.63	113.69
24	G	605	CHL	C4B-CHC-C1C	6.85	126.97	112.37
24	G	608	CHL	CMB-C2B-C3B	6.86	129.65	113.69
24	7	609	CHL	CMB-C2B-C3B	6.88	129.69	113.69
24	3	609	CHL	CMB-C2B-C3B	6.88	129.71	113.69
24	5	607	CHL	C4B-CHC-C1C	6.90	127.08	112.37
24	1	607	CHL	C4B-CHC-C1C	6.90	127.08	112.37
24	y	607	CHL	C4B-CHC-C1C	6.91	127.08	112.37
24	8	609	CHL	C4B-CHC-C1C	6.91	127.10	112.37
24	4	609	CHL	C4B-CHC-C1C	6.92	127.11	112.37
24	Y	607	CHL	C4B-CHC-C1C	6.92	127.12	112.37
24	7	608	CHL	CMB-C2B-C3B	6.92	129.79	113.69
24	S	606	CHL	C4B-CHC-C1C	6.93	127.14	112.37
24	y	605	CHL	C4B-CHC-C1C	6.93	127.14	112.37
24	3	608	CHL	CMB-C2B-C3B	6.93	129.82	113.69
24	Y	605	CHL	C4B-CHC-C1C	6.94	127.16	112.37
24	s	606	CHL	C4B-CHC-C1C	6.94	127.16	112.37
24	g	607	CHL	C4B-CHC-C1C	6.95	127.19	112.37
24	N	609	CHL	CMB-C2B-C3B	6.97	129.90	113.69
24	G	607	CHL	C4B-CHC-C1C	6.97	127.23	112.37
24	n	609	CHL	CMB-C2B-C3B	6.98	129.92	113.69
24	R	614	CHL	C4B-CHC-C1C	6.99	127.26	112.37
24	r	614	CHL	C4B-CHC-C1C	6.99	127.27	112.37
24	3	606	CHL	CMB-C2B-C3B	6.99	129.96	113.69
24	7	609	CHL	C4B-CHC-C1C	7.00	127.28	112.37
24	3	609	CHL	C4B-CHC-C1C	7.01	127.31	112.37
24	7	606	CHL	CMB-C2B-C3B	7.01	130.00	113.69
24	8	606	CHL	CMB-C2B-C3B	7.02	130.03	113.69
24	n	607	CHL	CMB-C2B-C3B	7.03	130.05	113.69
24	6	606	CHL	CMB-C2B-C3B	7.03	130.05	113.69
24	4	606	CHL	CMB-C2B-C3B	7.03	130.05	113.69
24	N	607	CHL	CMB-C2B-C3B	7.04	130.06	113.69
24	2	606	CHL	CMB-C2B-C3B	7.04	130.06	113.69
27	Y	1622	XAT	O24-C25-C24	7.04	118.44	113.33
27	R	622	XAT	O4-C5-C4	7.05	118.45	113.33
24	n	605	CHL	C4B-CHC-C1C	7.07	127.43	112.37
24	N	605	CHL	C4B-CHC-C1C	7.07	127.44	112.37
27	r	622	XAT	O4-C5-C4	7.10	118.48	113.33
27	y	1622	XAT	O24-C25-C24	7.12	118.49	113.33
24	6	609	CHL	CMB-C2B-C3B	7.12	130.26	113.69
24	r	608	CHL	C4B-CHC-C1C	7.13	127.56	112.37
24	2	609	CHL	CMB-C2B-C3B	7.14	130.29	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	608	CHL	C4B-CHC-C1C	7.14	127.59	112.37
24	7	608	CHL	C4B-CHC-C1C	7.18	127.67	112.37
24	3	608	CHL	C4B-CHC-C1C	7.19	127.68	112.37
24	2	601	CHL	C4B-CHC-C1C	7.22	127.75	112.37
24	6	601	CHL	C4B-CHC-C1C	7.23	127.79	112.37
24	n	609	CHL	C4B-CHC-C1C	7.24	127.81	112.37
24	N	609	CHL	C4B-CHC-C1C	7.24	127.81	112.37
24	N	606	CHL	CMB-C2B-C3B	7.25	130.56	113.69
24	y	601	CHL	C4B-CHC-C1C	7.26	127.83	112.37
24	n	606	CHL	CMB-C2B-C3B	7.26	130.59	113.69
24	y	607	CHL	CMB-C2B-C3B	7.27	130.59	113.69
24	Y	601	CHL	C4B-CHC-C1C	7.27	127.86	112.37
24	Y	607	CHL	CMB-C2B-C3B	7.28	130.62	113.69
24	S	608	CHL	C4B-CHC-C1C	7.30	127.92	112.37
24	g	609	CHL	C4B-CHC-C1C	7.30	127.94	112.37
24	s	608	CHL	C4B-CHC-C1C	7.31	127.94	112.37
24	G	609	CHL	C4B-CHC-C1C	7.32	127.97	112.37
24	4	608	CHL	C4B-CHC-C1C	7.33	127.99	112.37
24	8	608	CHL	C4B-CHC-C1C	7.34	128.01	112.37
24	n	601	CHL	C4B-CHC-C1C	7.34	128.02	112.37
24	N	601	CHL	C4B-CHC-C1C	7.34	128.02	112.37
34	a	418	SQD	O7-S-C6	7.36	113.12	106.83
34	A	418	SQD	O7-S-C6	7.38	113.13	106.83
24	g	601	CHL	C4B-CHC-C1C	7.43	128.21	112.37
24	G	601	CHL	C4B-CHC-C1C	7.43	128.21	112.37
24	R	607	CHL	C4B-CHC-C1C	7.47	128.29	112.37
24	r	607	CHL	C4B-CHC-C1C	7.49	128.32	112.37
24	G	606	CHL	CMB-C2B-C3B	7.52	131.19	113.69
24	g	606	CHL	CMB-C2B-C3B	7.53	131.22	113.69
24	y	609	CHL	C4B-CHC-C1C	7.54	128.43	112.37
24	Y	609	CHL	C4B-CHC-C1C	7.54	128.44	112.37
24	g	608	CHL	C4B-CHC-C1C	7.54	128.44	112.37
24	G	608	CHL	C4B-CHC-C1C	7.55	128.45	112.37
34	b	621	SQD	O9-S-C6	7.56	113.28	106.83
28	r	623	NEX	O24-C25-C24	7.56	118.81	113.33
27	N	1622	XAT	O4-C5-C4	7.58	118.83	113.33
34	B	621	SQD	O9-S-C6	7.59	113.31	106.83
28	R	623	NEX	O24-C25-C24	7.60	118.84	113.33
27	n	1622	XAT	O4-C5-C4	7.61	118.85	113.33
24	y	608	CHL	C4B-CHC-C1C	7.62	128.61	112.37
24	Y	608	CHL	C4B-CHC-C1C	7.62	128.62	112.37
24	n	608	CHL	C4B-CHC-C1C	7.64	128.65	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	608	CHL	C4B-CHC-C1C	7.66	128.70	112.37
24	5	609	CHL	CMB-C2B-C3B	7.67	131.52	113.69
24	1	609	CHL	CMB-C2B-C3B	7.68	131.55	113.69
27	r	622	XAT	O24-C25-C24	7.70	118.91	113.33
24	5	608	CHL	C4B-CHC-C1C	7.71	128.79	112.37
24	1	608	CHL	C4B-CHC-C1C	7.72	128.82	112.37
27	R	622	XAT	O24-C25-C24	7.73	118.94	113.33
24	7	606	CHL	C4B-CHC-C1C	8.01	129.43	112.37
24	3	606	CHL	C4B-CHC-C1C	8.01	129.44	112.37
27	N	1622	XAT	O24-C25-C24	8.04	119.17	113.33
27	n	1622	XAT	O24-C25-C24	8.08	119.19	113.33
27	5	1622	XAT	O4-C5-C4	8.10	119.20	113.33
28	s	1623	NEX	O24-C25-C24	8.14	119.23	113.33
27	1	1622	XAT	O4-C5-C4	8.16	119.25	113.33
28	S	1623	NEX	O24-C25-C24	8.16	119.25	113.33
28	N	1623	NEX	O24-C25-C24	8.77	119.69	113.33
28	n	1623	NEX	O24-C25-C24	8.78	119.70	113.33
27	7	1622	XAT	O4-C5-C4	9.17	119.98	113.33
27	3	1622	XAT	O4-C5-C4	9.19	120.00	113.33
27	g	1622	XAT	O24-C25-C24	9.62	120.31	113.33
27	G	1622	XAT	O24-C25-C24	9.62	120.31	113.33
28	7	1623	NEX	O24-C25-C24	9.67	120.35	113.33
28	3	1623	NEX	O24-C25-C24	9.68	120.35	113.33
27	6	1622	XAT	O24-C25-C24	9.78	120.42	113.33
27	2	1622	XAT	O24-C25-C24	9.81	120.45	113.33
28	1	1623	NEX	O24-C25-C24	9.93	120.53	113.33
28	5	1623	NEX	O24-C25-C24	9.98	120.57	113.33
28	2	1623	NEX	O24-C25-C24	10.15	120.69	113.33
28	g	1623	NEX	O24-C25-C24	10.20	120.73	113.33
28	G	1623	NEX	O24-C25-C24	10.20	120.73	113.33
27	6	1622	XAT	O4-C5-C4	10.23	120.75	113.33
27	2	1622	XAT	O4-C5-C4	10.24	120.75	113.33
28	6	1623	NEX	O24-C25-C24	10.25	120.76	113.33
27	1	1622	XAT	O24-C25-C24	10.96	121.28	113.33
27	5	1622	XAT	O24-C25-C24	10.96	121.28	113.33

All (620) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	410	CLA	NC
25	A	410	CLA	ND
25	A	410	CLA	NA

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Mol	Chain	Res	Type	Atom
25	B	606	CLA	NC
25	B	606	CLA	ND
25	B	606	CLA	NA
25	b	611	CLA	NC
25	b	611	CLA	NA
25	b	611	CLA	ND
25	3	613	CLA	NC
25	3	613	CLA	ND
25	3	613	CLA	NA
25	7	604	CLA	NC
25	7	604	CLA	ND
25	7	604	CLA	NA
25	b	610	CLA	NC
25	b	610	CLA	NA
25	B	611	CLA	NC
25	B	611	CLA	NA
25	B	611	CLA	ND
25	3	614	CLA	NC
25	3	614	CLA	ND
25	3	614	CLA	NA
25	g	610	CLA	NC
25	g	610	CLA	NA
25	g	610	CLA	ND
25	Y	612	CLA	NC
25	Y	612	CLA	ND
25	Y	612	CLA	NA
25	6	610	CLA	NC
25	6	610	CLA	ND
25	6	610	CLA	NA
25	5	612	CLA	NC
25	5	612	CLA	NA
25	5	612	CLA	ND
25	b	615	CLA	NC
25	b	615	CLA	ND
25	b	615	CLA	NA
25	B	605	CLA	NC
25	B	605	CLA	ND
25	B	605	CLA	NA
25	1	602	CLA	NC
25	1	602	CLA	ND
25	1	602	CLA	NA
25	R	616	CLA	NC

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Mol	Chain	Res	Type	Atom
25	R	616	CLA	NA
25	c	503	CLA	NC
25	c	503	CLA	ND
25	c	503	CLA	NA
25	c	513	CLA	NC
25	c	513	CLA	NA
25	N	602	CLA	NC
25	N	602	CLA	ND
25	N	602	CLA	NA
25	n	610	CLA	NC
25	n	610	CLA	NA
25	n	610	CLA	ND
25	a	407	CLA	NC
25	a	407	CLA	ND
25	a	407	CLA	NA
25	Y	604	CLA	NC
25	Y	604	CLA	ND
25	Y	604	CLA	NA
25	Y	614	CLA	NC
25	Y	614	CLA	ND
25	Y	614	CLA	NA
25	N	612	CLA	NC
25	N	612	CLA	ND
25	N	612	CLA	NA
25	B	609	CLA	NC
25	B	609	CLA	ND
25	B	609	CLA	NA
25	c	505	CLA	NC
25	c	505	CLA	NA
25	s	602	CLA	NC
25	s	602	CLA	ND
25	s	602	CLA	NA
25	7	613	CLA	NC
25	7	613	CLA	ND
25	7	613	CLA	NA
25	B	614	CLA	NC
25	B	614	CLA	ND
25	B	614	CLA	NA
25	6	603	CLA	NC
25	6	603	CLA	NA
25	6	603	CLA	ND
25	S	609	CLA	NC

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Mol	Chain	Res	Type	Atom
25	S	609	CLA	ND
25	S	609	CLA	NA
25	G	610	CLA	NC
25	G	610	CLA	NA
25	G	610	CLA	ND
25	B	604	CLA	NC
25	B	604	CLA	ND
25	B	604	CLA	NA
25	B	607	CLA	NC
25	B	607	CLA	ND
25	B	607	CLA	NA
25	s	603	CLA	NC
25	s	603	CLA	ND
25	s	603	CLA	NA
25	d	403	CLA	NC
25	d	403	CLA	NA
25	s	604	CLA	NC
25	s	604	CLA	ND
25	s	604	CLA	NA
25	g	612	CLA	NC
25	g	612	CLA	ND
25	g	612	CLA	NA
25	7	611	CLA	NC
25	7	611	CLA	ND
25	7	611	CLA	NA
25	G	612	CLA	NC
25	G	612	CLA	ND
25	G	612	CLA	NA
25	S	602	CLA	NC
25	S	602	CLA	ND
25	S	602	CLA	NA
25	c	512	CLA	NC
25	c	512	CLA	ND
25	c	512	CLA	NA
25	n	611	CLA	NC
25	n	611	CLA	ND
25	n	611	CLA	NA
25	2	610	CLA	NC
25	2	610	CLA	ND
25	2	610	CLA	NA
25	5	613	CLA	NC
25	5	613	CLA	NA

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Mol	Chain	Res	Type	Atom
25	R	611	CLA	NC
25	R	611	CLA	ND
25	R	611	CLA	NA
25	B	617	CLA	NC
25	B	617	CLA	ND
25	B	617	CLA	NA
25	G	603	CLA	NC
25	G	603	CLA	ND
25	G	603	CLA	NA
25	N	603	CLA	NC
25	N	603	CLA	ND
25	N	603	CLA	NA
25	C	504	CLA	NC
25	C	504	CLA	ND
25	C	504	CLA	NA
25	C	502	CLA	NC
25	C	502	CLA	ND
25	C	502	CLA	NA
25	n	602	CLA	NC
25	n	602	CLA	ND
25	n	602	CLA	NA
25	4	604	CLA	NC
25	4	604	CLA	NA
25	G	602	CLA	NC
25	G	602	CLA	ND
25	G	602	CLA	NA
25	R	603	CLA	NC
25	R	603	CLA	NA
25	R	603	CLA	ND
25	y	612	CLA	NC
25	y	612	CLA	ND
25	y	612	CLA	NA
25	r	610	CLA	NC
25	r	610	CLA	ND
25	r	610	CLA	NA
25	C	511	CLA	NC
25	C	511	CLA	NA
25	8	602	CLA	NC
25	8	602	CLA	ND
25	8	602	CLA	NA
25	b	604	CLA	NC
25	b	604	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	604	CLA	NA
25	1	614	CLA	NC
25	1	614	CLA	ND
25	1	614	CLA	NA
25	Y	603	CLA	NC
25	Y	603	CLA	NA
25	Y	603	CLA	ND
25	3	602	CLA	NC
25	3	602	CLA	ND
25	3	602	CLA	NA
25	N	611	CLA	NC
25	N	611	CLA	ND
25	N	611	CLA	NA
25	c	506	CLA	NC
25	c	506	CLA	NA
25	D	402	CLA	NC
25	D	402	CLA	ND
25	D	402	CLA	NA
25	5	602	CLA	NC
25	5	602	CLA	ND
25	5	602	CLA	NA
25	3	604	CLA	NC
25	3	604	CLA	ND
25	3	604	CLA	NA
25	7	602	CLA	NC
25	7	602	CLA	ND
25	7	602	CLA	NA
25	y	614	CLA	NC
25	y	614	CLA	ND
25	y	614	CLA	NA
25	6	602	CLA	NC
25	6	602	CLA	ND
25	6	602	CLA	NA
25	n	614	CLA	NC
25	n	614	CLA	ND
25	n	614	CLA	NA
25	n	603	CLA	NC
25	n	603	CLA	ND
25	n	603	CLA	NA
25	G	611	CLA	NC
25	G	611	CLA	ND
25	G	611	CLA	NA

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Mol	Chain	Res	Type	Atom
25	b	607	CLA	NC
25	b	607	CLA	ND
25	b	607	CLA	NA
25	S	604	CLA	NC
25	S	604	CLA	ND
25	S	604	CLA	NA
25	b	616	CLA	NC
25	b	616	CLA	ND
25	b	616	CLA	NA
25	s	610	CLA	NC
25	s	610	CLA	ND
25	s	610	CLA	NA
25	c	501	CLA	NC
25	c	501	CLA	ND
25	c	501	CLA	NA
25	r	609	CLA	NC
25	r	609	CLA	ND
25	r	609	CLA	NA
25	b	605	CLA	NC
25	b	605	CLA	ND
25	b	605	CLA	NA
25	5	614	CLA	NC
25	5	614	CLA	ND
25	5	614	CLA	NA
25	R	602	CLA	NC
25	R	602	CLA	ND
25	R	602	CLA	NA
25	y	611	CLA	NC
25	y	611	CLA	ND
25	y	611	CLA	NA
25	4	603	CLA	NC
25	4	603	CLA	ND
25	4	603	CLA	NA
25	N	604	CLA	NC
25	N	604	CLA	ND
25	N	604	CLA	NA
25	G	614	CLA	NC
25	G	614	CLA	ND
25	G	614	CLA	NA
25	C	501	CLA	NC
25	C	501	CLA	ND
25	C	501	CLA	NA

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Mol	Chain	Res	Type	Atom
25	C	507	CLA	NC
25	C	507	CLA	ND
25	C	507	CLA	NA
25	B	610	CLA	NC
25	B	610	CLA	NA
25	r	601	CLA	NC
25	r	601	CLA	ND
25	r	601	CLA	NA
25	5	603	CLA	NC
25	5	603	CLA	NA
25	5	603	CLA	ND
25	R	601	CLA	NC
25	R	601	CLA	ND
25	R	601	CLA	NA
25	B	616	CLA	NC
25	B	616	CLA	ND
25	B	616	CLA	NA
25	1	604	CLA	NC
25	1	604	CLA	ND
25	1	604	CLA	NA
25	c	510	CLA	NC
25	c	510	CLA	ND
25	c	510	CLA	NA
25	g	613	CLA	NC
25	g	613	CLA	NA
25	Y	611	CLA	NC
25	Y	611	CLA	ND
25	Y	611	CLA	NA
25	C	505	CLA	NC
25	C	505	CLA	NA
25	4	602	CLA	NC
25	4	602	CLA	ND
25	4	602	CLA	NA
25	S	614	CLA	NC
25	S	614	CLA	ND
25	S	614	CLA	NA
25	6	614	CLA	NC
25	6	614	CLA	NA
25	B	608	CLA	NC
25	B	608	CLA	ND
25	B	608	CLA	NA
25	N	613	CLA	NC

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Mol	Chain	Res	Type	Atom
25	N	613	CLA	ND
25	N	613	CLA	NA
25	y	610	CLA	NC
25	y	610	CLA	NA
25	y	610	CLA	ND
25	3	611	CLA	NC
25	3	611	CLA	ND
25	3	611	CLA	NA
25	s	609	CLA	NC
25	s	609	CLA	ND
25	s	609	CLA	NA
25	8	603	CLA	NC
25	8	603	CLA	ND
25	8	603	CLA	NA
25	S	610	CLA	NC
25	S	610	CLA	ND
25	S	610	CLA	NA
25	g	611	CLA	NC
25	g	611	CLA	ND
25	g	611	CLA	NA
25	D	403	CLA	NC
25	D	403	CLA	NA
25	7	612	CLA	NC
25	7	612	CLA	ND
25	7	612	CLA	NA
25	6	612	CLA	NC
25	6	612	CLA	ND
25	6	612	CLA	NA
25	b	608	CLA	NC
25	b	608	CLA	ND
25	b	608	CLA	NA
25	r	616	CLA	NC
25	r	616	CLA	NA
25	y	602	CLA	NC
25	y	602	CLA	ND
25	y	602	CLA	NA
25	5	610	CLA	NC
25	5	610	CLA	ND
25	5	610	CLA	NA
25	A	407	CLA	NC
25	A	407	CLA	ND
25	A	407	CLA	NA

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Mol	Chain	Res	Type	Atom
25	1	612	CLA	NC
25	1	612	CLA	NA
25	1	612	CLA	ND
25	r	613	CLA	NC
25	r	613	CLA	ND
25	r	613	CLA	NA
25	7	610	CLA	NC
25	7	610	CLA	ND
25	7	610	CLA	NA
25	8	610	CLA	NC
25	8	610	CLA	ND
25	8	610	CLA	NA
25	s	612	CLA	NC
25	s	612	CLA	ND
25	s	612	CLA	NA
25	R	612	CLA	NC
25	R	612	CLA	ND
25	R	612	CLA	NA
25	b	609	CLA	NC
25	b	609	CLA	ND
25	b	609	CLA	NA
25	2	602	CLA	NC
25	2	602	CLA	ND
25	2	602	CLA	NA
25	b	603	CLA	NC
25	b	603	CLA	ND
25	b	603	CLA	NA
25	Y	610	CLA	NC
25	Y	610	CLA	NA
25	Y	610	CLA	ND
25	S	613	CLA	NC
25	S	613	CLA	ND
25	S	613	CLA	NA
25	C	506	CLA	NC
25	C	506	CLA	NA
25	B	612	CLA	NC
25	B	612	CLA	ND
25	B	612	CLA	NA
25	c	507	CLA	NC
25	c	507	CLA	ND
25	c	507	CLA	NA
25	2	611	CLA	NC

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Mol	Chain	Res	Type	Atom
25	2	611	CLA	ND
25	2	611	CLA	NA
25	r	604	CLA	NC
25	r	604	CLA	ND
25	r	604	CLA	NA
25	G	604	CLA	NC
25	G	604	CLA	NA
25	c	502	CLA	NC
25	c	502	CLA	ND
25	c	502	CLA	NA
25	y	603	CLA	NC
25	y	603	CLA	NA
25	y	603	CLA	ND
25	c	509	CLA	NC
25	c	509	CLA	ND
25	c	509	CLA	NA
25	r	611	CLA	NC
25	r	611	CLA	ND
25	r	611	CLA	NA
25	b	602	CLA	NC
25	b	602	CLA	ND
25	b	602	CLA	NA
25	R	609	CLA	NC
25	R	609	CLA	ND
25	R	609	CLA	NA
25	6	613	CLA	NC
25	6	613	CLA	NA
25	b	606	CLA	NC
25	b	606	CLA	ND
25	b	606	CLA	NA
25	N	610	CLA	NC
25	N	610	CLA	NA
25	N	610	CLA	ND
25	7	603	CLA	NC
25	7	603	CLA	ND
25	7	603	CLA	NA
25	r	603	CLA	NC
25	r	603	CLA	NA
25	r	603	CLA	ND
25	S	611	CLA	NC
25	S	611	CLA	ND
25	S	611	CLA	NA

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Mol	Chain	Res	Type	Atom
25	1	603	CLA	NC
25	1	603	CLA	NA
25	1	603	CLA	ND
25	S	603	CLA	NC
25	S	603	CLA	ND
25	S	603	CLA	NA
25	b	614	CLA	NC
25	b	614	CLA	ND
25	b	614	CLA	NA
25	3	612	CLA	NC
25	3	612	CLA	ND
25	3	612	CLA	NA
25	b	617	CLA	NC
25	b	617	CLA	ND
25	b	617	CLA	NA
25	b	612	CLA	NC
25	b	612	CLA	ND
25	b	612	CLA	NA
25	6	604	CLA	NC
25	6	604	CLA	NA
25	C	510	CLA	NC
25	C	510	CLA	ND
25	C	510	CLA	NA
25	R	604	CLA	NC
25	R	604	CLA	ND
25	R	604	CLA	NA
25	y	613	CLA	NC
25	y	613	CLA	ND
25	y	613	CLA	NA
25	d	402	CLA	NC
25	d	402	CLA	ND
25	d	402	CLA	NA
25	Y	602	CLA	NC
25	Y	602	CLA	ND
25	Y	602	CLA	NA
25	B	613	CLA	NC
25	B	613	CLA	ND
25	B	613	CLA	NA
25	4	612	CLA	NC
25	4	612	CLA	ND
25	4	612	CLA	NA
25	3	610	CLA	NC

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Mol	Chain	Res	Type	Atom
25	3	610	CLA	ND
25	3	610	CLA	NA
25	5	611	CLA	NC
25	5	611	CLA	ND
25	5	611	CLA	NA
25	B	615	CLA	NC
25	B	615	CLA	ND
25	B	615	CLA	NA
25	N	614	CLA	NC
25	N	614	CLA	ND
25	N	614	CLA	NA
25	7	614	CLA	NC
25	7	614	CLA	ND
25	7	614	CLA	NA
25	6	611	CLA	NC
25	6	611	CLA	ND
25	6	611	CLA	NA
25	8	604	CLA	NC
25	8	604	CLA	NA
25	A	406	CLA	NC
25	A	406	CLA	ND
25	A	406	CLA	NA
25	n	604	CLA	NC
25	n	604	CLA	ND
25	n	604	CLA	NA
25	r	612	CLA	NC
25	r	612	CLA	ND
25	r	612	CLA	NA
25	C	512	CLA	NC
25	C	512	CLA	ND
25	C	512	CLA	NA
25	A	405	CLA	NC
25	A	405	CLA	ND
25	A	405	CLA	NA
25	n	612	CLA	NC
25	n	612	CLA	ND
25	n	612	CLA	NA
25	s	613	CLA	NC
25	s	613	CLA	ND
25	s	613	CLA	NA
25	2	604	CLA	NC
25	2	604	CLA	NA

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Mol	Chain	Res	Type	Atom
25	Y	613	CLA	NC
25	Y	613	CLA	ND
25	Y	613	CLA	NA
25	s	611	CLA	NC
25	s	611	CLA	ND
25	s	611	CLA	NA
25	c	508	CLA	NC
25	c	508	CLA	ND
25	c	508	CLA	NA
25	S	612	CLA	NC
25	S	612	CLA	ND
25	S	612	CLA	NA
25	2	613	CLA	NC
25	2	613	CLA	NA
25	C	509	CLA	NC
25	C	509	CLA	ND
25	C	509	CLA	NA
25	g	604	CLA	NC
25	g	604	CLA	NA
25	5	604	CLA	NC
25	5	604	CLA	ND
25	5	604	CLA	NA
25	2	614	CLA	NC
25	2	614	CLA	NA
25	1	610	CLA	NC
25	1	610	CLA	ND
25	1	610	CLA	NA
25	b	613	CLA	NC
25	b	613	CLA	ND
25	b	613	CLA	NA
25	y	604	CLA	NC
25	y	604	CLA	ND
25	y	604	CLA	NA
25	a	406	CLA	NC
25	a	406	CLA	ND
25	a	406	CLA	NA
25	8	612	CLA	NC
25	8	612	CLA	ND
25	8	612	CLA	NA
25	g	603	CLA	NC
25	g	603	CLA	ND
25	g	603	CLA	NA

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Mol	Chain	Res	Type	Atom
25	4	611	CLA	NC
25	4	611	CLA	ND
25	4	611	CLA	NA
25	c	504	CLA	NC
25	c	504	CLA	ND
25	c	504	CLA	NA
25	C	503	CLA	NC
25	C	503	CLA	ND
25	C	503	CLA	NA
25	1	613	CLA	NC
25	1	613	CLA	NA
25	n	613	CLA	NC
25	n	613	CLA	ND
25	n	613	CLA	NA
25	B	602	CLA	NC
25	B	602	CLA	ND
25	B	602	CLA	NA
25	2	612	CLA	NC
25	2	612	CLA	ND
25	2	612	CLA	NA
25	G	613	CLA	NC
25	G	613	CLA	NA
25	C	513	CLA	NC
25	C	513	CLA	NA
25	B	603	CLA	NC
25	B	603	CLA	ND
25	B	603	CLA	NA
25	g	614	CLA	NC
25	g	614	CLA	ND
25	g	614	CLA	NA
25	R	610	CLA	NC
25	R	610	CLA	ND
25	R	610	CLA	NA
25	c	511	CLA	NC
25	c	511	CLA	NA
25	C	508	CLA	NC
25	C	508	CLA	ND
25	C	508	CLA	NA
25	8	611	CLA	NC
25	8	611	CLA	ND
25	8	611	CLA	NA
25	R	613	CLA	NC

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Mol	Chain	Res	Type	Atom
25	R	613	CLA	ND
25	R	613	CLA	NA
25	a	410	CLA	NC
25	a	410	CLA	ND
25	a	410	CLA	NA
25	4	610	CLA	NC
25	4	610	CLA	ND
25	4	610	CLA	NA
25	s	614	CLA	NC
25	s	614	CLA	ND
25	s	614	CLA	NA
25	a	405	CLA	NC
25	a	405	CLA	ND
25	a	405	CLA	NA
25	g	602	CLA	NC
25	g	602	CLA	ND
25	g	602	CLA	NA
25	1	611	CLA	NC
25	1	611	CLA	ND
25	1	611	CLA	NA
25	r	602	CLA	NC
25	r	602	CLA	ND
25	r	602	CLA	NA
25	3	603	CLA	NC
25	3	603	CLA	ND
25	3	603	CLA	NA
25	2	603	CLA	NC
25	2	603	CLA	NA
25	2	603	CLA	ND

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	s	606	CHL	OMC-CMC-C2C-C1C
24	S	606	CHL	OMC-CMC-C2C-C1C

There are no ring outliers.

286 monomers are involved in 763 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	1620	LUT	6	0
26	1	1621	LUT	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	1	1622	XAT	4	0
28	1	1623	NEX	3	0
24	1	601	CHL	1	0
25	1	602	CLA	5	0
25	1	603	CLA	3	0
25	1	604	CLA	1	0
24	1	606	CHL	1	0
24	1	607	CHL	4	0
24	1	608	CHL	1	0
24	1	609	CHL	2	0
25	1	610	CLA	2	0
25	1	612	CLA	2	0
25	1	613	CLA	2	0
25	1	614	CLA	1	0
26	2	1620	LUT	4	0
26	2	1621	LUT	2	0
27	2	1622	XAT	6	0
28	2	1623	NEX	2	0
29	2	2630	LHG	2	0
24	2	601	CHL	1	0
25	2	602	CLA	3	0
25	2	603	CLA	3	0
25	2	604	CLA	1	0
24	2	605	CHL	1	0
24	2	606	CHL	3	0
24	2	607	CHL	2	0
24	2	608	CHL	2	0
24	2	609	CHL	5	0
25	2	610	CLA	3	0
25	2	612	CLA	2	0
25	2	613	CLA	3	0
25	2	614	CLA	2	0
26	3	1620	LUT	8	0
26	3	1621	LUT	4	0
27	3	1622	XAT	4	0
28	3	1623	NEX	2	0
29	3	2630	LHG	5	0
24	3	601	CHL	2	0
25	3	602	CLA	4	0
25	3	603	CLA	2	0
25	3	604	CLA	1	0
24	3	605	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3	606	CHL	4	0
24	3	607	CHL	6	0
24	3	608	CHL	2	0
24	3	609	CHL	4	0
25	3	610	CLA	2	0
25	3	611	CLA	5	0
25	3	613	CLA	4	0
25	3	614	CLA	1	0
29	4	2630	LHG	1	0
24	4	601	CHL	1	0
25	4	603	CLA	1	0
24	4	606	CHL	1	0
24	4	608	CHL	1	0
25	4	610	CLA	1	0
25	4	611	CLA	1	0
25	4	612	CLA	2	0
26	4	620	LUT	4	0
27	4	622	XAT	4	0
30	4	623	BCR	3	0
26	5	1620	LUT	7	0
26	5	1621	LUT	4	0
27	5	1622	XAT	4	0
28	5	1623	NEX	3	0
24	5	601	CHL	1	0
25	5	602	CLA	5	0
25	5	603	CLA	2	0
25	5	604	CLA	1	0
24	5	605	CHL	1	0
24	5	606	CHL	1	0
24	5	607	CHL	4	0
24	5	608	CHL	1	0
24	5	609	CHL	4	0
25	5	610	CLA	2	0
25	5	612	CLA	2	0
25	5	613	CLA	2	0
25	5	614	CLA	1	0
26	6	1620	LUT	4	0
26	6	1621	LUT	2	0
27	6	1622	XAT	5	0
29	6	2630	LHG	2	0
24	6	601	CHL	1	0
25	6	602	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	603	CLA	2	0
25	6	604	CLA	2	0
24	6	605	CHL	1	0
24	6	606	CHL	3	0
24	6	607	CHL	2	0
24	6	608	CHL	2	0
24	6	609	CHL	6	0
25	6	610	CLA	3	0
25	6	612	CLA	2	0
25	6	613	CLA	3	0
25	6	614	CLA	2	0
26	7	1620	LUT	7	0
26	7	1621	LUT	3	0
27	7	1622	XAT	7	0
28	7	1623	NEX	2	0
29	7	2630	LHG	6	0
24	7	601	CHL	2	0
25	7	602	CLA	5	0
25	7	603	CLA	3	0
25	7	604	CLA	1	0
24	7	605	CHL	1	0
24	7	606	CHL	4	0
24	7	607	CHL	6	0
24	7	608	CHL	3	0
24	7	609	CHL	6	0
25	7	610	CLA	3	0
25	7	611	CLA	5	0
25	7	613	CLA	3	0
25	7	614	CLA	1	0
29	8	2630	LHG	1	0
25	8	603	CLA	1	0
25	8	604	CLA	1	0
24	8	606	CHL	1	0
24	8	607	CHL	1	0
24	8	608	CHL	1	0
25	8	610	CLA	1	0
25	8	611	CLA	1	0
25	8	612	CLA	2	0
26	8	620	LUT	3	0
27	8	622	XAT	6	0
30	8	623	BCR	3	0
31	A	401	OEX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	405	CLA	5	0
25	A	406	CLA	4	0
25	A	407	CLA	2	0
33	A	408	PHO	8	0
33	A	409	PHO	6	0
25	A	410	CLA	7	0
30	A	411	BCR	4	0
34	A	412	SQD	2	0
35	A	413	LMG	2	0
34	A	418	SQD	6	0
29	B	2630	LHG	3	0
29	B	2631	LHG	5	0
35	B	2633	LMG	2	0
25	B	602	CLA	4	0
25	B	603	CLA	9	0
25	B	604	CLA	4	0
25	B	605	CLA	8	0
25	B	606	CLA	6	0
25	B	607	CLA	5	0
25	B	608	CLA	3	0
25	B	610	CLA	2	0
25	B	611	CLA	5	0
25	B	612	CLA	5	0
25	B	613	CLA	9	0
25	B	614	CLA	6	0
25	B	615	CLA	7	0
25	B	616	CLA	5	0
25	B	617	CLA	1	0
30	B	618	BCR	8	0
30	B	619	BCR	8	0
30	B	620	BCR	3	0
34	B	621	SQD	5	0
35	B	622	LMG	4	0
34	B	623	SQD	5	0
37	B	626	DGD	1	0
29	C	2630	LHG	5	0
25	C	501	CLA	5	0
25	C	502	CLA	1	0
25	C	503	CLA	2	0
25	C	504	CLA	1	0
25	C	505	CLA	1	0
25	C	506	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	507	CLA	5	0
25	C	508	CLA	2	0
25	C	509	CLA	1	0
25	C	510	CLA	5	0
25	C	511	CLA	9	0
25	C	512	CLA	4	0
25	C	513	CLA	4	0
30	C	514	BCR	3	0
30	C	515	BCR	2	0
30	C	516	BCR	2	0
30	C	517	BCR	10	0
37	C	518	DGD	3	0
37	C	519	DGD	3	0
37	C	520	DGD	3	0
35	C	521	LMG	1	0
29	C	522	LHG	3	0
29	C	523	LHG	1	0
38	D	401	BCT	1	0
25	D	402	CLA	8	0
25	D	403	CLA	2	0
30	D	404	BCR	7	0
36	D	405	PL9	6	0
29	D	408	LHG	4	0
29	D	409	LHG	11	0
29	D	410	LHG	4	0
35	D	411	LMG	3	0
26	G	1620	LUT	8	0
26	G	1621	LUT	5	0
27	G	1622	XAT	4	0
28	G	1623	NEX	4	0
29	G	2630	LHG	5	0
24	G	601	CHL	5	0
25	G	602	CLA	3	0
25	G	603	CLA	5	0
25	G	604	CLA	2	0
24	G	605	CHL	1	0
24	G	606	CHL	2	0
24	G	607	CHL	4	0
24	G	608	CHL	4	0
24	G	609	CHL	3	0
25	G	610	CLA	6	0
25	G	611	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	612	CLA	2	0
25	G	613	CLA	5	0
25	G	614	CLA	3	0
30	H	101	BCR	6	0
37	H	102	DGD	6	0
29	L	101	LHG	8	0
26	N	1620	LUT	5	0
26	N	1621	LUT	3	0
27	N	1622	XAT	7	0
28	N	1623	NEX	5	0
29	N	2630	LHG	4	0
24	N	601	CHL	2	0
25	N	602	CLA	8	0
25	N	603	CLA	6	0
25	N	604	CLA	1	0
24	N	606	CHL	4	0
24	N	607	CHL	5	0
24	N	608	CHL	3	0
24	N	609	CHL	5	0
25	N	610	CLA	5	0
25	N	611	CLA	2	0
25	N	612	CLA	4	0
25	N	613	CLA	4	0
29	R	2630	LHG	3	0
25	R	602	CLA	5	0
25	R	603	CLA	2	0
25	R	604	CLA	1	0
24	R	606	CHL	2	0
24	R	607	CHL	2	0
24	R	608	CHL	3	0
25	R	609	CLA	5	0
25	R	610	CLA	1	0
25	R	611	CLA	6	0
25	R	612	CLA	3	0
25	R	613	CLA	2	0
25	R	616	CLA	4	0
26	R	620	LUT	4	0
27	R	622	XAT	6	0
28	R	623	NEX	4	0
26	S	1620	LUT	4	0
26	S	1621	LUT	4	0
28	S	1623	NEX	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	S	2630	LHG	2	0
25	S	603	CLA	2	0
25	S	604	CLA	1	0
24	S	606	CHL	2	0
24	S	607	CHL	3	0
24	S	608	CHL	1	0
25	S	609	CLA	1	0
25	S	610	CLA	1	0
25	S	611	CLA	1	0
25	S	613	CLA	2	0
25	S	614	CLA	2	0
30	T	101	BCR	8	0
26	Y	1620	LUT	4	0
26	Y	1621	LUT	4	0
27	Y	1622	XAT	6	0
28	Y	1623	NEX	4	0
29	Y	2630	LHG	4	0
24	Y	601	CHL	8	0
25	Y	602	CLA	6	0
25	Y	603	CLA	10	0
25	Y	604	CLA	2	0
24	Y	605	CHL	1	0
24	Y	606	CHL	3	0
24	Y	607	CHL	4	0
24	Y	608	CHL	4	0
24	Y	609	CHL	3	0
25	Y	610	CLA	2	0
25	Y	611	CLA	4	0
25	Y	612	CLA	3	0
25	Y	613	CLA	2	0
25	Y	614	CLA	1	0
35	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.