



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 21, 2017 – 02:45 PM EDT

PDB ID : 5MDX
EMDB ID: : EMD-3491
Title : Cryo-EM structure of the PSII supercomplex from Arabidopsis thaliana
Authors : van Bezouwen, L.S.; Caffarri, S.; Kale, R.S.; Kouril, R.; Thunnissen, A.M.W.H.; Oostergetel, G.T.; Boekema, E.J.
Deposited on : unknown
Resolution : 5.30 Å(reported)

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

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

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

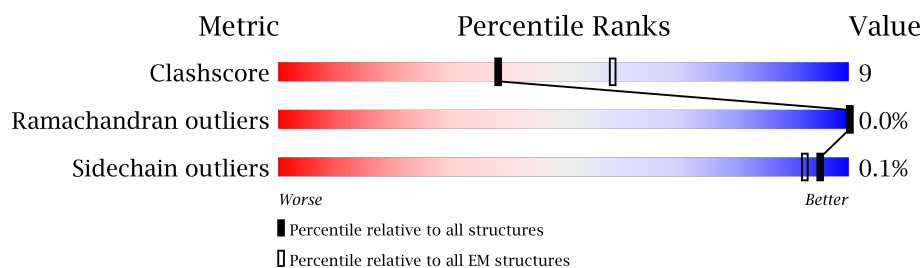
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.30 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	343	68% 22% 10%
1	a	343	96% .
2	B	507	65% 29% 6%
2	b	507	94% 6%
3	C	459	65% 29% 6%
3	c	459	94% 6%
4	D	352	68% 28% 5%
4	d	352	95% . 5%
5	E	83	70% 17% 13%

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Mol	Chain	Length	Quality of chain
5	e	83	
6	F	39	
6	f	39	
7	H	72	
7	h	72	
8	I	36	
8	i	36	
9	K	37	
9	k	37	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	O	247	
12	o	247	
13	T	33	
13	t	33	
14	W	54	
14	w	54	
15	X	116	
15	x	116	
16	Z	62	
16	z	62	
17	R	250	
17	r	250	

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Mol	Chain	Length	Quality of chain
18	S	232	
18	s	232	
19	1	224	
19	2	224	
19	3	224	
19	5	224	
19	6	224	
19	7	224	
19	G	224	
19	N	224	
19	Y	224	
19	g	224	
19	n	224	
19	y	224	
20	4	210	
20	8	210	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	2	602	X	-	-	-
22	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	604	X	-	-	-
22	CLA	2	609	X	-	-	-
22	CLA	2	610	X	-	-	-
22	CLA	2	611	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	613	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	314	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	314	X	-	-	-
22	CLA	8	302	X	-	-	-
22	CLA	8	303	X	-	-	-
22	CLA	8	304	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	A	402	X	-	-	-
22	CLA	A	403	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	501	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	G	602	X	-	-	-
22	CLA	G	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	G	604	X	-	-	-
22	CLA	G	610	X	-	-	-
22	CLA	G	611	X	-	-	-
22	CLA	G	612	X	-	-	-
22	CLA	G	613	X	-	-	-
22	CLA	G	614	X	-	-	-
22	CLA	N	602	X	-	-	-
22	CLA	N	603	X	-	-	-
22	CLA	N	604	X	-	-	-
22	CLA	N	610	X	-	-	-
22	CLA	N	611	X	-	-	-
22	CLA	N	612	X	-	-	-
22	CLA	N	613	X	-	-	-
22	CLA	N	614	X	-	-	-
22	CLA	R	301	X	-	-	-
22	CLA	R	302	X	-	X	-
22	CLA	R	303	X	-	-	-
22	CLA	R	307	X	-	-	-
22	CLA	R	308	X	-	-	-
22	CLA	R	309	X	-	-	-
22	CLA	R	310	X	-	-	-
22	CLA	R	311	X	-	-	-
22	CLA	R	312	X	-	X	-
22	CLA	S	301	X	-	X	-
22	CLA	S	303	X	-	-	-
22	CLA	S	304	X	-	-	-
22	CLA	S	305	X	-	-	-
22	CLA	S	309	X	-	-	-
22	CLA	S	310	X	-	-	-
22	CLA	S	311	X	-	-	-
22	CLA	S	312	X	-	-	-
22	CLA	S	313	X	-	-	-
22	CLA	S	314	X	-	-	-
22	CLA	Y	602	X	-	-	-
22	CLA	Y	603	X	-	-	-
22	CLA	Y	604	X	-	-	-
22	CLA	Y	610	X	-	-	-
22	CLA	Y	611	X	-	-	-
22	CLA	Y	612	X	-	-	-
22	CLA	Y	613	X	-	-	-
22	CLA	Y	614	X	-	-	-
22	CLA	a	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	a	403	X	-	-	-
22	CLA	a	405	X	-	-	-
22	CLA	b	601	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	-
22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	c	501	X	-	-	-
22	CLA	c	502	X	-	-	-
22	CLA	c	503	X	-	-	-
22	CLA	c	504	X	-	-	-
22	CLA	c	505	X	-	-	-
22	CLA	c	506	X	-	-	-
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	-
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	-
22	CLA	c	511	X	-	-	-
22	CLA	c	512	X	-	-	-
22	CLA	d	401	X	-	-	-
22	CLA	d	403	X	-	-	-
22	CLA	d	404	X	-	-	-
22	CLA	g	602	X	-	-	-
22	CLA	g	603	X	-	-	-
22	CLA	g	604	X	-	-	-
22	CLA	g	610	X	-	-	-
22	CLA	g	611	X	-	-	-
22	CLA	g	612	X	-	-	-
22	CLA	g	613	X	-	-	-
22	CLA	g	614	X	-	-	-
22	CLA	n	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	n	603	X	-	-	-
22	CLA	n	604	X	-	-	-
22	CLA	n	610	X	-	-	-
22	CLA	n	611	X	-	-	-
22	CLA	n	612	X	-	-	-
22	CLA	n	613	X	-	-	-
22	CLA	n	614	X	-	-	-
22	CLA	r	301	X	-	-	-
22	CLA	r	302	X	-	-	-
22	CLA	r	303	X	-	-	-
22	CLA	r	307	X	-	-	-
22	CLA	r	308	X	-	-	-
22	CLA	r	309	X	-	-	-
22	CLA	r	310	X	-	-	-
22	CLA	r	311	X	-	-	-
22	CLA	r	312	X	-	-	-
22	CLA	s	301	X	-	-	-
22	CLA	s	303	X	-	-	-
22	CLA	s	304	X	-	-	-
22	CLA	s	305	X	-	-	-
22	CLA	s	309	X	-	-	-
22	CLA	s	310	X	-	-	-
22	CLA	s	311	X	-	-	-
22	CLA	s	312	X	-	-	-
22	CLA	s	313	X	-	-	-
22	CLA	s	314	X	-	-	-
22	CLA	y	602	X	-	-	-
22	CLA	y	603	X	-	-	-
22	CLA	y	604	X	-	-	-
22	CLA	y	610	X	-	-	-
22	CLA	y	611	X	-	-	-
22	CLA	y	612	X	-	-	-
22	CLA	y	613	X	-	-	-
22	CLA	y	614	X	-	-	-

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 78324 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	308	Total	C	N	O	S	0	0
			2388	1558	392	426	12		
1	a	330	Total	C	N	O	S	0	0
			2584	1688	426	457	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		
2	b	478	Total	C	N	O	S	0	0
			3752	2459	635	646	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		
3	c	433	Total	C	N	O	S	0	0
			3373	2221	563	578	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		
4	d	336	Total	C	N	O	S	0	0
			2675	1770	438	455	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	72	Total	C	N	O	0	0
			586	386	93	107		
5	e	72	Total	C	N	O	0	0
			586	386	93	107		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	29	Total	C	N	O	S	0	0
			224	147	40	36	1		
6	f	29	Total	C	N	O	S	0	0
			224	147	40	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	52	Total	C	N	O	S	0	0
			389	257	61	69	2		
7	h	52	Total	C	N	O	S	0	0
			389	257	61	69	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	36	Total	C	N	O	S	0	0
			290	205	40	44	1		
9	k	36	Total	C	N	O	S	0	0
			290	205	40	44	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	36	Total	C	N	O	0	0
			302	200	47	55		

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	l	36	Total	C	N	O	0	0
			302	200	47	55		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	29	Total	C	N	O	0	0
			226	158	32	36		
11	m	29	Total	C	N	O	0	0
			226	158	32	36		

- Molecule 12 is a protein called Oxygen-evolving enhancer protein 1-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	193	Total	C	N	O	S	0	0
			1487	951	235	297	4		
12	o	193	Total	C	N	O	S	0	0
			1487	951	235	297	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	29	Total	C	N	O	S	0	0
			239	168	33	37	1		
13	t	29	Total	C	N	O	S	0	0
			239	168	33	37	1		

- Molecule 14 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	46	Total	C	N	O	S	0	0
			372	247	53	71	1		
14	w	46	Total	C	N	O	S	0	0
			372	247	53	71	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	X	32	Total	C	N	O	0	0
			226	149	35	42		
15	x	32	Total	C	N	O	0	0
			226	149	35	42		

- Molecule 16 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		
16	z	61	Total	C	N	O	S	0	0
			458	310	68	79	1		

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	188	Total	C	N	O	S	0	0
			1459	953	238	265	3		
17	r	188	Total	C	N	O	S	0	0
			1459	953	238	265	3		

- Molecule 18 is a protein called Chlorophyll a-b binding protein CP26, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		
18	s	214	Total	C	N	O	S	0	0
			1653	1082	270	297	4		

- Molecule 19 is a protein called Chlorophyll a-b binding protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	G	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	N	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	Y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	g	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	n	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	y	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	1	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	2	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	3	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	5	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	6	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		
19	7	219	Total	C	N	O	S	0	0
			1666	1078	273	310	5		

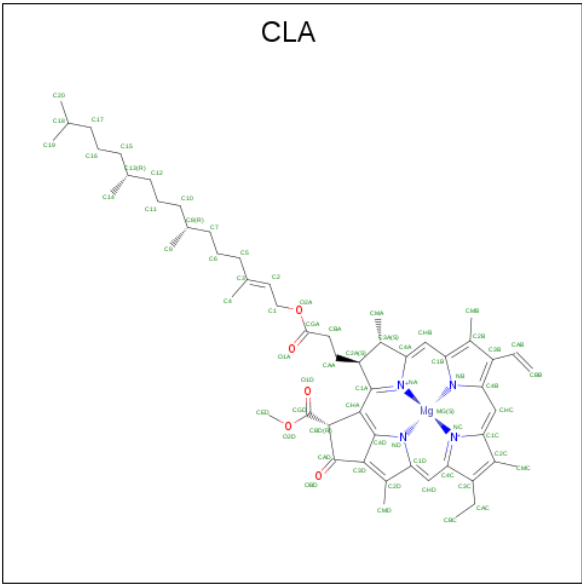
- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		
20	8	204	Total	C	N	O	S	0	0
			1597	1048	262	283	4		

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	A	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	B	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	C	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	D	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	D	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	D	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	a	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	a	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	a	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	b	1	Total	C	Mg	N	O	0
			720	560	16	64	80	
22	d	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	d	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	d	1	Total	C	Mg	N	O	0
			135	105	3	12	15	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	c	1	Total	C	Mg	N	O	0
			540	420	12	48	60	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	R	1	Total	C	Mg	N	O	0
			405	315	9	36	45	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	
22	S	1	Total	C	Mg	N	O	0
			450	350	10	40	50	

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Mol	Chain	Residues	Atoms					AltConf
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	S	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	G	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	N	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	Y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	r	1	Total 405	C 315	Mg 9	N 36	O 45	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	s	1	Total 450	C 350	Mg 10	N 40	O 50	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	g	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	n	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	y	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	1	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	3	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	4	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0

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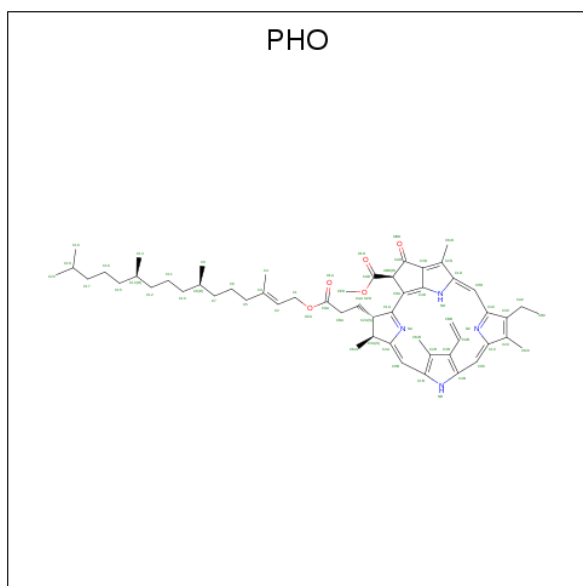
Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	6	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	7	1	Total 360	C 280	Mg 8	N 32	O 40	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0
22	8	1	Total 225	C 175	Mg 5	N 20	O 25	0

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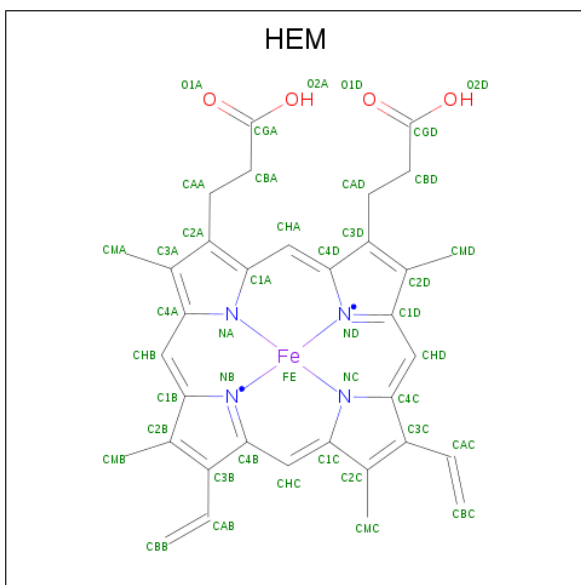
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	8	1	225	175	5	20	25	0

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



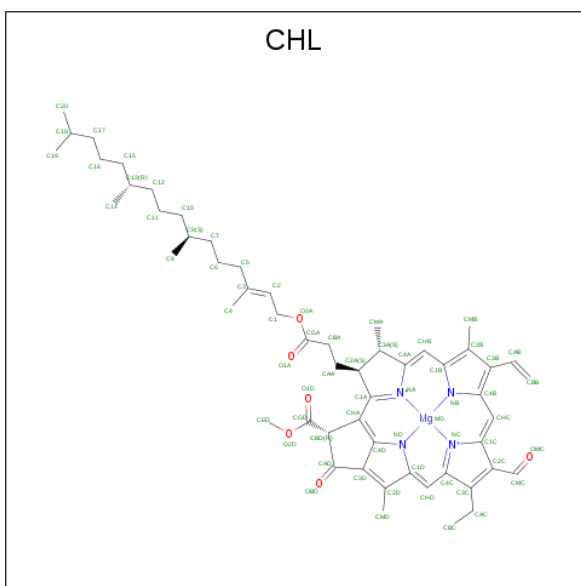
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
23	A	1	44	35	4	5	0
23	D	1	44	35	4	5	0
23	a	1	44	35	4	5	0
23	d	1	44	35	4	5	0

- Molecule 24 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms						AltConf
25	R	1	Total 138	C 105	Mg 3	N 12	O 18	0	
25	R	1	Total 138	C 105	Mg 3	N 12	O 18	0	

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Mol	Chain	Residues	Atoms					AltConf
25	R	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	S	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	G	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	N	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	

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Mol	Chain	Residues	Atoms					AltConf
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	Y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	r	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	r	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	r	1	Total	C	Mg	N	O	0
			138	105	3	12	18	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	s	1	Total	C	Mg	N	O	0
			184	140	4	16	24	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	g	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	n	1	Total	C	Mg	N	O	0
			272	208	6	24	34	

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	y	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	1	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	1	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	1	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	1	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	1	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	1	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	1	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	2	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	2	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	2	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	2	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	2	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	3	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	4	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	5	1	Total	C	Mg	N	O	0
			318	243	7	28	40	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	6	1	Total	C	Mg	N	O	0
			226	173	5	20	28	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	

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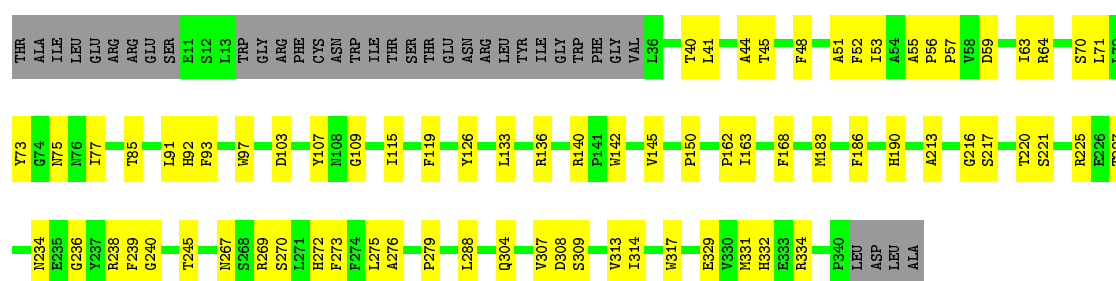
Mol	Chain	Residues	Atoms					AltConf
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	7	1	Total	C	Mg	N	O	0
			272	208	6	24	34	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	
25	8	1	Total	C	Mg	N	O	0
			230	175	5	20	30	

3 Residue-property plots

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

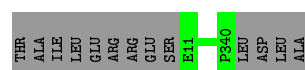
- Molecule 1: Photosystem II protein D1

Chain A: 



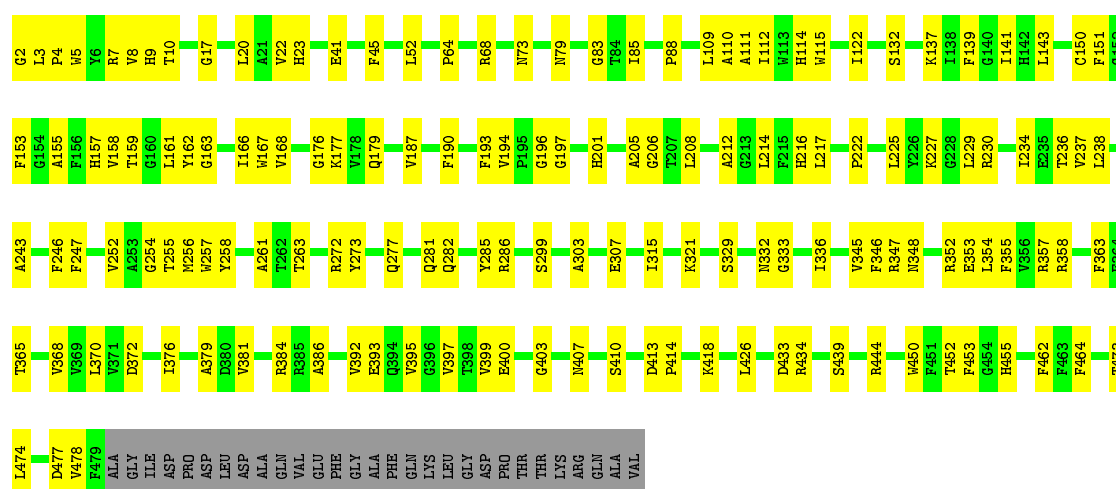
- Molecule 1: Photosystem II protein D1

Chain a: 



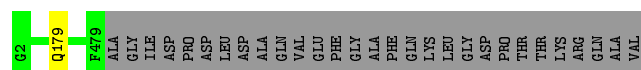
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 



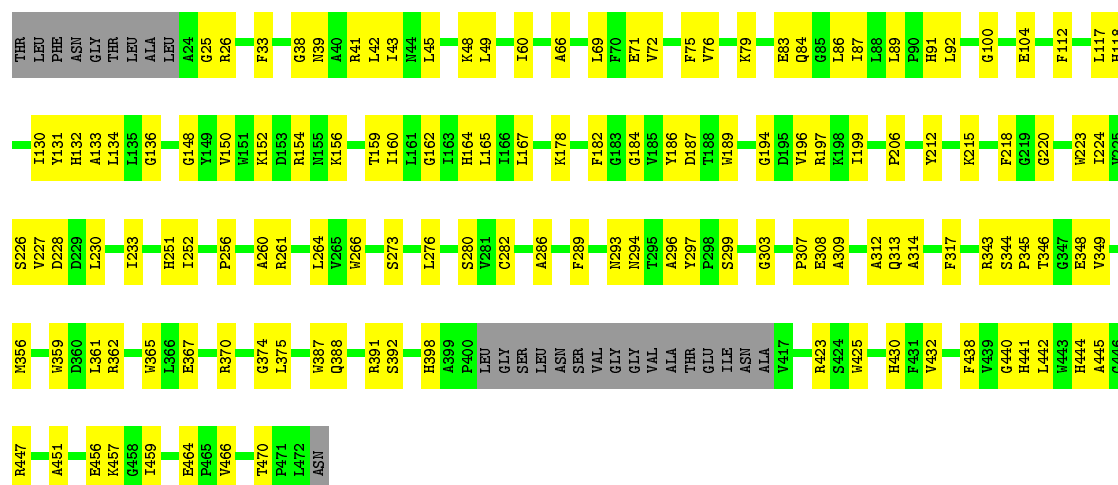
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  94% 6%



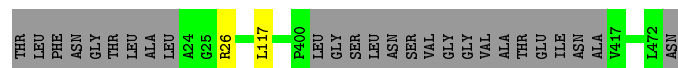
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:  65% 29% 6%



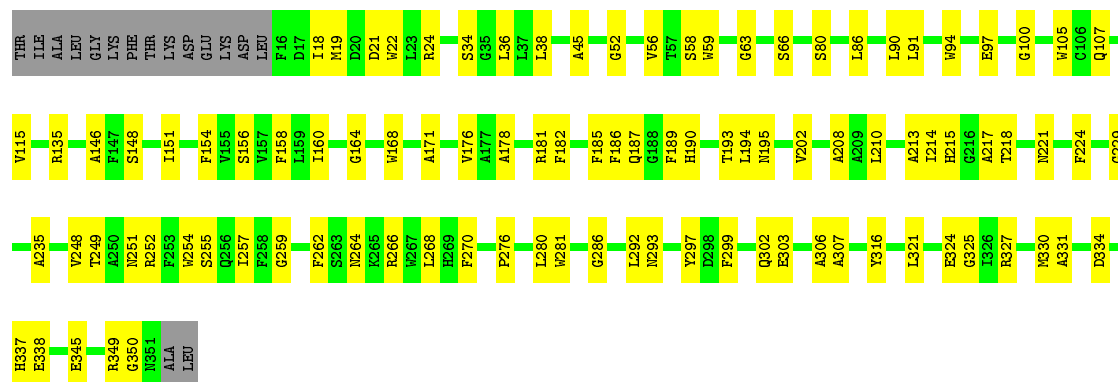
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c:  94% 6%



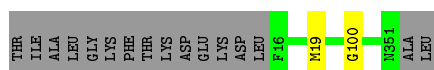
- Molecule 4: Photosystem II D2 protein

Chain D: 68% 28% 5%



- Molecule 4: Photosystem II D2 protein

Chain d:  95% . 5%



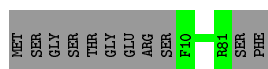
- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 70% 17% 13%



- Molecule 5: Cytochrome b559 subunit alpha

Chain e: 87% 13%



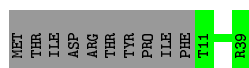
- Molecule 6: Cytochrome b559 subunit beta (PsbF)

Chain F: 51% 23% 26%



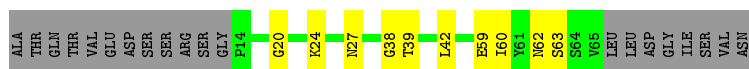
- Molecule 6: Cytochrome b559 subunit beta (PsbF)

Chain f: 74% 26%



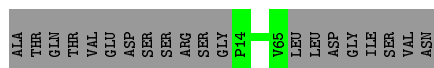
- Molecule 7: Photosystem II reaction center protein H

Chain H: 58% 14% 28%



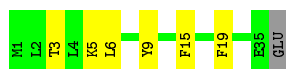
- Molecule 7: Photosystem II reaction center protein H

Chain h: 72% 28%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 81% 17% 2%



- Molecule 8: Photosystem II reaction center protein I

Chain i:  97%



- Molecule 9: Photosystem II reaction center protein K

Chain K:  68% 30%



- Molecule 9: Photosystem II reaction center protein K

Chain k:  97%




- Molecule 10: Photosystem II reaction center protein L

Chain L:  61% 32% 5%



- Molecule 10: Photosystem II reaction center protein L

Chain l:  92% 5%




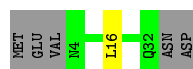
- Molecule 11: Photosystem II reaction center protein M

Chain M:  56% 29% 15%



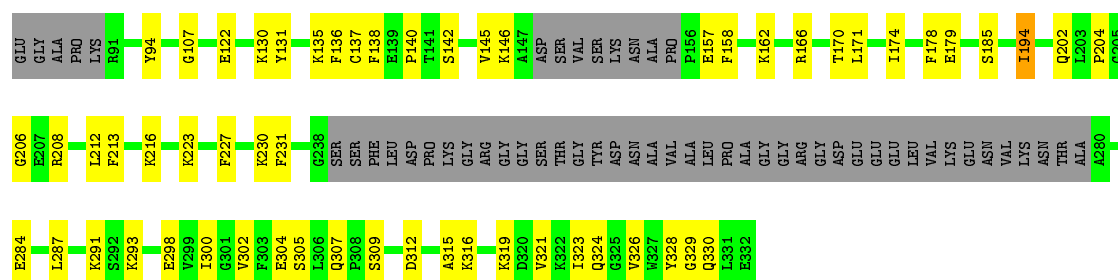
- Molecule 11: Photosystem II reaction center protein M

Chain m:  82% 15%



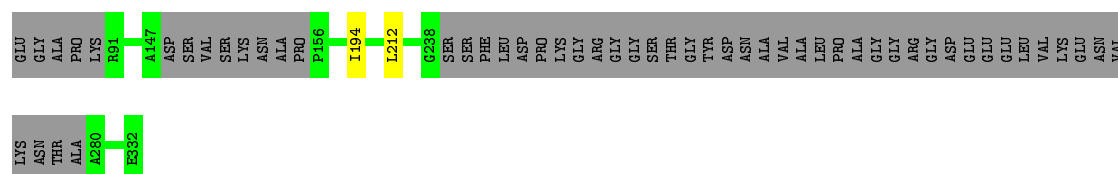
- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain O:  55% 23% 22%



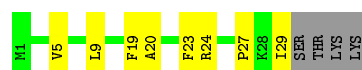
- Molecule 12: Oxygen-evolving enhancer protein 1-1, chloroplastic

Chain o: 77% 22%



- Molecule 13: Photosystem II reaction center protein T

Chain T: 64% 24% 12%



- Molecule 13: Photosystem II reaction center protein T

Chain t: 88% 12%



- Molecule 14: Photosystem II reaction center W protein, chloroplastic

Chain W: 63% 22% 15%



- Molecule 14: Photosystem II reaction center W protein, chloroplastic

Chain w: 85% 15%

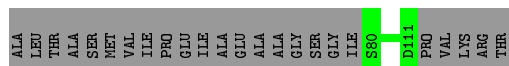


- Molecule 15: Photosystem II reaction center protein X

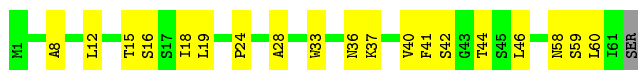
Chain X: 19% 9% 72%



- Molecule 15: Photosystem II reaction center protein X



- Molecule 16: Photosystem II reaction center protein Z



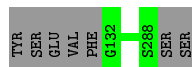
- Molecule 16: Photosystem II reaction center protein Z



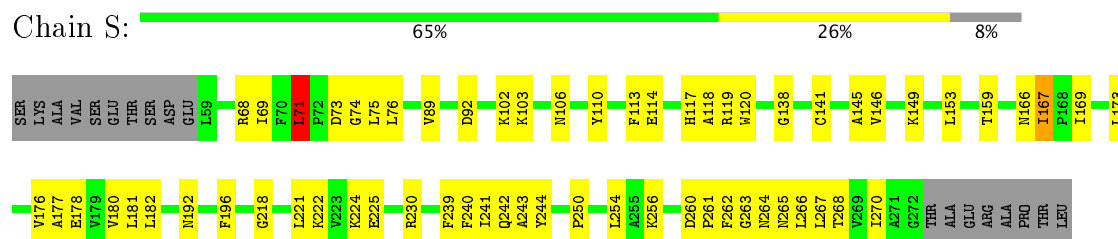
- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic



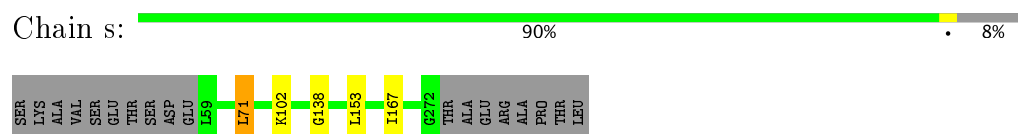
- Molecule 17: Chlorophyll a-b binding protein CP29.1, chloroplastic



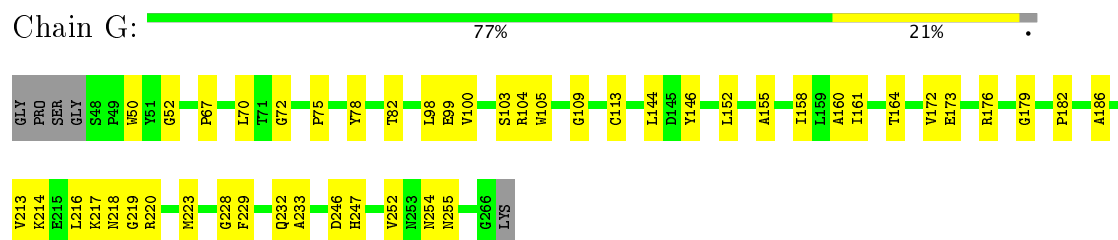
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic



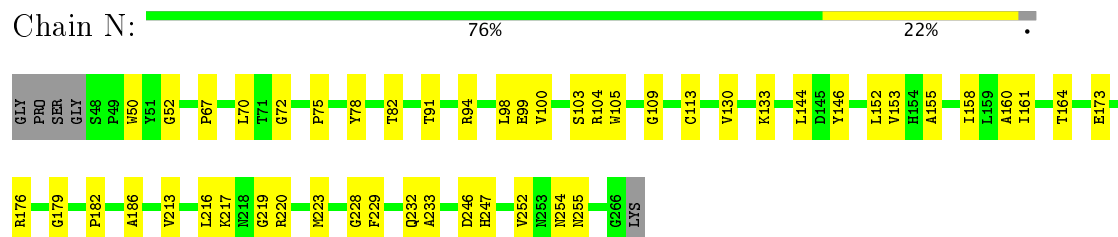
- Molecule 18: Chlorophyll a-b binding protein CP26, chloroplastic



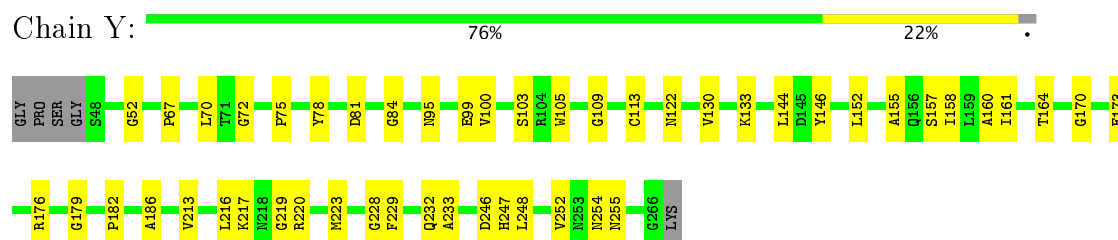
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

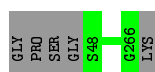


- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic



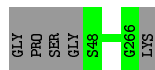
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic





- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain n: 98%



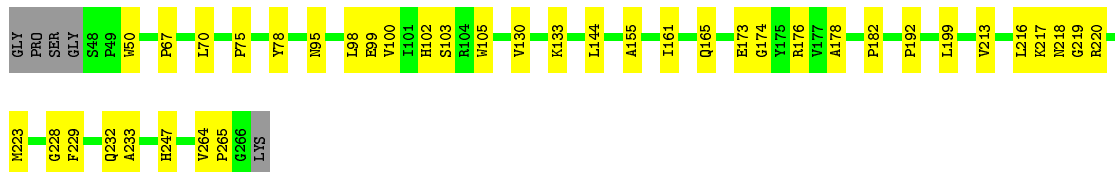
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain y: 98%



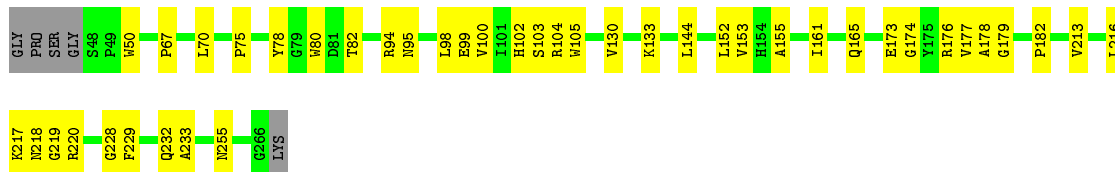
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 1: 80%



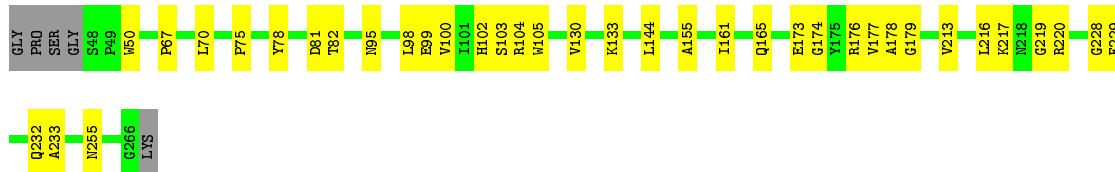
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 2: 79%



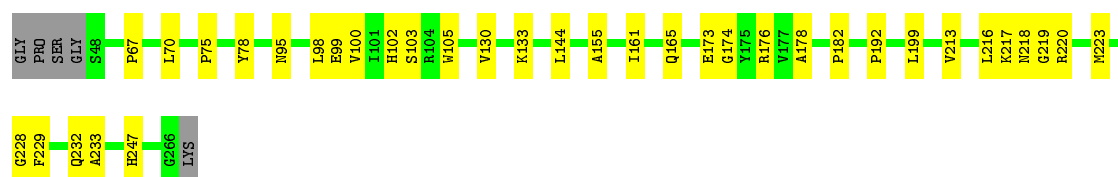
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 3: 81%



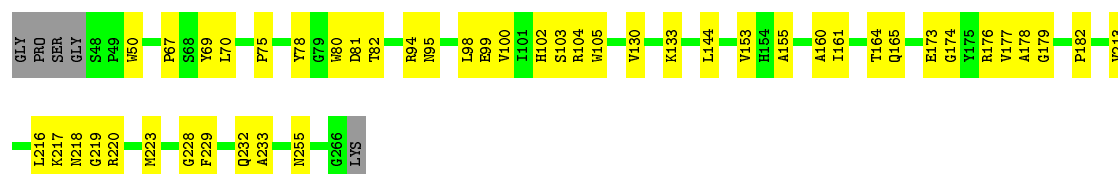
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 5: 82%



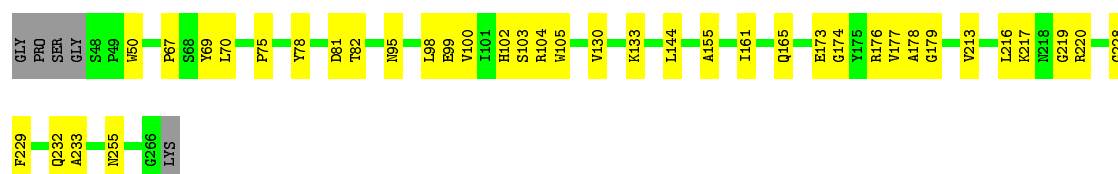
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 6: 77% 21%



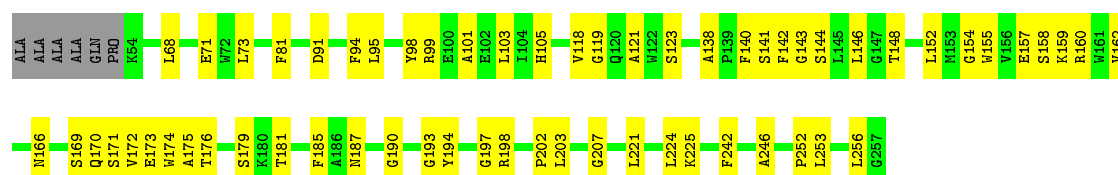
- Molecule 19: Chlorophyll a-b binding protein 1, chloroplastic

Chain 7: 81% 17%



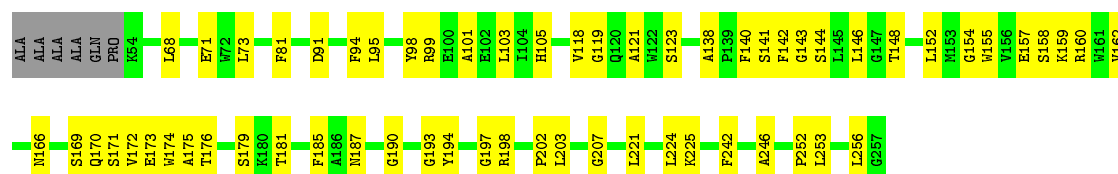
- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 68% 29%



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 68% 29%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	23434	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (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: CHL, HEM, PHO, CLA, FE2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.36	0/2458	0.58	0/3348
1	a	0.36	0/2665	0.58	0/3634
10	L	0.41	0/310	0.77	1/421 (0.2%)
10	l	0.41	0/310	0.77	1/421 (0.2%)
11	M	0.42	0/230	0.65	0/315
11	m	0.42	0/230	0.65	0/315
12	O	0.35	0/1518	0.68	1/2049 (0.0%)
12	o	0.35	0/1518	0.68	1/2049 (0.0%)
13	T	0.39	0/246	0.61	0/333
13	t	0.39	0/246	0.61	0/333
14	W	0.37	0/383	0.65	0/519
14	w	0.37	0/383	0.66	0/519
15	X	0.37	0/228	0.46	0/310
15	x	0.37	0/228	0.46	0/310
16	Z	0.31	0/468	0.50	0/641
16	z	0.32	0/468	0.50	0/641
17	R	0.35	0/1502	0.52	0/2047
17	r	0.35	0/1502	0.52	0/2047
18	S	0.37	0/1698	0.78	4/2305 (0.2%)
18	s	0.37	0/1698	0.78	4/2305 (0.2%)
19	1	0.31	0/1716	0.53	0/2336
19	2	0.31	0/1716	0.53	0/2336
19	3	0.31	0/1716	0.53	0/2336
19	5	0.31	0/1716	0.53	0/2336
19	6	0.31	0/1716	0.53	0/2336
19	7	0.31	0/1716	0.53	0/2336
19	G	0.36	0/1716	0.57	0/2336
19	N	0.36	0/1716	0.56	0/2336
19	Y	0.36	0/1716	0.57	0/2336
19	g	0.36	0/1716	0.57	0/2336
19	n	0.36	0/1716	0.56	0/2336
19	y	0.36	0/1716	0.57	0/2336

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	B	0.35	0/3881	0.58	0/5286
2	b	0.35	0/3881	0.58	0/5286
20	4	0.36	0/1652	0.97	3/2242 (0.1%)
20	8	0.36	0/1652	0.97	3/2242 (0.1%)
3	C	0.37	0/3487	0.60	1/4750 (0.0%)
3	c	0.37	0/3487	0.60	1/4750 (0.0%)
4	D	0.38	0/2768	0.60	1/3774 (0.0%)
4	d	0.38	0/2768	0.60	1/3774 (0.0%)
5	E	0.37	0/603	0.65	0/819
5	e	0.37	0/603	0.65	0/819
6	F	0.36	0/229	0.62	0/311
6	f	0.36	0/229	0.62	0/311
7	H	0.34	0/398	0.55	0/541
7	h	0.34	0/398	0.56	0/541
8	I	0.46	0/294	0.69	0/397
8	i	0.46	0/294	0.69	0/397
9	K	0.40	0/301	0.66	0/414
9	k	0.40	0/301	0.66	0/414
All	All	0.36	0/66107	0.62	22/89962 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	R	0	1
17	r	0	1
18	S	0	1
18	s	0	1
2	B	0	1
2	b	0	1
20	4	0	1
20	8	0	1
All	All	0	8

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	207	GLY	CA-C-N	-23.99	64.42	117.20
20	8	207	GLY	CA-C-N	-23.99	64.42	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	207	GLY	O-C-N	-21.84	87.76	122.70
20	8	207	GLY	O-C-N	-21.84	87.76	122.70
20	4	207	GLY	CA-C-O	17.55	152.19	120.60
20	8	207	GLY	CA-C-O	17.55	152.19	120.60
18	S	71	LEU	CA-CB-CG	7.85	133.37	115.30
18	s	71	LEU	CA-CB-CG	7.85	133.37	115.30
10	l	13	LEU	CA-CB-CG	5.72	128.45	115.30
10	L	13	LEU	CA-CB-CG	5.72	128.45	115.30
12	o	212	LEU	CA-CB-CG	5.70	128.42	115.30
12	O	212	LEU	CA-CB-CG	5.68	128.37	115.30
18	S	138	GLY	N-CA-C	5.62	127.15	113.10
18	s	138	GLY	N-CA-C	5.62	127.15	113.10
3	C	117	LEU	CA-CB-CG	5.38	127.67	115.30
3	c	117	LEU	CA-CB-CG	5.37	127.65	115.30
18	S	167	ILE	C-N-CD	-5.29	108.97	120.60
18	s	167	ILE	C-N-CD	-5.29	108.97	120.60
4	d	100	GLY	N-CA-C	-5.24	100.00	113.10
4	D	100	GLY	N-CA-C	-5.23	100.02	113.10
18	S	153	LEU	CA-CB-CG	5.18	127.22	115.30
18	s	153	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	4	176	THR	Peptide
20	8	176	THR	Peptide
2	B	179	GLN	Peptide
17	R	59	TYR	Peptide
18	S	71	LEU	Peptide
2	b	179	GLN	Peptide
17	r	59	TYR	Peptide
18	s	71	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2388	0	2309	70	0
1	a	2584	0	2490	0	0
2	B	3752	0	3636	152	0
2	b	3752	0	3636	0	0
3	C	3373	0	3302	143	0
3	c	3373	0	3302	0	0
4	D	2675	0	2565	99	0
4	d	2675	0	2565	0	0
5	E	586	0	566	17	0
5	e	586	0	566	0	0
6	F	224	0	233	6	0
6	f	224	0	233	0	0
7	H	389	0	411	11	0
7	h	389	0	411	0	0
8	I	286	0	295	5	0
8	i	286	0	295	0	0
9	K	290	0	300	7	0
9	k	290	0	300	0	0
10	L	302	0	291	16	0
10	l	302	0	291	0	0
11	M	226	0	252	10	0
11	m	226	0	252	0	0
12	O	1487	0	1462	39	0
12	o	1487	0	1462	0	0
13	T	239	0	255	8	0
13	t	239	0	255	0	0
14	W	372	0	346	8	0
14	w	372	0	346	0	0
15	X	226	0	244	8	0
15	x	226	0	244	0	0
16	Z	458	0	490	39	0
16	z	458	0	489	0	0
17	R	1459	0	1428	223	0
17	r	1459	0	1428	0	0
18	S	1653	0	1639	110	0
18	s	1653	0	1639	0	0
19	1	1666	0	1593	33	0
19	2	1666	0	1593	35	0
19	3	1666	0	1593	29	0
19	5	1666	0	1593	31	0
19	6	1666	0	1593	39	0
19	7	1666	0	1593	31	0
19	G	1666	0	1593	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	1666	0	1593	37	0
19	Y	1666	0	1593	37	0
19	g	1666	0	1593	0	0
19	n	1666	0	1593	0	0
19	y	1666	0	1593	0	0
20	4	1597	0	1526	155	0
20	8	1597	0	1526	157	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	1	360	0	264	4	0
22	2	360	0	264	21	0
22	3	360	0	264	2	0
22	4	225	0	165	7	0
22	5	360	0	264	4	0
22	6	360	0	264	21	0
22	7	360	0	264	2	0
22	8	225	0	165	8	0
22	A	135	0	99	4	0
22	B	720	0	528	39	0
22	C	540	0	396	23	0
22	D	135	0	99	4	0
22	G	360	0	264	12	0
22	N	360	0	264	5	0
22	R	405	0	295	101	0
22	S	450	0	330	32	0
22	Y	360	0	264	10	0
22	a	135	0	99	0	0
22	b	720	0	528	0	0
22	c	540	0	396	0	0
22	d	135	0	99	0	0
22	g	360	0	264	0	0
22	n	360	0	264	0	0
22	r	405	0	295	0	0
22	s	450	0	330	0	0
22	y	360	0	264	0	0
23	A	44	0	35	3	0
23	D	44	0	35	2	0
23	a	44	0	35	0	0
23	d	44	0	35	0	0
24	E	43	0	30	4	0
24	e	43	0	30	0	0
25	1	318	0	213	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	2	226	0	151	15	0
25	3	272	0	182	9	0
25	4	230	0	155	13	0
25	5	318	0	213	10	0
25	6	226	0	151	15	0
25	7	272	0	182	10	0
25	8	230	0	155	16	0
25	G	272	0	182	13	0
25	N	272	0	182	10	0
25	R	138	0	93	5	0
25	S	184	0	124	4	0
25	Y	272	0	182	13	0
25	g	272	0	182	0	0
25	n	272	0	182	0	0
25	r	138	0	93	0	0
25	s	184	0	124	0	0
25	y	272	0	182	0	0
All	All	78324	0	72516	1364	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 9.

All (1364) 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)
3:C:182:PHE:CZ	18:S:261:PRO:HG2	1.17	1.70
16:Z:59:SER:CB	18:S:267:LEU:CD2	1.74	1.58
17:R:280:HIS:HA	20:4:141:SER:N	167.28	1.48
16:Z:59:SER:CB	18:S:267:LEU:HD23	1.02	1.47
2:B:214:LEU:HD22	22:R:302:CLA:CED	105.31	1.47
3:C:182:PHE:CE1	18:S:261:PRO:HG2	1.47	1.46
17:R:280:HIS:HA	20:8:141:SER:N	1.20	1.44
3:C:182:PHE:CE1	18:S:261:PRO:CG	2.02	1.43
2:B:214:LEU:HB3	22:R:302:CLA:CED	105.65	1.40
18:S:74:GLY:N	22:S:301:CLA:HED2	3.74	1.40
16:Z:60:LEU:CD2	18:S:270:ILE:HG21	1.83	1.39
3:C:182:PHE:CZ	18:S:261:PRO:CG	2.07	1.38
2:B:214:LEU:CG	22:R:302:CLA:HED1	105.10	1.37
22:R:312:CLA:C1B	20:8:173:GLU:HG2	1.37	1.35
22:R:312:CLA:HMA1	20:4:159:LYS:CE	162.82	1.35
2:B:214:LEU:CB	22:R:302:CLA:HED1	105.04	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:312:CLA:HMA1	20:8:159:LYS:CE	1.55	1.34
17:R:285:ASP:CB	20:8:141:SER:HB3	1.45	1.32
3:C:131:TYR:OH	18:S:74:GLY:HA3	1.21	1.30
3:C:131:TYR:OH	18:S:74:GLY:CA	1.80	1.29
17:R:285:ASP:CB	20:4:141:SER:HB3	159.98	1.29
22:R:312:CLA:CHC	20:8:174:TRP:O	1.80	1.29
16:Z:59:SER:OG	18:S:267:LEU:CD2	1.71	1.28
22:R:312:CLA:CHC	20:4:174:TRP:O	162.14	1.28
22:R:312:CLA:HHC	20:4:174:TRP:O	162.73	1.28
22:R:312:CLA:C1B	20:4:173:GLU:HG2	160.58	1.27
2:B:214:LEU:CD2	22:R:302:CLA:CED	104.71	1.27
17:R:280:HIS:CA	20:8:141:SER:N	1.98	1.26
18:S:74:GLY:N	22:S:301:CLA:CED	3.40	1.26
17:R:280:HIS:CA	20:4:141:SER:N	167.40	1.26
22:R:312:CLA:C1B	20:8:173:GLU:CG	2.09	1.26
20:4:148:THR:OG1	25:4:301:CHL:CED	1.85	1.25
17:R:62:ALA:CB	20:8:172:VAL:CG2	2.15	1.24
20:8:148:THR:OG1	25:8:301:CHL:CED	1.85	1.24
17:R:62:ALA:CB	20:4:172:VAL:CG2	155.83	1.24
22:R:312:CLA:HHC	20:8:174:TRP:O	1.13	1.24
18:S:73:ASP:C	22:S:301:CLA:HED2	4.49	1.22
22:R:312:CLA:NB	20:8:173:GLU:HG2	1.52	1.22
17:R:285:ASP:OD1	20:8:142:PHE:N	1.71	1.21
22:R:312:CLA:NB	20:4:173:GLU:HG2	159.85	1.21
2:B:214:LEU:HD22	22:R:302:CLA:O2D	105.76	1.20
17:R:285:ASP:OD1	20:4:142:PHE:N	162.93	1.20
17:R:285:ASP:CB	20:8:141:SER:CB	2.18	1.20
16:Z:60:LEU:HD22	18:S:270:ILE:HG21	1.01	1.19
2:B:162:TYR:CE1	17:R:193:TRP:HZ2	100.71	1.19
22:R:312:CLA:C1B	20:4:173:GLU:CG	159.74	1.19
16:Z:59:SER:HB3	18:S:267:LEU:CD2	1.48	1.18
17:R:62:ALA:CB	20:4:172:VAL:HG23	156.43	1.18
17:R:280:HIS:CA	20:4:141:SER:H	167.21	1.17
17:R:285:ASP:CB	20:4:141:SER:CB	160.73	1.17
2:B:162:TYR:HE1	17:R:193:TRP:CZ2	102.10	1.17
17:R:285:ASP:HB2	20:4:141:SER:CB	160.83	1.17
22:R:312:CLA:NB	20:4:173:GLU:CG	159.00	1.17
17:R:285:ASP:HB2	20:8:141:SER:CB	1.75	1.16
17:R:56:PRO:N	20:4:174:TRP:HE1	161.27	1.16
17:R:280:HIS:CA	20:8:141:SER:H	1.55	1.15
17:R:59:TYR:HE1	20:8:170:GLN:N	1.42	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:59:TYR:HE1	20:4:170:GLN:N	162.10	1.15
17:R:62:ALA:CB	20:8:172:VAL:HG23	1.71	1.14
2:B:214:LEU:CG	22:R:302:CLA:CED	105.13	1.14
2:B:214:LEU:CD1	22:R:302:CLA:HED1	106.50	1.14
17:R:56:PRO:N	20:8:174:TRP:HE1	1.43	1.14
22:R:312:CLA:NB	20:8:173:GLU:CG	2.07	1.13
2:B:214:LEU:CB	22:R:302:CLA:CED	105.06	1.13
17:R:280:HIS:CE1	20:8:138:ALA:O	2.01	1.13
17:R:280:HIS:CE1	20:4:138:ALA:O	174.68	1.12
17:R:62:ALA:HB2	20:8:172:VAL:HG23	1.16	1.12
22:R:312:CLA:HBB1	20:8:173:GLU:O	1.37	1.11
22:R:312:CLA:HMA1	20:4:159:LYS:HE2	162.21	1.10
2:B:214:LEU:HD22	22:R:302:CLA:HED3	104.42	1.10
17:R:285:ASP:HB2	20:4:141:SER:HB3	160.08	1.10
22:2:613:CLA:HAB	25:4:301:CHL:HAB	1.29	1.10
17:R:62:ALA:HB2	20:4:172:VAL:HG23	157.18	1.09
22:R:312:CLA:C3B	20:8:175:ALA:HB2	1.83	1.09
22:6:613:CLA:HAB	25:8:301:CHL:HAB	1.29	1.08
22:R:312:CLA:HBB1	20:4:173:GLU:O	165.15	1.08
17:R:280:HIS:HE1	20:4:138:ALA:O	174.93	1.07
16:Z:60:LEU:HD22	18:S:270:ILE:CG2	1.82	1.07
22:R:312:CLA:C3B	20:4:175:ALA:HB2	164.40	1.06
16:Z:60:LEU:CD2	18:S:270:ILE:CG2	2.38	1.06
3:C:182:PHE:HZ	18:S:261:PRO:HG2	1.15	1.06
22:R:312:CLA:HMA1	20:8:159:LYS:HE2	1.12	1.06
20:4:148:THR:OG1	25:4:301:CHL:HED3	1.54	1.06
3:C:206:PRO:HG3	22:Y:614:CLA:HBB2	1.12	1.06
17:R:59:TYR:CE1	20:8:170:GLN:HA	1.91	1.05
17:R:62:ALA:HB2	20:8:172:VAL:CG2	1.82	1.05
17:R:62:ALA:HB1	20:4:172:VAL:CG2	155.66	1.05
3:C:182:PHE:CE1	18:S:261:PRO:CD	2.37	1.05
16:Z:59:SER:OG	18:S:267:LEU:HD21	1.41	1.05
17:R:59:TYR:CE1	20:4:170:GLN:HA	162.58	1.04
17:R:285:ASP:HB2	20:8:141:SER:HB3	1.31	1.04
17:R:56:PRO:N	20:4:174:TRP:NE1	161.79	1.03
20:8:148:THR:OG1	25:8:301:CHL:HED3	1.54	1.03
22:R:312:CLA:O2A	20:4:162:VAL:HG21	151.66	1.03
17:R:56:PRO:N	20:8:174:TRP:NE1	2.05	1.03
17:R:275:LEU:O	22:6:613:CLA:HMB1	1.59	1.03
17:R:62:ALA:HB1	20:8:172:VAL:CG2	1.85	1.02
17:R:62:ALA:HB2	20:4:172:VAL:CG2	156.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:312:CLA:O2A	20:8:162:VAL:HG21	1.58	1.01
17:R:62:ALA:HB1	20:8:172:VAL:HG21	1.40	1.01
17:R:280:HIS:HE1	20:8:138:ALA:O	1.33	1.01
17:R:62:ALA:HB1	20:4:172:VAL:HG21	154.76	1.01
15:X:82:SER:O	15:X:86:PHE:HB3	1.61	1.01
22:R:312:CLA:HMA1	20:8:159:LYS:HE3	1.38	1.00
17:R:275:LEU:O	22:2:613:CLA:HMB1	174.50	1.00
3:C:182:PHE:HE1	18:S:261:PRO:CG	1.67	1.00
16:Z:59:SER:HG	18:S:267:LEU:HD21	1.23	1.00
18:S:74:GLY:CA	22:S:301:CLA:HED2	3.79	0.99
22:R:312:CLA:C3B	20:4:175:ALA:CB	165.36	0.99
22:R:312:CLA:HMA1	20:4:159:LYS:HE3	162.34	0.98
17:R:62:ALA:CB	20:8:172:VAL:HG21	1.90	0.98
3:C:182:PHE:CE1	18:S:261:PRO:HD2	1.97	0.98
16:Z:59:SER:CB	18:S:267:LEU:HD21	1.85	0.97
20:8:148:THR:OG1	25:8:301:CHL:HED1	1.61	0.97
22:R:312:CLA:CBB	20:4:173:GLU:O	165.39	0.97
22:R:312:CLA:C3B	20:8:175:ALA:CB	2.38	0.97
3:C:182:PHE:CE1	18:S:261:PRO:CB	2.48	0.96
3:C:260:ALA:O	3:C:264:LEU:HB2	1.66	0.96
22:R:312:CLA:CBB	20:8:173:GLU:O	2.13	0.96
2:B:214:LEU:HD13	22:R:302:CLA:HED1	107.13	0.96
18:S:177:ALA:O	18:S:181:LEU:HB2	1.66	0.96
2:B:214:LEU:CD2	22:R:302:CLA:HED3	103.83	0.95
22:R:312:CLA:C2B	20:8:173:GLU:HG2	1.96	0.95
22:6:613:CLA:CAB	25:8:301:CHL:HAB	1.97	0.95
22:R:312:CLA:C2B	20:4:173:GLU:HG2	161.92	0.95
22:R:312:CLA:CGA	20:8:162:VAL:HG21	1.96	0.95
20:4:148:THR:OG1	25:4:301:CHL:HED1	1.61	0.95
17:R:285:ASP:HB2	20:4:141:SER:OG	160.72	0.95
17:R:191:LEU:O	17:R:195:GLU:HB2	1.67	0.95
17:R:62:ALA:CB	20:4:172:VAL:HG21	154.94	0.95
22:2:613:CLA:CAB	25:4:301:CHL:HAB	1.97	0.94
22:R:312:CLA:CGA	20:4:162:VAL:HG21	152.78	0.94
22:R:312:CLA:CMA	20:4:159:LYS:CE	161.96	0.94
17:R:278:PRO:CG	22:2:613:CLA:HBB2	175.25	0.94
2:B:161:LEU:HD21	25:R:305:CHL:HMD2	111.00	0.94
22:R:312:CLA:C4B	20:8:173:GLU:HG2	1.98	0.93
2:B:345:VAL:O	2:B:399:VAL:HA	1.69	0.93
22:R:312:CLA:CMA	20:8:159:LYS:CE	2.45	0.93
15:X:84:LYS:O	15:X:88:LEU:HB2	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:312:CLA:C4B	20:4:173:GLU:HG2	160.54	0.93
16:Z:36:ASN:O	16:Z:40:VAL:HB	1.68	0.93
2:B:346:PHE:O	2:B:354:LEU:HB2	1.69	0.92
17:R:285:ASP:HB2	20:8:141:SER:OG	1.67	0.92
17:R:278:PRO:CG	22:6:613:CLA:HBB2	1.98	0.92
18:S:74:GLY:CA	22:S:301:CLA:CED	3.81	0.92
20:8:148:THR:HG1	25:8:301:CHL:CED	1.76	0.92
17:R:59:TYR:CE1	20:4:170:GLN:N	161.80	0.92
17:R:59:TYR:CE1	20:4:170:GLN:CA	162.93	0.92
17:R:61:GLY:O	20:8:166:ASN:ND2	2.03	0.91
22:R:312:CLA:CMA	20:4:159:LYS:HE3	161.47	0.91
17:R:59:TYR:CE1	20:8:170:GLN:CA	2.53	0.91
16:Z:59:SER:HB2	18:S:267:LEU:CD2	1.99	0.91
17:R:61:GLY:O	20:4:166:ASN:ND2	152.97	0.91
22:R:312:CLA:CMA	20:8:159:LYS:HE3	2.00	0.90
17:R:278:PRO:CD	22:6:613:CLA:HBB2	2.01	0.90
17:R:278:PRO:CD	22:2:613:CLA:HBB2	175.53	0.90
17:R:61:GLY:HA2	20:4:169:SER:HB2	157.12	0.90
17:R:61:GLY:HA2	20:8:169:SER:HB2	1.52	0.90
17:R:288:SER:OG	20:8:142:PHE:HD2	1.56	0.89
3:C:206:PRO:CG	22:Y:614:CLA:HBB2	2.02	0.89
17:R:59:TYR:CE1	20:8:170:GLN:N	2.35	0.89
3:C:182:PHE:HE1	18:S:261:PRO:CD	1.80	0.89
1:A:51:ALA:O	1:A:55:ALA:HB2	1.73	0.88
17:R:255:GLY:O	17:R:259:GLN:HB3	1.73	0.88
3:C:131:TYR:OH	18:S:74:GLY:HA2	1.70	0.88
3:C:182:PHE:HZ	18:S:261:PRO:CG	1.78	0.87
17:R:288:SER:OG	20:4:142:PHE:HD2	157.98	0.87
20:4:148:THR:HG1	25:4:301:CHL:HED3	1.35	0.87
20:4:94:PHE:O	20:4:98:TYR:HB3	1.74	0.86
20:8:94:PHE:O	20:8:98:TYR:HB3	1.74	0.86
2:B:110:ALA:O	2:B:114:HIS:HB2	1.74	0.86
2:B:214:LEU:HB3	22:R:302:CLA:HED1	105.64	0.86
3:C:182:PHE:CE1	18:S:261:PRO:HB2	2.11	0.85
2:B:64:PRO:O	2:B:68:ARG:HB2	1.77	0.85
3:C:182:PHE:HE1	18:S:261:PRO:CB	1.85	0.85
17:R:280:HIS:HA	20:8:140:PHE:C	1.96	0.85
17:R:284:ILE:HG12	20:4:146:LEU:N	162.64	0.84
2:B:214:LEU:CD2	22:R:302:CLA:O2D	105.16	0.84
17:R:280:HIS:CA	20:4:140:PHE:C	168.62	0.84
17:R:280:HIS:HA	20:4:140:PHE:C	168.50	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:284:ILE:HG12	20:8:146:LEU:N	1.92	0.84
17:R:287:PHE:CZ	20:4:146:LEU:HD23	153.71	0.84
17:R:278:PRO:HD3	22:6:613:CLA:HBB2	1.59	0.84
17:R:59:TYR:HE1	20:8:170:GLN:CA	1.91	0.84
17:R:287:PHE:CZ	20:8:146:LEU:HD23	2.13	0.83
17:R:280:HIS:CA	20:8:140:PHE:C	2.44	0.83
17:R:56:PRO:N	20:8:174:TRP:CD1	2.47	0.83
2:B:214:LEU:HD13	22:R:302:CLA:CED	107.16	0.83
2:B:346:PHE:HB2	2:B:354:LEU:O	1.78	0.83
17:R:278:PRO:HD3	22:2:613:CLA:HBB2	175.67	0.83
17:R:58:TRP:C	20:4:173:GLU:HG3	155.23	0.83
17:R:56:PRO:N	20:4:174:TRP:CD1	161.42	0.83
17:R:58:TRP:C	20:8:173:GLU:HG3	1.98	0.82
17:R:285:ASP:CA	20:4:141:SER:HB3	158.97	0.82
20:4:144:SER:O	25:4:301:CHL:CED	2.28	0.82
3:C:130:ILE:O	3:C:134:LEU:HB2	1.78	0.82
20:8:144:SER:O	25:8:301:CHL:CED	2.28	0.81
17:R:285:ASP:CA	20:8:141:SER:HB3	2.09	0.81
17:R:280:HIS:CA	20:4:140:PHE:CA	169.73	0.81
18:S:178:GLU:O	18:S:182:LEU:HB3	1.81	0.81
2:B:247:PHE:HB2	22:B:608:CLA:HBC1	1.61	0.81
17:R:280:HIS:CA	20:8:140:PHE:CA	2.47	0.81
17:R:59:TYR:HE1	20:8:170:GLN:H	0.81	0.81
17:R:58:TRP:O	20:4:173:GLU:HG3	155.30	0.80
15:X:83:LEU:O	15:X:87:LEU:HB2	1.82	0.80
17:R:284:ILE:HG12	20:8:146:LEU:H	1.47	0.80
2:B:114:HIS:HE1	22:B:616:CLA:ND	1.79	0.79
16:Z:60:LEU:HD23	18:S:270:ILE:HG21	2.18	0.79
17:R:58:TRP:O	20:8:173:GLU:HG3	1.82	0.79
20:8:148:THR:HG1	25:8:301:CHL:HED3	1.34	0.79
5:E:72:SER:O	5:E:76:LEU:HB2	1.83	0.79
2:B:214:LEU:CB	22:R:302:CLA:HED3	104.18	0.78
17:R:280:HIS:CB	20:4:141:SER:N	167.82	0.78
3:C:182:PHE:CZ	18:S:261:PRO:CB	2.66	0.78
13:T:20:ALA:O	13:T:24:ARG:HB3	1.84	0.78
17:R:284:ILE:HG12	20:4:146:LEU:H	162.33	0.78
20:4:148:THR:HG1	25:4:301:CHL:CED	1.89	0.78
2:B:214:LEU:CD1	22:R:302:CLA:CED	106.54	0.78
17:R:59:TYR:HE1	20:4:170:GLN:CA	163.22	0.78
22:B:604:CLA:HBB1	22:B:607:CLA:HBB2	1.65	0.77
1:A:48:PHE:O	1:A:52:PHE:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:PHE:O	4:D:158:PHE:HB2	1.84	0.77
17:R:287:PHE:HZ	20:4:146:LEU:HD23	154.38	0.77
18:S:250:PRO:O	18:S:254:LEU:HB2	1.84	0.77
22:2:613:CLA:HAB	25:4:301:CHL:CAB	2.13	0.77
4:D:186:PHE:O	4:D:190:HIS:HB2	1.85	0.77
2:B:214:LEU:HB3	22:R:302:CLA:HED3	104.77	0.77
18:S:73:ASP:HB3	22:S:301:CLA:O2D	1.84	0.77
4:D:327:ARG:O	4:D:331:ALA:HB2	1.85	0.77
18:S:73:ASP:HB3	22:S:301:CLA:CED	2.68	0.77
17:R:288:SER:HG	20:8:142:PHE:HD2	0.78	0.76
5:E:33:ALA:O	5:E:37:PHE:HB2	1.86	0.76
17:R:287:PHE:HZ	20:8:146:LEU:HD23	1.49	0.76
17:R:59:TYR:HE1	20:4:170:GLN:H	161.37	0.76
18:S:225:GLU:HA	22:S:310:CLA:HBB1	1.67	0.76
22:6:613:CLA:HAB	25:8:301:CHL:CAB	2.13	0.75
22:R:312:CLA:NB	20:8:173:GLU:HG3	2.00	0.75
2:B:168:VAL:O	2:B:176:GLY:HA2	1.87	0.75
3:C:131:TYR:CZ	18:S:74:GLY:HA3	2.22	0.75
1:A:186:PHE:O	1:A:190:HIS:HB2	1.87	0.75
17:R:177:SER:O	17:R:183:PRO:HA	1.87	0.75
16:Z:60:LEU:CD2	18:S:270:ILE:HG22	2.17	0.75
17:R:285:ASP:CG	20:4:142:PHE:H	162.43	0.75
17:R:285:ASP:N	20:8:141:SER:HB3	2.02	0.75
22:R:312:CLA:C2B	20:8:175:ALA:CB	2.65	0.75
2:B:2:GLY:HA3	10:L:12:GLU:HG2	1.68	0.75
22:R:312:CLA:C2B	20:4:175:ALA:CB	165.36	0.74
3:C:182:PHE:CE1	18:S:262:PHE:HD2	2.78	0.74
17:R:280:HIS:CB	20:8:141:SER:N	2.42	0.74
16:Z:37:LYS:O	16:Z:41:PHE:HB2	1.87	0.74
22:R:312:CLA:CMA	20:4:159:LYS:HE2	161.34	0.74
17:R:285:ASP:CG	20:8:142:PHE:N	2.41	0.74
4:D:181:ARG:O	4:D:185:PHE:HB2	1.88	0.74
18:S:73:ASP:HB2	22:S:301:CLA:HBD	1.69	0.74
2:B:282:GLN:O	2:B:286:ARG:HB2	1.88	0.73
9:K:31:ALA:O	9:K:34:ASN:HB2	1.88	0.73
4:D:178:ALA:O	4:D:182:PHE:HB2	1.88	0.73
17:R:285:ASP:CG	20:4:142:PHE:N	162.85	0.73
12:O:136:PHE:HB3	12:O:174:ILE:HB	1.71	0.73
12:O:137:CYS:HB3	12:O:328:TYR:HB3	1.70	0.73
22:R:312:CLA:NB	20:4:173:GLU:HG3	158.35	0.73
19:1:228:GLY:O	19:1:232:GLN:HB3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:285:ASP:N	20:4:141:SER:HB3	159.33	0.73
19:5:228:GLY:O	19:5:232:GLN:HB3	1.89	0.73
17:R:285:ASP:CG	20:8:142:PHE:H	1.88	0.73
19:7:228:GLY:O	19:7:232:GLN:HB3	1.89	0.72
22:R:312:CLA:CMA	20:8:159:LYS:HE2	2.07	0.72
16:Z:60:LEU:HD21	18:S:270:ILE:CG2	2.40	0.72
19:3:228:GLY:O	19:3:232:GLN:HB3	1.89	0.72
16:Z:42:SER:O	16:Z:46:LEU:HB2	1.89	0.72
16:Z:60:LEU:HD21	18:S:270:ILE:HG21	2.17	0.72
4:D:302:GLN:O	4:D:306:ALA:HB3	1.90	0.72
2:B:333:GLY:HA2	2:B:444:ARG:HH11	1.55	0.72
19:6:228:GLY:O	19:6:232:GLN:HB3	1.89	0.72
17:R:288:SER:HG	20:4:142:PHE:HD2	158.75	0.71
1:A:331:MET:HG3	4:D:325:GLY:HA3	1.72	0.71
3:C:224:ILE:O	3:C:227:VAL:HB	1.90	0.71
2:B:157:HIS:HE1	22:B:606:CLA:NA	2.34	0.71
20:4:95:LEU:O	20:4:99:ARG:HB2	1.91	0.71
19:2:228:GLY:O	19:2:232:GLN:HB3	1.89	0.71
10:L:36:PHE:HB3	11:M:7:ALA:HB1	2.71	0.71
16:Z:33:TRP:O	16:Z:37:LYS:HB2	1.91	0.70
4:D:330:MET:O	4:D:334:ASP:HB2	1.92	0.70
16:Z:59:SER:OG	18:S:267:LEU:HD23	1.57	0.70
20:8:95:LEU:O	20:8:99:ARG:HB2	1.91	0.70
2:B:212:ALA:O	2:B:216:HIS:HB2	1.91	0.70
20:4:187:ASN:HD22	20:4:197:GLY:H	1.40	0.70
20:8:187:ASN:HD22	20:8:197:GLY:H	1.40	0.70
1:A:75:ASN:OD1	4:D:302:GLN:NE2	2.26	0.69
2:B:162:TYR:CE1	17:R:193:TRP:CZ2	101.43	0.69
1:A:272:HIS:HD2	4:D:215:HIS:NE2	1.90	0.69
3:C:276:LEU:HD21	22:C:508:CLA:HAB	1.75	0.69
22:R:312:CLA:O2A	20:4:162:VAL:CG2	151.71	0.68
3:C:165:LEU:HD21	22:C:506:CLA:HAB	1.74	0.68
17:R:209:GLU:HB2	25:R:306:CHL:HBC1	1.75	0.68
17:R:59:TYR:O	20:8:173:GLU:OE1	2.11	0.68
22:R:312:CLA:C2B	20:4:175:ALA:HB3	165.62	0.68
1:A:288:LEU:HD22	3:C:432:VAL:HG22	2.56	0.68
2:B:214:LEU:HD22	22:R:302:CLA:CGD	105.90	0.68
25:R:304:CHL:HBB2	25:R:305:CHL:HAB	1.76	0.68
12:O:227:PHE:HB2	12:O:287:LEU:HB2	1.75	0.68
19:Y:182:PRO:HD2	25:Y:608:CHL:HBB2	1.76	0.68
20:8:144:SER:O	25:8:301:CHL:HED1	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:59:TYR:O	20:4:173:GLU:OE1	155.19	0.67
22:R:312:CLA:C2B	20:8:175:ALA:HB2	2.25	0.67
4:D:280:LEU:HD22	23:D:402:PHO:HBC3	1.76	0.67
25:G:606:CHL:HBB2	25:G:607:CHL:HBB1	1.77	0.67
16:Z:59:SER:HB3	18:S:267:LEU:CG	2.24	0.67
17:R:56:PRO:CD	20:8:174:TRP:HE1	2.07	0.67
22:R:312:CLA:C2B	20:8:175:ALA:HB3	2.24	0.67
19:3:161:ILE:HG12	25:3:306:CHL:HAC1	1.78	0.66
17:R:56:PRO:CD	20:4:174:TRP:HE1	161.17	0.66
3:C:466:VAL:HG21	4:D:249:THR:HA	1.77	0.66
20:4:144:SER:O	25:4:301:CHL:HED1	1.94	0.66
4:D:210:LEU:O	4:D:214:ILE:HB	1.96	0.66
18:S:159:THR:O	18:S:166:ASN:ND2	2.29	0.66
22:R:312:CLA:C2B	20:4:175:ALA:HB2	164.40	0.66
19:N:182:PRO:HD2	25:N:608:CHL:HBB2	1.77	0.66
3:C:251:HIS:CE1	22:C:506:CLA:NA	2.67	0.66
18:S:74:GLY:H	22:S:301:CLA:CED	3.14	0.66
19:7:161:ILE:HG12	25:7:306:CHL:HAC1	1.78	0.65
3:C:440:GLY:O	3:C:444:HIS:HB2	1.97	0.65
22:G:611:CLA:HMB2	19:5:199:LEU:HD23	1.78	0.65
12:O:230:LYS:HG2	12:O:284:GLU:HG2	1.78	0.65
20:4:121:ALA:HA	20:4:253:LEU:HD22	1.78	0.65
17:R:191:LEU:O	17:R:195:GLU:CB	2.44	0.65
18:S:256:LYS:HB3	18:S:264:ASN:HD21	1.62	0.65
18:S:74:GLY:CA	22:S:301:CLA:HED3	4.76	0.65
13:T:5:VAL:O	13:T:9:LEU:HB2	1.97	0.65
19:G:182:PRO:HD2	25:G:608:CHL:HBB2	1.79	0.65
20:8:121:ALA:HA	20:8:253:LEU:HD22	1.78	0.65
3:C:79:LYS:HB2	3:C:84:GLN:HE21	1.61	0.65
20:8:94:PHE:O	20:8:98:TYR:CB	2.45	0.65
3:C:39:ASN:O	3:C:42:LEU:HB2	1.97	0.65
2:B:111:ALA:O	2:B:115:TRP:HB2	1.96	0.65
22:G:611:CLA:HMB2	19:1:199:LEU:HD23	212.05	0.64
1:A:85:THR:HA	1:A:109:GLY:HA3	1.79	0.64
2:B:273:TYR:O	2:B:277:GLN:HB2	1.96	0.64
3:C:289:PHE:O	3:C:293:ASN:HB3	1.98	0.64
2:B:52:LEU:HD21	2:B:307:GLU:HB3	1.80	0.64
3:C:227:VAL:HG11	3:C:233:ILE:HD11	1.80	0.64
12:O:138:PHE:HB2	12:O:171:LEU:HB2	1.80	0.64
17:R:61:GLY:CA	20:8:169:SER:HB2	2.26	0.64
17:R:61:GLY:CA	20:4:169:SER:HB2	156.17	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:312:CLA:C3B	20:4:173:GLU:HG2	161.90	0.64
1:A:145:VAL:HG22	3:C:442:LEU:HB3	2.31	0.64
1:A:334:ARG:HB2	4:D:350:GLY:HA2	1.96	0.63
22:R:312:CLA:C3B	20:8:173:GLU:HG2	2.28	0.63
11:M:24:ILE:HG23	11:M:27:VAL:HG21	5.54	0.63
12:O:213:PHE:HA	12:O:307:GLN:HE22	1.64	0.63
19:2:161:ILE:HG12	25:2:605:CHL:HAC1	1.81	0.63
20:4:94:PHE:O	20:4:98:TYR:CB	2.45	0.63
2:B:329:SER:H	2:B:332:ASN:HD22	1.46	0.63
12:O:216:LYS:H	12:O:231:PHE:HB2	1.63	0.63
4:D:181:ARG:NH2	4:D:334:ASP:OD1	2.32	0.63
19:6:179:GLY:HA2	25:6:607:CHL:HMC	1.81	0.62
3:C:345:PRO:HB3	12:O:166:ARG:HE	1.63	0.62
22:R:312:CLA:O2A	20:8:162:VAL:CG2	2.40	0.62
19:6:161:ILE:HG12	25:6:605:CHL:HAC1	1.81	0.62
3:C:459:ILE:H	4:D:224:PHE:HA	1.65	0.62
2:B:336:ILE:HB	2:B:433:ASP:HB3	1.81	0.62
12:O:202:GLN:HE21	12:O:206:GLY:HA2	1.64	0.62
17:R:73:VAL:HB	17:R:137:ARG:HH12	1.64	0.62
2:B:357:ARG:NH2	4:D:338:GLU:OE1	2.33	0.62
17:R:275:LEU:O	22:2:613:CLA:HBB1	175.62	0.62
16:Z:37:LYS:O	16:Z:41:PHE:CB	2.47	0.62
2:B:41:GLU:O	2:B:45:PHE:HB2	2.00	0.62
3:C:132:HIS:CE1	22:S:301:CLA:NA	2.74	0.62
1:A:133:LEU:HD23	4:D:257:ILE:HG12	1.82	0.62
17:R:275:LEU:O	22:6:613:CLA:HBB1	2.00	0.62
19:2:179:GLY:HA2	25:2:607:CHL:HMC	1.81	0.61
3:C:282:CYS:O	3:C:286:ALA:HB2	2.00	0.61
18:S:73:ASP:C	22:S:301:CLA:CED	4.00	0.61
2:B:254:GLY:O	2:B:258:TYR:HB2	2.01	0.61
3:C:349:VAL:H	3:C:374:GLY:HA3	1.65	0.61
18:S:192:ASN:HB3	18:S:196:PHE:HB2	1.83	0.61
3:C:150:VAL:HG13	3:C:152:LYS:H	1.66	0.61
18:S:75:LEU:CD1	22:S:301:CLA:HMD1	2.30	0.61
3:C:251:HIS:HE1	22:C:506:CLA:NA	2.10	0.61
3:C:75:PHE:O	9:K:25:LYS:NZ	2.33	0.61
10:L:16:THR:O	10:L:20:TRP:HB3	2.01	0.61
22:R:312:CLA:CMB	20:4:175:ALA:HB3	166.72	0.61
19:1:182:PRO:HD2	25:1:608:CHL:HBB2	1.82	0.61
2:B:208:LEU:HD12	22:B:602:CLA:HAC2	1.83	0.61
19:G:82:THR:HG21	25:Y:609:CHL:HAA1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:103:SER:HB3	19:1:219:GLY:HA3	1.83	0.61
3:C:160:ILE:HD13	22:C:512:CLA:HAC2	1.89	0.61
1:A:317:TRP:HE3	4:D:181:ARG:HD3	1.75	0.60
2:B:347:ARG:O	2:B:397:VAL:HA	2.02	0.60
3:C:444:HIS:CE1	22:C:508:CLA:NA	2.69	0.60
17:R:275:LEU:O	22:2:613:CLA:CMB	175.07	0.60
22:R:312:CLA:CMB	20:8:175:ALA:HB3	2.31	0.60
19:3:103:SER:HB3	19:3:219:GLY:HA3	1.83	0.60
3:C:441:HIS:O	3:C:445:ALA:HB3	2.01	0.60
25:S:306:CHL:HBA1	25:S:306:CHL:HBD	1.83	0.60
12:O:107:GLY:HA3	14:W:90:THR:HG22	1.98	0.60
17:R:72:LEU:HD13	17:R:137:ARG:HD2	1.84	0.60
19:5:103:SER:HB3	19:5:219:GLY:HA3	1.83	0.60
3:C:361:LEU:O	3:C:370:ARG:NH2	2.35	0.60
19:6:229:PHE:O	19:6:233:ALA:HB3	2.02	0.60
19:N:94:ARG:NH1	19:Y:81:ASP:O	2.35	0.60
13:T:19:PHE:O	13:T:23:PHE:HB2	2.02	0.60
17:R:275:LEU:HB3	22:2:613:CLA:CMB	173.79	0.60
19:3:229:PHE:O	19:3:233:ALA:HB3	2.02	0.60
19:7:103:SER:HB3	19:7:219:GLY:HA3	1.83	0.60
18:S:242:GLN:OE1	22:S:313:CLA:ND	2.35	0.60
16:Z:59:SER:CB	18:S:267:LEU:CG	2.74	0.59
19:2:229:PHE:O	19:2:233:ALA:HB3	2.02	0.59
19:6:103:SER:HB3	19:6:219:GLY:HA3	1.83	0.59
17:R:275:LEU:HB3	22:6:613:CLA:CMB	2.32	0.59
19:2:103:SER:HB3	19:2:219:GLY:HA3	1.83	0.59
22:R:312:CLA:C3B	20:4:173:GLU:O	163.86	0.59
19:5:182:PRO:HD2	25:5:608:CHL:HBB2	1.82	0.59
19:7:229:PHE:O	19:7:233:ALA:HB3	2.02	0.59
3:C:25:GLY:O	3:C:41:ARG:NH1	2.35	0.59
22:R:312:CLA:C3B	20:8:173:GLU:O	2.50	0.59
2:B:227:LYS:O	2:B:230:ARG:NH1	2.36	0.59
2:B:256:MET:HA	2:B:263:THR:HG21	1.85	0.59
20:4:171:SER:HA	20:4:179:SER:HB2	1.83	0.59
22:R:312:CLA:HHC	20:8:174:TRP:C	2.10	0.59
19:1:229:PHE:O	19:1:233:ALA:HB3	2.02	0.59
18:S:176:VAL:O	18:S:180:VAL:HB	2.03	0.59
19:5:229:PHE:O	19:5:233:ALA:HB3	2.02	0.59
3:C:43:ILE:HG12	22:C:509:CLA:HAC2	1.91	0.58
3:C:76:VAL:O	3:C:84:GLN:NE2	2.36	0.58
4:D:327:ARG:O	4:D:331:ALA:CB	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:78:TYR:OH	19:1:217:LYS:NZ	2.36	0.58
19:3:78:TYR:OH	19:3:217:LYS:NZ	2.36	0.58
2:B:214:LEU:HB3	22:R:302:CLA:HED2	106.28	0.58
3:C:118:HIS:CE1	22:C:502:CLA:NA	2.78	0.58
19:2:78:TYR:OH	19:2:217:LYS:NZ	2.36	0.58
19:6:78:TYR:OH	19:6:217:LYS:NZ	2.36	0.58
4:D:21:ASP:OD1	4:D:24:ARG:NH2	2.37	0.58
20:8:171:SER:HA	20:8:179:SER:HB2	1.83	0.58
17:R:285:ASP:CB	20:8:141:SER:OG	2.40	0.58
2:B:79:ASN:H	2:B:83:GLY:H	1.52	0.58
19:7:161:ILE:O	19:7:165:GLN:HB2	2.04	0.58
3:C:33:PHE:O	3:C:41:ARG:NH2	2.30	0.58
4:D:217:ALA:O	4:D:221:ASN:HB2	2.03	0.58
19:G:67:PRO:HG2	19:G:70:LEU:HD12	1.86	0.58
17:R:152:LEU:O	17:R:156:SER:HB3	2.04	0.58
22:R:312:CLA:C4B	20:4:175:ALA:HB2	163.05	0.58
16:Z:60:LEU:HD21	18:S:270:ILE:HG22	1.85	0.58
17:R:280:HIS:HA	20:8:141:SER:H	0.61	0.58
22:R:312:CLA:C4B	20:8:175:ALA:HB2	2.33	0.58
2:B:368:VAL:HB	2:B:381:VAL:HB	1.84	0.58
3:C:83:GLU:OE2	3:C:398:HIS:NE2	2.37	0.58
2:B:161:LEU:CD2	25:R:305:CHL:HMD2	110.15	0.58
18:S:71:LEU:HB2	18:S:75:LEU:HD22	1.86	0.58
20:4:81:PHE:HB2	22:4:302:CLA:HMD1	1.86	0.58
19:5:161:ILE:O	19:5:165:GLN:HB2	2.04	0.58
19:7:78:TYR:OH	19:7:217:LYS:NZ	2.36	0.58
20:8:81:PHE:HB2	22:8:302:CLA:HMD1	1.86	0.58
1:A:307:VAL:HG22	1:A:313:VAL:HG22	1.86	0.58
3:C:307:PRO:HB2	3:C:361:LEU:HD13	1.86	0.58
19:6:161:ILE:O	19:6:165:GLN:HB2	2.04	0.57
3:C:297:TYR:O	3:C:423:ARG:NH2	2.35	0.57
19:3:161:ILE:O	19:3:165:GLN:HB2	2.04	0.57
2:B:158:VAL:HG22	2:B:166:ILE:HD11	1.86	0.57
3:C:131:TYR:O	3:C:136:GLY:N	2.36	0.57
3:C:365:TRP:HB2	3:C:388:GLN:HG2	1.86	0.57
1:A:225:ARG:NH2	2:B:477:ASP:O	2.37	0.57
16:Z:59:SER:HB3	18:S:267:LEU:HD23	0.58	0.57
19:1:161:ILE:O	19:1:165:GLN:HB2	2.04	0.57
19:5:78:TYR:OH	19:5:217:LYS:NZ	2.36	0.57
1:A:245:THR:OG1	4:D:266:ARG:NH2	2.37	0.57
4:D:36:LEU:HD21	15:X:104:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:236:ALA:O	17:R:240:LEU:HB2	2.05	0.57
1:A:225:ARG:HH21	2:B:478:VAL:HA	1.70	0.57
2:B:474:LEU:O	4:D:135:ARG:NH1	2.96	0.57
1:A:317:TRP:HE1	4:D:66:SER:HB3	1.70	0.57
3:C:346:THR:OG1	3:C:348:GLU:OE1	2.23	0.57
18:S:250:PRO:O	18:S:254:LEU:CB	2.53	0.57
25:6:606:CHL:HBB2	25:7:301:CHL:HBB1	1.87	0.57
17:R:267:PRO:O	17:R:271:TRP:CB	2.53	0.57
17:R:283:ILE:N	20:8:144:SER:OG	2.20	0.57
19:2:161:ILE:O	19:2:165:GLN:HB2	2.04	0.56
17:R:62:ALA:CA	20:4:172:VAL:HG21	153.70	0.56
3:C:441:HIS:O	3:C:445:ALA:CB	2.53	0.56
19:1:100:VAL:HG22	19:1:216:LEU:HD21	1.88	0.56
19:2:100:VAL:HG22	19:2:216:LEU:HD21	1.88	0.56
19:6:104:ARG:NH1	25:6:607:CHL:OBD	2.38	0.56
1:A:217:SER:O	1:A:221:SER:CB	2.54	0.56
2:B:355:PHE:O	2:B:370:LEU:HA	2.04	0.56
2:B:22:VAL:HG22	22:B:614:CLA:HMB3	1.88	0.56
19:N:67:PRO:HG2	19:N:70:LEU:HD12	1.86	0.56
17:R:283:ILE:N	20:4:144:SER:OG	158.36	0.56
2:B:41:GLU:O	2:B:45:PHE:CB	2.54	0.56
5:E:19:TYR:O	5:E:23:HIS:ND1	2.39	0.56
19:Y:67:PRO:HG2	19:Y:70:LEU:HD12	1.86	0.56
19:2:177:VAL:HG21	25:2:608:CHL:HMA3	1.87	0.56
22:R:312:CLA:C3B	20:4:173:GLU:C	162.94	0.56
19:6:177:VAL:HG21	25:6:608:CHL:HMA3	1.87	0.56
14:W:97:SER:H	14:W:101:LEU:HD22	1.71	0.56
1:A:53:ILE:HG12	1:A:71:LEU:HD12	1.88	0.56
2:B:384:ARG:HH21	4:D:345:GLU:HA	1.70	0.56
4:D:59:TRP:CE2	5:E:64:PRO:HG3	2.96	0.56
19:N:179:GLY:HA3	19:N:186:ALA:HB2	1.87	0.56
18:S:113:PHE:O	18:S:117:HIS:HB2	2.06	0.56
18:S:74:GLY:HA3	22:S:301:CLA:CED	3.75	0.56
19:Y:179:GLY:HA3	19:Y:186:ALA:HB2	1.87	0.56
25:2:608:CHL:HAA1	19:3:82:THR:HG21	1.88	0.56
17:R:62:ALA:CA	20:8:172:VAL:HG21	2.35	0.56
20:8:148:THR:HG1	25:8:301:CHL:HED1	1.53	0.56
12:O:293:LYS:HD3	12:O:298:GLU:HB2	1.88	0.56
20:8:224:LEU:HB2	22:8:309:CLA:HMA1	1.88	0.56
1:A:234:ASN:O	4:D:264:ASN:ND2	3.03	0.56
19:N:176:ARG:NH1	25:N:608:CHL:O1D	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:GLY:O	3:C:156:LYS:NZ	2.39	0.56
3:C:256:PRO:O	3:C:261:ARG:NH1	2.39	0.56
19:G:179:GLY:HA3	19:G:186:ALA:HB2	1.87	0.56
12:O:298:GLU:HG2	12:O:330:GLN:HG2	1.88	0.56
18:S:68:ARG:HH11	25:S:302:CHL:HBC1	1.71	0.56
19:Y:144:LEU:HD23	25:Y:606:CHL:HMD2	1.88	0.56
2:B:321:LYS:NZ	2:B:363:PHE:O	2.39	0.56
22:R:312:CLA:C3B	20:8:173:GLU:C	2.74	0.56
17:R:63:ILE:HG13	20:4:166:ASN:ND2	150.43	0.56
2:B:167:TRP:HA	2:B:177:LYS:O	2.07	0.55
7:H:20:GLY:O	7:H:24:LYS:HB2	2.06	0.55
10:L:15:ARG:NH2	11:M:26:TYR:OH	2.56	0.55
19:N:103:SER:HB3	19:N:219:GLY:HA3	1.88	0.55
25:6:608:CHL:HAA1	19:7:82:THR:HG21	1.88	0.55
1:A:56:PRO:HB2	12:O:208:ARG:HH22	1.71	0.55
17:R:168:ALA:O	17:R:172:GLU:HB2	2.06	0.55
7:H:39:THR:HG22	7:H:42:LEU:HB3	1.89	0.55
19:5:100:VAL:HG22	19:5:216:LEU:HD21	1.88	0.55
3:C:187:ASP:O	3:C:194:GLY:HA2	2.06	0.55
25:N:606:CHL:HBB2	25:N:607:CHL:HBB1	1.88	0.55
18:S:74:GLY:N	22:S:301:CLA:HED1	3.13	0.55
25:2:606:CHL:HBB2	25:3:301:CHL:HBB1	1.87	0.55
19:6:100:VAL:HG22	19:6:216:LEU:HD21	1.88	0.55
19:7:100:VAL:HG22	19:7:216:LEU:HD21	1.88	0.55
1:A:217:SER:O	1:A:221:SER:HB2	2.07	0.55
1:A:150:PRO:HD3	23:A:404:PHO:HBC2	1.89	0.55
19:3:100:VAL:HG22	19:3:216:LEU:HD21	1.88	0.55
19:7:67:PRO:HG2	19:7:70:LEU:HD12	1.89	0.55
11:M:22:LEU:HD23	11:M:25:ILE:HD12	1.89	0.55
17:R:63:ILE:HG13	20:8:166:ASN:ND2	2.21	0.55
16:Z:8:ALA:O	16:Z:12:LEU:HB2	2.07	0.55
19:5:67:PRO:HG2	19:5:70:LEU:HD12	1.89	0.55
3:C:344:SER:OG	3:C:348:GLU:N	2.40	0.55
1:A:48:PHE:O	1:A:52:PHE:CB	2.55	0.55
18:S:218:GLY:O	18:S:222:LYS:HB2	2.07	0.55
14:W:93:PRO:HB2	14:W:96:LEU:HB2	1.88	0.55
14:W:99:ASN:ND2	19:Y:122:ASN:O	2.40	0.55
19:Y:229:PHE:O	19:Y:233:ALA:CB	2.55	0.55
17:R:63:ILE:HD11	20:8:166:ASN:ND2	2.22	0.55
4:D:297:TYR:O	4:D:316:TYR:OH	2.25	0.55
19:G:229:PHE:O	19:G:233:ALA:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:229:PHE:O	19:N:233:ALA:CB	2.55	0.55
17:R:280:HIS:HA	20:4:141:SER:H	167.09	0.54
2:B:8:VAL:HG12	10:L:11:VAL:HG21	1.89	0.54
4:D:259:GLY:O	13:T:24:ARG:NH1	2.40	0.54
19:G:103:SER:HB3	19:G:219:GLY:HA3	1.88	0.54
25:G:601:CHL:HBA1	25:G:601:CHL:HED3	1.89	0.54
19:2:229:PHE:O	19:2:233:ALA:CB	2.56	0.54
19:2:104:ARG:NH1	25:2:607:CHL:OBD	2.38	0.54
19:2:67:PRO:HG2	19:2:70:LEU:HD12	1.89	0.54
19:5:229:PHE:O	19:5:233:ALA:CB	2.56	0.54
19:3:179:GLY:HA2	25:3:308:CHL:HMC	1.89	0.54
3:C:456:GLU:HG2	3:C:457:LYS:HD2	1.90	0.54
4:D:195:ASN:HD21	4:D:286:GLY:HA3	1.73	0.54
19:N:246:ASP:O	19:N:254:ASN:ND2	2.40	0.54
19:3:67:PRO:HG2	19:3:70:LEU:HD12	1.89	0.54
20:4:224:LEU:HB2	22:4:309:CLA:HMA1	1.88	0.54
1:A:238:ARG:NH1	1:A:239:PHE:O	2.40	0.54
18:S:119:ARG:NH1	25:S:308:CHL:OBD	2.41	0.54
19:Y:103:SER:HB3	19:Y:219:GLY:HA3	1.88	0.54
19:3:229:PHE:O	19:3:233:ALA:CB	2.56	0.54
19:6:182:PRO:HD2	25:6:607:CHL:HBB2	1.89	0.54
17:R:275:LEU:C	22:6:613:CLA:HMB1	2.27	0.54
2:B:162:TYR:HD2	22:B:606:CLA:HAC2	1.73	0.54
4:D:330:MET:O	4:D:334:ASP:CB	2.56	0.54
4:D:337:HIS:HA	5:E:65:LEU:HD21	1.90	0.54
19:N:228:GLY:O	19:N:232:GLN:HB3	2.08	0.54
12:O:136:PHE:HA	12:O:329:GLY:HA2	1.90	0.54
17:R:275:LEU:O	22:6:613:CLA:CMB	2.44	0.54
19:3:75:PRO:HB3	19:3:213:VAL:HG22	1.90	0.54
20:4:95:LEU:O	20:4:99:ARG:CB	2.56	0.54
20:8:252:PRO:O	20:8:256:LEU:HB3	2.07	0.54
19:G:228:GLY:O	19:G:232:GLN:HB3	2.08	0.54
17:R:63:ILE:HD11	20:4:166:ASN:ND2	150.13	0.54
19:7:229:PHE:O	19:7:233:ALA:CB	2.56	0.54
18:S:73:ASP:HB3	22:S:301:CLA:HED1	2.73	0.54
19:2:182:PRO:HD2	25:2:607:CHL:HBB2	1.89	0.54
19:6:229:PHE:O	19:6:233:ALA:CB	2.56	0.54
19:6:67:PRO:HG2	19:6:70:LEU:HD12	1.89	0.54
19:7:176:ARG:HH22	25:7:308:CHL:HED2	1.73	0.54
1:A:103:ASP:O	1:A:107:TYR:HB2	2.08	0.54
2:B:153:PHE:HB2	22:B:606:CLA:HAB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:238:LEU:HB3	22:R:308:CLA:HMA1	1.89	0.54
17:R:58:TRP:O	20:8:173:GLU:CG	2.55	0.54
19:3:176:ARG:HH22	25:3:308:CHL:HED2	1.73	0.53
2:B:122:ILE:HG12	7:H:24:LYS:HA	1.90	0.53
22:G:611:CLA:HMB2	19:1:199:LEU:CD2	212.89	0.53
19:7:75:PRO:HB3	19:7:213:VAL:HG22	1.90	0.53
2:B:73:ASN:HB3	2:B:88:PRO:HB3	1.89	0.53
3:C:87:ILE:O	3:C:91:HIS:ND1	2.38	0.53
25:G:601:CHL:HBD	25:G:601:CHL:O1A	2.09	0.53
19:Y:228:GLY:O	19:Y:232:GLN:HB3	2.08	0.53
20:8:91:ASP:HB2	20:8:94:PHE:HD2	1.73	0.53
3:C:230:LEU:HA	3:C:233:ILE:HB	1.90	0.53
19:G:99:GLU:OE2	19:G:220:ARG:NE	2.33	0.53
25:N:606:CHL:HBC2	25:N:607:CHL:HAC2	1.90	0.53
19:Y:247:HIS:NE2	22:Y:614:CLA:ND	2.56	0.53
19:1:229:PHE:O	19:1:233:ALA:CB	2.56	0.53
19:1:75:PRO:HB3	19:1:213:VAL:HG22	1.90	0.53
17:R:275:LEU:C	22:2:613:CLA:HMB1	173.28	0.53
19:1:67:PRO:HG2	19:1:70:LEU:HD12	1.89	0.53
17:R:278:PRO:HG2	22:2:613:CLA:HBB2	176.08	0.53
19:7:179:GLY:HA2	25:7:308:CHL:HMC	1.89	0.53
2:B:299:SER:O	2:B:303:ALA:HB2	2.09	0.53
3:C:303:GLY:O	3:C:423:ARG:NE	2.37	0.53
4:D:34:SER:O	4:D:38:LEU:HB3	2.08	0.53
12:O:312:ASP:HB3	12:O:315:ALA:HB3	1.90	0.53
19:6:75:PRO:HB3	19:6:213:VAL:HG22	1.90	0.53
4:D:189:PHE:HE1	4:D:327:ARG:HA	1.74	0.53
18:S:75:LEU:HD12	22:S:301:CLA:HMD1	1.89	0.53
19:5:75:PRO:HB3	19:5:213:VAL:HG22	1.90	0.53
4:D:302:GLN:O	4:D:306:ALA:CB	2.57	0.53
17:R:58:TRP:O	20:4:173:GLU:CG	155.94	0.53
20:4:252:PRO:O	20:4:256:LEU:HB3	2.07	0.53
20:4:91:ASP:HB2	20:4:94:PHE:HD2	1.73	0.53
22:G:611:CLA:HMB2	19:5:199:LEU:CD2	2.39	0.53
17:R:285:ASP:CB	20:4:141:SER:OG	160.61	0.53
2:B:281:GLN:O	2:B:285:TYR:HB3	2.09	0.53
3:C:178:LYS:NZ	3:C:182:PHE:O	2.42	0.53
17:R:256:PHE:O	17:R:260:ALA:HB3	2.09	0.53
18:S:178:GLU:O	18:S:182:LEU:CB	2.55	0.53
19:Y:99:GLU:OE2	19:Y:220:ARG:NE	2.33	0.53
3:C:130:ILE:HA	3:C:134:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:HIS:CE1	22:B:609:CLA:NA	2.76	0.52
2:B:225:LEU:O	2:B:229:LEU:HB2	2.09	0.52
3:C:45:LEU:O	3:C:49:LEU:HB2	2.10	0.52
17:R:284:ILE:CG1	20:4:146:LEU:H	162.63	0.52
2:B:201:HIS:CE1	22:B:602:CLA:ND	2.77	0.52
12:O:122:GLU:HG2	12:O:291:LYS:HG2	1.90	0.52
10:L:30:VAL:HG22	13:T:9:LEU:HG	1.90	0.52
3:C:289:PHE:O	3:C:293:ASN:CB	2.58	0.52
12:O:312:ASP:HB2	12:O:316:LYS:HG2	1.91	0.52
19:Y:246:ASP:O	19:Y:254:ASN:ND2	2.40	0.52
22:R:312:CLA:C4B	20:8:174:TRP:O	2.42	0.52
2:B:111:ALA:O	2:B:115:TRP:CB	2.56	0.52
19:2:98:LEU:O	19:2:102:HIS:ND1	2.42	0.52
20:8:95:LEU:O	20:8:99:ARG:CB	2.56	0.52
2:B:197:GLY:O	2:B:201:HIS:CB	2.58	0.52
3:C:212:TYR:HB3	3:C:224:ILE:HG22	1.91	0.52
1:A:279:PRO:HG2	4:D:213:ALA:HB2	1.91	0.52
5:E:33:ALA:O	5:E:37:PHE:CB	2.58	0.52
4:D:255:SER:HB3	13:T:24:ARG:HH22	1.73	0.52
19:2:75:PRO:HB3	19:2:213:VAL:HG22	1.90	0.52
20:8:68:LEU:HB3	20:8:71:GLU:HB2	1.92	0.52
1:A:93:PHE:HB2	3:C:218:PHE:CG	2.71	0.52
3:C:349:VAL:HB	3:C:375:LEU:H	1.74	0.52
19:N:176:ARG:HH22	25:N:608:CHL:HED2	1.75	0.52
16:Z:60:LEU:HD23	18:S:270:ILE:CG2	2.56	0.52
2:B:400:GLU:HA	2:B:410:SER:HA	1.92	0.52
4:D:262:PHE:HB2	4:D:268:LEU:HD12	1.91	0.52
17:R:56:PRO:CA	20:4:174:TRP:CD1	160.70	0.52
18:S:75:LEU:HD11	22:S:301:CLA:HMD1	2.00	0.52
2:B:193:PHE:HA	2:B:261:ALA:HB2	1.91	0.52
19:G:246:ASP:O	19:G:254:ASN:ND2	2.40	0.52
17:R:63:ILE:CD1	20:8:166:ASN:ND2	2.73	0.52
22:R:312:CLA:C4B	20:8:173:GLU:CG	2.71	0.52
3:C:215:LYS:NZ	3:C:226:SER:OG	2.42	0.52
3:C:162:GLY:HA3	3:C:252:ILE:HG13	1.92	0.52
4:D:148:SER:HA	4:D:151:ILE:HD12	1.91	0.52
10:L:13:LEU:HD23	10:L:14:ASN:H	1.76	0.52
19:N:78:TYR:OH	19:N:217:LYS:NZ	2.43	0.52
12:O:140:PRO:HD2	12:O:170:THR:HG22	1.92	0.52
19:1:176:ARG:NH1	25:1:608:CHL:O1D	2.43	0.51
17:R:275:LEU:HB3	22:6:613:CLA:HMB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:78:TYR:OH	19:G:217:LYS:NZ	2.43	0.51
18:S:167:ILE:HD12	18:S:169:ILE:HG12	1.91	0.51
19:5:176:ARG:NH1	25:5:608:CHL:O1D	2.43	0.51
17:R:62:ALA:CA	20:8:172:VAL:CG2	2.88	0.51
3:C:447:ARG:O	3:C:451:ALA:HB2	2.10	0.51
17:R:56:PRO:CA	20:8:174:TRP:CD1	2.93	0.51
17:R:63:ILE:CD1	20:4:166:ASN:ND2	149.43	0.51
19:Y:78:TYR:OH	19:Y:217:LYS:NZ	2.43	0.51
19:3:176:ARG:NH1	25:3:308:CHL:O1D	2.44	0.51
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.93	0.51
2:B:4:PRO:HG2	2:B:7:ARG:HD2	1.93	0.51
2:B:23:HIS:ND1	22:B:615:CLA:OBD	2.39	0.51
9:K:47:PHE:O	9:K:50:LEU:HB3	2.10	0.51
20:4:119:GLY:O	20:4:123:SER:CB	2.59	0.51
19:G:176:ARG:NH1	25:G:608:CHL:O1D	2.44	0.51
19:N:99:GLU:OE2	19:N:220:ARG:NE	2.33	0.51
22:R:312:CLA:C4B	20:4:173:GLU:CG	159.69	0.51
19:7:176:ARG:NH1	25:7:308:CHL:O1D	2.44	0.51
4:D:97:GLU:OE2	5:E:69:ARG:NH2	2.70	0.51
6:F:24:THR:O	6:F:28:LEU:HB2	2.11	0.51
17:R:265:LYS:HB3	17:R:269:ASN:HB3	1.93	0.51
25:Y:601:CHL:CGA	25:Y:601:CHL:HBD	2.41	0.51
1:A:55:ALA:HB3	1:A:70:SER:HB3	1.93	0.51
19:G:50:TRP:HE1	22:G:611:CLA:HED2	1.75	0.51
22:4:303:CLA:HMD1	25:4:308:CHL:HBA2	1.92	0.51
2:B:403:GLY:H	2:B:407:ASN:HA	1.75	0.51
2:B:143:LEU:HD11	22:B:609:CLA:HBB1	2.37	0.51
3:C:164:HIS:HD2	3:C:167:LEU:HD21	1.75	0.51
10:L:10:SER:OG	11:M:32:GLN:NE2	2.38	0.51
3:C:131:TYR:HH	18:S:74:GLY:HA3	1.89	0.51
20:4:154:GLY:O	20:4:158:SER:CB	2.59	0.51
20:4:68:LEU:HB3	20:4:71:GLU:HB2	1.92	0.51
2:B:236:THR:HB	2:B:473:THR:HG21	1.93	0.51
1:A:245:THR:O	4:D:266:ARG:NH2	2.44	0.51
25:G:609:CHL:HAA1	19:N:82:THR:HG21	1.93	0.51
17:R:58:TRP:C	20:8:173:GLU:CG	2.77	0.51
17:R:278:PRO:N	20:4:140:PHE:HE1	173.28	0.50
20:4:252:PRO:O	20:4:256:LEU:CB	2.59	0.50
20:8:119:GLY:O	20:8:123:SER:CB	2.59	0.50
20:8:154:GLY:O	20:8:158:SER:CB	2.59	0.50
1:A:276:ALA:HA	4:D:213:ALA:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:146:TYR:HD2	19:Y:152:LEU:HD13	1.76	0.50
19:2:95:ASN:HA	19:2:98:LEU:HD12	1.94	0.50
17:R:288:SER:OG	20:4:142:PHE:CD2	158.82	0.50
19:5:98:LEU:O	19:5:102:HIS:ND1	2.42	0.50
2:B:222:PRO:HG3	7:H:38:GLY:HA3	1.93	0.50
19:1:95:ASN:HA	19:1:98:LEU:HD12	1.94	0.50
17:R:278:PRO:CA	20:8:140:PHE:HE1	2.02	0.50
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.94	0.50
4:D:168:TRP:O	4:D:171:ALA:HB3	2.11	0.50
4:D:185:PHE:O	4:D:189:PHE:HB2	2.12	0.50
4:D:34:SER:O	4:D:38:LEU:CB	2.60	0.50
12:O:291:LYS:HB2	12:O:300:ILE:HG22	1.94	0.50
17:R:275:LEU:HB3	22:2:613:CLA:HMB2	173.30	0.50
2:B:151:PHE:O	2:B:155:ALA:HB3	2.12	0.50
19:6:174:GLY:O	19:6:178:ALA:HB3	2.12	0.50
22:8:303:CLA:HMD1	25:8:308:CHL:HBA2	1.92	0.50
2:B:392:VAL:HG13	2:B:397:VAL:HB	1.94	0.50
3:C:182:PHE:CZ	18:S:261:PRO:HD2	3.04	0.50
17:R:278:PRO:N	20:8:140:PHE:HE1	2.09	0.50
2:B:139:PHE:O	2:B:143:LEU:HB2	2.12	0.50
2:B:379:ALA:HB2	2:B:395:VAL:HG11	1.94	0.50
2:B:205:ALA:HA	22:B:602:CLA:HBC2	1.97	0.50
20:8:118:VAL:HG11	22:8:304:CLA:HAC2	1.94	0.50
19:G:146:TYR:HD2	19:G:152:LEU:HD13	1.76	0.50
19:G:160:ALA:O	19:G:164:THR:OG1	2.27	0.50
17:R:256:PHE:O	17:R:260:ALA:CB	2.60	0.50
19:1:174:GLY:O	19:1:178:ALA:HB3	2.12	0.50
20:4:118:VAL:HG11	22:4:304:CLA:HAC2	1.94	0.50
2:B:7:ARG:HG2	22:B:611:CLA:HED2	1.93	0.50
3:C:182:PHE:CE1	18:S:262:PHE:CD2	3.45	0.50
2:B:122:ILE:HD11	7:H:20:GLY:HA2	1.93	0.50
12:O:130:LYS:HG2	12:O:179:GLU:HG2	1.94	0.50
17:R:144:GLY:HA3	17:R:246:ALA:HB1	1.93	0.50
22:R:312:CLA:O1A	20:4:162:VAL:HG11	154.19	0.50
19:1:98:LEU:O	19:1:102:HIS:ND1	2.42	0.50
20:4:157:GLU:OE1	20:4:160:ARG:NH2	2.36	0.50
20:4:242:PHE:O	20:4:246:ALA:CB	2.60	0.50
20:8:242:PHE:O	20:8:246:ALA:CB	2.60	0.50
2:B:8:VAL:HB	22:B:614:CLA:HED1	3.13	0.50
3:C:444:HIS:HE1	22:C:508:CLA:NA	2.15	0.50
4:D:303:GLU:O	4:D:307:ALA:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:PHE:HB2	3:C:41:ARG:HE	1.77	0.49
17:R:279:LEU:HB3	20:4:140:PHE:N	175.44	0.49
1:A:240:GLY:HA2	13:T:29:ILE:HB	1.94	0.49
19:2:174:GLY:O	19:2:178:ALA:HB3	2.12	0.49
19:2:94:ARG:NH1	19:3:81:ASP:O	2.45	0.49
17:R:284:ILE:CG1	20:8:146:LEU:H	2.21	0.49
1:A:334:ARG:HH22	4:D:321:LEU:HD13	1.76	0.49
19:N:146:TYR:HD2	19:N:152:LEU:HD13	1.76	0.49
25:N:601:CHL:HBD	25:N:601:CHL:O1A	2.13	0.49
19:Y:157:SER:N	25:Y:605:CHL:OMC	2.36	0.49
17:R:62:ALA:CA	20:4:172:VAL:CG2	154.59	0.49
19:5:174:GLY:O	19:5:178:ALA:HB3	2.12	0.49
19:7:174:GLY:O	19:7:178:ALA:HB3	2.12	0.49
20:8:252:PRO:O	20:8:256:LEU:CB	2.59	0.49
2:B:372:ASP:OD1	2:B:376:ILE:N	2.46	0.49
22:R:312:CLA:O1A	20:8:162:VAL:HG11	2.12	0.49
19:6:95:ASN:HA	19:6:98:LEU:HD12	1.94	0.49
2:B:3:LEU:H	10:L:12:GLU:H	1.59	0.49
4:D:45:ALA:HA	4:D:115:VAL:HG22	1.95	0.49
24:E:101:HEM:HHC	24:E:101:HEM:HBB2	2.01	0.49
17:R:267:PRO:O	17:R:271:TRP:HB2	2.12	0.49
18:S:146:VAL:HG23	18:S:149:LYS:HB2	1.94	0.49
17:R:287:PHE:CE2	20:4:146:LEU:HD23	153.19	0.49
3:C:39:ASN:HD21	22:C:511:CLA:C1C	2.30	0.49
18:S:69:ILE:HG21	18:S:76:LEU:HD21	1.95	0.49
19:3:174:GLY:O	19:3:178:ALA:HB3	2.12	0.49
19:3:95:ASN:HA	19:3:98:LEU:HD12	1.94	0.49
5:E:72:SER:O	5:E:76:LEU:CB	2.58	0.49
19:N:75:PRO:HB3	19:N:213:VAL:HG22	1.95	0.49
12:O:302:VAL:HG22	12:O:326:VAL:HG12	1.94	0.49
25:Y:601:CHL:O1A	25:Y:601:CHL:HBD	2.13	0.49
19:2:50:TRP:HE1	22:2:610:CLA:HED2	1.77	0.49
1:A:272:HIS:HA	1:A:275:LEU:HD12	1.95	0.49
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.94	0.49
2:B:3:LEU:HB2	10:L:11:VAL:HG22	1.93	0.49
10:L:16:THR:O	10:L:20:TRP:CB	2.60	0.49
3:C:112:PHE:HZ	16:Z:58:ASN:HD21	1.60	0.49
22:1:613:CLA:HMB2	22:1:614:CLA:HAC2	1.95	0.49
19:7:98:LEU:O	19:7:102:HIS:ND1	2.42	0.49
20:8:103:LEU:HD13	20:8:193:GLY:HA3	1.95	0.49
2:B:187:VAL:HG12	22:B:601:CLA:HBC3	2.03	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:LYS:HG2	3:C:182:PHE:HB2	1.94	0.49
17:R:146:TRP:CD1	22:R:307:CLA:HMD3	2.48	0.49
17:R:279:LEU:HB3	20:8:140:PHE:N	2.27	0.49
14:W:111:LEU:O	14:W:114:THR:OG1	2.26	0.49
19:Y:176:ARG:NH1	25:Y:608:CHL:O1D	2.46	0.49
19:Y:75:PRO:HB3	19:Y:213:VAL:HG22	1.95	0.49
22:5:613:CLA:HMB2	22:5:614:CLA:HAC2	1.95	0.49
19:5:95:ASN:HA	19:5:98:LEU:HD12	1.94	0.49
3:C:92:LEU:HD21	22:C:502:CLA:H2A	1.93	0.49
17:R:287:PHE:CE2	20:8:146:LEU:HD23	2.48	0.49
17:R:58:TRP:C	20:4:173:GLU:CG	155.88	0.49
19:3:98:LEU:O	19:3:102:HIS:ND1	2.42	0.49
2:B:257:TRP:HB2	2:B:452:THR:HG21	1.95	0.49
3:C:356:MET:O	3:C:359:TRP:HB3	2.13	0.49
6:F:12:VAL:O	6:F:16:ALA:HB2	2.13	0.49
12:O:305:SER:N	12:O:323:ILE:O	2.46	0.49
19:6:50:TRP:HE1	22:6:610:CLA:HED2	1.77	0.48
19:7:95:ASN:HA	19:7:98:LEU:HD12	1.94	0.48
20:8:119:GLY:O	20:8:123:SER:OG	2.30	0.48
19:G:75:PRO:HB3	19:G:213:VAL:HG22	1.95	0.48
19:6:94:ARG:NH1	19:7:81:ASP:O	2.45	0.48
3:C:189:TRP:HZ3	3:C:367:GLU:HG3	1.78	0.48
19:N:91:THR:OG1	19:Y:84:GLY:O	2.27	0.48
16:Z:40:VAL:O	16:Z:44:THR:CB	2.61	0.48
22:A:405:CLA:HBA1	22:A:405:CLA:H3A	1.51	0.48
2:B:216:HIS:HE1	22:B:609:CLA:C1A	2.26	0.48
25:1:609:CHL:HAA1	19:2:82:THR:HG21	1.95	0.48
19:5:192:PRO:HG3	25:5:608:CHL:HMD2	1.95	0.48
3:C:182:PHE:CZ	18:S:261:PRO:CD	3.09	0.48
16:Z:24:PRO:O	16:Z:28:ALA:CB	2.62	0.48
22:8:309:CLA:HED2	22:8:309:CLA:HAA1	1.95	0.48
3:C:182:PHE:HE1	18:S:261:PRO:HD2	1.50	0.48
2:B:282:GLN:O	2:B:286:ARG:CB	2.61	0.48
2:B:384:ARG:HG2	2:B:386:ALA:H	1.79	0.48
3:C:447:ARG:HD3	22:C:508:CLA:HED3	1.96	0.48
12:O:142:SER:HB2	12:O:324:GLN:HB3	1.95	0.48
18:S:74:GLY:HA3	22:S:301:CLA:HED2	3.62	0.48
2:B:190:PHE:HB3	7:H:60:ILE:HG21	1.96	0.48
4:D:18:ILE:O	4:D:22:TRP:CB	2.62	0.48
19:1:247:HIS:NE2	22:1:614:CLA:ND	2.61	0.48
22:S:303:CLA:HBA2	22:S:303:CLA:H3A	1.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5:609:CHL:HAA1	19:6:82:THR:HG21	1.95	0.48
19:6:98:LEU:O	19:6:102:HIS:ND1	2.42	0.48
3:C:39:ASN:ND2	22:C:508:CLA:O2A	2.39	0.48
4:D:187:GLN:HB2	22:D:403:CLA:HBC1	1.96	0.48
17:R:145:ARG:NH2	17:R:216:LEU:O	2.47	0.48
17:R:269:ASN:O	17:R:273:THR:OG1	2.25	0.48
3:C:187:ASP:O	3:C:194:GLY:CA	2.62	0.48
3:C:38:GLY:HA3	22:C:511:CLA:HMD3	1.95	0.48
4:D:187:GLN:OE1	4:D:193:THR:N	2.45	0.48
5:E:76:LEU:O	5:E:80:SER:HB2	2.14	0.48
19:Y:247:HIS:HB2	22:Y:613:CLA:HAA2	1.96	0.48
2:B:197:GLY:O	2:B:201:HIS:HB2	2.14	0.47
2:B:9:HIS:CE1	22:B:614:CLA:NC	2.82	0.47
3:C:60:ILE:HG23	22:C:510:CLA:HMC2	1.96	0.47
12:O:305:SER:HB3	12:O:323:ILE:HB	1.96	0.47
17:R:278:PRO:HD3	22:6:613:CLA:CBB	2.39	0.47
20:4:103:LEU:HD13	20:4:193:GLY:HA3	1.95	0.47
23:A:404:PHO:H2A	23:A:404:PHO:HED2	1.99	0.47
5:E:69:ARG:NH2	7:H:63:SER:O	4.31	0.47
19:5:247:HIS:NE2	22:5:614:CLA:ND	2.61	0.47
3:C:132:HIS:HE1	22:S:301:CLA:NA	2.26	0.47
19:1:144:LEU:HB3	19:1:155:ALA:HB3	1.97	0.47
19:3:144:LEU:HB3	19:3:155:ALA:HB3	1.97	0.47
19:6:80:TRP:NE1	25:6:601:CHL:O2A	2.47	0.47
19:6:69:TYR:OH	19:6:81:ASP:OD2	2.26	0.47
19:N:98:LEU:HD23	25:N:609:CHL:HED3	1.97	0.47
12:O:94:TYR:CZ	12:O:135:LYS:HE3	2.50	0.47
19:2:80:TRP:NE1	25:2:601:CHL:O2A	2.47	0.47
19:7:144:LEU:HB3	19:7:155:ALA:HB3	1.97	0.47
4:D:86:LEU:HD13	4:D:91:LEU:HD11	1.96	0.47
19:G:158:ILE:HA	19:G:161:ILE:HD12	1.97	0.47
3:C:66:ALA:HB1	9:K:40:MET:HG3	1.95	0.47
19:N:158:ILE:HA	19:N:161:ILE:HD12	1.97	0.47
17:R:68:LEU:HD13	17:R:77:GLY:HA2	1.97	0.47
19:1:192:PRO:HG3	25:1:608:CHL:HMD2	1.95	0.47
22:4:309:CLA:HAA1	22:4:309:CLA:HED2	1.95	0.47
1:A:92:HIS:CE1	3:C:220:GLY:HA3	2.74	0.47
3:C:464:GLU:OE2	4:D:249:THR:OG1	2.33	0.47
24:E:101:HEM:HBC2	24:E:101:HEM:HHD	1.97	0.47
12:O:146:LYS:HE3	12:O:157:GLU:HA	1.97	0.47
19:5:161:ILE:HG12	25:5:605:CHL:HAC1	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:6:176:ARG:HH22	25:6:607:CHL:HED2	1.80	0.47
1:A:317:TRP:CE3	4:D:181:ARG:HD3	2.63	0.47
12:O:304:GLU:HG2	12:O:324:GLN:HG3	1.96	0.47
22:Y:613:CLA:HMB2	22:Y:614:CLA:HAC2	1.97	0.47
16:Z:37:LYS:HD2	18:S:75:LEU:O	2.22	0.47
20:8:146:LEU:HD13	25:8:306:CHL:HAC2	1.97	0.47
20:8:194:TYR:CZ	20:8:225:LYS:HG2	2.50	0.47
2:B:151:PHE:O	2:B:155:ALA:CB	2.63	0.47
2:B:381:VAL:HG13	2:B:418:LYS:HD3	1.97	0.47
3:C:48:LYS:HA	3:C:133:ALA:HA	1.96	0.47
3:C:447:ARG:O	3:C:451:ALA:CB	2.63	0.47
3:C:164:HIS:ND1	22:C:507:CLA:OBD	2.48	0.47
8:I:5:LYS:NZ	8:I:9:TYR:OH	2.46	0.47
18:S:120:TRP:HH2	18:S:182:LEU:HD11	1.80	0.47
19:Y:158:ILE:HA	19:Y:161:ILE:HD12	1.97	0.47
17:R:288:SER:OG	20:8:142:PHE:CD2	2.44	0.47
15:X:80:SER:HB3	15:X:83:LEU:HG	1.97	0.47
2:B:5:TRP:HD1	10:L:13:LEU:HD11	1.79	0.47
22:C:509:CLA:HMB1	22:C:511:CLA:HBB1	2.03	0.47
18:S:221:LEU:HD23	18:S:224:LYS:HD2	1.97	0.47
18:S:241:ILE:HG21	22:S:313:CLA:HAC2	1.96	0.47
3:C:312:ALA:HB1	3:C:392:SER:HA	1.97	0.46
19:1:105:TRP:CD1	25:1:609:CHL:HMD3	2.50	0.46
19:2:144:LEU:HB3	19:2:155:ALA:HB3	1.97	0.46
20:4:146:LEU:HD13	25:4:306:CHL:HAC2	1.97	0.46
19:5:105:TRP:CD1	25:5:609:CHL:HMD3	2.50	0.46
2:B:315:ILE:HG21	2:B:426:LEU:HD22	1.97	0.46
2:B:384:ARG:HE	4:D:345:GLU:HA	1.80	0.46
3:C:260:ALA:HA	3:C:264:LEU:HD13	1.97	0.46
3:C:294:ASN:HD21	3:C:362:ARG:HB2	1.80	0.46
3:C:430:HIS:CE1	22:C:501:CLA:NA	2.82	0.46
19:G:109:GLY:O	19:G:113:CYS:HB2	2.14	0.46
19:G:176:ARG:HH22	25:G:608:CHL:HED2	1.80	0.46
19:N:109:GLY:O	19:N:113:CYS:HB2	2.15	0.46
19:Y:109:GLY:O	19:Y:113:CYS:HB2	2.15	0.46
20:4:194:TYR:CZ	20:4:225:LYS:HG2	2.50	0.46
2:B:347:ARG:HG2	2:B:353:GLU:HA	1.98	0.46
3:C:294:ASN:ND2	3:C:362:ARG:O	2.49	0.46
4:D:156:SER:HA	4:D:160:ILE:HD12	1.98	0.46
4:D:178:ALA:O	4:D:182:PHE:CB	2.61	0.46
4:D:91:LEU:O	4:D:105:TRP:NE1	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:95:ASN:HB3	22:Y:602:CLA:HBB	1.98	0.46
19:2:176:ARG:HH22	25:2:607:CHL:HED2	1.80	0.46
20:8:157:GLU:OE1	20:8:160:ARG:NH2	2.36	0.46
2:B:238:LEU:HD11	22:B:611:CLA:HMB3	1.98	0.46
2:B:150:CYS:HB2	22:B:603:CLA:HMC3	1.97	0.46
3:C:206:PRO:HG3	22:Y:614:CLA:CBB	2.08	0.46
7:H:59:GLU:HG2	15:X:86:PHE:HZ	1.79	0.46
17:R:172:GLU:OE2	17:R:178:SER:N	2.49	0.46
17:R:63:ILE:HG13	20:8:166:ASN:HD21	1.81	0.46
25:6:606:CHL:HBA2	25:6:606:CHL:H3A	1.81	0.46
1:A:272:HIS:HD2	4:D:215:HIS:CD2	2.33	0.46
14:W:117:PHE:O	14:W:121:SER:CB	2.63	0.46
19:7:255:ASN:HA	22:7:313:CLA:HAA1	1.98	0.46
1:A:288:LEU:HD13	3:C:432:VAL:HG13	2.33	0.46
3:C:71:GLU:HG2	3:C:86:LEU:HD22	1.98	0.46
17:R:168:ALA:HB1	22:R:303:CLA:HED1	1.97	0.46
19:6:144:LEU:HB3	19:6:155:ALA:HB3	1.97	0.46
1:A:308:ASP:HB3	1:A:314:ILE:HD11	1.98	0.46
22:Y:611:CLA:HBA2	22:Y:611:CLA:H3A	1.75	0.46
19:1:161:ILE:HG12	25:1:605:CHL:HAC1	1.97	0.46
19:3:104:ARG:NH1	25:3:308:CHL:OBD	2.44	0.46
3:C:276:LEU:O	3:C:280:SER:HB2	2.16	0.46
17:R:135:ARG:NH1	22:R:302:CLA:O1A	2.49	0.46
18:S:266:LEU:HD13	22:S:313:CLA:HMD1	1.98	0.46
19:5:144:LEU:HB3	19:5:155:ALA:HB3	1.97	0.46
1:A:216:GLY:O	1:A:220:THR:CB	2.64	0.46
4:D:331:ALA:HA	4:D:334:ASP:HB3	1.98	0.46
6:F:23:PRO:O	6:F:27:PHE:HB2	2.16	0.46
19:G:172:VAL:HG12	25:G:608:CHL:HMB3	1.98	0.46
19:N:144:LEU:HB3	19:N:155:ALA:HB3	1.98	0.46
17:R:236:ALA:O	17:R:240:LEU:CB	2.64	0.46
14:W:119:TYR:O	14:W:122:SER:OG	2.27	0.46
15:X:85:ASN:O	15:X:89:SER:OG	2.25	0.46
3:C:159:THR:HG23	3:C:252:ILE:HG23	1.98	0.45
5:E:76:LEU:O	5:E:80:SER:CB	2.64	0.45
12:O:146:LYS:HB2	12:O:158:PHE:HB3	1.98	0.45
17:R:267:PRO:O	17:R:271:TRP:HB3	2.16	0.45
18:S:103:LYS:HD3	18:S:106:ASN:HD22	1.81	0.45
18:S:169:ILE:HD13	18:S:173:LEU:HB3	1.98	0.45
16:Z:42:SER:O	16:Z:46:LEU:CB	2.63	0.45
17:R:275:LEU:O	22:6:613:CLA:CBB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:8:119:GLY:O	20:8:123:SER:HB3	2.16	0.45
2:B:393:GLU:HG3	2:B:414:PRO:HG2	1.98	0.45
4:D:193:THR:HG23	22:D:403:CLA:HBC2	2.03	0.45
22:G:613:CLA:HMB2	22:G:614:CLA:HAC2	1.99	0.45
19:2:218:ASN:OD1	22:2:611:CLA:NB	2.49	0.45
19:3:177:VAL:HG21	25:3:309:CHL:HMA3	1.98	0.45
17:R:278:PRO:HG2	22:6:613:CLA:HBB2	1.90	0.45
17:R:59:TYR:N	20:8:173:GLU:CA	2.79	0.45
3:C:233:ILE:HA	3:C:233:ILE:HD13	1.82	0.45
19:N:229:PHE:O	19:N:233:ALA:HB3	2.17	0.45
12:O:130:LYS:HA	12:O:179:GLU:HA	1.98	0.45
19:Y:144:LEU:HB3	19:Y:155:ALA:HB3	1.98	0.45
19:6:218:ASN:OD1	22:6:611:CLA:NB	2.49	0.45
17:R:278:PRO:HG3	22:6:613:CLA:HBB2	1.94	0.45
20:8:154:GLY:O	20:8:158:SER:HB2	2.16	0.45
1:A:103:ASP:O	1:A:107:TYR:CB	2.65	0.45
2:B:272:ARG:HH12	4:D:293:ASN:ND2	2.56	0.45
2:B:64:PRO:O	2:B:68:ARG:CB	2.58	0.45
4:D:254:TRP:O	4:D:259:GLY:N	2.45	0.45
16:Z:40:VAL:O	16:Z:44:THR:OG1	2.29	0.45
17:R:63:ILE:HG13	20:4:166:ASN:HD21	150.34	0.45
3:C:470:THR:O	4:D:252:ARG:NH1	2.49	0.45
19:N:153:VAL:HA	25:N:605:CHL:C4D	2.47	0.45
17:R:278:PRO:CA	20:4:140:PHE:HE1	172.71	0.45
19:3:255:ASN:HA	22:3:313:CLA:HAA1	1.98	0.45
3:C:314:ALA:HA	3:C:317:PHE:HD2	1.81	0.45
19:G:144:LEU:HB3	19:G:155:ALA:HB3	1.98	0.45
19:Y:248:LEU:HD21	22:Y:614:CLA:HMC3	1.98	0.45
20:4:101:ALA:O	20:4:105:HIS:ND1	2.38	0.45
20:4:119:GLY:O	20:4:123:SER:HB3	2.16	0.45
20:4:185:PHE:HA	20:4:190:GLY:HA2	1.98	0.45
19:5:176:ARG:HH22	25:5:608:CHL:HED2	1.81	0.45
25:5:606:CHL:H3A	25:5:606:CHL:HBA2	1.83	0.45
20:8:154:GLY:O	20:8:158:SER:OG	2.30	0.45
20:8:185:PHE:HA	20:8:190:GLY:HA2	1.98	0.45
1:A:59:ASP:OD2	1:A:63:ILE:N	2.50	0.45
2:B:455:HIS:CD2	22:B:604:CLA:NC	3.14	0.45
3:C:86:LEU:HD13	3:C:89:LEU:HD12	1.99	0.45
25:2:606:CHL:H3A	25:2:606:CHL:HBA2	1.81	0.45
20:4:119:GLY:O	20:4:123:SER:OG	2.30	0.45
1:A:97:TRP:CG	8:I:5:LYS:HD2	3.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:90:LEU:HG	7:H:62:ASN:HD21	2.87	0.45
8:I:15:PHE:O	8:I:19:PHE:HB2	2.17	0.45
8:I:3:THR:HA	8:I:6:LEU:HD12	1.99	0.45
17:R:206:ARG:HA	25:R:306:CHL:HBC3	1.98	0.45
19:1:174:GLY:O	19:1:178:ALA:CB	2.65	0.45
19:2:255:ASN:HA	22:2:612:CLA:HAA1	1.99	0.45
19:7:177:VAL:HG21	25:7:309:CHL:HMA3	1.98	0.45
22:B:609:CLA:HMD1	7:H:39:THR:HB	1.98	0.45
12:O:131:TYR:HB2	12:O:178:PHE:HB3	1.99	0.45
17:R:146:TRP:CD2	22:R:307:CLA:HAC2	2.52	0.45
1:A:40:THR:O	1:A:44:ALA:HB3	2.17	0.45
2:B:194:VAL:HG12	2:B:196:GLY:H	1.82	0.45
2:B:214:LEU:HD13	22:R:302:CLA:O2D	107.60	0.45
19:G:229:PHE:O	19:G:233:ALA:HB3	2.17	0.45
18:S:74:GLY:CA	22:S:301:CLA:OBD	2.64	0.45
19:6:160:ALA:O	19:6:164:THR:OG1	2.32	0.44
19:6:174:GLY:O	19:6:178:ALA:CB	2.65	0.44
20:8:221:LEU:HG	20:8:225:LYS:HE3	1.99	0.44
2:B:299:SER:O	2:B:303:ALA:CB	2.66	0.44
22:B:602:CLA:H2A	22:B:602:CLA:HED3	2.35	0.44
19:G:98:LEU:HD23	25:G:609:CHL:HED3	1.99	0.44
19:N:160:ALA:O	19:N:164:THR:OG1	2.27	0.44
19:7:69:TYR:OH	19:7:81:ASP:OD2	2.26	0.44
20:8:144:SER:O	25:8:301:CHL:HED3	2.16	0.44
2:B:255:THR:HG21	22:B:602:CLA:HED1	1.99	0.44
3:C:199:ILE:HD11	3:C:230:LEU:HB2	2.00	0.44
22:A:403:CLA:HED2	4:D:176:VAL:HG13	1.99	0.44
4:D:303:GLU:O	4:D:307:ALA:CB	2.66	0.44
1:A:334:ARG:HH12	4:D:321:LEU:HD13	1.81	0.44
19:G:214:LYS:HD3	22:G:612:CLA:HAA2	1.99	0.44
19:G:218:ASN:OD1	22:G:612:CLA:NB	2.51	0.44
19:Y:229:PHE:O	19:Y:233:ALA:HB3	2.17	0.44
17:R:182:GLN:NE2	25:Y:605:CHL:HHB	2.33	0.44
19:3:105:TRP:CD1	25:3:309:CHL:HMD3	2.52	0.44
19:3:174:GLY:O	19:3:178:ALA:CB	2.65	0.44
22:R:312:CLA:CAB	20:8:173:GLU:O	2.64	0.44
3:C:69:LEU:HA	3:C:72:VAL:HG12	1.99	0.44
3:C:343:ARG:NE	12:O:170:THR:O	2.49	0.44
17:R:59:TYR:N	20:4:173:GLU:CA	156.63	0.44
19:5:174:GLY:O	19:5:178:ALA:CB	2.65	0.44
19:7:174:GLY:O	19:7:178:ALA:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:7:104:ARG:NH1	25:7:308:CHL:OBD	2.44	0.44
3:C:261:ARG:HA	3:C:266:TRP:HE1	1.82	0.44
1:A:309:SER:H	5:E:55:TYR:HD2	1.66	0.44
17:R:62:ALA:HB2	20:4:172:VAL:CB	156.54	0.44
19:1:176:ARG:HH22	25:1:608:CHL:HED2	1.81	0.44
20:4:154:GLY:O	20:4:158:SER:HB2	2.16	0.44
19:6:255:ASN:HA	22:6:612:CLA:HAA1	1.99	0.44
19:6:75:PRO:HB2	19:6:216:LEU:HD12	2.00	0.44
19:7:105:TRP:CD1	25:7:309:CHL:HMD3	2.52	0.44
2:B:413:ASP:OD1	2:B:413:ASP:N	2.51	0.44
2:B:197:GLY:HA2	22:B:602:CLA:HMB3	2.00	0.44
19:N:100:VAL:HG22	19:N:216:LEU:HD21	2.00	0.44
17:R:275:LEU:O	22:2:613:CLA:CBB	175.56	0.44
19:Y:100:VAL:HG22	19:Y:216:LEU:HD21	2.00	0.44
1:A:115:ILE:O	1:A:119:PHE:HB2	2.18	0.44
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.00	0.44
2:B:357:ARG:NH1	2:B:358:ARG:O	2.51	0.44
22:B:612:CLA:HMB3	22:B:613:CLA:HAA2	2.00	0.44
22:G:602:CLA:HBA2	22:G:602:CLA:H3A	1.80	0.44
19:Y:99:GLU:HG3	19:Y:223:MET:HE1	2.01	0.44
19:6:173:GLU:HA	19:6:176:ARG:HG2	2.00	0.44
2:B:281:GLN:O	2:B:285:TYR:CB	2.66	0.44
2:B:462:PHE:HE2	22:B:604:CLA:HAC2	1.91	0.44
3:C:309:ALA:O	3:C:313:GLN:HB2	2.18	0.44
19:G:100:VAL:HG22	19:G:216:LEU:HD21	1.99	0.44
22:N:610:CLA:HBA2	22:N:610:CLA:H3A	1.84	0.44
18:S:74:GLY:HA3	22:S:301:CLA:OBD	2.18	0.44
2:B:201:HIS:HE1	22:B:602:CLA:ND	2.15	0.44
4:D:208:ALA:HB2	4:D:276:PRO:HB3	1.99	0.44
9:K:35:PRO:O	9:K:38:ASP:HB2	2.18	0.44
18:S:260:ASP:HB3	18:S:263:GLY:HA3	2.00	0.44
19:Y:160:ALA:O	19:Y:164:THR:CB	2.66	0.44
20:8:73:LEU:HD21	22:8:302:CLA:HAA1	2.00	0.44
6:F:12:VAL:O	6:F:16:ALA:CB	2.66	0.44
19:G:160:ALA:O	19:G:164:THR:CB	2.66	0.44
19:N:160:ALA:O	19:N:164:THR:CB	2.66	0.44
4:D:251:ASN:HD21	13:T:27:PRO:HB2	1.83	0.44
19:2:174:GLY:O	19:2:178:ALA:CB	2.65	0.43
2:B:155:ALA:O	2:B:159:THR:OG1	2.32	0.43
2:B:257:TRP:NE1	4:D:164:GLY:O	2.52	0.43
25:G:606:CHL:HBA2	25:G:606:CHL:H3A	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:194:ILE:HG13	12:O:194:ILE:H	1.52	0.43
16:Z:24:PRO:O	16:Z:28:ALA:HB3	2.18	0.43
19:1:75:PRO:HB2	19:1:216:LEU:HD12	2.00	0.43
19:2:75:PRO:HB2	19:2:216:LEU:HD12	2.00	0.43
22:6:602:CLA:H3A	22:6:602:CLA:HBA2	1.69	0.43
19:7:173:GLU:HA	19:7:176:ARG:HG2	2.00	0.43
17:R:285:ASP:H	20:8:141:SER:HB3	1.81	0.43
4:D:266:ARG:O	4:D:270:PHE:HB2	2.19	0.43
4:D:58:SER:O	4:D:63:GLY:N	2.51	0.43
19:G:105:TRP:CD1	25:G:609:CHL:HMD3	2.53	0.43
19:N:99:GLU:HG3	19:N:223:MET:HE1	2.00	0.43
19:Y:170:GLY:N	25:Y:609:CHL:HAB	2.33	0.43
19:1:173:GLU:HA	19:1:176:ARG:HG2	2.00	0.43
19:5:173:GLU:HA	19:5:176:ARG:HG2	2.00	0.43
19:7:75:PRO:HB2	19:7:216:LEU:HD12	2.00	0.43
2:B:85:ILE:HD11	12:O:204:PRO:HD3	67.63	0.43
1:A:213:ALA:HB1	4:D:146:ALA:HB1	1.98	0.43
12:O:185:SER:HA	12:O:223:LYS:HA	2.00	0.43
17:R:240:LEU:HA	17:R:243:ILE:HG22	2.01	0.43
3:C:182:PHE:CD1	18:S:261:PRO:HD2	2.48	0.43
20:4:221:LEU:HG	20:4:225:LYS:HE3	1.99	0.43
2:B:109:LEU:HA	2:B:112:ILE:HD12	2.00	0.43
19:G:99:GLU:HG3	19:G:223:MET:HE1	2.00	0.43
25:N:606:CHL:HBA2	25:N:606:CHL:H3A	1.83	0.43
19:1:218:ASN:OD1	22:1:612:CLA:NB	2.51	0.43
19:2:173:GLU:HA	19:2:176:ARG:HG2	2.00	0.43
22:2:609:CLA:HBA2	22:2:609:CLA:H3A	1.82	0.43
19:3:173:GLU:HA	19:3:176:ARG:HG2	2.00	0.43
2:B:141:ILE:HG13	2:B:217:LEU:HD21	2.01	0.43
3:C:186:TYR:HA	3:C:196:VAL:HA	2.01	0.43
17:R:241:ALA:O	17:R:245:HIS:ND1	2.48	0.43
17:R:62:ALA:HA	20:4:172:VAL:HG21	153.56	0.43
25:1:601:CHL:HAA1	25:3:309:CHL:HMB2	2.00	0.43
25:5:601:CHL:HAA1	25:7:309:CHL:HMB2	2.00	0.43
1:A:269:ARG:NH1	4:D:235:ALA:O	2.86	0.43
1:A:77:ILE:HB	10:L:34:ASN:HD21	1.83	0.43
18:S:110:TYR:HA	18:S:113:PHE:HD2	1.83	0.43
19:5:75:PRO:HB2	19:5:216:LEU:HD12	2.00	0.43
1:A:216:GLY:O	1:A:220:THR:OG1	2.31	0.43
18:S:114:GLU:O	18:S:118:ALA:CB	2.66	0.43
19:3:50:TRP:HE1	22:3:311:CLA:HED2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:218:ASN:OD1	22:5:612:CLA:NB	2.51	0.43
17:R:284:ILE:CG2	20:8:141:SER:O	2.67	0.43
3:C:430:HIS:CD2	22:C:501:CLA:NC	2.87	0.43
2:B:384:ARG:HH22	4:D:349:ARG:NE	2.16	0.43
18:S:114:GLU:O	18:S:118:ALA:HB2	2.19	0.43
18:S:239:PHE:O	18:S:243:ALA:HB3	2.19	0.43
19:6:176:ARG:NH1	25:6:607:CHL:O1D	2.52	0.43
1:A:133:LEU:HD12	1:A:136:ARG:HB2	2.01	0.43
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.53	0.43
5:E:23:HIS:CD2	24:E:101:HEM:NC	2.87	0.43
22:R:312:CLA:CAB	20:4:173:GLU:O	164.85	0.43
1:A:56:PRO:HA	1:A:73:TYR:HE2	1.84	0.43
1:A:91:LEU:HD11	1:A:163:ILE:HA	2.01	0.43
10:L:18:LEU:HD22	11:M:26:TYR:CD1	2.53	0.43
12:O:162:LYS:HE2	12:O:202:GLN:HB3	2.01	0.43
22:Y:610:CLA:H3A	22:Y:610:CLA:HBA2	1.81	0.43
17:R:62:ALA:HA	20:4:172:VAL:HB	154.10	0.42
19:6:216:LEU:HD23	19:6:216:LEU:HA	1.87	0.42
20:8:101:ALA:O	20:8:105:HIS:ND1	2.38	0.42
19:G:104:ARG:NH1	25:G:608:CHL:OBD	2.51	0.42
17:R:284:ILE:CG2	20:4:141:SER:O	164.52	0.42
18:S:73:ASP:HB2	22:S:301:CLA:CBF	2.45	0.42
19:2:176:ARG:NH1	25:2:607:CHL:O1D	2.52	0.42
19:7:50:TRP:HE1	22:7:311:CLA:HED2	1.84	0.42
20:8:152:LEU:HA	20:8:155:TRP:HD1	1.85	0.42
17:R:62:ALA:HB1	20:8:172:VAL:HG23	1.64	0.42
1:A:304:GLN:HA	1:A:313:VAL:HG11	2.02	0.42
2:B:201:HIS:HE2	22:B:603:CLA:C1B	2.52	0.42
3:C:154:ARG:HB3	3:C:256:PRO:HG2	2.00	0.42
3:C:308:GLU:O	3:C:312:ALA:CB	2.67	0.42
4:D:52:GLY:HA2	4:D:56:VAL:HB	2.01	0.42
6:F:11:THR:OG1	6:F:12:VAL:N	2.51	0.42
17:R:278:PRO:HD3	22:2:613:CLA:CBB	176.04	0.42
22:S:303:CLA:HBB2	22:S:304:CLA:HHB	2.01	0.42
16:Z:15:THR:HA	16:Z:18:ILE:HD12	2.01	0.42
19:1:99:GLU:HG3	19:1:223:MET:HE1	2.00	0.42
25:6:601:CHL:HBC2	22:6:610:CLA:C4B	2.49	0.42
2:B:114:HIS:HE1	22:B:616:CLA:C1D	2.31	0.42
25:Y:606:CHL:H3A	25:Y:606:CHL:HBA2	1.66	0.42
20:4:144:SER:O	20:4:148:THR:OG1	2.30	0.42
20:4:152:LEU:HA	20:4:155:TRP:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:5:99:GLU:HG3	19:5:223:MET:HE1	2.02	0.42
19:6:130:VAL:HB	19:6:133:LYS:HB2	2.02	0.42
1:A:41:LEU:O	1:A:45:THR:OG1	2.28	0.42
20:4:73:LEU:HD21	22:4:302:CLA:HAA1	2.00	0.42
2:B:139:PHE:O	2:B:143:LEU:CB	2.68	0.42
9:K:28:GLU:O	9:K:31:ALA:HB3	2.19	0.42
18:S:120:TRP:CD1	22:S:309:CLA:HMD3	2.55	0.42
19:2:78:TYR:HH	19:2:217:LYS:NZ	2.17	0.42
19:2:105:TRP:CD1	25:2:608:CHL:HMD3	2.55	0.42
25:4:305:CHL:HMC	25:4:306:CHL:C4C	2.50	0.42
19:6:99:GLU:HG3	19:6:223:MET:HE1	2.02	0.42
17:R:62:ALA:HA	20:8:172:VAL:HB	2.01	0.42
22:A:402:CLA:HAB	22:A:402:CLA:HHC	1.85	0.42
1:A:126:TYR:OH	23:A:404:PHO:O1D	2.73	0.42
2:B:151:PHE:HB2	2:B:206:GLY:HA3	2.00	0.42
3:C:42:LEU:HD23	3:C:45:LEU:HD12	2.01	0.42
4:D:194:LEU:O	10:L:35:TYR:OH	2.26	0.42
23:D:402:PHO:H2A	23:D:402:PHO:HED2	2.19	0.42
19:N:50:TRP:HE1	22:N:611:CLA:HED2	1.84	0.42
17:R:145:ARG:HD3	22:R:308:CLA:HAC2	2.01	0.42
18:S:240:PHE:O	18:S:244:TYR:HB2	2.20	0.42
16:Z:19:LEU:HD11	16:Z:44:THR:HA	2.01	0.42
25:1:606:CHL:HBA2	25:1:606:CHL:H3A	1.83	0.42
25:2:601:CHL:HBC2	22:2:610:CLA:C4B	2.49	0.42
17:R:59:TYR:N	20:4:173:GLU:HA	155.96	0.42
20:8:202:PRO:HG2	20:8:203:LEU:HD12	2.01	0.42
20:8:224:LEU:HB3	22:8:309:CLA:HHC	2.02	0.42
1:A:217:SER:O	1:A:221:SER:OG	2.32	0.42
2:B:348:ASN:OD1	2:B:352:ARG:N	2.53	0.42
3:C:184:GLY:HA3	3:C:197:ARG:O	2.20	0.42
9:K:52:PHE:O	9:K:55:GLN:HB2	2.20	0.42
11:M:16:LEU:HD23	11:M:16:LEU:HD23	0.00	0.42
19:N:105:TRP:CD1	25:N:609:CHL:HMD3	2.55	0.42
18:S:167:ILE:HB	18:S:169:ILE:H	1.84	0.42
17:R:56:PRO:HA	20:4:174:TRP:CD1	161.20	0.42
19:7:130:VAL:HB	19:7:133:LYS:HB2	2.02	0.42
19:7:228:GLY:O	19:7:232:GLN:CB	2.65	0.42
3:C:299:SER:OG	3:C:308:GLU:OE1	2.29	0.42
5:E:28:PRO:HA	5:E:31:PHE:HB3	2.02	0.42
12:O:309:SER:N	12:O:319:LYS:O	2.49	0.42
22:R:312:CLA:HHC	20:4:174:TRP:C	163.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:602:CLA:H3A	22:2:602:CLA:HBA2	1.69	0.42
17:R:280:HIS:HA	20:4:140:PHE:CA	169.61	0.42
17:R:63:ILE:CG1	20:4:166:ASN:ND2	149.54	0.42
25:5:601:CHL:HBA1	25:5:601:CHL:HED3	2.02	0.42
1:A:140:ARG:HE	1:A:142:TRP:HZ3	1.67	0.42
2:B:252:VAL:HG12	22:B:603:CLA:CGA	2.50	0.42
19:G:247:HIS:HB2	22:G:613:CLA:HAA2	2.02	0.42
19:N:252:VAL:O	19:N:255:ASN:ND2	2.53	0.42
17:R:56:PRO:HA	20:8:174:TRP:CD1	2.55	0.42
19:Y:252:VAL:O	19:Y:255:ASN:ND2	2.53	0.42
19:2:152:LEU:HA	19:2:152:LEU:HD23	1.90	0.42
19:3:130:VAL:HB	19:3:133:LYS:HB2	2.02	0.42
19:3:75:PRO:HB2	19:3:216:LEU:HD12	2.00	0.42
19:6:228:GLY:O	19:6:232:GLN:CB	2.65	0.42
1:A:41:LEU:O	1:A:45:THR:CB	2.68	0.42
2:B:109:LEU:HD23	2:B:112:ILE:HD12	2.01	0.42
2:B:453:PHE:HB2	4:D:292:LEU:HD12	2.01	0.42
4:D:299:PHE:HD2	4:D:316:TYR:CZ	2.38	0.42
4:D:107:GLN:HE21	5:E:48:GLY:HA3	1.84	0.42
17:R:255:GLY:O	17:R:259:GLN:CB	2.57	0.42
17:R:166:GLN:HE22	17:R:267:PRO:HD3	1.84	0.42
17:R:274:HIS:CG	22:R:311:CLA:HAA2	2.55	0.42
17:R:59:TYR:N	20:8:173:GLU:HA	2.35	0.42
17:R:59:TYR:N	20:4:173:GLU:CG	156.16	0.41
20:4:202:PRO:HG2	20:4:203:LEU:HD12	2.01	0.41
2:B:187:VAL:HG13	22:B:601:CLA:HMD3	2.01	0.41
3:C:42:LEU:HB3	3:C:49:LEU:HD13	2.01	0.41
4:D:168:TRP:O	4:D:171:ALA:CB	2.69	0.41
4:D:214:ILE:O	4:D:218:THR:OG1	2.32	0.41
2:B:464:PHE:HB2	4:D:281:TRP:CZ3	3.10	0.41
4:D:58:SER:OG	4:D:80:SER:OG	2.38	0.41
22:N:602:CLA:H3A	22:N:602:CLA:HBA2	1.83	0.41
12:O:145:VAL:HG22	12:O:321:VAL:HG22	2.02	0.41
22:R:312:CLA:HBB	20:4:159:LYS:HE2	162.29	0.41
19:Y:152:LEU:HA	19:Y:152:LEU:HD23	1.86	0.41
19:Y:161:ILE:HG12	25:Y:605:CHL:HAC1	2.02	0.41
19:2:130:VAL:HB	19:2:133:LYS:HB2	2.02	0.41
19:3:99:GLU:OE2	19:3:220:ARG:NE	2.54	0.41
17:R:63:ILE:CG1	20:8:166:ASN:ND2	2.82	0.41
3:C:273:SER:HA	3:C:276:LEU:HD12	2.02	0.41
19:G:252:VAL:O	19:G:255:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:610:CLA:HBA2	22:G:610:CLA:H3A	1.79	0.41
17:R:61:GLY:CA	20:4:169:SER:CB	156.46	0.41
20:4:224:LEU:HB3	22:4:309:CLA:HBB	2.02	0.41
19:5:130:VAL:HB	19:5:133:LYS:HB2	2.02	0.41
17:R:59:TYR:N	20:8:173:GLU:CG	2.79	0.41
2:B:450:TRP:HB3	22:B:607:CLA:HMB2	2.41	0.41
4:D:107:GLN:NE2	5:E:48:GLY:HA3	2.35	0.41
18:S:141:CYS:HA	18:S:145:ALA:HB2	2.01	0.41
19:6:99:GLU:OE2	19:6:220:ARG:NE	2.54	0.41
1:A:269:ARG:O	1:A:273:PHE:HB2	2.21	0.41
1:A:59:ASP:OD2	1:A:64:ARG:N	2.53	0.41
3:C:228:ASP:HA	3:C:362:ARG:NH2	2.36	0.41
3:C:425:TRP:HB3	22:C:504:CLA:HMB2	2.02	0.41
4:D:189:PHE:HD1	4:D:327:ARG:HG2	1.86	0.41
19:1:130:VAL:HB	19:1:133:LYS:HB2	2.02	0.41
19:2:99:GLU:OE2	19:2:220:ARG:NE	2.54	0.41
17:R:285:ASP:H	20:4:141:SER:HB3	159.59	0.41
20:4:242:PHE:O	20:4:246:ALA:HB3	2.21	0.41
2:B:137:LYS:HE2	2:B:137:LYS:HB2	1.91	0.41
19:N:173:GLU:HA	19:N:176:ARG:HG2	2.03	0.41
22:R:312:CLA:H3A	22:R:312:CLA:HBA2	1.85	0.41
19:1:265:PRO:HD3	25:1:615:CHL:HAA2	2.03	0.41
25:2:601:CHL:HBD	25:2:601:CHL:O1A	2.21	0.41
19:6:105:TRP:CD1	25:6:608:CHL:HMD3	2.55	0.41
25:8:305:CHL:HMC	25:8:306:CHL:C4C	2.50	0.41
1:A:269:ARG:O	1:A:273:PHE:CB	2.69	0.41
2:B:237:VAL:HG22	22:B:610:CLA:HBC2	2.10	0.41
3:C:215:LYS:NZ	3:C:223:TRP:O	2.47	0.41
3:C:293:ASN:HD21	3:C:296:ALA:HB3	1.86	0.41
19:G:229:PHE:O	19:G:233:ALA:HB2	2.21	0.41
19:G:161:ILE:HG12	25:G:605:CHL:HAC1	2.02	0.41
1:A:97:TRP:CD1	8:I:5:LYS:HD2	3.10	0.41
19:N:229:PHE:O	19:N:233:ALA:HB2	2.21	0.41
18:S:89:VAL:HB	18:S:92:ASP:HB2	2.03	0.41
16:Z:12:LEU:O	16:Z:16:SER:OG	2.34	0.41
19:7:99:GLU:OE2	19:7:220:ARG:NE	2.54	0.41
17:R:62:ALA:HA	20:8:172:VAL:HG21	2.01	0.41
3:C:100:GLY:N	3:C:104:GLU:O	2.36	0.41
3:C:43:ILE:HG13	22:C:509:CLA:HMC1	2.24	0.41
22:B:614:CLA:HHD	11:M:21:PHE:CZ	2.82	0.41
19:N:104:ARG:HD3	22:N:610:CLA:HAC2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:230:ARG:NH2	22:S:303:CLA:O2D	2.54	0.41
19:Y:229:PHE:O	19:Y:233:ALA:HB2	2.21	0.41
19:5:99:GLU:OE2	19:5:220:ARG:NE	2.53	0.41
25:7:307:CHL:H3A	25:7:307:CHL:HBA2	1.87	0.41
1:A:57:PRO:O	12:O:208:ARG:NH1	2.47	0.41
4:D:181:ARG:O	4:D:185:PHE:CB	2.65	0.41
4:D:251:ASN:O	4:D:255:SER:OG	2.29	0.41
17:R:168:ALA:O	17:R:172:GLU:CB	2.67	0.41
22:R:311:CLA:H2A	22:R:311:CLA:HED3	2.03	0.41
25:1:601:CHL:HED3	25:1:601:CHL:HBA1	2.02	0.41
19:1:50:TRP:HE1	22:1:611:CLA:HED2	1.86	0.41
20:4:181:THR:HG21	20:4:198:ARG:HD2	2.02	0.41
22:B:616:CLA:HHC	22:B:616:CLA:HAB	1.86	0.41
4:D:257:ILE:HD13	4:D:257:ILE:HA	1.91	0.41
10:L:12:GLU:HA	11:M:29:THR:HA	2.02	0.41
17:R:157:VAL:O	17:R:161:THR:OG1	2.34	0.41
17:R:61:GLY:CA	20:8:169:SER:CB	2.96	0.41
18:S:196:PHE:HA	25:S:308:CHL:HBC1	2.03	0.41
14:W:117:PHE:O	14:W:121:SER:OG	2.32	0.41
25:8:307:CHL:HBA2	22:8:309:CLA:HMD2	2.03	0.41
2:B:132:SER:O	7:H:27:ASN:ND2	2.54	0.41
2:B:434:ARG:HA	2:B:439:SER:HB2	2.03	0.41
5:E:19:TYR:HE1	24:E:101:HEM:C4D	3.71	0.41
3:C:131:TYR:HH	18:S:74:GLY:HA2	1.80	0.41
25:6:601:CHL:HBD	25:6:601:CHL:O1A	2.21	0.41
2:B:234:ILE:HG23	22:B:612:CLA:HBC1	2.03	0.41
3:C:466:VAL:HG11	4:D:248:VAL:HG12	2.03	0.41
4:D:189:PHE:CD1	4:D:327:ARG:HG2	2.56	0.41
19:G:173:GLU:HA	19:G:176:ARG:HG2	2.03	0.41
19:N:130:VAL:HB	19:N:133:LYS:HB2	2.03	0.41
17:R:283:ILE:O	20:8:143:GLY:HA3	2.21	0.41
4:D:94:TRP:CD1	15:X:86:PHE:HA	2.64	0.41
19:Y:105:TRP:CD1	25:Y:609:CHL:HMD3	2.56	0.41
16:Z:40:VAL:O	16:Z:44:THR:HB	2.21	0.41
19:2:153:VAL:HA	25:2:605:CHL:C4D	2.51	0.40
17:R:283:ILE:O	20:4:143:GLY:HA3	154.56	0.40
19:6:153:VAL:HA	25:6:605:CHL:C4D	2.51	0.40
3:C:387:TRP:O	3:C:391:ARG:HG2	2.21	0.40
4:D:202:VAL:HG22	22:D:403:CLA:C1B	2.51	0.40
6:F:14:TRP:O	6:F:18:HIS:ND1	2.51	0.40
19:N:52:GLY:H	19:N:72:GLY:HA3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1:264:VAL:HG13	25:1:615:CHL:HED1	2.03	0.40
22:5:610:CLA:H3A	22:5:610:CLA:HBA2	1.82	0.40
20:8:181:THR:HG21	20:8:198:ARG:HD2	2.02	0.40
2:B:365:THR:HG21	4:D:324:GLU:HG2	2.02	0.40
3:C:457:LYS:HG2	4:D:229:GLY:HA2	2.03	0.40
22:D:403:CLA:HHC	22:D:403:CLA:HAB	1.85	0.40
19:G:52:GLY:H	19:G:72:GLY:HA3	1.86	0.40
12:O:135:LYS:O	12:O:330:GLN:N	2.53	0.40
22:R:312:CLA:HHB	20:8:159:LYS:HE2	2.02	0.40
18:S:73:ASP:CB	22:S:301:CLA:CED	3.64	0.40
19:Y:173:GLU:HA	19:Y:176:ARG:HG2	2.03	0.40
19:1:67:PRO:HB2	19:1:70:LEU:HB2	2.04	0.40
19:5:216:LEU:HD23	19:5:216:LEU:HA	1.87	0.40
19:5:67:PRO:HB2	19:5:70:LEU:HB2	2.04	0.40
1:A:227:THR:HG21	1:A:236:GLY:HA3	2.03	0.40
1:A:329:GLU:HA	1:A:332:HIS:CE1	2.56	0.40
22:C:501:CLA:HBA1	22:C:502:CLA:HMD1	2.04	0.40
3:C:438:PHE:CE1	22:C:505:CLA:HAB	2.63	0.40
19:1:99:GLU:OE2	19:1:220:ARG:NE	2.53	0.40
19:6:67:PRO:HB2	19:6:70:LEU:HB2	2.04	0.40
2:B:7:ARG:O	2:B:10:THR:OG1	2.28	0.40
2:B:230:ARG:HH21	4:D:135:ARG:HH21	3.14	0.40
22:G:611:CLA:H2A	22:G:611:CLA:HED3	2.04	0.40
19:N:247:HIS:HB2	22:N:613:CLA:HAA2	2.04	0.40
17:R:156:SER:O	17:R:160:LEU:HB2	2.22	0.40
18:S:240:PHE:O	18:S:244:TYR:CB	2.70	0.40
19:Y:52:GLY:H	19:Y:72:GLY:HA3	1.86	0.40
20:8:242:PHE:O	20:8:246:ALA:HB3	2.21	0.40
2:B:17:GLY:HA2	2:B:20:LEU:HD12	2.04	0.40
2:B:9:HIS:HB2	22:B:611:CLA:CGA	2.54	0.40
22:B:614:CLA:HHD	11:M:21:PHE:HZ	2.11	0.40
19:N:152:LEU:HD23	19:N:152:LEU:HA	1.86	0.40
19:N:75:PRO:HB2	19:N:216:LEU:HD12	2.04	0.40
18:S:265:ASN:O	18:S:268:THR:OG1	2.39	0.40
19:Y:130:VAL:HB	19:Y:133:LYS:HB2	2.03	0.40
25:Y:606:CHL:HBB2	25:Y:607:CHL:HBB1	2.04	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	A	303/343 (88%)	282 (93%)	21 (7%)	0	100	100
1	a	328/343 (96%)	306 (93%)	22 (7%)	0	100	100
2	B	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
2	b	476/507 (94%)	448 (94%)	28 (6%)	0	100	100
3	C	429/459 (94%)	401 (94%)	28 (6%)	0	100	100
3	c	429/459 (94%)	402 (94%)	27 (6%)	0	100	100
4	D	334/352 (95%)	308 (92%)	26 (8%)	0	100	100
4	d	334/352 (95%)	307 (92%)	27 (8%)	0	100	100
5	E	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
5	e	68/83 (82%)	59 (87%)	9 (13%)	0	100	100
6	F	27/39 (69%)	27 (100%)	0	0	100	100
6	f	27/39 (69%)	27 (100%)	0	0	100	100
7	H	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
7	h	50/72 (69%)	44 (88%)	6 (12%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
9	K	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
9	k	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
10	L	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
10	l	34/38 (90%)	28 (82%)	6 (18%)	0	100	100
11	M	27/34 (79%)	27 (100%)	0	0	100	100
11	m	27/34 (79%)	27 (100%)	0	0	100	100
12	O	187/247 (76%)	162 (87%)	24 (13%)	1 (0%)	32	74
12	o	187/247 (76%)	163 (87%)	23 (12%)	1 (0%)	32	74
13	T	27/33 (82%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	t	27/33 (82%)	27 (100%)	0	0	100	100
14	W	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
14	w	44/54 (82%)	39 (89%)	5 (11%)	0	100	100
15	X	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
15	x	30/116 (26%)	29 (97%)	1 (3%)	0	100	100
16	Z	59/62 (95%)	59 (100%)	0	0	100	100
16	z	59/62 (95%)	59 (100%)	0	0	100	100
17	R	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
17	r	184/250 (74%)	172 (94%)	12 (6%)	0	100	100
18	S	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
18	s	212/232 (91%)	171 (81%)	41 (19%)	0	100	100
19	1	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	2	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	3	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	5	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	6	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	7	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	G	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	N	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	Y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	g	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	n	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
19	y	217/224 (97%)	203 (94%)	14 (6%)	0	100	100
20	4	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
20	8	202/210 (96%)	184 (91%)	18 (9%)	0	100	100
All	All	8149/9096 (90%)	7521 (92%)	626 (8%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	O	194	ILE
12	o	194	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/278 (89%)	247 (100%)	0	100	100
1	a	267/278 (96%)	267 (100%)	0	100	100
2	B	379/401 (94%)	379 (100%)	0	100	100
2	b	379/401 (94%)	379 (100%)	0	100	100
3	C	340/359 (95%)	339 (100%)	1 (0%)	94	96
3	c	340/359 (95%)	339 (100%)	1 (0%)	94	96
4	D	269/282 (95%)	268 (100%)	1 (0%)	93	95
4	d	269/282 (95%)	268 (100%)	1 (0%)	93	95
5	E	63/73 (86%)	63 (100%)	0	100	100
5	e	63/73 (86%)	63 (100%)	0	100	100
6	F	24/34 (71%)	24 (100%)	0	100	100
6	f	24/34 (71%)	24 (100%)	0	100	100
7	H	43/60 (72%)	43 (100%)	0	100	100
7	h	43/60 (72%)	43 (100%)	0	100	100
8	I	32/33 (97%)	32 (100%)	0	100	100
8	i	32/33 (97%)	32 (100%)	0	100	100
9	K	31/32 (97%)	31 (100%)	0	100	100
9	k	31/32 (97%)	31 (100%)	0	100	100
10	L	34/36 (94%)	34 (100%)	0	100	100
10	l	34/36 (94%)	34 (100%)	0	100	100
11	M	25/30 (83%)	25 (100%)	0	100	100
11	m	25/30 (83%)	24 (96%)	1 (4%)	36	65
12	O	164/204 (80%)	164 (100%)	0	100	100
12	o	164/204 (80%)	164 (100%)	0	100	100
13	T	26/30 (87%)	26 (100%)	0	100	100
13	t	26/30 (87%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	W	40/47 (85%)	40 (100%)	0	100	100
14	w	40/47 (85%)	40 (100%)	0	100	100
15	X	27/92 (29%)	27 (100%)	0	100	100
15	x	27/92 (29%)	27 (100%)	0	100	100
16	Z	53/54 (98%)	53 (100%)	0	100	100
16	z	53/54 (98%)	53 (100%)	0	100	100
17	R	150/201 (75%)	150 (100%)	0	100	100
17	r	150/201 (75%)	150 (100%)	0	100	100
18	S	165/180 (92%)	164 (99%)	1 (1%)	89	94
18	s	165/180 (92%)	164 (99%)	1 (1%)	89	94
19	1	167/170 (98%)	167 (100%)	0	100	100
19	2	167/170 (98%)	167 (100%)	0	100	100
19	3	167/170 (98%)	167 (100%)	0	100	100
19	5	167/170 (98%)	167 (100%)	0	100	100
19	6	167/170 (98%)	167 (100%)	0	100	100
19	7	167/170 (98%)	167 (100%)	0	100	100
19	G	167/170 (98%)	167 (100%)	0	100	100
19	N	167/170 (98%)	167 (100%)	0	100	100
19	Y	167/170 (98%)	167 (100%)	0	100	100
19	g	167/170 (98%)	167 (100%)	0	100	100
19	n	167/170 (98%)	167 (100%)	0	100	100
19	y	167/170 (98%)	167 (100%)	0	100	100
20	4	156/158 (99%)	156 (100%)	0	100	100
20	8	156/158 (99%)	156 (100%)	0	100	100
All	All	6560/7208 (91%)	6553 (100%)	7 (0%)	95	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	26	ARG
4	D	19	MET
4	d	19	MET
11	m	16	LEU
3	c	26	ARG

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Mol	Chain	Res	Type
18	S	102	LYS
18	s	102	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	303	ASN
2	B	332	ASN
3	C	84	GLN
4	D	84	ASN
4	D	88	HIS
4	D	251	ASN
4	D	302	GLN
11	M	32	GLN
12	O	202	GLN
12	O	307	GLN
14	W	99	ASN
16	Z	58	ASN
1	a	296	ASN
1	a	303	ASN
2	b	332	ASN
4	d	84	ASN
4	d	351	ASN
12	o	202	GLN
12	o	307	GLN
3	c	84	GLN
17	R	182	GLN
18	S	106	ASN
18	S	117	HIS
18	S	140	ASN
18	S	264	ASN
19	G	122	ASN
19	G	156	GLN
19	N	122	ASN
19	N	156	GLN
19	Y	122	ASN
19	Y	156	GLN
19	Y	165	GLN
17	r	182	GLN
18	s	106	ASN
18	s	117	HIS

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Mol	Chain	Res	Type
18	s	140	ASN
18	s	264	ASN
19	g	122	ASN
19	g	156	GLN
19	n	122	ASN
19	n	156	GLN
19	y	122	ASN
19	y	156	GLN
19	y	165	GLN
19	1	95	ASN
19	1	156	GLN
19	2	95	ASN
19	2	156	GLN
19	3	95	ASN
19	3	156	GLN
20	4	166	ASN
19	5	95	ASN
19	5	156	GLN
19	6	95	ASN
19	6	156	GLN
19	7	95	ASN
19	7	156	GLN
20	8	166	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 316 ligands modelled in this entry, 2 are monoatomic - leaving 314 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
25	CHL	1	601	19	41,54,74	5.27	24 (58%)	24,90,114	3.64	14 (58%)
22	CLA	1	602	19	33,53,73	2.18	10 (30%)	37,89,113	3.41	18 (48%)
22	CLA	1	603	-	33,53,73	2.21	10 (30%)	37,89,113	3.37	19 (51%)
22	CLA	1	604	-	33,53,73	2.16	9 (27%)	37,89,113	3.39	17 (45%)
25	CHL	1	605	19	40,50,74	5.42	23 (57%)	25,85,114	3.43	15 (60%)
25	CHL	1	606	-	41,54,74	5.34	24 (58%)	24,90,114	3.65	14 (58%)
25	CHL	1	607	-	41,54,74	5.33	24 (58%)	24,90,114	3.76	16 (66%)
25	CHL	1	608	-	41,54,74	5.31	24 (58%)	24,90,114	3.55	14 (58%)
25	CHL	1	609	19	41,54,74	5.36	24 (58%)	24,90,114	3.63	13 (54%)
22	CLA	1	610	19	33,53,73	2.25	8 (24%)	37,89,113	3.39	16 (43%)
22	CLA	1	611	-	33,53,73	2.20	9 (27%)	37,89,113	3.42	17 (45%)
22	CLA	1	612	19	33,53,73	2.17	9 (27%)	37,89,113	3.29	20 (54%)
22	CLA	1	613	19	33,53,73	2.19	9 (27%)	37,89,113	3.35	17 (45%)
22	CLA	1	614	-	33,53,73	2.21	11 (33%)	37,89,113	3.53	19 (51%)
25	CHL	1	615	-	41,54,74	5.31	24 (58%)	24,90,114	3.64	15 (62%)
25	CHL	2	601	19	41,54,74	5.32	24 (58%)	24,90,114	3.64	13 (54%)
22	CLA	2	602	19	33,53,73	2.17	11 (33%)	37,89,113	3.39	17 (45%)
22	CLA	2	603	-	33,53,73	2.19	9 (27%)	37,89,113	3.31	17 (45%)
22	CLA	2	604	-	33,53,73	2.19	10 (30%)	37,89,113	3.37	19 (51%)
25	CHL	2	605	19	40,50,74	5.34	23 (57%)	25,85,114	3.39	14 (56%)
25	CHL	2	606	-	41,54,74	5.36	24 (58%)	24,90,114	3.68	16 (66%)
25	CHL	2	607	-	41,54,74	5.26	24 (58%)	24,90,114	3.60	14 (58%)
25	CHL	2	608	19	41,54,74	5.40	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	2	609	19	33,53,73	2.26	9 (27%)	37,89,113	3.31	18 (48%)
22	CLA	2	610	-	33,53,73	2.23	10 (30%)	37,89,113	3.35	18 (48%)
22	CLA	2	611	19	33,53,73	2.21	9 (27%)	37,89,113	3.25	16 (43%)
22	CLA	2	612	19	33,53,73	2.18	10 (30%)	37,89,113	3.49	16 (43%)
22	CLA	2	613	-	33,53,73	2.28	11 (33%)	37,89,113	3.24	16 (43%)
25	CHL	3	301	-	41,54,74	5.32	24 (58%)	24,90,114	3.59	15 (62%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	3	302	19	41,54,74	5.32	25 (60%)	24,90,114	3.67	13 (54%)
22	CLA	3	303	19	33,53,73	2.19	10 (30%)	37,89,113	3.37	18 (48%)
22	CLA	3	304	-	33,53,73	2.18	11 (33%)	37,89,113	3.32	19 (51%)
22	CLA	3	305	-	33,53,73	2.19	11 (33%)	37,89,113	3.36	19 (51%)
25	CHL	3	306	19	40,50,74	5.32	23 (57%)	25,85,114	3.38	13 (52%)
25	CHL	3	307	-	41,54,74	5.27	24 (58%)	24,90,114	3.69	14 (58%)
25	CHL	3	308	-	41,54,74	5.31	24 (58%)	24,90,114	3.56	12 (50%)
25	CHL	3	309	19	41,54,74	5.37	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	3	310	19	33,53,73	2.30	10 (30%)	37,89,113	3.35	17 (45%)
22	CLA	3	311	-	33,53,73	2.23	11 (33%)	37,89,113	3.36	18 (48%)
22	CLA	3	312	19	33,53,73	2.22	9 (27%)	37,89,113	3.41	17 (45%)
22	CLA	3	313	19	33,53,73	2.22	10 (30%)	37,89,113	3.40	17 (45%)
22	CLA	3	314	-	33,53,73	2.26	11 (33%)	37,89,113	3.13	16 (43%)
25	CHL	4	301	-	41,54,74	5.36	24 (58%)	24,90,114	3.52	15 (62%)
22	CLA	4	302	20	33,53,73	2.21	10 (30%)	37,89,113	3.72	19 (51%)
22	CLA	4	303	-	33,53,73	2.23	10 (30%)	37,89,113	3.33	19 (51%)
22	CLA	4	304	-	33,53,73	2.19	11 (33%)	37,89,113	3.39	18 (48%)
25	CHL	4	305	20	41,54,74	5.32	24 (58%)	24,90,114	3.84	14 (58%)
25	CHL	4	306	-	41,54,74	5.33	24 (58%)	24,90,114	3.68	14 (58%)
25	CHL	4	307	-	41,54,74	5.35	24 (58%)	24,90,114	8.23	16 (66%)
25	CHL	4	308	20	41,54,74	5.36	24 (58%)	24,90,114	3.59	14 (58%)
22	CLA	4	309	20	33,53,73	2.23	10 (30%)	37,89,113	3.26	19 (51%)
22	CLA	4	310	-	33,53,73	2.24	11 (33%)	37,89,113	3.26	19 (51%)
25	CHL	5	601	19	41,54,74	5.27	24 (58%)	24,90,114	3.64	14 (58%)
22	CLA	5	602	19	33,53,73	2.18	10 (30%)	37,89,113	3.41	18 (48%)
22	CLA	5	603	-	33,53,73	2.21	10 (30%)	37,89,113	3.37	19 (51%)
22	CLA	5	604	-	33,53,73	2.16	9 (27%)	37,89,113	3.39	17 (45%)
25	CHL	5	605	19	40,50,74	5.42	23 (57%)	25,85,114	3.43	15 (60%)
25	CHL	5	606	-	41,54,74	5.34	24 (58%)	24,90,114	3.65	14 (58%)
25	CHL	5	607	-	41,54,74	5.33	24 (58%)	24,90,114	3.76	16 (66%)
25	CHL	5	608	-	41,54,74	5.31	24 (58%)	24,90,114	3.55	14 (58%)
25	CHL	5	609	19	41,54,74	5.36	24 (58%)	24,90,114	3.63	13 (54%)
22	CLA	5	610	19	33,53,73	2.25	8 (24%)	37,89,113	3.39	16 (43%)
22	CLA	5	611	-	33,53,73	2.20	9 (27%)	37,89,113	3.42	17 (45%)
22	CLA	5	612	19	33,53,73	2.17	9 (27%)	37,89,113	3.29	20 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	613	19	33,53,73	2.19	9 (27%)	37,89,113	3.35	17 (45%)
22	CLA	5	614	-	33,53,73	2.21	11 (33%)	37,89,113	3.53	19 (51%)
25	CHL	5	615	-	41,54,74	5.31	24 (58%)	24,90,114	3.64	15 (62%)
25	CHL	6	601	19	41,54,74	5.32	24 (58%)	24,90,114	3.64	13 (54%)
22	CLA	6	602	19	33,53,73	2.17	11 (33%)	37,89,113	3.39	17 (45%)
22	CLA	6	603	-	33,53,73	2.19	9 (27%)	37,89,113	3.31	17 (45%)
22	CLA	6	604	-	33,53,73	2.19	10 (30%)	37,89,113	3.37	19 (51%)
25	CHL	6	605	19	40,50,74	5.34	23 (57%)	25,85,114	3.39	14 (56%)
25	CHL	6	606	-	41,54,74	5.36	24 (58%)	24,90,114	3.68	16 (66%)
25	CHL	6	607	-	41,54,74	5.26	24 (58%)	24,90,114	3.60	14 (58%)
25	CHL	6	608	19	41,54,74	5.40	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	6	609	19	33,53,73	2.26	9 (27%)	37,89,113	3.31	18 (48%)
22	CLA	6	610	-	33,53,73	2.23	10 (30%)	37,89,113	3.35	18 (48%)
22	CLA	6	611	19	33,53,73	2.21	9 (27%)	37,89,113	3.25	16 (43%)
22	CLA	6	612	19	33,53,73	2.18	10 (30%)	37,89,113	3.49	16 (43%)
22	CLA	6	613	-	33,53,73	2.28	11 (33%)	37,89,113	3.24	16 (43%)
25	CHL	7	301	-	41,54,74	5.32	24 (58%)	24,90,114	3.59	15 (62%)
25	CHL	7	302	19	41,54,74	5.32	25 (60%)	24,90,114	3.67	13 (54%)
22	CLA	7	303	19	33,53,73	2.19	10 (30%)	37,89,113	3.37	18 (48%)
22	CLA	7	304	-	33,53,73	2.18	11 (33%)	37,89,113	3.32	19 (51%)
22	CLA	7	305	-	33,53,73	2.19	11 (33%)	37,89,113	3.36	19 (51%)
25	CHL	7	306	19	40,50,74	5.32	23 (57%)	25,85,114	3.38	13 (52%)
25	CHL	7	307	-	41,54,74	5.27	24 (58%)	24,90,114	3.69	14 (58%)
25	CHL	7	308	-	41,54,74	5.31	24 (58%)	24,90,114	3.56	12 (50%)
25	CHL	7	309	19	41,54,74	5.37	24 (58%)	24,90,114	3.61	13 (54%)
22	CLA	7	310	19	33,53,73	2.30	10 (30%)	37,89,113	3.35	17 (45%)
22	CLA	7	311	-	33,53,73	2.23	11 (33%)	37,89,113	3.36	18 (48%)
22	CLA	7	312	19	33,53,73	2.22	9 (27%)	37,89,113	3.41	17 (45%)
22	CLA	7	313	19	33,53,73	2.22	10 (30%)	37,89,113	3.40	17 (45%)
22	CLA	7	314	-	33,53,73	2.26	11 (33%)	37,89,113	3.13	16 (43%)
25	CHL	8	301	-	41,54,74	5.36	24 (58%)	24,90,114	3.52	15 (62%)
22	CLA	8	302	20	33,53,73	2.21	10 (30%)	37,89,113	3.72	19 (51%)
22	CLA	8	303	-	33,53,73	2.23	10 (30%)	37,89,113	3.33	19 (51%)
22	CLA	8	304	-	33,53,73	2.19	11 (33%)	37,89,113	3.39	18 (48%)
25	CHL	8	305	20	41,54,74	5.32	24 (58%)	24,90,114	3.84	14 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	8	306	-	41,54,74	5.33	24 (58%)	24,90,114	3.68	14 (58%)
25	CHL	8	307	-	41,54,74	5.35	24 (58%)	24,90,114	8.23	16 (66%)
25	CHL	8	308	20	41,54,74	5.36	24 (58%)	24,90,114	3.59	14 (58%)
22	CLA	8	309	20	33,53,73	2.23	10 (30%)	37,89,113	3.26	19 (51%)
22	CLA	8	310	-	33,53,73	2.24	11 (33%)	37,89,113	3.26	19 (51%)
22	CLA	A	402	-	33,53,73	2.11	7 (21%)	37,89,113	3.55	19 (51%)
22	CLA	A	403	-	33,53,73	2.15	9 (27%)	37,89,113	3.37	19 (51%)
23	PHO	A	404	-	44,49,69	2.02	13 (29%)	59,75,99	2.27	16 (27%)
22	CLA	A	405	-	33,53,73	2.10	8 (24%)	37,89,113	3.51	18 (48%)
22	CLA	B	601	-	33,53,73	2.14	8 (24%)	37,89,113	3.20	16 (43%)
22	CLA	B	602	-	33,53,73	2.16	8 (24%)	37,89,113	3.51	18 (48%)
22	CLA	B	603	-	33,53,73	2.06	7 (21%)	37,89,113	3.51	20 (54%)
22	CLA	B	604	-	33,53,73	1.98	8 (24%)	37,89,113	3.70	19 (51%)
22	CLA	B	605	-	33,53,73	2.03	9 (27%)	37,89,113	3.45	19 (51%)
22	CLA	B	606	-	33,53,73	2.03	7 (21%)	37,89,113	3.34	18 (48%)
22	CLA	B	607	-	33,53,73	2.06	9 (27%)	37,89,113	3.49	19 (51%)
22	CLA	B	608	-	33,53,73	2.11	9 (27%)	37,89,113	3.70	18 (48%)
22	CLA	B	609	-	33,53,73	2.09	9 (27%)	37,89,113	3.59	20 (54%)
22	CLA	B	610	-	33,53,73	2.11	8 (24%)	37,89,113	3.35	18 (48%)
22	CLA	B	611	-	33,53,73	2.13	9 (27%)	37,89,113	3.34	19 (51%)
22	CLA	B	612	-	33,53,73	2.17	8 (24%)	37,89,113	3.62	18 (48%)
22	CLA	B	613	-	33,53,73	2.12	9 (27%)	37,89,113	3.38	21 (56%)
22	CLA	B	614	-	33,53,73	2.19	8 (24%)	37,89,113	3.45	19 (51%)
22	CLA	B	615	-	33,53,73	2.10	8 (24%)	37,89,113	3.82	20 (54%)
22	CLA	B	616	-	33,53,73	2.26	9 (27%)	37,89,113	3.61	21 (56%)
22	CLA	C	501	-	33,53,73	2.08	8 (24%)	37,89,113	3.53	23 (62%)
22	CLA	C	502	-	33,53,73	2.07	8 (24%)	37,89,113	3.09	19 (51%)
22	CLA	C	503	-	33,53,73	2.04	7 (21%)	37,89,113	3.34	20 (54%)
22	CLA	C	504	-	33,53,73	2.12	9 (27%)	37,89,113	3.48	18 (48%)
22	CLA	C	505	-	33,53,73	2.02	8 (24%)	37,89,113	3.43	19 (51%)
22	CLA	C	506	-	33,53,73	2.07	9 (27%)	37,89,113	3.73	18 (48%)
22	CLA	C	507	-	33,53,73	2.04	8 (24%)	37,89,113	3.50	18 (48%)
22	CLA	C	508	-	33,53,73	2.06	9 (27%)	37,89,113	3.74	20 (54%)
22	CLA	C	509	-	33,53,73	2.16	9 (27%)	37,89,113	3.35	20 (54%)
22	CLA	C	510	-	33,53,73	2.09	8 (24%)	37,89,113	3.67	20 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	511	3	33,53,73	2.11	10 (30%)	37,89,113	3.44	20 (54%)
22	CLA	C	512	-	33,53,73	2.16	10 (30%)	37,89,113	3.23	19 (51%)
22	CLA	D	401	-	33,53,73	2.03	8 (24%)	37,89,113	3.43	19 (51%)
23	PHO	D	402	-	44,49,69	2.01	11 (25%)	59,75,99	2.27	18 (30%)
22	CLA	D	403	-	33,53,73	2.13	8 (24%)	37,89,113	3.63	21 (56%)
22	CLA	D	404	-	33,53,73	2.13	9 (27%)	37,89,113	3.42	17 (45%)
24	HEM	E	101	5,6	28,50,50	2.06	4 (14%)	17,82,82	1.28	1 (5%)
25	CHL	G	601	19	41,54,74	5.45	26 (63%)	24,90,114	3.60	15 (62%)
22	CLA	G	602	19	33,53,73	2.09	9 (27%)	37,89,113	3.41	17 (45%)
22	CLA	G	603	-	33,53,73	2.07	9 (27%)	37,89,113	3.35	19 (51%)
22	CLA	G	604	-	33,53,73	2.07	9 (27%)	37,89,113	3.45	19 (51%)
25	CHL	G	605	19	40,50,74	5.37	23 (57%)	25,85,114	3.38	15 (60%)
25	CHL	G	606	-	41,54,74	5.49	24 (58%)	24,90,114	3.65	16 (66%)
25	CHL	G	607	-	41,54,74	5.39	24 (58%)	24,90,114	3.64	16 (66%)
25	CHL	G	608	-	41,54,74	5.52	24 (58%)	24,90,114	3.57	14 (58%)
25	CHL	G	609	19	41,54,74	5.54	25 (60%)	24,90,114	3.58	12 (50%)
22	CLA	G	610	19	33,53,73	2.19	7 (21%)	37,89,113	3.33	18 (48%)
22	CLA	G	611	-	33,53,73	2.11	8 (24%)	37,89,113	3.44	20 (54%)
22	CLA	G	612	19	33,53,73	2.10	8 (24%)	37,89,113	3.35	20 (54%)
22	CLA	G	613	19	33,53,73	2.06	8 (24%)	37,89,113	3.44	18 (48%)
22	CLA	G	614	-	33,53,73	2.18	10 (30%)	37,89,113	3.29	20 (54%)
25	CHL	N	601	19	41,54,74	5.49	24 (58%)	24,90,114	3.59	15 (62%)
22	CLA	N	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.44	17 (45%)
22	CLA	N	603	-	33,53,73	2.01	8 (24%)	37,89,113	3.37	19 (51%)
22	CLA	N	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.38	18 (48%)
25	CHL	N	605	19	40,50,74	5.54	24 (60%)	25,85,114	3.43	16 (64%)
25	CHL	N	606	-	41,54,74	5.55	23 (56%)	24,90,114	3.67	15 (62%)
25	CHL	N	607	-	41,54,74	5.57	25 (60%)	24,90,114	3.69	17 (70%)
25	CHL	N	608	-	41,54,74	5.54	24 (58%)	24,90,114	3.54	15 (62%)
25	CHL	N	609	19	41,54,74	5.64	25 (60%)	24,90,114	3.52	14 (58%)
22	CLA	N	610	19	33,53,73	2.15	8 (24%)	37,89,113	3.34	17 (45%)
22	CLA	N	611	-	33,53,73	2.13	8 (24%)	37,89,113	3.47	21 (56%)
22	CLA	N	612	19	33,53,73	2.09	8 (24%)	37,89,113	3.36	18 (48%)
22	CLA	N	613	19	33,53,73	2.04	9 (27%)	37,89,113	3.47	17 (45%)
22	CLA	N	614	-	33,53,73	2.24	11 (33%)	37,89,113	3.25	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	R	301	17	33,53,73	2.14	8 (24%)	37,89,113	3.42	19 (51%)
22	CLA	R	302	-	33,53,73	2.19	8 (24%)	37,89,113	3.35	16 (43%)
22	CLA	R	303	-	33,53,73	2.07	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	R	304	-	41,54,74	5.47	24 (58%)	24,90,114	3.79	16 (66%)
25	CHL	R	305	-	41,54,74	5.48	24 (58%)	24,90,114	3.78	16 (66%)
25	CHL	R	306	-	41,54,74	5.40	25 (60%)	24,90,114	3.62	15 (62%)
22	CLA	R	307	17	33,53,73	2.12	9 (27%)	37,89,113	3.39	17 (45%)
22	CLA	R	308	17	33,53,73	2.19	9 (27%)	37,89,113	3.30	19 (51%)
22	CLA	R	309	-	33,53,73	2.10	8 (24%)	37,89,113	3.41	19 (51%)
22	CLA	R	310	-	33,53,73	2.15	8 (24%)	37,89,113	3.30	17 (45%)
22	CLA	R	311	17	33,53,73	2.14	9 (27%)	37,89,113	3.50	17 (45%)
22	CLA	R	312	20,17	33,53,73	2.18	11 (33%)	37,89,113	3.36	20 (54%)
22	CLA	S	301	-	33,53,73	2.19	8 (24%)	37,89,113	3.53	18 (48%)
25	CHL	S	302	18	41,54,74	5.54	25 (60%)	24,90,114	3.58	14 (58%)
22	CLA	S	303	18	33,53,73	2.12	9 (27%)	37,89,113	3.41	19 (51%)
22	CLA	S	304	-	33,53,73	2.19	9 (27%)	37,89,113	3.09	17 (45%)
22	CLA	S	305	-	33,53,73	2.12	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	S	306	18	41,54,74	5.42	24 (58%)	24,90,114	3.79	15 (62%)
25	CHL	S	307	-	41,54,74	5.53	24 (58%)	24,90,114	8.30	17 (70%)
25	CHL	S	308	-	41,54,74	5.50	26 (63%)	24,90,114	3.52	15 (62%)
22	CLA	S	309	18	33,53,73	2.16	9 (27%)	37,89,113	3.32	19 (51%)
22	CLA	S	310	18	33,53,73	2.06	9 (27%)	37,89,113	3.37	19 (51%)
22	CLA	S	311	-	33,53,73	2.07	7 (21%)	37,89,113	3.43	19 (51%)
22	CLA	S	312	18	33,53,73	2.08	9 (27%)	37,89,113	3.44	20 (54%)
22	CLA	S	313	18	33,53,73	2.03	8 (24%)	37,89,113	3.42	21 (56%)
22	CLA	S	314	-	33,53,73	2.05	8 (24%)	37,89,113	3.53	19 (51%)
25	CHL	Y	601	19	41,54,74	5.46	25 (60%)	24,90,114	3.56	15 (62%)
22	CLA	Y	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.46	17 (45%)
22	CLA	Y	603	-	33,53,73	2.00	8 (24%)	37,89,113	3.45	20 (54%)
22	CLA	Y	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.66	19 (51%)
25	CHL	Y	605	19	40,50,74	5.68	24 (60%)	25,85,114	3.43	18 (72%)
25	CHL	Y	606	-	41,54,74	5.47	23 (56%)	24,90,114	3.83	14 (58%)
25	CHL	Y	607	-	41,54,74	5.53	25 (60%)	24,90,114	3.67	17 (70%)
25	CHL	Y	608	-	41,54,74	5.55	25 (60%)	24,90,114	3.53	15 (62%)
25	CHL	Y	609	19	41,54,74	5.67	24 (58%)	24,90,114	3.67	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Y	610	19	33,53,73	2.13	8 (24%)	37,89,113	3.42	18 (48%)
22	CLA	Y	611	-	33,53,73	2.05	8 (24%)	37,89,113	3.54	18 (48%)
22	CLA	Y	612	19	33,53,73	1.99	8 (24%)	37,89,113	3.29	20 (54%)
22	CLA	Y	613	19	33,53,73	2.02	9 (27%)	37,89,113	3.60	17 (45%)
22	CLA	Y	614	-	33,53,73	2.07	7 (21%)	37,89,113	3.46	21 (56%)
22	CLA	a	402	-	33,53,73	2.12	10 (30%)	37,89,113	3.33	19 (51%)
22	CLA	a	403	-	33,53,73	2.09	8 (24%)	37,89,113	3.52	19 (51%)
23	PHO	a	404	-	44,49,69	2.02	12 (27%)	59,75,99	2.19	17 (28%)
22	CLA	a	405	-	33,53,73	2.10	7 (21%)	37,89,113	3.62	20 (54%)
22	CLA	b	601	-	33,53,73	2.15	8 (24%)	37,89,113	3.25	18 (48%)
22	CLA	b	602	-	33,53,73	2.06	8 (24%)	37,89,113	3.44	16 (43%)
22	CLA	b	603	-	33,53,73	2.09	9 (27%)	37,89,113	3.37	20 (54%)
22	CLA	b	604	-	33,53,73	2.06	8 (24%)	37,89,113	3.42	18 (48%)
22	CLA	b	605	-	33,53,73	2.13	8 (24%)	37,89,113	3.29	18 (48%)
22	CLA	b	606	-	33,53,73	2.25	11 (33%)	37,89,113	2.98	18 (48%)
22	CLA	b	607	-	33,53,73	2.06	9 (27%)	37,89,113	3.44	19 (51%)
22	CLA	b	608	-	33,53,73	2.07	8 (24%)	37,89,113	3.28	20 (54%)
22	CLA	b	609	-	33,53,73	2.05	8 (24%)	37,89,113	3.63	20 (54%)
22	CLA	b	610	-	33,53,73	2.15	10 (30%)	37,89,113	3.48	19 (51%)
22	CLA	b	611	-	33,53,73	2.11	8 (24%)	37,89,113	3.52	21 (56%)
22	CLA	b	612	-	33,53,73	2.24	10 (30%)	37,89,113	3.24	19 (51%)
22	CLA	b	613	-	33,53,73	2.13	9 (27%)	37,89,113	3.73	23 (62%)
22	CLA	b	614	-	33,53,73	2.08	9 (27%)	37,89,113	3.43	18 (48%)
22	CLA	b	615	-	33,53,73	2.11	8 (24%)	37,89,113	3.13	18 (48%)
22	CLA	b	616	-	33,53,73	2.00	9 (27%)	37,89,113	3.65	24 (64%)
22	CLA	c	501	-	33,53,73	2.13	8 (24%)	37,89,113	3.47	20 (54%)
22	CLA	c	502	-	33,53,73	2.02	8 (24%)	37,89,113	3.42	20 (54%)
22	CLA	c	503	-	33,53,73	2.03	7 (21%)	37,89,113	3.51	19 (51%)
22	CLA	c	504	-	33,53,73	2.14	9 (27%)	37,89,113	3.34	17 (45%)
22	CLA	c	505	-	33,53,73	2.03	7 (21%)	37,89,113	3.49	21 (56%)
22	CLA	c	506	-	33,53,73	2.09	9 (27%)	37,89,113	3.68	19 (51%)
22	CLA	c	507	-	33,53,73	1.99	7 (21%)	37,89,113	3.50	19 (51%)
22	CLA	c	508	-	33,53,73	2.06	9 (27%)	37,89,113	3.64	20 (54%)
22	CLA	c	509	-	33,53,73	2.16	8 (24%)	37,89,113	3.29	18 (48%)
22	CLA	c	510	-	33,53,73	2.18	8 (24%)	37,89,113	3.44	19 (51%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	c	511	3	33,53,73	2.08	9 (27%)	37,89,113	3.33	18 (48%)
22	CLA	c	512	-	33,53,73	2.10	9 (27%)	37,89,113	3.63	20 (54%)
22	CLA	d	401	-	33,53,73	2.07	8 (24%)	37,89,113	3.39	19 (51%)
23	PHO	d	402	-	44,49,69	2.04	11 (25%)	59,75,99	2.22	17 (28%)
22	CLA	d	403	-	33,53,73	2.15	8 (24%)	37,89,113	3.60	22 (59%)
22	CLA	d	404	-	33,53,73	2.15	9 (27%)	37,89,113	3.25	17 (45%)
24	HEM	e	101	5,6	28,50,50	2.12	4 (14%)	17,82,82	1.49	3 (17%)
25	CHL	g	601	19	41,54,74	5.45	26 (63%)	24,90,114	3.60	15 (62%)
22	CLA	g	602	19	33,53,73	2.09	9 (27%)	37,89,113	3.41	17 (45%)
22	CLA	g	603	-	33,53,73	2.07	9 (27%)	37,89,113	3.35	19 (51%)
22	CLA	g	604	-	33,53,73	2.07	9 (27%)	37,89,113	3.45	19 (51%)
25	CHL	g	605	19	40,50,74	5.37	23 (57%)	25,85,114	3.38	15 (60%)
25	CHL	g	606	-	41,54,74	5.49	24 (58%)	24,90,114	3.65	16 (66%)
25	CHL	g	607	-	41,54,74	5.39	24 (58%)	24,90,114	3.64	16 (66%)
25	CHL	g	608	-	41,54,74	5.52	24 (58%)	24,90,114	3.57	14 (58%)
25	CHL	g	609	19	41,54,74	5.54	25 (60%)	24,90,114	3.58	12 (50%)
22	CLA	g	610	19	33,53,73	2.19	7 (21%)	37,89,113	3.33	18 (48%)
22	CLA	g	611	-	33,53,73	2.11	8 (24%)	37,89,113	3.44	20 (54%)
22	CLA	g	612	19	33,53,73	2.10	8 (24%)	37,89,113	3.35	20 (54%)
22	CLA	g	613	19	33,53,73	2.06	8 (24%)	37,89,113	3.44	18 (48%)
22	CLA	g	614	-	33,53,73	2.18	10 (30%)	37,89,113	3.29	20 (54%)
25	CHL	n	601	19	41,54,74	5.49	24 (58%)	24,90,114	3.59	15 (62%)
22	CLA	n	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.44	17 (45%)
22	CLA	n	603	-	33,53,73	2.01	8 (24%)	37,89,113	3.37	19 (51%)
22	CLA	n	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.38	18 (48%)
25	CHL	n	605	19	40,50,74	5.54	24 (60%)	25,85,114	3.43	16 (64%)
25	CHL	n	606	-	41,54,74	5.55	23 (56%)	24,90,114	3.67	15 (62%)
25	CHL	n	607	-	41,54,74	5.57	25 (60%)	24,90,114	3.69	17 (70%)
25	CHL	n	608	-	41,54,74	5.54	24 (58%)	24,90,114	3.54	15 (62%)
25	CHL	n	609	19	41,54,74	5.64	25 (60%)	24,90,114	3.52	14 (58%)
22	CLA	n	610	19	33,53,73	2.15	8 (24%)	37,89,113	3.34	17 (45%)
22	CLA	n	611	-	33,53,73	2.13	8 (24%)	37,89,113	3.47	21 (56%)
22	CLA	n	612	19	33,53,73	2.09	8 (24%)	37,89,113	3.36	18 (48%)
22	CLA	n	613	19	33,53,73	2.04	9 (27%)	37,89,113	3.47	17 (45%)
22	CLA	n	614	-	33,53,73	2.24	11 (33%)	37,89,113	3.25	17 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	r	301	17	33,53,73	2.14	8 (24%)	37,89,113	3.42	19 (51%)
22	CLA	r	302	-	33,53,73	2.19	8 (24%)	37,89,113	3.35	16 (43%)
22	CLA	r	303	-	33,53,73	2.07	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	r	304	-	41,54,74	5.47	24 (58%)	24,90,114	3.79	16 (66%)
25	CHL	r	305	-	41,54,74	5.48	24 (58%)	24,90,114	3.78	16 (66%)
25	CHL	r	306	-	41,54,74	5.40	25 (60%)	24,90,114	3.62	15 (62%)
22	CLA	r	307	17	33,53,73	2.12	9 (27%)	37,89,113	3.39	17 (45%)
22	CLA	r	308	17	33,53,73	2.19	9 (27%)	37,89,113	3.30	19 (51%)
22	CLA	r	309	-	33,53,73	2.10	8 (24%)	37,89,113	3.41	19 (51%)
22	CLA	r	310	-	33,53,73	2.15	8 (24%)	37,89,113	3.30	17 (45%)
22	CLA	r	311	17	33,53,73	2.14	9 (27%)	37,89,113	3.50	17 (45%)
22	CLA	r	312	20,17	33,53,73	2.18	11 (33%)	37,89,113	3.36	20 (54%)
22	CLA	s	301	-	33,53,73	2.17	9 (27%)	37,89,113	3.22	19 (51%)
25	CHL	s	302	18	41,54,74	5.54	25 (60%)	24,90,114	3.58	14 (58%)
22	CLA	s	303	18	33,53,73	2.12	9 (27%)	37,89,113	3.41	19 (51%)
22	CLA	s	304	-	33,53,73	2.19	9 (27%)	37,89,113	3.09	17 (45%)
22	CLA	s	305	-	33,53,73	2.12	8 (24%)	37,89,113	3.48	19 (51%)
25	CHL	s	306	18	41,54,74	5.42	24 (58%)	24,90,114	3.79	15 (62%)
25	CHL	s	307	-	41,54,74	5.53	24 (58%)	24,90,114	8.30	17 (70%)
25	CHL	s	308	-	41,54,74	5.50	26 (63%)	24,90,114	3.52	15 (62%)
22	CLA	s	309	18	33,53,73	2.16	9 (27%)	37,89,113	3.32	19 (51%)
22	CLA	s	310	18	33,53,73	2.06	9 (27%)	37,89,113	3.37	19 (51%)
22	CLA	s	311	-	33,53,73	2.07	7 (21%)	37,89,113	3.43	19 (51%)
22	CLA	s	312	18	33,53,73	2.08	9 (27%)	37,89,113	3.44	20 (54%)
22	CLA	s	313	18	33,53,73	2.03	8 (24%)	37,89,113	3.42	21 (56%)
22	CLA	s	314	-	33,53,73	2.05	8 (24%)	37,89,113	3.53	19 (51%)
25	CHL	y	601	19	41,54,74	5.46	25 (60%)	24,90,114	3.56	15 (62%)
22	CLA	y	602	19	33,53,73	2.11	9 (27%)	37,89,113	3.46	17 (45%)
22	CLA	y	603	-	33,53,73	2.00	8 (24%)	37,89,113	3.45	20 (54%)
22	CLA	y	604	-	33,53,73	2.04	8 (24%)	37,89,113	3.66	19 (51%)
25	CHL	y	605	19	40,50,74	5.68	24 (60%)	25,85,114	3.43	18 (72%)
25	CHL	y	606	-	41,54,74	5.47	23 (56%)	24,90,114	3.83	14 (58%)
25	CHL	y	607	-	41,54,74	5.53	25 (60%)	24,90,114	3.67	17 (70%)
25	CHL	y	608	-	41,54,74	5.55	25 (60%)	24,90,114	3.53	15 (62%)
25	CHL	y	609	19	41,54,74	5.67	24 (58%)	24,90,114	3.67	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	y	610	19	33,53,73	2.13	8 (24%)	37,89,113	3.42	18 (48%)
22	CLA	y	611	-	33,53,73	2.05	8 (24%)	37,89,113	3.54	18 (48%)
22	CLA	y	612	19	33,53,73	1.99	8 (24%)	37,89,113	3.29	20 (54%)
22	CLA	y	613	19	33,53,73	2.02	9 (27%)	37,89,113	3.60	17 (45%)
22	CLA	y	614	-	33,53,73	2.07	7 (21%)	37,89,113	3.46	21 (56%)

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
25	CHL	1	601	19	-	0/15/153/177	0/0/9/9
22	CLA	1	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	1	605	19	-	0/12/148/177	0/0/9/9
25	CHL	1	606	-	-	1/15/153/177	0/0/9/9
25	CHL	1	607	-	-	0/15/153/177	0/0/9/9
25	CHL	1	608	-	-	0/15/153/177	0/0/9/9
25	CHL	1	609	19	-	0/15/153/177	0/0/9/9
22	CLA	1	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	1	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	1	615	-	-	0/15/153/177	0/0/9/9
25	CHL	2	601	19	-	0/15/153/177	0/0/9/9
22	CLA	2	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	2	605	19	-	0/12/148/177	0/0/9/9
25	CHL	2	606	-	-	1/15/153/177	0/0/9/9
25	CHL	2	607	-	-	0/15/153/177	0/0/9/9
25	CHL	2	608	19	-	0/15/153/177	0/0/9/9
22	CLA	2	609	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	611	19	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	2	613	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	3	301	-	-	0/15/153/177	0/0/9/9
25	CHL	3	302	19	-	0/15/153/177	0/0/9/9
22	CLA	3	303	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	3	306	19	-	0/12/148/177	0/0/9/9
25	CHL	3	307	-	-	1/15/153/177	0/0/9/9
25	CHL	3	308	-	-	0/15/153/177	0/0/9/9
25	CHL	3	309	19	-	0/15/153/177	0/0/9/9
22	CLA	3	310	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	312	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	313	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	3	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	4	301	-	-	0/15/153/177	0/0/9/9
22	CLA	4	302	20	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	4	303	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	4	304	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	4	305	20	-	0/15/153/177	0/0/9/9
25	CHL	4	306	-	-	0/15/153/177	0/0/9/9
25	CHL	4	307	-	-	0/15/153/177	0/0/9/9
25	CHL	4	308	20	-	0/15/153/177	0/0/9/9
22	CLA	4	309	20	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	4	310	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	5	601	19	-	0/15/153/177	0/0/9/9
22	CLA	5	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	5	605	19	-	0/12/148/177	0/0/9/9
25	CHL	5	606	-	-	1/15/153/177	0/0/9/9
25	CHL	5	607	-	-	0/15/153/177	0/0/9/9
25	CHL	5	608	-	-	0/15/153/177	0/0/9/9
25	CHL	5	609	19	-	0/15/153/177	0/0/9/9
22	CLA	5	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	611	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	5	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	5	615	-	-	0/15/153/177	0/0/9/9
25	CHL	6	601	19	-	0/15/153/177	0/0/9/9
22	CLA	6	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	6	605	19	-	0/12/148/177	0/0/9/9
25	CHL	6	606	-	-	1/15/153/177	0/0/9/9
25	CHL	6	607	-	-	0/15/153/177	0/0/9/9
25	CHL	6	608	19	-	0/15/153/177	0/0/9/9
22	CLA	6	609	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	611	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	6	613	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	7	301	-	-	0/15/153/177	0/0/9/9
25	CHL	7	302	19	-	0/15/153/177	0/0/9/9
22	CLA	7	303	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	7	306	19	-	0/12/148/177	0/0/9/9
25	CHL	7	307	-	-	1/15/153/177	0/0/9/9
25	CHL	7	308	-	-	0/15/153/177	0/0/9/9
25	CHL	7	309	19	-	0/15/153/177	0/0/9/9
22	CLA	7	310	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	312	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	313	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	7	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	8	301	-	-	0/15/153/177	0/0/9/9
22	CLA	8	302	20	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	8	303	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	8	304	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	8	305	20	-	0/15/153/177	0/0/9/9
25	CHL	8	306	-	-	0/15/153/177	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	8	307	-	-	0/15/153/177	0/0/9/9
25	CHL	8	308	20	-	0/15/153/177	0/0/9/9
22	CLA	8	309	20	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	8	310	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	A	402	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	A	403	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	A	404	-	-	0/27/79/103	0/1/6/6
22	CLA	A	405	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	601	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	602	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	603	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	604	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	605	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	606	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	607	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	608	-	1/1/16/25	0/11/111/135	0/0/9/9
22	CLA	B	609	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	B	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	612	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	613	-	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	B	614	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	615	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	B	616	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	501	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	502	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	503	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	504	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	505	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	C	506	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	507	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	508	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	509	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	510	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	C	511	3	1/1/16/25	1/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	512	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	D	401	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	D	402	-	-	0/27/79/103	0/1/6/6
22	CLA	D	403	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	D	404	-	3/3/16/25	0/11/111/135	0/0/9/9
24	HEM	E	101	5,6	-	0/6/54/54	0/0/8/8
25	CHL	G	601	19	-	0/15/153/177	0/0/9/9
22	CLA	G	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	G	605	19	-	0/12/148/177	0/0/9/9
25	CHL	G	606	-	-	1/15/153/177	0/0/9/9
25	CHL	G	607	-	-	0/15/153/177	0/0/9/9
25	CHL	G	608	-	-	0/15/153/177	0/0/9/9
25	CHL	G	609	19	-	0/15/153/177	0/0/9/9
22	CLA	G	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	G	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	N	601	19	-	0/15/153/177	0/0/9/9
22	CLA	N	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	N	605	19	-	0/12/148/177	0/0/9/9
25	CHL	N	606	-	-	1/15/153/177	0/0/9/9
25	CHL	N	607	-	-	0/15/153/177	0/0/9/9
25	CHL	N	608	-	-	0/15/153/177	0/0/9/9
25	CHL	N	609	19	-	0/15/153/177	0/0/9/9
22	CLA	N	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	N	614	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	301	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	302	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	303	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	R	304	-	-	0/15/153/177	0/0/9/9
25	CHL	R	305	-	-	1/15/153/177	0/0/9/9
25	CHL	R	306	-	-	0/15/153/177	0/0/9/9
22	CLA	R	307	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	308	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	309	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	310	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	311	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	R	312	20,17	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	S	301	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	S	302	18	-	0/15/153/177	0/0/9/9
22	CLA	S	303	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	S	306	18	-	0/15/153/177	0/0/9/9
25	CHL	S	307	-	-	0/15/153/177	0/0/9/9
25	CHL	S	308	-	-	0/15/153/177	0/0/9/9
22	CLA	S	309	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	310	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	S	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	312	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	S	313	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	S	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	Y	601	19	-	0/15/153/177	0/0/9/9
22	CLA	Y	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	Y	605	19	-	0/12/148/177	0/0/9/9
25	CHL	Y	606	-	-	1/15/153/177	0/0/9/9
25	CHL	Y	607	-	-	0/15/153/177	0/0/9/9
25	CHL	Y	608	-	-	0/15/153/177	0/0/9/9
25	CHL	Y	609	19	-	0/15/153/177	0/0/9/9
22	CLA	Y	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	Y	614	-	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	402	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	a	403	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	a	404	-	-	0/27/79/103	0/1/6/6
22	CLA	a	405	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	601	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	602	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	603	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	604	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	605	-	1/1/16/25	0/11/111/135	0/0/9/9
22	CLA	b	606	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	607	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	608	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	609	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	610	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	611	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	612	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	613	-	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	b	614	-	2/2/16/25	0/11/111/135	0/0/9/9
22	CLA	b	615	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	b	616	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	501	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	502	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	503	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	504	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	505	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	506	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	507	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	508	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	509	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	510	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	c	511	3	1/1/16/25	1/11/111/135	0/0/9/9
22	CLA	c	512	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	d	401	-	3/3/16/25	0/11/111/135	0/0/9/9
23	PHO	d	402	-	-	0/27/79/103	0/1/6/6
22	CLA	d	403	-	2/2/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	404	-	3/3/16/25	0/11/111/135	0/0/9/9
24	HEM	e	101	5,6	-	0/6/54/54	0/0/8/8
25	CHL	g	601	19	-	0/15/153/177	0/0/9/9
22	CLA	g	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	g	605	19	-	0/12/148/177	0/0/9/9
25	CHL	g	606	-	-	1/15/153/177	0/0/9/9
25	CHL	g	607	-	-	0/15/153/177	0/0/9/9
25	CHL	g	608	-	-	0/15/153/177	0/0/9/9
25	CHL	g	609	19	-	0/15/153/177	0/0/9/9
22	CLA	g	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	g	614	-	3/3/16/25	1/11/111/135	0/0/9/9
25	CHL	n	601	19	-	0/15/153/177	0/0/9/9
22	CLA	n	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	n	605	19	-	0/12/148/177	0/0/9/9
25	CHL	n	606	-	-	1/15/153/177	0/0/9/9
25	CHL	n	607	-	-	0/15/153/177	0/0/9/9
25	CHL	n	608	-	-	0/15/153/177	0/0/9/9
25	CHL	n	609	19	-	0/15/153/177	0/0/9/9
22	CLA	n	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	n	614	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	301	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	302	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	303	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	r	304	-	-	0/15/153/177	0/0/9/9
25	CHL	r	305	-	-	1/15/153/177	0/0/9/9
25	CHL	r	306	-	-	0/15/153/177	0/0/9/9
22	CLA	r	307	17	3/3/16/25	0/11/111/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	r	308	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	309	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	310	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	311	17	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	r	312	20,17	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	s	301	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	s	302	18	-	0/15/153/177	0/0/9/9
22	CLA	s	303	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	304	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	305	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	s	306	18	-	0/15/153/177	0/0/9/9
25	CHL	s	307	-	-	0/15/153/177	0/0/9/9
25	CHL	s	308	-	-	0/15/153/177	0/0/9/9
22	CLA	s	309	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	310	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	s	311	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	312	18	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	s	313	18	3/3/16/25	1/11/111/135	0/0/9/9
22	CLA	s	314	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	y	601	19	-	0/15/153/177	0/0/9/9
22	CLA	y	602	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	603	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	604	-	3/3/16/25	0/11/111/135	0/0/9/9
25	CHL	y	605	19	-	0/12/148/177	0/0/9/9
25	CHL	y	606	-	-	1/15/153/177	0/0/9/9
25	CHL	y	607	-	-	0/15/153/177	0/0/9/9
25	CHL	y	608	-	-	0/15/153/177	0/0/9/9
25	CHL	y	609	19	-	0/15/153/177	0/0/9/9
22	CLA	y	610	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	611	-	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	612	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	613	19	3/3/16/25	0/11/111/135	0/0/9/9
22	CLA	y	614	-	3/3/16/25	0/11/111/135	0/0/9/9

All (4253) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	608	CHL	C3B-C2B	-15.86	1.35	1.55
25	G	608	CHL	C3B-C2B	-15.86	1.35	1.55
25	g	606	CHL	C3B-C2B	-15.69	1.36	1.55
25	G	606	CHL	C3B-C2B	-15.69	1.36	1.55
25	y	608	CHL	C3B-C2B	-15.63	1.36	1.55
25	Y	608	CHL	C3B-C2B	-15.63	1.36	1.55
25	n	606	CHL	C3B-C2B	-15.46	1.36	1.55
25	N	606	CHL	C3B-C2B	-15.46	1.36	1.55
25	Y	605	CHL	C3B-C2B	-15.44	1.36	1.55
25	y	605	CHL	C3B-C2B	-15.44	1.36	1.55
25	S	302	CHL	C3B-C2B	-15.33	1.36	1.55
25	s	302	CHL	C3B-C2B	-15.33	1.36	1.55
25	N	608	CHL	C3B-C2B	-15.31	1.36	1.55
25	n	608	CHL	C3B-C2B	-15.31	1.36	1.55
25	s	307	CHL	C3B-C2B	-15.23	1.36	1.55
25	S	307	CHL	C3B-C2B	-15.23	1.36	1.55
25	y	609	CHL	C3B-C2B	-15.22	1.36	1.55
25	Y	609	CHL	C3B-C2B	-15.22	1.36	1.55
25	2	606	CHL	C3B-C2B	-15.21	1.36	1.55
25	6	606	CHL	C3B-C2B	-15.21	1.36	1.55
25	S	308	CHL	C3B-C2B	-15.17	1.36	1.55
25	s	308	CHL	C3B-C2B	-15.17	1.36	1.55
25	N	601	CHL	C3B-C2B	-15.16	1.36	1.55
25	n	601	CHL	C3B-C2B	-15.16	1.36	1.55
25	1	608	CHL	C3B-C2B	-15.15	1.36	1.55
25	r	305	CHL	C3B-C2B	-15.15	1.36	1.55
25	5	608	CHL	C3B-C2B	-15.15	1.36	1.55
25	R	305	CHL	C3B-C2B	-15.15	1.36	1.55
25	R	304	CHL	C3B-C2B	-15.15	1.36	1.55
25	r	304	CHL	C3B-C2B	-15.15	1.36	1.55
25	n	607	CHL	C3B-C2B	-15.12	1.36	1.55
25	N	607	CHL	C3B-C2B	-15.12	1.36	1.55
25	Y	607	CHL	C3B-C2B	-15.11	1.36	1.55
25	y	607	CHL	C3B-C2B	-15.11	1.36	1.55
25	8	308	CHL	C3B-C2B	-15.04	1.36	1.55
25	4	308	CHL	C3B-C2B	-15.04	1.36	1.55
25	s	306	CHL	C3B-C2B	-15.01	1.36	1.55
25	S	306	CHL	C3B-C2B	-15.01	1.36	1.55
25	N	605	CHL	C3B-C2B	-14.99	1.36	1.55
25	n	605	CHL	C3B-C2B	-14.99	1.36	1.55
25	6	608	CHL	C3B-C2B	-14.96	1.36	1.55
25	2	608	CHL	C3B-C2B	-14.96	1.36	1.55
25	3	302	CHL	C3B-C2B	-14.95	1.36	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	302	CHL	C3B-C2B	-14.95	1.36	1.55
25	y	606	CHL	C3B-C2B	-14.95	1.36	1.55
25	Y	606	CHL	C3B-C2B	-14.95	1.36	1.55
25	n	609	CHL	C3B-C2B	-14.94	1.36	1.55
25	N	609	CHL	C3B-C2B	-14.94	1.36	1.55
25	6	601	CHL	C3B-C2B	-14.94	1.36	1.55
25	2	601	CHL	C3B-C2B	-14.94	1.36	1.55
25	4	307	CHL	C3B-C2B	-14.93	1.36	1.55
25	8	307	CHL	C3B-C2B	-14.93	1.36	1.55
25	4	306	CHL	C3B-C2B	-14.92	1.36	1.55
25	8	306	CHL	C3B-C2B	-14.92	1.36	1.55
25	g	601	CHL	C3B-C2B	-14.90	1.37	1.55
25	G	601	CHL	C3B-C2B	-14.90	1.37	1.55
25	2	607	CHL	C3B-C2B	-14.90	1.37	1.55
25	6	607	CHL	C3B-C2B	-14.90	1.37	1.55
25	1	607	CHL	C3B-C2B	-14.88	1.37	1.55
25	5	607	CHL	C3B-C2B	-14.88	1.37	1.55
25	r	306	CHL	C3B-C2B	-14.87	1.37	1.55
25	R	306	CHL	C3B-C2B	-14.87	1.37	1.55
25	G	609	CHL	C3B-C2B	-14.85	1.37	1.55
25	g	609	CHL	C3B-C2B	-14.85	1.37	1.55
25	1	605	CHL	C3B-C2B	-14.85	1.37	1.55
25	4	301	CHL	C3B-C2B	-14.85	1.37	1.55
25	5	605	CHL	C3B-C2B	-14.85	1.37	1.55
25	8	301	CHL	C3B-C2B	-14.85	1.37	1.55
25	7	308	CHL	C3B-C2B	-14.85	1.37	1.55
25	3	308	CHL	C3B-C2B	-14.85	1.37	1.55
25	7	309	CHL	C3B-C2B	-14.84	1.37	1.55
25	3	309	CHL	C3B-C2B	-14.84	1.37	1.55
25	G	607	CHL	C3B-C2B	-14.82	1.37	1.55
25	g	607	CHL	C3B-C2B	-14.82	1.37	1.55
25	5	615	CHL	C3B-C2B	-14.82	1.37	1.55
25	1	615	CHL	C3B-C2B	-14.82	1.37	1.55
25	8	305	CHL	C3B-C2B	-14.81	1.37	1.55
25	4	305	CHL	C3B-C2B	-14.81	1.37	1.55
25	g	605	CHL	C3B-C2B	-14.80	1.37	1.55
25	G	605	CHL	C3B-C2B	-14.80	1.37	1.55
25	3	306	CHL	C3B-C2B	-14.80	1.37	1.55
25	7	306	CHL	C3B-C2B	-14.80	1.37	1.55
25	1	606	CHL	C3B-C2B	-14.78	1.37	1.55
25	5	606	CHL	C3B-C2B	-14.78	1.37	1.55
25	7	307	CHL	C3B-C2B	-14.75	1.37	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	307	CHL	C3B-C2B	-14.75	1.37	1.55
25	3	301	CHL	C3B-C2B	-14.72	1.37	1.55
25	7	301	CHL	C3B-C2B	-14.72	1.37	1.55
25	2	605	CHL	C3B-C2B	-14.71	1.37	1.55
25	6	605	CHL	C3B-C2B	-14.71	1.37	1.55
25	1	609	CHL	C3B-C2B	-14.70	1.37	1.55
25	5	609	CHL	C3B-C2B	-14.70	1.37	1.55
25	1	601	CHL	C3B-C2B	-14.69	1.37	1.55
25	5	601	CHL	C3B-C2B	-14.69	1.37	1.55
25	Y	601	CHL	C3B-C2B	-14.67	1.37	1.55
25	y	601	CHL	C3B-C2B	-14.67	1.37	1.55
25	N	608	CHL	C3D-C4D	-11.13	1.41	1.54
25	n	608	CHL	C3D-C4D	-11.13	1.41	1.54
25	n	606	CHL	C3D-C4D	-11.08	1.41	1.54
25	N	606	CHL	C3D-C4D	-11.08	1.41	1.54
25	n	609	CHL	C3D-C4D	-10.98	1.42	1.54
25	N	609	CHL	C3D-C4D	-10.98	1.42	1.54
25	g	608	CHL	C3D-C4D	-10.98	1.42	1.54
25	G	608	CHL	C3D-C4D	-10.98	1.42	1.54
25	y	606	CHL	C3D-C4D	-10.97	1.42	1.54
25	Y	606	CHL	C3D-C4D	-10.97	1.42	1.54
25	3	301	CHL	C3D-C4D	-10.95	1.42	1.54
25	7	301	CHL	C3D-C4D	-10.95	1.42	1.54
25	4	301	CHL	C3D-C4D	-10.90	1.42	1.54
25	8	301	CHL	C3D-C4D	-10.90	1.42	1.54
25	y	609	CHL	C3D-C4D	-10.89	1.42	1.54
25	Y	609	CHL	C3D-C4D	-10.89	1.42	1.54
25	s	306	CHL	C3D-C4D	-10.89	1.42	1.54
25	S	306	CHL	C3D-C4D	-10.89	1.42	1.54
25	S	302	CHL	C3D-C4D	-10.83	1.42	1.54
25	s	302	CHL	C3D-C4D	-10.83	1.42	1.54
25	y	608	CHL	C3D-C4D	-10.82	1.42	1.54
25	g	606	CHL	C3D-C4D	-10.82	1.42	1.54
25	Y	608	CHL	C3D-C4D	-10.82	1.42	1.54
25	G	606	CHL	C3D-C4D	-10.82	1.42	1.54
25	N	605	CHL	C3D-C4D	-10.80	1.42	1.54
25	n	605	CHL	C3D-C4D	-10.80	1.42	1.54
25	R	304	CHL	C3D-C4D	-10.80	1.42	1.54
25	r	304	CHL	C3D-C4D	-10.80	1.42	1.54
25	n	607	CHL	C3D-C4D	-10.78	1.42	1.54
25	N	607	CHL	C3D-C4D	-10.78	1.42	1.54
25	Y	605	CHL	C3D-C4D	-10.76	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	605	CHL	C3D-C4D	-10.76	1.42	1.54
25	G	609	CHL	C3D-C4D	-10.76	1.42	1.54
25	g	609	CHL	C3D-C4D	-10.76	1.42	1.54
25	r	305	CHL	C3D-C4D	-10.71	1.42	1.54
25	R	305	CHL	C3D-C4D	-10.71	1.42	1.54
25	8	305	CHL	C3D-C4D	-10.71	1.42	1.54
25	4	305	CHL	C3D-C4D	-10.71	1.42	1.54
25	g	601	CHL	C3D-C4D	-10.64	1.42	1.54
25	G	601	CHL	C3D-C4D	-10.64	1.42	1.54
25	1	609	CHL	C3D-C4D	-10.63	1.42	1.54
25	y	609	CHL	C3B-C4B	-10.63	1.42	1.54
25	5	609	CHL	C3D-C4D	-10.63	1.42	1.54
25	Y	609	CHL	C3B-C4B	-10.63	1.42	1.54
25	Y	607	CHL	C3D-C4D	-10.63	1.42	1.54
25	y	607	CHL	C3D-C4D	-10.63	1.42	1.54
25	G	607	CHL	C3D-C4D	-10.62	1.42	1.54
25	g	607	CHL	C3D-C4D	-10.62	1.42	1.54
25	7	308	CHL	C3D-C4D	-10.62	1.42	1.54
25	3	308	CHL	C3D-C4D	-10.62	1.42	1.54
25	1	606	CHL	C3D-C4D	-10.59	1.42	1.54
25	5	606	CHL	C3D-C4D	-10.59	1.42	1.54
25	r	306	CHL	C3D-C4D	-10.57	1.42	1.54
25	R	306	CHL	C3D-C4D	-10.57	1.42	1.54
25	Y	601	CHL	C3D-C4D	-10.57	1.42	1.54
25	y	601	CHL	C3D-C4D	-10.57	1.42	1.54
25	S	308	CHL	C3D-C4D	-10.55	1.42	1.54
25	s	308	CHL	C3D-C4D	-10.55	1.42	1.54
25	1	605	CHL	C3D-C4D	-10.52	1.42	1.54
25	5	605	CHL	C3D-C4D	-10.52	1.42	1.54
25	N	601	CHL	C3D-C4D	-10.51	1.42	1.54
25	n	601	CHL	C3D-C4D	-10.51	1.42	1.54
25	6	608	CHL	C3D-C4D	-10.50	1.42	1.54
25	2	608	CHL	C3D-C4D	-10.50	1.42	1.54
25	8	308	CHL	C3D-C4D	-10.49	1.42	1.54
25	4	308	CHL	C3D-C4D	-10.49	1.42	1.54
25	s	307	CHL	C3D-C4D	-10.44	1.42	1.54
25	S	307	CHL	C3D-C4D	-10.44	1.42	1.54
25	2	606	CHL	C3D-C4D	-10.42	1.42	1.54
25	6	606	CHL	C3D-C4D	-10.42	1.42	1.54
25	1	608	CHL	C3D-C4D	-10.39	1.42	1.54
25	5	608	CHL	C3D-C4D	-10.39	1.42	1.54
25	1	607	CHL	C3D-C4D	-10.37	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	607	CHL	C3D-C4D	-10.37	1.42	1.54
25	4	306	CHL	C3D-C4D	-10.35	1.42	1.54
25	8	306	CHL	C3D-C4D	-10.35	1.42	1.54
25	7	309	CHL	C3D-C4D	-10.32	1.42	1.54
25	3	309	CHL	C3D-C4D	-10.32	1.42	1.54
25	7	307	CHL	C3D-C4D	-10.32	1.42	1.54
25	3	307	CHL	C3D-C4D	-10.32	1.42	1.54
25	4	307	CHL	C3D-C4D	-10.30	1.42	1.54
25	8	307	CHL	C3D-C4D	-10.30	1.42	1.54
25	3	302	CHL	C3D-C4D	-10.28	1.42	1.54
25	7	302	CHL	C3D-C4D	-10.28	1.42	1.54
25	g	605	CHL	C3D-C4D	-10.27	1.42	1.54
25	G	605	CHL	C3D-C4D	-10.27	1.42	1.54
25	2	607	CHL	C3D-C4D	-10.26	1.42	1.54
25	6	607	CHL	C3D-C4D	-10.26	1.42	1.54
25	5	615	CHL	C3D-C4D	-10.25	1.42	1.54
25	1	615	CHL	C3D-C4D	-10.25	1.42	1.54
25	g	606	CHL	C3B-C4B	-10.23	1.42	1.54
25	G	606	CHL	C3B-C4B	-10.23	1.42	1.54
25	n	606	CHL	C3B-C4B	-10.19	1.42	1.54
25	N	606	CHL	C3B-C4B	-10.19	1.42	1.54
25	6	601	CHL	C3D-C4D	-10.19	1.42	1.54
25	2	601	CHL	C3D-C4D	-10.19	1.42	1.54
25	2	605	CHL	C3D-C4D	-10.18	1.42	1.54
25	6	605	CHL	C3D-C4D	-10.18	1.42	1.54
25	3	306	CHL	C3D-C4D	-10.17	1.42	1.54
25	7	306	CHL	C3D-C4D	-10.17	1.42	1.54
25	1	601	CHL	C3D-C4D	-10.15	1.42	1.54
25	5	601	CHL	C3D-C4D	-10.15	1.42	1.54
25	Y	605	CHL	C3B-C4B	-10.03	1.43	1.54
25	y	605	CHL	C3B-C4B	-10.03	1.43	1.54
25	n	609	CHL	C3B-C4B	-9.89	1.43	1.54
25	N	609	CHL	C3B-C4B	-9.89	1.43	1.54
25	R	304	CHL	C3B-C4B	-9.86	1.43	1.54
25	r	304	CHL	C3B-C4B	-9.86	1.43	1.54
25	n	609	CHL	CHD-C1D	-9.82	1.37	1.53
25	N	609	CHL	CHD-C1D	-9.82	1.37	1.53
25	Y	607	CHL	C3B-C4B	-9.72	1.43	1.54
25	y	607	CHL	C3B-C4B	-9.72	1.43	1.54
25	y	609	CHL	CHC-C4B	-9.69	1.37	1.53
25	Y	609	CHL	CHC-C4B	-9.69	1.37	1.53
25	G	609	CHL	CHD-C1D	-9.63	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	609	CHL	CHD-C1D	-9.63	1.38	1.53
25	y	606	CHL	C3B-C4B	-9.57	1.43	1.54
25	Y	606	CHL	C3B-C4B	-9.57	1.43	1.54
25	Y	605	CHL	CHC-C4B	-9.56	1.38	1.53
25	y	605	CHL	CHC-C4B	-9.56	1.38	1.53
25	y	608	CHL	CHB-C1B	-9.55	1.38	1.53
25	Y	608	CHL	CHB-C1B	-9.55	1.38	1.53
25	n	607	CHL	CHD-C1D	-9.54	1.38	1.53
25	N	607	CHL	CHD-C1D	-9.54	1.38	1.53
25	s	307	CHL	C3B-C4B	-9.53	1.43	1.54
25	S	307	CHL	C3B-C4B	-9.53	1.43	1.54
25	Y	605	CHL	CHD-C1D	-9.52	1.38	1.53
25	y	605	CHL	CHD-C1D	-9.52	1.38	1.53
25	n	606	CHL	CHC-C4B	-9.49	1.38	1.53
25	N	606	CHL	CHC-C4B	-9.49	1.38	1.53
25	Y	601	CHL	CHD-C1D	-9.49	1.38	1.53
25	y	601	CHL	CHD-C1D	-9.49	1.38	1.53
25	n	607	CHL	C3B-C4B	-9.47	1.43	1.54
25	N	607	CHL	C3B-C4B	-9.47	1.43	1.54
25	G	609	CHL	C3B-C4B	-9.45	1.43	1.54
25	g	609	CHL	C3B-C4B	-9.45	1.43	1.54
25	2	606	CHL	C3B-C4B	-9.39	1.43	1.54
25	6	606	CHL	C3B-C4B	-9.39	1.43	1.54
25	G	607	CHL	CHD-C1D	-9.39	1.38	1.53
25	g	607	CHL	CHD-C1D	-9.39	1.38	1.53
25	S	308	CHL	CHD-C1D	-9.38	1.38	1.53
25	s	308	CHL	CHD-C1D	-9.38	1.38	1.53
25	r	305	CHL	C3B-C4B	-9.35	1.43	1.54
25	R	305	CHL	C3B-C4B	-9.35	1.43	1.54
25	N	605	CHL	CHD-C1D	-9.34	1.38	1.53
25	n	605	CHL	CHD-C1D	-9.34	1.38	1.53
25	Y	607	CHL	CHD-C1D	-9.34	1.38	1.53
25	y	607	CHL	CHD-C1D	-9.34	1.38	1.53
25	n	609	CHL	CHC-C4B	-9.32	1.38	1.53
25	N	609	CHL	CHC-C4B	-9.32	1.38	1.53
25	7	309	CHL	C3B-C4B	-9.32	1.43	1.54
25	3	309	CHL	C3B-C4B	-9.32	1.43	1.54
25	N	601	CHL	C3B-C4B	-9.31	1.43	1.54
25	n	601	CHL	C3B-C4B	-9.31	1.43	1.54
25	y	609	CHL	CHD-C1D	-9.27	1.38	1.53
25	Y	609	CHL	CHD-C1D	-9.27	1.38	1.53
25	Y	607	CHL	CHC-C4B	-9.27	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	607	CHL	CHC-C4B	-9.27	1.38	1.53
25	N	608	CHL	CHC-C4B	-9.24	1.38	1.53
25	n	608	CHL	CHC-C4B	-9.24	1.38	1.53
25	g	606	CHL	CHC-C4B	-9.24	1.38	1.53
25	G	606	CHL	CHC-C4B	-9.24	1.38	1.53
25	y	606	CHL	CHC-C4B	-9.23	1.38	1.53
25	Y	606	CHL	CHC-C4B	-9.23	1.38	1.53
25	6	608	CHL	C3B-C4B	-9.22	1.44	1.54
25	2	608	CHL	C3B-C4B	-9.22	1.44	1.54
25	S	302	CHL	CHB-C1B	-9.20	1.38	1.53
25	s	302	CHL	CHB-C1B	-9.20	1.38	1.53
25	N	601	CHL	CHD-C1D	-9.19	1.38	1.53
25	n	601	CHL	CHD-C1D	-9.19	1.38	1.53
25	S	308	CHL	CHB-C1B	-9.17	1.38	1.53
25	s	308	CHL	CHB-C1B	-9.17	1.38	1.53
25	R	304	CHL	CHC-C4B	-9.16	1.38	1.53
25	r	304	CHL	CHC-C4B	-9.16	1.38	1.53
25	s	306	CHL	C3B-C4B	-9.15	1.44	1.54
25	S	306	CHL	C3B-C4B	-9.15	1.44	1.54
25	1	609	CHL	C3B-C4B	-9.15	1.44	1.54
25	5	609	CHL	C3B-C4B	-9.15	1.44	1.54
25	r	305	CHL	CHD-C1D	-9.15	1.38	1.53
25	R	305	CHL	CHD-C1D	-9.15	1.38	1.53
25	n	607	CHL	CHC-C4B	-9.14	1.38	1.53
25	N	607	CHL	CHC-C4B	-9.14	1.38	1.53
25	1	606	CHL	C3B-C4B	-9.12	1.44	1.54
25	5	606	CHL	C3B-C4B	-9.12	1.44	1.54
25	g	608	CHL	CHC-C4B	-9.12	1.38	1.53
25	G	608	CHL	CHC-C4B	-9.12	1.38	1.53
25	r	306	CHL	CHD-C1D	-9.12	1.38	1.53
25	S	302	CHL	CHD-C1D	-9.12	1.38	1.53
25	R	306	CHL	CHD-C1D	-9.12	1.38	1.53
25	s	302	CHL	CHD-C1D	-9.12	1.38	1.53
25	N	605	CHL	C3B-C4B	-9.11	1.44	1.54
25	n	605	CHL	C3B-C4B	-9.11	1.44	1.54
25	s	307	CHL	CHC-C4B	-9.11	1.38	1.53
25	S	307	CHL	CHC-C4B	-9.11	1.38	1.53
25	G	609	CHL	CHC-C4B	-9.09	1.38	1.53
25	g	609	CHL	CHC-C4B	-9.09	1.38	1.53
25	1	607	CHL	C3B-C4B	-9.08	1.44	1.54
25	5	607	CHL	C3B-C4B	-9.08	1.44	1.54
25	n	609	CHL	CHD-C4C	-9.07	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	609	CHL	CHD-C4C	-9.07	1.37	1.53
25	7	309	CHL	CHD-C1D	-9.07	1.38	1.53
25	3	309	CHL	CHD-C1D	-9.07	1.38	1.53
25	y	608	CHL	CHC-C4B	-9.05	1.39	1.53
25	Y	608	CHL	CHC-C4B	-9.05	1.39	1.53
25	s	307	CHL	CHD-C1D	-9.04	1.39	1.53
25	S	307	CHL	CHD-C1D	-9.04	1.39	1.53
25	N	608	CHL	C3B-C4B	-9.04	1.44	1.54
25	n	608	CHL	C3B-C4B	-9.04	1.44	1.54
25	N	601	CHL	CHC-C4B	-9.03	1.39	1.53
25	n	601	CHL	CHC-C4B	-9.03	1.39	1.53
25	8	308	CHL	CHC-C4B	-9.02	1.39	1.53
25	4	308	CHL	CHC-C4B	-9.02	1.39	1.53
25	2	605	CHL	CHD-C1D	-9.02	1.39	1.53
25	6	605	CHL	CHD-C1D	-9.02	1.39	1.53
25	g	601	CHL	CHD-C1D	-9.02	1.39	1.53
25	G	601	CHL	CHD-C1D	-9.02	1.39	1.53
25	g	608	CHL	CHB-C1B	-9.01	1.39	1.53
25	G	608	CHL	CHB-C1B	-9.01	1.39	1.53
25	1	605	CHL	CHD-C1D	-9.01	1.39	1.53
25	5	605	CHL	CHD-C1D	-9.01	1.39	1.53
25	S	308	CHL	CHC-C4B	-8.99	1.39	1.53
25	s	308	CHL	CHC-C4B	-8.99	1.39	1.53
25	s	307	CHL	CHB-C1B	-8.99	1.39	1.53
25	S	307	CHL	CHB-C1B	-8.99	1.39	1.53
25	6	608	CHL	CHD-C1D	-8.98	1.39	1.53
25	N	605	CHL	CHC-C4B	-8.98	1.39	1.53
25	n	605	CHL	CHC-C4B	-8.98	1.39	1.53
25	2	608	CHL	CHD-C1D	-8.98	1.39	1.53
25	4	306	CHL	C3B-C4B	-8.97	1.44	1.54
25	8	306	CHL	C3B-C4B	-8.97	1.44	1.54
25	S	302	CHL	C3B-C4B	-8.97	1.44	1.54
25	s	302	CHL	C3B-C4B	-8.97	1.44	1.54
25	g	605	CHL	C3B-C4B	-8.97	1.44	1.54
25	G	605	CHL	C3B-C4B	-8.97	1.44	1.54
25	N	608	CHL	CHB-C1B	-8.96	1.39	1.53
25	n	608	CHL	CHB-C1B	-8.96	1.39	1.53
25	1	605	CHL	CHC-C4B	-8.96	1.39	1.53
25	5	605	CHL	CHC-C4B	-8.96	1.39	1.53
25	3	306	CHL	CHD-C1D	-8.96	1.39	1.53
25	7	306	CHL	CHD-C1D	-8.96	1.39	1.53
25	1	609	CHL	CHD-C1D	-8.96	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	609	CHL	CHD-C1D	-8.96	1.39	1.53
25	G	609	CHL	CHD-C4C	-8.95	1.37	1.53
25	g	609	CHL	CHD-C4C	-8.95	1.37	1.53
25	g	601	CHL	C3B-C4B	-8.94	1.44	1.54
25	G	601	CHL	C3B-C4B	-8.94	1.44	1.54
25	r	305	CHL	CHC-C4B	-8.93	1.39	1.53
25	R	305	CHL	CHC-C4B	-8.93	1.39	1.53
25	4	301	CHL	CHC-C4B	-8.93	1.39	1.53
25	8	301	CHL	CHC-C4B	-8.93	1.39	1.53
25	g	601	CHL	CHC-C4B	-8.93	1.39	1.53
25	G	601	CHL	CHC-C4B	-8.93	1.39	1.53
25	1	601	CHL	CHD-C1D	-8.92	1.39	1.53
25	5	601	CHL	CHD-C1D	-8.92	1.39	1.53
25	3	302	CHL	CHB-C1B	-8.92	1.39	1.53
25	7	302	CHL	CHB-C1B	-8.92	1.39	1.53
25	g	601	CHL	CHB-C1B	-8.92	1.39	1.53
25	2	606	CHL	CHC-C4B	-8.92	1.39	1.53
25	6	606	CHL	CHC-C4B	-8.92	1.39	1.53
25	G	601	CHL	CHB-C1B	-8.92	1.39	1.53
25	5	615	CHL	CHD-C1D	-8.90	1.39	1.53
25	1	615	CHL	CHD-C1D	-8.90	1.39	1.53
25	N	601	CHL	CHB-C1B	-8.90	1.39	1.53
25	n	601	CHL	CHB-C1B	-8.90	1.39	1.53
25	1	601	CHL	C3B-C4B	-8.89	1.44	1.54
25	5	601	CHL	C3B-C4B	-8.89	1.44	1.54
25	6	608	CHL	CHC-C4B	-8.89	1.39	1.53
25	2	608	CHL	CHC-C4B	-8.89	1.39	1.53
25	6	601	CHL	CHD-C1D	-8.88	1.39	1.53
25	2	601	CHL	CHD-C1D	-8.88	1.39	1.53
25	3	306	CHL	C3B-C4B	-8.87	1.44	1.54
25	7	306	CHL	C3B-C4B	-8.87	1.44	1.54
25	n	607	CHL	CHB-C1B	-8.87	1.39	1.53
25	N	607	CHL	CHB-C1B	-8.87	1.39	1.53
25	Y	601	CHL	C3B-C4B	-8.86	1.44	1.54
25	y	601	CHL	C3B-C4B	-8.86	1.44	1.54
25	7	309	CHL	CHC-C4B	-8.86	1.39	1.53
25	3	309	CHL	CHC-C4B	-8.86	1.39	1.53
25	4	307	CHL	CHD-C1D	-8.86	1.39	1.53
25	8	307	CHL	CHD-C1D	-8.86	1.39	1.53
25	S	308	CHL	C3B-C4B	-8.86	1.44	1.54
25	s	308	CHL	C3B-C4B	-8.86	1.44	1.54
25	1	605	CHL	C3B-C4B	-8.86	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	605	CHL	C3B-C4B	-8.86	1.44	1.54
25	g	608	CHL	C3B-C4B	-8.85	1.44	1.54
25	G	608	CHL	C3B-C4B	-8.85	1.44	1.54
25	7	307	CHL	C3B-C4B	-8.85	1.44	1.54
25	3	307	CHL	C3B-C4B	-8.85	1.44	1.54
25	8	305	CHL	CHC-C4B	-8.85	1.39	1.53
25	4	305	CHL	CHC-C4B	-8.85	1.39	1.53
25	4	301	CHL	C3B-C4B	-8.85	1.44	1.54
25	8	301	CHL	C3B-C4B	-8.85	1.44	1.54
25	2	605	CHL	C3B-C4B	-8.85	1.44	1.54
25	6	605	CHL	C3B-C4B	-8.85	1.44	1.54
25	4	307	CHL	C3B-C4B	-8.84	1.44	1.54
25	8	307	CHL	C3B-C4B	-8.84	1.44	1.54
25	7	308	CHL	CHD-C1D	-8.84	1.39	1.53
25	3	308	CHL	CHD-C1D	-8.84	1.39	1.53
25	s	306	CHL	CHC-C4B	-8.84	1.39	1.53
25	S	306	CHL	CHC-C4B	-8.84	1.39	1.53
25	g	605	CHL	CHD-C1D	-8.84	1.39	1.53
25	G	605	CHL	CHD-C1D	-8.84	1.39	1.53
25	8	308	CHL	C3B-C4B	-8.83	1.44	1.54
25	4	308	CHL	C3B-C4B	-8.83	1.44	1.54
25	y	608	CHL	C3B-C4B	-8.83	1.44	1.54
25	Y	608	CHL	C3B-C4B	-8.83	1.44	1.54
25	6	601	CHL	CHC-C4B	-8.83	1.39	1.53
25	2	601	CHL	CHC-C4B	-8.83	1.39	1.53
25	3	301	CHL	CHD-C1D	-8.82	1.39	1.53
25	7	301	CHL	CHD-C1D	-8.82	1.39	1.53
25	y	609	CHL	CHB-C1B	-8.82	1.39	1.53
25	Y	609	CHL	CHB-C1B	-8.82	1.39	1.53
25	5	615	CHL	C3B-C4B	-8.82	1.44	1.54
25	1	615	CHL	C3B-C4B	-8.82	1.44	1.54
25	s	306	CHL	CHD-C1D	-8.81	1.39	1.53
25	S	306	CHL	CHD-C1D	-8.81	1.39	1.53
25	1	606	CHL	CHC-C4B	-8.81	1.39	1.53
25	5	606	CHL	CHC-C4B	-8.81	1.39	1.53
25	1	607	CHL	CHC-C4B	-8.80	1.39	1.53
25	g	605	CHL	CHC-C4B	-8.80	1.39	1.53
25	G	605	CHL	CHC-C4B	-8.80	1.39	1.53
25	5	607	CHL	CHC-C4B	-8.80	1.39	1.53
25	S	302	CHL	CHC-C4B	-8.78	1.39	1.53
25	s	302	CHL	CHC-C4B	-8.78	1.39	1.53
25	r	306	CHL	CHC-C4B	-8.78	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	306	CHL	CHC-C4B	-8.78	1.39	1.53
25	n	606	CHL	CHD-C1D	-8.78	1.39	1.53
25	N	606	CHL	CHD-C1D	-8.78	1.39	1.53
25	1	607	CHL	CHD-C1D	-8.77	1.39	1.53
25	5	607	CHL	CHD-C1D	-8.77	1.39	1.53
25	6	608	CHL	CHB-C1B	-8.76	1.39	1.53
25	2	606	CHL	CHD-C1D	-8.76	1.39	1.53
25	6	606	CHL	CHD-C1D	-8.76	1.39	1.53
25	2	608	CHL	CHB-C1B	-8.76	1.39	1.53
25	2	607	CHL	CHC-C4B	-8.76	1.39	1.53
25	4	307	CHL	CHC-C4B	-8.76	1.39	1.53
25	6	607	CHL	CHC-C4B	-8.76	1.39	1.53
25	8	307	CHL	CHC-C4B	-8.76	1.39	1.53
25	2	607	CHL	CHD-C1D	-8.76	1.39	1.53
25	N	608	CHL	CHD-C1D	-8.76	1.39	1.53
25	n	608	CHL	CHD-C1D	-8.76	1.39	1.53
25	6	607	CHL	CHD-C1D	-8.76	1.39	1.53
25	6	601	CHL	C3B-C4B	-8.76	1.44	1.54
25	2	601	CHL	C3B-C4B	-8.76	1.44	1.54
25	Y	601	CHL	CHB-C1B	-8.75	1.39	1.53
25	y	601	CHL	CHB-C1B	-8.75	1.39	1.53
25	3	302	CHL	CHC-C4B	-8.74	1.39	1.53
25	7	302	CHL	CHC-C4B	-8.74	1.39	1.53
25	1	609	CHL	CHC-C4B	-8.73	1.39	1.53
25	5	609	CHL	CHC-C4B	-8.73	1.39	1.53
25	G	607	CHL	CHC-C4B	-8.72	1.39	1.53
25	g	607	CHL	CHC-C4B	-8.72	1.39	1.53
25	G	607	CHL	C3B-C4B	-8.72	1.44	1.54
25	g	607	CHL	C3B-C4B	-8.72	1.44	1.54
25	8	305	CHL	C3B-C4B	-8.72	1.44	1.54
25	4	305	CHL	C3B-C4B	-8.72	1.44	1.54
25	7	307	CHL	CHC-C4B	-8.71	1.39	1.53
25	3	307	CHL	CHC-C4B	-8.71	1.39	1.53
25	r	306	CHL	CHB-C1B	-8.71	1.39	1.53
25	R	306	CHL	CHB-C1B	-8.71	1.39	1.53
25	N	605	CHL	CHB-C1B	-8.70	1.39	1.53
25	4	306	CHL	CHC-C4B	-8.70	1.39	1.53
25	8	306	CHL	CHC-C4B	-8.70	1.39	1.53
25	n	605	CHL	CHB-C1B	-8.70	1.39	1.53
25	4	306	CHL	CHD-C1D	-8.70	1.39	1.53
25	8	306	CHL	CHD-C1D	-8.70	1.39	1.53
25	Y	601	CHL	CHC-C4B	-8.70	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	601	CHL	CHC-C4B	-8.70	1.39	1.53
25	y	606	CHL	CHD-C1D	-8.70	1.39	1.53
25	Y	606	CHL	CHD-C1D	-8.70	1.39	1.53
25	4	301	CHL	CHD-C1D	-8.69	1.39	1.53
25	8	301	CHL	CHD-C1D	-8.69	1.39	1.53
25	8	308	CHL	CHB-C1B	-8.68	1.39	1.53
25	4	308	CHL	CHB-C1B	-8.68	1.39	1.53
25	Y	605	CHL	CHD-C4C	-8.68	1.37	1.53
25	y	605	CHL	CHD-C4C	-8.68	1.37	1.53
25	Y	607	CHL	CHB-C1B	-8.68	1.39	1.53
25	y	607	CHL	CHB-C1B	-8.68	1.39	1.53
25	y	609	CHL	CHD-C4C	-8.68	1.37	1.53
25	Y	609	CHL	CHD-C4C	-8.68	1.37	1.53
25	n	609	CHL	CHB-C1B	-8.67	1.39	1.53
25	N	609	CHL	CHB-C1B	-8.67	1.39	1.53
25	8	308	CHL	CHD-C1D	-8.67	1.39	1.53
25	4	308	CHL	CHD-C1D	-8.67	1.39	1.53
25	s	306	CHL	CHB-C1B	-8.67	1.39	1.53
25	S	306	CHL	CHB-C1B	-8.67	1.39	1.53
25	3	301	CHL	C3B-C4B	-8.67	1.44	1.54
25	7	301	CHL	C3B-C4B	-8.67	1.44	1.54
25	n	607	CHL	CHD-C4C	-8.66	1.37	1.53
25	N	607	CHL	CHD-C4C	-8.66	1.37	1.53
25	7	307	CHL	CHD-C1D	-8.66	1.39	1.53
25	3	307	CHL	CHD-C1D	-8.66	1.39	1.53
25	1	606	CHL	CHD-C1D	-8.65	1.39	1.53
25	5	606	CHL	CHD-C1D	-8.65	1.39	1.53
25	y	608	CHL	CHD-C1D	-8.65	1.39	1.53
25	Y	608	CHL	CHD-C1D	-8.65	1.39	1.53
25	1	608	CHL	CHD-C1D	-8.64	1.39	1.53
25	5	608	CHL	CHD-C1D	-8.64	1.39	1.53
25	r	306	CHL	C3B-C4B	-8.64	1.44	1.54
25	R	306	CHL	C3B-C4B	-8.64	1.44	1.54
25	4	301	CHL	CHB-C1B	-8.64	1.39	1.53
25	6	601	CHL	CHB-C1B	-8.64	1.39	1.53
25	8	301	CHL	CHB-C1B	-8.64	1.39	1.53
25	2	601	CHL	CHB-C1B	-8.64	1.39	1.53
25	8	305	CHL	CHB-C1B	-8.63	1.39	1.53
25	4	305	CHL	CHB-C1B	-8.63	1.39	1.53
25	2	605	CHL	CHC-C4B	-8.62	1.39	1.53
25	6	605	CHL	CHC-C4B	-8.62	1.39	1.53
25	5	615	CHL	CHC-C4B	-8.62	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	615	CHL	CHC-C4B	-8.62	1.39	1.53
25	g	608	CHL	CHD-C1D	-8.60	1.39	1.53
25	G	608	CHL	CHD-C1D	-8.60	1.39	1.53
25	G	607	CHL	CHB-C1B	-8.60	1.39	1.53
25	g	607	CHL	CHB-C1B	-8.60	1.39	1.53
25	3	302	CHL	C3B-C4B	-8.60	1.44	1.54
25	7	302	CHL	C3B-C4B	-8.60	1.44	1.54
25	1	608	CHL	CHB-C1B	-8.60	1.39	1.53
25	5	608	CHL	CHB-C1B	-8.60	1.39	1.53
25	1	608	CHL	CHC-C4B	-8.59	1.39	1.53
25	5	608	CHL	CHC-C4B	-8.59	1.39	1.53
25	1	605	CHL	CHB-C1B	-8.59	1.39	1.53
25	4	307	CHL	CHB-C1B	-8.59	1.39	1.53
25	5	605	CHL	CHB-C1B	-8.59	1.39	1.53
25	8	307	CHL	CHB-C1B	-8.59	1.39	1.53
25	7	308	CHL	CHC-C4B	-8.58	1.39	1.53
25	r	305	CHL	CHB-C1B	-8.58	1.39	1.53
25	R	305	CHL	CHB-C1B	-8.58	1.39	1.53
25	3	308	CHL	CHC-C4B	-8.58	1.39	1.53
25	Y	605	CHL	CHB-C1B	-8.58	1.39	1.53
25	y	605	CHL	CHB-C1B	-8.58	1.39	1.53
25	3	302	CHL	CHD-C1D	-8.58	1.39	1.53
25	7	302	CHL	CHD-C1D	-8.58	1.39	1.53
25	R	304	CHL	CHD-C1D	-8.57	1.39	1.53
25	r	304	CHL	CHD-C1D	-8.57	1.39	1.53
25	8	305	CHL	CHD-C1D	-8.57	1.39	1.53
25	4	305	CHL	CHD-C1D	-8.57	1.39	1.53
25	4	306	CHL	CHB-C1B	-8.56	1.39	1.53
25	8	306	CHL	CHB-C1B	-8.56	1.39	1.53
25	2	607	CHL	CHB-C1B	-8.56	1.39	1.53
25	6	607	CHL	CHB-C1B	-8.56	1.39	1.53
25	1	609	CHL	CHB-C1B	-8.55	1.39	1.53
25	5	609	CHL	CHB-C1B	-8.55	1.39	1.53
25	3	306	CHL	CHC-C4B	-8.55	1.39	1.53
25	7	306	CHL	CHC-C4B	-8.55	1.39	1.53
25	1	601	CHL	CHC-C4B	-8.55	1.39	1.53
25	5	601	CHL	CHC-C4B	-8.55	1.39	1.53
25	7	309	CHL	CHB-C1B	-8.54	1.39	1.53
25	3	309	CHL	CHB-C1B	-8.54	1.39	1.53
25	G	607	CHL	CHD-C4C	-8.54	1.38	1.53
25	g	607	CHL	CHD-C4C	-8.54	1.38	1.53
25	5	615	CHL	CHB-C1B	-8.53	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	615	CHL	CHB-C1B	-8.53	1.39	1.53
25	3	301	CHL	CHC-C4B	-8.52	1.39	1.53
25	7	301	CHL	CHC-C4B	-8.52	1.39	1.53
25	G	609	CHL	CHB-C1B	-8.52	1.39	1.53
25	g	609	CHL	CHB-C1B	-8.52	1.39	1.53
25	Y	601	CHL	CHD-C4C	-8.52	1.38	1.53
25	y	601	CHL	CHD-C4C	-8.52	1.38	1.53
25	S	308	CHL	CHD-C4C	-8.52	1.38	1.53
25	s	308	CHL	CHD-C4C	-8.52	1.38	1.53
25	1	607	CHL	CHB-C1B	-8.52	1.39	1.53
25	5	607	CHL	CHB-C1B	-8.52	1.39	1.53
25	N	605	CHL	CHD-C4C	-8.50	1.38	1.53
25	n	605	CHL	CHD-C4C	-8.50	1.38	1.53
25	7	308	CHL	CHB-C1B	-8.49	1.39	1.53
25	3	308	CHL	CHB-C1B	-8.49	1.39	1.53
25	Y	607	CHL	CHD-C4C	-8.47	1.38	1.53
25	y	607	CHL	CHD-C4C	-8.47	1.38	1.53
25	g	606	CHL	CHD-C1D	-8.46	1.39	1.53
25	G	606	CHL	CHD-C1D	-8.46	1.39	1.53
25	y	606	CHL	CHB-C1B	-8.42	1.40	1.53
25	Y	606	CHL	CHB-C1B	-8.42	1.40	1.53
25	g	605	CHL	CHB-C1B	-8.42	1.40	1.53
25	G	605	CHL	CHB-C1B	-8.42	1.40	1.53
25	1	606	CHL	CHB-C1B	-8.41	1.40	1.53
25	5	606	CHL	CHB-C1B	-8.41	1.40	1.53
25	r	306	CHL	CHD-C4C	-8.40	1.38	1.53
25	R	306	CHL	CHD-C4C	-8.40	1.38	1.53
25	7	307	CHL	CHB-C1B	-8.39	1.40	1.53
25	3	307	CHL	CHB-C1B	-8.39	1.40	1.53
25	2	605	CHL	CHB-C1B	-8.38	1.40	1.53
25	6	605	CHL	CHB-C1B	-8.38	1.40	1.53
25	3	301	CHL	CHB-C1B	-8.38	1.40	1.53
25	7	301	CHL	CHB-C1B	-8.38	1.40	1.53
25	y	609	CHL	CHC-C1C	-8.37	1.38	1.53
25	Y	609	CHL	CHC-C1C	-8.37	1.38	1.53
25	1	608	CHL	C3B-C4B	-8.36	1.44	1.54
25	5	608	CHL	C3B-C4B	-8.36	1.44	1.54
25	n	606	CHL	CHB-C1B	-8.34	1.40	1.53
25	N	606	CHL	CHB-C1B	-8.34	1.40	1.53
25	R	304	CHL	CHB-C1B	-8.33	1.40	1.53
25	r	304	CHL	CHB-C1B	-8.33	1.40	1.53
25	N	608	CHL	C1A-CHA	-8.31	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	608	CHL	C1A-CHA	-8.31	1.40	1.53
25	7	308	CHL	C3B-C4B	-8.30	1.45	1.54
25	3	308	CHL	C3B-C4B	-8.30	1.45	1.54
25	3	306	CHL	CHB-C1B	-8.30	1.40	1.53
25	7	306	CHL	CHB-C1B	-8.30	1.40	1.53
25	7	309	CHL	CHD-C4C	-8.29	1.38	1.53
25	3	309	CHL	CHD-C4C	-8.29	1.38	1.53
25	s	307	CHL	CHD-C4C	-8.28	1.38	1.53
25	S	307	CHL	CHD-C4C	-8.28	1.38	1.53
25	N	601	CHL	CHD-C4C	-8.27	1.38	1.53
25	n	601	CHL	CHD-C4C	-8.27	1.38	1.53
25	1	601	CHL	CHB-C1B	-8.27	1.40	1.53
25	5	601	CHL	CHB-C1B	-8.27	1.40	1.53
25	2	606	CHL	CHB-C1B	-8.25	1.40	1.53
25	6	606	CHL	CHB-C1B	-8.25	1.40	1.53
25	3	306	CHL	CHD-C4C	-8.25	1.38	1.53
25	7	306	CHL	CHD-C4C	-8.25	1.38	1.53
25	S	302	CHL	CHD-C4C	-8.25	1.38	1.53
25	s	302	CHL	CHD-C4C	-8.25	1.38	1.53
25	Y	601	CHL	C1A-CHA	-8.25	1.40	1.53
25	y	601	CHL	C1A-CHA	-8.25	1.40	1.53
25	g	606	CHL	CHB-C1B	-8.24	1.40	1.53
25	G	606	CHL	CHB-C1B	-8.24	1.40	1.53
25	n	606	CHL	CHC-C1C	-8.24	1.38	1.53
25	N	606	CHL	CHC-C1C	-8.24	1.38	1.53
25	1	605	CHL	CHD-C4C	-8.23	1.38	1.53
25	5	605	CHL	CHD-C4C	-8.23	1.38	1.53
25	r	305	CHL	CHD-C4C	-8.22	1.38	1.53
25	R	305	CHL	CHD-C4C	-8.22	1.38	1.53
25	S	302	CHL	C1A-CHA	-8.21	1.40	1.53
25	s	302	CHL	C1A-CHA	-8.21	1.40	1.53
25	1	609	CHL	CHD-C4C	-8.19	1.38	1.53
25	5	609	CHL	CHD-C4C	-8.19	1.38	1.53
25	2	605	CHL	CHD-C4C	-8.19	1.38	1.53
25	6	605	CHL	CHD-C4C	-8.19	1.38	1.53
25	N	608	CHL	CHC-C1C	-8.18	1.38	1.53
25	n	608	CHL	CHC-C1C	-8.18	1.38	1.53
25	7	308	CHL	CHD-C4C	-8.17	1.38	1.53
25	3	308	CHL	CHD-C4C	-8.17	1.38	1.53
25	6	608	CHL	CHD-C4C	-8.17	1.38	1.53
25	2	608	CHL	CHD-C4C	-8.17	1.38	1.53
25	n	609	CHL	CHC-C1C	-8.14	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	609	CHL	CHC-C1C	-8.14	1.38	1.53
25	2	607	CHL	C3B-C4B	-8.14	1.45	1.54
25	6	607	CHL	C3B-C4B	-8.14	1.45	1.54
25	5	615	CHL	CHD-C4C	-8.13	1.38	1.53
25	1	615	CHL	CHD-C4C	-8.13	1.38	1.53
25	s	306	CHL	CHD-C4C	-8.11	1.38	1.53
25	S	306	CHL	CHD-C4C	-8.11	1.38	1.53
25	g	605	CHL	CHD-C4C	-8.09	1.38	1.53
25	G	605	CHL	CHD-C4C	-8.09	1.38	1.53
25	g	601	CHL	CHD-C4C	-8.09	1.38	1.53
25	G	601	CHL	CHD-C4C	-8.09	1.38	1.53
25	3	301	CHL	CHD-C4C	-8.08	1.38	1.53
25	7	301	CHL	CHD-C4C	-8.08	1.38	1.53
25	1	607	CHL	CHD-C4C	-8.08	1.38	1.53
25	5	607	CHL	CHD-C4C	-8.08	1.38	1.53
25	y	608	CHL	CHD-C4C	-8.06	1.38	1.53
25	Y	608	CHL	CHD-C4C	-8.06	1.38	1.53
25	N	608	CHL	CHD-C4C	-8.06	1.38	1.53
25	n	608	CHL	CHD-C4C	-8.06	1.38	1.53
25	4	307	CHL	CHD-C4C	-8.05	1.38	1.53
25	2	606	CHL	CHD-C4C	-8.05	1.38	1.53
25	8	307	CHL	CHD-C4C	-8.05	1.38	1.53
25	6	606	CHL	CHD-C4C	-8.05	1.38	1.53
25	g	606	CHL	CHC-C1C	-8.04	1.39	1.53
25	G	606	CHL	CHC-C1C	-8.04	1.39	1.53
25	y	606	CHL	C1A-CHA	-8.04	1.41	1.53
25	Y	606	CHL	C1A-CHA	-8.04	1.41	1.53
25	6	601	CHL	CHD-C4C	-8.03	1.39	1.53
25	2	601	CHL	CHD-C4C	-8.03	1.39	1.53
25	n	606	CHL	C1A-CHA	-8.03	1.41	1.53
25	N	606	CHL	C1A-CHA	-8.03	1.41	1.53
25	n	606	CHL	CHD-C4C	-8.02	1.39	1.53
25	N	606	CHL	CHD-C4C	-8.02	1.39	1.53
25	g	608	CHL	CHD-C4C	-8.02	1.39	1.53
25	G	608	CHL	CHD-C4C	-8.02	1.39	1.53
25	Y	605	CHL	CHC-C1C	-8.01	1.39	1.53
25	y	605	CHL	CHC-C1C	-8.01	1.39	1.53
25	2	607	CHL	CHD-C4C	-8.01	1.39	1.53
25	6	607	CHL	CHD-C4C	-8.01	1.39	1.53
25	y	606	CHL	CHC-C1C	-8.00	1.39	1.53
25	Y	606	CHL	CHC-C1C	-8.00	1.39	1.53
25	1	601	CHL	CHD-C4C	-8.00	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	601	CHL	CHD-C4C	-8.00	1.39	1.53
25	y	606	CHL	CHD-C4C	-7.98	1.39	1.53
25	Y	606	CHL	CHD-C4C	-7.98	1.39	1.53
25	8	308	CHL	CHD-C4C	-7.96	1.39	1.53
25	4	308	CHL	CHD-C4C	-7.96	1.39	1.53
25	1	608	CHL	CHD-C4C	-7.95	1.39	1.53
25	5	608	CHL	CHD-C4C	-7.95	1.39	1.53
25	R	304	CHL	CHD-C4C	-7.95	1.39	1.53
25	r	304	CHL	CHD-C4C	-7.95	1.39	1.53
25	R	304	CHL	C1A-CHA	-7.93	1.41	1.53
25	r	304	CHL	C1A-CHA	-7.93	1.41	1.53
25	Y	605	CHL	C1A-CHA	-7.93	1.41	1.53
25	y	605	CHL	C1A-CHA	-7.93	1.41	1.53
25	y	608	CHL	CHC-C1C	-7.93	1.39	1.53
25	Y	608	CHL	CHC-C1C	-7.93	1.39	1.53
25	g	601	CHL	C1A-CHA	-7.93	1.41	1.53
25	G	601	CHL	C1A-CHA	-7.93	1.41	1.53
25	4	306	CHL	CHD-C4C	-7.91	1.39	1.53
25	8	306	CHL	CHD-C4C	-7.91	1.39	1.53
25	Y	607	CHL	CHC-C1C	-7.91	1.39	1.53
25	y	607	CHL	CHC-C1C	-7.91	1.39	1.53
25	7	307	CHL	CHD-C4C	-7.91	1.39	1.53
25	3	307	CHL	CHD-C4C	-7.91	1.39	1.53
25	1	606	CHL	CHD-C4C	-7.89	1.39	1.53
25	5	606	CHL	CHD-C4C	-7.89	1.39	1.53
25	g	608	CHL	CHC-C1C	-7.88	1.39	1.53
25	G	608	CHL	CHC-C1C	-7.88	1.39	1.53
25	G	609	CHL	CHC-C1C	-7.87	1.39	1.53
25	g	609	CHL	CHC-C1C	-7.87	1.39	1.53
25	R	304	CHL	CHC-C1C	-7.86	1.39	1.53
25	r	304	CHL	CHC-C1C	-7.86	1.39	1.53
25	g	606	CHL	C1A-CHA	-7.85	1.41	1.53
25	G	606	CHL	C1A-CHA	-7.85	1.41	1.53
25	y	608	CHL	C1A-CHA	-7.84	1.41	1.53
25	Y	608	CHL	C1A-CHA	-7.84	1.41	1.53
25	8	305	CHL	CHD-C4C	-7.83	1.39	1.53
25	4	305	CHL	CHD-C4C	-7.83	1.39	1.53
25	3	302	CHL	CHD-C4C	-7.80	1.39	1.53
25	7	302	CHL	CHD-C4C	-7.80	1.39	1.53
25	g	606	CHL	CHD-C4C	-7.79	1.39	1.53
25	G	606	CHL	CHD-C4C	-7.79	1.39	1.53
25	4	301	CHL	C1A-CHA	-7.79	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	301	CHL	C1A-CHA	-7.79	1.41	1.53
25	4	301	CHL	CHD-C4C	-7.79	1.39	1.53
25	8	301	CHL	CHD-C4C	-7.79	1.39	1.53
25	g	608	CHL	C1A-CHA	-7.79	1.41	1.53
25	G	608	CHL	C1A-CHA	-7.79	1.41	1.53
25	r	305	CHL	C1A-CHA	-7.78	1.41	1.53
25	R	305	CHL	C1A-CHA	-7.78	1.41	1.53
25	N	601	CHL	C1A-CHA	-7.77	1.41	1.53
25	n	601	CHL	C1A-CHA	-7.77	1.41	1.53
25	s	307	CHL	C1A-CHA	-7.75	1.41	1.53
25	S	307	CHL	C1A-CHA	-7.75	1.41	1.53
25	n	607	CHL	CHC-C1C	-7.75	1.39	1.53
25	N	607	CHL	CHC-C1C	-7.75	1.39	1.53
25	n	607	CHL	C1A-CHA	-7.74	1.41	1.53
25	N	607	CHL	C1A-CHA	-7.74	1.41	1.53
25	S	308	CHL	C1A-CHA	-7.72	1.41	1.53
25	s	308	CHL	C1A-CHA	-7.72	1.41	1.53
25	r	306	CHL	C1A-CHA	-7.69	1.41	1.53
25	R	306	CHL	C1A-CHA	-7.69	1.41	1.53
25	7	309	CHL	CHC-C1C	-7.68	1.39	1.53
25	3	309	CHL	CHC-C1C	-7.68	1.39	1.53
25	s	307	CHL	CHC-C1C	-7.66	1.39	1.53
25	S	307	CHL	CHC-C1C	-7.66	1.39	1.53
25	N	605	CHL	CHC-C1C	-7.65	1.39	1.53
25	n	605	CHL	CHC-C1C	-7.65	1.39	1.53
25	s	306	CHL	C1A-CHA	-7.63	1.41	1.53
25	S	306	CHL	C1A-CHA	-7.63	1.41	1.53
25	1	606	CHL	C1A-CHA	-7.62	1.41	1.53
25	5	606	CHL	C1A-CHA	-7.62	1.41	1.53
25	s	306	CHL	CHC-C1C	-7.62	1.39	1.53
25	S	306	CHL	CHC-C1C	-7.62	1.39	1.53
25	2	606	CHL	CHC-C1C	-7.61	1.39	1.53
25	6	606	CHL	CHC-C1C	-7.61	1.39	1.53
25	N	605	CHL	C1A-CHA	-7.61	1.41	1.53
25	n	605	CHL	C1A-CHA	-7.61	1.41	1.53
25	r	305	CHL	CHC-C1C	-7.60	1.39	1.53
25	R	305	CHL	CHC-C1C	-7.60	1.39	1.53
25	3	301	CHL	C3D-C2D	-7.59	1.35	1.55
25	7	301	CHL	C3D-C2D	-7.59	1.35	1.55
25	8	308	CHL	C1A-CHA	-7.57	1.41	1.53
25	4	308	CHL	C1A-CHA	-7.57	1.41	1.53
25	7	308	CHL	C1A-CHA	-7.55	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	308	CHL	C1A-CHA	-7.55	1.41	1.53
25	1	609	CHL	CHC-C1C	-7.53	1.39	1.53
25	5	609	CHL	CHC-C1C	-7.53	1.39	1.53
25	6	608	CHL	CHC-C1C	-7.52	1.39	1.53
25	2	608	CHL	CHC-C1C	-7.52	1.39	1.53
25	3	301	CHL	C1A-CHA	-7.50	1.41	1.53
25	7	301	CHL	C1A-CHA	-7.50	1.41	1.53
25	1	601	CHL	C1A-CHA	-7.50	1.41	1.53
25	5	601	CHL	C1A-CHA	-7.50	1.41	1.53
25	Y	607	CHL	C1A-CHA	-7.50	1.41	1.53
25	y	607	CHL	C1A-CHA	-7.50	1.41	1.53
25	y	609	CHL	C1A-CHA	-7.49	1.41	1.53
25	Y	609	CHL	C1A-CHA	-7.49	1.41	1.53
25	4	306	CHL	C1A-CHA	-7.48	1.41	1.53
25	8	306	CHL	C1A-CHA	-7.48	1.41	1.53
25	1	608	CHL	C1A-CHA	-7.47	1.42	1.53
25	5	608	CHL	C1A-CHA	-7.47	1.42	1.53
25	G	609	CHL	C3D-C2D	-7.47	1.35	1.55
25	g	609	CHL	C3D-C2D	-7.47	1.35	1.55
25	7	307	CHL	C1A-CHA	-7.46	1.42	1.53
25	3	307	CHL	C1A-CHA	-7.46	1.42	1.53
25	1	607	CHL	C1A-CHA	-7.45	1.42	1.53
25	5	607	CHL	C1A-CHA	-7.45	1.42	1.53
25	1	605	CHL	C1A-CHA	-7.44	1.42	1.53
25	5	605	CHL	C1A-CHA	-7.44	1.42	1.53
25	N	601	CHL	CHC-C1C	-7.44	1.40	1.53
25	n	601	CHL	CHC-C1C	-7.44	1.40	1.53
25	n	609	CHL	C3D-C2D	-7.44	1.35	1.55
25	N	609	CHL	C3D-C2D	-7.44	1.35	1.55
25	7	308	CHL	CHC-C1C	-7.43	1.40	1.53
25	3	308	CHL	CHC-C1C	-7.43	1.40	1.53
25	2	606	CHL	C1A-CHA	-7.42	1.42	1.53
25	6	606	CHL	C1A-CHA	-7.42	1.42	1.53
25	8	308	CHL	CHC-C1C	-7.41	1.40	1.53
25	4	308	CHL	CHC-C1C	-7.41	1.40	1.53
25	1	606	CHL	CHC-C1C	-7.41	1.40	1.53
25	5	606	CHL	CHC-C1C	-7.41	1.40	1.53
25	4	307	CHL	C1A-CHA	-7.41	1.42	1.53
25	8	307	CHL	C1A-CHA	-7.41	1.42	1.53
25	4	307	CHL	CHC-C1C	-7.40	1.40	1.53
25	8	307	CHL	CHC-C1C	-7.40	1.40	1.53
25	2	607	CHL	CHC-C1C	-7.40	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	301	CHL	CHC-C1C	-7.40	1.40	1.53
25	8	301	CHL	CHC-C1C	-7.40	1.40	1.53
25	6	607	CHL	CHC-C1C	-7.40	1.40	1.53
25	8	305	CHL	CHC-C1C	-7.39	1.40	1.53
25	4	305	CHL	CHC-C1C	-7.39	1.40	1.53
25	3	302	CHL	C1A-CHA	-7.39	1.42	1.53
25	7	302	CHL	C1A-CHA	-7.39	1.42	1.53
25	G	607	CHL	CHC-C1C	-7.39	1.40	1.53
25	g	607	CHL	CHC-C1C	-7.39	1.40	1.53
25	1	605	CHL	CHC-C1C	-7.38	1.40	1.53
25	5	605	CHL	CHC-C1C	-7.38	1.40	1.53
25	1	607	CHL	CHC-C1C	-7.36	1.40	1.53
25	5	607	CHL	CHC-C1C	-7.36	1.40	1.53
25	8	305	CHL	C1A-CHA	-7.35	1.42	1.53
25	4	305	CHL	C1A-CHA	-7.35	1.42	1.53
25	G	607	CHL	C1A-CHA	-7.35	1.42	1.53
25	g	607	CHL	C1A-CHA	-7.35	1.42	1.53
25	r	306	CHL	CHC-C1C	-7.35	1.40	1.53
25	R	306	CHL	CHC-C1C	-7.35	1.40	1.53
25	n	607	CHL	C3D-C2D	-7.34	1.35	1.55
25	N	607	CHL	C3D-C2D	-7.34	1.35	1.55
25	4	306	CHL	CHC-C1C	-7.33	1.40	1.53
25	8	306	CHL	CHC-C1C	-7.33	1.40	1.53
25	7	307	CHL	CHC-C1C	-7.33	1.40	1.53
25	3	307	CHL	CHC-C1C	-7.33	1.40	1.53
25	6	601	CHL	C1A-CHA	-7.33	1.42	1.53
25	2	601	CHL	C1A-CHA	-7.33	1.42	1.53
25	6	601	CHL	CHC-C1C	-7.32	1.40	1.53
25	2	601	CHL	CHC-C1C	-7.32	1.40	1.53
25	g	601	CHL	CHC-C1C	-7.31	1.40	1.53
25	G	601	CHL	CHC-C1C	-7.31	1.40	1.53
25	Y	601	CHL	CHC-C1C	-7.31	1.40	1.53
25	y	601	CHL	CHC-C1C	-7.31	1.40	1.53
25	5	615	CHL	C1A-CHA	-7.31	1.42	1.53
25	1	615	CHL	C1A-CHA	-7.31	1.42	1.53
25	1	608	CHL	CHC-C1C	-7.30	1.40	1.53
25	5	608	CHL	CHC-C1C	-7.30	1.40	1.53
25	5	615	CHL	CHC-C1C	-7.30	1.40	1.53
25	1	615	CHL	CHC-C1C	-7.30	1.40	1.53
25	S	302	CHL	CHC-C1C	-7.28	1.40	1.53
25	s	302	CHL	CHC-C1C	-7.28	1.40	1.53
25	G	607	CHL	C3D-C2D	-7.27	1.35	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	607	CHL	C3D-C2D	-7.27	1.35	1.55
25	n	609	CHL	C1A-CHA	-7.27	1.42	1.53
25	N	609	CHL	C1A-CHA	-7.27	1.42	1.53
25	Y	605	CHL	C4D-ND	-7.27	1.34	1.50
25	y	605	CHL	C4D-ND	-7.27	1.34	1.50
25	4	301	CHL	C3D-C2D	-7.27	1.35	1.55
25	8	301	CHL	C3D-C2D	-7.27	1.35	1.55
25	2	605	CHL	CHC-C1C	-7.27	1.40	1.53
25	6	605	CHL	CHC-C1C	-7.27	1.40	1.53
25	g	605	CHL	CHC-C1C	-7.26	1.40	1.53
25	G	605	CHL	CHC-C1C	-7.26	1.40	1.53
25	g	605	CHL	C1A-CHA	-7.25	1.42	1.53
25	G	605	CHL	C1A-CHA	-7.25	1.42	1.53
25	y	609	CHL	C3D-C2D	-7.25	1.36	1.55
25	Y	609	CHL	C3D-C2D	-7.25	1.36	1.55
25	Y	607	CHL	C3D-C2D	-7.24	1.36	1.55
25	y	607	CHL	C3D-C2D	-7.24	1.36	1.55
25	Y	601	CHL	C3D-C2D	-7.23	1.36	1.55
25	y	601	CHL	C3D-C2D	-7.23	1.36	1.55
25	n	606	CHL	C3D-C2D	-7.22	1.36	1.55
25	N	606	CHL	C3D-C2D	-7.22	1.36	1.55
25	2	607	CHL	C1A-CHA	-7.20	1.42	1.53
25	6	607	CHL	C1A-CHA	-7.20	1.42	1.53
25	3	306	CHL	CHC-C1C	-7.20	1.40	1.53
25	7	306	CHL	CHC-C1C	-7.20	1.40	1.53
25	3	301	CHL	CHC-C1C	-7.20	1.40	1.53
25	7	301	CHL	CHC-C1C	-7.20	1.40	1.53
25	1	609	CHL	C3D-C2D	-7.18	1.36	1.55
25	5	609	CHL	C3D-C2D	-7.18	1.36	1.55
25	7	309	CHL	C3D-C2D	-7.18	1.36	1.55
25	N	605	CHL	C3D-C2D	-7.18	1.36	1.55
25	3	309	CHL	C3D-C2D	-7.18	1.36	1.55
25	n	605	CHL	C3D-C2D	-7.18	1.36	1.55
25	y	606	CHL	C3D-C2D	-7.18	1.36	1.55
25	Y	606	CHL	C3D-C2D	-7.18	1.36	1.55
25	6	608	CHL	C3D-C2D	-7.17	1.36	1.55
25	2	608	CHL	C3D-C2D	-7.17	1.36	1.55
25	S	302	CHL	C4D-ND	-7.17	1.34	1.50
25	s	302	CHL	C4D-ND	-7.17	1.34	1.50
25	1	601	CHL	CHC-C1C	-7.17	1.40	1.53
25	5	601	CHL	CHC-C1C	-7.17	1.40	1.53
25	S	308	CHL	CHC-C1C	-7.16	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	308	CHL	CHC-C1C	-7.16	1.40	1.53
25	Y	605	CHL	C3D-C2D	-7.16	1.36	1.55
25	y	605	CHL	C3D-C2D	-7.16	1.36	1.55
25	g	608	CHL	C3D-C2D	-7.16	1.36	1.55
25	G	608	CHL	C3D-C2D	-7.16	1.36	1.55
25	7	308	CHL	C3D-C2D	-7.15	1.36	1.55
25	3	308	CHL	C3D-C2D	-7.15	1.36	1.55
25	3	302	CHL	CHC-C1C	-7.15	1.40	1.53
25	7	302	CHL	CHC-C1C	-7.15	1.40	1.53
25	1	609	CHL	C1A-CHA	-7.13	1.42	1.53
25	5	609	CHL	C1A-CHA	-7.13	1.42	1.53
25	2	605	CHL	C1A-CHA	-7.13	1.42	1.53
25	6	605	CHL	C1A-CHA	-7.13	1.42	1.53
25	N	601	CHL	C4D-ND	-7.12	1.35	1.50
25	n	601	CHL	C4D-ND	-7.12	1.35	1.50
25	g	601	CHL	C4D-ND	-7.12	1.35	1.50
25	G	601	CHL	C4D-ND	-7.12	1.35	1.50
25	s	307	CHL	C4D-ND	-7.12	1.35	1.50
25	S	307	CHL	C4D-ND	-7.12	1.35	1.50
25	8	305	CHL	C3D-C2D	-7.11	1.36	1.55
25	4	305	CHL	C3D-C2D	-7.11	1.36	1.55
25	n	607	CHL	C4D-ND	-7.11	1.35	1.50
25	N	607	CHL	C4D-ND	-7.11	1.35	1.50
25	r	305	CHL	C3D-C2D	-7.09	1.36	1.55
25	R	305	CHL	C3D-C2D	-7.09	1.36	1.55
25	N	608	CHL	C4D-ND	-7.09	1.35	1.50
25	n	608	CHL	C4D-ND	-7.09	1.35	1.50
25	S	308	CHL	C3D-C2D	-7.09	1.36	1.55
25	s	308	CHL	C3D-C2D	-7.09	1.36	1.55
25	Y	601	CHL	C4D-ND	-7.08	1.35	1.50
25	y	601	CHL	C4D-ND	-7.08	1.35	1.50
25	Y	607	CHL	C4D-ND	-7.08	1.35	1.50
25	y	607	CHL	C4D-ND	-7.08	1.35	1.50
25	g	601	CHL	C3D-C2D	-7.08	1.36	1.55
25	G	601	CHL	C3D-C2D	-7.08	1.36	1.55
25	S	308	CHL	C4D-ND	-7.07	1.35	1.50
25	s	308	CHL	C4D-ND	-7.07	1.35	1.50
25	S	302	CHL	C3D-C2D	-7.07	1.36	1.55
25	s	302	CHL	C3D-C2D	-7.07	1.36	1.55
25	4	307	CHL	C3D-C2D	-7.07	1.36	1.55
25	8	307	CHL	C3D-C2D	-7.07	1.36	1.55
25	N	605	CHL	C4D-ND	-7.06	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	605	CHL	C4D-ND	-7.06	1.35	1.50
25	N	608	CHL	C3D-C2D	-7.06	1.36	1.55
25	n	608	CHL	C3D-C2D	-7.06	1.36	1.55
25	1	606	CHL	C3D-C2D	-7.06	1.36	1.55
25	5	606	CHL	C3D-C2D	-7.06	1.36	1.55
25	s	306	CHL	C3D-C2D	-7.05	1.36	1.55
25	S	306	CHL	C3D-C2D	-7.05	1.36	1.55
25	r	306	CHL	C3D-C2D	-7.05	1.36	1.55
25	R	306	CHL	C3D-C2D	-7.05	1.36	1.55
25	g	606	CHL	C3D-C2D	-7.04	1.36	1.55
25	G	606	CHL	C3D-C2D	-7.04	1.36	1.55
25	g	605	CHL	C3D-C2D	-7.04	1.36	1.55
25	G	605	CHL	C3D-C2D	-7.04	1.36	1.55
25	n	609	CHL	C4D-ND	-7.02	1.35	1.50
25	N	609	CHL	C4D-ND	-7.02	1.35	1.50
25	3	306	CHL	C1A-CHA	-7.01	1.42	1.53
25	7	306	CHL	C1A-CHA	-7.01	1.42	1.53
25	N	601	CHL	C3D-C2D	-7.01	1.36	1.55
25	n	601	CHL	C3D-C2D	-7.01	1.36	1.55
25	3	306	CHL	C3D-C2D	-7.00	1.36	1.55
25	7	306	CHL	C3D-C2D	-7.00	1.36	1.55
25	2	605	CHL	C3D-C2D	-7.00	1.36	1.55
25	6	605	CHL	C3D-C2D	-7.00	1.36	1.55
25	2	607	CHL	C3D-C2D	-7.00	1.36	1.55
25	6	607	CHL	C3D-C2D	-7.00	1.36	1.55
25	r	305	CHL	C4D-ND	-7.00	1.35	1.50
25	R	305	CHL	C4D-ND	-7.00	1.35	1.50
25	1	608	CHL	C3D-C2D	-7.00	1.36	1.55
25	5	608	CHL	C3D-C2D	-7.00	1.36	1.55
25	1	607	CHL	C3D-C2D	-6.98	1.36	1.55
25	5	607	CHL	C3D-C2D	-6.98	1.36	1.55
25	4	306	CHL	C3D-C2D	-6.98	1.36	1.55
25	8	306	CHL	C3D-C2D	-6.98	1.36	1.55
25	6	601	CHL	C3D-C2D	-6.97	1.36	1.55
25	2	601	CHL	C3D-C2D	-6.97	1.36	1.55
25	s	307	CHL	C3D-C2D	-6.97	1.36	1.55
25	S	307	CHL	C3D-C2D	-6.97	1.36	1.55
25	2	606	CHL	C3D-C2D	-6.96	1.36	1.55
25	6	606	CHL	C3D-C2D	-6.96	1.36	1.55
25	n	606	CHL	C4D-ND	-6.96	1.35	1.50
25	N	606	CHL	C4D-ND	-6.96	1.35	1.50
25	y	609	CHL	C4D-ND	-6.96	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	609	CHL	C4D-ND	-6.96	1.35	1.50
25	y	608	CHL	C3D-C2D	-6.95	1.36	1.55
25	Y	608	CHL	C3D-C2D	-6.95	1.36	1.55
25	R	304	CHL	C3D-C2D	-6.94	1.36	1.55
25	r	304	CHL	C3D-C2D	-6.94	1.36	1.55
25	y	606	CHL	C4D-ND	-6.93	1.35	1.50
25	Y	606	CHL	C4D-ND	-6.93	1.35	1.50
25	1	601	CHL	C3D-C2D	-6.93	1.36	1.55
25	5	601	CHL	C3D-C2D	-6.93	1.36	1.55
25	7	307	CHL	C3D-C2D	-6.93	1.36	1.55
25	3	307	CHL	C3D-C2D	-6.93	1.36	1.55
25	g	608	CHL	C4D-ND	-6.93	1.35	1.50
25	G	608	CHL	C4D-ND	-6.93	1.35	1.50
25	5	615	CHL	C3D-C2D	-6.92	1.36	1.55
25	1	615	CHL	C3D-C2D	-6.92	1.36	1.55
25	8	308	CHL	C3D-C2D	-6.91	1.36	1.55
25	4	308	CHL	C3D-C2D	-6.91	1.36	1.55
25	G	609	CHL	C4D-ND	-6.91	1.35	1.50
25	g	609	CHL	C4D-ND	-6.91	1.35	1.50
25	1	605	CHL	C3D-C2D	-6.91	1.36	1.55
25	5	605	CHL	C3D-C2D	-6.91	1.36	1.55
25	r	306	CHL	C4D-ND	-6.90	1.35	1.50
25	R	306	CHL	C4D-ND	-6.90	1.35	1.50
25	1	605	CHL	C4D-ND	-6.89	1.35	1.50
25	5	605	CHL	C4D-ND	-6.89	1.35	1.50
25	3	302	CHL	C3D-C2D	-6.88	1.36	1.55
25	7	302	CHL	C3D-C2D	-6.88	1.36	1.55
25	y	608	CHL	C4D-ND	-6.88	1.35	1.50
25	Y	608	CHL	C4D-ND	-6.88	1.35	1.50
25	G	609	CHL	C1A-CHA	-6.88	1.42	1.53
25	g	609	CHL	C1A-CHA	-6.88	1.42	1.53
25	g	606	CHL	C4D-ND	-6.83	1.35	1.50
25	G	606	CHL	C4D-ND	-6.83	1.35	1.50
25	1	609	CHL	C4D-ND	-6.82	1.35	1.50
25	5	609	CHL	C4D-ND	-6.82	1.35	1.50
25	4	301	CHL	C4D-ND	-6.81	1.35	1.50
25	8	301	CHL	C4D-ND	-6.81	1.35	1.50
25	R	304	CHL	C4D-ND	-6.80	1.35	1.50
25	r	304	CHL	C4D-ND	-6.80	1.35	1.50
25	G	607	CHL	C4D-ND	-6.79	1.35	1.50
25	g	607	CHL	C4D-ND	-6.79	1.35	1.50
25	4	306	CHL	C4D-ND	-6.77	1.35	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	306	CHL	C4D-ND	-6.77	1.35	1.50
25	1	607	CHL	C4D-ND	-6.76	1.35	1.50
25	5	607	CHL	C4D-ND	-6.76	1.35	1.50
25	s	306	CHL	C4D-ND	-6.75	1.35	1.50
25	S	306	CHL	C4D-ND	-6.75	1.35	1.50
25	1	606	CHL	C4D-ND	-6.74	1.35	1.50
25	5	606	CHL	C4D-ND	-6.74	1.35	1.50
25	5	615	CHL	C4D-ND	-6.74	1.35	1.50
25	1	615	CHL	C4D-ND	-6.74	1.35	1.50
25	6	601	CHL	C4D-ND	-6.71	1.35	1.50
25	2	601	CHL	C4D-ND	-6.71	1.35	1.50
25	4	307	CHL	C4D-ND	-6.71	1.35	1.50
25	8	307	CHL	C4D-ND	-6.71	1.35	1.50
25	7	308	CHL	C4D-ND	-6.71	1.35	1.50
25	3	308	CHL	C4D-ND	-6.71	1.35	1.50
25	2	606	CHL	C4D-ND	-6.70	1.35	1.50
25	6	606	CHL	C4D-ND	-6.70	1.35	1.50
25	3	302	CHL	C4D-ND	-6.69	1.35	1.50
25	7	302	CHL	C4D-ND	-6.69	1.35	1.50
25	8	308	CHL	C4D-ND	-6.68	1.36	1.50
25	4	308	CHL	C4D-ND	-6.68	1.36	1.50
25	1	608	CHL	C4D-ND	-6.66	1.36	1.50
25	5	608	CHL	C4D-ND	-6.66	1.36	1.50
25	6	608	CHL	C1A-CHA	-6.66	1.43	1.53
25	2	608	CHL	C1A-CHA	-6.66	1.43	1.53
25	1	601	CHL	C4D-ND	-6.65	1.36	1.50
25	5	601	CHL	C4D-ND	-6.65	1.36	1.50
25	2	607	CHL	C4D-ND	-6.63	1.36	1.50
25	6	607	CHL	C4D-ND	-6.63	1.36	1.50
25	7	307	CHL	C4D-ND	-6.61	1.36	1.50
25	3	307	CHL	C4D-ND	-6.61	1.36	1.50
25	7	309	CHL	C4D-ND	-6.60	1.36	1.50
25	3	309	CHL	C4D-ND	-6.60	1.36	1.50
25	8	305	CHL	C4D-ND	-6.58	1.36	1.50
25	4	305	CHL	C4D-ND	-6.58	1.36	1.50
25	6	608	CHL	C4D-ND	-6.57	1.36	1.50
25	2	608	CHL	C4D-ND	-6.57	1.36	1.50
25	3	301	CHL	C4D-ND	-6.57	1.36	1.50
25	7	301	CHL	C4D-ND	-6.57	1.36	1.50
25	7	309	CHL	C1A-CHA	-6.55	1.43	1.53
25	3	309	CHL	C1A-CHA	-6.55	1.43	1.53
25	g	605	CHL	C4D-ND	-6.55	1.36	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	605	CHL	C4D-ND	-6.55	1.36	1.50
25	3	306	CHL	C4D-ND	-6.48	1.36	1.50
25	7	306	CHL	C4D-ND	-6.48	1.36	1.50
25	2	605	CHL	C4D-ND	-6.45	1.36	1.50
25	6	605	CHL	C4D-ND	-6.45	1.36	1.50
25	n	607	CHL	C1D-ND	-6.43	1.36	1.50
25	N	607	CHL	C1D-ND	-6.43	1.36	1.50
25	Y	605	CHL	C1D-ND	-6.35	1.36	1.50
25	y	605	CHL	C1D-ND	-6.35	1.36	1.50
25	y	609	CHL	C3B-CAB	-6.35	1.44	1.50
25	Y	609	CHL	C3B-CAB	-6.35	1.44	1.50
25	y	609	CHL	C1D-ND	-6.34	1.36	1.50
25	Y	609	CHL	C1D-ND	-6.34	1.36	1.50
25	Y	607	CHL	C1D-ND	-6.32	1.36	1.50
25	y	607	CHL	C1D-ND	-6.32	1.36	1.50
25	N	605	CHL	C1D-ND	-6.31	1.36	1.50
25	n	605	CHL	C1D-ND	-6.31	1.36	1.50
25	n	606	CHL	C1D-ND	-6.29	1.36	1.50
25	N	606	CHL	C1D-ND	-6.29	1.36	1.50
25	y	609	CHL	C4B-NB	-6.26	1.36	1.50
25	Y	609	CHL	C4B-NB	-6.26	1.36	1.50
25	r	305	CHL	C1D-ND	-6.25	1.36	1.50
25	R	305	CHL	C1D-ND	-6.25	1.36	1.50
25	G	607	CHL	C1D-ND	-6.24	1.36	1.50
25	g	607	CHL	C1D-ND	-6.24	1.36	1.50
25	n	609	CHL	C3B-CAB	-6.24	1.44	1.50
25	N	609	CHL	C3B-CAB	-6.24	1.44	1.50
25	n	609	CHL	C1D-ND	-6.23	1.36	1.50
25	N	609	CHL	C1D-ND	-6.23	1.36	1.50
25	G	609	CHL	C1D-ND	-6.23	1.36	1.50
25	g	609	CHL	C1D-ND	-6.23	1.36	1.50
25	S	302	CHL	C1D-ND	-6.22	1.36	1.50
25	s	302	CHL	C1D-ND	-6.22	1.36	1.50
25	N	608	CHL	C1D-ND	-6.20	1.37	1.50
25	n	608	CHL	C1D-ND	-6.20	1.37	1.50
25	y	606	CHL	C1D-ND	-6.19	1.37	1.50
25	Y	606	CHL	C1D-ND	-6.19	1.37	1.50
25	y	608	CHL	CHB-C4A	-6.19	1.37	1.52
25	Y	608	CHL	CHB-C4A	-6.19	1.37	1.52
25	S	308	CHL	C1D-ND	-6.18	1.37	1.50
25	s	308	CHL	C1D-ND	-6.18	1.37	1.50
25	r	306	CHL	C1D-ND	-6.18	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	306	CHL	C1D-ND	-6.18	1.37	1.50
25	s	306	CHL	C1D-ND	-6.18	1.37	1.50
25	S	306	CHL	C1D-ND	-6.18	1.37	1.50
25	Y	601	CHL	C1D-ND	-6.16	1.37	1.50
25	y	601	CHL	C1D-ND	-6.16	1.37	1.50
25	s	307	CHL	C1D-ND	-6.15	1.37	1.50
25	S	307	CHL	C1D-ND	-6.15	1.37	1.50
25	R	304	CHL	C1D-ND	-6.15	1.37	1.50
25	r	304	CHL	C1D-ND	-6.15	1.37	1.50
25	Y	601	CHL	C1B-NB	-6.15	1.37	1.50
25	y	601	CHL	C1B-NB	-6.15	1.37	1.50
25	y	608	CHL	C4B-NB	-6.14	1.37	1.50
25	Y	608	CHL	C4B-NB	-6.14	1.37	1.50
25	g	606	CHL	C1D-ND	-6.12	1.37	1.50
25	G	606	CHL	C1D-ND	-6.12	1.37	1.50
25	y	609	CHL	C1B-NB	-6.12	1.37	1.50
25	Y	609	CHL	C1B-NB	-6.12	1.37	1.50
25	y	608	CHL	C1D-ND	-6.10	1.37	1.50
25	Y	608	CHL	C1D-ND	-6.10	1.37	1.50
25	n	609	CHL	C4B-NB	-6.09	1.37	1.50
25	N	609	CHL	C4B-NB	-6.09	1.37	1.50
25	n	609	CHL	C1B-NB	-6.09	1.37	1.50
25	N	609	CHL	C1B-NB	-6.09	1.37	1.50
25	S	302	CHL	C1B-NB	-6.08	1.37	1.50
25	s	302	CHL	C1B-NB	-6.08	1.37	1.50
25	s	306	CHL	C1B-NB	-6.08	1.37	1.50
25	S	306	CHL	C1B-NB	-6.08	1.37	1.50
25	l	605	CHL	C1D-ND	-6.07	1.37	1.50
25	l	605	CHL	C1D-ND	-6.07	1.37	1.50
25	S	302	CHL	CHB-C4A	-6.07	1.38	1.52
25	s	302	CHL	CHB-C4A	-6.07	1.38	1.52
25	y	608	CHL	C1B-NB	-6.07	1.37	1.50
25	Y	608	CHL	C1B-NB	-6.07	1.37	1.50
25	n	607	CHL	C1B-NB	-6.06	1.37	1.50
25	N	607	CHL	C1B-NB	-6.06	1.37	1.50
25	N	608	CHL	C1B-NB	-6.06	1.37	1.50
25	n	608	CHL	C1B-NB	-6.06	1.37	1.50
25	N	601	CHL	C1D-ND	-6.06	1.37	1.50
25	n	601	CHL	C1D-ND	-6.06	1.37	1.50
25	Y	605	CHL	C4B-NB	-6.05	1.37	1.50
25	y	605	CHL	C4B-NB	-6.05	1.37	1.50
25	Y	601	CHL	C4B-NB	-6.04	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	601	CHL	C4B-NB	-6.04	1.37	1.50
25	6	608	CHL	C1B-NB	-6.04	1.37	1.50
25	y	606	CHL	C4B-NB	-6.04	1.37	1.50
25	Y	606	CHL	C4B-NB	-6.04	1.37	1.50
25	2	608	CHL	C1B-NB	-6.04	1.37	1.50
25	8	305	CHL	C1B-NB	-6.03	1.37	1.50
25	4	305	CHL	C1B-NB	-6.03	1.37	1.50
25	1	606	CHL	C1D-ND	-6.03	1.37	1.50
25	5	606	CHL	C1D-ND	-6.03	1.37	1.50
25	g	608	CHL	C4B-NB	-6.03	1.37	1.50
25	G	608	CHL	C4B-NB	-6.03	1.37	1.50
25	g	601	CHL	C1D-ND	-6.03	1.37	1.50
25	G	601	CHL	C1D-ND	-6.03	1.37	1.50
25	s	307	CHL	C4B-NB	-6.02	1.37	1.50
25	S	307	CHL	C4B-NB	-6.02	1.37	1.50
25	n	606	CHL	C1B-NB	-6.02	1.37	1.50
25	N	606	CHL	C1B-NB	-6.02	1.37	1.50
25	3	301	CHL	C1D-ND	-6.02	1.37	1.50
25	7	301	CHL	C1D-ND	-6.02	1.37	1.50
25	S	308	CHL	C1B-NB	-6.01	1.37	1.50
25	s	308	CHL	C1B-NB	-6.01	1.37	1.50
25	n	607	CHL	C3B-CAB	-6.01	1.44	1.50
25	N	607	CHL	C3B-CAB	-6.01	1.44	1.50
25	2	606	CHL	C1D-ND	-6.01	1.37	1.50
25	6	606	CHL	C1D-ND	-6.01	1.37	1.50
25	5	615	CHL	C1D-ND	-6.01	1.37	1.50
25	1	615	CHL	C1D-ND	-6.01	1.37	1.50
25	s	307	CHL	C1B-NB	-6.01	1.37	1.50
25	S	307	CHL	C1B-NB	-6.01	1.37	1.50
25	4	307	CHL	C1D-ND	-6.00	1.37	1.50
25	8	307	CHL	C1D-ND	-6.00	1.37	1.50
25	G	609	CHL	C3B-CAB	-6.00	1.44	1.50
25	g	609	CHL	C3B-CAB	-6.00	1.44	1.50
25	Y	607	CHL	C1B-NB	-6.00	1.37	1.50
25	y	607	CHL	C1B-NB	-6.00	1.37	1.50
25	N	608	CHL	C4B-NB	-6.00	1.37	1.50
25	n	608	CHL	C4B-NB	-6.00	1.37	1.50
25	g	608	CHL	C1D-ND	-6.00	1.37	1.50
25	G	608	CHL	C1D-ND	-6.00	1.37	1.50
25	4	306	CHL	C1D-ND	-5.99	1.37	1.50
25	8	306	CHL	C1D-ND	-5.99	1.37	1.50
25	S	302	CHL	C4B-NB	-5.99	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	302	CHL	C4B-NB	-5.99	1.37	1.50
25	r	306	CHL	C1B-NB	-5.98	1.37	1.50
25	R	306	CHL	C1B-NB	-5.98	1.37	1.50
25	n	607	CHL	C4B-NB	-5.98	1.37	1.50
25	N	607	CHL	C4B-NB	-5.98	1.37	1.50
25	S	308	CHL	CHB-C4A	-5.98	1.38	1.52
25	s	308	CHL	CHB-C4A	-5.98	1.38	1.52
25	Y	607	CHL	C4B-NB	-5.98	1.37	1.50
25	y	607	CHL	C4B-NB	-5.98	1.37	1.50
25	y	608	CHL	C3B-CAB	-5.97	1.44	1.50
25	Y	608	CHL	C3B-CAB	-5.97	1.44	1.50
25	1	607	CHL	C1D-ND	-5.97	1.37	1.50
25	5	607	CHL	C1D-ND	-5.97	1.37	1.50
25	N	601	CHL	C1B-NB	-5.97	1.37	1.50
25	n	601	CHL	C1B-NB	-5.97	1.37	1.50
25	g	608	CHL	C3B-CAB	-5.96	1.44	1.50
25	G	608	CHL	C3B-CAB	-5.96	1.44	1.50
25	N	601	CHL	C4B-NB	-5.96	1.37	1.50
25	n	601	CHL	C4B-NB	-5.96	1.37	1.50
25	G	609	CHL	C4B-NB	-5.96	1.37	1.50
25	g	609	CHL	C4B-NB	-5.96	1.37	1.50
25	S	308	CHL	C4B-NB	-5.96	1.37	1.50
25	s	308	CHL	C4B-NB	-5.96	1.37	1.50
25	Y	605	CHL	C1B-NB	-5.96	1.37	1.50
25	y	605	CHL	C1B-NB	-5.96	1.37	1.50
25	6	601	CHL	C1D-ND	-5.95	1.37	1.50
25	2	601	CHL	C1D-ND	-5.95	1.37	1.50
25	4	301	CHL	C1D-ND	-5.95	1.37	1.50
25	8	301	CHL	C1D-ND	-5.95	1.37	1.50
25	N	605	CHL	C4B-NB	-5.94	1.37	1.50
25	n	605	CHL	C4B-NB	-5.94	1.37	1.50
25	G	609	CHL	C1B-NB	-5.93	1.37	1.50
25	g	609	CHL	C1B-NB	-5.93	1.37	1.50
25	7	307	CHL	C1D-ND	-5.93	1.37	1.50
25	3	307	CHL	C1D-ND	-5.93	1.37	1.50
25	G	607	CHL	C1B-NB	-5.93	1.37	1.50
25	g	607	CHL	C1B-NB	-5.93	1.37	1.50
25	N	605	CHL	C1B-NB	-5.93	1.37	1.50
25	n	605	CHL	C1B-NB	-5.93	1.37	1.50
25	R	304	CHL	C4B-NB	-5.92	1.37	1.50
25	r	304	CHL	C4B-NB	-5.92	1.37	1.50
25	g	606	CHL	C1B-NB	-5.92	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	605	CHL	C1B-NB	-5.92	1.37	1.50
25	G	606	CHL	C1B-NB	-5.92	1.37	1.50
25	G	605	CHL	C1B-NB	-5.92	1.37	1.50
25	R	304	CHL	C3B-CAB	-5.91	1.44	1.50
25	s	307	CHL	C3B-CAB	-5.91	1.44	1.50
25	r	304	CHL	C3B-CAB	-5.91	1.44	1.50
25	S	307	CHL	C3B-CAB	-5.91	1.44	1.50
25	2	605	CHL	C1D-ND	-5.91	1.37	1.50
25	6	605	CHL	C1D-ND	-5.91	1.37	1.50
25	g	605	CHL	C1D-ND	-5.91	1.37	1.50
25	G	605	CHL	C1D-ND	-5.91	1.37	1.50
25	1	608	CHL	C1D-ND	-5.90	1.37	1.50
25	5	608	CHL	C1D-ND	-5.90	1.37	1.50
25	g	601	CHL	CHB-C4A	-5.90	1.38	1.52
25	G	601	CHL	CHB-C4A	-5.90	1.38	1.52
25	3	302	CHL	C1D-ND	-5.90	1.37	1.50
25	7	302	CHL	C1D-ND	-5.90	1.37	1.50
25	r	305	CHL	C1B-NB	-5.89	1.37	1.50
25	R	305	CHL	C1B-NB	-5.89	1.37	1.50
25	g	601	CHL	C1B-NB	-5.89	1.37	1.50
25	G	601	CHL	C1B-NB	-5.89	1.37	1.50
25	8	308	CHL	C1B-NB	-5.89	1.37	1.50
25	4	308	CHL	C1B-NB	-5.89	1.37	1.50
25	7	308	CHL	C1D-ND	-5.89	1.37	1.50
25	3	308	CHL	C1D-ND	-5.89	1.37	1.50
25	3	306	CHL	C1D-ND	-5.88	1.37	1.50
25	7	306	CHL	C1D-ND	-5.88	1.37	1.50
25	Y	601	CHL	CHB-C4A	-5.88	1.38	1.52
25	y	601	CHL	CHB-C4A	-5.88	1.38	1.52
25	2	607	CHL	C1D-ND	-5.88	1.37	1.50
25	6	607	CHL	C1D-ND	-5.88	1.37	1.50
25	R	304	CHL	C1B-NB	-5.88	1.37	1.50
25	r	304	CHL	C1B-NB	-5.88	1.37	1.50
25	g	601	CHL	C4B-NB	-5.87	1.37	1.50
25	G	601	CHL	C4B-NB	-5.87	1.37	1.50
25	2	605	CHL	C1B-NB	-5.87	1.37	1.50
25	6	605	CHL	C1B-NB	-5.87	1.37	1.50
25	r	305	CHL	C4B-NB	-5.86	1.37	1.50
25	R	305	CHL	C4B-NB	-5.86	1.37	1.50
25	3	301	CHL	C1B-NB	-5.85	1.37	1.50
25	7	301	CHL	C1B-NB	-5.85	1.37	1.50
25	3	306	CHL	C1B-NB	-5.85	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	306	CHL	C1B-NB	-5.85	1.37	1.50
25	1	609	CHL	C1D-ND	-5.85	1.37	1.50
25	5	609	CHL	C1D-ND	-5.85	1.37	1.50
25	n	606	CHL	C4B-NB	-5.85	1.37	1.50
25	N	606	CHL	C4B-NB	-5.85	1.37	1.50
25	N	601	CHL	C3B-CAB	-5.84	1.44	1.50
25	n	601	CHL	C3B-CAB	-5.84	1.44	1.50
25	8	308	CHL	C1D-ND	-5.83	1.37	1.50
25	4	308	CHL	C1D-ND	-5.83	1.37	1.50
25	2	607	CHL	C1B-NB	-5.83	1.37	1.50
25	6	607	CHL	C1B-NB	-5.83	1.37	1.50
25	g	608	CHL	C1B-NB	-5.83	1.37	1.50
25	G	608	CHL	C1B-NB	-5.83	1.37	1.50
25	g	608	CHL	CHB-C4A	-5.83	1.38	1.52
25	G	608	CHL	CHB-C4A	-5.83	1.38	1.52
25	4	301	CHL	C4B-NB	-5.82	1.37	1.50
25	8	301	CHL	C4B-NB	-5.82	1.37	1.50
25	N	608	CHL	CHB-C4A	-5.82	1.38	1.52
25	n	608	CHL	CHB-C4A	-5.82	1.38	1.52
25	6	608	CHL	C4B-NB	-5.82	1.37	1.50
25	2	608	CHL	C4B-NB	-5.82	1.37	1.50
25	8	305	CHL	C1D-ND	-5.82	1.37	1.50
25	4	305	CHL	C1D-ND	-5.82	1.37	1.50
25	s	307	CHL	CHB-C4A	-5.81	1.38	1.52
25	S	307	CHL	CHB-C4A	-5.81	1.38	1.52
25	7	308	CHL	C1B-NB	-5.81	1.37	1.50
25	3	308	CHL	C1B-NB	-5.81	1.37	1.50
25	1	601	CHL	C1D-ND	-5.81	1.37	1.50
25	5	601	CHL	C1D-ND	-5.81	1.37	1.50
25	7	309	CHL	C1B-NB	-5.81	1.37	1.50
25	3	309	CHL	C1B-NB	-5.81	1.37	1.50
25	r	305	CHL	C3B-CAB	-5.80	1.44	1.50
25	R	305	CHL	C3B-CAB	-5.80	1.44	1.50
25	1	608	CHL	C1B-NB	-5.80	1.37	1.50
25	5	608	CHL	C1B-NB	-5.80	1.37	1.50
25	1	607	CHL	C1B-NB	-5.80	1.37	1.50
25	5	607	CHL	C1B-NB	-5.80	1.37	1.50
25	7	309	CHL	C3B-CAB	-5.80	1.44	1.50
25	3	309	CHL	C3B-CAB	-5.80	1.44	1.50
25	4	307	CHL	C1B-NB	-5.80	1.37	1.50
25	8	307	CHL	C1B-NB	-5.80	1.37	1.50
25	7	309	CHL	C1D-ND	-5.79	1.37	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	309	CHL	C1D-ND	-5.79	1.37	1.50
25	6	601	CHL	C1B-NB	-5.79	1.37	1.50
25	2	601	CHL	C1B-NB	-5.79	1.37	1.50
25	N	601	CHL	CHB-C4A	-5.79	1.38	1.52
25	n	601	CHL	CHB-C4A	-5.79	1.38	1.52
25	4	301	CHL	C1B-NB	-5.78	1.37	1.50
25	8	301	CHL	C1B-NB	-5.78	1.37	1.50
25	6	608	CHL	C1D-ND	-5.78	1.37	1.50
25	2	608	CHL	C1D-ND	-5.78	1.37	1.50
25	G	607	CHL	C4B-NB	-5.78	1.37	1.50
25	g	607	CHL	C4B-NB	-5.78	1.37	1.50
25	Y	607	CHL	C3B-CAB	-5.77	1.44	1.50
25	y	607	CHL	C3B-CAB	-5.77	1.44	1.50
25	1	605	CHL	C1B-NB	-5.77	1.37	1.50
25	5	605	CHL	C1B-NB	-5.77	1.37	1.50
25	r	306	CHL	C4B-NB	-5.77	1.37	1.50
25	R	306	CHL	C4B-NB	-5.77	1.37	1.50
25	y	606	CHL	C1B-NB	-5.77	1.37	1.50
25	Y	606	CHL	C1B-NB	-5.77	1.37	1.50
25	g	605	CHL	C4B-NB	-5.76	1.37	1.50
25	G	605	CHL	C4B-NB	-5.76	1.37	1.50
25	1	601	CHL	C1B-NB	-5.76	1.37	1.50
25	5	601	CHL	C1B-NB	-5.76	1.37	1.50
25	6	608	CHL	C3B-CAB	-5.76	1.45	1.50
25	2	608	CHL	C3B-CAB	-5.76	1.45	1.50
25	5	615	CHL	C1B-NB	-5.76	1.37	1.50
25	1	615	CHL	C1B-NB	-5.76	1.37	1.50
25	2	606	CHL	C1B-NB	-5.75	1.37	1.50
25	6	606	CHL	C1B-NB	-5.75	1.37	1.50
25	1	607	CHL	C4B-NB	-5.75	1.37	1.50
25	5	607	CHL	C4B-NB	-5.75	1.37	1.50
25	1	606	CHL	C1B-NB	-5.75	1.37	1.50
25	6	601	CHL	C4B-NB	-5.75	1.37	1.50
25	5	606	CHL	C1B-NB	-5.75	1.37	1.50
25	2	601	CHL	C4B-NB	-5.75	1.37	1.50
25	g	606	CHL	C4B-NB	-5.75	1.37	1.50
25	G	606	CHL	C4B-NB	-5.75	1.37	1.50
25	s	306	CHL	C4B-NB	-5.74	1.38	1.50
25	S	306	CHL	C4B-NB	-5.74	1.38	1.50
25	4	306	CHL	C1B-NB	-5.74	1.38	1.50
25	8	306	CHL	C1B-NB	-5.74	1.38	1.50
25	1	609	CHL	C4B-NB	-5.74	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	609	CHL	C4B-NB	-5.74	1.38	1.50
25	N	605	CHL	CHB-C4A	-5.73	1.38	1.52
25	n	605	CHL	CHB-C4A	-5.73	1.38	1.52
25	r	306	CHL	CHB-C4A	-5.73	1.39	1.52
25	R	306	CHL	CHB-C4A	-5.73	1.39	1.52
25	n	607	CHL	CHB-C4A	-5.73	1.39	1.52
25	N	607	CHL	CHB-C4A	-5.73	1.39	1.52
25	3	302	CHL	CHB-C4A	-5.73	1.39	1.52
25	7	302	CHL	CHB-C4A	-5.73	1.39	1.52
25	4	307	CHL	C4B-NB	-5.72	1.38	1.50
25	8	307	CHL	C4B-NB	-5.72	1.38	1.50
25	1	609	CHL	C3B-CAB	-5.72	1.45	1.50
25	5	609	CHL	C3B-CAB	-5.72	1.45	1.50
25	7	309	CHL	C4B-NB	-5.71	1.38	1.50
25	3	309	CHL	C4B-NB	-5.71	1.38	1.50
25	4	306	CHL	C4B-NB	-5.71	1.38	1.50
25	8	306	CHL	C4B-NB	-5.71	1.38	1.50
25	1	606	CHL	C4B-NB	-5.71	1.38	1.50
25	5	606	CHL	C4B-NB	-5.71	1.38	1.50
25	7	307	CHL	C1B-NB	-5.71	1.38	1.50
25	3	307	CHL	C1B-NB	-5.71	1.38	1.50
25	3	302	CHL	C1B-NB	-5.71	1.38	1.50
25	7	302	CHL	C1B-NB	-5.71	1.38	1.50
25	1	609	CHL	C1B-NB	-5.70	1.38	1.50
25	5	609	CHL	C1B-NB	-5.70	1.38	1.50
25	Y	607	CHL	CHB-C4A	-5.70	1.39	1.52
25	y	607	CHL	CHB-C4A	-5.70	1.39	1.52
25	1	601	CHL	C4B-NB	-5.69	1.38	1.50
25	5	601	CHL	C4B-NB	-5.69	1.38	1.50
25	S	302	CHL	C3B-CAB	-5.69	1.45	1.50
25	s	302	CHL	C3B-CAB	-5.69	1.45	1.50
25	r	305	CHL	CHB-C4A	-5.68	1.39	1.52
25	R	305	CHL	CHB-C4A	-5.68	1.39	1.52
25	g	606	CHL	C3B-CAB	-5.68	1.45	1.50
25	G	606	CHL	C3B-CAB	-5.68	1.45	1.50
25	Y	605	CHL	C3B-CAB	-5.67	1.45	1.50
25	y	605	CHL	C3B-CAB	-5.67	1.45	1.50
25	8	305	CHL	C4B-NB	-5.67	1.38	1.50
25	2	605	CHL	C4B-NB	-5.67	1.38	1.50
25	4	305	CHL	C4B-NB	-5.67	1.38	1.50
25	6	605	CHL	C4B-NB	-5.67	1.38	1.50
25	5	615	CHL	C4B-NB	-5.67	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	615	CHL	C4B-NB	-5.67	1.38	1.50
25	2	606	CHL	C4B-NB	-5.66	1.38	1.50
25	6	606	CHL	C4B-NB	-5.66	1.38	1.50
25	3	302	CHL	C4B-NB	-5.65	1.38	1.50
25	7	302	CHL	C4B-NB	-5.65	1.38	1.50
25	1	605	CHL	C4B-NB	-5.64	1.38	1.50
25	5	605	CHL	C4B-NB	-5.64	1.38	1.50
25	8	308	CHL	C4B-NB	-5.64	1.38	1.50
25	4	308	CHL	C4B-NB	-5.64	1.38	1.50
25	8	308	CHL	CHB-C4A	-5.63	1.39	1.52
25	4	308	CHL	CHB-C4A	-5.63	1.39	1.52
25	8	305	CHL	CHB-C4A	-5.63	1.39	1.52
25	4	305	CHL	CHB-C4A	-5.63	1.39	1.52
25	3	301	CHL	C4B-NB	-5.63	1.38	1.50
25	7	301	CHL	C4B-NB	-5.63	1.38	1.50
25	s	306	CHL	CHB-C4A	-5.62	1.39	1.52
25	S	306	CHL	CHB-C4A	-5.62	1.39	1.52
25	1	608	CHL	CHB-C4A	-5.62	1.39	1.52
25	5	608	CHL	CHB-C4A	-5.62	1.39	1.52
25	6	601	CHL	CHB-C4A	-5.62	1.39	1.52
25	2	601	CHL	CHB-C4A	-5.62	1.39	1.52
25	4	301	CHL	CHB-C4A	-5.62	1.39	1.52
25	8	301	CHL	CHB-C4A	-5.62	1.39	1.52
25	1	608	CHL	C4B-NB	-5.61	1.38	1.50
25	5	608	CHL	C4B-NB	-5.61	1.38	1.50
25	7	307	CHL	C4B-NB	-5.61	1.38	1.50
25	3	307	CHL	C4B-NB	-5.61	1.38	1.50
25	1	607	CHL	CHB-C4A	-5.61	1.39	1.52
25	5	607	CHL	CHB-C4A	-5.61	1.39	1.52
25	3	306	CHL	C4B-NB	-5.60	1.38	1.50
25	7	306	CHL	C4B-NB	-5.60	1.38	1.50
25	1	605	CHL	CHB-C4A	-5.60	1.39	1.52
25	5	605	CHL	CHB-C4A	-5.60	1.39	1.52
25	Y	605	CHL	CHB-C4A	-5.60	1.39	1.52
25	y	605	CHL	CHB-C4A	-5.60	1.39	1.52
25	4	306	CHL	CHB-C4A	-5.59	1.39	1.52
25	8	306	CHL	CHB-C4A	-5.59	1.39	1.52
25	5	615	CHL	CHB-C4A	-5.58	1.39	1.52
25	1	615	CHL	CHB-C4A	-5.58	1.39	1.52
25	7	308	CHL	C4B-NB	-5.57	1.38	1.50
25	3	308	CHL	C4B-NB	-5.57	1.38	1.50
25	6	608	CHL	CHB-C4A	-5.56	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	608	CHL	CHB-C4A	-5.56	1.39	1.52
25	4	307	CHL	CHB-C4A	-5.55	1.39	1.52
25	8	307	CHL	CHB-C4A	-5.55	1.39	1.52
25	2	607	CHL	C4B-NB	-5.55	1.38	1.50
25	6	607	CHL	C4B-NB	-5.55	1.38	1.50
25	G	607	CHL	CHB-C4A	-5.54	1.39	1.52
25	g	607	CHL	CHB-C4A	-5.54	1.39	1.52
25	S	308	CHL	C3B-CAB	-5.53	1.45	1.50
25	s	308	CHL	C3B-CAB	-5.53	1.45	1.50
25	2	607	CHL	CHB-C4A	-5.53	1.39	1.52
25	6	607	CHL	CHB-C4A	-5.53	1.39	1.52
25	1	606	CHL	CHB-C4A	-5.52	1.39	1.52
25	5	606	CHL	CHB-C4A	-5.52	1.39	1.52
25	7	308	CHL	CHB-C4A	-5.52	1.39	1.52
25	3	308	CHL	CHB-C4A	-5.52	1.39	1.52
25	s	306	CHL	C3B-CAB	-5.51	1.45	1.50
25	S	306	CHL	C3B-CAB	-5.51	1.45	1.50
25	g	606	CHL	CHB-C4A	-5.50	1.39	1.52
25	G	606	CHL	CHB-C4A	-5.50	1.39	1.52
25	g	601	CHL	C3B-CAB	-5.50	1.45	1.50
25	G	601	CHL	C3B-CAB	-5.50	1.45	1.50
25	3	302	CHL	C3B-CAB	-5.49	1.45	1.50
25	7	302	CHL	C3B-CAB	-5.49	1.45	1.50
25	n	606	CHL	CHB-C4A	-5.49	1.39	1.52
25	N	606	CHL	CHB-C4A	-5.49	1.39	1.52
25	N	605	CHL	C3B-CAB	-5.46	1.45	1.50
25	n	605	CHL	C3B-CAB	-5.46	1.45	1.50
25	y	606	CHL	CHB-C4A	-5.46	1.39	1.52
25	Y	606	CHL	CHB-C4A	-5.46	1.39	1.52
25	R	304	CHL	CHB-C4A	-5.46	1.39	1.52
25	r	304	CHL	CHB-C4A	-5.46	1.39	1.52
25	4	306	CHL	C3B-CAB	-5.46	1.45	1.50
25	8	306	CHL	C3B-CAB	-5.46	1.45	1.50
25	2	605	CHL	CHB-C4A	-5.46	1.39	1.52
25	6	605	CHL	CHB-C4A	-5.46	1.39	1.52
25	3	301	CHL	CHB-C4A	-5.45	1.39	1.52
25	7	301	CHL	CHB-C4A	-5.45	1.39	1.52
25	n	606	CHL	C3B-CAB	-5.45	1.45	1.50
25	N	606	CHL	C3B-CAB	-5.45	1.45	1.50
25	1	601	CHL	CHB-C4A	-5.44	1.39	1.52
25	5	601	CHL	CHB-C4A	-5.44	1.39	1.52
25	2	606	CHL	C3B-CAB	-5.43	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	606	CHL	C3B-CAB	-5.43	1.45	1.50
25	y	606	CHL	C3B-CAB	-5.43	1.45	1.50
25	Y	606	CHL	C3B-CAB	-5.43	1.45	1.50
25	n	609	CHL	CHB-C4A	-5.42	1.39	1.52
25	N	609	CHL	CHB-C4A	-5.42	1.39	1.52
25	g	605	CHL	CHB-C4A	-5.41	1.39	1.52
25	G	605	CHL	CHB-C4A	-5.41	1.39	1.52
25	1	607	CHL	C3B-CAB	-5.41	1.45	1.50
25	5	607	CHL	C3B-CAB	-5.41	1.45	1.50
25	7	307	CHL	CHB-C4A	-5.40	1.39	1.52
25	3	307	CHL	CHB-C4A	-5.40	1.39	1.52
25	2	606	CHL	CHB-C4A	-5.39	1.39	1.52
25	6	606	CHL	CHB-C4A	-5.39	1.39	1.52
25	g	605	CHL	C3B-CAB	-5.39	1.45	1.50
25	G	605	CHL	C3B-CAB	-5.39	1.45	1.50
25	y	609	CHL	CHB-C4A	-5.39	1.39	1.52
25	Y	609	CHL	CHB-C4A	-5.39	1.39	1.52
25	4	301	CHL	C3B-CAB	-5.38	1.45	1.50
25	8	301	CHL	C3B-CAB	-5.38	1.45	1.50
25	7	307	CHL	C3B-CAB	-5.37	1.45	1.50
25	3	307	CHL	C3B-CAB	-5.37	1.45	1.50
25	N	608	CHL	C3B-CAB	-5.36	1.45	1.50
25	n	608	CHL	C3B-CAB	-5.36	1.45	1.50
25	1	606	CHL	C3B-CAB	-5.35	1.45	1.50
25	5	606	CHL	C3B-CAB	-5.35	1.45	1.50
25	3	306	CHL	CHB-C4A	-5.34	1.39	1.52
25	7	306	CHL	CHB-C4A	-5.34	1.39	1.52
25	G	609	CHL	CHB-C4A	-5.34	1.39	1.52
25	g	609	CHL	CHB-C4A	-5.34	1.39	1.52
25	1	609	CHL	CHB-C4A	-5.34	1.39	1.52
25	5	609	CHL	CHB-C4A	-5.34	1.39	1.52
25	2	605	CHL	C3B-CAB	-5.32	1.45	1.50
25	6	605	CHL	C3B-CAB	-5.32	1.45	1.50
25	G	607	CHL	C3B-CAB	-5.31	1.45	1.50
25	g	607	CHL	C3B-CAB	-5.31	1.45	1.50
25	4	307	CHL	C3B-CAB	-5.30	1.45	1.50
25	8	307	CHL	C3B-CAB	-5.30	1.45	1.50
25	7	309	CHL	CHB-C4A	-5.30	1.40	1.52
25	3	309	CHL	CHB-C4A	-5.30	1.40	1.52
25	3	306	CHL	C3B-CAB	-5.29	1.45	1.50
25	7	306	CHL	C3B-CAB	-5.29	1.45	1.50
24	E	101	HEM	C3C-C2C	-5.26	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	608	CHL	C3B-CAB	-5.25	1.45	1.50
25	5	608	CHL	C3B-CAB	-5.25	1.45	1.50
24	e	101	HEM	C3C-C2C	-5.25	1.33	1.40
24	E	101	HEM	C3B-C2B	-5.24	1.33	1.40
25	5	615	CHL	C3B-CAB	-5.23	1.45	1.50
25	1	615	CHL	C3B-CAB	-5.23	1.45	1.50
25	1	601	CHL	C3B-CAB	-5.23	1.45	1.50
25	5	601	CHL	C3B-CAB	-5.23	1.45	1.50
25	r	306	CHL	C3B-CAB	-5.23	1.45	1.50
25	R	306	CHL	C3B-CAB	-5.23	1.45	1.50
24	e	101	HEM	C3B-C2B	-5.19	1.33	1.40
25	6	601	CHL	C3B-CAB	-5.16	1.45	1.50
25	2	601	CHL	C3B-CAB	-5.16	1.45	1.50
25	1	605	CHL	C3B-CAB	-5.16	1.45	1.50
25	5	605	CHL	C3B-CAB	-5.16	1.45	1.50
25	3	301	CHL	C3B-CAB	-5.16	1.45	1.50
25	7	301	CHL	C3B-CAB	-5.16	1.45	1.50
25	8	305	CHL	C3B-CAB	-5.10	1.45	1.50
25	4	305	CHL	C3B-CAB	-5.10	1.45	1.50
25	y	608	CHL	C2B-C1B	-5.10	1.43	1.53
25	Y	608	CHL	C2B-C1B	-5.10	1.43	1.53
25	Y	601	CHL	C3B-CAB	-5.09	1.45	1.50
25	y	601	CHL	C3B-CAB	-5.09	1.45	1.50
25	6	608	CHL	C2B-C1B	-4.96	1.43	1.53
25	2	608	CHL	C2B-C1B	-4.96	1.43	1.53
25	8	308	CHL	C3B-CAB	-4.93	1.45	1.50
25	4	308	CHL	C3B-CAB	-4.93	1.45	1.50
25	n	609	CHL	C2D-C1D	-4.86	1.43	1.53
25	N	609	CHL	C2D-C1D	-4.86	1.43	1.53
25	7	308	CHL	C3B-CAB	-4.86	1.45	1.50
25	3	308	CHL	C3B-CAB	-4.86	1.45	1.50
25	S	302	CHL	C2B-C1B	-4.77	1.43	1.53
25	s	302	CHL	C2B-C1B	-4.77	1.43	1.53
25	8	305	CHL	C2B-C1B	-4.71	1.44	1.53
25	4	305	CHL	C2B-C1B	-4.71	1.44	1.53
25	2	607	CHL	C3B-CAB	-4.70	1.46	1.50
25	6	607	CHL	C3B-CAB	-4.70	1.46	1.50
25	g	601	CHL	C2B-C1B	-4.67	1.44	1.53
25	G	601	CHL	C2B-C1B	-4.67	1.44	1.53
25	s	307	CHL	C2B-C1B	-4.67	1.44	1.53
25	S	307	CHL	C2B-C1B	-4.67	1.44	1.53
25	S	308	CHL	C2B-C1B	-4.66	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	308	CHL	C2B-C1B	-4.66	1.44	1.53
25	G	609	CHL	C2D-C1D	-4.65	1.44	1.53
25	g	609	CHL	C2D-C1D	-4.65	1.44	1.53
25	N	608	CHL	C2B-C1B	-4.64	1.44	1.53
25	n	608	CHL	C2B-C1B	-4.64	1.44	1.53
25	n	607	CHL	C2B-C1B	-4.64	1.44	1.53
25	N	607	CHL	C2B-C1B	-4.64	1.44	1.53
25	g	608	CHL	C2B-C1B	-4.61	1.44	1.53
25	G	608	CHL	C2B-C1B	-4.61	1.44	1.53
25	Y	601	CHL	C2B-C1B	-4.59	1.44	1.53
25	y	601	CHL	C2B-C1B	-4.59	1.44	1.53
25	N	601	CHL	C2B-C1B	-4.52	1.44	1.53
25	n	601	CHL	C2B-C1B	-4.52	1.44	1.53
25	y	609	CHL	C2D-C1D	-4.51	1.44	1.53
25	Y	609	CHL	C2D-C1D	-4.51	1.44	1.53
25	3	302	CHL	C2B-C1B	-4.48	1.44	1.53
25	7	302	CHL	C2B-C1B	-4.48	1.44	1.53
25	1	608	CHL	C2B-C1B	-4.47	1.44	1.53
25	5	608	CHL	C2B-C1B	-4.47	1.44	1.53
25	y	606	CHL	C2B-C1B	-4.46	1.44	1.53
25	Y	606	CHL	C2B-C1B	-4.46	1.44	1.53
25	Y	601	CHL	C2D-C1D	-4.43	1.44	1.53
25	y	601	CHL	C2D-C1D	-4.43	1.44	1.53
25	y	609	CHL	C2B-C1B	-4.42	1.44	1.53
25	Y	609	CHL	C2B-C1B	-4.42	1.44	1.53
25	2	607	CHL	C2B-C1B	-4.42	1.44	1.53
25	6	607	CHL	C2B-C1B	-4.42	1.44	1.53
25	R	304	CHL	C2B-C1B	-4.42	1.44	1.53
25	r	304	CHL	C2B-C1B	-4.42	1.44	1.53
25	r	305	CHL	C2B-C1B	-4.41	1.44	1.53
25	R	305	CHL	C2B-C1B	-4.41	1.44	1.53
25	1	607	CHL	C2B-C1B	-4.41	1.44	1.53
25	5	607	CHL	C2B-C1B	-4.41	1.44	1.53
25	Y	605	CHL	C2D-C1D	-4.41	1.44	1.53
25	y	605	CHL	C2D-C1D	-4.41	1.44	1.53
25	7	308	CHL	C2B-C1B	-4.41	1.44	1.53
25	3	308	CHL	C2B-C1B	-4.41	1.44	1.53
25	n	609	CHL	C2B-C1B	-4.40	1.44	1.53
25	N	609	CHL	C2B-C1B	-4.40	1.44	1.53
25	G	607	CHL	C2B-C1B	-4.40	1.44	1.53
25	g	607	CHL	C2B-C1B	-4.40	1.44	1.53
25	5	615	CHL	C2B-C1B	-4.40	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	615	CHL	C2B-C1B	-4.40	1.44	1.53
25	r	306	CHL	C2B-C1B	-4.40	1.44	1.53
25	R	306	CHL	C2B-C1B	-4.40	1.44	1.53
25	7	309	CHL	C2B-C1B	-4.39	1.44	1.53
25	3	309	CHL	C2B-C1B	-4.39	1.44	1.53
25	1	605	CHL	C2B-C1B	-4.38	1.44	1.53
25	5	605	CHL	C2B-C1B	-4.38	1.44	1.53
25	N	605	CHL	C2B-C1B	-4.37	1.44	1.53
25	n	605	CHL	C2B-C1B	-4.37	1.44	1.53
25	n	607	CHL	C2D-C1D	-4.36	1.44	1.53
25	N	607	CHL	C2D-C1D	-4.36	1.44	1.53
25	6	601	CHL	C2B-C1B	-4.36	1.44	1.53
25	2	601	CHL	C2B-C1B	-4.36	1.44	1.53
25	G	607	CHL	C2D-C1D	-4.36	1.44	1.53
25	g	607	CHL	C2D-C1D	-4.36	1.44	1.53
25	s	306	CHL	C2B-C1B	-4.35	1.44	1.53
25	S	306	CHL	C2B-C1B	-4.35	1.44	1.53
25	g	605	CHL	C2B-C1B	-4.34	1.44	1.53
25	G	605	CHL	C2B-C1B	-4.34	1.44	1.53
25	4	306	CHL	C2B-C1B	-4.33	1.44	1.53
25	8	306	CHL	C2B-C1B	-4.33	1.44	1.53
25	r	306	CHL	C2D-C1D	-4.33	1.44	1.53
25	R	306	CHL	C2D-C1D	-4.33	1.44	1.53
25	Y	607	CHL	C2B-C1B	-4.33	1.44	1.53
25	y	607	CHL	C2B-C1B	-4.33	1.44	1.53
25	N	605	CHL	C2D-C1D	-4.33	1.44	1.53
25	n	605	CHL	C2D-C1D	-4.33	1.44	1.53
25	G	609	CHL	C2B-C1B	-4.33	1.44	1.53
25	g	609	CHL	C2B-C1B	-4.33	1.44	1.53
25	4	301	CHL	C2B-C1B	-4.33	1.44	1.53
25	8	301	CHL	C2B-C1B	-4.33	1.44	1.53
25	4	307	CHL	C2B-C1B	-4.32	1.44	1.53
25	8	307	CHL	C2B-C1B	-4.32	1.44	1.53
25	2	605	CHL	C2B-C1B	-4.30	1.44	1.53
25	6	605	CHL	C2B-C1B	-4.30	1.44	1.53
25	3	301	CHL	C2B-C1B	-4.30	1.44	1.53
25	7	301	CHL	C2B-C1B	-4.30	1.44	1.53
25	1	609	CHL	C2B-C1B	-4.30	1.44	1.53
25	5	609	CHL	C2B-C1B	-4.30	1.44	1.53
25	G	609	CHL	C3D-CAD	-4.29	1.43	1.51
25	g	609	CHL	C3D-CAD	-4.29	1.43	1.51
25	r	305	CHL	C2D-C1D	-4.28	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	305	CHL	C2D-C1D	-4.28	1.44	1.53
25	Y	607	CHL	C2D-C1D	-4.28	1.44	1.53
25	y	607	CHL	C2D-C1D	-4.28	1.44	1.53
25	1	601	CHL	C2B-C1B	-4.27	1.44	1.53
25	5	601	CHL	C2B-C1B	-4.27	1.44	1.53
25	8	308	CHL	C2B-C1B	-4.27	1.44	1.53
25	4	308	CHL	C2B-C1B	-4.27	1.44	1.53
25	S	302	CHL	C2D-C1D	-4.27	1.44	1.53
25	s	302	CHL	C2D-C1D	-4.27	1.44	1.53
25	n	606	CHL	C2B-C1B	-4.26	1.44	1.53
25	N	606	CHL	C2B-C1B	-4.26	1.44	1.53
25	g	606	CHL	C2B-C1B	-4.26	1.44	1.53
25	G	606	CHL	C2B-C1B	-4.26	1.44	1.53
25	N	601	CHL	C2D-C1D	-4.25	1.44	1.53
25	n	601	CHL	C2D-C1D	-4.25	1.44	1.53
25	1	606	CHL	C2B-C1B	-4.25	1.44	1.53
25	5	606	CHL	C2B-C1B	-4.25	1.44	1.53
25	S	308	CHL	C2D-C1D	-4.24	1.44	1.53
25	s	308	CHL	C2D-C1D	-4.24	1.44	1.53
25	n	609	CHL	C3D-CAD	-4.24	1.43	1.51
25	N	609	CHL	C3D-CAD	-4.24	1.43	1.51
25	7	309	CHL	C2D-C1D	-4.22	1.45	1.53
25	3	309	CHL	C2D-C1D	-4.22	1.45	1.53
25	7	307	CHL	C2B-C1B	-4.22	1.45	1.53
25	3	307	CHL	C2B-C1B	-4.22	1.45	1.53
25	3	306	CHL	C2B-C1B	-4.21	1.45	1.53
25	7	306	CHL	C2B-C1B	-4.21	1.45	1.53
25	g	601	CHL	C2D-C1D	-4.21	1.45	1.53
25	G	601	CHL	C2D-C1D	-4.21	1.45	1.53
25	2	606	CHL	C2B-C1B	-4.19	1.45	1.53
25	6	606	CHL	C2B-C1B	-4.19	1.45	1.53
25	6	608	CHL	C2D-C1D	-4.19	1.45	1.53
25	2	608	CHL	C2D-C1D	-4.19	1.45	1.53
25	n	606	CHL	C2D-C1D	-4.16	1.45	1.53
25	N	606	CHL	C2D-C1D	-4.16	1.45	1.53
25	3	301	CHL	C2D-C1D	-4.15	1.45	1.53
25	7	301	CHL	C2D-C1D	-4.15	1.45	1.53
25	Y	605	CHL	C2B-C1B	-4.14	1.45	1.53
25	y	605	CHL	C2B-C1B	-4.14	1.45	1.53
25	7	308	CHL	C2D-C1D	-4.13	1.45	1.53
25	3	308	CHL	C2D-C1D	-4.13	1.45	1.53
25	5	615	CHL	C2D-C1D	-4.11	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	605	CHL	C2D-C1D	-4.11	1.45	1.53
25	5	605	CHL	C2D-C1D	-4.11	1.45	1.53
25	1	615	CHL	C2D-C1D	-4.11	1.45	1.53
25	1	609	CHL	C2D-C1D	-4.10	1.45	1.53
25	5	609	CHL	C2D-C1D	-4.10	1.45	1.53
25	N	608	CHL	C2D-C1D	-4.09	1.45	1.53
25	n	608	CHL	C2D-C1D	-4.09	1.45	1.53
25	y	606	CHL	C2D-C1D	-4.06	1.45	1.53
25	Y	606	CHL	C2D-C1D	-4.06	1.45	1.53
25	3	306	CHL	C2D-C1D	-4.06	1.45	1.53
25	7	306	CHL	C2D-C1D	-4.06	1.45	1.53
25	s	307	CHL	C2D-C1D	-4.05	1.45	1.53
25	S	307	CHL	C2D-C1D	-4.05	1.45	1.53
25	s	306	CHL	C2D-C1D	-4.04	1.45	1.53
25	S	306	CHL	C2D-C1D	-4.04	1.45	1.53
25	2	605	CHL	C2D-C1D	-4.04	1.45	1.53
25	2	606	CHL	C2D-C1D	-4.04	1.45	1.53
25	6	606	CHL	C2D-C1D	-4.04	1.45	1.53
25	6	605	CHL	C2D-C1D	-4.04	1.45	1.53
25	g	605	CHL	C2D-C1D	-4.02	1.45	1.53
25	G	605	CHL	C2D-C1D	-4.02	1.45	1.53
25	2	607	CHL	C2D-C1D	-4.01	1.45	1.53
25	6	607	CHL	C2D-C1D	-4.01	1.45	1.53
25	1	606	CHL	C2D-C1D	-3.99	1.45	1.53
25	5	606	CHL	C2D-C1D	-3.99	1.45	1.53
25	4	307	CHL	C2D-C1D	-3.99	1.45	1.53
25	8	307	CHL	C2D-C1D	-3.99	1.45	1.53
25	6	601	CHL	C2D-C1D	-3.99	1.45	1.53
25	2	601	CHL	C2D-C1D	-3.99	1.45	1.53
25	g	608	CHL	C2D-C1D	-3.99	1.45	1.53
25	G	608	CHL	C2D-C1D	-3.99	1.45	1.53
25	R	304	CHL	C2D-C1D	-3.98	1.45	1.53
25	r	304	CHL	C2D-C1D	-3.98	1.45	1.53
25	8	308	CHL	C2D-C1D	-3.95	1.45	1.53
25	4	308	CHL	C2D-C1D	-3.95	1.45	1.53
25	7	308	CHL	C3D-CAD	-3.94	1.44	1.51
25	3	308	CHL	C3D-CAD	-3.94	1.44	1.51
25	y	608	CHL	C2D-C1D	-3.94	1.45	1.53
25	Y	608	CHL	C2D-C1D	-3.94	1.45	1.53
25	n	607	CHL	C3D-CAD	-3.94	1.44	1.51
25	N	607	CHL	C3D-CAD	-3.94	1.44	1.51
25	g	606	CHL	C2D-C1D	-3.91	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	606	CHL	C2D-C1D	-3.91	1.45	1.53
25	1	601	CHL	C2D-C1D	-3.91	1.45	1.53
25	5	601	CHL	C2D-C1D	-3.91	1.45	1.53
25	N	605	CHL	C3D-CAD	-3.91	1.44	1.51
25	n	605	CHL	C3D-CAD	-3.91	1.44	1.51
25	3	302	CHL	C2D-C1D	-3.91	1.45	1.53
25	7	302	CHL	C2D-C1D	-3.91	1.45	1.53
25	4	306	CHL	C2D-C1D	-3.90	1.45	1.53
25	8	306	CHL	C2D-C1D	-3.90	1.45	1.53
25	Y	607	CHL	C3D-CAD	-3.89	1.44	1.51
25	y	607	CHL	C3D-CAD	-3.89	1.44	1.51
25	y	609	CHL	C3D-CAD	-3.89	1.44	1.51
25	Y	609	CHL	C3D-CAD	-3.89	1.44	1.51
25	7	307	CHL	C2D-C1D	-3.89	1.45	1.53
25	3	307	CHL	C2D-C1D	-3.89	1.45	1.53
25	1	608	CHL	C2D-C1D	-3.88	1.45	1.53
25	5	608	CHL	C2D-C1D	-3.88	1.45	1.53
25	1	607	CHL	C2D-C1D	-3.87	1.45	1.53
25	5	607	CHL	C2D-C1D	-3.87	1.45	1.53
25	6	608	CHL	C3D-CAD	-3.85	1.44	1.51
25	2	608	CHL	C3D-CAD	-3.85	1.44	1.51
25	7	309	CHL	C3D-CAD	-3.84	1.44	1.51
25	3	309	CHL	C3D-CAD	-3.84	1.44	1.51
25	3	301	CHL	C3D-CAD	-3.84	1.44	1.51
25	7	301	CHL	C3D-CAD	-3.84	1.44	1.51
25	Y	601	CHL	C3D-CAD	-3.83	1.44	1.51
25	y	601	CHL	C3D-CAD	-3.83	1.44	1.51
25	g	601	CHL	C3D-CAD	-3.83	1.44	1.51
25	G	601	CHL	C3D-CAD	-3.83	1.44	1.51
25	G	607	CHL	C3D-CAD	-3.78	1.44	1.51
25	g	607	CHL	C3D-CAD	-3.78	1.44	1.51
25	1	609	CHL	C3D-CAD	-3.78	1.44	1.51
25	5	609	CHL	C3D-CAD	-3.78	1.44	1.51
25	Y	605	CHL	C3D-CAD	-3.77	1.44	1.51
25	y	605	CHL	C3D-CAD	-3.77	1.44	1.51
25	8	305	CHL	C2D-C1D	-3.76	1.45	1.53
25	4	305	CHL	C2D-C1D	-3.76	1.45	1.53
25	4	301	CHL	C2D-C1D	-3.75	1.45	1.53
25	8	301	CHL	C2D-C1D	-3.75	1.45	1.53
25	4	301	CHL	C3D-CAD	-3.71	1.44	1.51
25	8	301	CHL	C3D-CAD	-3.71	1.44	1.51
25	r	306	CHL	C3D-CAD	-3.69	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	306	CHL	C3D-CAD	-3.69	1.44	1.51
25	n	606	CHL	C3D-CAD	-3.69	1.44	1.51
25	N	606	CHL	C3D-CAD	-3.69	1.44	1.51
25	y	606	CHL	C3D-CAD	-3.66	1.44	1.51
25	Y	606	CHL	C3D-CAD	-3.66	1.44	1.51
25	N	601	CHL	C3D-CAD	-3.65	1.44	1.51
25	n	601	CHL	C3D-CAD	-3.65	1.44	1.51
25	S	302	CHL	C3D-CAD	-3.65	1.44	1.51
25	s	302	CHL	C3D-CAD	-3.65	1.44	1.51
25	8	305	CHL	C3D-CAD	-3.65	1.44	1.51
25	4	305	CHL	C3D-CAD	-3.65	1.44	1.51
25	N	608	CHL	C3D-CAD	-3.62	1.44	1.51
25	n	608	CHL	C3D-CAD	-3.62	1.44	1.51
25	g	608	CHL	C3D-CAD	-3.61	1.44	1.51
25	G	608	CHL	C3D-CAD	-3.61	1.44	1.51
25	g	606	CHL	C3D-CAD	-3.61	1.44	1.51
25	G	606	CHL	C3D-CAD	-3.61	1.44	1.51
25	S	308	CHL	C3D-CAD	-3.60	1.44	1.51
25	s	308	CHL	C3D-CAD	-3.60	1.44	1.51
25	r	305	CHL	C3D-CAD	-3.55	1.44	1.51
25	R	305	CHL	C3D-CAD	-3.55	1.44	1.51
25	2	605	CHL	C3D-CAD	-3.54	1.44	1.51
25	6	605	CHL	C3D-CAD	-3.54	1.44	1.51
25	1	605	CHL	C3D-CAD	-3.52	1.44	1.51
25	5	605	CHL	C3D-CAD	-3.52	1.44	1.51
25	R	304	CHL	C3D-CAD	-3.52	1.44	1.51
25	r	304	CHL	C3D-CAD	-3.52	1.44	1.51
25	4	306	CHL	C3D-CAD	-3.52	1.44	1.51
25	8	306	CHL	C3D-CAD	-3.52	1.44	1.51
25	s	307	CHL	C3D-CAD	-3.50	1.44	1.51
25	S	307	CHL	C3D-CAD	-3.50	1.44	1.51
25	s	306	CHL	C3D-CAD	-3.50	1.44	1.51
25	S	306	CHL	C3D-CAD	-3.50	1.44	1.51
25	3	306	CHL	C3D-CAD	-3.48	1.44	1.51
25	7	306	CHL	C3D-CAD	-3.48	1.44	1.51
25	y	608	CHL	C3D-CAD	-3.48	1.44	1.51
25	1	608	CHL	C3D-CAD	-3.48	1.44	1.51
25	Y	608	CHL	C3D-CAD	-3.48	1.44	1.51
25	5	608	CHL	C3D-CAD	-3.48	1.44	1.51
25	g	605	CHL	C3D-CAD	-3.48	1.44	1.51
25	G	605	CHL	C3D-CAD	-3.48	1.44	1.51
25	1	607	CHL	C3D-CAD	-3.48	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	607	CHL	C3D-CAD	-3.48	1.44	1.51
25	6	601	CHL	C3D-CAD	-3.46	1.44	1.51
25	2	601	CHL	C3D-CAD	-3.46	1.44	1.51
25	2	607	CHL	C3D-CAD	-3.44	1.44	1.51
25	6	607	CHL	C3D-CAD	-3.44	1.44	1.51
25	1	606	CHL	C3D-CAD	-3.43	1.44	1.51
25	5	606	CHL	C3D-CAD	-3.43	1.44	1.51
25	5	615	CHL	C3D-CAD	-3.42	1.45	1.51
25	1	615	CHL	C3D-CAD	-3.42	1.45	1.51
25	1	601	CHL	C3D-CAD	-3.37	1.45	1.51
25	5	601	CHL	C3D-CAD	-3.37	1.45	1.51
25	8	308	CHL	C3D-CAD	-3.36	1.45	1.51
25	4	308	CHL	C3D-CAD	-3.36	1.45	1.51
25	2	606	CHL	C3D-CAD	-3.35	1.45	1.51
25	6	606	CHL	C3D-CAD	-3.35	1.45	1.51
25	7	307	CHL	C3D-CAD	-3.34	1.45	1.51
25	3	307	CHL	C3D-CAD	-3.34	1.45	1.51
25	3	302	CHL	C3D-CAD	-3.33	1.45	1.51
25	7	302	CHL	C3D-CAD	-3.33	1.45	1.51
25	4	307	CHL	C3D-CAD	-3.25	1.45	1.51
25	8	307	CHL	C3D-CAD	-3.25	1.45	1.51
23	d	402	PHO	C1A-NA	-3.16	1.30	1.37
23	A	404	PHO	C1C-NC	-3.12	1.31	1.38
23	D	402	PHO	C1A-NA	-3.12	1.30	1.37
23	A	404	PHO	C1A-NA	-3.11	1.30	1.37
23	a	404	PHO	C1A-NA	-2.98	1.31	1.37
23	D	402	PHO	C1C-NC	-2.89	1.32	1.38
23	d	402	PHO	C1C-NC	-2.88	1.32	1.38
23	a	404	PHO	C1C-NC	-2.86	1.32	1.38
25	7	308	CHL	O2D-CED	-2.83	1.38	1.45
25	3	308	CHL	O2D-CED	-2.83	1.38	1.45
25	8	308	CHL	C2A-C3A	-2.79	1.49	1.55
25	4	308	CHL	C2A-C3A	-2.79	1.49	1.55
25	g	601	CHL	O2D-CED	-2.78	1.38	1.45
25	G	601	CHL	O2D-CED	-2.78	1.38	1.45
25	Y	605	CHL	O2D-CED	-2.76	1.38	1.45
25	y	605	CHL	O2D-CED	-2.76	1.38	1.45
25	Y	601	CHL	O2D-CED	-2.73	1.38	1.45
25	y	601	CHL	O2D-CED	-2.73	1.38	1.45
25	N	608	CHL	O2D-CED	-2.73	1.38	1.45
25	n	608	CHL	O2D-CED	-2.73	1.38	1.45
25	s	307	CHL	O2D-CED	-2.72	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	307	CHL	O2D-CED	-2.72	1.38	1.45
25	R	304	CHL	C2A-C3A	-2.72	1.49	1.55
25	r	304	CHL	C2A-C3A	-2.72	1.49	1.55
25	g	608	CHL	O2D-CED	-2.71	1.38	1.45
25	G	608	CHL	O2D-CED	-2.71	1.38	1.45
25	y	608	CHL	O2D-CED	-2.69	1.38	1.45
25	Y	608	CHL	O2D-CED	-2.69	1.38	1.45
25	S	302	CHL	O2D-CED	-2.68	1.38	1.45
25	s	302	CHL	O2D-CED	-2.68	1.38	1.45
25	5	615	CHL	O2D-CED	-2.67	1.38	1.45
25	1	615	CHL	O2D-CED	-2.67	1.38	1.45
25	n	607	CHL	O2D-CED	-2.67	1.38	1.45
25	N	607	CHL	O2D-CED	-2.67	1.38	1.45
25	G	607	CHL	O2D-CED	-2.67	1.38	1.45
25	g	607	CHL	O2D-CED	-2.67	1.38	1.45
25	N	601	CHL	O2D-CED	-2.67	1.38	1.45
25	n	601	CHL	O2D-CED	-2.67	1.38	1.45
25	y	606	CHL	O2D-CED	-2.66	1.38	1.45
25	Y	606	CHL	O2D-CED	-2.66	1.38	1.45
25	6	608	CHL	O2D-CED	-2.65	1.38	1.45
25	2	608	CHL	O2D-CED	-2.65	1.38	1.45
23	a	404	PHO	C3D-C4D	-2.65	1.35	1.43
25	R	304	CHL	O2D-CED	-2.65	1.38	1.45
25	r	304	CHL	O2D-CED	-2.65	1.38	1.45
25	1	605	CHL	O2D-CED	-2.63	1.39	1.45
25	5	605	CHL	O2D-CED	-2.63	1.39	1.45
25	S	308	CHL	O2D-CED	-2.63	1.39	1.45
25	s	308	CHL	O2D-CED	-2.63	1.39	1.45
25	1	607	CHL	O2D-CED	-2.63	1.39	1.45
25	5	607	CHL	O2D-CED	-2.63	1.39	1.45
25	Y	607	CHL	O2D-CED	-2.62	1.39	1.45
25	y	607	CHL	O2D-CED	-2.62	1.39	1.45
25	8	308	CHL	O2D-CED	-2.62	1.39	1.45
25	4	308	CHL	O2D-CED	-2.62	1.39	1.45
25	n	606	CHL	O2D-CED	-2.62	1.39	1.45
25	N	606	CHL	O2D-CED	-2.62	1.39	1.45
25	8	305	CHL	O2D-CED	-2.62	1.39	1.45
25	4	305	CHL	O2D-CED	-2.62	1.39	1.45
25	2	607	CHL	O2D-CED	-2.61	1.39	1.45
25	6	607	CHL	O2D-CED	-2.61	1.39	1.45
25	7	307	CHL	O2D-CED	-2.61	1.39	1.45
25	3	307	CHL	O2D-CED	-2.61	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	301	CHL	O2D-CED	-2.61	1.39	1.45
25	7	301	CHL	O2D-CED	-2.61	1.39	1.45
25	6	601	CHL	O2D-CED	-2.61	1.39	1.45
25	2	601	CHL	O2D-CED	-2.61	1.39	1.45
25	S	302	CHL	C2A-C3A	-2.61	1.49	1.55
25	s	302	CHL	C2A-C3A	-2.61	1.49	1.55
25	3	302	CHL	O2D-CED	-2.60	1.39	1.45
25	7	302	CHL	O2D-CED	-2.60	1.39	1.45
25	1	601	CHL	O2D-CED	-2.60	1.39	1.45
25	5	601	CHL	O2D-CED	-2.60	1.39	1.45
25	s	306	CHL	O2D-CED	-2.60	1.39	1.45
25	S	306	CHL	O2D-CED	-2.60	1.39	1.45
25	N	605	CHL	O2D-CED	-2.59	1.39	1.45
25	r	306	CHL	O2D-CED	-2.59	1.39	1.45
25	R	306	CHL	O2D-CED	-2.59	1.39	1.45
25	n	605	CHL	O2D-CED	-2.59	1.39	1.45
25	3	302	CHL	C2A-C3A	-2.59	1.49	1.55
25	7	302	CHL	C2A-C3A	-2.59	1.49	1.55
23	d	402	PHO	C3D-C4D	-2.59	1.35	1.43
25	2	606	CHL	O2D-CED	-2.59	1.39	1.45
25	6	606	CHL	O2D-CED	-2.59	1.39	1.45
25	4	301	CHL	O2D-CED	-2.58	1.39	1.45
25	8	301	CHL	O2D-CED	-2.58	1.39	1.45
25	g	606	CHL	O2D-CED	-2.57	1.39	1.45
25	G	606	CHL	O2D-CED	-2.57	1.39	1.45
25	1	608	CHL	O2D-CED	-2.57	1.39	1.45
25	5	608	CHL	O2D-CED	-2.57	1.39	1.45
23	A	404	PHO	C3D-C4D	-2.56	1.35	1.43
25	1	606	CHL	O2D-CED	-2.56	1.39	1.45
25	5	606	CHL	O2D-CED	-2.56	1.39	1.45
25	4	306	CHL	O2D-CED	-2.55	1.39	1.45
25	8	306	CHL	O2D-CED	-2.55	1.39	1.45
25	g	605	CHL	O2D-CED	-2.55	1.39	1.45
25	G	605	CHL	O2D-CED	-2.55	1.39	1.45
25	y	608	CHL	C2A-C3A	-2.54	1.50	1.55
25	Y	608	CHL	C2A-C3A	-2.54	1.50	1.55
25	4	307	CHL	O2D-CED	-2.54	1.39	1.45
25	8	307	CHL	O2D-CED	-2.54	1.39	1.45
23	D	402	PHO	C3D-C4D	-2.53	1.35	1.43
25	7	309	CHL	O2D-CED	-2.53	1.39	1.45
25	3	309	CHL	O2D-CED	-2.53	1.39	1.45
25	r	305	CHL	O2D-CED	-2.52	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	305	CHL	O2D-CED	-2.52	1.39	1.45
25	1	609	CHL	O2D-CED	-2.52	1.39	1.45
25	5	609	CHL	O2D-CED	-2.52	1.39	1.45
25	y	606	CHL	C2A-C3A	-2.51	1.50	1.55
25	Y	606	CHL	C2A-C3A	-2.51	1.50	1.55
25	g	601	CHL	C2A-C3A	-2.51	1.50	1.55
25	G	601	CHL	C2A-C3A	-2.51	1.50	1.55
25	3	306	CHL	O2D-CED	-2.50	1.39	1.45
25	7	306	CHL	O2D-CED	-2.50	1.39	1.45
25	s	306	CHL	C2A-C3A	-2.49	1.50	1.55
25	S	306	CHL	C2A-C3A	-2.49	1.50	1.55
25	2	605	CHL	O2D-CED	-2.49	1.39	1.45
25	6	605	CHL	O2D-CED	-2.49	1.39	1.45
25	y	609	CHL	O2D-CED	-2.49	1.39	1.45
25	Y	609	CHL	O2D-CED	-2.49	1.39	1.45
25	y	609	CHL	C2A-C3A	-2.49	1.50	1.55
25	Y	609	CHL	C2A-C3A	-2.49	1.50	1.55
25	n	606	CHL	C2A-C3A	-2.49	1.50	1.55
25	N	606	CHL	C2A-C3A	-2.49	1.50	1.55
25	r	305	CHL	C2A-C3A	-2.48	1.50	1.55
25	R	305	CHL	C2A-C3A	-2.48	1.50	1.55
25	N	608	CHL	C2A-C3A	-2.48	1.50	1.55
25	n	608	CHL	C2A-C3A	-2.48	1.50	1.55
25	S	308	CHL	C2A-C3A	-2.46	1.50	1.55
25	s	308	CHL	C2A-C3A	-2.46	1.50	1.55
25	G	609	CHL	O2D-CED	-2.44	1.39	1.45
25	g	609	CHL	O2D-CED	-2.44	1.39	1.45
25	n	609	CHL	O2D-CED	-2.44	1.39	1.45
25	N	609	CHL	O2D-CED	-2.44	1.39	1.45
25	Y	601	CHL	C2A-C3A	-2.42	1.50	1.55
25	y	601	CHL	C2A-C3A	-2.42	1.50	1.55
25	G	609	CHL	C2A-C3A	-2.39	1.50	1.55
25	g	609	CHL	C2A-C3A	-2.39	1.50	1.55
25	r	306	CHL	C2A-C3A	-2.38	1.50	1.55
25	R	306	CHL	C2A-C3A	-2.38	1.50	1.55
25	N	601	CHL	C2A-C3A	-2.37	1.50	1.55
25	n	601	CHL	C2A-C3A	-2.37	1.50	1.55
25	s	307	CHL	C2A-C3A	-2.36	1.50	1.55
25	S	307	CHL	C2A-C3A	-2.36	1.50	1.55
25	n	609	CHL	C2A-C3A	-2.34	1.50	1.55
25	N	609	CHL	C2A-C3A	-2.34	1.50	1.55
25	g	608	CHL	C2A-C3A	-2.33	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	608	CHL	C2A-C3A	-2.33	1.50	1.55
25	1	609	CHL	C2A-C3A	-2.31	1.50	1.55
25	5	609	CHL	C2A-C3A	-2.31	1.50	1.55
25	1	608	CHL	C2A-C3A	-2.29	1.50	1.55
25	5	608	CHL	C2A-C3A	-2.29	1.50	1.55
25	4	301	CHL	C2A-C3A	-2.28	1.50	1.55
25	8	301	CHL	C2A-C3A	-2.28	1.50	1.55
25	g	601	CHL	C4A-C3A	-2.28	1.51	1.53
25	G	601	CHL	C4A-C3A	-2.28	1.51	1.53
25	3	302	CHL	C4A-C3A	-2.26	1.51	1.53
25	7	302	CHL	C4A-C3A	-2.26	1.51	1.53
25	g	606	CHL	C2A-C3A	-2.26	1.50	1.55
25	G	606	CHL	C2A-C3A	-2.26	1.50	1.55
25	y	608	CHL	C4A-C3A	-2.25	1.51	1.53
25	Y	608	CHL	C4A-C3A	-2.25	1.51	1.53
25	8	305	CHL	C2A-C3A	-2.25	1.50	1.55
25	4	305	CHL	C2A-C3A	-2.25	1.50	1.55
25	1	606	CHL	C2A-C3A	-2.25	1.50	1.55
25	5	606	CHL	C2A-C3A	-2.25	1.50	1.55
25	7	309	CHL	C2A-C3A	-2.24	1.50	1.55
25	3	309	CHL	C2A-C3A	-2.24	1.50	1.55
25	4	306	CHL	C2A-C3A	-2.24	1.50	1.55
25	8	306	CHL	C2A-C3A	-2.24	1.50	1.55
25	4	307	CHL	C2A-C3A	-2.23	1.50	1.55
25	8	307	CHL	C2A-C3A	-2.23	1.50	1.55
25	n	609	CHL	C4C-C3C	-2.23	1.43	1.50
25	N	609	CHL	C4C-C3C	-2.23	1.43	1.50
25	2	607	CHL	C2A-C3A	-2.22	1.50	1.55
25	6	607	CHL	C2A-C3A	-2.22	1.50	1.55
23	A	404	PHO	CBD-CGD	-2.22	1.45	1.52
25	Y	605	CHL	C4C-C3C	-2.21	1.43	1.50
25	y	605	CHL	C4C-C3C	-2.21	1.43	1.50
25	6	601	CHL	C2A-C3A	-2.21	1.50	1.55
25	2	601	CHL	C2A-C3A	-2.21	1.50	1.55
25	Y	607	CHL	C2A-C3A	-2.20	1.50	1.55
25	y	607	CHL	C2A-C3A	-2.20	1.50	1.55
25	7	308	CHL	C2A-C3A	-2.20	1.50	1.55
25	3	308	CHL	C2A-C3A	-2.20	1.50	1.55
25	5	615	CHL	C2A-C3A	-2.20	1.50	1.55
25	1	615	CHL	C2A-C3A	-2.20	1.50	1.55
25	1	601	CHL	C2A-C3A	-2.17	1.50	1.55
25	5	601	CHL	C2A-C3A	-2.17	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	609	CHL	C4C-C3C	-2.16	1.43	1.50
25	g	609	CHL	C4C-C3C	-2.16	1.43	1.50
25	3	301	CHL	C2A-C3A	-2.14	1.50	1.55
25	7	301	CHL	C2A-C3A	-2.14	1.50	1.55
25	1	607	CHL	C2A-C3A	-2.13	1.50	1.55
25	5	607	CHL	C2A-C3A	-2.13	1.50	1.55
25	S	308	CHL	C4C-C3C	-2.13	1.43	1.50
25	s	308	CHL	C4C-C3C	-2.13	1.43	1.50
25	2	606	CHL	C2A-C3A	-2.12	1.50	1.55
25	6	606	CHL	C2A-C3A	-2.12	1.50	1.55
25	S	308	CHL	C4A-C3A	-2.10	1.51	1.53
25	s	308	CHL	C4A-C3A	-2.10	1.51	1.53
25	6	608	CHL	C2A-C3A	-2.09	1.50	1.55
25	2	608	CHL	C2A-C3A	-2.09	1.50	1.55
25	S	302	CHL	C4A-C3A	-2.09	1.51	1.53
25	s	302	CHL	C4A-C3A	-2.09	1.51	1.53
25	7	307	CHL	C2A-C3A	-2.07	1.51	1.55
25	3	307	CHL	C2A-C3A	-2.07	1.51	1.55
25	N	605	CHL	C4C-C3C	-2.07	1.44	1.50
25	n	605	CHL	C4C-C3C	-2.07	1.44	1.50
25	Y	607	CHL	C4C-C3C	-2.06	1.44	1.50
25	y	607	CHL	C4C-C3C	-2.06	1.44	1.50
25	n	607	CHL	C2A-C3A	-2.06	1.51	1.55
25	N	607	CHL	C2A-C3A	-2.06	1.51	1.55
25	n	607	CHL	C4C-C3C	-2.06	1.44	1.50
25	N	607	CHL	C4C-C3C	-2.06	1.44	1.50
23	a	404	PHO	CBD-CGD	-2.05	1.46	1.52
25	g	601	CHL	C1A-C2A	-2.03	1.51	1.53
25	G	601	CHL	C1A-C2A	-2.03	1.51	1.53
25	Y	601	CHL	C4A-C3A	-2.02	1.51	1.53
25	y	601	CHL	C4A-C3A	-2.02	1.51	1.53
23	A	404	PHO	C1D-ND	-2.02	1.34	1.38
25	r	306	CHL	C4C-C3C	-2.01	1.44	1.50
25	R	306	CHL	C4C-C3C	-2.01	1.44	1.50
25	Y	601	CHL	C4C-C3C	-2.01	1.44	1.50
25	y	601	CHL	C4C-C3C	-2.01	1.44	1.50
25	G	607	CHL	C4C-C3C	-2.01	1.44	1.50
25	g	607	CHL	C4C-C3C	-2.01	1.44	1.50
22	2	612	CLA	CMC-C2C	2.00	1.55	1.50
22	6	612	CLA	CMC-C2C	2.00	1.55	1.50
23	D	402	PHO	CHC-C4B	2.00	1.45	1.40
22	C	504	CLA	C4C-C3C	2.00	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	CAA-C2A	2.00	1.58	1.54
22	4	304	CLA	CMC-C2C	2.00	1.55	1.50
22	8	304	CLA	CMC-C2C	2.00	1.55	1.50
22	R	312	CLA	CMC-C2C	2.00	1.55	1.50
22	r	312	CLA	CMC-C2C	2.00	1.55	1.50
22	B	608	CLA	CAA-C2A	2.01	1.58	1.54
22	D	404	CLA	C4C-C3C	2.01	1.48	1.45
25	g	601	CHL	CBD-CGD	2.01	1.55	1.52
25	G	601	CHL	CBD-CGD	2.01	1.55	1.52
22	G	614	CLA	CAA-C2A	2.01	1.58	1.54
22	g	614	CLA	CAA-C2A	2.01	1.58	1.54
22	c	509	CLA	C3D-C2D	2.01	1.44	1.39
22	n	613	CLA	C4C-C3C	2.01	1.48	1.45
22	N	613	CLA	C4C-C3C	2.01	1.48	1.45
22	A	403	CLA	CAA-C2A	2.01	1.58	1.54
22	S	310	CLA	CAA-C2A	2.01	1.58	1.54
22	s	310	CLA	CAA-C2A	2.01	1.58	1.54
22	5	614	CLA	CMC-C2C	2.01	1.55	1.50
22	2	602	CLA	CMC-C2C	2.01	1.55	1.50
22	1	614	CLA	CMC-C2C	2.01	1.55	1.50
22	6	602	CLA	CMC-C2C	2.01	1.55	1.50
22	a	402	CLA	C4C-C3C	2.02	1.48	1.45
22	y	613	CLA	C3D-C2D	2.02	1.44	1.39
22	Y	613	CLA	C3D-C2D	2.02	1.44	1.39
22	7	303	CLA	CAA-C2A	2.02	1.58	1.54
22	3	303	CLA	CAA-C2A	2.02	1.58	1.54
22	S	311	CLA	O2D-CGD	2.02	1.38	1.33
22	s	311	CLA	O2D-CGD	2.02	1.38	1.33
22	B	610	CLA	O2D-CGD	2.02	1.38	1.33
22	y	613	CLA	CMC-C2C	2.02	1.55	1.50
22	Y	613	CLA	CMC-C2C	2.02	1.55	1.50
25	Y	605	CHL	CBD-CGD	2.02	1.55	1.52
25	y	605	CHL	CBD-CGD	2.02	1.55	1.52
22	B	611	CLA	O2D-CGD	2.02	1.38	1.33
22	Y	604	CLA	C3D-C2D	2.02	1.44	1.39
22	y	604	CLA	C3D-C2D	2.02	1.44	1.39
22	a	402	CLA	C3B-CAB	2.03	1.51	1.47
22	G	614	CLA	C3B-CAB	2.03	1.51	1.47
22	g	614	CLA	C3B-CAB	2.03	1.51	1.47
22	3	304	CLA	CMC-C2C	2.03	1.55	1.50
22	7	304	CLA	CMC-C2C	2.03	1.55	1.50
25	n	607	CHL	CBD-CGD	2.03	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	607	CHL	CBD-CGD	2.03	1.55	1.52
22	S	310	CLA	C3D-C2D	2.03	1.44	1.39
22	s	310	CLA	C3D-C2D	2.03	1.44	1.39
22	B	604	CLA	C4C-C3C	2.03	1.48	1.45
22	C	501	CLA	C3D-C2D	2.03	1.44	1.39
22	7	311	CLA	CMC-C2C	2.03	1.55	1.50
22	3	311	CLA	CMC-C2C	2.03	1.55	1.50
22	r	307	CLA	C4C-C3C	2.03	1.48	1.45
22	R	307	CLA	C4C-C3C	2.03	1.48	1.45
22	7	313	CLA	CMC-C2C	2.03	1.55	1.50
22	3	313	CLA	CMC-C2C	2.03	1.55	1.50
22	2	602	CLA	CAA-C2A	2.03	1.58	1.54
22	6	602	CLA	CAA-C2A	2.03	1.58	1.54
22	B	603	CLA	O2D-CGD	2.03	1.38	1.33
22	a	402	CLA	O2D-CGD	2.03	1.38	1.33
22	8	310	CLA	C3B-CAB	2.03	1.51	1.47
22	4	310	CLA	C3B-CAB	2.03	1.51	1.47
22	A	405	CLA	C4C-C3C	2.03	1.48	1.45
22	N	614	CLA	CAA-C2A	2.03	1.58	1.54
22	n	614	CLA	CAA-C2A	2.03	1.58	1.54
22	B	607	CLA	C3D-C2D	2.04	1.44	1.39
22	7	305	CLA	CMC-C2C	2.04	1.55	1.50
22	3	305	CLA	CMC-C2C	2.04	1.55	1.50
22	2	610	CLA	C4C-C3C	2.04	1.48	1.45
22	6	610	CLA	C4C-C3C	2.04	1.48	1.45
22	6	609	CLA	C3D-C2D	2.04	1.44	1.39
22	2	609	CLA	C3D-C2D	2.04	1.44	1.39
22	D	403	CLA	C3B-CAB	2.04	1.51	1.47
22	c	512	CLA	C4C-C3C	2.04	1.48	1.45
22	G	602	CLA	CAA-C2A	2.04	1.58	1.54
22	g	602	CLA	CAA-C2A	2.04	1.58	1.54
22	R	311	CLA	CMC-C2C	2.04	1.55	1.50
22	r	311	CLA	CMC-C2C	2.04	1.55	1.50
22	s	303	CLA	C3B-CAB	2.04	1.51	1.47
22	S	303	CLA	C3B-CAB	2.04	1.51	1.47
22	4	304	CLA	CAA-C2A	2.04	1.58	1.54
22	8	304	CLA	CAA-C2A	2.04	1.58	1.54
22	C	509	CLA	CMC-C2C	2.04	1.55	1.50
22	6	611	CLA	CMC-C2C	2.04	1.55	1.50
22	2	611	CLA	CMC-C2C	2.04	1.55	1.50
22	8	310	CLA	CMC-C2C	2.04	1.55	1.50
22	4	310	CLA	CMC-C2C	2.04	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	602	CLA	CAA-C2A	2.05	1.58	1.54
22	5	602	CLA	CAA-C2A	2.05	1.58	1.54
22	n	610	CLA	C3D-C2D	2.05	1.44	1.39
22	N	610	CLA	C3D-C2D	2.05	1.44	1.39
22	3	310	CLA	C3B-CAB	2.05	1.51	1.47
22	7	311	CLA	C3B-CAB	2.05	1.51	1.47
22	7	310	CLA	C3B-CAB	2.05	1.51	1.47
22	3	311	CLA	C3B-CAB	2.05	1.51	1.47
22	y	611	CLA	C3D-C2D	2.05	1.44	1.39
22	b	602	CLA	C3D-C2D	2.05	1.44	1.39
22	Y	611	CLA	C3D-C2D	2.05	1.44	1.39
22	c	511	CLA	C4C-C3C	2.05	1.48	1.45
22	R	308	CLA	C3D-C2D	2.05	1.44	1.39
22	r	308	CLA	C3D-C2D	2.05	1.44	1.39
22	B	607	CLA	C4C-C3C	2.05	1.48	1.45
22	4	303	CLA	C3B-CAB	2.05	1.52	1.47
22	8	303	CLA	C3B-CAB	2.05	1.52	1.47
22	D	403	CLA	C3D-C2D	2.05	1.44	1.39
22	b	613	CLA	C4C-C3C	2.05	1.48	1.45
22	N	602	CLA	C3D-C2D	2.06	1.44	1.39
22	n	602	CLA	C3D-C2D	2.06	1.44	1.39
22	1	603	CLA	C3B-CAB	2.06	1.52	1.47
22	5	603	CLA	C3B-CAB	2.06	1.52	1.47
22	C	512	CLA	O2D-CGD	2.06	1.38	1.33
22	N	614	CLA	C3B-CAB	2.06	1.52	1.47
22	n	614	CLA	C3B-CAB	2.06	1.52	1.47
22	d	404	CLA	C4C-C3C	2.06	1.48	1.45
22	b	611	CLA	O2D-CGD	2.06	1.38	1.33
22	Y	603	CLA	C3D-C2D	2.06	1.44	1.39
22	y	603	CLA	C3D-C2D	2.06	1.44	1.39
22	4	309	CLA	C3B-CAB	2.06	1.52	1.47
22	8	309	CLA	C3B-CAB	2.06	1.52	1.47
22	s	309	CLA	C4C-C3C	2.06	1.48	1.45
22	S	309	CLA	C4C-C3C	2.06	1.48	1.45
22	b	610	CLA	CMC-C2C	2.07	1.55	1.50
22	7	314	CLA	C3B-CAB	2.07	1.52	1.47
22	3	314	CLA	C3B-CAB	2.07	1.52	1.47
22	B	602	CLA	O2D-CGD	2.07	1.38	1.33
22	g	613	CLA	C3D-C2D	2.07	1.44	1.39
22	G	613	CLA	C3D-C2D	2.07	1.44	1.39
22	b	603	CLA	C3D-C2D	2.07	1.44	1.39
22	A	403	CLA	C3D-C2D	2.07	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	PHO	CHC-C4B	2.07	1.45	1.40
22	B	611	CLA	C3D-C2D	2.07	1.44	1.39
22	d	403	CLA	C3D-C2D	2.07	1.44	1.39
22	7	314	CLA	CAA-C2A	2.08	1.58	1.54
22	3	314	CLA	CAA-C2A	2.08	1.58	1.54
22	n	603	CLA	C3D-C2D	2.08	1.44	1.39
22	N	603	CLA	C3D-C2D	2.08	1.44	1.39
22	2	610	CLA	C3B-CAB	2.08	1.52	1.47
22	6	610	CLA	C3B-CAB	2.08	1.52	1.47
22	s	309	CLA	C3B-CAB	2.08	1.52	1.47
22	S	309	CLA	C3B-CAB	2.08	1.52	1.47
22	c	511	CLA	C3D-C2D	2.08	1.44	1.39
22	R	312	CLA	C3B-CAB	2.08	1.52	1.47
22	r	312	CLA	C3B-CAB	2.08	1.52	1.47
22	b	609	CLA	C4C-C3C	2.08	1.48	1.45
22	s	303	CLA	C3D-C2D	2.09	1.44	1.39
22	S	303	CLA	C3D-C2D	2.09	1.44	1.39
22	B	613	CLA	C4C-C3C	2.09	1.48	1.45
22	3	312	CLA	C4C-C3C	2.09	1.48	1.45
22	7	312	CLA	C4C-C3C	2.09	1.48	1.45
22	B	609	CLA	C3D-C2D	2.09	1.44	1.39
22	C	511	CLA	CAA-C2A	2.09	1.58	1.54
22	B	604	CLA	C4B-CHC	2.09	1.45	1.40
22	B	612	CLA	C3D-C2D	2.10	1.44	1.39
22	n	612	CLA	C3D-C2D	2.10	1.44	1.39
22	N	612	CLA	C3D-C2D	2.10	1.44	1.39
22	b	608	CLA	O2D-CGD	2.10	1.38	1.33
22	5	614	CLA	C3B-CAB	2.10	1.52	1.47
22	1	614	CLA	C3B-CAB	2.10	1.52	1.47
22	C	505	CLA	O2D-CGD	2.10	1.38	1.33
22	c	503	CLA	O2D-CGD	2.10	1.38	1.33
22	c	504	CLA	C4C-C3C	2.10	1.48	1.45
22	2	613	CLA	CAA-C2A	2.10	1.58	1.54
22	6	613	CLA	CAA-C2A	2.10	1.58	1.54
22	B	614	CLA	C3D-C2D	2.10	1.44	1.39
22	g	612	CLA	C3D-C2D	2.10	1.44	1.39
22	G	612	CLA	C3D-C2D	2.10	1.44	1.39
22	6	609	CLA	C1C-C2C	2.10	1.48	1.44
22	2	609	CLA	C1C-C2C	2.10	1.48	1.44
22	C	512	CLA	CMC-C2C	2.10	1.55	1.50
22	b	602	CLA	O2D-CGD	2.10	1.38	1.33
22	8	302	CLA	CAA-C2A	2.10	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4	302	CLA	CAA-C2A	2.10	1.58	1.54
22	3	304	CLA	C3B-CAB	2.11	1.52	1.47
22	7	304	CLA	C3B-CAB	2.11	1.52	1.47
22	7	303	CLA	C4C-C3C	2.11	1.48	1.45
22	3	303	CLA	C4C-C3C	2.11	1.48	1.45
22	d	401	CLA	O2D-CGD	2.11	1.38	1.33
22	3	310	CLA	C1C-C2C	2.11	1.48	1.44
22	7	310	CLA	C1C-C2C	2.11	1.48	1.44
22	D	401	CLA	C4C-C3C	2.11	1.48	1.45
22	6	603	CLA	C4C-C3C	2.11	1.48	1.45
22	2	603	CLA	C4C-C3C	2.11	1.48	1.45
22	b	611	CLA	C3B-CAB	2.11	1.52	1.47
22	b	607	CLA	C3D-C2D	2.11	1.44	1.39
22	B	609	CLA	C4C-C3C	2.12	1.48	1.45
22	B	608	CLA	C3D-C2D	2.12	1.44	1.39
22	B	605	CLA	C3D-C2D	2.12	1.44	1.39
22	b	612	CLA	C3B-CAB	2.12	1.52	1.47
22	b	612	CLA	O2D-CGD	2.12	1.38	1.33
22	S	304	CLA	C3B-CAB	2.12	1.52	1.47
22	s	304	CLA	C3B-CAB	2.12	1.52	1.47
22	B	605	CLA	CAA-C2A	2.12	1.58	1.54
23	d	402	PHO	CHC-C4B	2.12	1.45	1.40
22	2	602	CLA	C4C-C3C	2.12	1.48	1.45
22	6	602	CLA	C4C-C3C	2.12	1.48	1.45
22	Y	604	CLA	O2D-CGD	2.13	1.38	1.33
22	y	604	CLA	O2D-CGD	2.13	1.38	1.33
22	4	309	CLA	CAA-C2A	2.13	1.58	1.54
22	8	309	CLA	CAA-C2A	2.13	1.58	1.54
22	S	301	CLA	C3D-C2D	2.13	1.44	1.39
22	S	312	CLA	CMC-C2C	2.13	1.55	1.50
22	s	312	CLA	CMC-C2C	2.13	1.55	1.50
22	8	302	CLA	C4C-C3C	2.13	1.48	1.45
22	4	302	CLA	C4C-C3C	2.13	1.48	1.45
22	2	612	CLA	C4C-C3C	2.13	1.48	1.45
22	6	612	CLA	C4C-C3C	2.13	1.48	1.45
22	s	301	CLA	C4C-C3C	2.13	1.48	1.45
22	B	612	CLA	C3B-CAB	2.13	1.52	1.47
22	n	610	CLA	O2D-CGD	2.13	1.38	1.33
22	N	610	CLA	O2D-CGD	2.13	1.38	1.33
22	2	613	CLA	C3B-CAB	2.13	1.52	1.47
22	6	613	CLA	C3B-CAB	2.13	1.52	1.47
22	n	613	CLA	O2D-CGD	2.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	613	CLA	O2D-CGD	2.13	1.38	1.33
22	c	507	CLA	C3D-C2D	2.13	1.44	1.39
22	b	612	CLA	C4C-C3C	2.14	1.48	1.45
22	g	611	CLA	C3D-C2D	2.14	1.44	1.39
22	r	310	CLA	C3D-C2D	2.14	1.44	1.39
22	G	611	CLA	C3D-C2D	2.14	1.44	1.39
22	R	310	CLA	C3D-C2D	2.14	1.44	1.39
22	D	401	CLA	C3D-C2D	2.14	1.44	1.39
22	c	501	CLA	C3D-C2D	2.14	1.44	1.39
22	b	613	CLA	C3D-C2D	2.14	1.44	1.39
22	y	611	CLA	O2D-CGD	2.14	1.38	1.33
22	Y	611	CLA	O2D-CGD	2.14	1.38	1.33
25	N	608	CHL	CBD-CGD	2.14	1.55	1.52
25	n	608	CHL	CBD-CGD	2.14	1.55	1.52
22	n	604	CLA	C3D-C2D	2.14	1.44	1.39
22	N	604	CLA	C3D-C2D	2.14	1.44	1.39
22	c	512	CLA	O2D-CGD	2.15	1.38	1.33
22	S	305	CLA	O2D-CGD	2.15	1.38	1.33
22	s	305	CLA	O2D-CGD	2.15	1.38	1.33
22	N	602	CLA	CAA-C2A	2.15	1.58	1.54
22	n	602	CLA	CAA-C2A	2.15	1.58	1.54
22	c	501	CLA	O2D-CGD	2.15	1.38	1.33
22	a	403	CLA	C3D-C2D	2.15	1.44	1.39
22	N	614	CLA	C4C-C3C	2.16	1.48	1.45
22	n	614	CLA	C4C-C3C	2.16	1.48	1.45
22	G	604	CLA	C4C-C3C	2.16	1.48	1.45
22	g	604	CLA	C4C-C3C	2.16	1.48	1.45
22	a	402	CLA	C3D-C2D	2.16	1.44	1.39
22	B	607	CLA	O2D-CGD	2.16	1.38	1.33
22	C	502	CLA	C3D-C2D	2.16	1.44	1.39
22	D	404	CLA	O2D-CGD	2.16	1.38	1.33
22	r	307	CLA	C3D-C2D	2.17	1.44	1.39
22	R	307	CLA	C3D-C2D	2.17	1.44	1.39
22	Y	602	CLA	CAA-C2A	2.17	1.58	1.54
22	y	602	CLA	CAA-C2A	2.17	1.58	1.54
22	b	607	CLA	C4C-C3C	2.17	1.48	1.45
22	5	604	CLA	C4C-C3C	2.17	1.48	1.45
22	1	604	CLA	C4C-C3C	2.17	1.48	1.45
22	2	604	CLA	CAA-C2A	2.17	1.58	1.54
22	6	604	CLA	CAA-C2A	2.17	1.58	1.54
22	1	602	CLA	C4C-C3C	2.17	1.48	1.45
22	5	602	CLA	C4C-C3C	2.17	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	314	CLA	C3D-C2D	2.17	1.44	1.39
22	s	314	CLA	C3D-C2D	2.17	1.44	1.39
22	b	610	CLA	O2D-CGD	2.17	1.38	1.33
22	y	610	CLA	C3D-C2D	2.18	1.44	1.39
22	Y	610	CLA	C3D-C2D	2.18	1.44	1.39
22	R	308	CLA	CAA-C2A	2.18	1.58	1.54
22	r	308	CLA	CAA-C2A	2.18	1.58	1.54
22	A	402	CLA	O2D-CGD	2.18	1.38	1.33
22	R	303	CLA	C3D-C2D	2.18	1.44	1.39
22	r	303	CLA	C3D-C2D	2.18	1.44	1.39
22	B	601	CLA	C3D-C2D	2.18	1.44	1.39
22	b	606	CLA	O2D-CGD	2.18	1.38	1.33
22	c	506	CLA	C4C-C3C	2.18	1.48	1.45
22	C	507	CLA	C3D-C2D	2.19	1.44	1.39
22	n	613	CLA	C3D-C2D	2.19	1.44	1.39
22	N	613	CLA	C3D-C2D	2.19	1.44	1.39
22	G	602	CLA	O2D-CGD	2.19	1.38	1.33
22	g	602	CLA	O2D-CGD	2.19	1.38	1.33
22	B	611	CLA	C3B-CAB	2.19	1.52	1.47
22	8	310	CLA	C4C-C3C	2.19	1.48	1.45
22	4	310	CLA	C4C-C3C	2.19	1.48	1.45
22	c	510	CLA	C3D-C2D	2.19	1.44	1.39
25	1	607	CHL	CBD-CGD	2.19	1.55	1.52
25	5	607	CHL	CBD-CGD	2.19	1.55	1.52
23	A	404	PHO	CHC-C4B	2.19	1.45	1.40
25	Y	607	CHL	CBD-CGD	2.19	1.55	1.52
25	y	607	CHL	CBD-CGD	2.19	1.55	1.52
22	d	403	CLA	C4C-C3C	2.19	1.48	1.45
22	y	610	CLA	O2D-CGD	2.19	1.38	1.33
22	Y	610	CLA	O2D-CGD	2.19	1.38	1.33
22	7	305	CLA	CAA-C2A	2.20	1.58	1.54
22	3	305	CLA	CAA-C2A	2.20	1.58	1.54
22	b	604	CLA	C3D-C2D	2.20	1.44	1.39
25	N	605	CHL	CBD-CGD	2.20	1.55	1.52
25	n	605	CHL	CBD-CGD	2.20	1.55	1.52
22	n	611	CLA	O2D-CGD	2.20	1.38	1.33
22	N	611	CLA	O2D-CGD	2.20	1.38	1.33
22	R	303	CLA	O2D-CGD	2.20	1.38	1.33
22	r	303	CLA	O2D-CGD	2.20	1.38	1.33
22	G	610	CLA	O2D-CGD	2.20	1.38	1.33
22	g	610	CLA	O2D-CGD	2.20	1.38	1.33
22	R	311	CLA	C3D-C2D	2.20	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	311	CLA	C3D-C2D	2.20	1.44	1.39
22	c	505	CLA	C3D-C2D	2.20	1.44	1.39
22	5	611	CLA	C4C-C3C	2.20	1.48	1.45
22	1	611	CLA	C4C-C3C	2.20	1.48	1.45
22	R	309	CLA	C3D-C2D	2.20	1.44	1.39
22	r	309	CLA	C3D-C2D	2.20	1.44	1.39
22	C	510	CLA	C3D-C2D	2.21	1.44	1.39
22	C	506	CLA	C4C-C3C	2.21	1.48	1.45
22	y	613	CLA	O2D-CGD	2.21	1.38	1.33
22	Y	613	CLA	O2D-CGD	2.21	1.38	1.33
22	C	507	CLA	O2D-CGD	2.21	1.38	1.33
22	c	512	CLA	C3D-C2D	2.21	1.44	1.39
22	D	404	CLA	C3D-C2D	2.21	1.44	1.39
22	C	508	CLA	C3D-C2D	2.21	1.44	1.39
22	b	601	CLA	C3D-C2D	2.21	1.44	1.39
22	b	604	CLA	O2D-CGD	2.21	1.38	1.33
22	N	602	CLA	O2D-CGD	2.21	1.38	1.33
22	n	602	CLA	O2D-CGD	2.21	1.38	1.33
22	B	610	CLA	C4C-C3C	2.21	1.48	1.45
22	2	602	CLA	C3D-C2D	2.21	1.44	1.39
22	6	602	CLA	C3D-C2D	2.21	1.44	1.39
22	S	305	CLA	C3D-C2D	2.21	1.44	1.39
22	s	305	CLA	C3D-C2D	2.21	1.44	1.39
22	B	616	CLA	C4C-C3C	2.22	1.48	1.45
22	2	613	CLA	C4C-C3C	2.22	1.49	1.45
22	6	613	CLA	C4C-C3C	2.22	1.49	1.45
25	N	601	CHL	CBD-CGD	2.22	1.55	1.52
25	n	601	CHL	CBD-CGD	2.22	1.55	1.52
22	G	603	CLA	C4C-C3C	2.22	1.49	1.45
22	g	603	CLA	C4C-C3C	2.22	1.49	1.45
22	g	613	CLA	O2D-CGD	2.23	1.38	1.33
22	G	613	CLA	O2D-CGD	2.23	1.38	1.33
22	b	615	CLA	O2D-CGD	2.23	1.38	1.33
22	C	509	CLA	C3D-C2D	2.23	1.44	1.39
22	b	614	CLA	O2D-CGD	2.23	1.38	1.33
22	8	302	CLA	O2D-CGD	2.23	1.38	1.33
22	4	302	CLA	O2D-CGD	2.23	1.38	1.33
22	B	615	CLA	C3D-C2D	2.23	1.44	1.39
22	7	314	CLA	C4C-C3C	2.23	1.49	1.45
22	4	304	CLA	C4C-C3C	2.23	1.49	1.45
22	4	303	CLA	C4C-C3C	2.23	1.49	1.45
22	3	314	CLA	C4C-C3C	2.23	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	8	304	CLA	C4C-C3C	2.23	1.49	1.45
22	8	303	CLA	C4C-C3C	2.23	1.49	1.45
22	1	612	CLA	C4C-C3C	2.23	1.49	1.45
22	5	612	CLA	C4C-C3C	2.23	1.49	1.45
22	1	603	CLA	C4C-C3C	2.23	1.49	1.45
22	R	312	CLA	C4C-C3C	2.23	1.49	1.45
22	5	603	CLA	C4C-C3C	2.23	1.49	1.45
22	r	312	CLA	C4C-C3C	2.23	1.49	1.45
22	s	309	CLA	O2D-CGD	2.23	1.38	1.33
22	S	309	CLA	O2D-CGD	2.23	1.38	1.33
25	3	301	CHL	CBD-CGD	2.24	1.55	1.52
25	7	301	CHL	CBD-CGD	2.24	1.55	1.52
22	C	512	CLA	C3D-C2D	2.24	1.44	1.39
22	7	311	CLA	C4C-C3C	2.24	1.49	1.45
22	3	311	CLA	C4C-C3C	2.24	1.49	1.45
22	r	307	CLA	O2D-CGD	2.24	1.38	1.33
22	R	307	CLA	O2D-CGD	2.24	1.38	1.33
22	G	614	CLA	C3D-C2D	2.24	1.44	1.39
22	g	614	CLA	C3D-C2D	2.24	1.44	1.39
22	C	506	CLA	O2D-CGD	2.24	1.38	1.33
22	C	504	CLA	C3D-C2D	2.24	1.44	1.39
22	A	405	CLA	O2D-CGD	2.24	1.38	1.33
22	G	602	CLA	C3D-C2D	2.24	1.44	1.39
22	g	602	CLA	C3D-C2D	2.24	1.44	1.39
22	B	605	CLA	O2D-CGD	2.24	1.38	1.33
22	C	503	CLA	O2D-CGD	2.24	1.38	1.33
22	S	304	CLA	C3D-C2D	2.24	1.44	1.39
22	s	304	CLA	C3D-C2D	2.24	1.44	1.39
22	B	609	CLA	O2D-CGD	2.24	1.38	1.33
22	b	614	CLA	C3D-C2D	2.24	1.44	1.39
25	y	608	CHL	CBD-CGD	2.24	1.55	1.52
25	Y	608	CHL	CBD-CGD	2.24	1.55	1.52
22	2	613	CLA	C3D-C2D	2.24	1.44	1.39
22	6	613	CLA	C3D-C2D	2.24	1.44	1.39
22	C	511	CLA	C4C-C3C	2.25	1.49	1.45
22	B	604	CLA	C3D-C2D	2.25	1.44	1.39
22	d	404	CLA	O2D-CGD	2.25	1.38	1.33
25	Y	601	CHL	CBD-CAD	2.25	1.56	1.53
25	y	601	CHL	CBD-CAD	2.25	1.56	1.53
22	b	606	CLA	C3B-CAB	2.25	1.52	1.47
22	Y	614	CLA	O2D-CGD	2.25	1.38	1.33
22	y	614	CLA	O2D-CGD	2.25	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	O2D-CGD	2.25	1.38	1.33
22	b	614	CLA	CAA-C2A	2.25	1.58	1.54
22	C	504	CLA	O2D-CGD	2.25	1.38	1.33
22	c	504	CLA	C3D-C2D	2.25	1.44	1.39
22	b	612	CLA	C3D-C2D	2.25	1.44	1.39
22	R	301	CLA	O2D-CGD	2.25	1.38	1.33
22	r	301	CLA	O2D-CGD	2.25	1.38	1.33
22	b	605	CLA	C3D-C2D	2.25	1.44	1.39
22	G	603	CLA	O2D-CGD	2.25	1.38	1.33
22	g	603	CLA	O2D-CGD	2.25	1.38	1.33
22	c	511	CLA	O2D-CGD	2.26	1.38	1.33
22	C	502	CLA	O2D-CGD	2.26	1.38	1.33
25	S	302	CHL	CBD-CGD	2.26	1.55	1.52
25	s	302	CHL	CBD-CGD	2.26	1.55	1.52
22	R	301	CLA	C3D-C2D	2.26	1.44	1.39
22	r	301	CLA	C3D-C2D	2.26	1.44	1.39
22	B	604	CLA	O2D-CGD	2.26	1.38	1.33
22	7	313	CLA	C4C-C3C	2.26	1.49	1.45
22	3	313	CLA	C4C-C3C	2.26	1.49	1.45
22	B	613	CLA	C3D-C2D	2.26	1.44	1.39
22	R	309	CLA	O2D-CGD	2.27	1.38	1.33
22	r	309	CLA	O2D-CGD	2.27	1.38	1.33
25	G	607	CHL	CBD-CGD	2.27	1.55	1.52
25	g	607	CHL	CBD-CGD	2.27	1.55	1.52
22	c	509	CLA	C3B-CAB	2.27	1.52	1.47
22	B	615	CLA	O2D-CGD	2.27	1.38	1.33
25	n	607	CHL	CBD-CAD	2.27	1.56	1.53
25	N	607	CHL	CBD-CAD	2.27	1.56	1.53
22	b	601	CLA	O2D-CGD	2.27	1.38	1.33
22	a	405	CLA	O2D-CGD	2.27	1.38	1.33
22	b	606	CLA	C4C-C3C	2.27	1.49	1.45
22	3	310	CLA	C3D-C2D	2.27	1.44	1.39
22	7	310	CLA	C3D-C2D	2.27	1.44	1.39
22	c	502	CLA	O2D-CGD	2.27	1.39	1.33
22	1	610	CLA	C3D-C2D	2.27	1.44	1.39
22	5	610	CLA	C3D-C2D	2.27	1.44	1.39
22	7	305	CLA	O2D-CGD	2.27	1.39	1.33
22	3	305	CLA	O2D-CGD	2.27	1.39	1.33
22	B	606	CLA	O2D-CGD	2.28	1.39	1.33
22	n	611	CLA	C3D-C2D	2.28	1.44	1.39
22	N	611	CLA	C3D-C2D	2.28	1.44	1.39
22	n	604	CLA	O2D-CGD	2.28	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	604	CLA	O2D-CGD	2.28	1.39	1.33
22	B	614	CLA	CAA-C2A	2.28	1.58	1.54
22	2	612	CLA	O2D-CGD	2.28	1.39	1.33
22	6	612	CLA	O2D-CGD	2.28	1.39	1.33
22	c	502	CLA	C3D-C2D	2.28	1.44	1.39
22	C	501	CLA	O2D-CGD	2.28	1.39	1.33
22	c	508	CLA	C3D-C2D	2.28	1.44	1.39
22	g	611	CLA	O2D-CGD	2.29	1.39	1.33
22	G	611	CLA	O2D-CGD	2.29	1.39	1.33
22	G	604	CLA	O2D-CGD	2.29	1.39	1.33
22	g	604	CLA	O2D-CGD	2.29	1.39	1.33
22	R	312	CLA	C3D-C2D	2.29	1.44	1.39
22	r	312	CLA	C3D-C2D	2.29	1.44	1.39
22	s	301	CLA	O2D-CGD	2.29	1.39	1.33
22	G	614	CLA	O2D-CGD	2.29	1.39	1.33
22	g	614	CLA	O2D-CGD	2.29	1.39	1.33
22	1	613	CLA	C4C-C3C	2.29	1.49	1.45
22	5	613	CLA	C4C-C3C	2.29	1.49	1.45
22	s	301	CLA	C3D-C2D	2.29	1.44	1.39
22	s	313	CLA	O2D-CGD	2.29	1.39	1.33
22	S	314	CLA	O2D-CGD	2.29	1.39	1.33
22	s	314	CLA	O2D-CGD	2.29	1.39	1.33
22	S	313	CLA	O2D-CGD	2.29	1.39	1.33
22	s	313	CLA	C3D-C2D	2.29	1.44	1.39
22	S	313	CLA	C3D-C2D	2.29	1.44	1.39
22	C	512	CLA	C4C-C3C	2.29	1.49	1.45
22	C	509	CLA	C3B-CAB	2.29	1.52	1.47
22	4	309	CLA	C3D-C2D	2.30	1.44	1.39
22	8	309	CLA	C3D-C2D	2.30	1.44	1.39
22	B	601	CLA	O2D-CGD	2.30	1.39	1.33
22	3	304	CLA	C4C-C3C	2.30	1.49	1.45
22	7	304	CLA	C4C-C3C	2.30	1.49	1.45
25	S	308	CHL	CBD-CGD	2.30	1.56	1.52
25	s	308	CHL	CBD-CGD	2.30	1.56	1.52
22	n	603	CLA	O2D-CGD	2.30	1.39	1.33
22	N	603	CLA	O2D-CGD	2.30	1.39	1.33
22	7	313	CLA	O2D-CGD	2.30	1.39	1.33
22	3	313	CLA	O2D-CGD	2.30	1.39	1.33
22	5	604	CLA	O2D-CGD	2.30	1.39	1.33
22	1	604	CLA	O2D-CGD	2.30	1.39	1.33
22	r	310	CLA	O2D-CGD	2.30	1.39	1.33
22	R	310	CLA	O2D-CGD	2.30	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	C3D-C2D	2.30	1.44	1.39
22	S	312	CLA	C3D-C2D	2.30	1.44	1.39
22	s	312	CLA	C3D-C2D	2.30	1.44	1.39
22	c	510	CLA	O2D-CGD	2.30	1.39	1.33
22	y	612	CLA	O2D-CGD	2.31	1.39	1.33
22	Y	612	CLA	O2D-CGD	2.31	1.39	1.33
22	R	312	CLA	O2D-CGD	2.31	1.39	1.33
22	r	312	CLA	O2D-CGD	2.31	1.39	1.33
22	d	401	CLA	C3D-C2D	2.31	1.44	1.39
22	b	603	CLA	C4C-C3C	2.31	1.49	1.45
22	S	312	CLA	O2D-CGD	2.31	1.39	1.33
22	s	312	CLA	O2D-CGD	2.31	1.39	1.33
22	c	504	CLA	O2D-CGD	2.31	1.39	1.33
22	S	310	CLA	O2D-CGD	2.32	1.39	1.33
22	s	310	CLA	O2D-CGD	2.32	1.39	1.33
22	c	506	CLA	O2D-CGD	2.32	1.39	1.33
22	R	308	CLA	O2D-CGD	2.32	1.39	1.33
22	r	308	CLA	O2D-CGD	2.32	1.39	1.33
22	4	303	CLA	O2D-CGD	2.32	1.39	1.33
22	8	303	CLA	O2D-CGD	2.32	1.39	1.33
23	A	404	PHO	CHD-C1D	2.32	1.43	1.38
22	3	304	CLA	O2D-CGD	2.32	1.39	1.33
22	7	304	CLA	O2D-CGD	2.32	1.39	1.33
22	1	603	CLA	C3D-C2D	2.32	1.44	1.39
22	5	603	CLA	C3D-C2D	2.32	1.44	1.39
22	B	616	CLA	O2D-CGD	2.32	1.39	1.33
22	6	603	CLA	C3D-C2D	2.33	1.44	1.39
22	2	603	CLA	C3D-C2D	2.33	1.44	1.39
22	G	603	CLA	C3D-C2D	2.33	1.44	1.39
22	g	603	CLA	C3D-C2D	2.33	1.44	1.39
22	Y	603	CLA	O2D-CGD	2.33	1.39	1.33
22	y	603	CLA	O2D-CGD	2.33	1.39	1.33
22	7	311	CLA	O2D-CGD	2.33	1.39	1.33
22	3	311	CLA	O2D-CGD	2.33	1.39	1.33
22	1	603	CLA	O2D-CGD	2.33	1.39	1.33
22	5	603	CLA	O2D-CGD	2.33	1.39	1.33
22	5	611	CLA	O2D-CGD	2.33	1.39	1.33
22	1	611	CLA	O2D-CGD	2.33	1.39	1.33
22	b	606	CLA	C3D-C2D	2.33	1.44	1.39
25	3	301	CHL	CBD-CAD	2.33	1.56	1.53
25	7	301	CHL	CBD-CAD	2.33	1.56	1.53
22	b	609	CLA	O2D-CGD	2.33	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	301	CLA	O2D-CGD	2.34	1.39	1.33
22	8	310	CLA	O2D-CGD	2.34	1.39	1.33
22	4	310	CLA	O2D-CGD	2.34	1.39	1.33
22	c	508	CLA	C4C-C3C	2.34	1.49	1.45
22	S	304	CLA	O2D-CGD	2.34	1.39	1.33
22	s	304	CLA	O2D-CGD	2.34	1.39	1.33
22	7	303	CLA	C3D-C2D	2.34	1.44	1.39
22	3	303	CLA	C3D-C2D	2.34	1.44	1.39
22	6	611	CLA	O2D-CGD	2.34	1.39	1.33
22	2	611	CLA	O2D-CGD	2.34	1.39	1.33
22	b	607	CLA	C3B-C2B	2.34	1.43	1.40
22	C	511	CLA	O2D-CGD	2.34	1.39	1.33
22	2	610	CLA	O2D-CGD	2.34	1.39	1.33
22	6	610	CLA	O2D-CGD	2.34	1.39	1.33
22	2	604	CLA	O2D-CGD	2.35	1.39	1.33
22	6	604	CLA	O2D-CGD	2.35	1.39	1.33
22	C	506	CLA	C3D-C2D	2.35	1.44	1.39
22	d	404	CLA	C3D-C2D	2.35	1.44	1.39
25	N	608	CHL	CBD-CAD	2.35	1.56	1.53
25	n	608	CHL	CBD-CAD	2.35	1.56	1.53
22	4	304	CLA	O2D-CGD	2.35	1.39	1.33
22	8	304	CLA	O2D-CGD	2.35	1.39	1.33
22	N	614	CLA	O2D-CGD	2.35	1.39	1.33
22	n	614	CLA	O2D-CGD	2.35	1.39	1.33
22	1	602	CLA	O2D-CGD	2.36	1.39	1.33
22	5	602	CLA	O2D-CGD	2.36	1.39	1.33
22	b	607	CLA	O2D-CGD	2.36	1.39	1.33
22	n	612	CLA	O2D-CGD	2.36	1.39	1.33
22	N	612	CLA	O2D-CGD	2.36	1.39	1.33
22	6	603	CLA	O2D-CGD	2.36	1.39	1.33
22	2	603	CLA	O2D-CGD	2.36	1.39	1.33
22	1	610	CLA	O2D-CGD	2.36	1.39	1.33
22	5	610	CLA	O2D-CGD	2.36	1.39	1.33
22	1	613	CLA	O2D-CGD	2.36	1.39	1.33
22	c	508	CLA	O2D-CGD	2.36	1.39	1.33
22	5	613	CLA	O2D-CGD	2.36	1.39	1.33
22	C	508	CLA	O2D-CGD	2.36	1.39	1.33
22	C	505	CLA	C3D-C2D	2.37	1.45	1.39
22	y	612	CLA	C3D-C2D	2.37	1.45	1.39
22	Y	612	CLA	C3D-C2D	2.37	1.45	1.39
25	g	606	CHL	CBD-CGD	2.37	1.56	1.52
25	G	606	CHL	CBD-CGD	2.37	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	303	CLA	O2D-CGD	2.37	1.39	1.33
22	3	303	CLA	O2D-CGD	2.37	1.39	1.33
22	2	602	CLA	O2D-CGD	2.37	1.39	1.33
22	1	612	CLA	O2D-CGD	2.37	1.39	1.33
22	5	612	CLA	O2D-CGD	2.37	1.39	1.33
22	6	602	CLA	O2D-CGD	2.37	1.39	1.33
22	3	310	CLA	O2D-CGD	2.37	1.39	1.33
22	7	310	CLA	O2D-CGD	2.37	1.39	1.33
22	r	302	CLA	O2D-CGD	2.37	1.39	1.33
22	R	302	CLA	O2D-CGD	2.37	1.39	1.33
22	7	314	CLA	O2D-CGD	2.38	1.39	1.33
22	3	314	CLA	O2D-CGD	2.38	1.39	1.33
22	5	614	CLA	C3D-C2D	2.38	1.45	1.39
22	1	614	CLA	C3D-C2D	2.38	1.45	1.39
22	C	510	CLA	O2D-CGD	2.38	1.39	1.33
22	3	312	CLA	O2D-CGD	2.38	1.39	1.33
22	7	312	CLA	O2D-CGD	2.38	1.39	1.33
22	2	613	CLA	O2D-CGD	2.38	1.39	1.33
22	6	613	CLA	O2D-CGD	2.38	1.39	1.33
22	7	305	CLA	C4C-C3C	2.39	1.49	1.45
22	3	305	CLA	C4C-C3C	2.39	1.49	1.45
22	2	604	CLA	C4C-C3C	2.39	1.49	1.45
22	6	604	CLA	C4C-C3C	2.39	1.49	1.45
25	g	608	CHL	CBD-CGD	2.40	1.56	1.52
25	G	608	CHL	CBD-CGD	2.40	1.56	1.52
22	b	615	CLA	C3D-C2D	2.40	1.45	1.39
22	g	612	CLA	O2D-CGD	2.40	1.39	1.33
22	G	612	CLA	O2D-CGD	2.40	1.39	1.33
22	b	616	CLA	C3D-C2D	2.40	1.45	1.39
22	c	506	CLA	C3D-C2D	2.40	1.45	1.39
22	6	611	CLA	C3D-C2D	2.40	1.45	1.39
22	2	611	CLA	C3D-C2D	2.40	1.45	1.39
22	b	616	CLA	O2D-CGD	2.41	1.39	1.33
22	b	613	CLA	O2D-CGD	2.41	1.39	1.33
22	1	602	CLA	C3D-C2D	2.41	1.45	1.39
22	5	602	CLA	C3D-C2D	2.41	1.45	1.39
22	2	612	CLA	C3D-C2D	2.41	1.45	1.39
22	6	612	CLA	C3D-C2D	2.41	1.45	1.39
22	G	604	CLA	C3D-C2D	2.41	1.45	1.39
22	g	604	CLA	C3D-C2D	2.41	1.45	1.39
22	2	610	CLA	C3D-C2D	2.41	1.45	1.39
22	6	610	CLA	C3D-C2D	2.41	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	301	CHL	CBD-CGD	2.41	1.56	1.52
25	8	301	CHL	CBD-CGD	2.41	1.56	1.52
22	r	302	CLA	C3D-C2D	2.42	1.45	1.39
22	R	302	CLA	C3D-C2D	2.42	1.45	1.39
25	G	607	CHL	CBD-CAD	2.42	1.56	1.53
25	g	607	CHL	CBD-CAD	2.42	1.56	1.53
22	4	309	CLA	O2D-CGD	2.42	1.39	1.33
22	8	309	CLA	O2D-CGD	2.42	1.39	1.33
22	b	608	CLA	C3D-C2D	2.42	1.45	1.39
22	b	610	CLA	C3D-C2D	2.43	1.45	1.39
22	6	609	CLA	O2D-CGD	2.43	1.39	1.33
22	2	609	CLA	O2D-CGD	2.43	1.39	1.33
22	4	304	CLA	C3D-C2D	2.43	1.45	1.39
22	8	304	CLA	C3D-C2D	2.43	1.45	1.39
22	b	616	CLA	C4C-C3C	2.44	1.49	1.45
22	5	611	CLA	C3D-C2D	2.44	1.45	1.39
22	1	611	CLA	C3D-C2D	2.44	1.45	1.39
22	8	310	CLA	C3D-C2D	2.44	1.45	1.39
22	4	310	CLA	C3D-C2D	2.44	1.45	1.39
22	B	613	CLA	O2D-CGD	2.44	1.39	1.33
22	8	302	CLA	C3D-C2D	2.45	1.45	1.39
22	4	302	CLA	C3D-C2D	2.45	1.45	1.39
22	3	312	CLA	C3D-C2D	2.46	1.45	1.39
22	7	312	CLA	C3D-C2D	2.46	1.45	1.39
22	N	614	CLA	C3D-C2D	2.46	1.45	1.39
22	n	614	CLA	C3D-C2D	2.46	1.45	1.39
22	5	614	CLA	O2D-CGD	2.46	1.39	1.33
22	1	614	CLA	O2D-CGD	2.46	1.39	1.33
23	A	404	PHO	O2D-CGD	2.47	1.39	1.33
22	C	508	CLA	C4C-C3C	2.48	1.49	1.45
22	b	610	CLA	C4C-C3C	2.48	1.49	1.45
22	7	311	CLA	C3D-C2D	2.48	1.45	1.39
22	3	311	CLA	C3D-C2D	2.48	1.45	1.39
22	B	616	CLA	C3B-CAB	2.48	1.52	1.47
22	3	304	CLA	C3D-C2D	2.49	1.45	1.39
22	7	304	CLA	C3D-C2D	2.49	1.45	1.39
22	A	403	CLA	O2D-CGD	2.49	1.39	1.33
22	R	311	CLA	O2D-CGD	2.49	1.39	1.33
22	r	311	CLA	O2D-CGD	2.49	1.39	1.33
22	C	506	CLA	C3B-C2B	2.49	1.43	1.40
22	B	602	CLA	C3D-C2D	2.49	1.45	1.39
22	b	603	CLA	O2D-CGD	2.49	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	PHO	O2D-CGD	2.50	1.39	1.33
22	5	614	CLA	C4C-C3C	2.51	1.49	1.45
22	1	614	CLA	C4C-C3C	2.51	1.49	1.45
22	Y	602	CLA	O2D-CGD	2.51	1.39	1.33
22	y	602	CLA	O2D-CGD	2.51	1.39	1.33
22	7	314	CLA	C3D-C2D	2.52	1.45	1.39
22	3	314	CLA	C3D-C2D	2.52	1.45	1.39
22	1	613	CLA	C3D-C2D	2.52	1.45	1.39
22	5	613	CLA	C3D-C2D	2.52	1.45	1.39
22	7	305	CLA	C3D-C2D	2.52	1.45	1.39
22	3	305	CLA	C3D-C2D	2.52	1.45	1.39
22	a	403	CLA	O2D-CGD	2.53	1.39	1.33
25	n	606	CHL	CBD-CAD	2.54	1.56	1.53
25	N	606	CHL	CBD-CAD	2.54	1.56	1.53
22	2	604	CLA	C3D-C2D	2.54	1.45	1.39
22	6	604	CLA	C3D-C2D	2.54	1.45	1.39
22	B	609	CLA	C3B-C2B	2.54	1.43	1.40
22	7	313	CLA	C3D-C2D	2.55	1.45	1.39
22	3	313	CLA	C3D-C2D	2.55	1.45	1.39
25	r	305	CHL	CBD-CGD	2.55	1.56	1.52
25	R	305	CHL	CBD-CGD	2.55	1.56	1.52
22	C	508	CLA	C4B-CHC	2.56	1.47	1.40
22	4	303	CLA	C3D-C2D	2.57	1.45	1.39
22	8	303	CLA	C3D-C2D	2.57	1.45	1.39
22	5	604	CLA	C3D-C2D	2.58	1.45	1.39
22	1	604	CLA	C3D-C2D	2.58	1.45	1.39
22	b	605	CLA	O2D-CGD	2.58	1.39	1.33
25	y	606	CHL	CBD-CAD	2.58	1.56	1.53
25	Y	606	CHL	CBD-CAD	2.58	1.56	1.53
25	g	601	CHL	CBD-CAD	2.58	1.56	1.53
25	G	601	CHL	CBD-CAD	2.58	1.56	1.53
25	g	608	CHL	CBD-CAD	2.59	1.56	1.53
25	G	608	CHL	CBD-CAD	2.59	1.56	1.53
22	1	612	CLA	C3D-C2D	2.59	1.45	1.39
22	5	612	CLA	C3D-C2D	2.59	1.45	1.39
25	Y	607	CHL	CBD-CAD	2.60	1.56	1.53
25	y	607	CHL	CBD-CAD	2.60	1.56	1.53
22	Y	602	CLA	C3D-C2D	2.60	1.45	1.39
22	y	602	CLA	C3D-C2D	2.60	1.45	1.39
25	s	306	CHL	CBD-CGD	2.61	1.56	1.52
25	S	306	CHL	CBD-CGD	2.61	1.56	1.52
25	N	605	CHL	CBD-CAD	2.61	1.56	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	605	CHL	CBD-CAD	2.61	1.56	1.53
25	5	615	CHL	CBD-CGD	2.62	1.56	1.52
25	1	615	CHL	CBD-CGD	2.62	1.56	1.52
22	c	506	CLA	C3B-C2B	2.62	1.43	1.40
22	c	507	CLA	C4B-CHC	2.62	1.47	1.40
25	y	608	CHL	CBD-CAD	2.62	1.57	1.53
25	Y	608	CHL	CBD-CAD	2.62	1.57	1.53
25	1	605	CHL	CBD-CGD	2.62	1.56	1.52
25	5	605	CHL	CBD-CGD	2.62	1.56	1.52
22	b	609	CLA	C3B-C2B	2.63	1.43	1.40
25	1	606	CHL	CBD-CGD	2.63	1.56	1.52
25	5	606	CHL	CBD-CGD	2.63	1.56	1.52
25	S	302	CHL	CBD-CAD	2.63	1.57	1.53
25	s	302	CHL	CBD-CAD	2.63	1.57	1.53
25	Y	601	CHL	O2D-CGD	2.64	1.39	1.33
25	y	601	CHL	O2D-CGD	2.64	1.39	1.33
22	C	506	CLA	C4B-CHC	2.65	1.47	1.40
25	g	606	CHL	CBD-CAD	2.65	1.57	1.53
25	G	606	CHL	CBD-CAD	2.65	1.57	1.53
25	8	305	CHL	CBD-CGD	2.66	1.56	1.52
25	4	305	CHL	CBD-CGD	2.66	1.56	1.52
25	4	301	CHL	CBD-CAD	2.66	1.57	1.53
25	8	301	CHL	CBD-CAD	2.66	1.57	1.53
25	r	306	CHL	CBD-CGD	2.66	1.56	1.52
25	R	306	CHL	CBD-CGD	2.66	1.56	1.52
25	2	606	CHL	CBD-CGD	2.66	1.56	1.52
25	6	606	CHL	CBD-CGD	2.66	1.56	1.52
22	c	501	CLA	C4B-CHC	2.66	1.47	1.40
25	1	607	CHL	CBD-CAD	2.67	1.57	1.53
25	5	607	CHL	CBD-CAD	2.67	1.57	1.53
25	7	307	CHL	CBD-CGD	2.67	1.56	1.52
25	3	307	CHL	CBD-CGD	2.67	1.56	1.52
22	C	501	CLA	C4B-CHC	2.67	1.47	1.40
22	b	616	CLA	C4B-CHC	2.67	1.47	1.40
25	N	605	CHL	O2D-CGD	2.67	1.40	1.33
25	n	605	CHL	O2D-CGD	2.67	1.40	1.33
22	Y	604	CLA	C4B-CHC	2.68	1.47	1.40
22	y	604	CLA	C4B-CHC	2.68	1.47	1.40
25	S	308	CHL	CBD-CAD	2.69	1.57	1.53
25	s	308	CHL	CBD-CAD	2.69	1.57	1.53
25	Y	605	CHL	CBD-CAD	2.69	1.57	1.53
25	y	605	CHL	CBD-CAD	2.69	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	601	CHL	O2D-CGD	2.69	1.40	1.33
25	G	601	CHL	O2D-CGD	2.69	1.40	1.33
23	d	402	PHO	O2D-CGD	2.70	1.40	1.33
25	N	601	CHL	CBD-CAD	2.70	1.57	1.53
25	n	601	CHL	CBD-CAD	2.70	1.57	1.53
25	R	304	CHL	CBD-CGD	2.71	1.56	1.52
25	r	304	CHL	CBD-CGD	2.71	1.56	1.52
25	N	608	CHL	O2D-CGD	2.71	1.40	1.33
25	n	608	CHL	O2D-CGD	2.71	1.40	1.33
22	B	608	CLA	C4B-CHC	2.71	1.47	1.40
22	C	504	CLA	C4B-CHC	2.71	1.47	1.40
25	Y	605	CHL	O2D-CGD	2.72	1.40	1.33
25	y	605	CHL	O2D-CGD	2.72	1.40	1.33
25	6	601	CHL	CBD-CGD	2.72	1.56	1.52
25	2	601	CHL	CBD-CGD	2.72	1.56	1.52
23	D	402	PHO	O2D-CGD	2.73	1.40	1.33
22	y	612	CLA	C4B-CHC	2.73	1.47	1.40
22	Y	612	CLA	C4B-CHC	2.73	1.47	1.40
22	s	303	CLA	O2D-CGD	2.74	1.40	1.33
22	S	303	CLA	O2D-CGD	2.74	1.40	1.33
22	B	607	CLA	C4B-CHC	2.74	1.47	1.40
22	n	604	CLA	C4B-CHC	2.74	1.47	1.40
22	N	604	CLA	C4B-CHC	2.74	1.47	1.40
22	y	612	CLA	C3B-C2B	2.74	1.44	1.40
22	Y	612	CLA	C3B-C2B	2.74	1.44	1.40
22	G	604	CLA	C4B-CHC	2.74	1.47	1.40
22	g	604	CLA	C4B-CHC	2.74	1.47	1.40
25	g	608	CHL	O2D-CGD	2.75	1.40	1.33
25	G	608	CHL	O2D-CGD	2.75	1.40	1.33
25	4	306	CHL	CBD-CGD	2.75	1.56	1.52
25	8	306	CHL	CBD-CGD	2.75	1.56	1.52
25	8	308	CHL	CBD-CGD	2.75	1.56	1.52
25	4	308	CHL	CBD-CGD	2.75	1.56	1.52
22	c	508	CLA	C4B-CHC	2.75	1.47	1.40
25	n	606	CHL	O2D-CGD	2.75	1.40	1.33
25	N	606	CHL	O2D-CGD	2.75	1.40	1.33
25	y	606	CHL	O2D-CGD	2.75	1.40	1.33
25	Y	606	CHL	O2D-CGD	2.75	1.40	1.33
25	R	304	CHL	CBD-CAD	2.76	1.57	1.53
25	r	304	CHL	CBD-CAD	2.76	1.57	1.53
22	B	615	CLA	C4B-CHC	2.77	1.47	1.40
22	s	309	CLA	C4B-CHC	2.77	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	309	CLA	C4B-CHC	2.77	1.47	1.40
25	7	308	CHL	O2D-CGD	2.77	1.40	1.33
25	3	308	CHL	O2D-CGD	2.77	1.40	1.33
25	y	608	CHL	O2D-CGD	2.78	1.40	1.33
25	Y	608	CHL	O2D-CGD	2.78	1.40	1.33
22	b	604	CLA	C4B-CHC	2.78	1.47	1.40
22	d	403	CLA	C4B-CHC	2.79	1.47	1.40
22	b	611	CLA	C4B-CHC	2.79	1.47	1.40
22	b	613	CLA	C4B-CHC	2.79	1.47	1.40
25	7	308	CHL	CBD-CGD	2.79	1.56	1.52
25	3	308	CHL	CBD-CGD	2.79	1.56	1.52
22	C	510	CLA	C4B-CHC	2.79	1.47	1.40
25	s	306	CHL	CBD-CAD	2.79	1.57	1.53
25	S	306	CHL	CBD-CAD	2.79	1.57	1.53
25	s	307	CHL	O2D-CGD	2.79	1.40	1.33
25	S	307	CHL	O2D-CGD	2.79	1.40	1.33
25	6	608	CHL	O2D-CGD	2.80	1.40	1.33
25	2	608	CHL	O2D-CGD	2.80	1.40	1.33
25	y	609	CHL	O2D-CGD	2.81	1.40	1.33
25	Y	609	CHL	O2D-CGD	2.81	1.40	1.33
22	c	505	CLA	C4B-CHC	2.81	1.47	1.40
22	D	403	CLA	C4B-CHC	2.81	1.47	1.40
25	N	601	CHL	O2D-CGD	2.81	1.40	1.33
25	n	601	CHL	O2D-CGD	2.81	1.40	1.33
25	G	607	CHL	O2D-CGD	2.82	1.40	1.33
25	g	607	CHL	O2D-CGD	2.82	1.40	1.33
25	l	601	CHL	CBD-CGD	2.82	1.56	1.52
25	5	601	CHL	CBD-CGD	2.82	1.56	1.52
25	R	304	CHL	O2D-CGD	2.82	1.40	1.33
25	r	304	CHL	O2D-CGD	2.82	1.40	1.33
22	C	505	CLA	C4B-CHC	2.83	1.47	1.40
25	r	306	CHL	O2D-CGD	2.83	1.40	1.33
25	R	306	CHL	O2D-CGD	2.83	1.40	1.33
22	b	609	CLA	C4B-CHC	2.84	1.47	1.40
22	b	604	CLA	C3B-C2B	2.84	1.44	1.40
25	n	609	CHL	O2D-CGD	2.84	1.40	1.33
25	N	609	CHL	O2D-CGD	2.84	1.40	1.33
25	r	306	CHL	CBD-CAD	2.84	1.57	1.53
25	R	306	CHL	CBD-CAD	2.84	1.57	1.53
22	S	312	CLA	C4B-CHC	2.85	1.47	1.40
22	s	312	CLA	C4B-CHC	2.85	1.47	1.40
25	r	305	CHL	CBD-CAD	2.85	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	305	CHL	CBD-CAD	2.85	1.57	1.53
25	3	306	CHL	CBD-CGD	2.85	1.56	1.52
25	7	306	CHL	CBD-CGD	2.85	1.56	1.52
22	R	303	CLA	C4B-CHC	2.85	1.47	1.40
22	r	303	CLA	C4B-CHC	2.85	1.47	1.40
22	B	606	CLA	C4B-CHC	2.85	1.47	1.40
25	4	306	CHL	CBD-CAD	2.86	1.57	1.53
25	8	306	CHL	CBD-CAD	2.86	1.57	1.53
25	S	302	CHL	O2D-CGD	2.86	1.40	1.33
25	s	302	CHL	O2D-CGD	2.86	1.40	1.33
25	4	301	CHL	O2D-CGD	2.86	1.40	1.33
25	8	301	CHL	O2D-CGD	2.86	1.40	1.33
22	n	603	CLA	C4B-CHC	2.87	1.47	1.40
22	N	603	CLA	C4B-CHC	2.87	1.47	1.40
22	S	312	CLA	C3B-C2B	2.87	1.44	1.40
22	s	312	CLA	C3B-C2B	2.87	1.44	1.40
22	Y	614	CLA	C4B-CHC	2.87	1.47	1.40
22	y	614	CLA	C4B-CHC	2.87	1.47	1.40
22	G	603	CLA	C4B-CHC	2.87	1.47	1.40
22	g	603	CLA	C4B-CHC	2.87	1.47	1.40
22	Y	603	CLA	C4B-CHC	2.87	1.47	1.40
22	y	603	CLA	C4B-CHC	2.87	1.47	1.40
22	Y	603	CLA	C3B-C2B	2.88	1.44	1.40
22	y	603	CLA	C3B-C2B	2.88	1.44	1.40
25	1	608	CHL	CBD-CGD	2.88	1.56	1.52
25	5	608	CHL	CBD-CGD	2.88	1.56	1.52
22	b	607	CLA	C4B-CHC	2.88	1.47	1.40
22	C	505	CLA	C3B-C2B	2.88	1.44	1.40
22	B	603	CLA	C4B-CHC	2.88	1.47	1.40
22	B	605	CLA	C4B-CHC	2.89	1.47	1.40
25	3	302	CHL	CBD-CGD	2.89	1.57	1.52
25	7	302	CHL	CBD-CGD	2.89	1.57	1.52
22	G	603	CLA	C3B-C2B	2.89	1.44	1.40
22	g	603	CLA	C3B-C2B	2.89	1.44	1.40
22	c	503	CLA	C4B-CHC	2.89	1.47	1.40
25	g	606	CHL	O2D-CGD	2.90	1.40	1.33
25	G	606	CHL	O2D-CGD	2.90	1.40	1.33
25	n	607	CHL	O2D-CGD	2.90	1.40	1.33
25	N	607	CHL	O2D-CGD	2.90	1.40	1.33
25	Y	607	CHL	O2D-CGD	2.90	1.40	1.33
25	y	607	CHL	O2D-CGD	2.90	1.40	1.33
22	C	507	CLA	C4B-CHC	2.90	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	609	CHL	O2D-CGD	2.90	1.40	1.33
25	g	609	CHL	O2D-CGD	2.90	1.40	1.33
22	D	401	CLA	C4B-CHC	2.90	1.47	1.40
22	c	504	CLA	C4B-CHC	2.90	1.47	1.40
22	c	506	CLA	C4B-CHC	2.90	1.47	1.40
25	8	305	CHL	CBD-CAD	2.91	1.57	1.53
25	4	305	CHL	CBD-CAD	2.91	1.57	1.53
22	b	602	CLA	C3B-C2B	2.91	1.44	1.40
22	S	314	CLA	C4B-CHC	2.91	1.47	1.40
22	s	314	CLA	C4B-CHC	2.91	1.47	1.40
25	2	606	CHL	O2D-CGD	2.91	1.40	1.33
25	6	606	CHL	O2D-CGD	2.91	1.40	1.33
25	3	306	CHL	CBD-CAD	2.91	1.57	1.53
25	7	306	CHL	CBD-CAD	2.91	1.57	1.53
25	1	606	CHL	O2D-CGD	2.91	1.40	1.33
25	5	606	CHL	O2D-CGD	2.91	1.40	1.33
22	S	305	CLA	C4B-CHC	2.91	1.47	1.40
22	s	305	CLA	C4B-CHC	2.91	1.47	1.40
22	c	512	CLA	C4B-CHC	2.92	1.47	1.40
25	S	308	CHL	O2D-CGD	2.92	1.40	1.33
25	s	308	CHL	O2D-CGD	2.92	1.40	1.33
22	a	405	CLA	C4B-CHC	2.93	1.47	1.40
22	s	313	CLA	C4B-CHC	2.93	1.47	1.40
22	S	313	CLA	C4B-CHC	2.93	1.47	1.40
22	B	610	CLA	C4B-CHC	2.93	1.47	1.40
25	7	307	CHL	O2D-CGD	2.93	1.40	1.33
25	3	307	CHL	O2D-CGD	2.93	1.40	1.33
22	b	614	CLA	C4B-CHC	2.93	1.47	1.40
25	1	607	CHL	O2D-CGD	2.93	1.40	1.33
25	5	607	CHL	O2D-CGD	2.93	1.40	1.33
25	2	607	CHL	O2D-CGD	2.93	1.40	1.33
25	6	607	CHL	O2D-CGD	2.93	1.40	1.33
22	n	612	CLA	C4B-CHC	2.93	1.47	1.40
22	N	612	CLA	C4B-CHC	2.93	1.47	1.40
25	5	615	CHL	O2D-CGD	2.93	1.40	1.33
25	1	615	CHL	O2D-CGD	2.93	1.40	1.33
22	n	604	CLA	C3B-C2B	2.93	1.44	1.40
22	N	604	CLA	C3B-C2B	2.93	1.44	1.40
22	A	402	CLA	C4B-CHC	2.94	1.47	1.40
22	y	611	CLA	C4B-CHC	2.94	1.47	1.40
22	Y	611	CLA	C4B-CHC	2.94	1.47	1.40
25	1	605	CHL	O2D-CGD	2.94	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	605	CHL	O2D-CGD	2.94	1.40	1.33
22	c	502	CLA	C4B-CHC	2.94	1.48	1.40
25	s	306	CHL	O2D-CGD	2.95	1.40	1.33
25	S	306	CHL	O2D-CGD	2.95	1.40	1.33
25	1	609	CHL	O2D-CGD	2.95	1.40	1.33
25	5	609	CHL	O2D-CGD	2.95	1.40	1.33
22	G	604	CLA	C3B-C2B	2.95	1.44	1.40
22	g	604	CLA	C3B-C2B	2.95	1.44	1.40
25	1	601	CHL	O2D-CGD	2.95	1.40	1.33
25	5	601	CHL	O2D-CGD	2.95	1.40	1.33
25	g	605	CHL	CBD-CGD	2.96	1.57	1.52
25	G	605	CHL	CBD-CGD	2.96	1.57	1.52
25	7	309	CHL	O2D-CGD	2.96	1.40	1.33
25	3	309	CHL	O2D-CGD	2.96	1.40	1.33
25	y	609	CHL	CBD-CGD	2.96	1.57	1.52
25	Y	609	CHL	CBD-CGD	2.96	1.57	1.52
25	1	609	CHL	CBD-CGD	2.96	1.57	1.52
25	5	609	CHL	CBD-CGD	2.96	1.57	1.52
25	7	307	CHL	CBD-CAD	2.96	1.57	1.53
25	3	307	CHL	CBD-CAD	2.96	1.57	1.53
22	n	603	CLA	C3B-C2B	2.96	1.44	1.40
22	N	603	CLA	C3B-C2B	2.96	1.44	1.40
25	6	601	CHL	O2D-CGD	2.96	1.40	1.33
25	2	601	CHL	O2D-CGD	2.96	1.40	1.33
22	n	611	CLA	C4B-CHC	2.97	1.48	1.40
22	N	611	CLA	C4B-CHC	2.97	1.48	1.40
25	2	605	CHL	CBD-CGD	2.97	1.57	1.52
25	6	605	CHL	CBD-CGD	2.97	1.57	1.52
22	R	303	CLA	C3B-C2B	2.97	1.44	1.40
22	r	303	CLA	C3B-C2B	2.97	1.44	1.40
22	c	510	CLA	C4B-CHC	2.97	1.48	1.40
25	3	301	CHL	O2D-CGD	2.97	1.40	1.33
25	7	301	CHL	O2D-CGD	2.97	1.40	1.33
22	C	511	CLA	C4B-CHC	2.97	1.48	1.40
22	g	611	CLA	C4B-CHC	2.97	1.48	1.40
22	G	611	CLA	C4B-CHC	2.97	1.48	1.40
25	8	308	CHL	O2D-CGD	2.98	1.40	1.33
25	4	308	CHL	O2D-CGD	2.98	1.40	1.33
25	r	305	CHL	O2D-CGD	2.98	1.40	1.33
25	R	305	CHL	O2D-CGD	2.98	1.40	1.33
22	b	603	CLA	C4B-CHC	2.98	1.48	1.40
23	A	404	PHO	CHD-C4C	2.98	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	302	CHL	O2D-CGD	2.98	1.40	1.33
25	7	302	CHL	O2D-CGD	2.98	1.40	1.33
22	d	401	CLA	C4B-CHC	2.98	1.48	1.40
22	b	610	CLA	C4B-CHC	2.99	1.48	1.40
22	N	602	CLA	C4B-CHC	2.99	1.48	1.40
22	n	602	CLA	C4B-CHC	2.99	1.48	1.40
22	5	604	CLA	C4B-CHC	2.99	1.48	1.40
22	1	604	CLA	C4B-CHC	2.99	1.48	1.40
22	C	507	CLA	C3B-C2B	2.99	1.44	1.40
25	8	305	CHL	O2D-CGD	2.99	1.40	1.33
25	4	305	CHL	O2D-CGD	2.99	1.40	1.33
25	5	615	CHL	CBD-CAD	3.00	1.57	1.53
25	1	615	CHL	CBD-CAD	3.00	1.57	1.53
22	R	311	CLA	C3B-C2B	3.00	1.44	1.40
22	r	311	CLA	C3B-C2B	3.00	1.44	1.40
22	S	310	CLA	C3B-C2B	3.00	1.44	1.40
22	s	310	CLA	C3B-C2B	3.00	1.44	1.40
22	5	614	CLA	C4B-CHC	3.00	1.48	1.40
22	1	614	CLA	C4B-CHC	3.00	1.48	1.40
22	B	612	CLA	C4B-CHC	3.00	1.48	1.40
25	1	608	CHL	O2D-CGD	3.01	1.40	1.33
25	5	608	CHL	O2D-CGD	3.01	1.40	1.33
22	n	613	CLA	C4B-CHC	3.01	1.48	1.40
22	Y	602	CLA	C4B-CHC	3.01	1.48	1.40
22	N	613	CLA	C4B-CHC	3.01	1.48	1.40
22	y	602	CLA	C4B-CHC	3.01	1.48	1.40
25	7	308	CHL	CBD-CAD	3.01	1.57	1.53
25	3	308	CHL	CBD-CAD	3.01	1.57	1.53
22	g	613	CLA	C4B-CHC	3.01	1.48	1.40
22	G	613	CLA	C4B-CHC	3.01	1.48	1.40
25	2	606	CHL	CBD-CAD	3.01	1.57	1.53
25	6	606	CHL	CBD-CAD	3.01	1.57	1.53
25	1	605	CHL	CBD-CAD	3.01	1.57	1.53
25	5	605	CHL	CBD-CAD	3.01	1.57	1.53
22	D	404	CLA	C4B-CHC	3.02	1.48	1.40
25	4	307	CHL	O2D-CGD	3.02	1.40	1.33
25	8	307	CHL	O2D-CGD	3.02	1.40	1.33
22	C	508	CLA	C3B-C2B	3.02	1.44	1.40
22	B	611	CLA	C4B-CHC	3.02	1.48	1.40
22	b	608	CLA	C4B-CHC	3.02	1.48	1.40
25	4	306	CHL	O2D-CGD	3.03	1.40	1.33
25	8	306	CHL	O2D-CGD	3.03	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	C3B-C2B	3.03	1.44	1.40
22	r	307	CLA	C4B-CHC	3.03	1.48	1.40
22	R	307	CLA	C4B-CHC	3.03	1.48	1.40
22	y	610	CLA	C4B-CHC	3.03	1.48	1.40
22	Y	610	CLA	C4B-CHC	3.03	1.48	1.40
25	8	308	CHL	CBD-CAD	3.03	1.57	1.53
25	4	308	CHL	CBD-CAD	3.03	1.57	1.53
22	c	507	CLA	C3B-C2B	3.03	1.44	1.40
22	A	405	CLA	C4B-CHC	3.04	1.48	1.40
22	R	309	CLA	C4B-CHC	3.04	1.48	1.40
22	r	309	CLA	C4B-CHC	3.04	1.48	1.40
22	8	302	CLA	C3B-C2B	3.04	1.44	1.40
22	4	302	CLA	C3B-C2B	3.04	1.44	1.40
25	2	607	CHL	CBD-CGD	3.05	1.57	1.52
25	6	607	CHL	CBD-CGD	3.05	1.57	1.52
25	g	605	CHL	O2D-CGD	3.05	1.40	1.33
25	G	605	CHL	O2D-CGD	3.05	1.40	1.33
22	S	301	CLA	C4B-CHC	3.05	1.48	1.40
22	a	402	CLA	C4B-CHC	3.06	1.48	1.40
22	D	401	CLA	C3B-C2B	3.06	1.44	1.40
22	y	613	CLA	C4B-CHC	3.06	1.48	1.40
22	Y	613	CLA	C4B-CHC	3.06	1.48	1.40
22	C	511	CLA	C3B-C2B	3.06	1.44	1.40
22	B	609	CLA	C4B-CHC	3.06	1.48	1.40
25	1	601	CHL	CBD-CAD	3.07	1.57	1.53
25	5	601	CHL	CBD-CAD	3.07	1.57	1.53
22	c	511	CLA	C4B-CHC	3.07	1.48	1.40
25	2	605	CHL	O2D-CGD	3.07	1.41	1.33
25	6	605	CHL	O2D-CGD	3.07	1.41	1.33
25	2	605	CHL	CBD-CAD	3.07	1.57	1.53
25	6	605	CHL	CBD-CAD	3.07	1.57	1.53
22	G	602	CLA	C4B-CHC	3.07	1.48	1.40
22	g	602	CLA	C4B-CHC	3.07	1.48	1.40
25	3	306	CHL	O2D-CGD	3.07	1.41	1.33
25	7	306	CHL	O2D-CGD	3.07	1.41	1.33
22	2	604	CLA	C4B-CHC	3.08	1.48	1.40
22	6	604	CLA	C4B-CHC	3.08	1.48	1.40
22	C	504	CLA	C3B-C2B	3.08	1.44	1.40
22	N	614	CLA	C4B-CHC	3.08	1.48	1.40
22	n	614	CLA	C4B-CHC	3.08	1.48	1.40
22	8	302	CLA	C4B-CHC	3.08	1.48	1.40
22	4	302	CLA	C4B-CHC	3.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	605	CHL	CBD-CAD	3.09	1.57	1.53
25	G	605	CHL	CBD-CAD	3.09	1.57	1.53
22	B	616	CLA	C4B-CHC	3.09	1.48	1.40
25	6	601	CHL	CBD-CAD	3.09	1.57	1.53
25	2	601	CHL	CBD-CAD	3.09	1.57	1.53
22	d	404	CLA	C4B-CHC	3.09	1.48	1.40
22	s	313	CLA	C3B-C2B	3.09	1.44	1.40
22	S	313	CLA	C3B-C2B	3.09	1.44	1.40
22	c	505	CLA	C3B-C2B	3.10	1.44	1.40
22	S	311	CLA	C4B-CHC	3.10	1.48	1.40
22	s	311	CLA	C4B-CHC	3.10	1.48	1.40
25	2	607	CHL	CBD-CAD	3.11	1.57	1.53
25	6	607	CHL	CBD-CAD	3.11	1.57	1.53
22	c	508	CLA	C3B-C2B	3.11	1.44	1.40
25	1	606	CHL	CBD-CAD	3.11	1.57	1.53
25	5	606	CHL	CBD-CAD	3.11	1.57	1.53
22	S	310	CLA	C4B-CHC	3.12	1.48	1.40
22	s	310	CLA	C4B-CHC	3.12	1.48	1.40
22	B	607	CLA	C3B-C2B	3.13	1.44	1.40
22	7	305	CLA	C4B-CHC	3.13	1.48	1.40
22	3	305	CLA	C4B-CHC	3.13	1.48	1.40
22	g	612	CLA	C4B-CHC	3.14	1.48	1.40
22	G	612	CLA	C4B-CHC	3.14	1.48	1.40
22	3	304	CLA	C4B-CHC	3.14	1.48	1.40
22	7	304	CLA	C4B-CHC	3.14	1.48	1.40
22	C	503	CLA	C4B-CHC	3.14	1.48	1.40
22	B	613	CLA	C4B-CHC	3.14	1.48	1.40
25	1	608	CHL	CBD-CAD	3.15	1.57	1.53
25	5	608	CHL	CBD-CAD	3.15	1.57	1.53
22	g	613	CLA	C3B-C2B	3.15	1.44	1.40
22	G	613	CLA	C3B-C2B	3.15	1.44	1.40
22	d	401	CLA	C3B-C2B	3.15	1.44	1.40
22	s	301	CLA	C4B-CHC	3.16	1.48	1.40
22	R	311	CLA	C4B-CHC	3.16	1.48	1.40
22	s	303	CLA	C4B-CHC	3.16	1.48	1.40
22	S	303	CLA	C4B-CHC	3.16	1.48	1.40
22	r	311	CLA	C4B-CHC	3.16	1.48	1.40
22	Y	602	CLA	C3B-C2B	3.16	1.44	1.40
22	c	503	CLA	C3B-C2B	3.16	1.44	1.40
22	b	614	CLA	C3B-C2B	3.16	1.44	1.40
22	y	602	CLA	C3B-C2B	3.16	1.44	1.40
22	S	304	CLA	C4B-CHC	3.16	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	s	304	CLA	C4B-CHC	3.16	1.48	1.40
22	B	604	CLA	CHC-C1C	3.16	1.44	1.35
25	1	609	CHL	CBD-CAD	3.17	1.57	1.53
25	5	609	CHL	CBD-CAD	3.17	1.57	1.53
22	c	502	CLA	C3B-C2B	3.17	1.44	1.40
22	b	602	CLA	C4B-CHC	3.17	1.48	1.40
22	5	611	CLA	C4B-CHC	3.17	1.48	1.40
22	1	611	CLA	C4B-CHC	3.17	1.48	1.40
22	C	509	CLA	C4B-CHC	3.17	1.48	1.40
22	y	613	CLA	C3B-C2B	3.17	1.44	1.40
22	Y	613	CLA	C3B-C2B	3.17	1.44	1.40
22	1	603	CLA	C4B-CHC	3.17	1.48	1.40
22	5	603	CLA	C4B-CHC	3.17	1.48	1.40
22	b	603	CLA	C3B-C2B	3.18	1.44	1.40
22	4	304	CLA	C4B-CHC	3.19	1.48	1.40
22	8	304	CLA	C4B-CHC	3.19	1.48	1.40
22	B	606	CLA	C3B-C2B	3.19	1.44	1.40
22	r	310	CLA	C4B-CHC	3.19	1.48	1.40
22	R	310	CLA	C4B-CHC	3.19	1.48	1.40
22	S	314	CLA	C3B-C2B	3.20	1.44	1.40
22	s	314	CLA	C3B-C2B	3.20	1.44	1.40
22	b	601	CLA	C4B-CHC	3.20	1.48	1.40
22	1	613	CLA	C4B-CHC	3.21	1.48	1.40
22	5	613	CLA	C4B-CHC	3.21	1.48	1.40
22	6	603	CLA	C4B-CHC	3.21	1.48	1.40
22	2	603	CLA	C4B-CHC	3.21	1.48	1.40
25	s	307	CHL	CBD-CAD	3.21	1.57	1.53
25	S	307	CHL	CBD-CAD	3.21	1.57	1.53
25	n	609	CHL	CBD-CGD	3.21	1.57	1.52
25	N	609	CHL	CBD-CGD	3.21	1.57	1.52
25	6	608	CHL	CBD-CGD	3.21	1.57	1.52
25	2	608	CHL	CBD-CGD	3.21	1.57	1.52
22	G	614	CLA	C4B-CHC	3.21	1.48	1.40
22	g	614	CLA	C4B-CHC	3.21	1.48	1.40
22	1	612	CLA	C4B-CHC	3.21	1.48	1.40
22	5	612	CLA	C4B-CHC	3.21	1.48	1.40
25	y	609	CHL	CBD-CAD	3.22	1.57	1.53
25	Y	609	CHL	CBD-CAD	3.22	1.57	1.53
22	2	604	CLA	C3B-C2B	3.22	1.44	1.40
22	6	604	CLA	C3B-C2B	3.22	1.44	1.40
22	C	502	CLA	C4B-CHC	3.22	1.48	1.40
22	R	312	CLA	C4B-CHC	3.22	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	312	CLA	C4B-CHC	3.22	1.48	1.40
22	B	605	CLA	C3B-C2B	3.22	1.44	1.40
22	c	509	CLA	C4B-CHC	3.22	1.48	1.40
22	a	403	CLA	C4B-CHC	3.22	1.48	1.40
22	c	512	CLA	C3B-C2B	3.22	1.44	1.40
22	r	302	CLA	C4B-CHC	3.23	1.48	1.40
22	R	302	CLA	C4B-CHC	3.23	1.48	1.40
22	C	512	CLA	C4B-CHC	3.23	1.48	1.40
22	S	304	CLA	C3B-C2B	3.23	1.44	1.40
22	s	304	CLA	C3B-C2B	3.23	1.44	1.40
22	b	615	CLA	C4B-CHC	3.23	1.48	1.40
22	2	602	CLA	C4B-CHC	3.23	1.48	1.40
22	6	602	CLA	C4B-CHC	3.23	1.48	1.40
22	n	610	CLA	C4B-CHC	3.23	1.48	1.40
22	N	610	CLA	C4B-CHC	3.23	1.48	1.40
22	2	612	CLA	C4B-CHC	3.24	1.48	1.40
22	6	612	CLA	C4B-CHC	3.24	1.48	1.40
22	8	310	CLA	C4B-CHC	3.24	1.48	1.40
22	4	310	CLA	C4B-CHC	3.24	1.48	1.40
22	b	616	CLA	C3B-C2B	3.25	1.44	1.40
23	d	402	PHO	CHD-C1D	3.25	1.45	1.38
23	a	404	PHO	CHD-C1D	3.25	1.45	1.38
22	b	605	CLA	C4B-CHC	3.25	1.48	1.40
22	B	602	CLA	C4B-CHC	3.25	1.48	1.40
22	1	613	CLA	C3B-C2B	3.26	1.44	1.40
22	2	602	CLA	C3B-C2B	3.26	1.44	1.40
22	6	602	CLA	C3B-C2B	3.26	1.44	1.40
22	5	613	CLA	C3B-C2B	3.26	1.44	1.40
22	A	403	CLA	C4B-CHC	3.26	1.48	1.40
23	D	402	PHO	CHD-C1D	3.26	1.45	1.38
22	R	301	CLA	C4B-CHC	3.26	1.48	1.40
22	r	301	CLA	C4B-CHC	3.26	1.48	1.40
22	r	307	CLA	C3B-C2B	3.26	1.44	1.40
22	R	307	CLA	C3B-C2B	3.26	1.44	1.40
22	4	309	CLA	C4B-CHC	3.27	1.48	1.40
22	8	309	CLA	C4B-CHC	3.27	1.48	1.40
22	Y	604	CLA	C3B-C2B	3.27	1.44	1.40
22	y	604	CLA	C3B-C2B	3.27	1.44	1.40
22	1	602	CLA	C4B-CHC	3.27	1.48	1.40
22	2	610	CLA	C4B-CHC	3.27	1.48	1.40
22	4	303	CLA	C4B-CHC	3.27	1.48	1.40
22	5	602	CLA	C4B-CHC	3.27	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	610	CLA	C4B-CHC	3.27	1.48	1.40
22	8	303	CLA	C4B-CHC	3.27	1.48	1.40
22	R	308	CLA	C4B-CHC	3.27	1.48	1.40
22	r	308	CLA	C4B-CHC	3.27	1.48	1.40
22	7	313	CLA	C4B-CHC	3.27	1.48	1.40
22	3	313	CLA	C4B-CHC	3.27	1.48	1.40
22	B	601	CLA	C4B-CHC	3.28	1.48	1.40
25	3	302	CHL	CBD-CAD	3.28	1.57	1.53
25	7	302	CHL	CBD-CAD	3.28	1.57	1.53
22	2	613	CLA	C4B-CHC	3.28	1.48	1.40
22	6	613	CLA	C4B-CHC	3.28	1.48	1.40
22	7	303	CLA	C4B-CHC	3.28	1.48	1.40
22	3	303	CLA	C4B-CHC	3.28	1.48	1.40
22	7	311	CLA	C4B-CHC	3.28	1.48	1.40
22	3	311	CLA	C4B-CHC	3.28	1.48	1.40
22	s	301	CLA	C3B-C2B	3.29	1.44	1.40
22	b	601	CLA	C3B-C2B	3.29	1.44	1.40
22	R	309	CLA	C3B-C2B	3.30	1.44	1.40
22	r	309	CLA	C3B-C2B	3.30	1.44	1.40
22	B	615	CLA	C3B-C2B	3.31	1.44	1.40
25	7	309	CHL	CBD-CAD	3.31	1.58	1.53
25	3	309	CHL	CBD-CAD	3.31	1.58	1.53
22	G	610	CLA	C4B-CHC	3.31	1.48	1.40
22	g	610	CLA	C4B-CHC	3.31	1.48	1.40
22	n	613	CLA	C3B-C2B	3.32	1.44	1.40
22	N	613	CLA	C3B-C2B	3.32	1.44	1.40
22	3	312	CLA	C4B-CHC	3.33	1.49	1.40
22	7	312	CLA	C4B-CHC	3.33	1.49	1.40
22	6	611	CLA	C4B-CHC	3.33	1.49	1.40
22	2	611	CLA	C4B-CHC	3.33	1.49	1.40
22	b	613	CLA	C3B-C2B	3.33	1.44	1.40
22	S	305	CLA	C3B-C2B	3.33	1.44	1.40
22	s	305	CLA	C3B-C2B	3.33	1.44	1.40
22	7	314	CLA	C4B-CHC	3.33	1.49	1.40
22	3	314	CLA	C4B-CHC	3.33	1.49	1.40
22	d	404	CLA	C3B-C2B	3.33	1.44	1.40
22	1	612	CLA	C3B-C2B	3.34	1.44	1.40
22	5	612	CLA	C3B-C2B	3.34	1.44	1.40
25	4	307	CHL	CBD-CAD	3.34	1.58	1.53
25	8	307	CHL	CBD-CAD	3.34	1.58	1.53
22	C	502	CLA	C3B-C2B	3.34	1.44	1.40
25	n	609	CHL	CBD-CAD	3.35	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	609	CHL	CBD-CAD	3.35	1.58	1.53
25	7	309	CHL	CBD-CGD	3.35	1.57	1.52
25	3	309	CHL	CBD-CGD	3.35	1.57	1.52
22	b	608	CLA	C3B-C2B	3.35	1.44	1.40
22	1	610	CLA	C4B-CHC	3.35	1.49	1.40
22	5	610	CLA	C4B-CHC	3.35	1.49	1.40
22	7	303	CLA	C3B-C2B	3.35	1.44	1.40
22	3	303	CLA	C3B-C2B	3.35	1.44	1.40
22	n	612	CLA	C3B-C2B	3.35	1.44	1.40
22	N	612	CLA	C3B-C2B	3.35	1.44	1.40
23	a	404	PHO	CHD-C4C	3.36	1.48	1.40
22	b	615	CLA	C3B-C2B	3.36	1.44	1.40
22	G	602	CLA	C3B-C2B	3.36	1.44	1.40
22	N	602	CLA	C3B-C2B	3.36	1.44	1.40
22	g	602	CLA	C3B-C2B	3.36	1.44	1.40
22	n	602	CLA	C3B-C2B	3.36	1.44	1.40
22	b	606	CLA	C4B-CHC	3.36	1.49	1.40
22	c	511	CLA	C3B-C2B	3.37	1.44	1.40
22	S	301	CLA	C3B-C2B	3.38	1.44	1.40
22	B	608	CLA	C3B-C2B	3.38	1.44	1.40
22	b	610	CLA	C3B-C2B	3.38	1.44	1.40
22	B	610	CLA	C3B-C2B	3.39	1.44	1.40
25	G	609	CHL	CBD-CGD	3.39	1.57	1.52
25	g	609	CHL	CBD-CGD	3.39	1.57	1.52
22	b	616	CLA	CHB-C4A	3.40	1.37	1.33
25	6	608	CHL	CBD-CAD	3.40	1.58	1.53
25	2	608	CHL	CBD-CAD	3.40	1.58	1.53
23	d	402	PHO	CHD-C4C	3.40	1.48	1.40
22	D	404	CLA	C3B-C2B	3.40	1.44	1.40
22	7	305	CLA	C3B-C2B	3.40	1.44	1.40
22	3	305	CLA	C3B-C2B	3.40	1.44	1.40
22	S	311	CLA	C3B-C2B	3.40	1.44	1.40
22	s	311	CLA	C3B-C2B	3.40	1.44	1.40
22	6	603	CLA	C3B-C2B	3.41	1.44	1.40
22	2	603	CLA	C3B-C2B	3.41	1.44	1.40
22	5	604	CLA	C3B-C2B	3.42	1.44	1.40
22	1	604	CLA	C3B-C2B	3.42	1.44	1.40
22	c	507	CLA	CHC-C1C	3.42	1.45	1.35
23	D	402	PHO	CHD-C4C	3.43	1.48	1.40
22	B	601	CLA	C3B-C2B	3.44	1.44	1.40
22	b	612	CLA	C4B-CHC	3.44	1.49	1.40
25	G	609	CHL	CBD-CAD	3.46	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	609	CHL	CBD-CAD	3.46	1.58	1.53
22	D	403	CLA	C3C-C2C	3.46	1.44	1.36
22	1	603	CLA	C3B-C2B	3.46	1.44	1.40
22	5	603	CLA	C3B-C2B	3.46	1.44	1.40
22	3	304	CLA	C3B-C2B	3.47	1.44	1.40
22	7	304	CLA	C3B-C2B	3.47	1.44	1.40
22	C	512	CLA	C3B-C2B	3.47	1.44	1.40
22	6	611	CLA	C3B-C2B	3.47	1.44	1.40
22	2	611	CLA	C3B-C2B	3.47	1.44	1.40
22	y	611	CLA	C3B-C2B	3.48	1.44	1.40
22	Y	611	CLA	C3B-C2B	3.48	1.44	1.40
22	s	309	CLA	C3B-C2B	3.48	1.44	1.40
22	4	309	CLA	C3B-C2B	3.48	1.44	1.40
22	8	309	CLA	C3B-C2B	3.48	1.44	1.40
22	S	309	CLA	C3B-C2B	3.48	1.44	1.40
22	B	613	CLA	C3B-C2B	3.48	1.44	1.40
22	g	612	CLA	C3B-C2B	3.49	1.45	1.40
22	G	612	CLA	C3B-C2B	3.49	1.45	1.40
22	B	614	CLA	C4B-CHC	3.49	1.49	1.40
22	1	602	CLA	C3B-C2B	3.49	1.45	1.40
22	5	602	CLA	C3B-C2B	3.49	1.45	1.40
22	4	304	CLA	C3B-C2B	3.51	1.45	1.40
22	8	304	CLA	C3B-C2B	3.51	1.45	1.40
22	R	301	CLA	C3B-C2B	3.51	1.45	1.40
22	r	301	CLA	C3B-C2B	3.51	1.45	1.40
22	3	312	CLA	C3B-C2B	3.52	1.45	1.40
22	7	312	CLA	C3B-C2B	3.52	1.45	1.40
22	5	614	CLA	C3B-C2B	3.52	1.45	1.40
22	1	614	CLA	C3B-C2B	3.52	1.45	1.40
22	6	609	CLA	C4B-CHC	3.52	1.49	1.40
22	2	609	CLA	C4B-CHC	3.52	1.49	1.40
22	b	605	CLA	C3B-C2B	3.53	1.45	1.40
22	c	501	CLA	CHC-C1C	3.53	1.45	1.35
22	2	612	CLA	C3B-C2B	3.53	1.45	1.40
22	6	612	CLA	C3B-C2B	3.53	1.45	1.40
22	r	302	CLA	C3B-C2B	3.54	1.45	1.40
22	R	302	CLA	C3B-C2B	3.54	1.45	1.40
22	3	310	CLA	C4B-CHC	3.54	1.49	1.40
22	7	310	CLA	C4B-CHC	3.54	1.49	1.40
22	B	605	CLA	C3C-C2C	3.54	1.44	1.36
22	a	403	CLA	C3B-C2B	3.55	1.45	1.40
22	C	508	CLA	CHC-C1C	3.56	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	C3C-C2C	3.56	1.44	1.36
22	C	510	CLA	C3B-C2B	3.57	1.45	1.40
22	C	506	CLA	CHC-C1C	3.57	1.45	1.35
22	B	608	CLA	CHC-C1C	3.58	1.45	1.35
22	B	615	CLA	C3C-C2C	3.58	1.44	1.36
22	Y	614	CLA	C3B-C2B	3.60	1.45	1.40
22	y	614	CLA	C3B-C2B	3.60	1.45	1.40
22	B	603	CLA	C3B-C2B	3.61	1.45	1.40
22	r	310	CLA	C3B-C2B	3.61	1.45	1.40
22	R	310	CLA	C3B-C2B	3.61	1.45	1.40
22	5	611	CLA	C3B-C2B	3.61	1.45	1.40
22	1	611	CLA	C3B-C2B	3.61	1.45	1.40
22	b	616	CLA	CHC-C1C	3.61	1.45	1.35
22	b	614	CLA	C3C-C2C	3.62	1.44	1.36
22	C	501	CLA	CHC-C1C	3.62	1.45	1.35
22	c	504	CLA	C3B-C2B	3.63	1.45	1.40
22	C	504	CLA	CHC-C1C	3.63	1.45	1.35
22	7	313	CLA	C3B-C2B	3.63	1.45	1.40
22	3	313	CLA	C3B-C2B	3.63	1.45	1.40
22	b	604	CLA	CHC-C1C	3.64	1.45	1.35
22	g	611	CLA	C3B-C2B	3.65	1.45	1.40
22	G	611	CLA	C3B-C2B	3.65	1.45	1.40
22	a	405	CLA	C3B-C2B	3.65	1.45	1.40
22	C	507	CLA	CHC-C1C	3.66	1.46	1.35
22	C	510	CLA	CHC-C1C	3.66	1.46	1.35
23	D	402	PHO	CHC-C1C	3.66	1.45	1.38
22	B	602	CLA	C3B-C2B	3.67	1.45	1.40
22	c	503	CLA	C3C-C2C	3.67	1.44	1.36
22	B	614	CLA	C3B-C2B	3.67	1.45	1.40
22	4	303	CLA	C3B-C2B	3.67	1.45	1.40
22	n	611	CLA	C3B-C2B	3.67	1.45	1.40
22	8	303	CLA	C3B-C2B	3.67	1.45	1.40
22	N	611	CLA	C3B-C2B	3.67	1.45	1.40
22	b	611	CLA	C3C-C2C	3.67	1.44	1.36
22	d	403	CLA	C3C-C2C	3.68	1.44	1.36
22	R	312	CLA	C3B-C2B	3.68	1.45	1.40
22	r	312	CLA	C3B-C2B	3.68	1.45	1.40
22	Y	604	CLA	CHC-C1C	3.68	1.46	1.35
22	y	604	CLA	CHC-C1C	3.68	1.46	1.35
22	d	403	CLA	CHC-C1C	3.69	1.46	1.35
22	C	505	CLA	CHC-C1C	3.69	1.46	1.35
22	c	506	CLA	CHC-C1C	3.71	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	CHC-C1C	3.71	1.46	1.35
22	R	308	CLA	C3B-C2B	3.71	1.45	1.40
22	r	308	CLA	C3B-C2B	3.71	1.45	1.40
22	G	614	CLA	C3B-C2B	3.71	1.45	1.40
22	g	614	CLA	C3B-C2B	3.71	1.45	1.40
22	D	403	CLA	CHC-C1C	3.71	1.46	1.35
22	Y	604	CLA	C3C-C2C	3.72	1.44	1.36
22	y	604	CLA	C3C-C2C	3.72	1.44	1.36
22	c	508	CLA	CHC-C1C	3.73	1.46	1.35
22	B	611	CLA	C3C-C2C	3.73	1.44	1.36
22	7	311	CLA	C3B-C2B	3.73	1.45	1.40
22	3	311	CLA	C3B-C2B	3.73	1.45	1.40
22	y	611	CLA	C3C-C2C	3.73	1.44	1.36
22	Y	611	CLA	C3C-C2C	3.73	1.44	1.36
22	y	612	CLA	CHC-C1C	3.73	1.46	1.35
22	Y	612	CLA	CHC-C1C	3.73	1.46	1.35
22	S	312	CLA	CHC-C1C	3.73	1.46	1.35
22	s	312	CLA	CHC-C1C	3.73	1.46	1.35
22	s	303	CLA	C3B-C2B	3.73	1.45	1.40
22	S	303	CLA	C3B-C2B	3.73	1.45	1.40
22	s	313	CLA	C3C-C2C	3.73	1.44	1.36
22	S	313	CLA	C3C-C2C	3.73	1.44	1.36
22	B	607	CLA	CHC-C1C	3.73	1.46	1.35
22	B	605	CLA	CHC-C1C	3.74	1.46	1.35
22	b	613	CLA	CHC-C1C	3.74	1.46	1.35
23	A	404	PHO	CHC-C1C	3.74	1.46	1.38
22	A	405	CLA	C3B-C2B	3.75	1.45	1.40
22	a	405	CLA	CHC-C1C	3.75	1.46	1.35
22	n	610	CLA	C3B-C2B	3.76	1.45	1.40
22	N	610	CLA	C3B-C2B	3.76	1.45	1.40
22	S	314	CLA	CHC-C1C	3.76	1.46	1.35
22	s	314	CLA	CHC-C1C	3.76	1.46	1.35
22	C	501	CLA	C3B-C2B	3.76	1.45	1.40
22	b	609	CLA	CHC-C1C	3.77	1.46	1.35
22	c	505	CLA	CHC-C1C	3.77	1.46	1.35
22	G	604	CLA	CHC-C1C	3.77	1.46	1.35
22	g	604	CLA	CHC-C1C	3.77	1.46	1.35
22	A	402	CLA	C3C-C2C	3.77	1.44	1.36
22	a	405	CLA	C3C-C2C	3.77	1.44	1.36
22	2	610	CLA	C3B-C2B	3.77	1.45	1.40
22	6	610	CLA	C3B-C2B	3.77	1.45	1.40
22	s	309	CLA	CHC-C1C	3.78	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	309	CLA	CHC-C1C	3.78	1.46	1.35
22	8	310	CLA	C3B-C2B	3.79	1.45	1.40
22	4	310	CLA	C3B-C2B	3.79	1.45	1.40
22	C	511	CLA	CHC-C1C	3.79	1.46	1.35
23	a	404	PHO	CHC-C1C	3.79	1.46	1.38
22	b	607	CLA	CHC-C1C	3.79	1.46	1.35
22	y	613	CLA	CHC-C1C	3.79	1.46	1.35
22	Y	613	CLA	CHC-C1C	3.79	1.46	1.35
22	N	602	CLA	CHC-C1C	3.79	1.46	1.35
22	n	602	CLA	CHC-C1C	3.79	1.46	1.35
22	B	612	CLA	C3B-C2B	3.80	1.45	1.40
22	n	612	CLA	CHC-C1C	3.80	1.46	1.35
22	N	612	CLA	CHC-C1C	3.80	1.46	1.35
22	b	611	CLA	CHC-C1C	3.80	1.46	1.35
23	d	402	PHO	CHC-C1C	3.80	1.46	1.38
22	n	613	CLA	CHC-C1C	3.81	1.46	1.35
22	N	613	CLA	CHC-C1C	3.81	1.46	1.35
24	E	101	HEM	C3B-CAB	3.81	1.55	1.47
22	y	610	CLA	C3B-C2B	3.81	1.45	1.40
22	Y	610	CLA	C3B-C2B	3.81	1.45	1.40
22	y	611	CLA	CHC-C1C	3.81	1.46	1.35
22	Y	611	CLA	CHC-C1C	3.81	1.46	1.35
22	b	614	CLA	CHC-C1C	3.82	1.46	1.35
22	Y	614	CLA	CHC-C1C	3.82	1.46	1.35
22	y	614	CLA	CHC-C1C	3.82	1.46	1.35
22	B	616	CLA	C3C-C2C	3.82	1.44	1.36
22	D	401	CLA	CHC-C1C	3.82	1.46	1.35
22	8	302	CLA	CHC-C1C	3.82	1.46	1.35
22	4	302	CLA	CHC-C1C	3.82	1.46	1.35
22	A	405	CLA	CHC-C1C	3.82	1.46	1.35
22	c	502	CLA	CHC-C1C	3.82	1.46	1.35
22	c	504	CLA	CHC-C1C	3.83	1.46	1.35
24	E	101	HEM	C3C-CAC	3.83	1.55	1.47
22	B	603	CLA	C3C-C2C	3.83	1.44	1.36
22	g	613	CLA	CHC-C1C	3.83	1.46	1.35
22	G	613	CLA	CHC-C1C	3.83	1.46	1.35
22	G	602	CLA	CHC-C1C	3.83	1.46	1.35
22	g	602	CLA	CHC-C1C	3.83	1.46	1.35
22	a	402	CLA	C3B-C2B	3.84	1.45	1.40
22	b	610	CLA	CHC-C1C	3.84	1.46	1.35
22	n	604	CLA	CHC-C1C	3.85	1.46	1.35
22	N	604	CLA	CHC-C1C	3.85	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	512	CLA	CHC-C1C	3.85	1.46	1.35
22	B	610	CLA	CHC-C1C	3.85	1.46	1.35
22	Y	602	CLA	CHC-C1C	3.85	1.46	1.35
22	y	602	CLA	CHC-C1C	3.85	1.46	1.35
22	b	603	CLA	CHC-C1C	3.85	1.46	1.35
22	R	303	CLA	CHC-C1C	3.86	1.46	1.35
22	r	303	CLA	CHC-C1C	3.86	1.46	1.35
22	A	402	CLA	C3B-C2B	3.86	1.45	1.40
22	n	611	CLA	CHC-C1C	3.87	1.46	1.35
22	N	611	CLA	CHC-C1C	3.87	1.46	1.35
22	c	501	CLA	C3B-C2B	3.87	1.45	1.40
25	s	307	CHL	CBD-CGD	3.87	1.58	1.52
25	S	307	CHL	CBD-CGD	3.87	1.58	1.52
22	N	614	CLA	C3B-C2B	3.87	1.45	1.40
22	n	614	CLA	C3B-C2B	3.87	1.45	1.40
22	n	603	CLA	CHC-C1C	3.87	1.46	1.35
22	N	603	CLA	CHC-C1C	3.87	1.46	1.35
22	Y	603	CLA	CHC-C1C	3.87	1.46	1.35
22	y	603	CLA	CHC-C1C	3.87	1.46	1.35
22	g	611	CLA	CHC-C1C	3.87	1.46	1.35
22	G	611	CLA	CHC-C1C	3.87	1.46	1.35
22	y	610	CLA	CHC-C1C	3.87	1.46	1.35
22	Y	610	CLA	CHC-C1C	3.87	1.46	1.35
22	d	401	CLA	CHC-C1C	3.87	1.46	1.35
22	c	503	CLA	CHC-C1C	3.87	1.46	1.35
22	C	506	CLA	C3C-C2C	3.88	1.45	1.36
22	B	606	CLA	CHC-C1C	3.88	1.46	1.35
22	C	505	CLA	C3C-C2C	3.88	1.45	1.36
22	G	603	CLA	CHC-C1C	3.88	1.46	1.35
22	g	603	CLA	CHC-C1C	3.88	1.46	1.35
22	A	402	CLA	CHC-C1C	3.88	1.46	1.35
22	b	602	CLA	CHC-C1C	3.89	1.46	1.35
22	B	609	CLA	CHC-C1C	3.89	1.46	1.35
22	C	509	CLA	C3B-C2B	3.89	1.45	1.40
22	c	510	CLA	CHC-C1C	3.89	1.46	1.35
22	c	511	CLA	CHC-C1C	3.89	1.46	1.35
22	D	404	CLA	CHC-C1C	3.90	1.46	1.35
22	7	314	CLA	C3B-C2B	3.90	1.45	1.40
22	3	314	CLA	C3B-C2B	3.90	1.45	1.40
25	4	307	CHL	CBD-CGD	3.90	1.58	1.52
25	8	307	CHL	CBD-CGD	3.90	1.58	1.52
22	B	603	CLA	CHC-C1C	3.90	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	G	610	CLA	C3B-C2B	3.90	1.45	1.40
22	g	610	CLA	C3B-C2B	3.90	1.45	1.40
22	b	606	CLA	C3B-C2B	3.90	1.45	1.40
22	g	612	CLA	CHC-C1C	3.90	1.46	1.35
22	G	612	CLA	CHC-C1C	3.90	1.46	1.35
22	C	504	CLA	C3C-C2C	3.91	1.45	1.36
22	c	506	CLA	C3C-C2C	3.91	1.45	1.36
22	c	505	CLA	C3C-C2C	3.91	1.45	1.36
22	S	305	CLA	CHC-C1C	3.91	1.46	1.35
22	s	305	CLA	CHC-C1C	3.91	1.46	1.35
22	C	503	CLA	C3C-C2C	3.91	1.45	1.36
22	Y	614	CLA	C3C-C2C	3.91	1.45	1.36
22	y	614	CLA	C3C-C2C	3.91	1.45	1.36
22	6	609	CLA	C3C-C2C	3.92	1.45	1.36
22	2	609	CLA	C3C-C2C	3.92	1.45	1.36
22	B	608	CLA	C3C-C2C	3.92	1.45	1.36
22	1	610	CLA	C3B-C2B	3.92	1.45	1.40
22	5	610	CLA	C3B-C2B	3.92	1.45	1.40
22	S	310	CLA	CHC-C1C	3.93	1.46	1.35
22	s	310	CLA	CHC-C1C	3.93	1.46	1.35
22	B	609	CLA	C3C-C2C	3.93	1.45	1.36
24	e	101	HEM	C3C-CAC	3.93	1.55	1.47
22	N	602	CLA	C3C-C2C	3.93	1.45	1.36
22	n	602	CLA	C3C-C2C	3.93	1.45	1.36
22	C	510	CLA	C3C-C2C	3.94	1.45	1.36
22	b	609	CLA	C3C-C2C	3.94	1.45	1.36
22	S	301	CLA	CHC-C1C	3.94	1.46	1.35
22	a	402	CLA	CHC-C1C	3.94	1.46	1.35
22	B	612	CLA	CHC-C1C	3.94	1.46	1.35
22	s	313	CLA	CHC-C1C	3.95	1.46	1.35
22	S	313	CLA	CHC-C1C	3.95	1.46	1.35
22	S	314	CLA	C3C-C2C	3.95	1.45	1.36
22	s	314	CLA	C3C-C2C	3.95	1.45	1.36
22	G	602	CLA	C3C-C2C	3.95	1.45	1.36
22	g	602	CLA	C3C-C2C	3.95	1.45	1.36
22	c	501	CLA	C3C-C2C	3.95	1.45	1.36
22	3	310	CLA	C3C-C2C	3.95	1.45	1.36
22	7	310	CLA	C3C-C2C	3.95	1.45	1.36
22	5	614	CLA	CHC-C1C	3.95	1.46	1.35
22	1	614	CLA	CHC-C1C	3.95	1.46	1.35
22	B	602	CLA	CHC-C1C	3.95	1.46	1.35
22	b	608	CLA	CHC-C1C	3.96	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	g	611	CLA	C3C-C2C	3.96	1.45	1.36
22	G	611	CLA	C3C-C2C	3.96	1.45	1.36
22	5	604	CLA	CHC-C1C	3.96	1.46	1.35
22	1	604	CLA	CHC-C1C	3.96	1.46	1.35
22	n	611	CLA	C3C-C2C	3.96	1.45	1.36
22	N	611	CLA	C3C-C2C	3.96	1.45	1.36
22	2	613	CLA	C3B-C2B	3.96	1.45	1.40
22	6	613	CLA	C3B-C2B	3.96	1.45	1.40
22	6	609	CLA	C3B-C2B	3.96	1.45	1.40
22	2	609	CLA	C3B-C2B	3.96	1.45	1.40
22	B	611	CLA	CHC-C1C	3.96	1.46	1.35
22	b	602	CLA	C3C-C2C	3.96	1.45	1.36
22	B	602	CLA	C3C-C2C	3.96	1.45	1.36
22	4	309	CLA	C3C-C2C	3.97	1.45	1.36
22	8	309	CLA	C3C-C2C	3.97	1.45	1.36
22	d	404	CLA	CHC-C1C	3.97	1.46	1.35
22	c	502	CLA	C3C-C2C	3.97	1.45	1.36
22	R	309	CLA	CHC-C1C	3.97	1.46	1.35
22	r	309	CLA	CHC-C1C	3.97	1.46	1.35
22	r	307	CLA	CHC-C1C	3.97	1.46	1.35
22	R	307	CLA	CHC-C1C	3.97	1.46	1.35
22	A	405	CLA	C3C-C2C	3.98	1.45	1.36
22	y	610	CLA	C3C-C2C	3.98	1.45	1.36
22	Y	610	CLA	C3C-C2C	3.98	1.45	1.36
22	n	610	CLA	C3C-C2C	3.98	1.45	1.36
22	s	303	CLA	C3C-C2C	3.98	1.45	1.36
22	S	303	CLA	C3C-C2C	3.98	1.45	1.36
22	N	610	CLA	C3C-C2C	3.98	1.45	1.36
22	n	603	CLA	C3C-C2C	3.98	1.45	1.36
22	N	603	CLA	C3C-C2C	3.98	1.45	1.36
22	B	612	CLA	C3C-C2C	3.98	1.45	1.36
22	S	311	CLA	CHC-C1C	3.98	1.46	1.35
22	s	311	CLA	CHC-C1C	3.98	1.46	1.35
22	S	304	CLA	C3C-C2C	3.99	1.45	1.36
22	s	304	CLA	C3C-C2C	3.99	1.45	1.36
22	B	616	CLA	CHC-C1C	3.99	1.47	1.35
22	R	308	CLA	CHC-C1C	4.00	1.47	1.35
22	r	308	CLA	CHC-C1C	4.00	1.47	1.35
22	b	615	CLA	CHB-C4A	4.00	1.38	1.33
22	n	613	CLA	C3C-C2C	4.00	1.45	1.36
22	N	613	CLA	C3C-C2C	4.00	1.45	1.36
22	c	510	CLA	C3B-C2B	4.00	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	311	CLA	C3C-C2C	4.00	1.45	1.36
22	r	311	CLA	C3C-C2C	4.00	1.45	1.36
22	C	503	CLA	CHC-C1C	4.01	1.47	1.35
22	B	614	CLA	C3C-C2C	4.01	1.45	1.36
22	2	612	CLA	CHC-C1C	4.01	1.47	1.35
22	6	612	CLA	CHC-C1C	4.01	1.47	1.35
22	b	616	CLA	C3C-C2C	4.01	1.45	1.36
22	r	307	CLA	C3C-C2C	4.01	1.45	1.36
22	R	307	CLA	C3C-C2C	4.01	1.45	1.36
22	y	613	CLA	CHB-C4A	4.01	1.38	1.33
22	Y	613	CLA	CHB-C4A	4.01	1.38	1.33
22	R	308	CLA	C3C-C2C	4.02	1.45	1.36
22	r	308	CLA	C3C-C2C	4.02	1.45	1.36
22	y	613	CLA	C3C-C2C	4.02	1.45	1.36
22	Y	613	CLA	C3C-C2C	4.02	1.45	1.36
22	b	612	CLA	C3B-C2B	4.02	1.45	1.40
23	a	404	PHO	C3C-C2C	4.02	1.45	1.36
22	b	607	CLA	C3C-C2C	4.02	1.45	1.36
22	n	610	CLA	CHC-C1C	4.02	1.47	1.35
22	N	610	CLA	CHC-C1C	4.02	1.47	1.35
22	b	613	CLA	C3C-C2C	4.03	1.45	1.36
22	Y	603	CLA	C3C-C2C	4.03	1.45	1.36
22	y	603	CLA	C3C-C2C	4.03	1.45	1.36
22	G	610	CLA	C3C-C2C	4.03	1.45	1.36
22	g	610	CLA	C3C-C2C	4.03	1.45	1.36
22	R	309	CLA	C3C-C2C	4.03	1.45	1.36
22	Y	602	CLA	C3C-C2C	4.03	1.45	1.36
22	r	309	CLA	C3C-C2C	4.03	1.45	1.36
22	y	602	CLA	C3C-C2C	4.03	1.45	1.36
22	A	403	CLA	C3B-C2B	4.04	1.45	1.40
22	s	303	CLA	CHC-C1C	4.04	1.47	1.35
22	S	303	CLA	CHC-C1C	4.04	1.47	1.35
22	S	301	CLA	C3C-C2C	4.04	1.45	1.36
22	B	613	CLA	CHC-C1C	4.05	1.47	1.35
22	G	603	CLA	C3C-C2C	4.05	1.45	1.36
22	g	603	CLA	C3C-C2C	4.05	1.45	1.36
22	B	601	CLA	C3C-C2C	4.05	1.45	1.36
22	n	604	CLA	C3C-C2C	4.05	1.45	1.36
22	N	604	CLA	C3C-C2C	4.05	1.45	1.36
22	C	509	CLA	CHC-C1C	4.05	1.47	1.35
22	5	614	CLA	C3C-C2C	4.05	1.45	1.36
22	1	614	CLA	C3C-C2C	4.05	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	611	CLA	CHC-C1C	4.05	1.47	1.35
22	1	611	CLA	CHC-C1C	4.05	1.47	1.35
23	d	402	PHO	C3C-C2C	4.06	1.45	1.36
22	N	614	CLA	CHC-C1C	4.06	1.47	1.35
22	n	614	CLA	CHC-C1C	4.06	1.47	1.35
22	S	310	CLA	C3C-C2C	4.06	1.45	1.36
22	s	310	CLA	C3C-C2C	4.06	1.45	1.36
22	a	403	CLA	CHC-C1C	4.06	1.47	1.35
22	1	613	CLA	CHC-C1C	4.06	1.47	1.35
22	5	613	CLA	CHC-C1C	4.06	1.47	1.35
22	4	304	CLA	CHC-C1C	4.06	1.47	1.35
22	8	304	CLA	CHC-C1C	4.06	1.47	1.35
22	b	601	CLA	CHC-C1C	4.07	1.47	1.35
22	n	612	CLA	C3C-C2C	4.07	1.45	1.36
22	N	612	CLA	C3C-C2C	4.07	1.45	1.36
22	R	301	CLA	C3C-C2C	4.07	1.45	1.36
22	r	301	CLA	C3C-C2C	4.07	1.45	1.36
22	2	604	CLA	CHC-C1C	4.07	1.47	1.35
22	6	604	CLA	CHC-C1C	4.07	1.47	1.35
22	d	401	CLA	C3C-C2C	4.07	1.45	1.36
22	7	313	CLA	CHC-C1C	4.07	1.47	1.35
22	3	313	CLA	CHC-C1C	4.07	1.47	1.35
22	R	311	CLA	CHC-C1C	4.07	1.47	1.35
22	r	311	CLA	CHC-C1C	4.07	1.47	1.35
22	s	301	CLA	CHC-C1C	4.08	1.47	1.35
24	e	101	HEM	C3B-CAB	4.08	1.56	1.47
22	C	508	CLA	C3C-C2C	4.08	1.45	1.36
22	C	507	CLA	C3C-C2C	4.08	1.45	1.36
22	1	602	CLA	CHC-C1C	4.08	1.47	1.35
22	5	602	CLA	CHC-C1C	4.08	1.47	1.35
23	D	402	PHO	C3C-C2C	4.08	1.45	1.36
22	c	508	CLA	C3C-C2C	4.08	1.45	1.36
22	3	312	CLA	CHC-C1C	4.09	1.47	1.35
22	7	312	CLA	CHC-C1C	4.09	1.47	1.35
22	b	605	CLA	C3C-C2C	4.09	1.45	1.36
22	7	305	CLA	CHC-C1C	4.09	1.47	1.35
22	3	305	CLA	CHC-C1C	4.09	1.47	1.35
22	g	613	CLA	C3C-C2C	4.09	1.45	1.36
22	G	613	CLA	C3C-C2C	4.09	1.45	1.36
22	b	601	CLA	C3C-C2C	4.09	1.45	1.36
22	7	303	CLA	CHC-C1C	4.09	1.47	1.35
22	3	303	CLA	CHC-C1C	4.09	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	C3B-C2B	4.09	1.45	1.40
22	2	602	CLA	CHC-C1C	4.10	1.47	1.35
22	6	602	CLA	CHC-C1C	4.10	1.47	1.35
22	S	305	CLA	C3C-C2C	4.10	1.45	1.36
22	s	305	CLA	C3C-C2C	4.10	1.45	1.36
22	G	614	CLA	CHC-C1C	4.10	1.47	1.35
22	g	614	CLA	CHC-C1C	4.10	1.47	1.35
22	8	302	CLA	C3C-C2C	4.10	1.45	1.36
22	4	302	CLA	C3C-C2C	4.10	1.45	1.36
22	3	304	CLA	CHC-C1C	4.10	1.47	1.35
22	7	304	CLA	CHC-C1C	4.10	1.47	1.35
22	c	509	CLA	CHC-C1C	4.10	1.47	1.35
22	c	510	CLA	C3C-C2C	4.10	1.45	1.36
22	b	611	CLA	C3B-C2B	4.11	1.45	1.40
22	c	512	CLA	C3C-C2C	4.11	1.45	1.36
22	1	610	CLA	C3C-C2C	4.11	1.45	1.36
22	5	610	CLA	C3C-C2C	4.11	1.45	1.36
22	R	301	CLA	CHC-C1C	4.11	1.47	1.35
22	r	301	CLA	CHC-C1C	4.11	1.47	1.35
22	1	603	CLA	CHC-C1C	4.11	1.47	1.35
22	5	603	CLA	CHC-C1C	4.11	1.47	1.35
22	G	604	CLA	C3C-C2C	4.11	1.45	1.36
22	g	604	CLA	C3C-C2C	4.11	1.45	1.36
22	S	304	CLA	CHC-C1C	4.11	1.47	1.35
22	s	304	CLA	CHC-C1C	4.11	1.47	1.35
22	4	303	CLA	CHC-C1C	4.12	1.47	1.35
22	8	303	CLA	CHC-C1C	4.12	1.47	1.35
22	b	608	CLA	C3C-C2C	4.12	1.45	1.36
22	2	610	CLA	CHC-C1C	4.12	1.47	1.35
22	6	610	CLA	CHC-C1C	4.12	1.47	1.35
22	r	310	CLA	CHC-C1C	4.12	1.47	1.35
22	R	310	CLA	CHC-C1C	4.12	1.47	1.35
22	A	403	CLA	CHC-C1C	4.12	1.47	1.35
22	g	612	CLA	C3C-C2C	4.13	1.45	1.36
22	G	612	CLA	C3C-C2C	4.13	1.45	1.36
22	7	311	CLA	CHC-C1C	4.13	1.47	1.35
22	3	311	CLA	CHC-C1C	4.13	1.47	1.35
22	2	612	CLA	C3C-C2C	4.13	1.45	1.36
22	6	612	CLA	C3C-C2C	4.13	1.45	1.36
22	b	615	CLA	CHC-C1C	4.13	1.47	1.35
22	c	511	CLA	C3C-C2C	4.14	1.45	1.36
22	1	612	CLA	CHC-C1C	4.14	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	5	612	CLA	CHC-C1C	4.14	1.47	1.35
22	C	502	CLA	CHC-C1C	4.14	1.47	1.35
22	b	603	CLA	C3C-C2C	4.14	1.45	1.36
22	S	311	CLA	C3C-C2C	4.14	1.45	1.36
22	s	311	CLA	C3C-C2C	4.14	1.45	1.36
22	D	404	CLA	C3C-C2C	4.15	1.45	1.36
22	R	303	CLA	C3C-C2C	4.15	1.45	1.36
22	r	303	CLA	C3C-C2C	4.15	1.45	1.36
22	2	602	CLA	C3C-C2C	4.15	1.45	1.36
22	6	602	CLA	C3C-C2C	4.15	1.45	1.36
22	8	310	CLA	CHC-C1C	4.15	1.47	1.35
22	4	310	CLA	CHC-C1C	4.15	1.47	1.35
22	1	602	CLA	C3C-C2C	4.15	1.45	1.36
22	5	602	CLA	C3C-C2C	4.15	1.45	1.36
22	B	604	CLA	C3C-C2C	4.15	1.45	1.36
22	c	504	CLA	C3C-C2C	4.15	1.45	1.36
22	R	312	CLA	CHC-C1C	4.15	1.47	1.35
22	r	312	CLA	CHC-C1C	4.15	1.47	1.35
22	G	610	CLA	CHC-C1C	4.15	1.47	1.35
22	g	610	CLA	CHC-C1C	4.15	1.47	1.35
22	b	605	CLA	CHC-C1C	4.15	1.47	1.35
22	6	603	CLA	CHC-C1C	4.16	1.47	1.35
22	2	603	CLA	CHC-C1C	4.16	1.47	1.35
22	2	613	CLA	CHC-C1C	4.16	1.47	1.35
22	6	613	CLA	CHC-C1C	4.16	1.47	1.35
22	1	610	CLA	CHC-C1C	4.16	1.47	1.35
22	5	610	CLA	CHC-C1C	4.16	1.47	1.35
22	r	302	CLA	CHC-C1C	4.16	1.47	1.35
22	C	512	CLA	CHC-C1C	4.16	1.47	1.35
22	R	302	CLA	CHC-C1C	4.16	1.47	1.35
22	y	612	CLA	C3C-C2C	4.17	1.45	1.36
22	Y	612	CLA	C3C-C2C	4.17	1.45	1.36
22	B	601	CLA	CHC-C1C	4.17	1.47	1.35
22	1	603	CLA	C3C-C2C	4.17	1.45	1.36
22	G	614	CLA	C3C-C2C	4.17	1.45	1.36
22	g	614	CLA	C3C-C2C	4.17	1.45	1.36
22	5	603	CLA	C3C-C2C	4.17	1.45	1.36
22	s	301	CLA	C3C-C2C	4.17	1.45	1.36
22	4	309	CLA	CHC-C1C	4.17	1.47	1.35
22	8	309	CLA	CHC-C1C	4.17	1.47	1.35
22	B	613	CLA	C3C-C2C	4.18	1.45	1.36
22	b	603	CLA	CHB-C4A	4.18	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	C3C-C2C	4.18	1.45	1.36
22	B	610	CLA	C3C-C2C	4.19	1.45	1.36
22	1	613	CLA	C3C-C2C	4.19	1.45	1.36
22	5	613	CLA	C3C-C2C	4.19	1.45	1.36
22	5	611	CLA	C3C-C2C	4.20	1.45	1.36
22	1	611	CLA	C3C-C2C	4.20	1.45	1.36
22	a	403	CLA	C3C-C2C	4.20	1.45	1.36
22	7	303	CLA	C3C-C2C	4.20	1.45	1.36
22	3	303	CLA	C3C-C2C	4.20	1.45	1.36
22	6	611	CLA	CHC-C1C	4.21	1.47	1.35
22	2	611	CLA	CHC-C1C	4.21	1.47	1.35
22	B	611	CLA	C3B-C2B	4.21	1.45	1.40
22	C	511	CLA	C3C-C2C	4.22	1.45	1.36
22	6	603	CLA	C3C-C2C	4.22	1.45	1.36
22	2	603	CLA	C3C-C2C	4.22	1.45	1.36
22	B	614	CLA	CHC-C1C	4.22	1.47	1.35
22	S	311	CLA	CHB-C4A	4.22	1.38	1.33
22	s	311	CLA	CHB-C4A	4.22	1.38	1.33
22	n	604	CLA	CHB-C4A	4.23	1.38	1.33
22	N	604	CLA	CHB-C4A	4.23	1.38	1.33
22	y	612	CLA	CHB-C4A	4.23	1.38	1.33
22	Y	612	CLA	CHB-C4A	4.23	1.38	1.33
22	A	403	CLA	C3C-C2C	4.23	1.45	1.36
22	7	311	CLA	C3C-C2C	4.24	1.45	1.36
22	3	311	CLA	C3C-C2C	4.24	1.45	1.36
22	c	505	CLA	CHB-C4A	4.24	1.38	1.33
22	C	502	CLA	C3C-C2C	4.24	1.45	1.36
22	D	401	CLA	CHB-C4A	4.24	1.38	1.33
22	3	312	CLA	C3C-C2C	4.24	1.45	1.36
22	7	312	CLA	C3C-C2C	4.24	1.45	1.36
22	r	310	CLA	C3C-C2C	4.24	1.45	1.36
22	R	310	CLA	C3C-C2C	4.24	1.45	1.36
22	3	310	CLA	C3B-C2B	4.24	1.46	1.40
22	7	310	CLA	C3B-C2B	4.24	1.46	1.40
22	c	509	CLA	C3C-C2C	4.24	1.45	1.36
22	7	314	CLA	CHC-C1C	4.25	1.47	1.35
22	3	314	CLA	CHC-C1C	4.25	1.47	1.35
22	D	401	CLA	C3C-C2C	4.25	1.45	1.36
22	5	604	CLA	C3C-C2C	4.25	1.45	1.36
22	1	604	CLA	C3C-C2C	4.25	1.45	1.36
22	7	313	CLA	C3C-C2C	4.25	1.45	1.36
22	3	313	CLA	C3C-C2C	4.25	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	3	304	CLA	C3C-C2C	4.25	1.45	1.36
22	7	304	CLA	C3C-C2C	4.25	1.45	1.36
22	R	312	CLA	C3C-C2C	4.25	1.45	1.36
22	r	312	CLA	C3C-C2C	4.25	1.45	1.36
22	d	404	CLA	C3C-C2C	4.25	1.45	1.36
22	2	610	CLA	C3C-C2C	4.26	1.45	1.36
22	6	610	CLA	C3C-C2C	4.26	1.45	1.36
22	b	615	CLA	C3C-C2C	4.26	1.45	1.36
22	2	604	CLA	C3C-C2C	4.26	1.45	1.36
22	6	604	CLA	C3C-C2C	4.26	1.45	1.36
22	4	304	CLA	C3C-C2C	4.26	1.45	1.36
22	8	304	CLA	C3C-C2C	4.26	1.45	1.36
22	C	509	CLA	C3C-C2C	4.26	1.45	1.36
22	d	403	CLA	C3B-C2B	4.27	1.46	1.40
22	7	305	CLA	C3C-C2C	4.27	1.45	1.36
22	3	305	CLA	C3C-C2C	4.27	1.45	1.36
22	S	312	CLA	C3C-C2C	4.28	1.45	1.36
22	s	312	CLA	C3C-C2C	4.28	1.45	1.36
22	a	402	CLA	C3C-C2C	4.28	1.45	1.36
22	C	505	CLA	CHB-C4A	4.28	1.39	1.33
22	b	606	CLA	CHB-C4A	4.29	1.39	1.33
22	b	604	CLA	C3C-C2C	4.29	1.45	1.36
22	A	403	CLA	CHB-C4A	4.29	1.39	1.33
22	b	606	CLA	CHC-C1C	4.29	1.47	1.35
22	4	303	CLA	C3C-C2C	4.29	1.45	1.36
22	8	303	CLA	C3C-C2C	4.29	1.45	1.36
22	3	310	CLA	CHC-C1C	4.30	1.47	1.35
22	7	310	CLA	CHC-C1C	4.30	1.47	1.35
22	2	613	CLA	C3C-C2C	4.31	1.46	1.36
22	6	613	CLA	C3C-C2C	4.31	1.46	1.36
22	N	614	CLA	C3C-C2C	4.31	1.46	1.36
22	n	614	CLA	C3C-C2C	4.31	1.46	1.36
22	C	501	CLA	C3C-C2C	4.31	1.46	1.36
22	b	608	CLA	CHB-C4A	4.33	1.39	1.33
22	7	314	CLA	C3C-C2C	4.33	1.46	1.36
22	3	314	CLA	C3C-C2C	4.33	1.46	1.36
22	c	507	CLA	C3C-C2C	4.33	1.46	1.36
22	6	609	CLA	CHC-C1C	4.34	1.48	1.35
22	2	609	CLA	CHC-C1C	4.34	1.48	1.35
22	6	611	CLA	C3C-C2C	4.35	1.46	1.36
22	2	611	CLA	C3C-C2C	4.35	1.46	1.36
22	C	512	CLA	C3C-C2C	4.35	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	r	302	CLA	C3C-C2C	4.35	1.46	1.36
22	R	302	CLA	C3C-C2C	4.35	1.46	1.36
22	s	309	CLA	C3C-C2C	4.35	1.46	1.36
22	S	309	CLA	C3C-C2C	4.35	1.46	1.36
22	b	612	CLA	CHC-C1C	4.36	1.48	1.35
22	1	612	CLA	C3C-C2C	4.38	1.46	1.36
22	5	612	CLA	C3C-C2C	4.38	1.46	1.36
22	b	612	CLA	CHB-C4A	4.39	1.39	1.33
22	b	605	CLA	CHB-C4A	4.39	1.39	1.33
22	D	403	CLA	C3B-C2B	4.40	1.46	1.40
22	b	610	CLA	C3C-C2C	4.41	1.46	1.36
22	b	612	CLA	C3C-C2C	4.41	1.46	1.36
22	b	606	CLA	C3C-C2C	4.42	1.46	1.36
22	S	314	CLA	CHB-C4A	4.42	1.39	1.33
22	s	314	CLA	CHB-C4A	4.42	1.39	1.33
22	b	609	CLA	CHB-C4A	4.45	1.39	1.33
23	A	404	PHO	C3C-C2C	4.47	1.46	1.36
22	C	511	CLA	CHB-C4A	4.48	1.39	1.33
22	8	310	CLA	C3C-C2C	4.48	1.46	1.36
22	4	310	CLA	C3C-C2C	4.48	1.46	1.36
22	B	603	CLA	CHB-C4A	4.49	1.39	1.33
22	C	509	CLA	CHB-C4A	4.50	1.39	1.33
22	S	305	CLA	CHB-C4A	4.50	1.39	1.33
22	s	305	CLA	CHB-C4A	4.50	1.39	1.33
22	Y	603	CLA	CHB-C4A	4.53	1.39	1.33
22	c	507	CLA	CHB-C4A	4.53	1.39	1.33
22	y	603	CLA	CHB-C4A	4.53	1.39	1.33
22	G	604	CLA	CHB-C4A	4.54	1.39	1.33
22	g	604	CLA	CHB-C4A	4.54	1.39	1.33
22	n	613	CLA	CHB-C4A	4.54	1.39	1.33
22	N	613	CLA	CHB-C4A	4.54	1.39	1.33
22	s	313	CLA	CHB-C4A	4.56	1.39	1.33
22	S	313	CLA	CHB-C4A	4.56	1.39	1.33
22	A	405	CLA	CHB-C4A	4.56	1.39	1.33
22	n	603	CLA	CHB-C4A	4.56	1.39	1.33
22	N	603	CLA	CHB-C4A	4.56	1.39	1.33
22	Y	614	CLA	CHB-C4A	4.56	1.39	1.33
22	C	502	CLA	CHB-C4A	4.56	1.39	1.33
22	y	614	CLA	CHB-C4A	4.56	1.39	1.33
22	d	401	CLA	CHB-C4A	4.56	1.39	1.33
22	g	612	CLA	CHB-C4A	4.56	1.39	1.33
22	G	612	CLA	CHB-C4A	4.56	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	604	CLA	CHB-C4A	4.57	1.39	1.33
22	y	604	CLA	CHB-C4A	4.57	1.39	1.33
22	c	511	CLA	CHB-C4A	4.58	1.39	1.33
22	C	512	CLA	CHB-C4A	4.58	1.39	1.33
22	a	403	CLA	CHB-C4A	4.60	1.39	1.33
22	y	611	CLA	CHB-C4A	4.61	1.39	1.33
22	Y	611	CLA	CHB-C4A	4.61	1.39	1.33
22	C	503	CLA	CHB-C4A	4.63	1.39	1.33
22	a	402	CLA	CHB-C4A	4.63	1.39	1.33
22	C	507	CLA	CHB-C4A	4.64	1.39	1.33
22	Y	602	CLA	CHB-C4A	4.64	1.39	1.33
22	y	602	CLA	CHB-C4A	4.64	1.39	1.33
22	g	613	CLA	CHB-C4A	4.67	1.39	1.33
22	G	613	CLA	CHB-C4A	4.67	1.39	1.33
22	5	604	CLA	CHB-C4A	4.67	1.39	1.33
22	1	604	CLA	CHB-C4A	4.67	1.39	1.33
22	R	303	CLA	CHB-C4A	4.68	1.39	1.33
22	r	303	CLA	CHB-C4A	4.68	1.39	1.33
22	R	309	CLA	CHB-C4A	4.68	1.39	1.33
22	r	309	CLA	CHB-C4A	4.68	1.39	1.33
22	R	312	CLA	CHB-C4A	4.69	1.39	1.33
22	r	312	CLA	CHB-C4A	4.69	1.39	1.33
22	c	509	CLA	CHB-C4A	4.70	1.39	1.33
22	S	310	CLA	CHB-C4A	4.72	1.39	1.33
22	s	310	CLA	CHB-C4A	4.72	1.39	1.33
22	B	605	CLA	CHB-C4A	4.73	1.39	1.33
22	c	508	CLA	CHB-C4A	4.74	1.39	1.33
22	B	601	CLA	CHB-C4A	4.76	1.39	1.33
22	b	610	CLA	CHB-C4A	4.77	1.39	1.33
22	s	303	CLA	CHB-C4A	4.77	1.39	1.33
22	S	303	CLA	CHB-C4A	4.77	1.39	1.33
22	2	604	CLA	CHB-C4A	4.77	1.39	1.33
22	6	604	CLA	CHB-C4A	4.77	1.39	1.33
22	B	607	CLA	CHB-C4A	4.78	1.39	1.33
22	R	301	CLA	CHB-C4A	4.78	1.39	1.33
22	r	301	CLA	CHB-C4A	4.78	1.39	1.33
22	G	603	CLA	CHB-C4A	4.79	1.39	1.33
22	g	603	CLA	CHB-C4A	4.79	1.39	1.33
22	B	606	CLA	CHB-C4A	4.79	1.39	1.33
22	D	404	CLA	CHB-C4A	4.79	1.39	1.33
22	c	504	CLA	CHB-C4A	4.79	1.39	1.33
22	g	611	CLA	CHB-C4A	4.80	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	614	CLA	CHB-C4A	4.80	1.39	1.33
22	G	611	CLA	CHB-C4A	4.80	1.39	1.33
22	c	502	CLA	OBD-CAD	4.81	1.29	1.22
22	s	301	CLA	CHB-C4A	4.81	1.39	1.33
22	C	510	CLA	CHB-C4A	4.81	1.39	1.33
22	G	602	CLA	CHB-C4A	4.82	1.39	1.33
22	g	602	CLA	CHB-C4A	4.82	1.39	1.33
22	R	311	CLA	CHB-C4A	4.83	1.39	1.33
22	r	311	CLA	CHB-C4A	4.83	1.39	1.33
22	4	304	CLA	CHB-C4A	4.83	1.39	1.33
22	8	304	CLA	CHB-C4A	4.83	1.39	1.33
22	C	501	CLA	CHB-C4A	4.83	1.39	1.33
22	c	512	CLA	CHB-C4A	4.84	1.39	1.33
22	1	612	CLA	CHB-C4A	4.85	1.39	1.33
22	5	612	CLA	CHB-C4A	4.85	1.39	1.33
22	G	614	CLA	CHB-C4A	4.85	1.39	1.33
22	g	614	CLA	CHB-C4A	4.85	1.39	1.33
22	S	312	CLA	CHB-C4A	4.86	1.39	1.33
22	s	312	CLA	CHB-C4A	4.86	1.39	1.33
22	c	502	CLA	CHB-C4A	4.86	1.39	1.33
22	d	404	CLA	CHB-C4A	4.87	1.39	1.33
22	C	508	CLA	CHB-C4A	4.88	1.39	1.33
22	B	610	CLA	CHB-C4A	4.88	1.39	1.33
22	r	307	CLA	CHB-C4A	4.88	1.39	1.33
22	R	307	CLA	CHB-C4A	4.88	1.39	1.33
22	7	305	CLA	CHB-C4A	4.90	1.39	1.33
22	3	305	CLA	CHB-C4A	4.90	1.39	1.33
22	r	310	CLA	CHB-C4A	4.93	1.39	1.33
22	R	310	CLA	CHB-C4A	4.93	1.39	1.33
22	n	611	CLA	CHB-C4A	4.93	1.39	1.33
22	N	611	CLA	CHB-C4A	4.93	1.39	1.33
22	b	604	CLA	CHB-C4A	4.93	1.39	1.33
22	a	405	CLA	CHB-C4A	4.94	1.39	1.33
22	1	613	CLA	CHB-C4A	4.94	1.39	1.33
22	5	613	CLA	CHB-C4A	4.94	1.39	1.33
22	B	609	CLA	CHB-C4A	4.95	1.39	1.33
22	B	616	CLA	C3B-C2B	4.95	1.46	1.40
22	n	612	CLA	CHB-C4A	4.96	1.39	1.33
22	N	612	CLA	CHB-C4A	4.96	1.39	1.33
22	B	608	CLA	CHB-C4A	4.97	1.39	1.33
22	C	502	CLA	OBD-CAD	4.97	1.29	1.22
22	3	304	CLA	CHB-C4A	4.98	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	7	304	CLA	CHB-C4A	4.98	1.39	1.33
22	b	601	CLA	CHB-C4A	5.03	1.39	1.33
22	c	503	CLA	CHB-C4A	5.04	1.39	1.33
22	b	607	CLA	CHB-C4A	5.06	1.40	1.33
22	s	309	CLA	CHB-C4A	5.06	1.40	1.33
22	S	309	CLA	CHB-C4A	5.06	1.40	1.33
22	7	314	CLA	CHB-C4A	5.09	1.40	1.33
22	3	314	CLA	CHB-C4A	5.09	1.40	1.33
22	a	403	CLA	OBD-CAD	5.11	1.29	1.22
22	N	614	CLA	CHB-C4A	5.11	1.40	1.33
22	n	614	CLA	CHB-C4A	5.11	1.40	1.33
22	d	403	CLA	CHB-C4A	5.11	1.40	1.33
22	N	602	CLA	CHB-C4A	5.12	1.40	1.33
22	n	602	CLA	CHB-C4A	5.12	1.40	1.33
22	6	611	CLA	CHB-C4A	5.12	1.40	1.33
22	2	611	CLA	CHB-C4A	5.12	1.40	1.33
22	7	313	CLA	CHB-C4A	5.12	1.40	1.33
22	3	313	CLA	CHB-C4A	5.12	1.40	1.33
22	2	612	CLA	CHB-C4A	5.12	1.40	1.33
22	6	612	CLA	CHB-C4A	5.12	1.40	1.33
22	5	614	CLA	CHB-C4A	5.12	1.40	1.33
22	1	614	CLA	CHB-C4A	5.12	1.40	1.33
22	7	303	CLA	CHB-C4A	5.13	1.40	1.33
22	3	303	CLA	CHB-C4A	5.13	1.40	1.33
22	c	506	CLA	CHB-C4A	5.15	1.40	1.33
22	5	611	CLA	CHB-C4A	5.15	1.40	1.33
22	1	611	CLA	CHB-C4A	5.15	1.40	1.33
22	b	602	CLA	CHB-C4A	5.16	1.40	1.33
22	2	602	CLA	CHB-C4A	5.17	1.40	1.33
22	6	602	CLA	CHB-C4A	5.17	1.40	1.33
22	r	302	CLA	CHB-C4A	5.19	1.40	1.33
22	R	302	CLA	CHB-C4A	5.19	1.40	1.33
22	y	610	CLA	CHB-C4A	5.23	1.40	1.33
22	Y	610	CLA	CHB-C4A	5.23	1.40	1.33
22	n	610	CLA	CHB-C4A	5.23	1.40	1.33
22	N	610	CLA	CHB-C4A	5.23	1.40	1.33
22	D	403	CLA	CHB-C4A	5.23	1.40	1.33
22	6	603	CLA	CHB-C4A	5.24	1.40	1.33
22	2	603	CLA	CHB-C4A	5.24	1.40	1.33
22	C	501	CLA	OBD-CAD	5.24	1.29	1.22
22	B	611	CLA	CHB-C4A	5.24	1.40	1.33
22	B	612	CLA	CHB-C4A	5.25	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CHB-C4A	5.25	1.40	1.33
22	A	402	CLA	CHB-C4A	5.25	1.40	1.33
22	2	610	CLA	CHB-C4A	5.26	1.40	1.33
22	6	610	CLA	CHB-C4A	5.26	1.40	1.33
22	7	311	CLA	CHB-C4A	5.26	1.40	1.33
22	3	311	CLA	CHB-C4A	5.26	1.40	1.33
22	n	603	CLA	OBD-CAD	5.27	1.30	1.22
22	N	603	CLA	OBD-CAD	5.27	1.30	1.22
22	B	613	CLA	OBD-CAD	5.28	1.30	1.22
22	C	504	CLA	CHB-C4A	5.28	1.40	1.33
22	8	310	CLA	CHB-C4A	5.28	1.40	1.33
22	4	310	CLA	CHB-C4A	5.28	1.40	1.33
22	s	303	CLA	OBD-CAD	5.28	1.30	1.22
22	S	303	CLA	OBD-CAD	5.28	1.30	1.22
22	B	615	CLA	CHB-C4A	5.28	1.40	1.33
22	B	616	CLA	OBD-CAD	5.29	1.30	1.22
22	B	604	CLA	CHB-C4A	5.30	1.40	1.33
22	R	308	CLA	CHB-C4A	5.32	1.40	1.33
22	r	308	CLA	CHB-C4A	5.32	1.40	1.33
22	B	604	CLA	OBD-CAD	5.32	1.30	1.22
22	Y	603	CLA	OBD-CAD	5.32	1.30	1.22
22	y	603	CLA	OBD-CAD	5.32	1.30	1.22
22	c	510	CLA	CHB-C4A	5.35	1.40	1.33
22	1	603	CLA	CHB-C4A	5.35	1.40	1.33
22	5	603	CLA	CHB-C4A	5.35	1.40	1.33
22	3	312	CLA	CHB-C4A	5.36	1.40	1.33
22	7	312	CLA	CHB-C4A	5.36	1.40	1.33
22	B	614	CLA	CHB-C4A	5.36	1.40	1.33
22	1	602	CLA	CHB-C4A	5.37	1.40	1.33
22	5	602	CLA	CHB-C4A	5.37	1.40	1.33
22	1	602	CLA	OBD-CAD	5.38	1.30	1.22
22	5	602	CLA	OBD-CAD	5.38	1.30	1.22
22	C	506	CLA	CHB-C4A	5.38	1.40	1.33
22	S	310	CLA	OBD-CAD	5.38	1.30	1.22
22	s	310	CLA	OBD-CAD	5.38	1.30	1.22
22	c	511	CLA	OBD-CAD	5.40	1.30	1.22
23	D	402	PHO	CHB-C1B	5.41	1.49	1.38
22	y	613	CLA	OBD-CAD	5.41	1.30	1.22
22	Y	613	CLA	OBD-CAD	5.41	1.30	1.22
22	c	503	CLA	OBD-CAD	5.41	1.30	1.22
23	D	402	PHO	C3B-C2B	5.41	1.47	1.37
22	b	611	CLA	OBD-CAD	5.42	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	501	CLA	OBD-CAD	5.43	1.30	1.22
22	n	613	CLA	OBD-CAD	5.43	1.30	1.22
22	N	613	CLA	OBD-CAD	5.43	1.30	1.22
22	B	611	CLA	OBD-CAD	5.44	1.30	1.22
22	b	613	CLA	OBD-CAD	5.45	1.30	1.22
22	G	610	CLA	CHB-C4A	5.45	1.40	1.33
22	g	610	CLA	CHB-C4A	5.45	1.40	1.33
23	a	404	PHO	CHB-C1B	5.45	1.49	1.38
22	s	313	CLA	OBD-CAD	5.46	1.30	1.22
22	S	313	CLA	OBD-CAD	5.46	1.30	1.22
22	C	503	CLA	OBD-CAD	5.46	1.30	1.22
22	g	613	CLA	OBD-CAD	5.48	1.30	1.22
22	G	613	CLA	OBD-CAD	5.48	1.30	1.22
22	c	507	CLA	OBD-CAD	5.48	1.30	1.22
22	2	613	CLA	CHB-C4A	5.49	1.40	1.33
22	6	613	CLA	CHB-C4A	5.49	1.40	1.33
22	G	602	CLA	OBD-CAD	5.49	1.30	1.22
22	g	602	CLA	OBD-CAD	5.49	1.30	1.22
22	4	303	CLA	CHB-C4A	5.50	1.40	1.33
22	8	303	CLA	CHB-C4A	5.50	1.40	1.33
22	y	612	CLA	OBD-CAD	5.51	1.30	1.22
22	Y	612	CLA	OBD-CAD	5.51	1.30	1.22
22	c	501	CLA	CHB-C4A	5.51	1.40	1.33
22	b	608	CLA	OBD-CAD	5.51	1.30	1.22
22	y	610	CLA	OBD-CAD	5.52	1.30	1.22
22	Y	610	CLA	OBD-CAD	5.52	1.30	1.22
23	A	404	PHO	CHB-C1B	5.52	1.49	1.38
22	b	611	CLA	CHB-C4A	5.52	1.40	1.33
22	8	302	CLA	OBD-CAD	5.53	1.30	1.22
22	4	302	CLA	OBD-CAD	5.53	1.30	1.22
23	d	402	PHO	CHB-C1B	5.53	1.49	1.38
22	b	604	CLA	OBD-CAD	5.53	1.30	1.22
22	R	308	CLA	OBD-CAD	5.53	1.30	1.22
22	r	308	CLA	OBD-CAD	5.53	1.30	1.22
22	S	304	CLA	CHB-C4A	5.53	1.40	1.33
22	s	304	CLA	CHB-C4A	5.53	1.40	1.33
22	B	605	CLA	OBD-CAD	5.55	1.30	1.22
23	a	404	PHO	C3B-C2B	5.56	1.47	1.37
22	R	301	CLA	OBD-CAD	5.56	1.30	1.22
22	r	301	CLA	OBD-CAD	5.56	1.30	1.22
22	1	610	CLA	CHB-C4A	5.56	1.40	1.33
22	5	610	CLA	CHB-C4A	5.56	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	602	CLA	OBD-CAD	5.58	1.30	1.22
22	n	602	CLA	OBD-CAD	5.58	1.30	1.22
22	2	602	CLA	OBD-CAD	5.58	1.30	1.22
22	6	602	CLA	OBD-CAD	5.58	1.30	1.22
22	G	603	CLA	OBD-CAD	5.60	1.30	1.22
22	g	603	CLA	OBD-CAD	5.60	1.30	1.22
22	D	401	CLA	OBD-CAD	5.60	1.30	1.22
23	d	402	PHO	C3B-C2B	5.60	1.47	1.37
22	G	610	CLA	OBD-CAD	5.60	1.30	1.22
22	n	610	CLA	OBD-CAD	5.60	1.30	1.22
22	N	610	CLA	OBD-CAD	5.60	1.30	1.22
22	g	610	CLA	OBD-CAD	5.60	1.30	1.22
22	6	609	CLA	CHB-C4A	5.61	1.40	1.33
22	2	609	CLA	CHB-C4A	5.61	1.40	1.33
22	A	405	CLA	OBD-CAD	5.62	1.30	1.22
22	a	402	CLA	OBD-CAD	5.62	1.30	1.22
22	r	310	CLA	OBD-CAD	5.63	1.30	1.22
22	R	310	CLA	OBD-CAD	5.63	1.30	1.22
22	n	612	CLA	OBD-CAD	5.64	1.30	1.22
22	N	612	CLA	OBD-CAD	5.64	1.30	1.22
22	S	301	CLA	CHB-C4A	5.64	1.40	1.33
22	B	603	CLA	OBD-CAD	5.64	1.30	1.22
22	B	602	CLA	CHB-C4A	5.65	1.40	1.33
22	A	403	CLA	OBD-CAD	5.65	1.30	1.22
22	c	508	CLA	OBD-CAD	5.66	1.30	1.22
22	B	612	CLA	OBD-CAD	5.68	1.30	1.22
22	4	303	CLA	OBD-CAD	5.68	1.30	1.22
22	8	303	CLA	OBD-CAD	5.68	1.30	1.22
22	S	312	CLA	OBD-CAD	5.68	1.30	1.22
22	s	312	CLA	OBD-CAD	5.68	1.30	1.22
22	7	303	CLA	OBD-CAD	5.68	1.30	1.22
22	3	303	CLA	OBD-CAD	5.68	1.30	1.22
23	A	404	PHO	C3B-C2B	5.68	1.47	1.37
22	y	611	CLA	OBD-CAD	5.69	1.30	1.22
22	Y	611	CLA	OBD-CAD	5.69	1.30	1.22
22	b	607	CLA	OBD-CAD	5.69	1.30	1.22
22	b	613	CLA	CHB-C4A	5.69	1.40	1.33
22	B	602	CLA	OBD-CAD	5.70	1.30	1.22
22	3	310	CLA	CHB-C4A	5.70	1.40	1.33
22	7	310	CLA	CHB-C4A	5.70	1.40	1.33
22	b	605	CLA	OBD-CAD	5.71	1.30	1.22
22	c	509	CLA	OBD-CAD	5.71	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Y	602	CLA	OBD-CAD	5.71	1.30	1.22
22	A	402	CLA	OBD-CAD	5.71	1.30	1.22
22	y	602	CLA	OBD-CAD	5.71	1.30	1.22
22	C	508	CLA	OBD-CAD	5.72	1.30	1.22
22	b	602	CLA	OBD-CAD	5.73	1.30	1.22
22	B	614	CLA	OBD-CAD	5.73	1.30	1.22
22	R	303	CLA	OBD-CAD	5.73	1.30	1.22
22	r	303	CLA	OBD-CAD	5.73	1.30	1.22
22	4	309	CLA	CHB-C4A	5.74	1.40	1.33
22	8	309	CLA	CHB-C4A	5.74	1.40	1.33
22	B	608	CLA	OBD-CAD	5.75	1.30	1.22
22	S	314	CLA	OBD-CAD	5.75	1.30	1.22
22	s	314	CLA	OBD-CAD	5.75	1.30	1.22
22	S	311	CLA	OBD-CAD	5.76	1.30	1.22
22	s	311	CLA	OBD-CAD	5.76	1.30	1.22
22	Y	614	CLA	OBD-CAD	5.76	1.30	1.22
22	y	614	CLA	OBD-CAD	5.76	1.30	1.22
22	g	612	CLA	OBD-CAD	5.77	1.30	1.22
22	G	612	CLA	OBD-CAD	5.77	1.30	1.22
22	b	616	CLA	OBD-CAD	5.77	1.30	1.22
22	C	510	CLA	OBD-CAD	5.77	1.30	1.22
22	B	606	CLA	OBD-CAD	5.78	1.30	1.22
22	C	506	CLA	OBD-CAD	5.78	1.30	1.22
22	Y	604	CLA	OBD-CAD	5.78	1.30	1.22
22	y	604	CLA	OBD-CAD	5.78	1.30	1.22
22	c	505	CLA	OBD-CAD	5.78	1.30	1.22
22	g	611	CLA	OBD-CAD	5.79	1.30	1.22
22	G	611	CLA	OBD-CAD	5.79	1.30	1.22
22	b	614	CLA	OBD-CAD	5.79	1.30	1.22
22	C	507	CLA	OBD-CAD	5.79	1.30	1.22
22	b	612	CLA	OBD-CAD	5.80	1.30	1.22
22	a	405	CLA	OBD-CAD	5.80	1.30	1.22
22	c	512	CLA	OBD-CAD	5.81	1.30	1.22
22	C	509	CLA	OBD-CAD	5.82	1.30	1.22
22	d	403	CLA	OBD-CAD	5.82	1.30	1.22
22	D	403	CLA	OBD-CAD	5.82	1.30	1.22
22	B	607	CLA	OBD-CAD	5.82	1.30	1.22
22	c	510	CLA	OBD-CAD	5.82	1.30	1.22
22	C	504	CLA	OBD-CAD	5.83	1.30	1.22
22	d	401	CLA	OBD-CAD	5.83	1.30	1.22
22	1	612	CLA	OBD-CAD	5.83	1.30	1.22
22	5	612	CLA	OBD-CAD	5.83	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	6	609	CLA	OBD-CAD	5.84	1.30	1.22
22	2	609	CLA	OBD-CAD	5.84	1.30	1.22
22	2	612	CLA	OBD-CAD	5.84	1.30	1.22
22	6	612	CLA	OBD-CAD	5.84	1.30	1.22
22	B	616	CLA	CHB-C4A	5.85	1.41	1.33
22	G	604	CLA	OBD-CAD	5.86	1.30	1.22
22	g	604	CLA	OBD-CAD	5.86	1.30	1.22
22	1	610	CLA	OBD-CAD	5.86	1.30	1.22
22	5	610	CLA	OBD-CAD	5.86	1.30	1.22
22	R	309	CLA	OBD-CAD	5.87	1.30	1.22
22	C	512	CLA	OBD-CAD	5.87	1.30	1.22
22	r	309	CLA	OBD-CAD	5.87	1.30	1.22
22	G	614	CLA	OBD-CAD	5.87	1.30	1.22
22	g	614	CLA	OBD-CAD	5.87	1.30	1.22
22	b	615	CLA	OBD-CAD	5.88	1.30	1.22
22	c	506	CLA	OBD-CAD	5.88	1.30	1.22
22	C	511	CLA	OBD-CAD	5.88	1.30	1.22
22	3	304	CLA	OBD-CAD	5.88	1.30	1.22
22	7	304	CLA	OBD-CAD	5.88	1.30	1.22
22	b	603	CLA	OBD-CAD	5.89	1.30	1.22
22	B	609	CLA	OBD-CAD	5.90	1.30	1.22
22	R	312	CLA	OBD-CAD	5.90	1.30	1.22
22	r	312	CLA	OBD-CAD	5.90	1.30	1.22
22	D	404	CLA	OBD-CAD	5.90	1.30	1.22
22	b	610	CLA	OBD-CAD	5.91	1.30	1.22
22	7	305	CLA	OBD-CAD	5.91	1.30	1.22
22	3	305	CLA	OBD-CAD	5.91	1.30	1.22
22	n	604	CLA	OBD-CAD	5.91	1.30	1.22
22	N	604	CLA	OBD-CAD	5.91	1.30	1.22
22	d	404	CLA	OBD-CAD	5.91	1.30	1.22
22	1	613	CLA	OBD-CAD	5.92	1.30	1.22
22	5	613	CLA	OBD-CAD	5.92	1.30	1.22
22	2	610	CLA	OBD-CAD	5.92	1.30	1.22
22	6	610	CLA	OBD-CAD	5.92	1.30	1.22
22	B	601	CLA	OBD-CAD	5.93	1.30	1.22
22	B	610	CLA	OBD-CAD	5.93	1.30	1.22
22	r	307	CLA	OBD-CAD	5.93	1.30	1.22
22	R	307	CLA	OBD-CAD	5.93	1.30	1.22
22	7	314	CLA	OBD-CAD	5.93	1.30	1.22
22	3	314	CLA	OBD-CAD	5.93	1.30	1.22
22	8	310	CLA	OBD-CAD	5.94	1.30	1.22
22	4	310	CLA	OBD-CAD	5.94	1.30	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	504	CLA	OBD-CAD	5.94	1.30	1.22
22	n	611	CLA	OBD-CAD	5.94	1.30	1.22
22	N	611	CLA	OBD-CAD	5.94	1.30	1.22
22	b	609	CLA	OBD-CAD	5.94	1.30	1.22
22	s	309	CLA	OBD-CAD	5.94	1.30	1.22
22	S	309	CLA	OBD-CAD	5.94	1.30	1.22
22	C	505	CLA	OBD-CAD	5.95	1.31	1.22
22	4	304	CLA	OBD-CAD	5.96	1.31	1.22
22	8	304	CLA	OBD-CAD	5.96	1.31	1.22
22	4	309	CLA	OBD-CAD	5.96	1.31	1.22
22	S	301	CLA	OBD-CAD	5.96	1.31	1.22
22	8	309	CLA	OBD-CAD	5.96	1.31	1.22
22	2	613	CLA	OBD-CAD	5.97	1.31	1.22
22	6	613	CLA	OBD-CAD	5.97	1.31	1.22
22	6	603	CLA	OBD-CAD	5.97	1.31	1.22
22	2	603	CLA	OBD-CAD	5.97	1.31	1.22
22	5	611	CLA	OBD-CAD	5.97	1.31	1.22
22	1	611	CLA	OBD-CAD	5.97	1.31	1.22
22	7	313	CLA	OBD-CAD	5.98	1.31	1.22
22	3	313	CLA	OBD-CAD	5.98	1.31	1.22
22	1	603	CLA	OBD-CAD	5.98	1.31	1.22
22	5	603	CLA	OBD-CAD	5.98	1.31	1.22
22	R	311	CLA	OBD-CAD	5.98	1.31	1.22
22	r	311	CLA	OBD-CAD	5.98	1.31	1.22
22	N	614	CLA	OBD-CAD	5.99	1.31	1.22
22	n	614	CLA	OBD-CAD	5.99	1.31	1.22
22	7	311	CLA	OBD-CAD	5.99	1.31	1.22
22	3	311	CLA	OBD-CAD	5.99	1.31	1.22
22	3	310	CLA	OBD-CAD	6.00	1.31	1.22
22	7	310	CLA	OBD-CAD	6.00	1.31	1.22
22	b	601	CLA	OBD-CAD	6.00	1.31	1.22
22	3	312	CLA	OBD-CAD	6.01	1.31	1.22
22	7	312	CLA	OBD-CAD	6.01	1.31	1.22
22	6	611	CLA	OBD-CAD	6.02	1.31	1.22
22	2	611	CLA	OBD-CAD	6.02	1.31	1.22
22	s	301	CLA	OBD-CAD	6.02	1.31	1.22
22	5	604	CLA	OBD-CAD	6.02	1.31	1.22
22	1	604	CLA	OBD-CAD	6.02	1.31	1.22
22	B	615	CLA	OBD-CAD	6.03	1.31	1.22
22	r	302	CLA	OBD-CAD	6.04	1.31	1.22
22	R	302	CLA	OBD-CAD	6.04	1.31	1.22
22	5	614	CLA	OBD-CAD	6.06	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1	614	CLA	OBD-CAD	6.06	1.31	1.22
22	b	606	CLA	OBD-CAD	6.10	1.31	1.22
22	2	604	CLA	OBD-CAD	6.11	1.31	1.22
22	6	604	CLA	OBD-CAD	6.11	1.31	1.22
22	8	302	CLA	CHB-C4A	6.14	1.41	1.33
22	4	302	CLA	CHB-C4A	6.14	1.41	1.33
22	S	304	CLA	OBD-CAD	6.19	1.31	1.22
22	s	304	CLA	OBD-CAD	6.19	1.31	1.22
22	S	305	CLA	OBD-CAD	6.21	1.31	1.22
22	s	305	CLA	OBD-CAD	6.21	1.31	1.22

All (5412) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	307	CHL	O2D-CGD-O1D	-23.26	77.05	123.82
25	S	307	CHL	O2D-CGD-O1D	-23.26	77.05	123.82
25	4	307	CHL	O2D-CGD-O1D	-22.59	78.38	123.82
25	8	307	CHL	O2D-CGD-O1D	-22.59	78.38	123.82
25	4	307	CHL	O1D-CGD-CBD	-20.34	82.50	124.53
25	8	307	CHL	O1D-CGD-CBD	-20.34	82.50	124.53
25	s	307	CHL	O1D-CGD-CBD	-19.58	84.07	124.53
25	S	307	CHL	O1D-CGD-CBD	-19.58	84.07	124.53
22	B	615	CLA	C1C-NC-C4C	-9.83	101.40	107.06
22	B	602	CLA	C1C-NC-C4C	-9.83	101.40	107.06
22	C	506	CLA	C1C-NC-C4C	-9.83	101.40	107.06
22	c	512	CLA	C1C-NC-C4C	-9.67	101.49	107.06
22	c	506	CLA	C1C-NC-C4C	-9.67	101.49	107.06
22	B	616	CLA	C1C-NC-C4C	-9.66	101.50	107.06
22	C	510	CLA	C1C-NC-C4C	-9.63	101.52	107.06
22	a	405	CLA	C1C-NC-C4C	-9.50	101.59	107.06
22	8	302	CLA	C1C-NC-C4C	-9.49	101.60	107.06
22	4	302	CLA	C1C-NC-C4C	-9.49	101.60	107.06
22	b	610	CLA	C1C-NC-C4C	-9.38	101.66	107.06
22	b	609	CLA	C1C-NC-C4C	-9.38	101.66	107.06
22	C	508	CLA	C1C-NC-C4C	-9.36	101.67	107.06
22	b	613	CLA	C1C-NC-C4C	-9.32	101.69	107.06
22	B	612	CLA	C1C-NC-C4C	-9.31	101.70	107.06
22	S	301	CLA	C1C-NC-C4C	-9.26	101.73	107.06
22	Y	604	CLA	C1C-NC-C4C	-9.23	101.75	107.06
22	y	604	CLA	C1C-NC-C4C	-9.23	101.75	107.06
22	A	402	CLA	C1C-NC-C4C	-9.21	101.75	107.06
22	b	602	CLA	C1C-NC-C4C	-9.21	101.76	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	C1C-NC-C4C	-9.18	101.78	107.06
22	C	507	CLA	C1C-NC-C4C	-9.15	101.79	107.06
22	y	613	CLA	C1C-NC-C4C	-9.06	101.84	107.06
22	Y	613	CLA	C1C-NC-C4C	-9.06	101.84	107.06
22	B	614	CLA	C1C-NC-C4C	-9.05	101.85	107.06
22	c	503	CLA	C1C-NC-C4C	-9.04	101.86	107.06
22	2	612	CLA	C1C-NC-C4C	-9.01	101.88	107.06
22	6	612	CLA	C1C-NC-C4C	-9.01	101.88	107.06
22	c	507	CLA	C1C-NC-C4C	-8.86	101.96	107.06
22	B	607	CLA	C1C-NC-C4C	-8.84	101.97	107.06
22	c	508	CLA	C1C-NC-C4C	-8.75	102.02	107.06
22	R	311	CLA	C1C-NC-C4C	-8.74	102.03	107.06
22	r	311	CLA	C1C-NC-C4C	-8.74	102.03	107.06
22	A	405	CLA	C1C-NC-C4C	-8.70	102.05	107.06
22	a	403	CLA	C1C-NC-C4C	-8.61	102.10	107.06
22	3	312	CLA	C1C-NC-C4C	-8.60	102.11	107.06
22	B	609	CLA	C1C-NC-C4C	-8.60	102.11	107.06
22	7	312	CLA	C1C-NC-C4C	-8.60	102.11	107.06
22	1	602	CLA	C1C-NC-C4C	-8.59	102.11	107.06
22	5	602	CLA	C1C-NC-C4C	-8.59	102.11	107.06
22	n	613	CLA	C1C-NC-C4C	-8.57	102.13	107.06
22	N	613	CLA	C1C-NC-C4C	-8.57	102.13	107.06
22	B	604	CLA	C1C-NC-C4C	-8.54	102.14	107.06
22	S	314	CLA	C1C-NC-C4C	-8.54	102.14	107.06
22	s	314	CLA	C1C-NC-C4C	-8.54	102.14	107.06
22	c	510	CLA	C1C-NC-C4C	-8.52	102.16	107.06
22	B	610	CLA	C1C-NC-C4C	-8.52	102.16	107.06
22	7	313	CLA	C1C-NC-C4C	-8.49	102.17	107.06
22	3	313	CLA	C1C-NC-C4C	-8.49	102.17	107.06
22	N	602	CLA	C1C-NC-C4C	-8.46	102.19	107.06
22	n	602	CLA	C1C-NC-C4C	-8.46	102.19	107.06
22	C	504	CLA	C1C-NC-C4C	-8.44	102.20	107.06
22	B	603	CLA	C1C-NC-C4C	-8.44	102.20	107.06
22	D	401	CLA	C1C-NC-C4C	-8.43	102.21	107.06
22	5	611	CLA	C1C-NC-C4C	-8.41	102.22	107.06
22	1	611	CLA	C1C-NC-C4C	-8.41	102.22	107.06
22	2	602	CLA	C1C-NC-C4C	-8.41	102.22	107.06
22	6	602	CLA	C1C-NC-C4C	-8.41	102.22	107.06
22	Y	602	CLA	C1C-NC-C4C	-8.40	102.22	107.06
22	y	602	CLA	C1C-NC-C4C	-8.40	102.22	107.06
22	B	605	CLA	C1C-NC-C4C	-8.39	102.23	107.06
22	C	501	CLA	C1C-NC-C4C	-8.37	102.24	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	610	CLA	C1C-NC-C4C	-8.35	102.25	107.06
22	Y	610	CLA	C1C-NC-C4C	-8.35	102.25	107.06
22	b	607	CLA	C1C-NC-C4C	-8.34	102.26	107.06
22	b	614	CLA	C1C-NC-C4C	-8.33	102.26	107.06
22	g	613	CLA	C1C-NC-C4C	-8.33	102.27	107.06
22	G	613	CLA	C1C-NC-C4C	-8.33	102.27	107.06
22	C	511	CLA	C1C-NC-C4C	-8.32	102.27	107.06
22	1	610	CLA	C1C-NC-C4C	-8.32	102.27	107.06
22	5	610	CLA	C1C-NC-C4C	-8.32	102.27	107.06
22	D	403	CLA	C1C-NC-C4C	-8.31	102.28	107.06
22	c	502	CLA	C1C-NC-C4C	-8.28	102.29	107.06
22	G	602	CLA	C1C-NC-C4C	-8.24	102.31	107.06
22	g	602	CLA	C1C-NC-C4C	-8.24	102.31	107.06
22	y	611	CLA	C1C-NC-C4C	-8.21	102.33	107.06
22	Y	611	CLA	C1C-NC-C4C	-8.21	102.33	107.06
22	b	616	CLA	C1C-NC-C4C	-8.20	102.34	107.06
22	r	307	CLA	C1C-NC-C4C	-8.19	102.34	107.06
22	R	307	CLA	C1C-NC-C4C	-8.19	102.34	107.06
22	1	603	CLA	C1C-NC-C4C	-8.18	102.35	107.06
22	5	603	CLA	C1C-NC-C4C	-8.18	102.35	107.06
22	R	301	CLA	C1C-NC-C4C	-8.17	102.36	107.06
22	r	301	CLA	C1C-NC-C4C	-8.17	102.36	107.06
22	7	303	CLA	C1C-NC-C4C	-8.16	102.36	107.06
22	3	303	CLA	C1C-NC-C4C	-8.16	102.36	107.06
22	S	311	CLA	C1C-NC-C4C	-8.16	102.36	107.06
22	s	311	CLA	C1C-NC-C4C	-8.16	102.36	107.06
22	D	404	CLA	C1C-NC-C4C	-8.12	102.39	107.06
22	5	614	CLA	C1C-NC-C4C	-8.11	102.39	107.06
22	1	614	CLA	C1C-NC-C4C	-8.11	102.39	107.06
22	7	311	CLA	C1C-NC-C4C	-8.10	102.40	107.06
22	3	311	CLA	C1C-NC-C4C	-8.10	102.40	107.06
22	c	501	CLA	C1C-NC-C4C	-8.09	102.40	107.06
22	n	611	CLA	C1C-NC-C4C	-8.07	102.42	107.06
22	N	611	CLA	C1C-NC-C4C	-8.07	102.42	107.06
22	3	310	CLA	C1C-NC-C4C	-8.06	102.42	107.06
22	7	310	CLA	C1C-NC-C4C	-8.06	102.42	107.06
22	4	303	CLA	C1C-NC-C4C	-8.06	102.42	107.06
22	8	303	CLA	C1C-NC-C4C	-8.06	102.42	107.06
22	d	401	CLA	C1C-NC-C4C	-8.05	102.42	107.06
22	G	604	CLA	C1C-NC-C4C	-8.04	102.43	107.06
22	g	604	CLA	C1C-NC-C4C	-8.04	102.43	107.06
22	2	610	CLA	C1C-NC-C4C	-8.04	102.43	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	610	CLA	C1C-NC-C4C	-8.04	102.43	107.06
22	n	610	CLA	C1C-NC-C4C	-8.02	102.44	107.06
22	N	610	CLA	C1C-NC-C4C	-8.02	102.44	107.06
22	R	309	CLA	C1C-NC-C4C	-8.01	102.45	107.06
22	C	503	CLA	C1C-NC-C4C	-8.01	102.45	107.06
22	r	309	CLA	C1C-NC-C4C	-8.01	102.45	107.06
22	4	304	CLA	C1C-NC-C4C	-8.00	102.45	107.06
22	8	304	CLA	C1C-NC-C4C	-8.00	102.45	107.06
22	d	403	CLA	C1C-NC-C4C	-7.97	102.47	107.06
22	G	610	CLA	C1C-NC-C4C	-7.97	102.47	107.06
22	g	610	CLA	C1C-NC-C4C	-7.97	102.47	107.06
22	R	312	CLA	C1C-NC-C4C	-7.96	102.47	107.06
22	r	312	CLA	C1C-NC-C4C	-7.96	102.47	107.06
22	1	613	CLA	C1C-NC-C4C	-7.96	102.48	107.06
22	5	613	CLA	C1C-NC-C4C	-7.96	102.48	107.06
22	B	606	CLA	C1C-NC-C4C	-7.95	102.48	107.06
22	Y	614	CLA	C1C-NC-C4C	-7.93	102.50	107.06
22	y	614	CLA	C1C-NC-C4C	-7.93	102.50	107.06
22	C	505	CLA	C1C-NC-C4C	-7.92	102.50	107.06
22	2	604	CLA	C1C-NC-C4C	-7.90	102.51	107.06
22	6	604	CLA	C1C-NC-C4C	-7.90	102.51	107.06
22	r	302	CLA	C1C-NC-C4C	-7.88	102.52	107.06
22	R	302	CLA	C1C-NC-C4C	-7.88	102.52	107.06
22	a	402	CLA	C1C-NC-C4C	-7.86	102.53	107.06
22	c	504	CLA	C1C-NC-C4C	-7.85	102.54	107.06
22	C	509	CLA	C1C-NC-C4C	-7.85	102.54	107.06
22	g	611	CLA	C1C-NC-C4C	-7.83	102.55	107.06
22	G	611	CLA	C1C-NC-C4C	-7.83	102.55	107.06
22	6	609	CLA	C1C-NC-C4C	-7.83	102.55	107.06
22	2	609	CLA	C1C-NC-C4C	-7.83	102.55	107.06
22	S	310	CLA	C1C-NC-C4C	-7.82	102.56	107.06
22	b	611	CLA	C1C-NC-C4C	-7.82	102.56	107.06
22	s	310	CLA	C1C-NC-C4C	-7.82	102.56	107.06
22	Y	603	CLA	C1C-NC-C4C	-7.79	102.57	107.06
22	y	603	CLA	C1C-NC-C4C	-7.79	102.57	107.06
22	5	604	CLA	C1C-NC-C4C	-7.78	102.58	107.06
22	1	604	CLA	C1C-NC-C4C	-7.78	102.58	107.06
22	4	309	CLA	C1C-NC-C4C	-7.78	102.58	107.06
22	8	309	CLA	C1C-NC-C4C	-7.78	102.58	107.06
22	6	603	CLA	C1C-NC-C4C	-7.77	102.58	107.06
22	2	603	CLA	C1C-NC-C4C	-7.77	102.58	107.06
22	8	310	CLA	C1C-NC-C4C	-7.75	102.60	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	310	CLA	C1C-NC-C4C	-7.75	102.60	107.06
22	A	403	CLA	C1C-NC-C4C	-7.73	102.61	107.06
22	7	305	CLA	C1C-NC-C4C	-7.73	102.61	107.06
22	3	305	CLA	C1C-NC-C4C	-7.73	102.61	107.06
22	c	511	CLA	C1C-NC-C4C	-7.71	102.62	107.06
22	s	303	CLA	C1C-NC-C4C	-7.70	102.62	107.06
22	S	303	CLA	C1C-NC-C4C	-7.70	102.62	107.06
22	c	509	CLA	C1C-NC-C4C	-7.70	102.63	107.06
22	b	601	CLA	C1C-NC-C4C	-7.66	102.65	107.06
22	n	612	CLA	C1C-NC-C4C	-7.66	102.65	107.06
22	N	612	CLA	C1C-NC-C4C	-7.66	102.65	107.06
22	6	611	CLA	C1C-NC-C4C	-7.64	102.66	107.06
22	2	611	CLA	C1C-NC-C4C	-7.64	102.66	107.06
22	s	313	CLA	C1C-NC-C4C	-7.61	102.68	107.06
22	S	305	CLA	C1C-NC-C4C	-7.61	102.68	107.06
22	s	305	CLA	C1C-NC-C4C	-7.61	102.68	107.06
22	S	313	CLA	C1C-NC-C4C	-7.61	102.68	107.06
22	c	505	CLA	C1C-NC-C4C	-7.60	102.68	107.06
22	1	612	CLA	C1C-NC-C4C	-7.58	102.69	107.06
22	5	612	CLA	C1C-NC-C4C	-7.58	102.69	107.06
22	s	309	CLA	C1C-NC-C4C	-7.58	102.69	107.06
22	S	309	CLA	C1C-NC-C4C	-7.58	102.69	107.06
22	g	612	CLA	C1C-NC-C4C	-7.53	102.72	107.06
22	G	612	CLA	C1C-NC-C4C	-7.53	102.72	107.06
22	R	308	CLA	C1C-NC-C4C	-7.52	102.73	107.06
22	r	308	CLA	C1C-NC-C4C	-7.52	102.73	107.06
22	3	304	CLA	C1C-NC-C4C	-7.50	102.74	107.06
22	7	304	CLA	C1C-NC-C4C	-7.50	102.74	107.06
22	G	603	CLA	C1C-NC-C4C	-7.44	102.77	107.06
22	g	603	CLA	C1C-NC-C4C	-7.44	102.77	107.06
22	r	310	CLA	C1C-NC-C4C	-7.43	102.78	107.06
22	R	310	CLA	C1C-NC-C4C	-7.43	102.78	107.06
22	C	512	CLA	C1C-NC-C4C	-7.42	102.79	107.06
22	R	303	CLA	C1C-NC-C4C	-7.41	102.79	107.06
22	2	613	CLA	C1C-NC-C4C	-7.41	102.79	107.06
22	r	303	CLA	C1C-NC-C4C	-7.41	102.79	107.06
22	6	613	CLA	C1C-NC-C4C	-7.41	102.79	107.06
22	b	603	CLA	C1C-NC-C4C	-7.41	102.79	107.06
22	n	604	CLA	C1C-NC-C4C	-7.39	102.80	107.06
22	N	604	CLA	C1C-NC-C4C	-7.39	102.80	107.06
22	S	312	CLA	C1C-NC-C4C	-7.32	102.84	107.06
22	s	312	CLA	C1C-NC-C4C	-7.32	102.84	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	404	CLA	C1C-NC-C4C	-7.32	102.84	107.06
22	G	614	CLA	C1C-NC-C4C	-7.30	102.85	107.06
22	g	614	CLA	C1C-NC-C4C	-7.30	102.85	107.06
22	n	603	CLA	C1C-NC-C4C	-7.29	102.86	107.06
22	N	603	CLA	C1C-NC-C4C	-7.29	102.86	107.06
22	s	301	CLA	C1C-NC-C4C	-7.21	102.91	107.06
22	b	604	CLA	C1C-NC-C4C	-7.19	102.92	107.06
22	B	601	CLA	C1C-NC-C4C	-7.13	102.95	107.06
22	B	613	CLA	C1C-NC-C4C	-7.10	102.97	107.06
22	N	614	CLA	C1C-NC-C4C	-7.06	103.00	107.06
22	n	614	CLA	C1C-NC-C4C	-7.06	103.00	107.06
22	b	608	CLA	C1C-NC-C4C	-7.04	103.01	107.06
22	B	611	CLA	C1C-NC-C4C	-6.90	103.09	107.06
22	b	605	CLA	C1C-NC-C4C	-6.83	103.13	107.06
22	B	604	CLA	C1C-C2C-C3C	-6.77	99.41	106.92
22	y	612	CLA	C1C-NC-C4C	-6.75	103.17	107.06
22	Y	612	CLA	C1C-NC-C4C	-6.75	103.17	107.06
22	c	501	CLA	C1C-C2C-C3C	-6.63	99.56	106.92
23	A	404	PHO	C3D-C2D-C1D	-6.58	96.07	105.82
22	7	314	CLA	C1C-NC-C4C	-6.48	103.33	107.06
22	3	314	CLA	C1C-NC-C4C	-6.48	103.33	107.06
22	C	502	CLA	C1C-NC-C4C	-6.45	103.35	107.06
22	b	612	CLA	C1C-NC-C4C	-6.43	103.36	107.06
22	b	609	CLA	C1C-C2C-C3C	-6.36	99.86	106.92
22	b	604	CLA	C1C-C2C-C3C	-6.35	99.88	106.92
22	S	312	CLA	C1C-C2C-C3C	-6.24	99.99	106.92
22	s	312	CLA	C1C-C2C-C3C	-6.24	99.99	106.92
22	B	616	CLA	C1C-C2C-C3C	-6.23	100.00	106.92
22	B	608	CLA	C1C-C2C-C3C	-6.22	100.02	106.92
22	y	613	CLA	C1C-C2C-C3C	-6.18	100.06	106.92
22	Y	613	CLA	C1C-C2C-C3C	-6.18	100.06	106.92
22	C	501	CLA	C1C-C2C-C3C	-6.15	100.09	106.92
22	C	504	CLA	C1C-C2C-C3C	-6.14	100.10	106.92
22	C	510	CLA	C1C-C2C-C3C	-6.08	100.17	106.92
22	c	506	CLA	C1C-C2C-C3C	-6.06	100.19	106.92
23	a	404	PHO	C3D-C2D-C1D	-6.06	96.83	105.82
22	c	507	CLA	C1C-C2C-C3C	-6.06	100.19	106.92
23	D	402	PHO	C3D-C2D-C1D	-6.05	96.84	105.82
22	S	304	CLA	C1C-NC-C4C	-6.04	103.58	107.06
22	s	304	CLA	C1C-NC-C4C	-6.04	103.58	107.06
22	C	506	CLA	C1C-C2C-C3C	-6.02	100.24	106.92
22	Y	604	CLA	C1C-C2C-C3C	-6.01	100.25	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	604	CLA	C1C-C2C-C3C	-6.01	100.25	106.92
22	n	612	CLA	C1C-C2C-C3C	-6.00	100.26	106.92
22	N	612	CLA	C1C-C2C-C3C	-6.00	100.26	106.92
22	b	613	CLA	C1C-C2C-C3C	-6.00	100.26	106.92
22	G	602	CLA	C1C-C2C-C3C	-5.95	100.32	106.92
22	g	602	CLA	C1C-C2C-C3C	-5.95	100.32	106.92
22	b	615	CLA	C1C-NC-C4C	-5.93	103.64	107.06
22	5	614	CLA	C1C-C2C-C3C	-5.92	100.35	106.92
22	l	614	CLA	C1C-C2C-C3C	-5.92	100.35	106.92
22	N	602	CLA	C1C-C2C-C3C	-5.91	100.36	106.92
22	b	616	CLA	C1C-C2C-C3C	-5.91	100.36	106.92
22	n	602	CLA	C1C-C2C-C3C	-5.91	100.36	106.92
23	d	402	PHO	C3D-C2D-C1D	-5.91	97.05	105.82
22	c	510	CLA	C1C-C2C-C3C	-5.91	100.36	106.92
22	g	612	CLA	C1C-C2C-C3C	-5.91	100.36	106.92
22	G	612	CLA	C1C-C2C-C3C	-5.91	100.36	106.92
22	n	611	CLA	C1C-C2C-C3C	-5.90	100.37	106.92
22	N	611	CLA	C1C-C2C-C3C	-5.90	100.37	106.92
22	y	612	CLA	C1C-C2C-C3C	-5.90	100.38	106.92
22	Y	612	CLA	C1C-C2C-C3C	-5.90	100.38	106.92
22	b	602	CLA	CHD-C4C-C3C	-5.89	116.04	124.92
22	C	509	CLA	C1C-C2C-C3C	-5.89	100.39	106.92
22	b	603	CLA	C1C-C2C-C3C	-5.86	100.42	106.92
22	Y	603	CLA	C1C-C2C-C3C	-5.85	100.42	106.92
22	y	603	CLA	C1C-C2C-C3C	-5.85	100.42	106.92
22	C	511	CLA	C1C-C2C-C3C	-5.85	100.42	106.92
22	S	314	CLA	C1C-C2C-C3C	-5.85	100.43	106.92
22	s	314	CLA	C1C-C2C-C3C	-5.85	100.43	106.92
22	c	509	CLA	CHD-C4C-C3C	-5.84	116.12	124.92
22	C	508	CLA	C1C-C2C-C3C	-5.84	100.44	106.92
22	c	512	CLA	C1C-C2C-C3C	-5.84	100.44	106.92
22	G	604	CLA	C1C-C2C-C3C	-5.82	100.47	106.92
22	g	604	CLA	C1C-C2C-C3C	-5.82	100.47	106.92
22	c	511	CLA	C1C-C2C-C3C	-5.81	100.47	106.92
22	y	611	CLA	C1C-C2C-C3C	-5.81	100.47	106.92
22	Y	611	CLA	C1C-C2C-C3C	-5.81	100.47	106.92
22	8	302	CLA	C1C-C2C-C3C	-5.81	100.48	106.92
22	4	302	CLA	C1C-C2C-C3C	-5.81	100.48	106.92
22	S	305	CLA	C1C-C2C-C3C	-5.80	100.48	106.92
22	s	305	CLA	C1C-C2C-C3C	-5.80	100.48	106.92
22	Y	614	CLA	C1C-C2C-C3C	-5.79	100.50	106.92
22	y	614	CLA	C1C-C2C-C3C	-5.79	100.50	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	311	CLA	C1C-C2C-C3C	-5.78	100.50	106.92
22	r	311	CLA	C1C-C2C-C3C	-5.78	100.50	106.92
22	c	502	CLA	C1C-C2C-C3C	-5.78	100.51	106.92
25	Y	605	CHL	CAA-C2A-C3A	-5.77	103.66	115.37
25	y	605	CHL	CAA-C2A-C3A	-5.77	103.66	115.37
22	g	613	CLA	C1C-C2C-C3C	-5.77	100.52	106.92
22	G	613	CLA	C1C-C2C-C3C	-5.77	100.52	106.92
22	Y	602	CLA	C1C-C2C-C3C	-5.77	100.52	106.92
22	y	602	CLA	C1C-C2C-C3C	-5.77	100.52	106.92
22	g	611	CLA	C1C-C2C-C3C	-5.77	100.52	106.92
22	G	611	CLA	C1C-C2C-C3C	-5.77	100.52	106.92
22	n	603	CLA	C1C-C2C-C3C	-5.75	100.54	106.92
22	N	603	CLA	C1C-C2C-C3C	-5.75	100.54	106.92
22	A	402	CLA	CHD-C4C-C3C	-5.75	116.25	124.92
22	c	508	CLA	C1C-C2C-C3C	-5.75	100.54	106.92
22	2	612	CLA	C1C-C2C-C3C	-5.73	100.56	106.92
22	6	612	CLA	C1C-C2C-C3C	-5.73	100.56	106.92
22	R	309	CLA	C1C-C2C-C3C	-5.72	100.57	106.92
22	r	309	CLA	C1C-C2C-C3C	-5.72	100.57	106.92
22	B	603	CLA	C1C-C2C-C3C	-5.72	100.57	106.92
22	b	607	CLA	C1C-C2C-C3C	-5.72	100.57	106.92
22	d	403	CLA	C1C-C2C-C3C	-5.72	100.58	106.92
22	N	614	CLA	C1C-C2C-C3C	-5.71	100.58	106.92
22	n	614	CLA	C1C-C2C-C3C	-5.71	100.58	106.92
22	G	603	CLA	C1C-C2C-C3C	-5.71	100.58	106.92
22	g	603	CLA	C1C-C2C-C3C	-5.71	100.58	106.92
22	s	309	CLA	C1C-C2C-C3C	-5.71	100.59	106.92
22	S	309	CLA	C1C-C2C-C3C	-5.71	100.59	106.92
22	S	311	CLA	C1C-C2C-C3C	-5.71	100.59	106.92
22	s	311	CLA	C1C-C2C-C3C	-5.71	100.59	106.92
22	n	613	CLA	C1C-C2C-C3C	-5.70	100.59	106.92
22	N	613	CLA	C1C-C2C-C3C	-5.70	100.59	106.92
22	B	610	CLA	C1C-C2C-C3C	-5.70	100.59	106.92
22	S	310	CLA	C1C-C2C-C3C	-5.70	100.60	106.92
22	s	310	CLA	C1C-C2C-C3C	-5.70	100.60	106.92
22	B	607	CLA	C1C-C2C-C3C	-5.69	100.61	106.92
22	5	604	CLA	C1C-C2C-C3C	-5.68	100.62	106.92
22	1	604	CLA	C1C-C2C-C3C	-5.68	100.62	106.92
22	S	301	CLA	C1C-C2C-C3C	-5.68	100.62	106.92
22	7	313	CLA	C1C-C2C-C3C	-5.67	100.62	106.92
22	3	313	CLA	C1C-C2C-C3C	-5.67	100.62	106.92
22	n	604	CLA	C1C-C2C-C3C	-5.67	100.63	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	604	CLA	C1C-C2C-C3C	-5.67	100.63	106.92
22	1	613	CLA	C1C-C2C-C3C	-5.66	100.64	106.92
22	5	613	CLA	C1C-C2C-C3C	-5.66	100.64	106.92
22	c	509	CLA	C1C-C2C-C3C	-5.66	100.64	106.92
22	R	303	CLA	C1C-C2C-C3C	-5.65	100.65	106.92
22	r	303	CLA	C1C-C2C-C3C	-5.65	100.65	106.92
22	D	404	CLA	C1C-C2C-C3C	-5.65	100.65	106.92
22	C	507	CLA	C1C-C2C-C3C	-5.64	100.66	106.92
22	3	304	CLA	C1C-C2C-C3C	-5.64	100.67	106.92
22	7	304	CLA	C1C-C2C-C3C	-5.64	100.67	106.92
22	5	611	CLA	C1C-C2C-C3C	-5.63	100.67	106.92
22	1	611	CLA	C1C-C2C-C3C	-5.63	100.67	106.92
22	2	602	CLA	C1C-C2C-C3C	-5.63	100.68	106.92
22	6	602	CLA	C1C-C2C-C3C	-5.63	100.68	106.92
22	b	614	CLA	C1C-C2C-C3C	-5.62	100.69	106.92
22	8	310	CLA	C1C-C2C-C3C	-5.61	100.69	106.92
22	4	310	CLA	C1C-C2C-C3C	-5.61	100.69	106.92
22	B	609	CLA	C1C-C2C-C3C	-5.61	100.69	106.92
22	1	603	CLA	C1C-C2C-C3C	-5.61	100.70	106.92
22	5	603	CLA	C1C-C2C-C3C	-5.61	100.70	106.92
22	4	304	CLA	C1C-C2C-C3C	-5.60	100.70	106.92
22	8	304	CLA	C1C-C2C-C3C	-5.60	100.70	106.92
22	y	610	CLA	C1C-C2C-C3C	-5.59	100.72	106.92
22	Y	610	CLA	C1C-C2C-C3C	-5.59	100.72	106.92
22	7	305	CLA	C1C-C2C-C3C	-5.58	100.72	106.92
22	3	305	CLA	C1C-C2C-C3C	-5.58	100.72	106.92
22	7	303	CLA	C1C-C2C-C3C	-5.58	100.72	106.92
22	3	303	CLA	C1C-C2C-C3C	-5.58	100.72	106.92
22	A	405	CLA	C1C-C2C-C3C	-5.58	100.73	106.92
22	B	602	CLA	CHD-C4C-C3C	-5.58	116.51	124.92
22	4	303	CLA	C1C-C2C-C3C	-5.58	100.73	106.92
22	8	303	CLA	C1C-C2C-C3C	-5.58	100.73	106.92
22	b	615	CLA	C1C-C2C-C3C	-5.58	100.73	106.92
22	7	311	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	r	310	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	R	310	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	3	311	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	6	603	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	2	603	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	G	614	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	g	614	CLA	C1C-C2C-C3C	-5.57	100.74	106.92
22	D	403	CLA	C1C-C2C-C3C	-5.57	100.74	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	405	CLA	C1C-C2C-C3C	-5.57	100.75	106.92
22	2	604	CLA	C1C-C2C-C3C	-5.56	100.75	106.92
22	6	604	CLA	C1C-C2C-C3C	-5.56	100.75	106.92
22	s	301	CLA	C1C-C2C-C3C	-5.56	100.75	106.92
22	3	312	CLA	C1C-C2C-C3C	-5.55	100.76	106.92
22	7	312	CLA	C1C-C2C-C3C	-5.55	100.76	106.92
22	G	610	CLA	CHD-C4C-C3C	-5.55	116.55	124.92
22	g	610	CLA	CHD-C4C-C3C	-5.55	116.55	124.92
22	r	302	CLA	CHD-C4C-C3C	-5.55	116.55	124.92
22	R	302	CLA	CHD-C4C-C3C	-5.55	116.55	124.92
22	1	612	CLA	C1C-C2C-C3C	-5.54	100.77	106.92
22	5	612	CLA	C1C-C2C-C3C	-5.54	100.77	106.92
22	c	503	CLA	C1C-C2C-C3C	-5.53	100.78	106.92
22	b	610	CLA	C1C-C2C-C3C	-5.53	100.78	106.92
22	s	303	CLA	C1C-C2C-C3C	-5.53	100.78	106.92
22	S	303	CLA	C1C-C2C-C3C	-5.53	100.78	106.92
22	1	602	CLA	C1C-C2C-C3C	-5.53	100.78	106.92
22	5	602	CLA	C1C-C2C-C3C	-5.53	100.78	106.92
22	d	404	CLA	C1C-C2C-C3C	-5.52	100.79	106.92
22	6	611	CLA	C1C-C2C-C3C	-5.52	100.79	106.92
22	2	611	CLA	C1C-C2C-C3C	-5.52	100.79	106.92
22	B	601	CLA	CHD-C4C-C3C	-5.52	116.60	124.92
22	6	609	CLA	CHD-C4C-C3C	-5.50	116.62	124.92
22	2	609	CLA	CHD-C4C-C3C	-5.50	116.62	124.92
22	3	310	CLA	CHD-C4C-C3C	-5.50	116.64	124.92
22	7	310	CLA	CHD-C4C-C3C	-5.50	116.64	124.92
22	R	312	CLA	C1C-C2C-C3C	-5.50	100.82	106.92
22	r	312	CLA	C1C-C2C-C3C	-5.50	100.82	106.92
22	B	615	CLA	C1C-C2C-C3C	-5.49	100.82	106.92
22	n	610	CLA	CHD-C4C-C3C	-5.49	116.64	124.92
22	N	610	CLA	CHD-C4C-C3C	-5.49	116.64	124.92
22	2	610	CLA	C1C-C2C-C3C	-5.49	100.83	106.92
22	6	610	CLA	C1C-C2C-C3C	-5.49	100.83	106.92
22	b	602	CLA	C1C-C2C-C3C	-5.49	100.83	106.92
22	B	612	CLA	C1C-C2C-C3C	-5.48	100.84	106.92
22	C	512	CLA	C1C-C2C-C3C	-5.48	100.84	106.92
22	B	601	CLA	C1C-C2C-C3C	-5.48	100.84	106.92
22	C	503	CLA	C1C-C2C-C3C	-5.47	100.85	106.92
22	c	504	CLA	C1C-C2C-C3C	-5.47	100.85	106.92
22	C	505	CLA	C1C-C2C-C3C	-5.46	100.86	106.92
22	7	314	CLA	C1C-C2C-C3C	-5.44	100.88	106.92
22	3	314	CLA	C1C-C2C-C3C	-5.44	100.88	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	613	CLA	C1C-C2C-C3C	-5.43	100.90	106.92
22	6	613	CLA	C1C-C2C-C3C	-5.43	100.90	106.92
22	b	608	CLA	C1C-C2C-C3C	-5.42	100.90	106.92
25	y	609	CHL	C1C-C2C-C3C	-5.42	106.12	111.52
25	Y	609	CHL	C1C-C2C-C3C	-5.42	106.12	111.52
22	b	601	CLA	C1C-C2C-C3C	-5.41	100.92	106.92
22	C	502	CLA	C1C-C2C-C3C	-5.40	100.92	106.92
22	a	402	CLA	C1C-C2C-C3C	-5.40	100.93	106.92
22	r	302	CLA	C1C-C2C-C3C	-5.39	100.94	106.92
22	R	302	CLA	C1C-C2C-C3C	-5.39	100.94	106.92
25	N	608	CHL	C1C-C2C-C3C	-5.39	106.15	111.52
25	n	608	CHL	C1C-C2C-C3C	-5.39	106.15	111.52
22	a	403	CLA	C1C-C2C-C3C	-5.39	100.94	106.92
22	b	601	CLA	CHD-C4C-C3C	-5.37	116.83	124.92
22	B	613	CLA	C1C-C2C-C3C	-5.36	100.97	106.92
22	B	615	CLA	CHD-C4C-C3C	-5.35	116.85	124.92
22	S	311	CLA	CHD-C4C-C3C	-5.35	116.86	124.92
22	s	311	CLA	CHD-C4C-C3C	-5.35	116.86	124.92
25	g	606	CHL	C1C-C2C-C3C	-5.34	106.20	111.52
25	G	606	CHL	C1C-C2C-C3C	-5.34	106.20	111.52
22	B	614	CLA	C1C-C2C-C3C	-5.33	101.00	106.92
22	R	301	CLA	C1C-C2C-C3C	-5.33	101.01	106.92
22	r	301	CLA	C1C-C2C-C3C	-5.33	101.01	106.92
22	l	610	CLA	C1C-C2C-C3C	-5.32	101.02	106.92
22	5	610	CLA	C1C-C2C-C3C	-5.32	101.02	106.92
25	R	304	CHL	C1C-C2C-C3C	-5.31	106.22	111.52
25	r	304	CHL	C1C-C2C-C3C	-5.31	106.22	111.52
22	B	614	CLA	CHD-C4C-C3C	-5.31	116.91	124.92
22	B	605	CLA	C1C-C2C-C3C	-5.31	101.03	106.92
22	b	612	CLA	C1C-C2C-C3C	-5.31	101.03	106.92
22	c	505	CLA	C1C-C2C-C3C	-5.31	101.03	106.92
22	s	313	CLA	C1C-C2C-C3C	-5.31	101.03	106.92
22	S	313	CLA	C1C-C2C-C3C	-5.31	101.03	106.92
22	A	403	CLA	C1C-C2C-C3C	-5.30	101.04	106.92
22	r	307	CLA	C1C-C2C-C3C	-5.28	101.06	106.92
22	R	307	CLA	C1C-C2C-C3C	-5.28	101.06	106.92
22	S	304	CLA	C1C-C2C-C3C	-5.27	101.07	106.92
22	s	304	CLA	C1C-C2C-C3C	-5.27	101.07	106.92
25	g	608	CHL	C1C-C2C-C3C	-5.27	106.26	111.52
25	G	608	CHL	C1C-C2C-C3C	-5.27	106.26	111.52
22	y	610	CLA	CHD-C4C-C3C	-5.26	116.98	124.92
22	Y	610	CLA	CHD-C4C-C3C	-5.26	116.98	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	309	CHL	C1C-C2C-C3C	-5.26	106.28	111.52
25	3	309	CHL	C1C-C2C-C3C	-5.26	106.28	111.52
22	4	309	CLA	CHD-C4C-C3C	-5.25	117.01	124.92
22	8	309	CLA	CHD-C4C-C3C	-5.25	117.01	124.92
22	C	502	CLA	CHD-C4C-C3C	-5.25	117.01	124.92
22	1	610	CLA	CHD-C4C-C3C	-5.24	117.01	124.92
22	5	610	CLA	CHD-C4C-C3C	-5.24	117.01	124.92
22	R	308	CLA	CHD-C4C-C3C	-5.23	117.03	124.92
22	r	308	CLA	CHD-C4C-C3C	-5.23	117.03	124.92
22	y	611	CLA	CHD-C4C-C3C	-5.23	117.04	124.92
22	Y	611	CLA	CHD-C4C-C3C	-5.23	117.04	124.92
22	D	401	CLA	C1C-C2C-C3C	-5.22	101.13	106.92
25	n	609	CHL	C1C-C2C-C3C	-5.19	106.34	111.52
25	N	609	CHL	C1C-C2C-C3C	-5.19	106.34	111.52
25	6	608	CHL	C1C-C2C-C3C	-5.18	106.35	111.52
25	2	608	CHL	C1C-C2C-C3C	-5.18	106.35	111.52
22	b	605	CLA	C1C-C2C-C3C	-5.17	101.18	106.92
22	d	401	CLA	C1C-C2C-C3C	-5.17	101.18	106.92
22	a	403	CLA	CHD-C4C-C3C	-5.17	117.13	124.92
22	R	301	CLA	CHD-C4C-C3C	-5.16	117.15	124.92
22	r	301	CLA	CHD-C4C-C3C	-5.16	117.15	124.92
22	Y	604	CLA	CHD-C4C-C3C	-5.15	117.16	124.92
22	y	604	CLA	CHD-C4C-C3C	-5.15	117.16	124.92
22	c	505	CLA	CMA-C3A-C4A	-5.14	97.97	111.77
22	3	310	CLA	C1C-C2C-C3C	-5.13	101.23	106.92
22	7	310	CLA	C1C-C2C-C3C	-5.13	101.23	106.92
22	R	311	CLA	CHD-C4C-C3C	-5.11	117.22	124.92
22	r	311	CLA	CHD-C4C-C3C	-5.11	117.22	124.92
22	b	606	CLA	C1C-C2C-C3C	-5.11	101.25	106.92
22	c	512	CLA	CHD-C4C-C3C	-5.10	117.24	124.92
22	B	602	CLA	C1C-C2C-C3C	-5.10	101.27	106.92
22	C	507	CLA	CHD-C4C-C3C	-5.09	117.24	124.92
22	R	308	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
22	r	308	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
22	6	609	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
22	2	609	CLA	C1C-C2C-C3C	-5.09	101.27	106.92
25	n	606	CHL	C1C-C2C-C3C	-5.07	106.46	111.52
25	N	606	CHL	C1C-C2C-C3C	-5.07	106.46	111.52
22	G	610	CLA	C1C-C2C-C3C	-5.06	101.30	106.92
22	g	610	CLA	C1C-C2C-C3C	-5.06	101.30	106.92
25	3	306	CHL	CAA-C2A-C3A	-5.06	105.10	115.37
25	7	306	CHL	CAA-C2A-C3A	-5.06	105.10	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	503	CLA	CHD-C4C-C3C	-5.06	117.30	124.92
25	r	306	CHL	C1C-C2C-C3C	-5.05	106.48	111.52
25	R	306	CHL	C1C-C2C-C3C	-5.05	106.48	111.52
25	N	605	CHL	CAA-C2A-C3A	-5.05	105.12	115.37
25	n	605	CHL	CAA-C2A-C3A	-5.05	105.12	115.37
22	s	303	CLA	CHD-C4C-C3C	-5.04	117.31	124.92
22	S	303	CLA	CHD-C4C-C3C	-5.04	117.31	124.92
22	6	611	CLA	CHD-C4C-C3C	-5.04	117.32	124.92
22	2	611	CLA	CHD-C4C-C3C	-5.04	117.32	124.92
25	1	609	CHL	C1C-C2C-C3C	-5.03	106.51	111.52
25	5	609	CHL	C1C-C2C-C3C	-5.03	106.51	111.52
25	2	605	CHL	CAA-C2A-C3A	-5.03	105.16	115.37
25	6	605	CHL	CAA-C2A-C3A	-5.03	105.16	115.37
25	1	605	CHL	CAA-C2A-C3A	-5.00	105.21	115.37
25	5	605	CHL	CAA-C2A-C3A	-5.00	105.21	115.37
22	n	610	CLA	C1C-C2C-C3C	-5.00	101.38	106.92
22	N	610	CLA	C1C-C2C-C3C	-5.00	101.38	106.92
22	S	301	CLA	CHD-C4C-C3C	-4.95	117.45	124.92
22	Y	603	CLA	CHD-C4C-C3C	-4.95	117.46	124.92
22	y	603	CLA	CHD-C4C-C3C	-4.95	117.46	124.92
22	3	312	CLA	CHD-C4C-C3C	-4.94	117.47	124.92
22	7	312	CLA	CHD-C4C-C3C	-4.94	117.47	124.92
22	a	405	CLA	CHD-C4C-C3C	-4.93	117.49	124.92
22	8	302	CLA	CHD-C4C-C3C	-4.92	117.50	124.92
22	4	302	CLA	CHD-C4C-C3C	-4.92	117.50	124.92
22	C	510	CLA	CHD-C4C-C3C	-4.91	117.51	124.92
22	4	309	CLA	C1C-C2C-C3C	-4.91	101.47	106.92
22	8	309	CLA	C1C-C2C-C3C	-4.91	101.47	106.92
22	c	510	CLA	CHD-C4C-C3C	-4.90	117.53	124.92
22	G	602	CLA	CHD-C4C-C3C	-4.90	117.54	124.92
22	g	602	CLA	CHD-C4C-C3C	-4.90	117.54	124.92
22	c	502	CLA	CHD-C4C-C3C	-4.89	117.54	124.92
25	Y	607	CHL	C1C-C2C-C3C	-4.87	106.66	111.52
25	y	607	CHL	C1C-C2C-C3C	-4.87	106.66	111.52
25	N	605	CHL	C1C-C2C-C3C	-4.87	106.66	111.52
25	n	605	CHL	C1C-C2C-C3C	-4.87	106.66	111.52
22	c	507	CLA	CHD-C4C-C3C	-4.87	117.58	124.92
25	2	607	CHL	C1C-C2C-C3C	-4.87	106.67	111.52
25	6	607	CHL	C1C-C2C-C3C	-4.87	106.67	111.52
25	G	609	CHL	C1C-C2C-C3C	-4.86	106.67	111.52
25	g	609	CHL	C1C-C2C-C3C	-4.86	106.67	111.52
22	n	612	CLA	CHD-C4C-C3C	-4.86	117.60	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	612	CLA	CHD-C4C-C3C	-4.86	117.60	124.92
22	d	401	CLA	CHD-C4C-C3C	-4.85	117.61	124.92
25	Y	605	CHL	C1C-C2C-C3C	-4.85	106.69	111.52
25	y	605	CHL	C1C-C2C-C3C	-4.85	106.69	111.52
22	b	611	CLA	C1C-C2C-C3C	-4.84	101.55	106.92
25	1	608	CHL	C1C-C2C-C3C	-4.83	106.70	111.52
25	5	608	CHL	C1C-C2C-C3C	-4.83	106.70	111.52
25	7	308	CHL	C1C-C2C-C3C	-4.83	106.70	111.52
25	3	308	CHL	C1C-C2C-C3C	-4.83	106.70	111.52
25	y	606	CHL	C1C-C2C-C3C	-4.82	106.71	111.52
25	Y	606	CHL	C1C-C2C-C3C	-4.82	106.71	111.52
22	g	611	CLA	CHD-C4C-C3C	-4.81	117.66	124.92
22	G	611	CLA	CHD-C4C-C3C	-4.81	117.66	124.92
22	B	612	CLA	CHD-C4C-C3C	-4.81	117.67	124.92
22	B	606	CLA	C1C-C2C-C3C	-4.80	101.59	106.92
22	b	611	CLA	CHD-C4C-C3C	-4.80	117.68	124.92
25	G	607	CHL	C1C-C2C-C3C	-4.80	106.74	111.52
25	g	607	CHL	C1C-C2C-C3C	-4.80	106.74	111.52
23	d	402	PHO	C4C-C3C-C2C	-4.79	101.43	106.81
22	C	503	CLA	CHD-C4C-C3C	-4.79	117.69	124.92
25	g	605	CHL	CAA-C2A-C3A	-4.79	105.64	115.37
25	G	605	CHL	CAA-C2A-C3A	-4.79	105.64	115.37
22	2	612	CLA	CHD-C4C-C3C	-4.79	117.70	124.92
22	6	612	CLA	CHD-C4C-C3C	-4.79	117.70	124.92
22	D	403	CLA	CAC-C3C-C2C	-4.79	119.20	127.49
22	S	310	CLA	CHD-C4C-C3C	-4.78	117.71	124.92
22	s	310	CLA	CHD-C4C-C3C	-4.78	117.71	124.92
22	C	509	CLA	CHD-C4C-C3C	-4.78	117.72	124.92
22	n	611	CLA	CHD-C4C-C3C	-4.78	117.72	124.92
22	N	611	CLA	CHD-C4C-C3C	-4.78	117.72	124.92
22	r	310	CLA	CHD-C4C-C3C	-4.77	117.72	124.92
22	R	310	CLA	CHD-C4C-C3C	-4.77	117.72	124.92
25	2	605	CHL	C1C-C2C-C3C	-4.77	106.76	111.52
25	6	605	CHL	C1C-C2C-C3C	-4.77	106.76	111.52
22	y	613	CLA	CHD-C4C-C3C	-4.77	117.73	124.92
22	Y	613	CLA	CHD-C4C-C3C	-4.77	117.73	124.92
22	B	611	CLA	CHD-C4C-C3C	-4.76	117.74	124.92
22	7	303	CLA	CHD-C4C-C3C	-4.76	117.74	124.92
22	3	303	CLA	CHD-C4C-C3C	-4.76	117.74	124.92
23	D	402	PHO	C4C-C3C-C2C	-4.75	101.47	106.81
22	2	610	CLA	CHD-C4C-C3C	-4.75	117.76	124.92
22	6	610	CLA	CHD-C4C-C3C	-4.75	117.76	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	PHO	C4C-C3C-C2C	-4.75	101.48	106.81
22	b	613	CLA	CHD-C4C-C3C	-4.74	117.77	124.92
22	Y	614	CLA	CHD-C4C-C3C	-4.74	117.77	124.92
22	y	614	CLA	CHD-C4C-C3C	-4.74	117.77	124.92
22	S	314	CLA	CHD-C4C-C3C	-4.74	117.78	124.92
22	s	314	CLA	CHD-C4C-C3C	-4.74	117.78	124.92
25	4	306	CHL	C1C-C2C-C3C	-4.73	106.81	111.52
25	8	306	CHL	C1C-C2C-C3C	-4.73	106.81	111.52
22	B	608	CLA	CHD-C4C-C3C	-4.72	117.80	124.92
22	b	609	CLA	CHD-C4C-C3C	-4.72	117.80	124.92
22	a	402	CLA	CHD-C4C-C3C	-4.70	117.83	124.92
22	g	613	CLA	CHD-C4C-C3C	-4.70	117.83	124.92
22	G	613	CLA	CHD-C4C-C3C	-4.70	117.83	124.92
22	R	309	CLA	CHD-C4C-C3C	-4.70	117.83	124.92
22	r	309	CLA	CHD-C4C-C3C	-4.70	117.83	124.92
25	s	307	CHL	C1C-C2C-C3C	-4.70	106.84	111.52
25	S	307	CHL	C1C-C2C-C3C	-4.70	106.84	111.52
25	y	608	CHL	C1C-C2C-C3C	-4.69	106.84	111.52
25	Y	608	CHL	C1C-C2C-C3C	-4.69	106.84	111.52
22	n	613	CLA	CHD-C4C-C3C	-4.69	117.84	124.92
22	N	613	CLA	CHD-C4C-C3C	-4.69	117.84	124.92
23	a	404	PHO	C4C-C3C-C2C	-4.69	101.55	106.81
25	1	606	CHL	C1C-C2C-C3C	-4.69	106.85	111.52
25	5	606	CHL	C1C-C2C-C3C	-4.69	106.85	111.52
25	3	306	CHL	C1C-C2C-C3C	-4.68	106.86	111.52
25	7	306	CHL	C1C-C2C-C3C	-4.68	106.86	111.52
22	Y	602	CLA	CHD-C4C-C3C	-4.68	117.87	124.92
22	y	602	CLA	CHD-C4C-C3C	-4.68	117.87	124.92
22	1	602	CLA	CHD-C4C-C3C	-4.68	117.87	124.92
22	G	614	CLA	CHD-C4C-C3C	-4.68	117.87	124.92
22	g	614	CLA	CHD-C4C-C3C	-4.68	117.87	124.92
22	5	602	CLA	CHD-C4C-C3C	-4.68	117.87	124.92
22	g	612	CLA	CHD-C4C-C3C	-4.67	117.87	124.92
22	G	612	CLA	CHD-C4C-C3C	-4.67	117.87	124.92
22	B	611	CLA	C1C-C2C-C3C	-4.67	101.73	106.92
22	B	609	CLA	CHD-C4C-C3C	-4.67	117.88	124.92
25	s	306	CHL	C1C-C2C-C3C	-4.66	106.87	111.52
25	S	306	CHL	C1C-C2C-C3C	-4.66	106.87	111.52
22	A	403	CLA	CHD-C4C-C3C	-4.66	117.89	124.92
22	d	403	CLA	CAC-C3C-C2C	-4.66	119.42	127.49
22	N	602	CLA	CHD-C4C-C3C	-4.65	117.91	124.92
22	n	602	CLA	CHD-C4C-C3C	-4.65	117.91	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CHD-C4C-C3C	-4.65	117.92	124.92
22	R	312	CLA	CHD-C4C-C3C	-4.63	117.94	124.92
22	r	312	CLA	CHD-C4C-C3C	-4.63	117.94	124.92
25	2	606	CHL	C1C-C2C-C3C	-4.63	106.91	111.52
25	6	606	CHL	C1C-C2C-C3C	-4.63	106.91	111.52
22	S	305	CLA	CHD-C4C-C3C	-4.62	117.95	124.92
22	s	305	CLA	CHD-C4C-C3C	-4.62	117.95	124.92
22	b	614	CLA	CHD-C4C-C3C	-4.60	117.99	124.92
22	b	612	CLA	CMA-C3A-C4A	-4.60	99.42	111.77
22	7	313	CLA	CHD-C4C-C3C	-4.59	118.01	124.92
22	3	313	CLA	CHD-C4C-C3C	-4.59	118.01	124.92
22	b	610	CLA	CHD-C4C-C3C	-4.59	118.01	124.92
22	2	602	CLA	CHD-C4C-C3C	-4.58	118.01	124.92
22	6	602	CLA	CHD-C4C-C3C	-4.58	118.01	124.92
22	B	616	CLA	CHD-C4C-C3C	-4.57	118.02	124.92
22	4	303	CLA	CHD-C4C-C3C	-4.57	118.02	124.92
22	8	303	CLA	CHD-C4C-C3C	-4.57	118.02	124.92
22	D	404	CLA	CHD-C4C-C3C	-4.57	118.02	124.92
25	8	305	CHL	C1C-C2C-C3C	-4.57	106.96	111.52
25	4	305	CHL	C1C-C2C-C3C	-4.57	106.96	111.52
22	5	611	CLA	CHD-C4C-C3C	-4.57	118.03	124.92
22	1	611	CLA	CHD-C4C-C3C	-4.57	118.03	124.92
22	B	610	CLA	CHD-C4C-C3C	-4.56	118.04	124.92
22	D	401	CLA	CHD-C4C-C3C	-4.56	118.04	124.92
22	A	402	CLA	C1C-C2C-C3C	-4.56	101.86	106.92
25	7	307	CHL	C1C-C2C-C3C	-4.56	106.98	111.52
25	3	307	CHL	C1C-C2C-C3C	-4.56	106.98	111.52
22	B	608	CLA	CBC-CAC-C3C	-4.56	99.47	112.41
25	3	301	CHL	C1C-C2C-C3C	-4.56	106.98	111.52
25	7	301	CHL	C1C-C2C-C3C	-4.56	106.98	111.52
25	Y	601	CHL	C1C-C2C-C3C	-4.55	106.99	111.52
25	y	601	CHL	C1C-C2C-C3C	-4.55	106.99	111.52
25	4	307	CHL	C1C-C2C-C3C	-4.54	107.00	111.52
25	8	307	CHL	C1C-C2C-C3C	-4.54	107.00	111.52
22	s	309	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
22	S	309	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
22	1	603	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
22	5	603	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
22	B	606	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
22	7	311	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
22	3	311	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
22	R	303	CLA	CHD-C4C-C3C	-4.53	118.09	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	303	CLA	CHD-C4C-C3C	-4.53	118.09	124.92
25	1	601	CHL	C1C-C2C-C3C	-4.53	107.01	111.52
25	5	601	CHL	C1C-C2C-C3C	-4.53	107.01	111.52
22	B	604	CLA	C1D-CHD-C4C	-4.52	116.31	122.48
25	3	302	CHL	C1C-C2C-C3C	-4.52	107.02	111.52
25	7	302	CHL	C1C-C2C-C3C	-4.52	107.02	111.52
22	r	307	CLA	CHD-C4C-C3C	-4.51	118.12	124.92
22	R	307	CLA	CHD-C4C-C3C	-4.51	118.12	124.92
22	c	504	CLA	CHD-C4C-C3C	-4.50	118.13	124.92
25	4	301	CHL	C1C-C2C-C3C	-4.50	107.04	111.52
25	8	301	CHL	C1C-C2C-C3C	-4.50	107.04	111.52
22	8	310	CLA	CHD-C4C-C3C	-4.49	118.15	124.92
22	4	310	CLA	CHD-C4C-C3C	-4.49	118.15	124.92
22	n	603	CLA	CHD-C4C-C3C	-4.48	118.16	124.92
22	N	603	CLA	CHD-C4C-C3C	-4.48	118.16	124.92
22	4	304	CLA	CHD-C4C-C3C	-4.48	118.16	124.92
22	8	304	CLA	CHD-C4C-C3C	-4.48	118.16	124.92
25	g	605	CHL	C1C-C2C-C3C	-4.47	107.06	111.52
25	G	605	CHL	C1C-C2C-C3C	-4.47	107.06	111.52
25	5	615	CHL	C1C-C2C-C3C	-4.47	107.06	111.52
25	1	615	CHL	C1C-C2C-C3C	-4.47	107.06	111.52
22	A	402	CLA	C1D-CHD-C4C	-4.47	116.37	122.48
22	B	607	CLA	CHD-C4C-C3C	-4.47	118.18	124.92
22	B	604	CLA	CHC-C1C-C2C	-4.47	114.47	126.65
22	6	603	CLA	CHD-C4C-C3C	-4.46	118.19	124.92
22	2	603	CLA	CHD-C4C-C3C	-4.46	118.19	124.92
22	y	611	CLA	CBC-CAC-C3C	-4.46	99.75	112.41
22	Y	611	CLA	CBC-CAC-C3C	-4.46	99.75	112.41
25	g	601	CHL	C1C-C2C-C3C	-4.46	107.08	111.52
25	G	601	CHL	C1C-C2C-C3C	-4.46	107.08	111.52
22	n	604	CLA	CHD-C4C-C3C	-4.44	118.22	124.92
22	N	604	CLA	CHD-C4C-C3C	-4.44	118.22	124.92
25	1	607	CHL	C1C-C2C-C3C	-4.43	107.10	111.52
25	5	607	CHL	C1C-C2C-C3C	-4.43	107.10	111.52
22	c	511	CLA	CHD-C4C-C3C	-4.43	118.24	124.92
22	b	605	CLA	CHD-C4C-C3C	-4.43	118.25	124.92
22	2	613	CLA	CHD-C4C-C3C	-4.42	118.25	124.92
22	6	613	CLA	CHD-C4C-C3C	-4.42	118.25	124.92
22	s	313	CLA	CHD-C4C-C3C	-4.42	118.25	124.92
22	S	313	CLA	CHD-C4C-C3C	-4.42	118.25	124.92
25	8	308	CHL	C1C-C2C-C3C	-4.41	107.12	111.52
25	4	308	CHL	C1C-C2C-C3C	-4.41	107.12	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	506	CLA	CHD-C4C-C3C	-4.40	118.28	124.92
22	B	603	CLA	CHD-C4C-C3C	-4.40	118.28	124.92
22	c	501	CLA	CBC-CAC-C3C	-4.40	99.91	112.41
22	C	504	CLA	CHD-C4C-C3C	-4.39	118.30	124.92
22	B	615	CLA	C1D-CHD-C4C	-4.39	116.48	122.48
25	r	305	CHL	C1C-C2C-C3C	-4.39	107.14	111.52
25	R	305	CHL	C1C-C2C-C3C	-4.39	107.14	111.52
22	R	308	CLA	OBD-CAD-C3D	-4.39	119.94	128.03
22	r	308	CLA	OBD-CAD-C3D	-4.39	119.94	128.03
22	c	505	CLA	CHD-C4C-C3C	-4.38	118.31	124.92
22	S	304	CLA	CHD-C4C-C3C	-4.38	118.32	124.92
22	s	304	CLA	CHD-C4C-C3C	-4.38	118.32	124.92
22	l	613	CLA	CHD-C4C-C3C	-4.38	118.32	124.92
22	5	613	CLA	CHD-C4C-C3C	-4.38	118.32	124.92
22	d	404	CLA	CHD-C4C-C3C	-4.37	118.33	124.92
22	l	612	CLA	CHD-C4C-C3C	-4.37	118.33	124.92
22	5	612	CLA	CHD-C4C-C3C	-4.37	118.33	124.92
22	b	606	CLA	C1C-NC-C4C	-4.36	104.55	107.06
25	n	607	CHL	C1C-C2C-C3C	-4.36	107.18	111.52
25	6	601	CHL	C1C-C2C-C3C	-4.36	107.18	111.52
25	N	607	CHL	C1C-C2C-C3C	-4.36	107.18	111.52
25	2	601	CHL	C1C-C2C-C3C	-4.36	107.18	111.52
22	2	604	CLA	CHD-C4C-C3C	-4.36	118.35	124.92
22	6	604	CLA	CHD-C4C-C3C	-4.36	118.35	124.92
25	S	308	CHL	C1C-C2C-C3C	-4.35	107.18	111.52
25	s	308	CHL	C1C-C2C-C3C	-4.35	107.18	111.52
22	y	611	CLA	C1D-CHD-C4C	-4.35	116.54	122.48
22	Y	611	CLA	C1D-CHD-C4C	-4.35	116.54	122.48
25	S	302	CHL	C1C-C2C-C3C	-4.35	107.19	111.52
25	s	302	CHL	C1C-C2C-C3C	-4.35	107.19	111.52
22	C	512	CLA	CHD-C4C-C3C	-4.35	118.37	124.92
22	G	604	CLA	CHD-C4C-C3C	-4.33	118.39	124.92
22	g	604	CLA	CHD-C4C-C3C	-4.33	118.39	124.92
22	b	607	CLA	CHD-C4C-C3C	-4.33	118.39	124.92
22	S	311	CLA	C1D-CHD-C4C	-4.32	116.58	122.48
22	s	311	CLA	C1D-CHD-C4C	-4.32	116.58	122.48
22	C	505	CLA	CHD-C4C-C3C	-4.32	118.40	124.92
22	5	604	CLA	CHD-C4C-C3C	-4.32	118.41	124.92
22	l	604	CLA	CHD-C4C-C3C	-4.32	118.41	124.92
22	N	614	CLA	CHD-C4C-C3C	-4.31	118.42	124.92
22	n	614	CLA	CHD-C4C-C3C	-4.31	118.42	124.92
22	B	605	CLA	CHD-C4C-C3C	-4.30	118.44	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	CHD-C4C-C3C	-4.29	118.44	124.92
22	r	302	CLA	C1D-CHD-C4C	-4.29	116.62	122.48
22	R	302	CLA	C1D-CHD-C4C	-4.29	116.62	122.48
25	N	601	CHL	C1C-C2C-C3C	-4.27	107.27	111.52
25	n	601	CHL	C1C-C2C-C3C	-4.27	107.27	111.52
22	s	301	CLA	CHD-C4C-C3C	-4.26	118.50	124.92
22	7	305	CLA	CHD-C4C-C3C	-4.26	118.50	124.92
22	3	305	CLA	CHD-C4C-C3C	-4.26	118.50	124.92
22	a	403	CLA	OBD-CAD-C3D	-4.26	120.19	128.03
22	D	403	CLA	CHD-C4C-C3C	-4.23	118.54	124.92
22	R	303	CLA	OBD-CAD-C3D	-4.22	120.24	128.03
22	r	303	CLA	OBD-CAD-C3D	-4.22	120.24	128.03
22	b	608	CLA	CHD-C4C-C3C	-4.22	118.56	124.92
22	b	604	CLA	O2D-CGD-O1D	-4.21	115.35	123.82
22	b	615	CLA	CHD-C4C-C3C	-4.21	118.57	124.92
22	y	612	CLA	CHD-C4C-C3C	-4.20	118.59	124.92
22	Y	612	CLA	CHD-C4C-C3C	-4.20	118.59	124.92
22	S	305	CLA	O2D-CGD-O1D	-4.19	115.38	123.82
22	s	305	CLA	O2D-CGD-O1D	-4.19	115.38	123.82
22	G	603	CLA	CHD-C4C-C3C	-4.19	118.60	124.92
22	g	603	CLA	CHD-C4C-C3C	-4.19	118.60	124.92
22	B	613	CLA	CHD-C4C-C3C	-4.18	118.62	124.92
22	3	304	CLA	CHD-C4C-C3C	-4.17	118.63	124.92
22	7	304	CLA	CHD-C4C-C3C	-4.17	118.63	124.92
22	S	310	CLA	CBC-CAC-C3C	-4.17	100.56	112.41
22	s	310	CLA	CBC-CAC-C3C	-4.17	100.56	112.41
22	Y	604	CLA	C1D-CHD-C4C	-4.17	116.78	122.48
22	y	604	CLA	C1D-CHD-C4C	-4.17	116.78	122.48
22	c	503	CLA	C1D-CHD-C4C	-4.17	116.79	122.48
22	b	611	CLA	C1D-CHD-C4C	-4.16	116.79	122.48
22	B	612	CLA	C1D-CHD-C4C	-4.16	116.80	122.48
22	b	602	CLA	C1D-CHD-C4C	-4.16	116.80	122.48
22	Y	614	CLA	C1D-CHD-C4C	-4.14	116.83	122.48
22	y	614	CLA	C1D-CHD-C4C	-4.14	116.83	122.48
22	n	611	CLA	CBC-CAC-C3C	-4.13	100.68	112.41
22	N	611	CLA	CBC-CAC-C3C	-4.13	100.68	112.41
25	1	605	CHL	C1C-C2C-C3C	-4.12	107.42	111.52
25	5	605	CHL	C1C-C2C-C3C	-4.12	107.42	111.52
22	B	616	CLA	C1D-CHD-C4C	-4.10	116.88	122.48
22	8	302	CLA	CMA-C3A-C4A	-4.10	100.75	111.77
22	4	302	CLA	CMA-C3A-C4A	-4.10	100.75	111.77
22	c	501	CLA	CHD-C4C-C3C	-4.10	118.74	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	303	CLA	O2D-CGD-O1D	-4.09	115.58	123.82
22	r	303	CLA	O2D-CGD-O1D	-4.09	115.58	123.82
22	C	511	CLA	CHD-C4C-C3C	-4.09	118.75	124.92
22	S	312	CLA	CHD-C4C-C3C	-4.08	118.76	124.92
22	b	612	CLA	CHD-C4C-C3C	-4.08	118.76	124.92
22	s	312	CLA	CHD-C4C-C3C	-4.08	118.76	124.92
22	b	616	CLA	CAA-C2A-C3A	-4.08	101.61	112.81
22	g	611	CLA	CBC-CAC-C3C	-4.07	100.85	112.41
22	G	611	CLA	CBC-CAC-C3C	-4.07	100.85	112.41
22	B	611	CLA	C1D-CHD-C4C	-4.07	116.92	122.48
22	s	303	CLA	C1D-CHD-C4C	-4.06	116.93	122.48
22	S	303	CLA	C1D-CHD-C4C	-4.06	116.93	122.48
22	b	611	CLA	CGD-CBD-CAD	-4.05	97.16	110.71
22	a	403	CLA	C1D-CHD-C4C	-4.04	116.97	122.48
22	c	502	CLA	CBC-CAC-C3C	-4.04	100.95	112.41
22	7	314	CLA	CHD-C4C-C3C	-4.01	118.87	124.92
22	3	314	CLA	CHD-C4C-C3C	-4.01	118.87	124.92
22	y	613	CLA	C1D-CHD-C4C	-4.01	117.00	122.48
22	Y	613	CLA	C1D-CHD-C4C	-4.01	117.00	122.48
22	5	614	CLA	CAC-C3C-C2C	-4.00	120.56	127.49
22	1	614	CLA	CAC-C3C-C2C	-4.00	120.56	127.49
22	Y	603	CLA	CBC-CAC-C3C	-3.99	101.08	112.41
22	y	603	CLA	CBC-CAC-C3C	-3.99	101.08	112.41
22	D	401	CLA	C1D-CHD-C4C	-3.99	117.03	122.48
22	Y	603	CLA	C1D-CHD-C4C	-3.98	117.05	122.48
22	y	603	CLA	C1D-CHD-C4C	-3.98	117.05	122.48
22	C	508	CLA	CHC-C1C-C2C	-3.95	115.87	126.65
22	c	508	CLA	CHD-C4C-C3C	-3.95	118.96	124.92
22	C	506	CLA	CHC-C1C-C2C	-3.95	115.87	126.65
22	c	512	CLA	C1D-CHD-C4C	-3.94	117.09	122.48
22	a	405	CLA	CGD-CBD-CAD	-3.94	97.51	110.71
22	6	609	CLA	OBD-CAD-C3D	-3.94	120.77	128.03
22	2	609	CLA	OBD-CAD-C3D	-3.94	120.77	128.03
22	b	614	CLA	CAC-C3C-C2C	-3.93	120.67	127.49
22	B	605	CLA	C1D-CHD-C4C	-3.92	117.12	122.48
22	n	612	CLA	CBC-CAC-C3C	-3.92	101.28	112.41
22	N	612	CLA	CBC-CAC-C3C	-3.92	101.28	112.41
22	c	509	CLA	C1D-CHD-C4C	-3.92	117.13	122.48
22	d	401	CLA	C1D-CHD-C4C	-3.91	117.14	122.48
22	Y	614	CLA	CBC-CAC-C3C	-3.90	101.34	112.41
22	y	614	CLA	CBC-CAC-C3C	-3.90	101.34	112.41
22	r	307	CLA	C1D-CHD-C4C	-3.89	117.17	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	307	CLA	C1D-CHD-C4C	-3.89	117.17	122.48
22	B	601	CLA	C1D-CHD-C4C	-3.89	117.17	122.48
22	B	605	CLA	CBC-CAC-C3C	-3.88	101.39	112.41
22	D	401	CLA	OBD-CAD-C3D	-3.88	120.88	128.03
22	S	304	CLA	CBC-CAC-C3C	-3.88	101.40	112.41
22	s	304	CLA	CBC-CAC-C3C	-3.88	101.40	112.41
22	n	603	CLA	CBC-CAC-C3C	-3.87	101.42	112.41
22	N	603	CLA	CBC-CAC-C3C	-3.87	101.42	112.41
22	4	309	CLA	C1D-CHD-C4C	-3.87	117.20	122.48
22	8	309	CLA	C1D-CHD-C4C	-3.87	117.20	122.48
22	n	610	CLA	OBD-CAD-C3D	-3.86	120.91	128.03
22	N	610	CLA	OBD-CAD-C3D	-3.86	120.91	128.03
22	a	402	CLA	C1D-CHD-C4C	-3.85	117.23	122.48
22	S	314	CLA	C1D-CHD-C4C	-3.84	117.23	122.48
22	s	314	CLA	C1D-CHD-C4C	-3.84	117.23	122.48
22	S	312	CLA	CBC-CAC-C3C	-3.83	101.53	112.41
22	s	312	CLA	CBC-CAC-C3C	-3.83	101.53	112.41
22	C	502	CLA	C1D-CHD-C4C	-3.83	117.25	122.48
22	C	508	CLA	CHD-C4C-C3C	-3.83	119.14	124.92
22	B	613	CLA	CMA-C3A-C2A	-3.83	98.23	113.77
22	R	301	CLA	C1D-CHD-C4C	-3.83	117.25	122.48
22	r	301	CLA	C1D-CHD-C4C	-3.83	117.25	122.48
22	5	614	CLA	CHD-C4C-C3C	-3.83	119.15	124.92
22	l	614	CLA	CHD-C4C-C3C	-3.83	119.15	124.92
22	C	501	CLA	CHD-C4C-C3C	-3.82	119.15	124.92
22	B	611	CLA	CGD-CBD-CAD	-3.82	97.91	110.71
22	b	605	CLA	C1D-CHD-C4C	-3.82	117.27	122.48
22	n	604	CLA	CAA-C2A-C3A	-3.81	102.36	112.81
22	N	604	CLA	CAA-C2A-C3A	-3.81	102.36	112.81
22	B	604	CLA	CHD-C4C-C3C	-3.81	119.17	124.92
22	y	610	CLA	C1D-CHD-C4C	-3.81	117.28	122.48
22	Y	610	CLA	C1D-CHD-C4C	-3.81	117.28	122.48
22	R	311	CLA	C1D-CHD-C4C	-3.81	117.28	122.48
22	r	311	CLA	C1D-CHD-C4C	-3.81	117.28	122.48
22	Y	604	CLA	CBC-CAC-C3C	-3.80	101.63	112.41
22	y	604	CLA	CBC-CAC-C3C	-3.80	101.63	112.41
22	b	613	CLA	CBC-CAC-C3C	-3.80	101.63	112.41
22	d	403	CLA	CHD-C4C-C3C	-3.80	119.20	124.92
22	G	610	CLA	OBD-CAD-C3D	-3.79	121.05	128.03
22	g	610	CLA	OBD-CAD-C3D	-3.79	121.05	128.03
22	g	613	CLA	C1D-CHD-C4C	-3.78	117.31	122.48
22	G	613	CLA	C1D-CHD-C4C	-3.78	117.31	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	304	CLA	CAC-C3C-C2C	-3.78	120.93	127.49
22	s	304	CLA	CAC-C3C-C2C	-3.78	120.93	127.49
22	b	611	CLA	O2D-CGD-O1D	-3.78	116.22	123.82
22	G	610	CLA	C1D-CHD-C4C	-3.78	117.32	122.48
22	g	610	CLA	C1D-CHD-C4C	-3.78	117.32	122.48
22	b	613	CLA	OBD-CAD-C3D	-3.77	121.08	128.03
22	c	502	CLA	C1D-CHD-C4C	-3.77	117.33	122.48
22	b	605	CLA	CBC-CAC-C3C	-3.77	101.70	112.41
22	y	613	CLA	CBC-CAC-C3C	-3.77	101.71	112.41
22	Y	613	CLA	CBC-CAC-C3C	-3.77	101.71	112.41
22	b	603	CLA	CHD-C4C-C3C	-3.77	119.24	124.92
22	n	603	CLA	C1D-CHD-C4C	-3.77	117.34	122.48
22	N	603	CLA	C1D-CHD-C4C	-3.77	117.34	122.48
22	G	602	CLA	C1D-CHD-C4C	-3.76	117.35	122.48
22	g	602	CLA	C1D-CHD-C4C	-3.76	117.35	122.48
22	R	309	CLA	CBC-CAC-C3C	-3.76	101.74	112.41
22	r	309	CLA	CBC-CAC-C3C	-3.76	101.74	112.41
22	n	613	CLA	C1D-CHD-C4C	-3.76	117.35	122.48
22	N	613	CLA	C1D-CHD-C4C	-3.76	117.35	122.48
22	C	502	CLA	CBC-CAC-C3C	-3.75	101.77	112.41
22	C	503	CLA	C1D-CHD-C4C	-3.72	117.40	122.48
22	B	606	CLA	CAC-C3C-C2C	-3.72	121.05	127.49
22	B	615	CLA	CBC-CAC-C3C	-3.71	101.86	112.41
22	B	606	CLA	C1D-CHD-C4C	-3.71	117.41	122.48
22	6	603	CLA	CBC-CAC-C3C	-3.70	101.89	112.41
22	2	603	CLA	CBC-CAC-C3C	-3.70	101.89	112.41
22	r	302	CLA	CBC-CAC-C3C	-3.70	101.90	112.41
22	R	302	CLA	CBC-CAC-C3C	-3.70	101.90	112.41
22	C	506	CLA	C1D-CHD-C4C	-3.69	117.44	122.48
22	n	612	CLA	C1D-CHD-C4C	-3.69	117.44	122.48
22	N	612	CLA	C1D-CHD-C4C	-3.69	117.44	122.48
22	B	609	CLA	CMA-C3A-C4A	-3.69	101.85	111.77
22	b	606	CLA	CMA-C3A-C4A	-3.69	101.86	111.77
22	a	405	CLA	C1D-CHD-C4C	-3.69	117.44	122.48
22	g	612	CLA	CBC-CAC-C3C	-3.69	101.95	112.41
22	G	612	CLA	CBC-CAC-C3C	-3.69	101.95	112.41
22	s	313	CLA	CAC-C3C-C2C	-3.68	121.11	127.49
22	S	313	CLA	CAC-C3C-C2C	-3.68	121.11	127.49
22	S	311	CLA	CBC-CAC-C3C	-3.68	101.96	112.41
22	s	311	CLA	CBC-CAC-C3C	-3.68	101.96	112.41
22	C	501	CLA	CBC-CAC-C3C	-3.68	101.96	112.41
22	C	510	CLA	C1D-CHD-C4C	-3.68	117.46	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	C1D-CHD-C4C	-3.67	117.47	122.48
22	n	613	CLA	OBD-CAD-C3D	-3.67	121.27	128.03
22	N	613	CLA	OBD-CAD-C3D	-3.67	121.27	128.03
22	G	603	CLA	CBC-CAC-C3C	-3.66	102.01	112.41
22	g	603	CLA	CBC-CAC-C3C	-3.66	102.01	112.41
22	2	612	CLA	OBD-CAD-C3D	-3.66	121.28	128.03
22	6	612	CLA	OBD-CAD-C3D	-3.66	121.28	128.03
22	c	507	CLA	CHC-C1C-C2C	-3.66	116.67	126.65
22	B	609	CLA	C1D-CHD-C4C	-3.65	117.49	122.48
22	R	312	CLA	C1D-CHD-C4C	-3.65	117.49	122.48
22	r	312	CLA	C1D-CHD-C4C	-3.65	117.49	122.48
22	y	612	CLA	CBC-CAC-C3C	-3.65	102.06	112.41
22	Y	612	CLA	CBC-CAC-C3C	-3.65	102.06	112.41
22	g	612	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	G	612	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	S	310	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	G	614	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	g	614	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	s	310	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	8	302	CLA	C1D-CHD-C4C	-3.64	117.50	122.48
22	4	302	CLA	C1D-CHD-C4C	-3.64	117.50	122.48
22	S	305	CLA	CBC-CAC-C3C	-3.64	102.06	112.41
22	s	305	CLA	CBC-CAC-C3C	-3.64	102.06	112.41
22	C	510	CLA	CBC-CAC-C3C	-3.64	102.07	112.41
22	C	507	CLA	CBC-CAC-C3C	-3.64	102.07	112.41
22	A	403	CLA	C1D-CHD-C4C	-3.64	117.51	122.48
22	b	604	CLA	C1D-CHD-C4C	-3.63	117.52	122.48
22	D	403	CLA	C1D-CHD-C4C	-3.63	117.53	122.48
22	1	610	CLA	OBD-CAD-C3D	-3.63	121.34	128.03
22	5	610	CLA	OBD-CAD-C3D	-3.63	121.34	128.03
22	A	405	CLA	CGD-CBD-CAD	-3.62	98.57	110.71
22	b	616	CLA	CHD-C4C-C3C	-3.62	119.46	124.92
22	n	611	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
22	N	611	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
22	6	609	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
22	2	609	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
22	c	510	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
22	3	310	CLA	OBD-CAD-C3D	-3.62	121.36	128.03
22	7	310	CLA	OBD-CAD-C3D	-3.62	121.36	128.03
22	R	303	CLA	CBC-CAC-C3C	-3.61	102.17	112.41
22	r	303	CLA	CBC-CAC-C3C	-3.61	102.17	112.41
22	g	611	CLA	C1D-CHD-C4C	-3.61	117.56	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	611	CLA	C1D-CHD-C4C	-3.61	117.56	122.48
22	s	309	CLA	CGD-CBD-CAD	-3.60	98.63	110.71
22	S	309	CLA	CGD-CBD-CAD	-3.60	98.63	110.71
22	n	603	CLA	CAC-C3C-C2C	-3.60	121.25	127.49
22	N	603	CLA	CAC-C3C-C2C	-3.60	121.25	127.49
22	n	604	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
22	N	604	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
22	s	313	CLA	CBC-CAC-C3C	-3.60	102.19	112.41
22	S	313	CLA	CBC-CAC-C3C	-3.60	102.19	112.41
22	r	307	CLA	CAC-C3C-C2C	-3.60	121.26	127.49
22	R	307	CLA	CAC-C3C-C2C	-3.60	121.26	127.49
22	B	607	CLA	C1D-CHD-C4C	-3.60	117.57	122.48
22	B	609	CLA	OBD-CAD-C3D	-3.58	121.42	128.03
22	b	606	CLA	O2D-CGD-O1D	-3.58	116.61	123.82
22	6	609	CLA	CBC-CAC-C3C	-3.58	102.24	112.41
22	2	609	CLA	CBC-CAC-C3C	-3.58	102.24	112.41
22	B	615	CLA	O2D-CGD-O1D	-3.58	116.63	123.82
22	N	614	CLA	CBC-CAC-C3C	-3.57	102.26	112.41
22	n	614	CLA	CBC-CAC-C3C	-3.57	102.26	112.41
22	c	505	CLA	C1D-CHD-C4C	-3.57	117.60	122.48
22	c	508	CLA	CBC-CAC-C3C	-3.57	102.28	112.41
22	C	505	CLA	C1D-CHD-C4C	-3.57	117.61	122.48
22	1	610	CLA	C1D-CHD-C4C	-3.57	117.61	122.48
22	5	610	CLA	C1D-CHD-C4C	-3.57	117.61	122.48
25	1	607	CHL	CHA-CBD-CGD	-3.57	106.73	115.00
25	5	607	CHL	CHA-CBD-CGD	-3.57	106.73	115.00
22	B	609	CLA	CBC-CAC-C3C	-3.56	102.30	112.41
22	C	509	CLA	C1D-CHD-C4C	-3.56	117.62	122.48
22	C	508	CLA	C1D-CHD-C4C	-3.56	117.62	122.48
22	C	503	CLA	CBC-CAC-C3C	-3.56	102.31	112.41
22	c	506	CLA	CAC-C3C-C2C	-3.55	121.33	127.49
22	G	603	CLA	CAC-C3C-C2C	-3.55	121.34	127.49
22	g	603	CLA	CAC-C3C-C2C	-3.55	121.34	127.49
22	3	310	CLA	C1D-CHD-C4C	-3.55	117.63	122.48
22	7	310	CLA	C1D-CHD-C4C	-3.55	117.63	122.48
22	C	508	CLA	OBD-CAD-C3D	-3.55	121.49	128.03
22	B	608	CLA	C1D-CHD-C4C	-3.55	117.64	122.48
22	B	613	CLA	OBD-CAD-C3D	-3.55	121.49	128.03
22	c	509	CLA	CBC-CAC-C3C	-3.54	102.37	112.41
22	B	605	CLA	CAC-C3C-C2C	-3.54	121.36	127.49
22	B	606	CLA	OBD-CAD-C3D	-3.53	121.52	128.03
22	b	604	CLA	CHD-C4C-C3C	-3.53	119.60	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	314	CLA	CBC-CAC-C3C	-3.53	102.40	112.41
22	s	314	CLA	CBC-CAC-C3C	-3.53	102.40	112.41
22	2	612	CLA	C1D-CHD-C4C	-3.53	117.67	122.48
22	6	612	CLA	C1D-CHD-C4C	-3.53	117.67	122.48
22	C	507	CLA	CGD-CBD-CAD	-3.52	98.90	110.71
22	R	308	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
22	2	610	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
22	6	610	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
22	r	308	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
22	b	616	CLA	CAC-C3C-C2C	-3.52	121.39	127.49
22	n	613	CLA	CBC-CAC-C3C	-3.51	102.43	112.41
22	N	613	CLA	CBC-CAC-C3C	-3.51	102.43	112.41
22	C	504	CLA	CAC-C3C-C2C	-3.50	121.42	127.49
22	3	304	CLA	CBC-CAC-C3C	-3.50	102.47	112.41
22	7	304	CLA	CBC-CAC-C3C	-3.50	102.47	112.41
22	s	313	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
22	R	303	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
22	r	303	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
22	S	313	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
22	b	608	CLA	CBC-CAC-C3C	-3.49	102.49	112.41
22	c	508	CLA	CHC-C1C-C2C	-3.49	117.13	126.65
22	b	604	CLA	CHC-C1C-C2C	-3.49	117.13	126.65
22	r	310	CLA	CBC-CAC-C3C	-3.49	102.50	112.41
22	R	310	CLA	CBC-CAC-C3C	-3.49	102.50	112.41
22	c	503	CLA	CBC-CAC-C3C	-3.48	102.53	112.41
22	N	602	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
22	n	602	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
22	6	611	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
22	2	611	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
22	b	603	CLA	CGD-CBD-CAD	-3.47	99.09	110.71
22	g	613	CLA	CBC-CAC-C3C	-3.47	102.56	112.41
22	G	613	CLA	CBC-CAC-C3C	-3.47	102.56	112.41
22	R	303	CLA	CAA-C2A-C3A	-3.47	103.30	112.81
22	r	303	CLA	CAA-C2A-C3A	-3.47	103.30	112.81
22	y	612	CLA	C1D-CHD-C4C	-3.47	117.75	122.48
22	Y	612	CLA	C1D-CHD-C4C	-3.47	117.75	122.48
22	B	603	CLA	CBC-CAC-C3C	-3.46	102.57	112.41
22	B	613	CLA	CAA-C2A-C3A	-3.46	103.31	112.81
22	G	614	CLA	CBC-CAC-C3C	-3.46	102.58	112.41
22	g	614	CLA	CBC-CAC-C3C	-3.46	102.58	112.41
22	Y	602	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
22	y	602	CLA	C1D-CHD-C4C	-3.46	117.75	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	g	613	CLA	OBD-CAD-C3D	-3.46	121.64	128.03
22	G	613	CLA	OBD-CAD-C3D	-3.46	121.64	128.03
22	A	405	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
22	b	615	CLA	CBC-CAC-C3C	-3.46	102.58	112.41
22	B	614	CLA	C1D-CHD-C4C	-3.46	117.76	122.48
22	C	506	CLA	OBD-CAD-C3D	-3.46	121.66	128.03
22	Y	603	CLA	OBD-CAD-C3D	-3.46	121.66	128.03
22	y	603	CLA	OBD-CAD-C3D	-3.46	121.66	128.03
22	B	615	CLA	OBD-CAD-C3D	-3.45	121.67	128.03
22	G	602	CLA	CBC-CAC-C3C	-3.45	102.62	112.41
22	g	602	CLA	CBC-CAC-C3C	-3.45	102.62	112.41
22	c	507	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
22	l	613	CLA	OBD-CAD-C3D	-3.44	121.68	128.03
22	5	613	CLA	OBD-CAD-C3D	-3.44	121.68	128.03
22	C	508	CLA	CBC-CAC-C3C	-3.44	102.63	112.41
22	G	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.81
22	g	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.81
22	b	607	CLA	CAC-C3C-C2C	-3.44	121.52	127.49
22	Y	604	CLA	OBD-CAD-C3D	-3.44	121.68	128.03
22	y	604	CLA	OBD-CAD-C3D	-3.44	121.68	128.03
22	5	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.81
22	l	604	CLA	CAA-C2A-C3A	-3.44	103.37	112.81
22	R	309	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
22	r	309	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
22	a	405	CLA	OBD-CAD-C3D	-3.44	121.68	128.03
22	C	501	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
22	D	404	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
22	B	615	CLA	CAC-C3C-C2C	-3.44	121.53	127.49
22	C	509	CLA	CBC-CAC-C3C	-3.44	102.65	112.41
22	4	304	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
22	8	304	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
22	c	512	CLA	OBD-CAD-C3D	-3.43	121.70	128.03
22	3	304	CLA	CAC-C3C-C2C	-3.43	121.55	127.49
22	7	304	CLA	CAC-C3C-C2C	-3.43	121.55	127.49
22	B	613	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
22	N	602	CLA	CBC-CAC-C3C	-3.42	102.69	112.41
22	n	602	CLA	CBC-CAC-C3C	-3.42	102.69	112.41
22	s	309	CLA	OBD-CAD-C3D	-3.42	121.72	128.03
22	S	309	CLA	OBD-CAD-C3D	-3.42	121.72	128.03
22	l	603	CLA	CBC-CAC-C3C	-3.41	102.72	112.41
22	5	603	CLA	CBC-CAC-C3C	-3.41	102.72	112.41
22	c	508	CLA	OBD-CAD-C3D	-3.41	121.74	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	312	CLA	C1D-CHD-C4C	-3.41	117.83	122.48
22	7	312	CLA	C1D-CHD-C4C	-3.41	117.83	122.48
22	A	405	CLA	OBD-CAD-C3D	-3.40	121.75	128.03
22	b	611	CLA	OBD-CAD-C3D	-3.40	121.76	128.03
22	n	610	CLA	C1D-CHD-C4C	-3.40	117.84	122.48
22	N	610	CLA	C1D-CHD-C4C	-3.40	117.84	122.48
22	3	310	CLA	CBC-CAC-C3C	-3.40	102.77	112.41
22	7	310	CLA	CBC-CAC-C3C	-3.40	102.77	112.41
22	B	615	CLA	CAA-C2A-C3A	-3.40	103.50	112.81
22	R	301	CLA	CBC-CAC-C3C	-3.40	102.77	112.41
22	r	301	CLA	CBC-CAC-C3C	-3.40	102.77	112.41
22	B	616	CLA	CAC-C3C-C2C	-3.40	121.61	127.49
22	b	604	CLA	CBC-CAC-C3C	-3.39	102.77	112.41
22	B	607	CLA	CHC-C1C-C2C	-3.39	117.40	126.65
22	b	616	CLA	CHC-C1C-C2C	-3.39	117.41	126.65
22	b	613	CLA	CMA-C3A-C2A	-3.39	100.03	113.77
22	B	612	CLA	OBD-CAD-C3D	-3.38	121.80	128.03
22	b	601	CLA	C1D-CHD-C4C	-3.38	117.87	122.48
22	A	405	CLA	CBC-CAC-C3C	-3.38	102.82	112.41
22	4	303	CLA	C1D-CHD-C4C	-3.38	117.87	122.48
22	8	303	CLA	C1D-CHD-C4C	-3.38	117.87	122.48
22	b	614	CLA	CBC-CAC-C3C	-3.38	102.83	112.41
22	2	613	CLA	C1D-CHD-C4C	-3.37	117.87	122.48
22	6	613	CLA	C1D-CHD-C4C	-3.37	117.87	122.48
22	s	303	CLA	CBC-CAC-C3C	-3.37	102.84	112.41
22	S	303	CLA	CBC-CAC-C3C	-3.37	102.84	112.41
22	b	606	CLA	CAC-C3C-C2C	-3.37	121.65	127.49
22	B	611	CLA	O2D-CGD-O1D	-3.37	117.04	123.82
22	b	601	CLA	CBC-CAC-C3C	-3.37	102.85	112.41
23	A	404	PHO	C4D-ND-C1D	-3.37	100.91	106.98
22	1	602	CLA	C1D-CHD-C4C	-3.37	117.88	122.48
22	5	602	CLA	C1D-CHD-C4C	-3.37	117.88	122.48
22	b	606	CLA	OBD-CAD-C3D	-3.36	121.84	128.03
22	b	609	CLA	CBC-CAC-C3C	-3.36	102.88	112.41
22	B	616	CLA	CHC-C1C-C2C	-3.36	117.50	126.65
22	r	310	CLA	C1D-CHD-C4C	-3.36	117.90	122.48
22	R	310	CLA	C1D-CHD-C4C	-3.36	117.90	122.48
22	B	603	CLA	CAC-C3C-C2C	-3.36	121.68	127.49
22	7	303	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
22	3	303	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
22	7	311	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
22	3	311	CLA	C1D-CHD-C4C	-3.35	117.90	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	604	CLA	CBC-CAC-C3C	-3.35	102.90	112.41
22	N	604	CLA	CBC-CAC-C3C	-3.35	102.90	112.41
22	b	602	CLA	CBC-CAC-C3C	-3.35	102.90	112.41
22	c	510	CLA	CBC-CAC-C3C	-3.35	102.91	112.41
22	5	614	CLA	CBC-CAC-C3C	-3.35	102.91	112.41
22	1	614	CLA	CBC-CAC-C3C	-3.35	102.91	112.41
22	C	505	CLA	CAC-C3C-C2C	-3.34	121.70	127.49
22	7	313	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
22	3	313	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
22	5	611	CLA	CBC-CAC-C3C	-3.33	102.94	112.41
22	1	611	CLA	CBC-CAC-C3C	-3.33	102.94	112.41
22	c	501	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
22	b	616	CLA	CBC-CAC-C3C	-3.33	102.95	112.41
22	c	508	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
22	S	301	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
22	1	613	CLA	CBC-CAC-C3C	-3.33	102.96	112.41
22	5	613	CLA	CBC-CAC-C3C	-3.33	102.96	112.41
22	c	506	CLA	CHC-C1C-C2C	-3.33	117.58	126.65
22	c	505	CLA	CAC-C3C-C2C	-3.33	121.73	127.49
22	n	603	CLA	OBD-CAD-C3D	-3.32	121.90	128.03
22	N	603	CLA	OBD-CAD-C3D	-3.32	121.90	128.03
22	b	603	CLA	CAC-C3C-C2C	-3.32	121.73	127.49
22	B	608	CLA	OBD-CAD-C3D	-3.32	121.90	128.03
22	6	611	CLA	CBC-CAC-C3C	-3.32	102.98	112.41
22	2	611	CLA	CBC-CAC-C3C	-3.32	102.98	112.41
22	b	601	CLA	OBD-CAD-C3D	-3.32	121.91	128.03
22	2	612	CLA	CBC-CAC-C3C	-3.31	103.00	112.41
22	6	612	CLA	CBC-CAC-C3C	-3.31	103.00	112.41
22	c	511	CLA	C1D-CHD-C4C	-3.31	117.95	122.48
22	5	611	CLA	C1D-CHD-C4C	-3.31	117.96	122.48
22	1	611	CLA	C1D-CHD-C4C	-3.31	117.96	122.48
22	b	609	CLA	OBD-CAD-C3D	-3.31	121.93	128.03
22	c	511	CLA	CBC-CAC-C3C	-3.31	103.02	112.41
22	g	611	CLA	OBD-CAD-C3D	-3.31	121.93	128.03
22	y	610	CLA	OBD-CAD-C3D	-3.31	121.93	128.03
22	G	611	CLA	OBD-CAD-C3D	-3.31	121.93	128.03
22	Y	610	CLA	OBD-CAD-C3D	-3.31	121.93	128.03
22	D	401	CLA	CHC-C1C-C2C	-3.31	117.64	126.65
22	s	309	CLA	CHC-C1C-C2C	-3.30	117.64	126.65
22	S	309	CLA	CHC-C1C-C2C	-3.30	117.64	126.65
22	S	312	CLA	CHC-C1C-C2C	-3.30	117.64	126.65
22	s	312	CLA	CHC-C1C-C2C	-3.30	117.64	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	CBC-CAC-C3C	-3.30	103.04	112.41
22	c	511	CLA	OBD-CAD-C3D	-3.30	121.95	128.03
22	7	311	CLA	CBC-CAC-C3C	-3.30	103.04	112.41
22	3	311	CLA	CBC-CAC-C3C	-3.30	103.04	112.41
22	Y	602	CLA	CBC-CAC-C3C	-3.30	103.05	112.41
22	y	602	CLA	CBC-CAC-C3C	-3.30	103.05	112.41
22	B	613	CLA	CBC-CAC-C3C	-3.29	103.06	112.41
22	G	604	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
22	g	604	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
22	2	602	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
22	6	602	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
22	B	609	CLA	CAC-C3C-C2C	-3.29	121.79	127.49
22	C	506	CLA	CAC-C3C-C2C	-3.29	121.79	127.49
22	B	602	CLA	C1D-CHD-C4C	-3.29	117.99	122.48
22	S	301	CLA	CGD-CBD-CAD	-3.29	99.70	110.71
22	5	604	CLA	CBC-CAC-C3C	-3.28	103.09	112.41
22	1	604	CLA	CBC-CAC-C3C	-3.28	103.09	112.41
22	r	310	CLA	OBD-CAD-C3D	-3.28	121.98	128.03
22	R	310	CLA	OBD-CAD-C3D	-3.28	121.98	128.03
22	S	305	CLA	OBD-CAD-C3D	-3.28	121.98	128.03
22	s	305	CLA	OBD-CAD-C3D	-3.28	121.98	128.03
22	d	403	CLA	CHC-C1C-C2C	-3.28	117.71	126.65
22	C	511	CLA	CHC-C1C-C2C	-3.28	117.71	126.65
22	C	512	CLA	OBD-CAD-C3D	-3.28	121.99	128.03
22	B	607	CLA	OBD-CAD-C3D	-3.27	122.00	128.03
22	2	610	CLA	CBC-CAC-C3C	-3.27	103.12	112.41
22	6	610	CLA	CBC-CAC-C3C	-3.27	103.12	112.41
22	b	606	CLA	CBC-CAC-C3C	-3.27	103.13	112.41
22	6	603	CLA	OBD-CAD-C3D	-3.27	122.00	128.03
22	2	603	CLA	OBD-CAD-C3D	-3.27	122.00	128.03
22	4	303	CLA	CBC-CAC-C3C	-3.27	103.13	112.41
22	8	303	CLA	CBC-CAC-C3C	-3.27	103.13	112.41
22	G	604	CLA	CBC-CAC-C3C	-3.27	103.14	112.41
22	g	604	CLA	CBC-CAC-C3C	-3.27	103.14	112.41
22	c	505	CLA	OBD-CAD-C3D	-3.26	122.01	128.03
22	B	605	CLA	OBD-CAD-C3D	-3.26	122.01	128.03
22	a	405	CLA	CBC-CAC-C3C	-3.26	103.15	112.41
22	r	302	CLA	OBD-CAD-C3D	-3.26	122.02	128.03
22	R	302	CLA	OBD-CAD-C3D	-3.26	122.02	128.03
22	1	603	CLA	CAC-C3C-C2C	-3.26	121.84	127.49
22	5	603	CLA	CAC-C3C-C2C	-3.26	121.84	127.49
22	B	603	CLA	C1D-CHD-C4C	-3.26	118.03	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	612	CLA	CHC-C1C-C2C	-3.26	117.76	126.65
22	Y	612	CLA	CHC-C1C-C2C	-3.26	117.76	126.65
22	G	614	CLA	OBD-CAD-C3D	-3.26	122.02	128.03
22	g	614	CLA	OBD-CAD-C3D	-3.26	122.02	128.03
22	5	604	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
22	1	604	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
22	C	507	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
22	B	601	CLA	OBD-CAD-C3D	-3.26	122.03	128.03
22	C	508	CLA	CAC-C3C-C2C	-3.25	121.85	127.49
22	1	603	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
22	5	603	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
22	C	504	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
22	c	503	CLA	OBD-CAD-C3D	-3.25	122.04	128.03
22	s	309	CLA	C1D-CHD-C4C	-3.25	118.05	122.48
22	S	309	CLA	C1D-CHD-C4C	-3.25	118.05	122.48
22	S	314	CLA	OBD-CAD-C3D	-3.25	122.05	128.03
22	s	314	CLA	OBD-CAD-C3D	-3.25	122.05	128.03
22	6	603	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
22	2	603	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
22	c	508	CLA	CAC-C3C-C2C	-3.24	121.87	127.49
22	7	305	CLA	OBD-CAD-C3D	-3.24	122.05	128.03
22	3	305	CLA	OBD-CAD-C3D	-3.24	122.05	128.03
22	C	505	CLA	CHC-C1C-C2C	-3.24	117.81	126.65
22	B	603	CLA	OBD-CAD-C3D	-3.24	122.06	128.03
22	B	608	CLA	CHC-C1C-C2C	-3.24	117.81	126.65
22	d	401	CLA	CAA-C2A-C3A	-3.24	103.93	112.81
22	B	615	CLA	CGD-CBD-CAD	-3.24	99.86	110.71
22	7	314	CLA	CBC-CAC-C3C	-3.24	103.22	112.41
22	3	314	CLA	CBC-CAC-C3C	-3.24	103.22	112.41
22	S	301	CLA	OBD-CAD-C3D	-3.24	122.06	128.03
22	7	313	CLA	CBC-CAC-C3C	-3.23	103.23	112.41
22	3	313	CLA	CBC-CAC-C3C	-3.23	103.23	112.41
22	y	613	CLA	OBD-CAD-C3D	-3.23	122.07	128.03
22	Y	613	CLA	OBD-CAD-C3D	-3.23	122.07	128.03
22	b	612	CLA	OBD-CAD-C3D	-3.23	122.08	128.03
22	5	614	CLA	CHC-C1C-C2C	-3.23	117.85	126.65
22	1	614	CLA	CHC-C1C-C2C	-3.23	117.85	126.65
22	G	603	CLA	C1D-CHD-C4C	-3.23	118.08	122.48
22	g	603	CLA	C1D-CHD-C4C	-3.23	118.08	122.48
22	c	501	CLA	CHC-C1C-C2C	-3.23	117.85	126.65
22	C	504	CLA	CHC-C1C-C2C	-3.22	117.86	126.65
22	c	502	CLA	CHC-C1C-C2C	-3.22	117.86	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	611	CLA	OBD-CAD-C3D	-3.22	122.09	128.03
22	N	611	CLA	OBD-CAD-C3D	-3.22	122.09	128.03
22	S	312	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
22	s	312	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
22	Y	614	CLA	CAC-C3C-C2C	-3.22	121.91	127.49
22	y	614	CLA	CAC-C3C-C2C	-3.22	121.91	127.49
22	B	605	CLA	CHC-C1C-C2C	-3.22	117.88	126.65
22	c	504	CLA	C1D-CHD-C4C	-3.22	118.09	122.48
22	D	404	CLA	CBC-CAC-C3C	-3.22	103.28	112.41
22	1	612	CLA	CBC-CAC-C3C	-3.22	103.28	112.41
22	5	612	CLA	CBC-CAC-C3C	-3.22	103.28	112.41
22	R	311	CLA	CBC-CAC-C3C	-3.21	103.29	112.41
22	r	311	CLA	CBC-CAC-C3C	-3.21	103.29	112.41
22	4	304	CLA	CBC-CAC-C3C	-3.21	103.29	112.41
22	8	304	CLA	CBC-CAC-C3C	-3.21	103.29	112.41
22	y	611	CLA	OBD-CAD-C3D	-3.21	122.11	128.03
22	Y	611	CLA	OBD-CAD-C3D	-3.21	122.11	128.03
22	b	616	CLA	OBD-CAD-C3D	-3.21	122.11	128.03
22	D	403	CLA	CHC-C1C-C2C	-3.21	117.90	126.65
22	2	610	CLA	OBD-CAD-C3D	-3.21	122.11	128.03
22	6	610	CLA	OBD-CAD-C3D	-3.21	122.11	128.03
22	b	613	CLA	CMA-C3A-C4A	-3.21	103.15	111.77
22	R	309	CLA	CGD-CBD-CAD	-3.21	99.97	110.71
22	r	309	CLA	CGD-CBD-CAD	-3.21	99.97	110.71
22	Y	614	CLA	OBD-CAD-C3D	-3.21	122.12	128.03
22	y	614	CLA	OBD-CAD-C3D	-3.21	122.12	128.03
22	6	603	CLA	CAC-C3C-C2C	-3.21	121.94	127.49
22	2	603	CLA	CAC-C3C-C2C	-3.21	121.94	127.49
25	1	607	CHL	O1D-CGD-CBD	-3.20	117.91	124.53
25	5	607	CHL	O1D-CGD-CBD	-3.20	117.91	124.53
22	1	610	CLA	O2D-CGD-O1D	-3.20	117.37	123.82
22	5	610	CLA	O2D-CGD-O1D	-3.20	117.37	123.82
22	7	313	CLA	OBD-CAD-C3D	-3.20	122.12	128.03
22	3	313	CLA	OBD-CAD-C3D	-3.20	122.12	128.03
22	C	512	CLA	C1D-CHD-C4C	-3.20	118.11	122.48
22	3	312	CLA	CBC-CAC-C3C	-3.20	103.32	112.41
22	7	312	CLA	CBC-CAC-C3C	-3.20	103.32	112.41
22	R	311	CLA	CAC-C3C-C2C	-3.20	121.94	127.49
22	r	311	CLA	CAC-C3C-C2C	-3.20	121.94	127.49
22	5	611	CLA	OBD-CAD-C3D	-3.20	122.13	128.03
22	1	611	CLA	OBD-CAD-C3D	-3.20	122.13	128.03
22	c	506	CLA	CBC-CAC-C3C	-3.20	103.33	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	512	CLA	CBC-CAC-C3C	-3.20	103.33	112.41
22	c	512	CLA	CHC-C1C-C2C	-3.20	117.94	126.65
22	1	603	CLA	OBD-CAD-C3D	-3.19	122.14	128.03
22	5	603	CLA	OBD-CAD-C3D	-3.19	122.14	128.03
22	C	506	CLA	CBC-CAC-C3C	-3.19	103.35	112.41
22	3	304	CLA	OBD-CAD-C3D	-3.19	122.15	128.03
22	7	304	CLA	OBD-CAD-C3D	-3.19	122.15	128.03
22	2	604	CLA	OBD-CAD-C3D	-3.19	122.15	128.03
22	6	604	CLA	OBD-CAD-C3D	-3.19	122.15	128.03
22	8	302	CLA	CBC-CAC-C3C	-3.19	103.37	112.41
22	4	302	CLA	CBC-CAC-C3C	-3.19	103.37	112.41
22	s	301	CLA	CAC-C3C-C2C	-3.18	121.98	127.49
22	b	609	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
25	1	605	CHL	OMC-CMC-C2C	-3.18	120.23	124.29
25	5	605	CHL	OMC-CMC-C2C	-3.18	120.23	124.29
25	N	605	CHL	CHA-CBD-CGD	-3.18	107.63	115.00
25	n	605	CHL	CHA-CBD-CGD	-3.18	107.63	115.00
22	B	611	CLA	OBD-CAD-C3D	-3.17	122.18	128.03
22	c	507	CLA	CBC-CAC-C3C	-3.17	103.40	112.41
22	b	607	CLA	C1D-CHD-C4C	-3.17	118.15	122.48
22	c	505	CLA	CHC-C1C-C2C	-3.17	118.00	126.65
22	C	501	CLA	CHC-C1C-C2C	-3.17	118.01	126.65
22	G	603	CLA	OBD-CAD-C3D	-3.17	122.19	128.03
22	g	603	CLA	OBD-CAD-C3D	-3.17	122.19	128.03
22	2	604	CLA	CAC-C3C-C2C	-3.16	122.01	127.49
22	6	604	CLA	CAC-C3C-C2C	-3.16	122.01	127.49
22	8	310	CLA	CBC-CAC-C3C	-3.16	103.44	112.41
22	4	310	CLA	CBC-CAC-C3C	-3.16	103.44	112.41
22	8	302	CLA	O2D-CGD-O1D	-3.16	117.46	123.82
22	4	302	CLA	O2D-CGD-O1D	-3.16	117.46	123.82
22	G	604	CLA	CAC-C3C-C2C	-3.16	122.02	127.49
22	g	604	CLA	CAC-C3C-C2C	-3.16	122.02	127.49
22	c	503	CLA	CAC-C3C-C2C	-3.16	122.02	127.49
22	R	312	CLA	OBD-CAD-C3D	-3.16	122.21	128.03
22	r	312	CLA	OBD-CAD-C3D	-3.16	122.21	128.03
22	S	310	CLA	OBD-CAD-C3D	-3.16	122.21	128.03
22	s	310	CLA	OBD-CAD-C3D	-3.16	122.21	128.03
22	B	610	CLA	C1D-CHD-C4C	-3.16	118.17	122.48
22	1	612	CLA	OBD-CAD-C3D	-3.15	122.22	128.03
22	5	612	CLA	OBD-CAD-C3D	-3.15	122.22	128.03
22	B	615	CLA	CHC-C1C-C2C	-3.15	118.06	126.65
25	n	607	CHL	CHA-CBD-CGD	-3.15	107.69	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	607	CHL	CHA-CBD-CGD	-3.15	107.69	115.00
22	7	305	CLA	CAC-C3C-C2C	-3.15	122.03	127.49
22	3	305	CLA	CAC-C3C-C2C	-3.15	122.03	127.49
22	4	304	CLA	OBD-CAD-C3D	-3.15	122.23	128.03
22	8	304	CLA	OBD-CAD-C3D	-3.15	122.23	128.03
22	d	404	CLA	C1D-CHD-C4C	-3.15	118.19	122.48
22	b	609	CLA	CAC-C3C-C2C	-3.15	122.04	127.49
22	S	314	CLA	CAC-C3C-C2C	-3.14	122.05	127.49
22	s	314	CLA	CAC-C3C-C2C	-3.14	122.05	127.49
22	b	613	CLA	CHC-C1C-C2C	-3.14	118.08	126.65
22	B	603	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
22	R	311	CLA	OBD-CAD-C3D	-3.14	122.24	128.03
22	r	311	CLA	OBD-CAD-C3D	-3.14	122.24	128.03
22	1	613	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
22	5	613	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
22	D	403	CLA	CAA-C2A-C3A	-3.14	104.20	112.81
22	3	310	CLA	O2D-CGD-O1D	-3.14	117.50	123.82
22	7	310	CLA	O2D-CGD-O1D	-3.14	117.50	123.82
22	C	511	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
22	Y	604	CLA	CAC-C3C-C2C	-3.14	122.05	127.49
22	y	604	CLA	CAC-C3C-C2C	-3.14	122.05	127.49
22	C	510	CLA	CHC-C1C-C2C	-3.13	118.10	126.65
22	G	603	CLA	CHC-C1C-C2C	-3.13	118.11	126.65
22	g	603	CLA	CHC-C1C-C2C	-3.13	118.11	126.65
22	6	611	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	2	611	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	7	314	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	3	314	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	N	614	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	n	614	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	d	401	CLA	CBC-CAC-C3C	-3.13	103.52	112.41
22	7	311	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	3	311	CLA	OBD-CAD-C3D	-3.13	122.26	128.03
22	c	506	CLA	OBD-CAD-C3D	-3.13	122.27	128.03
22	B	611	CLA	CAA-C2A-C3A	-3.13	104.24	112.81
22	b	611	CLA	CBC-CAC-C3C	-3.12	103.54	112.41
22	B	611	CLA	CBC-CAC-C3C	-3.12	103.56	112.41
22	c	506	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
22	n	603	CLA	CHC-C1C-C2C	-3.11	118.16	126.65
22	N	603	CLA	CHC-C1C-C2C	-3.11	118.16	126.65
22	d	403	CLA	C1D-CHD-C4C	-3.11	118.23	122.48
22	7	305	CLA	C1D-CHD-C4C	-3.11	118.24	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	305	CLA	C1D-CHD-C4C	-3.11	118.24	122.48
22	8	310	CLA	OBD-CAD-C3D	-3.11	122.30	128.03
22	4	310	CLA	OBD-CAD-C3D	-3.11	122.30	128.03
22	G	604	CLA	OBD-CAD-C3D	-3.10	122.31	128.03
22	g	604	CLA	OBD-CAD-C3D	-3.10	122.31	128.03
22	B	610	CLA	CBC-CAC-C3C	-3.10	103.60	112.41
22	A	405	CLA	CAC-C3C-C2C	-3.10	122.12	127.49
22	b	611	CLA	CHC-C1C-C2C	-3.10	118.20	126.65
22	3	312	CLA	OBD-CAD-C3D	-3.10	122.32	128.03
22	7	312	CLA	OBD-CAD-C3D	-3.10	122.32	128.03
22	2	613	CLA	OBD-CAD-C3D	-3.10	122.32	128.03
22	6	613	CLA	OBD-CAD-C3D	-3.10	122.32	128.03
22	1	602	CLA	CBC-CAC-C3C	-3.09	103.62	112.41
22	R	312	CLA	CBC-CAC-C3C	-3.09	103.62	112.41
22	5	602	CLA	CBC-CAC-C3C	-3.09	103.62	112.41
22	r	312	CLA	CBC-CAC-C3C	-3.09	103.62	112.41
22	d	403	CLA	CAA-C2A-C3A	-3.09	104.34	112.81
22	S	304	CLA	C1D-CHD-C4C	-3.09	118.26	122.48
22	s	304	CLA	C1D-CHD-C4C	-3.09	118.26	122.48
25	8	308	CHL	OBD-CAD-CBD	-3.09	120.04	127.52
25	4	308	CHL	OBD-CAD-CBD	-3.09	120.04	127.52
22	C	511	CLA	OBD-CAD-C3D	-3.09	122.34	128.03
22	B	612	CLA	CHC-C1C-C2C	-3.09	118.23	126.65
22	7	305	CLA	CBC-CAC-C3C	-3.09	103.65	112.41
22	3	305	CLA	CBC-CAC-C3C	-3.09	103.65	112.41
22	r	310	CLA	CGD-CBD-CAD	-3.09	100.37	110.71
22	R	310	CLA	CGD-CBD-CAD	-3.09	100.37	110.71
22	2	604	CLA	C1D-CHD-C4C	-3.09	118.27	122.48
22	6	604	CLA	C1D-CHD-C4C	-3.09	118.27	122.48
22	B	607	CLA	CBC-CAC-C3C	-3.08	103.65	112.41
22	Y	603	CLA	CAC-C3C-C2C	-3.08	122.15	127.49
22	y	603	CLA	CAC-C3C-C2C	-3.08	122.15	127.49
22	d	403	CLA	CGD-CBD-CAD	-3.08	100.39	110.71
22	b	609	CLA	CHC-C1C-C2C	-3.08	118.25	126.65
22	2	613	CLA	CBC-CAC-C3C	-3.08	103.67	112.41
22	6	613	CLA	CBC-CAC-C3C	-3.08	103.67	112.41
22	c	509	CLA	OBD-CAD-C3D	-3.08	122.36	128.03
22	4	309	CLA	CAC-C3C-C2C	-3.08	122.16	127.49
22	8	309	CLA	CAC-C3C-C2C	-3.08	122.16	127.49
22	N	614	CLA	C1D-CHD-C4C	-3.07	118.28	122.48
22	n	614	CLA	C1D-CHD-C4C	-3.07	118.28	122.48
22	Y	604	CLA	CAA-C2A-C3A	-3.07	104.38	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	604	CLA	CAA-C2A-C3A	-3.07	104.38	112.81
22	n	604	CLA	CAC-C3C-C2C	-3.07	122.17	127.49
22	N	604	CLA	CAC-C3C-C2C	-3.07	122.17	127.49
22	B	611	CLA	CAC-C3C-C2C	-3.07	122.17	127.49
22	A	403	CLA	OBD-CAD-C3D	-3.07	122.37	128.03
22	N	602	CLA	CAC-C3C-C2C	-3.07	122.18	127.49
22	n	602	CLA	CAC-C3C-C2C	-3.07	122.18	127.49
22	4	304	CLA	CAC-C3C-C2C	-3.06	122.18	127.49
22	8	304	CLA	CAC-C3C-C2C	-3.06	122.18	127.49
22	A	403	CLA	CBC-CAC-C3C	-3.06	103.72	112.41
22	y	613	CLA	CHC-C1C-C2C	-3.06	118.30	126.65
22	Y	613	CLA	CHC-C1C-C2C	-3.06	118.30	126.65
22	B	606	CLA	O2D-CGD-O1D	-3.06	117.66	123.82
22	R	309	CLA	OBD-CAD-C3D	-3.06	122.39	128.03
22	8	302	CLA	OBD-CAD-C3D	-3.06	122.39	128.03
22	r	309	CLA	OBD-CAD-C3D	-3.06	122.39	128.03
22	4	302	CLA	OBD-CAD-C3D	-3.06	122.39	128.03
22	a	402	CLA	CBC-CAC-C3C	-3.06	103.73	112.41
22	c	504	CLA	CHC-C1C-C2C	-3.06	118.31	126.65
22	b	611	CLA	CAC-C3C-C2C	-3.06	122.19	127.49
22	8	310	CLA	C1D-CHD-C4C	-3.06	118.31	122.48
22	4	310	CLA	C1D-CHD-C4C	-3.06	118.31	122.48
22	S	304	CLA	CHC-C1C-C2C	-3.05	118.32	126.65
22	s	304	CLA	CHC-C1C-C2C	-3.05	118.32	126.65
22	s	313	CLA	OBD-CAD-C3D	-3.05	122.40	128.03
22	S	313	CLA	OBD-CAD-C3D	-3.05	122.40	128.03
25	R	304	CHL	OBD-CAD-CBD	-3.05	120.12	127.52
25	r	304	CHL	OBD-CAD-CBD	-3.05	120.12	127.52
22	1	612	CLA	C1D-CHD-C4C	-3.05	118.31	122.48
22	5	612	CLA	C1D-CHD-C4C	-3.05	118.31	122.48
22	s	303	CLA	CAC-C3C-C2C	-3.05	122.20	127.49
22	S	303	CLA	CAC-C3C-C2C	-3.05	122.20	127.49
22	S	312	CLA	CAC-C3C-C2C	-3.05	122.20	127.49
22	s	312	CLA	CAC-C3C-C2C	-3.05	122.20	127.49
22	g	613	CLA	CHC-C1C-C2C	-3.05	118.34	126.65
22	G	613	CLA	CHC-C1C-C2C	-3.05	118.34	126.65
22	Y	614	CLA	CHC-C1C-C2C	-3.05	118.34	126.65
22	y	614	CLA	CHC-C1C-C2C	-3.05	118.34	126.65
22	7	314	CLA	CAC-C3C-C2C	-3.05	122.21	127.49
22	3	314	CLA	CAC-C3C-C2C	-3.05	122.21	127.49
22	5	614	CLA	C1D-CHD-C4C	-3.05	118.32	122.48
22	1	614	CLA	C1D-CHD-C4C	-3.05	118.32	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	CLA	OBD-CAD-C3D	-3.04	122.42	128.03
22	c	510	CLA	CHC-C1C-C2C	-3.04	118.35	126.65
25	n	606	CHL	OBD-CAD-CBD	-3.04	120.15	127.52
25	N	606	CHL	OBD-CAD-CBD	-3.04	120.15	127.52
22	b	610	CLA	C1D-CHD-C4C	-3.04	118.33	122.48
22	d	403	CLA	OBD-CAD-C3D	-3.04	122.42	128.03
22	g	612	CLA	OBD-CAD-C3D	-3.04	122.42	128.03
22	G	612	CLA	OBD-CAD-C3D	-3.04	122.42	128.03
22	a	403	CLA	CBC-CAC-C3C	-3.04	103.78	112.41
22	c	502	CLA	OBD-CAD-C3D	-3.04	122.43	128.03
22	d	404	CLA	CBC-CAC-C3C	-3.04	103.79	112.41
22	2	602	CLA	CAC-C3C-C2C	-3.04	122.23	127.49
22	6	602	CLA	CAC-C3C-C2C	-3.04	122.23	127.49
22	b	613	CLA	CAC-C3C-C2C	-3.03	122.23	127.49
22	y	611	CLA	CAC-C3C-C2C	-3.03	122.23	127.49
22	b	608	CLA	CAC-C3C-C2C	-3.03	122.23	127.49
22	Y	611	CLA	CAC-C3C-C2C	-3.03	122.23	127.49
22	5	604	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	1	604	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	R	309	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	G	602	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	B	613	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	r	309	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	g	602	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	n	612	CLA	CHC-C1C-C2C	-3.03	118.38	126.65
22	N	612	CLA	CHC-C1C-C2C	-3.03	118.38	126.65
22	C	511	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	n	611	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	N	611	CLA	CAC-C3C-C2C	-3.03	122.24	127.49
22	C	504	CLA	CBC-CAC-C3C	-3.03	103.81	112.41
22	R	301	CLA	OBD-CAD-C3D	-3.03	122.44	128.03
22	r	301	CLA	OBD-CAD-C3D	-3.03	122.44	128.03
22	2	604	CLA	CBC-CAC-C3C	-3.03	103.81	112.41
22	6	604	CLA	CBC-CAC-C3C	-3.03	103.81	112.41
22	B	602	CLA	OBD-CAD-C3D	-3.03	122.45	128.03
22	C	503	CLA	CAC-C3C-C2C	-3.03	122.25	127.49
22	C	504	CLA	OBD-CAD-C3D	-3.02	122.45	128.03
25	y	608	CHL	OBD-CAD-CBD	-3.02	120.20	127.52
25	Y	608	CHL	OBD-CAD-CBD	-3.02	120.20	127.52
22	4	309	CLA	OBD-CAD-C3D	-3.02	122.46	128.03
22	8	309	CLA	OBD-CAD-C3D	-3.02	122.46	128.03
22	c	504	CLA	CAC-C3C-C2C	-3.02	122.26	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	604	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
22	g	604	CLA	CHC-C1C-C2C	-3.02	118.42	126.65
22	n	613	CLA	CAC-C3C-C2C	-3.02	122.26	127.49
22	N	613	CLA	CAC-C3C-C2C	-3.02	122.26	127.49
22	a	405	CLA	CAC-C3C-C2C	-3.02	122.26	127.49
22	r	307	CLA	OBD-CAD-C3D	-3.02	122.47	128.03
22	R	307	CLA	OBD-CAD-C3D	-3.02	122.47	128.03
22	b	606	CLA	CHD-C4C-C3C	-3.02	120.37	124.92
22	S	301	CLA	CAC-C3C-C2C	-3.02	122.27	127.49
22	S	311	CLA	OBD-CAD-C3D	-3.02	122.47	128.03
22	s	311	CLA	OBD-CAD-C3D	-3.02	122.47	128.03
22	S	305	CLA	C1D-CHD-C4C	-3.01	118.36	122.48
22	s	305	CLA	C1D-CHD-C4C	-3.01	118.36	122.48
22	s	301	CLA	CBC-CAC-C3C	-3.01	103.85	112.41
22	S	301	CLA	CBC-CAC-C3C	-3.01	103.86	112.41
22	n	604	CLA	OBD-CAD-C3D	-3.01	122.47	128.03
22	N	604	CLA	OBD-CAD-C3D	-3.01	122.47	128.03
22	5	611	CLA	CAC-C3C-C2C	-3.01	122.27	127.49
22	1	611	CLA	CAC-C3C-C2C	-3.01	122.27	127.49
22	N	614	CLA	CAC-C3C-C2C	-3.01	122.27	127.49
22	n	614	CLA	CAC-C3C-C2C	-3.01	122.27	127.49
22	C	510	CLA	OBD-CAD-C3D	-3.01	122.48	128.03
22	n	613	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
22	N	613	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
22	b	614	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
22	b	612	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
22	b	615	CLA	OBD-CAD-C3D	-3.01	122.48	128.03
22	r	307	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
22	R	307	CLA	CHC-C1C-C2C	-3.01	118.44	126.65
22	1	602	CLA	CAC-C3C-C2C	-3.01	122.28	127.49
22	5	602	CLA	CAC-C3C-C2C	-3.01	122.28	127.49
22	n	611	CLA	CHC-C1C-C2C	-3.01	118.45	126.65
22	N	611	CLA	CHC-C1C-C2C	-3.01	118.45	126.65
25	S	302	CHL	OBD-CAD-CBD	-3.01	120.24	127.52
25	s	302	CHL	OBD-CAD-CBD	-3.01	120.24	127.52
22	7	311	CLA	CAC-C3C-C2C	-3.00	122.28	127.49
22	3	311	CLA	CAC-C3C-C2C	-3.00	122.28	127.49
22	S	314	CLA	CHC-C1C-C2C	-3.00	118.46	126.65
22	s	314	CLA	CHC-C1C-C2C	-3.00	118.46	126.65
22	g	611	CLA	CAC-C3C-C2C	-3.00	122.29	127.49
22	G	611	CLA	CAC-C3C-C2C	-3.00	122.29	127.49
22	7	303	CLA	CBC-CAC-C3C	-3.00	103.89	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	303	CLA	CBC-CAC-C3C	-3.00	103.89	112.41
25	g	606	CHL	OBD-CAD-CBD	-3.00	120.26	127.52
25	G	606	CHL	OBD-CAD-CBD	-3.00	120.26	127.52
22	Y	603	CLA	CHC-C1C-C2C	-3.00	118.47	126.65
22	y	603	CLA	CHC-C1C-C2C	-3.00	118.47	126.65
22	1	613	CLA	CAC-C3C-C2C	-3.00	122.30	127.49
22	y	610	CLA	CAC-C3C-C2C	-3.00	122.30	127.49
22	5	613	CLA	CAC-C3C-C2C	-3.00	122.30	127.49
22	Y	610	CLA	CAC-C3C-C2C	-3.00	122.30	127.49
22	8	302	CLA	CAC-C3C-C2C	-3.00	122.30	127.49
22	4	302	CLA	CAC-C3C-C2C	-3.00	122.30	127.49
22	5	614	CLA	O2D-CGD-O1D	-3.00	117.79	123.82
22	1	614	CLA	O2D-CGD-O1D	-3.00	117.79	123.82
22	S	301	CLA	CHC-C1C-C2C	-2.99	118.48	126.65
22	3	304	CLA	C1D-CHD-C4C	-2.99	118.39	122.48
22	7	304	CLA	C1D-CHD-C4C	-2.99	118.39	122.48
22	b	608	CLA	C1D-CHD-C4C	-2.99	118.39	122.48
22	C	510	CLA	CAC-C3C-C2C	-2.99	122.30	127.49
22	g	611	CLA	CHC-C1C-C2C	-2.99	118.49	126.65
22	G	611	CLA	CHC-C1C-C2C	-2.99	118.49	126.65
22	2	602	CLA	CBC-CAC-C3C	-2.99	103.92	112.41
22	6	602	CLA	CBC-CAC-C3C	-2.99	103.92	112.41
22	b	607	CLA	CHC-C1C-C2C	-2.99	118.49	126.65
25	7	307	CHL	OBD-CAD-CBD	-2.99	120.28	127.52
25	3	307	CHL	OBD-CAD-CBD	-2.99	120.28	127.52
22	b	610	CLA	CHC-C1C-C2C	-2.99	118.50	126.65
25	Y	601	CHL	OBD-CAD-CBD	-2.99	120.28	127.52
25	y	601	CHL	OBD-CAD-CBD	-2.99	120.28	127.52
22	5	604	CLA	OBD-CAD-C3D	-2.99	122.53	128.03
22	1	604	CLA	OBD-CAD-C3D	-2.99	122.53	128.03
22	B	603	CLA	CHC-C1C-C2C	-2.98	118.51	126.65
22	B	609	CLA	CHC-C1C-C2C	-2.98	118.51	126.65
22	5	614	CLA	OBD-CAD-C3D	-2.98	122.53	128.03
22	1	614	CLA	OBD-CAD-C3D	-2.98	122.53	128.03
22	d	401	CLA	CHC-C1C-C2C	-2.98	118.52	126.65
22	s	309	CLA	O2D-CGD-O1D	-2.98	117.82	123.82
22	S	309	CLA	O2D-CGD-O1D	-2.98	117.82	123.82
22	B	612	CLA	CMA-C3A-C4A	-2.98	103.76	111.77
22	y	612	CLA	CAC-C3C-C2C	-2.98	122.33	127.49
22	Y	612	CLA	CAC-C3C-C2C	-2.98	122.33	127.49
22	c	504	CLA	OBD-CAD-C3D	-2.98	122.54	128.03
22	1	610	CLA	CBC-CAC-C3C	-2.98	103.95	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	5	610	CLA	CBC-CAC-C3C	-2.98	103.95	112.41
22	4	303	CLA	CAC-C3C-C2C	-2.98	122.33	127.49
22	8	303	CLA	CAC-C3C-C2C	-2.98	122.33	127.49
22	7	313	CLA	CAC-C3C-C2C	-2.98	122.33	127.49
22	3	313	CLA	CAC-C3C-C2C	-2.98	122.33	127.49
25	S	308	CHL	OBD-CAD-CBD	-2.98	120.31	127.52
25	s	308	CHL	OBD-CAD-CBD	-2.98	120.31	127.52
22	B	608	CLA	CAC-C3C-C2C	-2.97	122.34	127.49
22	C	507	CLA	CHC-C1C-C2C	-2.97	118.54	126.65
22	b	607	CLA	OBD-CAD-C3D	-2.97	122.55	128.03
22	7	303	CLA	OBD-CAD-C3D	-2.97	122.56	128.03
22	3	303	CLA	OBD-CAD-C3D	-2.97	122.56	128.03
22	6	609	CLA	CAC-C3C-C2C	-2.97	122.35	127.49
22	2	609	CLA	CAC-C3C-C2C	-2.97	122.35	127.49
22	3	310	CLA	CAC-C3C-C2C	-2.97	122.35	127.49
22	7	310	CLA	CAC-C3C-C2C	-2.97	122.35	127.49
22	D	404	CLA	CAC-C3C-C2C	-2.96	122.35	127.49
22	c	505	CLA	CBC-CAC-C3C	-2.96	104.00	112.41
22	c	507	CLA	CGD-CBD-CAD	-2.96	100.78	110.71
22	B	612	CLA	CBC-CAC-C3C	-2.96	104.00	112.41
22	A	402	CLA	CBC-CAC-C3C	-2.96	104.00	112.41
22	8	302	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
22	4	302	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
22	c	511	CLA	CAC-C3C-C2C	-2.96	122.36	127.49
22	b	603	CLA	CBC-CAC-C3C	-2.96	104.02	112.41
22	n	612	CLA	OBD-CAD-C3D	-2.95	122.58	128.03
22	N	612	CLA	OBD-CAD-C3D	-2.95	122.58	128.03
22	n	610	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
22	N	610	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
22	b	605	CLA	CAC-C3C-C2C	-2.95	122.38	127.49
22	c	503	CLA	CHC-C1C-C2C	-2.94	118.62	126.65
25	N	608	CHL	OBD-CAD-CBD	-2.94	120.39	127.52
25	n	608	CHL	OBD-CAD-CBD	-2.94	120.39	127.52
22	b	616	CLA	C1D-CHD-C4C	-2.94	118.46	122.48
25	4	306	CHL	OBD-CAD-CBD	-2.94	120.39	127.52
25	8	306	CHL	OBD-CAD-CBD	-2.94	120.39	127.52
22	D	403	CLA	OBD-CAD-C3D	-2.94	122.60	128.03
22	B	610	CLA	CHC-C1C-C2C	-2.94	118.62	126.65
22	S	310	CLA	CAA-C2A-C3A	-2.94	104.74	112.81
22	s	310	CLA	CAA-C2A-C3A	-2.94	104.74	112.81
22	2	612	CLA	CAC-C3C-C2C	-2.94	122.39	127.49
22	G	614	CLA	CAC-C3C-C2C	-2.94	122.39	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	g	614	CLA	CAC-C3C-C2C	-2.94	122.39	127.49
22	6	612	CLA	CAC-C3C-C2C	-2.94	122.39	127.49
22	B	610	CLA	OBD-CAD-C3D	-2.94	122.61	128.03
25	N	601	CHL	OBD-CAD-CBD	-2.94	120.40	127.52
25	n	601	CHL	OBD-CAD-CBD	-2.94	120.40	127.52
22	N	614	CLA	CHC-C1C-C2C	-2.94	118.64	126.65
22	n	614	CLA	CHC-C1C-C2C	-2.94	118.64	126.65
25	s	306	CHL	OBD-CAD-CBD	-2.94	120.40	127.52
25	S	306	CHL	OBD-CAD-CBD	-2.94	120.40	127.52
22	7	303	CLA	CAC-C3C-C2C	-2.94	122.40	127.49
22	3	303	CLA	CAC-C3C-C2C	-2.94	122.40	127.49
25	1	607	CHL	OBD-CAD-CBD	-2.94	120.41	127.52
25	5	607	CHL	OBD-CAD-CBD	-2.94	120.41	127.52
22	D	404	CLA	CHC-C1C-C2C	-2.93	118.65	126.65
22	b	615	CLA	C1D-CHD-C4C	-2.93	118.48	122.48
22	A	402	CLA	OBD-CAD-C3D	-2.93	122.62	128.03
22	2	602	CLA	OBD-CAD-C3D	-2.93	122.62	128.03
22	6	602	CLA	OBD-CAD-C3D	-2.93	122.62	128.03
22	a	402	CLA	OBD-CAD-C3D	-2.93	122.63	128.03
22	y	611	CLA	CHC-C1C-C2C	-2.93	118.66	126.65
22	Y	611	CLA	CHC-C1C-C2C	-2.93	118.66	126.65
22	c	510	CLA	OBD-CAD-C3D	-2.93	122.63	128.03
25	N	605	CHL	OBD-CAD-CBD	-2.93	120.43	127.52
25	n	605	CHL	OBD-CAD-CBD	-2.93	120.43	127.52
22	7	314	CLA	C1D-CHD-C4C	-2.93	118.48	122.48
22	3	314	CLA	C1D-CHD-C4C	-2.93	118.48	122.48
22	B	613	CLA	CMA-C3A-C4A	-2.93	103.91	111.77
22	3	304	CLA	CHC-C1C-C2C	-2.92	118.68	126.65
22	7	304	CLA	CHC-C1C-C2C	-2.92	118.68	126.65
22	S	310	CLA	CAC-C3C-C2C	-2.92	122.43	127.49
22	s	310	CLA	CAC-C3C-C2C	-2.92	122.43	127.49
25	1	601	CHL	OBD-CAD-CBD	-2.92	120.44	127.52
25	5	601	CHL	OBD-CAD-CBD	-2.92	120.44	127.52
22	B	606	CLA	CBC-CAC-C3C	-2.92	104.11	112.41
25	1	605	CHL	OBD-CAD-CBD	-2.92	120.45	127.52
25	5	605	CHL	OBD-CAD-CBD	-2.92	120.45	127.52
22	S	305	CLA	CAC-C3C-C2C	-2.92	122.43	127.49
22	s	305	CLA	CAC-C3C-C2C	-2.92	122.43	127.49
22	B	614	CLA	CBC-CAC-C3C	-2.92	104.13	112.41
25	4	307	CHL	OBD-CAD-CBD	-2.91	120.46	127.52
25	8	307	CHL	OBD-CAD-CBD	-2.91	120.46	127.52
22	6	603	CLA	CHC-C1C-C2C	-2.91	118.70	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	603	CLA	CHC-C1C-C2C	-2.91	118.70	126.65
22	N	602	CLA	CHC-C1C-C2C	-2.91	118.70	126.65
22	n	602	CLA	CHC-C1C-C2C	-2.91	118.70	126.65
22	S	305	CLA	CGD-CBD-CAD	-2.91	100.95	110.71
22	s	305	CLA	CGD-CBD-CAD	-2.91	100.95	110.71
25	3	301	CHL	O1D-CGD-CBD	-2.91	118.52	124.53
25	7	301	CHL	O1D-CGD-CBD	-2.91	118.52	124.53
22	S	305	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
22	s	305	CLA	CHC-C1C-C2C	-2.91	118.71	126.65
22	1	603	CLA	CHC-C1C-C2C	-2.91	118.72	126.65
22	5	603	CLA	CHC-C1C-C2C	-2.91	118.72	126.65
25	3	306	CHL	OBD-CAD-CBD	-2.91	120.47	127.52
25	7	306	CHL	OBD-CAD-CBD	-2.91	120.47	127.52
22	c	504	CLA	CBC-CAC-C3C	-2.91	104.16	112.41
22	s	303	CLA	OBD-CAD-C3D	-2.91	122.67	128.03
22	S	303	CLA	OBD-CAD-C3D	-2.91	122.67	128.03
25	Y	605	CHL	OBD-CAD-CBD	-2.91	120.48	127.52
25	y	605	CHL	OBD-CAD-CBD	-2.91	120.48	127.52
22	R	309	CLA	CHC-C1C-C2C	-2.91	118.72	126.65
22	r	309	CLA	CHC-C1C-C2C	-2.91	118.72	126.65
22	R	303	CLA	CHC-C1C-C2C	-2.90	118.73	126.65
22	r	303	CLA	CHC-C1C-C2C	-2.90	118.73	126.65
25	g	605	CHL	OBD-CAD-CBD	-2.90	120.49	127.52
25	G	605	CHL	OBD-CAD-CBD	-2.90	120.49	127.52
22	b	602	CLA	OBD-CAD-C3D	-2.90	122.68	128.03
25	2	606	CHL	OBD-CAD-CBD	-2.90	120.50	127.52
25	6	606	CHL	OBD-CAD-CBD	-2.90	120.50	127.52
25	r	305	CHL	OBD-CAD-CBD	-2.90	120.50	127.52
25	R	305	CHL	OBD-CAD-CBD	-2.90	120.50	127.52
22	8	310	CLA	CHC-C1C-C2C	-2.90	118.75	126.65
22	4	310	CLA	CHC-C1C-C2C	-2.90	118.75	126.65
22	c	511	CLA	CHC-C1C-C2C	-2.90	118.75	126.65
25	2	605	CHL	OBD-CAD-CBD	-2.89	120.51	127.52
25	6	605	CHL	OBD-CAD-CBD	-2.89	120.51	127.52
22	2	604	CLA	CAA-C2A-C3A	-2.89	104.88	112.81
22	6	604	CLA	CAA-C2A-C3A	-2.89	104.88	112.81
22	C	505	CLA	OBD-CAD-C3D	-2.89	122.70	128.03
22	C	511	CLA	CBC-CAC-C3C	-2.89	104.20	112.41
22	G	610	CLA	O2D-CGD-O1D	-2.89	118.00	123.82
22	g	610	CLA	O2D-CGD-O1D	-2.89	118.00	123.82
23	A	404	PHO	C1C-C2C-C3C	-2.89	103.16	106.51
22	g	612	CLA	CAC-C3C-C2C	-2.89	122.48	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	612	CLA	CAC-C3C-C2C	-2.89	122.48	127.49
25	y	606	CHL	OBD-CAD-CBD	-2.88	120.53	127.52
25	Y	606	CHL	OBD-CAD-CBD	-2.88	120.53	127.52
22	s	313	CLA	CHC-C1C-C2C	-2.88	118.79	126.65
22	S	313	CLA	CHC-C1C-C2C	-2.88	118.79	126.65
22	1	610	CLA	CAC-C3C-C2C	-2.88	122.50	127.49
22	5	610	CLA	CAC-C3C-C2C	-2.88	122.50	127.49
22	c	501	CLA	OBD-CAD-C3D	-2.88	122.72	128.03
22	2	613	CLA	CAC-C3C-C2C	-2.88	122.50	127.49
22	6	613	CLA	CAC-C3C-C2C	-2.88	122.50	127.49
25	5	615	CHL	OBD-CAD-CBD	-2.88	120.55	127.52
25	1	615	CHL	OBD-CAD-CBD	-2.88	120.55	127.52
25	G	607	CHL	OBD-CAD-CBD	-2.88	120.55	127.52
25	g	607	CHL	OBD-CAD-CBD	-2.88	120.55	127.52
22	B	604	CLA	OBD-CAD-C3D	-2.88	122.72	128.03
22	b	603	CLA	CHC-C1C-C2C	-2.88	118.80	126.65
23	a	404	PHO	C4D-ND-C1D	-2.88	101.79	106.98
25	2	607	CHL	OBD-CAD-CBD	-2.88	120.55	127.52
25	6	607	CHL	OBD-CAD-CBD	-2.88	120.55	127.52
22	b	604	CLA	CMA-C3A-C4A	-2.88	104.04	111.77
22	G	610	CLA	CAC-C3C-C2C	-2.88	122.51	127.49
22	g	610	CLA	CAC-C3C-C2C	-2.88	122.51	127.49
22	7	305	CLA	CAA-C2A-C3A	-2.87	104.93	112.81
22	3	305	CLA	CAA-C2A-C3A	-2.87	104.93	112.81
22	b	607	CLA	CBC-CAC-C3C	-2.87	104.25	112.41
22	R	308	CLA	O2D-CGD-O1D	-2.87	118.04	123.82
22	r	308	CLA	O2D-CGD-O1D	-2.87	118.04	123.82
22	b	605	CLA	O1D-CGD-CBD	-2.87	119.44	124.60
22	R	312	CLA	CAC-C3C-C2C	-2.87	122.52	127.49
22	r	312	CLA	CAC-C3C-C2C	-2.87	122.52	127.49
22	4	304	CLA	CAA-C2A-C3A	-2.87	104.94	112.81
22	8	304	CLA	CAA-C2A-C3A	-2.87	104.94	112.81
22	b	616	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
22	5	611	CLA	CHC-C1C-C2C	-2.87	118.83	126.65
22	1	611	CLA	CHC-C1C-C2C	-2.87	118.83	126.65
22	Y	614	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
22	y	614	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
22	b	603	CLA	OBD-CAD-C3D	-2.86	122.75	128.03
22	g	612	CLA	CHC-C1C-C2C	-2.86	118.85	126.65
22	G	612	CLA	CHC-C1C-C2C	-2.86	118.85	126.65
22	a	405	CLA	CHC-C1C-C2C	-2.86	118.85	126.65
22	d	401	CLA	OBD-CAD-C3D	-2.86	122.75	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	CBC-CAC-C3C	-2.86	104.30	112.41
22	d	404	CLA	CAC-C3C-C2C	-2.86	122.54	127.49
25	n	607	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
25	r	306	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
25	R	306	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
25	N	607	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
22	c	510	CLA	CAC-C3C-C2C	-2.85	122.55	127.49
22	C	509	CLA	OBD-CAD-C3D	-2.85	122.77	128.03
25	3	302	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
25	7	302	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
25	1	606	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
25	5	606	CHL	OBD-CAD-CBD	-2.85	120.61	127.52
22	7	313	CLA	CHC-C1C-C2C	-2.85	118.88	126.65
22	3	313	CLA	CHC-C1C-C2C	-2.85	118.88	126.65
22	n	610	CLA	CAC-C3C-C2C	-2.85	122.56	127.49
22	N	610	CLA	CAC-C3C-C2C	-2.85	122.56	127.49
22	B	601	CLA	CBC-CAC-C3C	-2.85	104.32	112.41
22	7	305	CLA	CHC-C1C-C2C	-2.85	118.88	126.65
22	3	305	CLA	CHC-C1C-C2C	-2.85	118.88	126.65
22	s	301	CLA	OBD-CAD-C3D	-2.85	122.78	128.03
22	y	613	CLA	CAC-C3C-C2C	-2.85	122.56	127.49
22	Y	613	CLA	CAC-C3C-C2C	-2.85	122.56	127.49
22	a	402	CLA	CHC-C1C-C2C	-2.85	118.89	126.65
22	r	310	CLA	CHC-C1C-C2C	-2.84	118.89	126.65
22	R	310	CLA	CHC-C1C-C2C	-2.84	118.89	126.65
25	6	601	CHL	OBD-CAD-CBD	-2.84	120.63	127.52
25	2	601	CHL	OBD-CAD-CBD	-2.84	120.63	127.52
22	Y	602	CLA	CHC-C1C-C2C	-2.84	118.90	126.65
22	y	602	CLA	CHC-C1C-C2C	-2.84	118.90	126.65
25	g	601	CHL	OBD-CAD-CBD	-2.84	120.64	127.52
25	G	601	CHL	OBD-CAD-CBD	-2.84	120.64	127.52
22	C	512	CLA	CHC-C1C-C2C	-2.84	118.90	126.65
22	b	615	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
22	b	610	CLA	CGD-CBD-CAD	-2.84	101.21	110.71
22	b	609	CLA	CMA-C3A-C4A	-2.84	104.15	111.77
22	S	312	CLA	OBD-CAD-C3D	-2.84	122.80	128.03
22	s	312	CLA	OBD-CAD-C3D	-2.84	122.80	128.03
22	g	612	CLA	CGD-CBD-CAD	-2.83	101.22	110.71
22	D	403	CLA	CGD-CBD-CAD	-2.83	101.22	110.71
22	G	612	CLA	CGD-CBD-CAD	-2.83	101.22	110.71
22	2	610	CLA	CHC-C1C-C2C	-2.83	118.92	126.65
22	6	610	CLA	CHC-C1C-C2C	-2.83	118.92	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1	613	CLA	CHC-C1C-C2C	-2.83	118.93	126.65
22	5	613	CLA	CHC-C1C-C2C	-2.83	118.93	126.65
22	B	609	CLA	O2D-CGD-O1D	-2.83	118.12	123.82
22	D	404	CLA	OBD-CAD-C3D	-2.83	122.81	128.03
22	R	301	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
22	r	301	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
25	1	608	CHL	OBD-CAD-CBD	-2.83	120.67	127.52
25	5	608	CHL	OBD-CAD-CBD	-2.83	120.67	127.52
22	b	614	CLA	OBD-CAD-C3D	-2.82	122.83	128.03
25	s	307	CHL	OBD-CAD-CBD	-2.82	120.68	127.52
25	S	307	CHL	OBD-CAD-CBD	-2.82	120.68	127.52
23	A	404	PHO	CHD-C4C-C3C	-2.82	118.91	124.59
22	d	404	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
22	d	404	CLA	OBD-CAD-C3D	-2.82	122.83	128.03
22	A	402	CLA	CAA-C2A-C3A	-2.82	105.08	112.81
22	B	602	CLA	CHC-C1C-C2C	-2.82	118.96	126.65
22	2	612	CLA	CHC-C1C-C2C	-2.82	118.96	126.65
22	6	612	CLA	CHC-C1C-C2C	-2.82	118.96	126.65
22	A	402	CLA	CAC-C3C-C2C	-2.82	122.61	127.49
22	d	404	CLA	CAA-C2A-C3A	-2.82	105.09	112.81
22	5	604	CLA	CHC-C1C-C2C	-2.82	118.97	126.65
22	1	604	CLA	CHC-C1C-C2C	-2.82	118.97	126.65
22	B	614	CLA	CAC-C3C-C2C	-2.82	122.61	127.49
22	a	403	CLA	CAA-C2A-C3A	-2.81	105.10	112.81
23	D	402	PHO	CBD-CHA-C4D	-2.81	105.37	108.54
22	s	313	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
22	S	313	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
24	e	101	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
22	A	402	CLA	CHC-C1C-C2C	-2.81	119.00	126.65
22	2	610	CLA	CAC-C3C-C2C	-2.81	122.63	127.49
22	6	610	CLA	CAC-C3C-C2C	-2.81	122.63	127.49
22	S	312	CLA	CGD-CBD-CAD	-2.81	101.31	110.71
22	s	312	CLA	CGD-CBD-CAD	-2.81	101.31	110.71
22	A	403	CLA	CAA-C2A-C3A	-2.80	105.12	112.81
22	4	304	CLA	CHC-C1C-C2C	-2.80	119.00	126.65
22	8	304	CLA	CHC-C1C-C2C	-2.80	119.00	126.65
22	4	303	CLA	CHC-C1C-C2C	-2.80	119.00	126.65
22	8	303	CLA	CHC-C1C-C2C	-2.80	119.00	126.65
25	4	301	CHL	OBD-CAD-CBD	-2.80	120.73	127.52
25	8	301	CHL	OBD-CAD-CBD	-2.80	120.73	127.52
22	1	612	CLA	CAC-C3C-C2C	-2.80	122.63	127.49
22	5	612	CLA	CAC-C3C-C2C	-2.80	122.63	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	608	CLA	CGD-CBD-CAD	-2.80	101.32	110.71
22	B	606	CLA	CHC-C1C-C2C	-2.80	119.01	126.65
22	b	612	CLA	CBC-CAC-C3C	-2.80	104.46	112.41
22	B	612	CLA	CAC-C3C-C2C	-2.80	122.64	127.49
22	A	405	CLA	CHC-C1C-C2C	-2.80	119.02	126.65
22	7	311	CLA	CHC-C1C-C2C	-2.80	119.02	126.65
22	3	311	CLA	CHC-C1C-C2C	-2.80	119.02	126.65
22	n	612	CLA	CGD-CBD-CAD	-2.80	101.35	110.71
22	N	612	CLA	CGD-CBD-CAD	-2.80	101.35	110.71
22	n	603	CLA	CAA-C2A-C3A	-2.79	105.15	112.81
22	N	603	CLA	CAA-C2A-C3A	-2.79	105.15	112.81
22	1	602	CLA	OBD-CAD-C3D	-2.79	122.88	128.03
22	5	602	CLA	OBD-CAD-C3D	-2.79	122.88	128.03
22	d	401	CLA	CGD-CBD-CAD	-2.79	101.35	110.71
23	d	402	PHO	C4D-ND-C1D	-2.79	101.94	106.98
22	b	610	CLA	OBD-CAD-C3D	-2.79	122.88	128.03
22	y	612	CLA	OBD-CAD-C3D	-2.79	122.89	128.03
22	Y	612	CLA	OBD-CAD-C3D	-2.79	122.89	128.03
22	b	608	CLA	OBD-CAD-C3D	-2.79	122.89	128.03
25	n	607	CHL	O1D-CGD-CBD	-2.79	118.77	124.53
25	N	607	CHL	O1D-CGD-CBD	-2.79	118.77	124.53
22	B	616	CLA	O2D-CGD-O1D	-2.79	118.21	123.82
22	b	615	CLA	CAC-C3C-C2C	-2.79	122.66	127.49
22	2	604	CLA	CHC-C1C-C2C	-2.78	119.06	126.65
22	6	604	CLA	CHC-C1C-C2C	-2.78	119.06	126.65
22	3	312	CLA	CAC-C3C-C2C	-2.78	122.67	127.49
22	7	312	CLA	CAC-C3C-C2C	-2.78	122.67	127.49
22	B	611	CLA	CHC-C1C-C2C	-2.78	119.07	126.65
22	B	610	CLA	CAC-C3C-C2C	-2.78	122.68	127.49
22	Y	602	CLA	CAC-C3C-C2C	-2.78	122.68	127.49
22	y	602	CLA	CAC-C3C-C2C	-2.78	122.68	127.49
22	y	610	CLA	CBC-CAC-C3C	-2.77	104.53	112.41
22	Y	610	CLA	CBC-CAC-C3C	-2.77	104.53	112.41
22	B	613	CLA	CHC-C1C-C2C	-2.77	119.08	126.65
25	g	608	CHL	OBD-CAD-CBD	-2.77	120.80	127.52
25	G	608	CHL	OBD-CAD-CBD	-2.77	120.80	127.52
22	1	612	CLA	CHC-C1C-C2C	-2.77	119.10	126.65
22	5	612	CLA	CHC-C1C-C2C	-2.77	119.10	126.65
22	y	610	CLA	CHC-C1C-C2C	-2.77	119.10	126.65
22	Y	610	CLA	CHC-C1C-C2C	-2.77	119.10	126.65
22	n	604	CLA	CHC-C1C-C2C	-2.77	119.10	126.65
22	N	604	CLA	CHC-C1C-C2C	-2.77	119.10	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	308	CLA	CAC-C3C-C2C	-2.76	122.70	127.49
22	r	308	CLA	CAC-C3C-C2C	-2.76	122.70	127.49
25	3	301	CHL	OBD-CAD-CBD	-2.76	120.83	127.52
25	7	301	CHL	OBD-CAD-CBD	-2.76	120.83	127.52
22	6	609	CLA	O2D-CGD-O1D	-2.76	118.26	123.82
22	y	610	CLA	O2D-CGD-O1D	-2.76	118.26	123.82
22	2	609	CLA	O2D-CGD-O1D	-2.76	118.26	123.82
22	Y	610	CLA	O2D-CGD-O1D	-2.76	118.26	123.82
22	G	614	CLA	CHC-C1C-C2C	-2.76	119.12	126.65
22	g	614	CLA	CHC-C1C-C2C	-2.76	119.12	126.65
22	D	404	CLA	O2D-CGD-O1D	-2.76	118.27	123.82
22	g	611	CLA	CGD-CBD-CAD	-2.76	101.46	110.71
22	G	611	CLA	CGD-CBD-CAD	-2.76	101.46	110.71
25	Y	607	CHL	CHA-CBD-CGD	-2.76	108.60	115.00
25	y	607	CHL	CHA-CBD-CGD	-2.76	108.60	115.00
25	8	305	CHL	OBD-CAD-CBD	-2.76	120.83	127.52
25	4	305	CHL	OBD-CAD-CBD	-2.76	120.83	127.52
22	Y	603	CLA	CGD-CBD-CAD	-2.76	101.47	110.71
22	y	603	CLA	CGD-CBD-CAD	-2.76	101.47	110.71
22	R	308	CLA	CMA-C3A-C2A	-2.76	102.58	113.77
22	r	308	CLA	CMA-C3A-C2A	-2.76	102.58	113.77
22	D	401	CLA	CAA-C2A-C3A	-2.75	105.26	112.81
22	G	602	CLA	CHC-C1C-C2C	-2.75	119.14	126.65
22	g	602	CLA	CHC-C1C-C2C	-2.75	119.14	126.65
22	b	606	CLA	CAA-C2A-C3A	-2.75	105.27	112.81
22	R	312	CLA	CHC-C1C-C2C	-2.75	119.15	126.65
22	r	312	CLA	CHC-C1C-C2C	-2.75	119.15	126.65
22	b	603	CLA	O2D-CGD-O1D	-2.75	118.29	123.82
22	b	614	CLA	CHC-C1C-C2C	-2.75	119.16	126.65
22	B	614	CLA	OBD-CAD-C3D	-2.74	122.97	128.03
22	b	608	CLA	CHC-C1C-C2C	-2.74	119.17	126.65
22	8	302	CLA	CMA-C3A-C2A	-2.74	102.64	113.77
22	4	302	CLA	CMA-C3A-C2A	-2.74	102.64	113.77
22	2	613	CLA	CHC-C1C-C2C	-2.74	119.17	126.65
22	6	613	CLA	CHC-C1C-C2C	-2.74	119.17	126.65
22	S	311	CLA	CHC-C1C-C2C	-2.74	119.18	126.65
22	s	311	CLA	CHC-C1C-C2C	-2.74	119.18	126.65
22	y	612	CLA	CGD-CBD-CAD	-2.74	101.54	110.71
22	Y	612	CLA	CGD-CBD-CAD	-2.74	101.54	110.71
22	N	602	CLA	OBD-CAD-C3D	-2.74	122.98	128.03
22	n	602	CLA	OBD-CAD-C3D	-2.74	122.98	128.03
22	3	312	CLA	CHC-C1C-C2C	-2.74	119.19	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	312	CLA	CHC-C1C-C2C	-2.74	119.19	126.65
22	A	403	CLA	CHC-C1C-C2C	-2.73	119.20	126.65
22	g	613	CLA	CAC-C3C-C2C	-2.73	122.76	127.49
22	G	613	CLA	CAC-C3C-C2C	-2.73	122.76	127.49
22	R	309	CLA	O2D-CGD-O1D	-2.73	118.33	123.82
22	r	309	CLA	O2D-CGD-O1D	-2.73	118.33	123.82
22	B	614	CLA	O1D-CGD-CBD	-2.73	119.70	124.60
22	s	301	CLA	C1D-CHD-C4C	-2.73	118.76	122.48
22	s	303	CLA	CHC-C1C-C2C	-2.72	119.22	126.65
22	S	303	CLA	CHC-C1C-C2C	-2.72	119.22	126.65
22	4	309	CLA	CBC-CAC-C3C	-2.72	104.68	112.41
22	8	309	CLA	CBC-CAC-C3C	-2.72	104.68	112.41
22	C	508	CLA	O2D-CGD-O1D	-2.72	118.34	123.82
22	Y	604	CLA	CHC-C1C-C2C	-2.72	119.22	126.65
22	y	604	CLA	CHC-C1C-C2C	-2.72	119.22	126.65
22	R	303	CLA	CAC-C3C-C2C	-2.72	122.78	127.49
22	r	303	CLA	CAC-C3C-C2C	-2.72	122.78	127.49
22	s	303	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
22	S	303	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
22	b	608	CLA	CGD-CBD-CAD	-2.72	101.60	110.71
22	G	610	CLA	CBC-CAC-C3C	-2.72	104.70	112.41
22	g	610	CLA	CBC-CAC-C3C	-2.72	104.70	112.41
22	S	310	CLA	CHC-C1C-C2C	-2.71	119.25	126.65
22	s	310	CLA	CHC-C1C-C2C	-2.71	119.25	126.65
22	c	507	CLA	OBD-CAD-C3D	-2.71	123.03	128.03
22	C	503	CLA	CHC-C1C-C2C	-2.71	119.26	126.65
22	C	501	CLA	CAA-C2A-C3A	-2.71	105.38	112.81
22	c	502	CLA	CAC-C3C-C2C	-2.71	122.80	127.49
25	Y	607	CHL	O1D-CGD-CBD	-2.71	118.94	124.53
25	y	607	CHL	O1D-CGD-CBD	-2.71	118.94	124.53
22	a	403	CLA	CHC-C1C-C2C	-2.71	119.26	126.65
22	S	311	CLA	CGD-CBD-CAD	-2.71	101.64	110.71
22	s	311	CLA	CGD-CBD-CAD	-2.71	101.64	110.71
22	r	310	CLA	O2D-CGD-O1D	-2.71	118.37	123.82
22	R	310	CLA	O2D-CGD-O1D	-2.71	118.37	123.82
22	R	301	CLA	CAC-C3C-C2C	-2.70	122.80	127.49
22	r	301	CLA	CAC-C3C-C2C	-2.70	122.80	127.49
22	7	305	CLA	O2D-CGD-O1D	-2.70	118.38	123.82
22	3	305	CLA	O2D-CGD-O1D	-2.70	118.38	123.82
22	Y	602	CLA	OBD-CAD-C3D	-2.70	123.05	128.03
22	y	602	CLA	OBD-CAD-C3D	-2.70	123.05	128.03
22	C	512	CLA	CAC-C3C-C2C	-2.70	122.82	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	CGD-CBD-CAD	-2.70	101.68	110.71
23	D	402	PHO	C4D-ND-C1D	-2.70	102.11	106.98
22	2	602	CLA	CHC-C1C-C2C	-2.70	119.30	126.65
22	6	602	CLA	CHC-C1C-C2C	-2.70	119.30	126.65
22	B	616	CLA	CBC-CAC-C3C	-2.69	104.76	112.41
22	d	403	CLA	O2D-CGD-O1D	-2.69	118.40	123.82
25	Y	607	CHL	OBD-CAD-CBD	-2.69	121.00	127.52
25	y	607	CHL	OBD-CAD-CBD	-2.69	121.00	127.52
22	c	512	CLA	CGD-CBD-CAD	-2.69	101.70	110.71
22	1	602	CLA	CHC-C1C-C2C	-2.69	119.33	126.65
22	5	602	CLA	CHC-C1C-C2C	-2.69	119.33	126.65
22	n	612	CLA	CAC-C3C-C2C	-2.68	122.84	127.49
22	N	612	CLA	CAC-C3C-C2C	-2.68	122.84	127.49
22	c	508	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
22	7	303	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
22	3	303	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
22	b	605	CLA	CHC-C1C-C2C	-2.67	119.36	126.65
25	g	606	CHL	C3B-CAB-CBB	-2.67	119.20	125.20
25	G	606	CHL	C3B-CAB-CBB	-2.67	119.20	125.20
22	D	403	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
22	A	402	CLA	CGD-CBD-CAD	-2.67	101.77	110.71
22	4	303	CLA	OBD-CAD-C3D	-2.67	123.11	128.03
22	8	303	CLA	OBD-CAD-C3D	-2.67	123.11	128.03
22	b	616	CLA	CGD-CBD-CAD	-2.67	101.77	110.71
22	C	509	CLA	CHC-C1C-C2C	-2.67	119.37	126.65
22	C	503	CLA	CGD-CBD-CAD	-2.67	101.78	110.71
22	c	501	CLA	CAC-C3C-C2C	-2.67	122.87	127.49
22	g	611	CLA	O1D-CGD-CBD	-2.66	119.81	124.60
22	G	611	CLA	O1D-CGD-CBD	-2.66	119.81	124.60
22	Y	614	CLA	CAA-C2A-C3A	-2.66	105.53	112.81
22	y	614	CLA	CAA-C2A-C3A	-2.66	105.53	112.81
22	b	601	CLA	O2D-CGD-O1D	-2.65	118.48	123.82
22	C	507	CLA	OBD-CAD-C3D	-2.65	123.14	128.03
22	B	609	CLA	CHA-C1A-NA	-2.65	120.02	126.18
22	b	612	CLA	CAC-C3C-C2C	-2.65	122.90	127.49
22	R	301	CLA	CHC-C1C-C2C	-2.65	119.43	126.65
22	r	301	CLA	CHC-C1C-C2C	-2.65	119.43	126.65
22	7	314	CLA	CHC-C1C-C2C	-2.65	119.43	126.65
22	3	314	CLA	CHC-C1C-C2C	-2.65	119.43	126.65
22	D	403	CLA	CBC-CAC-C3C	-2.64	104.90	112.41
22	R	301	CLA	CAA-C2A-C3A	-2.64	105.56	112.81
22	r	301	CLA	CAA-C2A-C3A	-2.64	105.56	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	602	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
22	6	602	CLA	O2D-CGD-O1D	-2.64	118.50	123.82
22	r	302	CLA	O2D-CGD-O1D	-2.64	118.51	123.82
22	R	302	CLA	O2D-CGD-O1D	-2.64	118.51	123.82
22	B	607	CLA	CAC-C3C-C2C	-2.64	122.92	127.49
22	Y	614	CLA	CGD-CBD-CAD	-2.64	101.88	110.71
22	y	614	CLA	CGD-CBD-CAD	-2.64	101.88	110.71
22	b	612	CLA	CMA-C3A-C2A	-2.64	103.08	113.77
22	B	602	CLA	CGD-CBD-CAD	-2.63	101.89	110.71
22	r	310	CLA	CAC-C3C-C2C	-2.63	122.93	127.49
22	R	310	CLA	CAC-C3C-C2C	-2.63	122.93	127.49
22	s	301	CLA	CHC-C1C-C2C	-2.63	119.48	126.65
22	2	604	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
22	6	604	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
22	a	402	CLA	CAA-C2A-C3A	-2.62	105.61	112.81
22	C	503	CLA	OBD-CAD-C3D	-2.62	123.19	128.03
22	S	304	CLA	OBD-CAD-C3D	-2.62	123.19	128.03
22	s	304	CLA	OBD-CAD-C3D	-2.62	123.19	128.03
22	N	602	CLA	CGD-CBD-CAD	-2.62	101.93	110.71
22	n	602	CLA	CGD-CBD-CAD	-2.62	101.93	110.71
22	a	402	CLA	CAC-C3C-C2C	-2.62	122.95	127.49
22	1	613	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
22	5	613	CLA	CMA-C3A-C4A	-2.62	104.74	111.77
22	1	603	CLA	CGD-CBD-CAD	-2.61	101.95	110.71
22	5	603	CLA	CGD-CBD-CAD	-2.61	101.95	110.71
22	b	606	CLA	CHC-C1C-C2C	-2.61	119.52	126.65
22	s	303	CLA	CGD-CBD-CAD	-2.61	101.96	110.71
22	S	303	CLA	CGD-CBD-CAD	-2.61	101.96	110.71
22	b	615	CLA	CHC-C1C-C2C	-2.61	119.53	126.65
22	R	311	CLA	CHC-C1C-C2C	-2.61	119.53	126.65
22	r	311	CLA	CHC-C1C-C2C	-2.61	119.53	126.65
22	n	611	CLA	CGD-CBD-CAD	-2.61	101.97	110.71
22	N	611	CLA	CGD-CBD-CAD	-2.61	101.97	110.71
22	D	404	CLA	CAA-C2A-C3A	-2.61	105.66	112.81
22	C	502	CLA	CHC-C1C-C2C	-2.60	119.55	126.65
22	b	607	CLA	CAA-C2A-C3A	-2.60	105.68	112.81
22	b	604	CLA	OBD-CAD-C3D	-2.59	123.25	128.03
22	A	403	CLA	CAC-C3C-C2C	-2.59	123.00	127.49
22	5	611	CLA	O2D-CGD-O1D	-2.59	118.61	123.82
22	1	611	CLA	O2D-CGD-O1D	-2.59	118.61	123.82
22	d	401	CLA	CAC-C3C-C2C	-2.59	123.01	127.49
23	d	402	PHO	CBD-CHA-C4D	-2.58	105.63	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	OBD-CAD-C3D	-2.58	123.28	128.03
22	c	506	CLA	O2D-CGD-O1D	-2.57	118.64	123.82
22	s	301	CLA	CAA-C2A-C3A	-2.57	105.75	112.81
23	D	402	PHO	O2D-CGD-O1D	-2.57	118.65	123.82
22	6	611	CLA	CHC-C1C-C2C	-2.57	119.64	126.65
22	2	611	CLA	CHC-C1C-C2C	-2.57	119.64	126.65
22	7	303	CLA	CHC-C1C-C2C	-2.56	119.66	126.65
22	3	303	CLA	CHC-C1C-C2C	-2.56	119.66	126.65
25	7	308	CHL	OBD-CAD-CBD	-2.56	121.31	127.52
25	3	308	CHL	OBD-CAD-CBD	-2.56	121.31	127.52
22	G	614	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
22	g	614	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
22	B	601	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
22	N	602	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
22	n	602	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
22	n	604	CLA	CGD-CBD-CAD	-2.56	102.14	110.71
22	N	604	CLA	CGD-CBD-CAD	-2.56	102.14	110.71
22	c	509	CLA	CHC-C1C-C2C	-2.56	119.68	126.65
22	B	603	CLA	CMA-C3A-C4A	-2.55	104.91	111.77
25	1	609	CHL	OBD-CAD-CBD	-2.55	121.33	127.52
25	5	609	CHL	OBD-CAD-CBD	-2.55	121.33	127.52
22	b	604	CLA	CAA-C2A-C3A	-2.55	105.81	112.81
22	d	401	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
25	G	607	CHL	CHA-CBD-CGD	-2.55	109.09	115.00
25	g	607	CHL	CHA-CBD-CGD	-2.55	109.09	115.00
22	S	304	CLA	CGD-CBD-CAD	-2.54	102.19	110.71
22	s	304	CLA	CGD-CBD-CAD	-2.54	102.19	110.71
23	A	404	PHO	CBD-CHA-C4D	-2.54	105.67	108.54
22	4	309	CLA	CAA-C2A-C3A	-2.54	105.84	112.81
22	8	309	CLA	CAA-C2A-C3A	-2.54	105.84	112.81
22	Y	602	CLA	O2D-CGD-O1D	-2.54	118.71	123.82
22	y	602	CLA	O2D-CGD-O1D	-2.54	118.71	123.82
22	B	609	CLA	CMA-C3A-C2A	-2.54	103.46	113.77
22	c	509	CLA	O2D-CGD-O1D	-2.54	118.71	123.82
22	b	615	CLA	CAA-C2A-C3A	-2.54	105.85	112.81
22	C	511	CLA	O2D-CGD-O1D	-2.53	118.72	123.82
22	4	309	CLA	CMA-C3A-C2A	-2.53	103.50	113.77
22	8	309	CLA	CMA-C3A-C2A	-2.53	103.50	113.77
25	Y	601	CHL	CHA-CBD-CGD	-2.53	109.13	115.00
25	y	601	CHL	CHA-CBD-CGD	-2.53	109.13	115.00
24	E	101	HEM	CMD-C2D-C1D	-2.53	124.58	128.46
22	n	603	CLA	CGD-CBD-CAD	-2.53	102.24	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	603	CLA	CGD-CBD-CAD	-2.53	102.24	110.71
22	N	614	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
22	n	614	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
22	b	612	CLA	CHC-C1C-C2C	-2.53	119.76	126.65
22	n	610	CLA	CBC-CAC-C3C	-2.53	105.24	112.41
22	N	610	CLA	CBC-CAC-C3C	-2.53	105.24	112.41
22	1	602	CLA	O2D-CGD-O1D	-2.53	118.74	123.82
22	5	602	CLA	O2D-CGD-O1D	-2.53	118.74	123.82
22	b	615	CLA	CGD-CBD-CAD	-2.52	102.26	110.71
22	7	311	CLA	O2D-CGD-O1D	-2.52	118.76	123.82
22	3	311	CLA	O2D-CGD-O1D	-2.52	118.76	123.82
22	b	602	CLA	CHC-C1C-C2C	-2.52	119.79	126.65
22	C	501	CLA	CMA-C3A-C4A	-2.52	105.01	111.77
22	B	601	CLA	CAC-C3C-C2C	-2.52	123.13	127.49
22	D	401	CLA	CBC-CAC-C3C	-2.51	105.28	112.41
22	G	603	CLA	CAA-C2A-C3A	-2.51	105.94	112.81
22	g	603	CLA	CAA-C2A-C3A	-2.51	105.94	112.81
22	b	602	CLA	CAA-C2A-C3A	-2.51	105.94	112.81
22	G	603	CLA	CGD-CBD-CAD	-2.51	102.32	110.71
22	g	603	CLA	CGD-CBD-CAD	-2.51	102.32	110.71
22	C	502	CLA	CAA-C2A-C3A	-2.50	105.94	112.81
23	a	404	PHO	CBD-CHA-C4D	-2.50	105.72	108.54
24	e	101	HEM	CMD-C2D-C1D	-2.50	124.62	128.46
25	y	609	CHL	OBD-CAD-CBD	-2.50	121.47	127.52
25	Y	609	CHL	OBD-CAD-CBD	-2.50	121.47	127.52
22	r	302	CLA	CHC-C1C-C2C	-2.49	119.84	126.65
22	R	302	CLA	CHC-C1C-C2C	-2.49	119.84	126.65
22	C	509	CLA	CAC-C3C-C2C	-2.49	123.17	127.49
22	2	610	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
22	6	610	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
22	b	603	CLA	CAA-C2A-C3A	-2.49	105.97	112.81
22	s	313	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
22	S	313	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
22	R	308	CLA	CMA-C3A-C4A	-2.49	105.09	111.77
22	r	308	CLA	CMA-C3A-C4A	-2.49	105.09	111.77
22	b	601	CLA	CHC-C1C-C2C	-2.49	119.87	126.65
22	4	304	CLA	O2D-CGD-O1D	-2.49	118.82	123.82
22	8	304	CLA	O2D-CGD-O1D	-2.49	118.82	123.82
22	C	504	CLA	CAA-C2A-C3A	-2.49	106.00	112.81
22	1	613	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
22	5	613	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
22	c	509	CLA	CAA-C2A-C3A	-2.48	106.02	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	y	611	CLA	O2D-CGD-O1D	-2.48	118.83	123.82
22	Y	611	CLA	O2D-CGD-O1D	-2.48	118.83	123.82
22	C	501	CLA	CAC-C3C-C2C	-2.47	123.21	127.49
22	S	310	CLA	CGD-CBD-CAD	-2.47	102.44	110.71
22	s	310	CLA	CGD-CBD-CAD	-2.47	102.44	110.71
22	B	616	CLA	OBD-CAD-C3D	-2.47	123.48	128.03
22	c	512	CLA	CAC-C3C-C2C	-2.47	123.22	127.49
22	G	602	CLA	OBD-CAD-C3D	-2.46	123.49	128.03
22	g	602	CLA	OBD-CAD-C3D	-2.46	123.49	128.03
22	1	610	CLA	CHC-C1C-C2C	-2.46	119.93	126.65
22	5	610	CLA	CHC-C1C-C2C	-2.46	119.93	126.65
22	S	314	CLA	CGD-CBD-CAD	-2.46	102.47	110.71
22	s	314	CLA	CGD-CBD-CAD	-2.46	102.47	110.71
25	g	601	CHL	CHA-CBD-CGD	-2.46	109.30	115.00
25	G	601	CHL	CHA-CBD-CGD	-2.46	109.30	115.00
25	S	308	CHL	CHA-CBD-CGD	-2.46	109.30	115.00
25	s	308	CHL	CHA-CBD-CGD	-2.46	109.30	115.00
22	B	614	CLA	O2D-CGD-O1D	-2.45	118.88	123.82
22	3	312	CLA	CGD-CBD-CAD	-2.45	102.50	110.71
22	7	312	CLA	CGD-CBD-CAD	-2.45	102.50	110.71
22	s	301	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
22	C	507	CLA	O2D-CGD-O1D	-2.45	118.90	123.82
22	5	604	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
22	1	604	CLA	O2D-CGD-O1D	-2.44	118.90	123.82
22	B	612	CLA	CGD-CBD-CAD	-2.44	102.52	110.71
22	c	504	CLA	CAA-C2A-C3A	-2.44	106.12	112.81
23	D	402	PHO	C1C-C2C-C3C	-2.44	103.68	106.51
22	4	303	CLA	O2D-CGD-O1D	-2.43	118.92	123.82
22	8	303	CLA	O2D-CGD-O1D	-2.43	118.92	123.82
22	4	309	CLA	CHC-C1C-C2C	-2.43	120.01	126.65
22	8	309	CLA	CHC-C1C-C2C	-2.43	120.01	126.65
22	C	501	CLA	CGD-CBD-CAD	-2.43	102.57	110.71
25	Y	605	CHL	CHA-CBD-CGD	-2.43	109.37	115.00
25	y	605	CHL	CHA-CBD-CGD	-2.43	109.37	115.00
22	b	616	CLA	CHA-C1A-NA	-2.43	120.54	126.18
22	7	314	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
22	3	314	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
23	a	404	PHO	C1C-C2C-C3C	-2.43	103.69	106.51
22	1	603	CLA	CAA-C2A-C3A	-2.43	106.16	112.81
22	5	603	CLA	CAA-C2A-C3A	-2.43	106.16	112.81
22	B	610	CLA	CGD-CBD-CAD	-2.43	102.59	110.71
22	B	608	CLA	O2D-CGD-O1D	-2.42	118.95	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CHA-C1A-NA	-2.42	120.56	126.18
22	R	301	CLA	CMA-C3A-C2A	-2.42	103.95	113.77
22	r	301	CLA	CMA-C3A-C2A	-2.42	103.95	113.77
22	C	505	CLA	O2D-CGD-O1D	-2.42	118.95	123.82
22	8	310	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
22	4	310	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
25	R	304	CHL	C3B-CAB-CBB	-2.41	119.78	125.20
25	r	304	CHL	C3B-CAB-CBB	-2.41	119.78	125.20
22	R	312	CLA	CAA-C2A-C3A	-2.41	106.20	112.81
22	r	312	CLA	CAA-C2A-C3A	-2.41	106.20	112.81
22	2	613	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
22	6	613	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
22	4	309	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
22	8	309	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
22	d	404	CLA	O2D-CGD-O1D	-2.41	118.97	123.82
22	b	603	CLA	C1D-CHD-C4C	-2.41	119.19	122.48
22	d	403	CLA	CMA-C3A-C4A	-2.41	105.30	111.77
22	C	506	CLA	O2D-CGD-O1D	-2.41	118.98	123.82
22	c	511	CLA	O2D-CGD-O1D	-2.41	118.98	123.82
22	B	609	CLA	CGD-CBD-CAD	-2.41	102.65	110.71
22	C	509	CLA	O2D-CGD-O1D	-2.41	118.98	123.82
22	7	303	CLA	CGD-CBD-CAD	-2.40	102.68	110.71
22	3	303	CLA	CGD-CBD-CAD	-2.40	102.68	110.71
22	n	611	CLA	O1D-CGD-CBD	-2.40	120.30	124.60
22	N	611	CLA	O1D-CGD-CBD	-2.40	120.30	124.60
22	a	403	CLA	CAC-C3C-C2C	-2.39	123.35	127.49
22	Y	602	CLA	CMA-C3A-C2A	-2.39	104.06	113.77
22	y	602	CLA	CMA-C3A-C2A	-2.39	104.06	113.77
22	7	313	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
22	3	313	CLA	O2D-CGD-O1D	-2.39	119.01	123.82
22	G	602	CLA	CGD-CBD-CAD	-2.39	102.71	110.71
22	g	602	CLA	CGD-CBD-CAD	-2.39	102.71	110.71
22	1	603	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
22	5	603	CLA	O2D-CGD-O1D	-2.39	119.02	123.82
22	C	508	CLA	CHA-C1A-NA	-2.39	120.64	126.18
22	A	403	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
22	2	602	CLA	CGD-CBD-CAD	-2.38	102.73	110.71
22	6	602	CLA	CGD-CBD-CAD	-2.38	102.73	110.71
22	C	502	CLA	OBD-CAD-C3D	-2.38	123.64	128.03
22	S	301	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
25	2	606	CHL	C3B-CAB-CBB	-2.38	119.86	125.20
25	6	606	CHL	C3B-CAB-CBB	-2.38	119.86	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	611	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
22	2	611	CLA	O2D-CGD-O1D	-2.38	119.03	123.82
22	n	610	CLA	CHC-C1C-C2C	-2.38	120.16	126.65
22	N	610	CLA	CHC-C1C-C2C	-2.38	120.16	126.65
22	b	605	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
22	S	304	CLA	CAA-C2A-C3A	-2.38	106.30	112.81
22	s	304	CLA	CAA-C2A-C3A	-2.38	106.30	112.81
22	G	610	CLA	CHC-C1C-C2C	-2.37	120.17	126.65
22	g	610	CLA	CHC-C1C-C2C	-2.37	120.17	126.65
22	8	310	CLA	CAC-C3C-C2C	-2.37	123.38	127.49
22	4	310	CLA	CAC-C3C-C2C	-2.37	123.38	127.49
22	G	610	CLA	CMA-C3A-C4A	-2.37	105.39	111.77
22	g	610	CLA	CMA-C3A-C4A	-2.37	105.39	111.77
25	4	301	CHL	O1D-CGD-CBD	-2.37	119.64	124.53
25	8	301	CHL	O1D-CGD-CBD	-2.37	119.64	124.53
22	C	508	CLA	CGD-CBD-CAD	-2.37	102.77	110.71
22	b	609	CLA	O2D-CGD-O1D	-2.37	119.06	123.82
22	c	508	CLA	CHA-C1A-NA	-2.37	120.68	126.18
25	Y	601	CHL	O1D-CGD-CBD	-2.37	119.65	124.53
25	y	601	CHL	O1D-CGD-CBD	-2.37	119.65	124.53
22	C	506	CLA	CAA-C2A-C3A	-2.36	106.33	112.81
22	c	504	CLA	O2D-CGD-O1D	-2.36	119.06	123.82
22	c	506	CLA	CHA-C1A-NA	-2.36	120.69	126.18
22	C	504	CLA	O2D-CGD-O1D	-2.36	119.07	123.82
22	g	612	CLA	CAA-C2A-C3A	-2.36	106.34	112.81
22	G	612	CLA	CAA-C2A-C3A	-2.36	106.34	112.81
25	n	607	CHL	C3B-CAB-CBB	-2.36	119.90	125.20
25	N	607	CHL	C3B-CAB-CBB	-2.36	119.90	125.20
23	d	402	PHO	C1C-C2C-C3C	-2.36	103.78	106.51
22	c	503	CLA	CGD-CBD-CAD	-2.35	102.83	110.71
22	A	402	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
22	y	611	CLA	CHA-C1A-NA	-2.35	120.72	126.18
22	Y	611	CLA	CHA-C1A-NA	-2.35	120.72	126.18
22	b	601	CLA	CAC-C3C-C2C	-2.35	123.42	127.49
22	D	401	CLA	CAC-C3C-C2C	-2.35	123.42	127.49
23	d	402	PHO	O2D-CGD-O1D	-2.35	119.09	123.82
22	S	305	CLA	CAA-C2A-C3A	-2.35	106.37	112.81
22	s	305	CLA	CAA-C2A-C3A	-2.35	106.37	112.81
22	S	314	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
22	s	314	CLA	O2D-CGD-O1D	-2.35	119.09	123.82
22	Y	603	CLA	CAA-C2A-C3A	-2.35	106.37	112.81
22	y	603	CLA	CAA-C2A-C3A	-2.35	106.37	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	311	CLA	CAC-C3C-C2C	-2.35	123.42	127.49
22	s	311	CLA	CAC-C3C-C2C	-2.35	123.42	127.49
22	6	611	CLA	CGD-CBD-CAD	-2.34	102.86	110.71
22	2	611	CLA	CGD-CBD-CAD	-2.34	102.86	110.71
22	c	505	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
22	B	604	CLA	CHA-C1A-NA	-2.34	120.75	126.18
23	D	402	PHO	C3B-C2B-C1B	-2.34	101.58	106.30
22	d	403	CLA	CMA-C3A-C2A	-2.34	104.29	113.77
22	S	311	CLA	CAA-C2A-C3A	-2.34	106.41	112.81
22	s	311	CLA	CAA-C2A-C3A	-2.34	106.41	112.81
22	C	502	CLA	CGD-CBD-CAD	-2.33	102.89	110.71
22	1	602	CLA	CMA-C3A-C2A	-2.33	104.31	113.77
22	5	602	CLA	CMA-C3A-C2A	-2.33	104.31	113.77
22	1	612	CLA	O2D-CGD-O1D	-2.33	119.14	123.82
22	5	612	CLA	O2D-CGD-O1D	-2.33	119.14	123.82
22	B	601	CLA	CHC-C1C-C2C	-2.33	120.31	126.65
22	b	609	CLA	CGD-CBD-CAD	-2.32	102.92	110.71
25	G	607	CHL	O1D-CGD-CBD	-2.32	119.73	124.53
25	g	607	CHL	O1D-CGD-CBD	-2.32	119.73	124.53
22	B	602	CLA	O2D-CGD-O1D	-2.32	119.14	123.82
22	y	612	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
22	Y	612	CLA	O2D-CGD-O1D	-2.32	119.16	123.82
22	8	310	CLA	CGD-CBD-CAD	-2.31	102.96	110.71
22	4	310	CLA	CGD-CBD-CAD	-2.31	102.96	110.71
22	C	503	CLA	CHA-C1A-NA	-2.31	120.81	126.18
22	n	604	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
22	N	604	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
22	6	603	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
22	2	603	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
22	C	510	CLA	O2D-CGD-O1D	-2.31	119.17	123.82
22	S	301	CLA	CHA-C1A-NA	-2.31	120.81	126.18
22	b	601	CLA	CGD-CBD-CAD	-2.31	102.97	110.71
22	R	308	CLA	CHC-C1C-C2C	-2.31	120.35	126.65
22	r	308	CLA	CHC-C1C-C2C	-2.31	120.35	126.65
25	y	606	CHL	O1D-CGD-CBD	-2.31	119.77	124.53
25	Y	606	CHL	O1D-CGD-CBD	-2.31	119.77	124.53
22	S	312	CLA	O2D-CGD-O1D	-2.31	119.18	123.82
22	s	312	CLA	O2D-CGD-O1D	-2.31	119.18	123.82
22	B	613	CLA	O2D-CGD-O1D	-2.30	119.18	123.82
25	6	608	CHL	OBD-CAD-CBD	-2.30	121.94	127.52
25	2	608	CHL	OBD-CAD-CBD	-2.30	121.94	127.52
25	Y	605	CHL	O1D-CGD-CBD	-2.30	119.78	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	605	CHL	O1D-CGD-CBD	-2.30	119.78	124.53
22	Y	604	CLA	CGD-CBD-CAD	-2.30	103.01	110.71
22	y	604	CLA	CGD-CBD-CAD	-2.30	103.01	110.71
22	3	304	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
22	7	304	CLA	O2D-CGD-O1D	-2.30	119.19	123.82
22	y	613	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
22	Y	613	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
22	C	506	CLA	CHA-C1A-NA	-2.30	120.85	126.18
22	b	612	CLA	O2D-CGD-O1D	-2.29	119.20	123.82
25	s	306	CHL	C3B-CAB-CBB	-2.29	120.05	125.20
25	S	306	CHL	C3B-CAB-CBB	-2.29	120.05	125.20
25	n	609	CHL	C3B-CAB-CBB	-2.29	120.06	125.20
25	N	609	CHL	C3B-CAB-CBB	-2.29	120.06	125.20
22	c	512	CLA	O2D-CGD-O1D	-2.29	119.22	123.82
22	a	405	CLA	CHA-C1A-NA	-2.29	120.87	126.18
22	B	610	CLA	CAA-C2A-C3A	-2.29	106.54	112.81
22	6	611	CLA	CAC-C3C-C2C	-2.28	123.53	127.49
22	2	611	CLA	CAC-C3C-C2C	-2.28	123.53	127.49
22	Y	604	CLA	CHA-C1A-NA	-2.28	120.87	126.18
22	y	604	CLA	CHA-C1A-NA	-2.28	120.87	126.18
22	B	602	CLA	CHA-C1A-NA	-2.28	120.87	126.18
22	R	311	CLA	O2D-CGD-O1D	-2.28	119.22	123.82
22	r	311	CLA	O2D-CGD-O1D	-2.28	119.22	123.82
22	c	501	CLA	CHA-C1A-NA	-2.28	120.88	126.18
22	b	610	CLA	CAC-C3C-C2C	-2.28	123.54	127.49
22	1	612	CLA	CAA-C2A-C3A	-2.28	106.56	112.81
22	5	612	CLA	CAA-C2A-C3A	-2.28	106.56	112.81
23	d	402	PHO	C3B-C2B-C1B	-2.28	101.70	106.30
22	3	312	CLA	O2D-CGD-O1D	-2.28	119.24	123.82
22	7	312	CLA	O2D-CGD-O1D	-2.28	119.24	123.82
22	c	502	CLA	CAA-C2A-C3A	-2.28	106.57	112.81
22	c	511	CLA	CGD-CBD-CAD	-2.27	103.09	110.71
22	d	403	CLA	CBC-CAC-C3C	-2.27	105.95	112.41
22	C	501	CLA	CHA-C1A-NA	-2.27	120.90	126.18
22	S	312	CLA	CAA-C2A-C3A	-2.27	106.58	112.81
22	s	312	CLA	CAA-C2A-C3A	-2.27	106.58	112.81
22	a	403	CLA	O2D-CGD-O1D	-2.27	119.25	123.82
22	C	511	CLA	CAA-C2A-C3A	-2.27	106.59	112.81
22	B	607	CLA	O2D-CGD-O1D	-2.27	119.26	123.82
22	S	311	CLA	O2D-CGD-O1D	-2.27	119.26	123.82
22	s	311	CLA	O2D-CGD-O1D	-2.27	119.26	123.82
22	C	507	CLA	CAC-C3C-C2C	-2.27	123.57	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	606	CHL	C3B-CAB-CBB	-2.26	120.12	125.20
25	N	606	CHL	C3B-CAB-CBB	-2.26	120.12	125.20
22	n	612	CLA	O2D-CGD-O1D	-2.26	119.27	123.82
22	N	612	CLA	O2D-CGD-O1D	-2.26	119.27	123.82
22	b	613	CLA	CAA-C2A-C3A	-2.26	106.61	112.81
25	5	615	CHL	O1D-CGD-CBD	-2.26	119.86	124.53
25	1	615	CHL	O1D-CGD-CBD	-2.26	119.86	124.53
22	b	615	CLA	CHA-C1A-NA	-2.26	120.93	126.18
22	c	503	CLA	CHA-C1A-NA	-2.26	120.94	126.18
22	b	605	CLA	CHA-C1A-NA	-2.26	120.94	126.18
22	B	614	CLA	CHA-C1A-NA	-2.25	120.94	126.18
22	R	308	CLA	CBC-CAC-C3C	-2.25	106.01	112.41
22	r	308	CLA	CBC-CAC-C3C	-2.25	106.01	112.41
25	Y	605	CHL	C3B-CAB-CBB	-2.25	120.14	125.20
25	y	605	CHL	C3B-CAB-CBB	-2.25	120.14	125.20
22	c	508	CLA	CGD-CBD-CAD	-2.25	103.17	110.71
25	g	606	CHL	O1D-CGD-CBD	-2.25	119.88	124.53
25	G	606	CHL	O1D-CGD-CBD	-2.25	119.88	124.53
22	B	605	CLA	CMA-C3A-C4A	-2.25	105.73	111.77
22	b	616	CLA	C4A-NA-C1A	-2.25	103.66	106.45
25	R	304	CHL	O1D-CGD-CBD	-2.25	119.89	124.53
25	r	304	CHL	O1D-CGD-CBD	-2.25	119.89	124.53
22	C	509	CLA	CAA-C2A-C3A	-2.25	106.64	112.81
22	4	303	CLA	CAA-C2A-C3A	-2.25	106.65	112.81
22	8	303	CLA	CAA-C2A-C3A	-2.25	106.65	112.81
22	C	512	CLA	CHA-C1A-NA	-2.24	120.97	126.18
22	r	307	CLA	CGD-CBD-CAD	-2.24	103.20	110.71
22	R	307	CLA	CGD-CBD-CAD	-2.24	103.20	110.71
22	c	505	CLA	CAA-C2A-C3A	-2.24	106.67	112.81
22	N	614	CLA	CAA-C2A-C3A	-2.24	106.68	112.81
22	n	614	CLA	CAA-C2A-C3A	-2.24	106.68	112.81
22	b	608	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
22	3	310	CLA	CHC-C1C-C2C	-2.24	120.55	126.65
22	7	310	CLA	CHC-C1C-C2C	-2.24	120.55	126.65
23	d	402	PHO	CAA-C2A-C3A	-2.24	106.68	112.81
22	c	510	CLA	O2D-CGD-O1D	-2.23	119.32	123.82
22	c	510	CLA	CHA-C1A-NA	-2.23	120.99	126.18
22	C	512	CLA	CGD-CBD-CAD	-2.23	103.23	110.71
22	B	603	CLA	CGD-CBD-CAD	-2.23	103.25	110.71
22	B	607	CLA	CHA-C1A-NA	-2.23	121.00	126.18
22	c	505	CLA	O1D-CGD-CBD	-2.23	120.60	124.60
22	c	509	CLA	CGD-CBD-CAD	-2.23	103.26	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	CAA-C2A-C3A	-2.22	106.71	112.81
22	y	612	CLA	CAA-C2A-C3A	-2.22	106.72	112.81
22	Y	612	CLA	CAA-C2A-C3A	-2.22	106.72	112.81
22	C	510	CLA	CHA-C1A-NA	-2.22	121.02	126.18
22	R	312	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
22	r	312	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
22	b	607	CLA	CGD-CBD-CAD	-2.22	103.29	110.71
25	Y	607	CHL	C3B-CAB-CBB	-2.21	120.23	125.20
25	y	607	CHL	C3B-CAB-CBB	-2.21	120.23	125.20
22	G	610	CLA	CMA-C3A-C2A	-2.21	104.79	113.77
22	g	610	CLA	CMA-C3A-C2A	-2.21	104.79	113.77
22	S	314	CLA	CAA-C2A-C3A	-2.21	106.75	112.81
22	s	314	CLA	CAA-C2A-C3A	-2.21	106.75	112.81
22	a	402	CLA	CHA-C1A-NA	-2.21	121.05	126.18
22	b	616	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
22	s	309	CLA	CAA-C2A-C3A	-2.21	106.76	112.81
22	S	309	CLA	CAA-C2A-C3A	-2.21	106.76	112.81
22	C	510	CLA	CGD-CBD-CAD	-2.20	103.33	110.71
22	c	501	CLA	CAA-C2A-C3A	-2.20	106.77	112.81
22	Y	603	CLA	O2D-CGD-O1D	-2.20	119.39	123.82
22	y	603	CLA	O2D-CGD-O1D	-2.20	119.39	123.82
25	n	606	CHL	O1D-CGD-CBD	-2.20	120.00	124.53
25	N	606	CHL	O1D-CGD-CBD	-2.20	120.00	124.53
22	n	603	CLA	O2D-CGD-O1D	-2.20	119.40	123.82
22	N	603	CLA	O2D-CGD-O1D	-2.20	119.40	123.82
22	c	512	CLA	CHA-C1A-NA	-2.20	121.08	126.18
25	7	309	CHL	OBD-CAD-CBD	-2.19	122.21	127.52
25	3	309	CHL	OBD-CAD-CBD	-2.19	122.21	127.52
23	D	402	PHO	CAA-C2A-C3A	-2.19	106.80	112.81
22	c	506	CLA	CAA-C2A-C3A	-2.19	106.80	112.81
22	R	309	CLA	CAA-C2A-C3A	-2.19	106.82	112.81
22	r	309	CLA	CAA-C2A-C3A	-2.19	106.82	112.81
23	a	404	PHO	C3B-C2B-C1B	-2.19	101.89	106.30
22	G	614	CLA	CAA-C2A-C3A	-2.18	106.83	112.81
22	g	614	CLA	CAA-C2A-C3A	-2.18	106.83	112.81
23	a	404	PHO	O2D-CGD-O1D	-2.18	119.43	123.82
25	g	601	CHL	O1D-CGD-CBD	-2.18	120.03	124.53
25	G	601	CHL	O1D-CGD-CBD	-2.18	120.03	124.53
22	b	602	CLA	O2D-CGD-O1D	-2.18	119.43	123.82
22	7	303	CLA	CMA-C3A-C2A	-2.18	104.94	113.77
22	3	303	CLA	CMA-C3A-C2A	-2.18	104.94	113.77
22	B	614	CLA	CHC-C1C-C2C	-2.17	120.72	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	6	609	CLA	CHC-C1C-C2C	-2.17	120.72	126.65
22	2	609	CLA	CHC-C1C-C2C	-2.17	120.72	126.65
22	g	611	CLA	CAA-C2A-C3A	-2.17	106.85	112.81
22	G	611	CLA	CAA-C2A-C3A	-2.17	106.85	112.81
22	c	507	CLA	CAA-C2A-C3A	-2.17	106.86	112.81
22	c	502	CLA	O2D-CGD-O1D	-2.17	119.45	123.82
22	D	401	CLA	CHA-C1A-NA	-2.17	121.14	126.18
22	a	405	CLA	O2D-CGD-O1D	-2.17	119.46	123.82
22	B	616	CLA	CGD-CBD-CAD	-2.17	103.45	110.71
22	7	303	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
22	3	303	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
22	b	614	CLA	CHA-C1A-NA	-2.17	121.15	126.18
22	B	602	CLA	CBC-CAC-C3C	-2.16	106.28	112.41
22	b	601	CLA	CAA-C2A-C3A	-2.16	106.89	112.81
25	N	601	CHL	O1D-CGD-CBD	-2.16	120.08	124.53
25	n	601	CHL	O1D-CGD-CBD	-2.16	120.08	124.53
22	b	613	CLA	O2D-CGD-O1D	-2.16	119.48	123.82
22	7	314	CLA	CAA-C2A-C3A	-2.15	106.91	112.81
22	3	314	CLA	CAA-C2A-C3A	-2.15	106.91	112.81
22	b	614	CLA	O2D-CGD-O1D	-2.15	119.49	123.82
22	b	610	CLA	CHA-C1A-NA	-2.15	121.19	126.18
22	B	613	CLA	CHA-C1A-NA	-2.15	121.19	126.18
22	Y	603	CLA	CHA-C1A-NA	-2.15	121.19	126.18
22	y	603	CLA	CHA-C1A-NA	-2.15	121.19	126.18
22	B	616	CLA	CHA-C1A-NA	-2.15	121.19	126.18
22	2	610	CLA	CGD-CBD-CAD	-2.15	103.52	110.71
22	6	610	CLA	CGD-CBD-CAD	-2.15	103.52	110.71
22	5	614	CLA	CHA-C1A-NA	-2.14	121.20	126.18
22	1	614	CLA	CHA-C1A-NA	-2.14	121.20	126.18
22	b	607	CLA	O2D-CGD-O1D	-2.14	119.50	123.82
22	2	612	CLA	O2D-CGD-O1D	-2.14	119.51	123.82
22	6	612	CLA	O2D-CGD-O1D	-2.14	119.51	123.82
22	G	603	CLA	CHA-C1A-NA	-2.14	121.20	126.18
22	g	603	CLA	CHA-C1A-NA	-2.14	121.20	126.18
25	s	306	CHL	CHA-CBD-CGD	-2.14	110.03	115.00
25	S	306	CHL	CHA-CBD-CGD	-2.14	110.03	115.00
22	R	311	CLA	CGD-CBD-CAD	-2.14	103.53	110.71
22	r	311	CLA	CGD-CBD-CAD	-2.14	103.53	110.71
22	B	610	CLA	CHA-C1A-NA	-2.14	121.20	126.18
25	N	605	CHL	C3B-CAB-CBB	-2.14	120.40	125.20
25	n	605	CHL	C3B-CAB-CBB	-2.14	120.40	125.20
22	B	604	CLA	CGD-CBD-CAD	-2.14	103.55	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	602	CLA	CAC-C3C-C2C	-2.13	123.79	127.49
22	D	403	CLA	CMA-C3A-C4A	-2.13	106.05	111.77
22	A	403	CLA	CGD-CBD-CAD	-2.13	103.58	110.71
22	y	613	CLA	CHA-C1A-NA	-2.13	121.24	126.18
22	Y	613	CLA	CHA-C1A-NA	-2.13	121.24	126.18
22	B	604	CLA	O1D-CGD-CBD	-2.13	120.78	124.60
25	r	305	CHL	O1D-CGD-CBD	-2.13	120.14	124.53
25	R	305	CHL	O1D-CGD-CBD	-2.13	120.14	124.53
22	G	602	CLA	O2D-CGD-O1D	-2.13	119.54	123.82
22	g	602	CLA	O2D-CGD-O1D	-2.13	119.54	123.82
22	n	611	CLA	O2D-CGD-O1D	-2.13	119.54	123.82
22	N	611	CLA	O2D-CGD-O1D	-2.13	119.54	123.82
22	2	602	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
22	6	602	CLA	CMA-C3A-C4A	-2.12	106.07	111.77
25	s	307	CHL	C3B-CAB-CBB	-2.12	120.43	125.20
25	S	307	CHL	C3B-CAB-CBB	-2.12	120.43	125.20
22	C	503	CLA	O2D-CGD-O1D	-2.12	119.56	123.82
22	B	604	CLA	CAC-C3C-C2C	-2.11	123.83	127.49
25	Y	605	CHL	CMA-C3A-C2A	-2.11	111.08	115.37
25	y	605	CHL	CMA-C3A-C2A	-2.11	111.08	115.37
22	b	612	CLA	CGD-CBD-CAD	-2.11	103.64	110.71
22	g	612	CLA	O2D-CGD-O1D	-2.11	119.58	123.82
22	G	612	CLA	O2D-CGD-O1D	-2.11	119.58	123.82
22	Y	602	CLA	CGD-CBD-CAD	-2.11	103.66	110.71
22	y	602	CLA	CGD-CBD-CAD	-2.11	103.66	110.71
23	a	404	PHO	CAA-C2A-C3A	-2.10	107.04	112.81
22	c	512	CLA	CAA-C2A-C3A	-2.10	107.04	112.81
22	C	502	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
25	S	308	CHL	C3B-CAB-CBB	-2.10	120.48	125.20
25	s	308	CHL	C3B-CAB-CBB	-2.10	120.48	125.20
22	r	302	CLA	CAA-C2A-C3A	-2.10	107.05	112.81
22	R	302	CLA	CAA-C2A-C3A	-2.10	107.05	112.81
22	y	613	CLA	CAA-C2A-C3A	-2.10	107.05	112.81
22	Y	613	CLA	CAA-C2A-C3A	-2.10	107.05	112.81
22	n	613	CLA	CHA-C1A-NA	-2.10	121.31	126.18
22	N	613	CLA	CHA-C1A-NA	-2.10	121.31	126.18
22	b	608	CLA	CHA-C1A-NA	-2.10	121.31	126.18
22	s	309	CLA	CAC-C3C-C2C	-2.10	123.86	127.49
22	S	309	CLA	CAC-C3C-C2C	-2.10	123.86	127.49
24	e	101	HEM	CAA-CBA-CGA	-2.09	109.08	112.66
25	N	601	CHL	C3B-CAB-CBB	-2.09	120.50	125.20
25	n	601	CHL	C3B-CAB-CBB	-2.09	120.50	125.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	311	CLA	CGD-CBD-CAD	-2.09	103.70	110.71
22	3	311	CLA	CGD-CBD-CAD	-2.09	103.70	110.71
22	C	505	CLA	O1D-CGD-CBD	-2.09	120.84	124.60
22	G	604	CLA	O2D-CGD-O1D	-2.09	119.61	123.82
22	g	604	CLA	O2D-CGD-O1D	-2.09	119.61	123.82
22	3	310	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
22	7	310	CLA	CMA-C3A-C4A	-2.09	106.16	111.77
22	s	313	CLA	CAA-C2A-C3A	-2.09	107.08	112.81
22	S	313	CLA	CAA-C2A-C3A	-2.09	107.08	112.81
23	A	404	PHO	CAA-C2A-C1A	-2.09	106.88	112.28
22	2	604	CLA	CHA-C1A-NA	-2.09	121.33	126.18
22	6	604	CLA	CHA-C1A-NA	-2.09	121.33	126.18
22	C	512	CLA	CAA-C2A-C3A	-2.08	107.09	112.81
22	B	607	CLA	CGD-CBD-CAD	-2.08	103.73	110.71
22	y	612	CLA	CHA-C1A-NA	-2.08	121.34	126.18
22	Y	612	CLA	CHA-C1A-NA	-2.08	121.34	126.18
25	y	608	CHL	O1D-CGD-CBD	-2.08	120.23	124.53
25	Y	608	CHL	O1D-CGD-CBD	-2.08	120.23	124.53
22	7	313	CLA	CAA-C2A-C3A	-2.08	107.11	112.81
22	3	313	CLA	CAA-C2A-C3A	-2.08	107.11	112.81
22	S	301	CLA	CAA-C2A-C3A	-2.08	107.12	112.81
22	c	505	CLA	CMA-C3A-C2A	-2.07	105.36	113.77
22	b	602	CLA	CGD-CBD-CAD	-2.07	103.77	110.71
22	1	602	CLA	CGD-CBD-CAD	-2.07	103.77	110.71
22	5	602	CLA	CGD-CBD-CAD	-2.07	103.77	110.71
22	6	603	CLA	CAA-C2A-C3A	-2.07	107.14	112.81
22	2	603	CLA	CAA-C2A-C3A	-2.07	107.14	112.81
22	a	403	CLA	CHA-C1A-NA	-2.07	121.37	126.18
22	c	501	CLA	CGD-CBD-CAD	-2.07	103.78	110.71
22	G	614	CLA	CHA-C1A-NA	-2.07	121.38	126.18
22	g	614	CLA	CHA-C1A-NA	-2.07	121.38	126.18
22	7	305	CLA	CHA-C1A-NA	-2.07	121.38	126.18
22	3	305	CLA	CHA-C1A-NA	-2.07	121.38	126.18
22	B	605	CLA	CAA-C2A-C3A	-2.07	107.15	112.81
22	B	605	CLA	CHA-C1A-NA	-2.07	121.38	126.18
22	n	613	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
22	S	310	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
22	N	613	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
22	s	310	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
22	C	501	CLA	O2D-CGD-O1D	-2.06	119.67	123.82
22	3	304	CLA	CHA-C1A-NA	-2.06	121.39	126.18
22	7	304	CLA	CHA-C1A-NA	-2.06	121.39	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	605	CHL	CHA-CBD-CGD	-2.06	110.22	115.00
25	5	605	CHL	CHA-CBD-CGD	-2.06	110.22	115.00
22	G	604	CLA	CHA-C1A-NA	-2.06	121.39	126.18
22	g	604	CLA	CHA-C1A-NA	-2.06	121.39	126.18
25	2	606	CHL	O1D-CGD-CBD	-2.06	120.28	124.53
25	6	606	CHL	O1D-CGD-CBD	-2.06	120.28	124.53
25	1	606	CHL	O1D-CGD-CBD	-2.06	120.28	124.53
25	5	606	CHL	O1D-CGD-CBD	-2.06	120.28	124.53
25	S	302	CHL	C3B-CAB-CBB	-2.05	120.59	125.20
25	s	302	CHL	C3B-CAB-CBB	-2.05	120.59	125.20
22	C	503	CLA	CAA-C2A-C3A	-2.05	107.19	112.81
22	r	307	CLA	O2D-CGD-O1D	-2.05	119.69	123.82
22	R	307	CLA	O2D-CGD-O1D	-2.05	119.69	123.82
22	B	603	CLA	CHA-C1A-NA	-2.05	121.42	126.18
22	s	301	CLA	CGD-CBD-CAD	-2.05	103.85	110.71
22	C	507	CLA	CHA-C1A-NA	-2.05	121.42	126.18
22	c	507	CLA	O2D-CGD-O1D	-2.05	119.70	123.82
23	a	404	PHO	CHC-C1C-C2C	-2.05	120.93	125.62
22	R	312	CLA	CHA-C1A-NA	-2.05	121.43	126.18
22	r	312	CLA	CHA-C1A-NA	-2.05	121.43	126.18
22	b	609	CLA	CHA-C1A-NA	-2.04	121.43	126.18
22	d	401	CLA	CHA-C1A-NA	-2.04	121.43	126.18
22	D	403	CLA	CHA-C1A-NA	-2.04	121.43	126.18
22	g	613	CLA	O2D-CGD-O1D	-2.04	119.71	123.82
22	G	613	CLA	O2D-CGD-O1D	-2.04	119.71	123.82
23	D	402	PHO	CHC-C1C-C2C	-2.04	120.94	125.62
22	C	511	CLA	CGD-CBD-CAD	-2.04	103.88	110.71
22	R	312	CLA	CGD-CBD-CAD	-2.04	103.88	110.71
22	r	312	CLA	CGD-CBD-CAD	-2.04	103.88	110.71
22	d	403	CLA	CHA-C1A-NA	-2.04	121.45	126.18
22	S	311	CLA	CHA-C1A-NA	-2.04	121.45	126.18
22	s	311	CLA	CHA-C1A-NA	-2.04	121.45	126.18
22	R	301	CLA	CGD-CBD-CAD	-2.04	103.89	110.71
22	r	301	CLA	CGD-CBD-CAD	-2.04	103.89	110.71
25	n	609	CHL	OBD-CAD-CBD	-2.03	122.60	127.52
25	N	609	CHL	OBD-CAD-CBD	-2.03	122.60	127.52
22	A	403	CLA	CHA-C1A-NA	-2.03	121.46	126.18
22	C	502	CLA	CAC-C3C-C2C	-2.03	123.97	127.49
22	1	612	CLA	CGD-CBD-CAD	-2.02	103.93	110.71
22	5	612	CLA	CGD-CBD-CAD	-2.02	103.93	110.71
22	b	608	CLA	CAA-C2A-C3A	-2.02	107.26	112.81
22	n	611	CLA	CAA-C2A-C3A	-2.02	107.26	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	611	CLA	CAA-C2A-C3A	-2.02	107.26	112.81
22	C	505	CLA	CHA-C1A-NA	-2.02	121.48	126.18
25	g	605	CHL	O1D-CGD-CBD	-2.02	120.36	124.53
25	G	605	CHL	O1D-CGD-CBD	-2.02	120.36	124.53
22	r	307	CLA	CBC-CAC-C3C	-2.02	106.68	112.41
22	R	307	CLA	CBC-CAC-C3C	-2.02	106.68	112.41
22	4	304	CLA	CHA-C1A-NA	-2.02	121.49	126.18
22	8	304	CLA	CHA-C1A-NA	-2.02	121.49	126.18
25	r	305	CHL	C3B-CAB-CBB	-2.02	120.67	125.20
25	R	305	CHL	C3B-CAB-CBB	-2.02	120.67	125.20
22	Y	614	CLA	CHA-C1A-NA	-2.02	121.49	126.18
22	y	614	CLA	CHA-C1A-NA	-2.02	121.49	126.18
22	b	613	CLA	CHA-C1A-NA	-2.02	121.50	126.18
22	B	612	CLA	CHA-C1A-NA	-2.02	121.50	126.18
22	b	611	CLA	CAA-C2A-C3A	-2.02	107.28	112.81
22	g	613	CLA	CGD-CBD-CAD	-2.02	103.96	110.71
22	G	613	CLA	CGD-CBD-CAD	-2.02	103.96	110.71
22	b	611	CLA	CHA-C1A-NA	-2.01	121.50	126.18
25	N	608	CHL	O1D-CGD-CBD	-2.01	120.37	124.53
25	n	608	CHL	O1D-CGD-CBD	-2.01	120.37	124.53
22	s	313	CLA	CHA-C1A-NA	-2.01	121.51	126.18
22	S	313	CLA	CHA-C1A-NA	-2.01	121.51	126.18
22	n	611	CLA	CHA-C1A-NA	-2.01	121.51	126.18
22	l	612	CLA	CHA-C1A-NA	-2.01	121.51	126.18
22	5	612	CLA	CHA-C1A-NA	-2.01	121.51	126.18
22	N	611	CLA	CHA-C1A-NA	-2.01	121.51	126.18
22	y	610	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
22	Y	610	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
22	C	509	CLA	CHA-C1A-NA	-2.01	121.52	126.18
22	r	302	CLA	CHA-C1A-NA	-2.01	121.52	126.18
22	b	604	CLA	CHA-C1A-NA	-2.01	121.52	126.18
22	R	302	CLA	CHA-C1A-NA	-2.01	121.52	126.18
22	b	610	CLA	CAA-C2A-C3A	-2.01	107.31	112.81
22	3	304	CLA	CAA-C2A-C3A	-2.00	107.31	112.81
22	7	304	CLA	CAA-C2A-C3A	-2.00	107.31	112.81
22	c	502	CLA	CGD-CBD-CAD	-2.00	104.00	110.71
22	g	612	CLA	CMC-C2C-C3C	2.00	131.63	126.09
22	G	612	CLA	CMC-C2C-C3C	2.00	131.63	126.09
22	c	509	CLA	CMC-C2C-C3C	2.01	131.64	126.09
22	g	612	CLA	C3B-C4B-NB	2.01	111.80	109.21
22	G	612	CLA	C3B-C4B-NB	2.01	111.80	109.21
22	b	613	CLA	CMC-C2C-C1C	2.01	128.06	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	306	CHL	O2D-CGD-CBD	2.01	116.10	111.20
25	8	306	CHL	O2D-CGD-CBD	2.01	116.10	111.20
22	4	309	CLA	C3B-C4B-NB	2.01	111.81	109.21
22	8	309	CLA	C3B-C4B-NB	2.01	111.81	109.21
22	c	506	CLA	C3D-CAD-CBD	2.01	110.44	107.60
22	C	504	CLA	CMC-C2C-C3C	2.01	131.66	126.09
22	4	303	CLA	C3B-C4B-NB	2.01	111.81	109.21
22	8	303	CLA	C3B-C4B-NB	2.01	111.81	109.21
22	b	613	CLA	CMC-C2C-C3C	2.02	131.67	126.09
22	G	614	CLA	CED-O2D-CGD	2.02	120.70	115.97
22	g	614	CLA	CED-O2D-CGD	2.02	120.70	115.97
22	c	503	CLA	C3D-CAD-CBD	2.02	110.45	107.60
22	n	612	CLA	CED-O2D-CGD	2.02	120.70	115.97
22	N	612	CLA	CED-O2D-CGD	2.02	120.70	115.97
22	4	303	CLA	C3D-CAD-CBD	2.02	110.45	107.60
22	8	303	CLA	C3D-CAD-CBD	2.02	110.45	107.60
22	7	305	CLA	C3D-CAD-CBD	2.02	110.45	107.60
22	3	305	CLA	C3D-CAD-CBD	2.02	110.45	107.60
22	4	303	CLA	CMC-C2C-C1C	2.02	128.09	125.02
22	8	303	CLA	CMC-C2C-C1C	2.02	128.09	125.02
22	B	605	CLA	C3D-CAD-CBD	2.02	110.45	107.60
22	c	503	CLA	C3B-C4B-NB	2.02	111.83	109.21
22	c	509	CLA	C3B-C4B-NB	2.03	111.83	109.21
22	D	401	CLA	OBD-CAD-CBD	2.03	129.00	125.94
25	8	305	CHL	O2D-CGD-CBD	2.03	116.15	111.20
25	4	305	CHL	O2D-CGD-CBD	2.03	116.15	111.20
22	G	603	CLA	CED-O2D-CGD	2.03	120.73	115.97
22	g	603	CLA	CED-O2D-CGD	2.03	120.73	115.97
22	G	603	CLA	CMC-C2C-C1C	2.03	128.10	125.02
22	g	603	CLA	CMC-C2C-C1C	2.03	128.10	125.02
22	C	508	CLA	C3D-CAD-CBD	2.03	110.47	107.60
22	b	603	CLA	CMC-C2C-C1C	2.03	128.10	125.02
22	6	603	CLA	CMC-C2C-C1C	2.03	128.10	125.02
22	2	603	CLA	CMC-C2C-C1C	2.03	128.10	125.02
22	c	510	CLA	C3B-C4B-NB	2.04	111.84	109.21
22	4	303	CLA	CMB-C2B-C3B	2.04	128.67	124.89
22	8	303	CLA	CMB-C2B-C3B	2.04	128.67	124.89
22	c	511	CLA	C3D-CAD-CBD	2.04	110.48	107.60
25	7	307	CHL	O2D-CGD-CBD	2.04	116.18	111.20
25	3	307	CHL	O2D-CGD-CBD	2.04	116.18	111.20
22	g	612	CLA	CED-O2D-CGD	2.04	120.76	115.97
22	G	612	CLA	CED-O2D-CGD	2.04	120.76	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	C3D-CAD-CBD	2.04	110.48	107.60
22	G	604	CLA	CMC-C2C-C3C	2.04	131.75	126.09
22	g	604	CLA	CMC-C2C-C3C	2.04	131.75	126.09
22	R	311	CLA	C3B-C4B-NB	2.04	111.85	109.21
22	r	311	CLA	C3B-C4B-NB	2.04	111.85	109.21
22	b	607	CLA	CMC-C2C-C1C	2.04	128.12	125.02
25	g	606	CHL	O2D-CGD-CBD	2.05	116.20	111.20
25	G	606	CHL	O2D-CGD-CBD	2.05	116.20	111.20
22	c	507	CLA	CMB-C2B-C3B	2.05	128.69	124.89
22	g	613	CLA	CMC-C2C-C3C	2.05	131.76	126.09
22	G	613	CLA	CMC-C2C-C3C	2.05	131.76	126.09
22	C	512	CLA	CMC-C2C-C3C	2.05	131.76	126.09
22	b	608	CLA	C3B-C4B-NB	2.05	111.86	109.21
22	2	610	CLA	CED-O2D-CGD	2.06	120.79	115.97
22	6	610	CLA	CED-O2D-CGD	2.06	120.79	115.97
22	s	309	CLA	CED-O2D-CGD	2.06	120.79	115.97
22	S	309	CLA	CED-O2D-CGD	2.06	120.79	115.97
22	c	502	CLA	C3B-C4B-NB	2.06	111.87	109.21
22	a	402	CLA	CMC-C2C-C3C	2.06	131.79	126.09
22	c	508	CLA	C3D-CAD-CBD	2.06	110.51	107.60
22	C	501	CLA	CED-O2D-CGD	2.06	120.80	115.97
23	d	402	PHO	CBD-CHA-C1A	2.06	131.21	126.36
22	8	310	CLA	C3B-C4B-NB	2.06	111.87	109.21
22	4	310	CLA	C3B-C4B-NB	2.06	111.87	109.21
22	y	610	CLA	C3B-C4B-NB	2.06	111.88	109.21
22	Y	610	CLA	C3B-C4B-NB	2.06	111.88	109.21
22	R	303	CLA	OBD-CAD-CBD	2.06	129.05	125.94
22	r	303	CLA	OBD-CAD-CBD	2.06	129.05	125.94
22	g	613	CLA	CMB-C2B-C3B	2.06	128.72	124.89
22	G	613	CLA	CMB-C2B-C3B	2.06	128.72	124.89
22	R	309	CLA	CMC-C2C-C1C	2.06	128.15	125.02
22	r	309	CLA	CMC-C2C-C1C	2.06	128.15	125.02
22	b	607	CLA	C3B-C4B-NB	2.06	111.88	109.21
25	N	605	CHL	O2D-CGD-CBD	2.07	116.25	111.20
25	n	605	CHL	O2D-CGD-CBD	2.07	116.25	111.20
25	g	608	CHL	OBD-CAD-C3D	2.07	130.35	126.75
25	G	608	CHL	OBD-CAD-C3D	2.07	130.35	126.75
22	G	614	CLA	CMC-C2C-C1C	2.07	128.16	125.02
22	g	614	CLA	CMC-C2C-C1C	2.07	128.16	125.02
22	8	310	CLA	CED-O2D-CGD	2.07	120.83	115.97
22	4	310	CLA	CED-O2D-CGD	2.07	120.83	115.97
22	7	311	CLA	CMC-C2C-C1C	2.07	128.16	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	311	CLA	CMC-C2C-C1C	2.07	128.16	125.02
22	b	610	CLA	CED-O2D-CGD	2.07	120.83	115.97
22	2	613	CLA	CED-O2D-CGD	2.08	120.84	115.97
22	6	613	CLA	CED-O2D-CGD	2.08	120.84	115.97
22	r	310	CLA	CMB-C2B-C3B	2.08	128.75	124.89
22	R	310	CLA	CMB-C2B-C3B	2.08	128.75	124.89
22	n	611	CLA	CMC-C2C-C1C	2.08	128.18	125.02
22	N	611	CLA	CMC-C2C-C1C	2.08	128.18	125.02
22	1	602	CLA	C3D-CAD-CBD	2.08	110.54	107.60
22	5	602	CLA	C3D-CAD-CBD	2.08	110.54	107.60
25	8	308	CHL	O2D-CGD-CBD	2.08	116.29	111.20
25	4	308	CHL	O2D-CGD-CBD	2.08	116.29	111.20
22	S	311	CLA	CMC-C2C-C1C	2.08	128.18	125.02
22	s	311	CLA	CMC-C2C-C1C	2.08	128.18	125.02
22	n	613	CLA	CMB-C2B-C3B	2.08	128.76	124.89
22	N	613	CLA	CMB-C2B-C3B	2.08	128.76	124.89
22	S	310	CLA	CMB-C2B-C3B	2.09	128.76	124.89
22	s	310	CLA	CMB-C2B-C3B	2.09	128.76	124.89
22	s	301	CLA	CED-O2D-CGD	2.09	120.86	115.97
22	1	603	CLA	CED-O2D-CGD	2.09	120.86	115.97
22	5	603	CLA	CED-O2D-CGD	2.09	120.86	115.97
22	c	510	CLA	CED-O2D-CGD	2.09	120.87	115.97
22	B	611	CLA	C3D-CAD-CBD	2.09	110.55	107.60
22	R	312	CLA	C3B-C4B-NB	2.09	111.92	109.21
22	r	312	CLA	C3B-C4B-NB	2.09	111.92	109.21
22	C	505	CLA	C3B-C4B-NB	2.09	111.92	109.21
22	g	611	CLA	CMC-C2C-C1C	2.10	128.20	125.02
22	G	611	CLA	CMC-C2C-C1C	2.10	128.20	125.02
22	5	611	CLA	CMC-C2C-C1C	2.10	128.20	125.02
22	1	611	CLA	CMC-C2C-C1C	2.10	128.20	125.02
25	y	608	CHL	CHB-C4A-C3A	2.10	122.79	117.08
25	Y	608	CHL	CHB-C4A-C3A	2.10	122.79	117.08
22	n	610	CLA	OBD-CAD-CBD	2.10	129.10	125.94
22	N	610	CLA	OBD-CAD-CBD	2.10	129.10	125.94
22	a	405	CLA	C3B-C4B-NB	2.10	111.92	109.21
22	R	308	CLA	CMB-C2B-C3B	2.10	128.79	124.89
22	r	308	CLA	CMB-C2B-C3B	2.10	128.79	124.89
22	6	611	CLA	CMB-C2B-C3B	2.10	128.79	124.89
22	2	611	CLA	CMB-C2B-C3B	2.10	128.79	124.89
22	R	301	CLA	CMC-C2C-C1C	2.10	128.21	125.02
22	r	301	CLA	CMC-C2C-C1C	2.10	128.21	125.02
22	S	314	CLA	C3B-C4B-NB	2.10	111.93	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	s	314	CLA	C3B-C4B-NB	2.10	111.93	109.21
22	n	612	CLA	CMC-C2C-C3C	2.10	131.91	126.09
22	N	612	CLA	CMC-C2C-C3C	2.10	131.91	126.09
23	D	402	PHO	CBD-CHA-C1A	2.10	131.32	126.36
22	7	313	CLA	CMB-C2B-C3B	2.11	128.80	124.89
22	3	313	CLA	CMB-C2B-C3B	2.11	128.80	124.89
22	4	304	CLA	C3B-C4B-NB	2.11	111.93	109.21
22	8	304	CLA	C3B-C4B-NB	2.11	111.93	109.21
22	C	510	CLA	CED-O2D-CGD	2.11	120.91	115.97
22	B	614	CLA	CMB-C2B-C3B	2.11	128.80	124.89
22	1	613	CLA	C3B-C4B-NB	2.11	111.94	109.21
22	5	613	CLA	C3B-C4B-NB	2.11	111.94	109.21
22	c	511	CLA	C3B-C4B-NB	2.11	111.94	109.21
22	G	614	CLA	C3B-C4B-NB	2.11	111.94	109.21
22	g	614	CLA	C3B-C4B-NB	2.11	111.94	109.21
22	Y	603	CLA	CED-O2D-CGD	2.11	120.92	115.97
22	y	603	CLA	CED-O2D-CGD	2.11	120.92	115.97
22	b	612	CLA	CED-O2D-CGD	2.11	120.92	115.97
22	8	302	CLA	C3B-C4B-NB	2.11	111.94	109.21
22	4	302	CLA	C3B-C4B-NB	2.11	111.94	109.21
25	r	305	CHL	O2D-CGD-CBD	2.11	116.36	111.20
25	R	305	CHL	O2D-CGD-CBD	2.11	116.36	111.20
22	b	611	CLA	CED-O2D-CGD	2.11	120.93	115.97
22	A	402	CLA	CED-O2D-CGD	2.12	120.94	115.97
22	5	614	CLA	CMB-C2B-C3B	2.12	128.82	124.89
22	1	614	CLA	CMB-C2B-C3B	2.12	128.82	124.89
22	r	310	CLA	C3B-C4B-NB	2.12	111.95	109.21
22	R	310	CLA	C3B-C4B-NB	2.12	111.95	109.21
22	2	604	CLA	CMC-C2C-C1C	2.12	128.24	125.02
22	6	604	CLA	CMC-C2C-C1C	2.12	128.24	125.02
22	8	302	CLA	CMC-C2C-C1C	2.12	128.24	125.02
22	4	302	CLA	CMC-C2C-C1C	2.12	128.24	125.02
25	2	606	CHL	O2D-CGD-CBD	2.12	116.38	111.20
25	6	606	CHL	O2D-CGD-CBD	2.12	116.38	111.20
22	C	504	CLA	CMC-C2C-C1C	2.12	128.24	125.02
22	b	610	CLA	C3B-C4B-NB	2.12	111.95	109.21
22	D	404	CLA	C3B-C4B-NB	2.12	111.96	109.21
22	Y	614	CLA	CED-O2D-CGD	2.13	120.95	115.97
22	y	614	CLA	CED-O2D-CGD	2.13	120.95	115.97
22	D	401	CLA	CED-O2D-CGD	2.13	120.95	115.97
22	7	313	CLA	CMC-C2C-C1C	2.13	128.24	125.02
22	3	313	CLA	CMC-C2C-C1C	2.13	128.24	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	606	CHL	CHC-C4B-C3B	2.13	123.27	118.23
25	N	606	CHL	CHC-C4B-C3B	2.13	123.27	118.23
22	g	611	CLA	CED-O2D-CGD	2.13	120.97	115.97
22	G	611	CLA	CED-O2D-CGD	2.13	120.97	115.97
25	1	601	CHL	O2D-CGD-CBD	2.13	116.41	111.20
25	5	601	CHL	O2D-CGD-CBD	2.13	116.41	111.20
22	n	613	CLA	C3B-C4B-NB	2.14	111.97	109.21
22	N	613	CLA	C3B-C4B-NB	2.14	111.97	109.21
22	B	603	CLA	C3B-C4B-NB	2.14	111.97	109.21
22	1	612	CLA	CED-O2D-CGD	2.14	120.98	115.97
22	5	612	CLA	CED-O2D-CGD	2.14	120.98	115.97
22	B	605	CLA	C3B-C4B-NB	2.14	111.98	109.21
22	C	503	CLA	CMC-C2C-C1C	2.14	128.27	125.02
22	R	312	CLA	CED-O2D-CGD	2.14	120.99	115.97
22	r	312	CLA	CED-O2D-CGD	2.14	120.99	115.97
22	B	607	CLA	C3B-C4B-NB	2.14	111.98	109.21
22	C	502	CLA	C3D-CAD-CBD	2.14	110.63	107.60
25	G	609	CHL	CHB-C4A-C3A	2.14	122.91	117.08
25	g	609	CHL	CHB-C4A-C3A	2.14	122.91	117.08
22	C	507	CLA	CED-O2D-CGD	2.15	121.00	115.97
22	6	609	CLA	OBD-CAD-CBD	2.15	129.17	125.94
22	2	609	CLA	OBD-CAD-CBD	2.15	129.17	125.94
22	y	612	CLA	C3D-CAD-CBD	2.15	110.63	107.60
22	Y	612	CLA	C3D-CAD-CBD	2.15	110.63	107.60
22	B	603	CLA	CMC-C2C-C1C	2.15	128.28	125.02
22	c	507	CLA	CED-O2D-CGD	2.15	121.01	115.97
22	C	512	CLA	C3B-C4B-NB	2.15	111.99	109.21
22	b	606	CLA	C3C-C4C-NC	2.15	112.39	110.21
22	1	612	CLA	C3B-C4B-NB	2.15	111.99	109.21
22	5	612	CLA	C3B-C4B-NB	2.15	111.99	109.21
22	1	613	CLA	CMC-C2C-C1C	2.15	128.29	125.02
22	5	613	CLA	CMC-C2C-C1C	2.15	128.29	125.02
22	B	608	CLA	CMC-C2C-C3C	2.15	132.05	126.09
25	Y	607	CHL	OBD-CAD-C3D	2.15	130.51	126.75
25	y	607	CHL	OBD-CAD-C3D	2.15	130.51	126.75
22	d	401	CLA	CMC-C2C-C3C	2.16	132.06	126.09
22	C	506	CLA	C3D-CAD-CBD	2.16	110.64	107.60
22	n	603	CLA	CMC-C2C-C1C	2.16	128.29	125.02
22	N	603	CLA	CMC-C2C-C1C	2.16	128.29	125.02
22	b	603	CLA	CED-O2D-CGD	2.16	121.03	115.97
22	s	309	CLA	CMB-C2B-C3B	2.16	128.90	124.89
22	S	309	CLA	CMB-C2B-C3B	2.16	128.90	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	s	313	CLA	C3B-C4B-NB	2.16	112.00	109.21
22	S	313	CLA	C3B-C4B-NB	2.16	112.00	109.21
22	D	404	CLA	CMB-C2B-C3B	2.16	128.90	124.89
22	b	611	CLA	C3D-CAD-CBD	2.16	110.65	107.60
22	C	505	CLA	CMC-C2C-C3C	2.16	132.07	126.09
25	1	605	CHL	OBD-CAD-C3D	2.16	130.52	126.75
25	5	605	CHL	OBD-CAD-C3D	2.16	130.52	126.75
25	g	606	CHL	CHC-C4B-C3B	2.17	123.36	118.23
25	G	606	CHL	CHC-C4B-C3B	2.17	123.36	118.23
22	c	505	CLA	CMC-C2C-C3C	2.17	132.09	126.09
22	s	303	CLA	C3B-C4B-NB	2.17	112.01	109.21
22	S	303	CLA	C3B-C4B-NB	2.17	112.01	109.21
22	S	314	CLA	CMC-C2C-C1C	2.17	128.31	125.02
22	s	314	CLA	CMC-C2C-C1C	2.17	128.31	125.02
22	S	312	CLA	C3D-CAD-CBD	2.17	110.66	107.60
22	s	312	CLA	C3D-CAD-CBD	2.17	110.66	107.60
22	3	312	CLA	CMC-C2C-C1C	2.17	128.31	125.02
22	7	312	CLA	CMC-C2C-C1C	2.17	128.31	125.02
22	A	405	CLA	CED-O2D-CGD	2.17	121.06	115.97
22	S	312	CLA	CMC-C2C-C3C	2.17	132.10	126.09
22	s	312	CLA	CMC-C2C-C3C	2.17	132.10	126.09
25	n	609	CHL	CHB-C4A-C3A	2.17	122.99	117.08
25	N	609	CHL	CHB-C4A-C3A	2.17	122.99	117.08
22	3	312	CLA	CMB-C2B-C3B	2.17	128.92	124.89
22	7	312	CLA	CMB-C2B-C3B	2.17	128.92	124.89
22	c	512	CLA	CMB-C2B-C3B	2.17	128.92	124.89
22	g	613	CLA	C3B-C4B-NB	2.17	112.02	109.21
22	G	613	CLA	C3B-C4B-NB	2.17	112.02	109.21
22	R	303	CLA	CMC-C2C-C3C	2.17	132.11	126.09
22	r	303	CLA	CMC-C2C-C3C	2.17	132.11	126.09
22	B	615	CLA	CMB-C2B-C3B	2.18	128.93	124.89
22	3	304	CLA	CMC-C2C-C1C	2.18	128.32	125.02
22	7	304	CLA	CMC-C2C-C1C	2.18	128.32	125.02
23	A	404	PHO	CBD-CHA-C1A	2.18	131.49	126.36
25	Y	605	CHL	O2D-CGD-CBD	2.18	116.52	111.20
25	y	605	CHL	O2D-CGD-CBD	2.18	116.52	111.20
22	n	603	CLA	C3D-CAD-CBD	2.18	110.68	107.60
22	N	603	CLA	C3D-CAD-CBD	2.18	110.68	107.60
22	y	613	CLA	CMC-C2C-C3C	2.18	132.13	126.09
22	Y	613	CLA	CMC-C2C-C3C	2.18	132.13	126.09
25	2	607	CHL	O2D-CGD-CBD	2.18	116.52	111.20
25	6	607	CHL	O2D-CGD-CBD	2.18	116.52	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	609	CHL	CHC-C4B-C3B	2.18	123.40	118.23
25	Y	609	CHL	CHC-C4B-C3B	2.18	123.40	118.23
25	2	607	CHL	OBD-CAD-C3D	2.18	130.55	126.75
25	6	607	CHL	OBD-CAD-C3D	2.18	130.55	126.75
25	N	608	CHL	OBD-CAD-C3D	2.18	130.56	126.75
25	n	608	CHL	OBD-CAD-C3D	2.18	130.56	126.75
25	8	305	CHL	OBD-CAD-C3D	2.18	130.56	126.75
25	4	305	CHL	OBD-CAD-C3D	2.18	130.56	126.75
25	3	302	CHL	OBD-CAD-C3D	2.18	130.56	126.75
25	7	302	CHL	OBD-CAD-C3D	2.18	130.56	126.75
22	2	604	CLA	C3B-C4B-NB	2.19	112.04	109.21
22	6	604	CLA	C3B-C4B-NB	2.19	112.04	109.21
22	B	609	CLA	C3D-CAD-CBD	2.19	110.69	107.60
22	s	301	CLA	CMB-C2B-C3B	2.19	128.95	124.89
22	c	506	CLA	CMC-C2C-C1C	2.19	128.34	125.02
22	c	510	CLA	CMC-C2C-C1C	2.19	128.34	125.02
22	2	612	CLA	CMB-C2B-C3B	2.19	128.96	124.89
22	6	612	CLA	CMB-C2B-C3B	2.19	128.96	124.89
25	r	306	CHL	OBD-CAD-C3D	2.19	130.57	126.75
25	R	306	CHL	OBD-CAD-C3D	2.19	130.57	126.75
22	B	604	CLA	CMB-C2B-C1B	2.19	131.84	128.46
25	S	302	CHL	CHB-C4A-C3A	2.19	123.05	117.08
25	s	302	CHL	CHB-C4A-C3A	2.19	123.05	117.08
25	1	608	CHL	O2D-CGD-CBD	2.19	116.56	111.20
25	5	608	CHL	O2D-CGD-CBD	2.19	116.56	111.20
22	Y	614	CLA	CMC-C2C-C1C	2.20	128.35	125.02
22	y	614	CLA	CMC-C2C-C1C	2.20	128.35	125.02
25	4	301	CHL	OBD-CAD-C3D	2.20	130.58	126.75
25	8	301	CHL	OBD-CAD-C3D	2.20	130.58	126.75
22	B	609	CLA	CMC-C2C-C1C	2.20	128.35	125.02
25	2	605	CHL	O2D-CGD-CBD	2.20	116.56	111.20
25	6	605	CHL	O2D-CGD-CBD	2.20	116.56	111.20
22	c	503	CLA	CMC-C2C-C1C	2.20	128.36	125.02
22	R	303	CLA	C3D-CAD-CBD	2.20	110.71	107.60
22	r	303	CLA	C3D-CAD-CBD	2.20	110.71	107.60
22	d	404	CLA	CMB-C2B-C3B	2.21	128.98	124.89
22	S	310	CLA	CMC-C2C-C1C	2.21	128.37	125.02
22	s	310	CLA	CMC-C2C-C1C	2.21	128.37	125.02
22	b	606	CLA	C3B-C4B-NB	2.21	112.06	109.21
22	c	502	CLA	CMB-C2B-C3B	2.21	128.99	124.89
22	C	510	CLA	CMC-C2C-C1C	2.21	128.37	125.02
22	7	311	CLA	C3B-C4B-NB	2.21	112.06	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	3	311	CLA	C3B-C4B-NB	2.21	112.06	109.21
25	y	608	CHL	O2D-CGD-CBD	2.21	116.59	111.20
25	Y	608	CHL	O2D-CGD-CBD	2.21	116.59	111.20
22	B	607	CLA	CMB-C2B-C3B	2.21	128.99	124.89
22	6	603	CLA	C3B-C4B-NB	2.21	112.07	109.21
22	2	603	CLA	C3B-C4B-NB	2.21	112.07	109.21
22	4	309	CLA	CED-O2D-CGD	2.21	121.16	115.97
22	8	309	CLA	CED-O2D-CGD	2.21	121.16	115.97
22	C	507	CLA	CMC-C2C-C3C	2.21	132.22	126.09
25	2	605	CHL	OBD-CAD-C3D	2.21	130.61	126.75
25	6	605	CHL	OBD-CAD-C3D	2.21	130.61	126.75
22	b	606	CLA	CMC-C2C-C3C	2.22	132.23	126.09
22	c	508	CLA	C3B-C4B-NB	2.22	112.08	109.21
25	1	608	CHL	OBD-CAD-C3D	2.22	130.62	126.75
25	5	608	CHL	OBD-CAD-C3D	2.22	130.62	126.75
25	S	308	CHL	CHB-C4A-C3A	2.22	123.12	117.08
25	s	308	CHL	CHB-C4A-C3A	2.22	123.12	117.08
22	n	612	CLA	C3B-C4B-NB	2.22	112.09	109.21
22	N	612	CLA	C3B-C4B-NB	2.22	112.09	109.21
22	8	310	CLA	CMC-C2C-C3C	2.22	132.25	126.09
22	4	310	CLA	CMC-C2C-C3C	2.22	132.25	126.09
22	A	405	CLA	CMC-C2C-C1C	2.23	128.40	125.02
22	a	405	CLA	CED-O2D-CGD	2.23	121.19	115.97
22	r	307	CLA	CMB-C2B-C3B	2.23	129.03	124.89
22	R	307	CLA	CMB-C2B-C3B	2.23	129.03	124.89
22	B	610	CLA	C3B-C4B-NB	2.23	112.09	109.21
25	5	615	CHL	O2D-CGD-CBD	2.23	116.64	111.20
25	1	615	CHL	O2D-CGD-CBD	2.23	116.64	111.20
22	d	404	CLA	CED-O2D-CGD	2.23	121.20	115.97
22	c	505	CLA	C3B-C4B-NB	2.23	112.10	109.21
22	b	613	CLA	CED-O2D-CGD	2.24	121.21	115.97
25	N	608	CHL	O2D-CGD-CBD	2.24	116.66	111.20
25	n	608	CHL	O2D-CGD-CBD	2.24	116.66	111.20
22	c	512	CLA	CMC-C2C-C3C	2.24	132.29	126.09
22	b	614	CLA	CMB-C2B-C3B	2.24	129.04	124.89
22	1	603	CLA	CMC-C2C-C1C	2.24	128.42	125.02
22	5	603	CLA	CMC-C2C-C1C	2.24	128.42	125.02
25	s	307	CHL	OBD-CAD-C3D	2.24	130.66	126.75
25	S	307	CHL	OBD-CAD-C3D	2.24	130.66	126.75
25	y	608	CHL	CHB-C1B-C2B	2.24	123.19	116.99
25	Y	608	CHL	CHB-C1B-C2B	2.24	123.19	116.99
22	B	605	CLA	CMB-C2B-C3B	2.24	129.05	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	601	CHL	OBD-CAD-C3D	2.24	130.66	126.75
25	2	601	CHL	OBD-CAD-C3D	2.24	130.66	126.75
22	r	307	CLA	C3B-C4B-NB	2.24	112.11	109.21
22	b	609	CLA	C3B-C4B-NB	2.24	112.11	109.21
22	R	307	CLA	C3B-C4B-NB	2.24	112.11	109.21
22	5	611	CLA	C3B-C4B-NB	2.25	112.11	109.21
22	1	611	CLA	C3B-C4B-NB	2.25	112.11	109.21
22	c	501	CLA	C3D-CAD-CBD	2.25	110.77	107.60
22	B	604	CLA	C3D-CAD-CBD	2.25	110.78	107.60
22	S	304	CLA	CMC-C2C-C1C	2.25	128.44	125.02
22	s	304	CLA	CMC-C2C-C1C	2.25	128.44	125.02
25	Y	605	CHL	CHC-C4B-C3B	2.25	123.56	118.23
25	y	605	CHL	CHC-C4B-C3B	2.25	123.56	118.23
22	b	603	CLA	CMB-C2B-C3B	2.26	129.08	124.89
25	6	608	CHL	CHB-C4A-C3A	2.26	123.23	117.08
25	2	608	CHL	CHB-C4A-C3A	2.26	123.23	117.08
22	B	616	CLA	C3B-C4B-NB	2.26	112.13	109.21
22	c	502	CLA	CED-O2D-CGD	2.26	121.27	115.97
22	b	610	CLA	CMC-C2C-C3C	2.26	132.36	126.09
25	3	306	CHL	OBD-CAD-C3D	2.26	130.70	126.75
25	7	306	CHL	OBD-CAD-C3D	2.26	130.70	126.75
22	b	601	CLA	CMB-C2B-C3B	2.26	129.09	124.89
22	s	313	CLA	CED-O2D-CGD	2.26	121.28	115.97
22	S	313	CLA	CED-O2D-CGD	2.26	121.28	115.97
22	C	503	CLA	CED-O2D-CGD	2.27	121.29	115.97
22	Y	602	CLA	CMB-C2B-C3B	2.27	129.10	124.89
22	y	602	CLA	CMB-C2B-C3B	2.27	129.10	124.89
25	3	302	CHL	CHB-C4A-C3A	2.27	123.26	117.08
25	7	302	CHL	CHB-C4A-C3A	2.27	123.26	117.08
25	5	615	CHL	OBD-CAD-C3D	2.27	130.71	126.75
25	1	615	CHL	OBD-CAD-C3D	2.27	130.71	126.75
22	5	611	CLA	CMB-C2B-C3B	2.27	129.11	124.89
22	1	611	CLA	CMB-C2B-C3B	2.27	129.11	124.89
22	6	609	CLA	CED-O2D-CGD	2.28	121.31	115.97
22	2	609	CLA	CED-O2D-CGD	2.28	121.31	115.97
22	G	604	CLA	CMB-C2B-C3B	2.28	129.12	124.89
22	g	604	CLA	CMB-C2B-C3B	2.28	129.12	124.89
22	R	301	CLA	CMB-C2B-C3B	2.28	129.12	124.89
22	r	301	CLA	CMB-C2B-C3B	2.28	129.12	124.89
25	g	608	CHL	O2D-CGD-CBD	2.28	116.77	111.20
25	G	608	CHL	O2D-CGD-CBD	2.28	116.77	111.20
22	b	616	CLA	C3D-CAD-CBD	2.28	110.82	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	405	CLA	CMC-C2C-C1C	2.28	128.48	125.02
22	C	511	CLA	C3B-C4B-NB	2.29	112.17	109.21
22	d	401	CLA	CMB-C2B-C3B	2.29	129.14	124.89
22	N	602	CLA	CMB-C2B-C3B	2.29	129.14	124.89
22	n	602	CLA	CMB-C2B-C3B	2.29	129.14	124.89
22	C	511	CLA	CMC-C2C-C3C	2.29	132.44	126.09
22	A	402	CLA	C3B-C4B-NB	2.30	112.18	109.21
22	B	616	CLA	CMC-C2C-C3C	2.30	132.45	126.09
22	3	304	CLA	CMB-C2B-C3B	2.30	129.16	124.89
22	7	304	CLA	CMB-C2B-C3B	2.30	129.16	124.89
25	g	605	CHL	OBD-CAD-C3D	2.30	130.76	126.75
25	G	605	CHL	OBD-CAD-C3D	2.30	130.76	126.75
25	1	609	CHL	O2D-CGD-CBD	2.30	116.81	111.20
25	5	609	CHL	O2D-CGD-CBD	2.30	116.81	111.20
25	s	306	CHL	CHB-C4A-C3A	2.30	123.34	117.08
25	S	306	CHL	CHB-C4A-C3A	2.30	123.34	117.08
22	Y	603	CLA	CMC-C2C-C1C	2.30	128.51	125.02
22	y	603	CLA	CMC-C2C-C1C	2.30	128.51	125.02
22	C	502	CLA	CED-O2D-CGD	2.30	121.37	115.97
22	S	305	CLA	CED-O2D-CGD	2.30	121.37	115.97
22	s	305	CLA	CED-O2D-CGD	2.30	121.37	115.97
22	5	614	CLA	CMC-C2C-C1C	2.30	128.51	125.02
22	1	614	CLA	CMC-C2C-C1C	2.30	128.51	125.02
22	R	309	CLA	CMB-C2B-C3B	2.30	129.17	124.89
22	r	309	CLA	CMB-C2B-C3B	2.30	129.17	124.89
22	Y	603	CLA	C3B-C4B-NB	2.30	112.19	109.21
22	y	603	CLA	C3B-C4B-NB	2.30	112.19	109.21
22	2	610	CLA	C3B-C4B-NB	2.31	112.20	109.21
22	6	610	CLA	C3B-C4B-NB	2.31	112.20	109.21
22	1	612	CLA	CMB-C2B-C3B	2.31	129.18	124.89
22	5	612	CLA	CMB-C2B-C3B	2.31	129.18	124.89
22	2	612	CLA	CMC-C2C-C1C	2.32	128.53	125.02
22	6	612	CLA	CMC-C2C-C1C	2.32	128.53	125.02
22	S	301	CLA	CMC-C2C-C1C	2.33	128.55	125.02
22	g	612	CLA	CMB-C2B-C3B	2.33	129.21	124.89
22	G	612	CLA	CMB-C2B-C3B	2.33	129.21	124.89
22	B	606	CLA	CMC-C2C-C1C	2.33	128.55	125.02
25	g	608	CHL	CHB-C4A-C3A	2.33	123.41	117.08
25	G	608	CHL	CHB-C4A-C3A	2.33	123.41	117.08
25	y	609	CHL	CHB-C4A-C3A	2.33	123.42	117.08
25	Y	609	CHL	CHB-C4A-C3A	2.33	123.42	117.08
25	4	307	CHL	OBD-CAD-C3D	2.33	130.81	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	307	CHL	OBD-CAD-C3D	2.33	130.81	126.75
22	c	504	CLA	C3B-C4B-NB	2.33	112.23	109.21
25	1	606	CHL	OBD-CAD-C3D	2.33	130.82	126.75
25	5	606	CHL	OBD-CAD-C3D	2.33	130.82	126.75
25	g	605	CHL	O2D-CGD-CBD	2.34	116.91	111.20
25	G	605	CHL	O2D-CGD-CBD	2.34	116.91	111.20
22	b	609	CLA	CED-O2D-CGD	2.34	121.46	115.97
22	b	616	CLA	CED-O2D-CGD	2.34	121.46	115.97
25	Y	607	CHL	O2D-CGD-CBD	2.34	116.92	111.20
25	y	607	CHL	O2D-CGD-CBD	2.34	116.92	111.20
25	R	304	CHL	OBD-CAD-C3D	2.34	130.84	126.75
25	r	304	CHL	OBD-CAD-C3D	2.34	130.84	126.75
22	Y	604	CLA	CMB-C2B-C3B	2.35	129.24	124.89
22	y	604	CLA	CMB-C2B-C3B	2.35	129.24	124.89
25	4	306	CHL	OBD-CAD-C3D	2.35	130.85	126.75
25	8	306	CHL	OBD-CAD-C3D	2.35	130.85	126.75
22	c	503	CLA	CMB-C2B-C3B	2.35	129.25	124.89
25	r	306	CHL	CHB-C4A-C3A	2.35	123.48	117.08
25	R	306	CHL	CHB-C4A-C3A	2.35	123.48	117.08
25	2	606	CHL	OBD-CAD-C3D	2.35	130.85	126.75
25	6	606	CHL	OBD-CAD-C3D	2.35	130.85	126.75
22	a	403	CLA	C3D-CAD-CBD	2.35	110.92	107.60
22	c	506	CLA	CED-O2D-CGD	2.35	121.49	115.97
22	1	603	CLA	C3B-C4B-NB	2.36	112.26	109.21
22	5	603	CLA	C3B-C4B-NB	2.36	112.26	109.21
25	n	607	CHL	CHB-C4A-C3A	2.36	123.50	117.08
25	N	607	CHL	CHB-C4A-C3A	2.36	123.50	117.08
22	7	311	CLA	CMB-C2B-C3B	2.37	129.28	124.89
22	3	311	CLA	CMB-C2B-C3B	2.37	129.28	124.89
22	a	402	CLA	CED-O2D-CGD	2.37	121.52	115.97
25	G	607	CHL	CHB-C4A-C3A	2.37	123.53	117.08
25	g	607	CHL	CHB-C4A-C3A	2.37	123.53	117.08
25	N	605	CHL	OBD-CAD-C3D	2.37	130.88	126.75
25	n	605	CHL	OBD-CAD-C3D	2.37	130.88	126.75
25	4	301	CHL	CHB-C4A-C3A	2.37	123.53	117.08
25	8	301	CHL	CHB-C4A-C3A	2.37	123.53	117.08
22	S	314	CLA	CMB-C2B-C3B	2.37	129.29	124.89
22	s	314	CLA	CMB-C2B-C3B	2.37	129.29	124.89
22	Y	614	CLA	C3B-C4B-NB	2.37	112.28	109.21
22	y	614	CLA	C3B-C4B-NB	2.37	112.28	109.21
25	S	302	CHL	OBD-CAD-C3D	2.37	130.89	126.75
25	s	302	CHL	OBD-CAD-C3D	2.37	130.89	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	301	CHL	O2D-CGD-CBD	2.37	117.00	111.20
25	8	301	CHL	O2D-CGD-CBD	2.37	117.00	111.20
25	7	309	CHL	CHB-C4A-C3A	2.38	123.54	117.08
25	3	309	CHL	CHB-C4A-C3A	2.38	123.54	117.08
22	R	303	CLA	C3B-C4B-NB	2.38	112.28	109.21
22	r	303	CLA	C3B-C4B-NB	2.38	112.28	109.21
25	G	607	CHL	O2D-CGD-CBD	2.38	117.01	111.20
25	g	607	CHL	O2D-CGD-CBD	2.38	117.01	111.20
25	s	307	CHL	CHB-C4A-C3A	2.38	123.56	117.08
25	S	307	CHL	CHB-C4A-C3A	2.38	123.56	117.08
25	8	308	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	4	308	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	g	601	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	N	601	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	n	601	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	G	601	CHL	OBD-CAD-C3D	2.38	130.90	126.75
22	b	616	CLA	CMC-C2C-C3C	2.38	132.68	126.09
25	r	305	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	R	305	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	S	308	CHL	OBD-CAD-C3D	2.38	130.90	126.75
25	s	308	CHL	OBD-CAD-C3D	2.38	130.90	126.75
22	S	305	CLA	C3B-C4B-NB	2.38	112.29	109.21
22	s	305	CLA	C3B-C4B-NB	2.38	112.29	109.21
22	5	604	CLA	C3B-C4B-NB	2.39	112.29	109.21
22	1	604	CLA	C3B-C4B-NB	2.39	112.29	109.21
25	1	601	CHL	OBD-CAD-C3D	2.39	130.91	126.75
25	5	601	CHL	OBD-CAD-C3D	2.39	130.91	126.75
22	y	612	CLA	CMC-C2C-C3C	2.39	132.70	126.09
22	Y	612	CLA	CMC-C2C-C3C	2.39	132.70	126.09
25	R	304	CHL	CHC-C4B-C3B	2.39	123.89	118.23
25	r	304	CHL	CHC-C4B-C3B	2.39	123.89	118.23
22	7	305	CLA	C3B-C4B-NB	2.39	112.31	109.21
22	3	305	CLA	C3B-C4B-NB	2.39	112.31	109.21
25	2	607	CHL	CHB-C4A-C3A	2.39	123.59	117.08
25	6	607	CHL	CHB-C4A-C3A	2.39	123.59	117.08
22	C	503	CLA	CMB-C2B-C3B	2.40	129.34	124.89
22	a	402	CLA	C3B-C4B-NB	2.40	112.31	109.21
22	g	611	CLA	C3B-C4B-NB	2.40	112.31	109.21
22	G	611	CLA	C3B-C4B-NB	2.40	112.31	109.21
25	1	607	CHL	OBD-CAD-C3D	2.40	130.94	126.75
25	5	607	CHL	OBD-CAD-C3D	2.40	130.94	126.75
22	y	611	CLA	C3B-C4B-NB	2.40	112.32	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	611	CLA	C3B-C4B-NB	2.40	112.32	109.21
25	g	606	CHL	OBD-CAD-C3D	2.41	130.95	126.75
25	G	606	CHL	OBD-CAD-C3D	2.41	130.95	126.75
22	s	301	CLA	CMC-C2C-C1C	2.41	128.67	125.02
25	r	306	CHL	O2D-CGD-CBD	2.41	117.08	111.20
25	R	306	CHL	O2D-CGD-CBD	2.41	117.08	111.20
25	N	605	CHL	CHB-C4A-C3A	2.41	123.64	117.08
25	n	605	CHL	CHB-C4A-C3A	2.41	123.64	117.08
22	y	610	CLA	CMC-C2C-C1C	2.41	128.68	125.02
22	Y	610	CLA	CMC-C2C-C1C	2.41	128.68	125.02
22	B	615	CLA	C3B-C4B-NB	2.42	112.33	109.21
22	r	302	CLA	CMB-C2B-C3B	2.42	129.38	124.89
22	R	302	CLA	CMB-C2B-C3B	2.42	129.38	124.89
25	Y	607	CHL	CHB-C4A-C3A	2.42	123.66	117.08
25	y	607	CHL	CHB-C4A-C3A	2.42	123.66	117.08
25	7	307	CHL	OBD-CAD-C3D	2.42	130.97	126.75
25	3	307	CHL	OBD-CAD-C3D	2.42	130.97	126.75
22	d	403	CLA	CMC-C2C-C1C	2.42	128.69	125.02
25	4	307	CHL	CHB-C4A-C3A	2.42	123.67	117.08
25	8	307	CHL	CHB-C4A-C3A	2.42	123.67	117.08
25	1	608	CHL	CHB-C4A-C3A	2.42	123.68	117.08
25	5	608	CHL	CHB-C4A-C3A	2.42	123.68	117.08
25	2	605	CHL	CHB-C4A-C3A	2.43	123.68	117.08
25	6	605	CHL	CHB-C4A-C3A	2.43	123.68	117.08
25	y	606	CHL	OBD-CAD-C3D	2.43	130.98	126.75
25	Y	606	CHL	OBD-CAD-C3D	2.43	130.98	126.75
22	B	602	CLA	CED-O2D-CGD	2.43	121.68	115.97
22	S	310	CLA	CED-O2D-CGD	2.44	121.68	115.97
22	s	310	CLA	CED-O2D-CGD	2.44	121.68	115.97
25	y	608	CHL	OBD-CAD-C3D	2.44	131.00	126.75
25	Y	608	CHL	OBD-CAD-C3D	2.44	131.00	126.75
25	s	306	CHL	OBD-CAD-C3D	2.44	131.00	126.75
25	S	306	CHL	OBD-CAD-C3D	2.44	131.00	126.75
25	4	306	CHL	CHB-C4A-C3A	2.44	123.71	117.08
25	8	306	CHL	CHB-C4A-C3A	2.44	123.71	117.08
22	s	313	CLA	CMB-C2B-C3B	2.44	129.41	124.89
22	2	613	CLA	CMB-C2B-C3B	2.44	129.41	124.89
22	S	313	CLA	CMB-C2B-C3B	2.44	129.41	124.89
22	6	613	CLA	CMB-C2B-C3B	2.44	129.41	124.89
25	Y	605	CHL	OBD-CAD-C3D	2.44	131.00	126.75
25	y	605	CHL	OBD-CAD-C3D	2.44	131.00	126.75
22	C	510	CLA	C3B-C4B-NB	2.44	112.36	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	8	310	CLA	CMB-C2B-C3B	2.44	129.42	124.89
22	4	310	CLA	CMB-C2B-C3B	2.44	129.42	124.89
22	C	511	CLA	CED-O2D-CGD	2.44	121.69	115.97
25	G	607	CHL	OBD-CAD-C3D	2.44	131.01	126.75
25	g	607	CHL	OBD-CAD-C3D	2.44	131.01	126.75
22	n	603	CLA	C3B-C4B-NB	2.45	112.37	109.21
22	N	603	CLA	C3B-C4B-NB	2.45	112.37	109.21
22	C	502	CLA	CMB-C2B-C3B	2.45	129.43	124.89
22	C	511	CLA	CMB-C2B-C3B	2.45	129.43	124.89
22	Y	604	CLA	C3B-C4B-NB	2.45	112.38	109.21
22	y	604	CLA	C3B-C4B-NB	2.45	112.38	109.21
22	B	612	CLA	CMB-C2B-C3B	2.45	129.44	124.89
22	B	613	CLA	C3D-CAD-CBD	2.45	111.06	107.60
22	y	611	CLA	CMC-C2C-C1C	2.45	128.73	125.02
22	Y	611	CLA	CMC-C2C-C1C	2.45	128.73	125.02
22	B	606	CLA	CMB-C2B-C3B	2.45	129.45	124.89
22	G	603	CLA	C3B-C4B-NB	2.46	112.39	109.21
22	g	603	CLA	C3B-C4B-NB	2.46	112.39	109.21
25	1	605	CHL	CHB-C4A-C3A	2.46	123.77	117.08
25	5	605	CHL	CHB-C4A-C3A	2.46	123.77	117.08
22	2	604	CLA	CMB-C2B-C3B	2.46	129.45	124.89
22	6	604	CLA	CMB-C2B-C3B	2.46	129.45	124.89
22	B	616	CLA	CED-O2D-CGD	2.46	121.73	115.97
22	2	610	CLA	CMB-C2B-C3B	2.46	129.46	124.89
22	6	610	CLA	CMB-C2B-C3B	2.46	129.46	124.89
22	S	312	CLA	CED-O2D-CGD	2.47	121.75	115.97
22	s	312	CLA	CED-O2D-CGD	2.47	121.75	115.97
22	G	604	CLA	C3B-C4B-NB	2.47	112.40	109.21
22	g	604	CLA	C3B-C4B-NB	2.47	112.40	109.21
22	B	616	CLA	C3D-CAD-CBD	2.47	111.08	107.60
22	S	304	CLA	C3C-C4C-NC	2.47	112.71	110.21
22	s	304	CLA	C3C-C4C-NC	2.47	112.71	110.21
22	C	509	CLA	CMC-C2C-C1C	2.47	128.76	125.02
25	8	308	CHL	CHB-C4A-C3A	2.47	123.81	117.08
25	4	308	CHL	CHB-C4A-C3A	2.47	123.81	117.08
22	C	509	CLA	C3B-C4B-NB	2.47	112.41	109.21
25	6	608	CHL	O2D-CGD-CBD	2.47	117.23	111.20
25	2	608	CHL	O2D-CGD-CBD	2.47	117.23	111.20
25	8	305	CHL	CHB-C4A-C3A	2.48	123.82	117.08
25	4	305	CHL	CHB-C4A-C3A	2.48	123.82	117.08
22	C	505	CLA	CMB-C2B-C3B	2.48	129.49	124.89
22	n	611	CLA	CMB-C2B-C3B	2.48	129.49	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	611	CLA	CMB-C2B-C3B	2.48	129.49	124.89
22	S	312	CLA	C3B-C4B-NB	2.48	112.42	109.21
22	s	312	CLA	C3B-C4B-NB	2.48	112.42	109.21
22	c	502	CLA	C3D-CAD-CBD	2.48	111.11	107.60
25	Y	601	CHL	CHB-C4A-C3A	2.49	123.85	117.08
25	y	601	CHL	CHB-C4A-C3A	2.49	123.85	117.08
22	B	615	CLA	CMC-C2C-C1C	2.49	128.80	125.02
25	g	605	CHL	CHB-C4A-C3A	2.49	123.86	117.08
25	G	605	CHL	CHB-C4A-C3A	2.49	123.86	117.08
22	R	309	CLA	C3B-C4B-NB	2.49	112.43	109.21
22	r	309	CLA	C3B-C4B-NB	2.49	112.43	109.21
22	7	305	CLA	CMB-C2B-C3B	2.49	129.52	124.89
22	3	305	CLA	CMB-C2B-C3B	2.49	129.52	124.89
25	g	601	CHL	CHB-C4A-C3A	2.49	123.87	117.08
25	G	601	CHL	CHB-C4A-C3A	2.49	123.87	117.08
22	s	303	CLA	CMB-C2B-C3B	2.50	129.52	124.89
22	S	303	CLA	CMB-C2B-C3B	2.50	129.52	124.89
25	6	601	CHL	CHB-C4A-C3A	2.50	123.87	117.08
25	2	601	CHL	CHB-C4A-C3A	2.50	123.87	117.08
22	s	303	CLA	CMC-C2C-C1C	2.50	128.81	125.02
22	S	303	CLA	CMC-C2C-C1C	2.50	128.81	125.02
25	3	301	CHL	OBD-CAD-C3D	2.50	131.11	126.75
25	7	301	CHL	OBD-CAD-C3D	2.50	131.11	126.75
22	B	616	CLA	CMB-C2B-C3B	2.50	129.53	124.89
22	2	602	CLA	CMC-C2C-C1C	2.50	128.81	125.02
22	N	602	CLA	CMC-C2C-C1C	2.50	128.81	125.02
22	6	602	CLA	CMC-C2C-C1C	2.50	128.81	125.02
22	n	602	CLA	CMC-C2C-C1C	2.50	128.81	125.02
25	1	607	CHL	CHB-C4A-C3A	2.50	123.89	117.08
25	5	607	CHL	CHB-C4A-C3A	2.50	123.89	117.08
25	r	306	CHL	OMC-CMC-C2C	2.51	127.48	124.29
25	R	306	CHL	OMC-CMC-C2C	2.51	127.48	124.29
22	n	604	CLA	CMB-C2B-C3B	2.51	129.54	124.89
22	N	604	CLA	CMB-C2B-C3B	2.51	129.54	124.89
25	N	608	CHL	CHB-C4A-C3A	2.51	123.90	117.08
25	n	608	CHL	CHB-C4A-C3A	2.51	123.90	117.08
22	c	512	CLA	C3B-C4B-NB	2.51	112.45	109.21
22	D	401	CLA	CMB-C2B-C3B	2.51	129.55	124.89
25	r	305	CHL	CHB-C4A-C3A	2.51	123.92	117.08
25	R	305	CHL	CHB-C4A-C3A	2.51	123.92	117.08
25	S	302	CHL	CHB-C1B-C2B	2.51	123.95	116.99
25	s	302	CHL	CHB-C1B-C2B	2.51	123.95	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	306	CHL	CHB-C4A-C3A	2.52	123.92	117.08
25	7	306	CHL	CHB-C4A-C3A	2.52	123.92	117.08
25	n	607	CHL	OBD-CAD-C3D	2.52	131.14	126.75
25	N	607	CHL	OBD-CAD-C3D	2.52	131.14	126.75
22	n	611	CLA	C3B-C4B-NB	2.52	112.46	109.21
22	N	611	CLA	C3B-C4B-NB	2.52	112.46	109.21
22	b	604	CLA	C3D-CAD-CBD	2.52	111.16	107.60
25	Y	607	CHL	CHC-C4B-C3B	2.52	124.20	118.23
25	y	607	CHL	CHC-C4B-C3B	2.52	124.20	118.23
22	6	609	CLA	CMB-C2B-C3B	2.52	129.57	124.89
22	2	609	CLA	CMB-C2B-C3B	2.52	129.57	124.89
25	g	601	CHL	CHB-C1B-C2B	2.52	123.98	116.99
25	G	601	CHL	CHB-C1B-C2B	2.52	123.98	116.99
22	R	308	CLA	OBD-CAD-CBD	2.52	129.75	125.94
22	r	308	CLA	OBD-CAD-CBD	2.52	129.75	125.94
22	D	403	CLA	C3B-C4B-NB	2.53	112.48	109.21
25	5	615	CHL	CHB-C4A-C3A	2.53	123.96	117.08
25	1	615	CHL	CHB-C4A-C3A	2.53	123.96	117.08
22	B	613	CLA	CED-O2D-CGD	2.53	121.90	115.97
22	1	602	CLA	CMC-C2C-C1C	2.53	128.86	125.02
22	R	311	CLA	CMC-C2C-C1C	2.53	128.86	125.02
22	5	602	CLA	CMC-C2C-C1C	2.53	128.86	125.02
22	r	311	CLA	CMC-C2C-C1C	2.53	128.86	125.02
25	y	609	CHL	O2D-CGD-CBD	2.53	117.38	111.20
25	Y	609	CHL	O2D-CGD-CBD	2.53	117.38	111.20
22	4	304	CLA	CMB-C2B-C3B	2.54	129.60	124.89
22	8	304	CLA	CMB-C2B-C3B	2.54	129.60	124.89
22	G	602	CLA	CMB-C2B-C3B	2.54	129.60	124.89
22	g	602	CLA	CMB-C2B-C3B	2.54	129.60	124.89
25	1	609	CHL	CHB-C4A-C3A	2.54	124.00	117.08
25	5	609	CHL	CHB-C4A-C3A	2.54	124.00	117.08
22	7	303	CLA	CMC-C2C-C1C	2.54	128.88	125.02
22	3	303	CLA	CMC-C2C-C1C	2.54	128.88	125.02
22	R	312	CLA	CMB-C2B-C3B	2.54	129.61	124.89
22	r	312	CLA	CMB-C2B-C3B	2.54	129.61	124.89
22	N	614	CLA	C3B-C4B-NB	2.55	112.50	109.21
22	n	614	CLA	C3B-C4B-NB	2.55	112.50	109.21
25	n	607	CHL	O2D-CGD-CBD	2.55	117.42	111.20
25	N	607	CHL	O2D-CGD-CBD	2.55	117.42	111.20
22	B	612	CLA	C3B-C4B-NB	2.55	112.51	109.21
25	7	308	CHL	CHB-C4A-C3A	2.55	124.03	117.08
25	3	308	CHL	CHB-C4A-C3A	2.55	124.03	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	CMC-C2C-C1C	2.55	128.89	125.02
22	b	607	CLA	CED-O2D-CGD	2.56	121.96	115.97
25	N	601	CHL	CHB-C4A-C3A	2.56	124.04	117.08
25	n	601	CHL	CHB-C4A-C3A	2.56	124.04	117.08
25	2	606	CHL	CHC-C4B-C3B	2.56	124.29	118.23
25	6	606	CHL	CHC-C4B-C3B	2.56	124.29	118.23
22	B	608	CLA	CMB-C2B-C3B	2.56	129.64	124.89
22	c	511	CLA	CMB-C2B-C3B	2.56	129.64	124.89
22	B	610	CLA	CMB-C2B-C3B	2.56	129.64	124.89
22	C	508	CLA	CMB-C2B-C3B	2.56	129.65	124.89
22	n	604	CLA	C3B-C4B-NB	2.56	112.53	109.21
22	N	604	CLA	C3B-C4B-NB	2.56	112.53	109.21
22	C	501	CLA	C3D-CAD-CBD	2.56	111.22	107.60
25	3	301	CHL	CHB-C4A-C3A	2.57	124.06	117.08
25	7	301	CHL	CHB-C4A-C3A	2.57	124.06	117.08
23	A	404	PHO	CMC-C2C-C3C	2.57	133.22	126.09
22	s	313	CLA	CMC-C2C-C1C	2.58	128.93	125.02
22	S	313	CLA	CMC-C2C-C1C	2.58	128.93	125.02
25	3	301	CHL	O2D-CGD-CBD	2.58	117.49	111.20
25	7	301	CHL	O2D-CGD-CBD	2.58	117.49	111.20
22	C	512	CLA	CMB-C2B-C3B	2.58	129.68	124.89
25	1	606	CHL	CHB-C4A-C3A	2.58	124.10	117.08
25	5	606	CHL	CHB-C4A-C3A	2.58	124.10	117.08
22	b	609	CLA	CMC-C2C-C1C	2.58	128.93	125.02
22	Y	614	CLA	CMB-C2B-C3B	2.58	129.68	124.89
22	y	614	CLA	CMB-C2B-C3B	2.58	129.68	124.89
22	C	501	CLA	C3B-C4B-NB	2.59	112.55	109.21
25	7	307	CHL	CHB-C4A-C3A	2.59	124.12	117.08
25	3	307	CHL	CHB-C4A-C3A	2.59	124.12	117.08
22	B	614	CLA	CMC-C2C-C1C	2.59	128.94	125.02
22	c	501	CLA	CMC-C2C-C3C	2.59	133.26	126.09
22	C	506	CLA	CMC-C2C-C3C	2.59	133.26	126.09
22	b	605	CLA	CMB-C2B-C3B	2.59	129.70	124.89
25	y	606	CHL	CHC-C4B-C3B	2.59	124.37	118.23
25	Y	606	CHL	CHC-C4B-C3B	2.59	124.37	118.23
22	b	614	CLA	C3B-C4B-NB	2.59	112.56	109.21
25	3	302	CHL	CHB-C1B-C2B	2.60	124.18	116.99
25	7	302	CHL	CHB-C1B-C2B	2.60	124.18	116.99
22	a	403	CLA	CMB-C2B-C3B	2.60	129.71	124.89
25	n	606	CHL	OBD-CAD-C3D	2.60	131.28	126.75
25	N	606	CHL	OBD-CAD-C3D	2.60	131.28	126.75
22	B	604	CLA	C3C-C4C-NC	2.60	112.85	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	508	CLA	CMC-C2C-C3C	2.60	133.30	126.09
22	5	604	CLA	CMB-C2B-C3B	2.60	129.72	124.89
22	1	604	CLA	CMB-C2B-C3B	2.60	129.72	124.89
22	B	611	CLA	C3B-C4B-NB	2.60	112.58	109.21
22	B	614	CLA	CAA-C2A-C1A	2.61	120.52	111.97
22	C	508	CLA	C3B-C4B-NB	2.61	112.58	109.21
22	g	611	CLA	CMB-C2B-C3B	2.61	129.74	124.89
22	G	611	CLA	CMB-C2B-C3B	2.61	129.74	124.89
25	7	309	CHL	C3B-C4B-NB	2.62	108.11	103.55
25	3	309	CHL	C3B-C4B-NB	2.62	108.11	103.55
22	B	607	CLA	CMC-C2C-C3C	2.62	133.34	126.09
25	R	304	CHL	O2D-CGD-CBD	2.62	117.60	111.20
25	r	304	CHL	O2D-CGD-CBD	2.62	117.60	111.20
22	b	601	CLA	CMC-C2C-C1C	2.62	129.00	125.02
22	3	304	CLA	C3B-C4B-NB	2.62	112.60	109.21
22	7	304	CLA	C3B-C4B-NB	2.62	112.60	109.21
25	R	304	CHL	CHB-C4A-C3A	2.62	124.22	117.08
25	r	304	CHL	CHB-C4A-C3A	2.62	124.22	117.08
22	y	612	CLA	C3B-C4B-NB	2.63	112.60	109.21
22	Y	612	CLA	C3B-C4B-NB	2.63	112.60	109.21
25	6	608	CHL	C3B-C4B-NB	2.63	108.14	103.55
25	2	608	CHL	C3B-C4B-NB	2.63	108.14	103.55
25	y	606	CHL	CHB-C4A-C3A	2.64	124.25	117.08
25	Y	606	CHL	CHB-C4A-C3A	2.64	124.25	117.08
25	n	609	CHL	CHC-C4B-C3B	2.64	124.47	118.23
25	N	609	CHL	CHC-C4B-C3B	2.64	124.47	118.23
25	8	305	CHL	CHB-C1B-C2B	2.64	124.29	116.99
25	4	305	CHL	CHB-C1B-C2B	2.64	124.29	116.99
25	y	608	CHL	C3B-C4B-NB	2.64	108.15	103.55
25	Y	608	CHL	C3B-C4B-NB	2.64	108.15	103.55
22	1	610	CLA	CMB-C2B-C3B	2.64	129.79	124.89
22	5	610	CLA	CMB-C2B-C3B	2.64	129.79	124.89
25	S	308	CHL	CHB-C1B-C2B	2.64	124.30	116.99
25	s	308	CHL	CHB-C1B-C2B	2.64	124.30	116.99
23	a	404	PHO	O2D-CGD-CBD	2.65	116.03	111.30
25	s	307	CHL	CHB-C1B-C2B	2.65	124.32	116.99
25	S	307	CHL	CHB-C1B-C2B	2.65	124.32	116.99
22	B	601	CLA	CMB-C2B-C3B	2.65	129.81	124.89
22	G	614	CLA	CMB-C2B-C3B	2.65	129.82	124.89
22	g	614	CLA	CMB-C2B-C3B	2.65	129.82	124.89
22	b	613	CLA	CMB-C2B-C3B	2.66	129.82	124.89
22	8	302	CLA	CAA-C2A-C1A	2.66	120.69	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	4	302	CLA	CAA-C2A-C1A	2.66	120.69	111.97
22	N	614	CLA	CMB-C2B-C3B	2.67	129.84	124.89
22	n	614	CLA	CMB-C2B-C3B	2.67	129.84	124.89
25	g	608	CHL	CHB-C1B-C2B	2.67	124.39	116.99
25	G	608	CHL	CHB-C1B-C2B	2.67	124.39	116.99
22	c	507	CLA	C3B-C4B-NB	2.67	112.66	109.21
23	A	404	PHO	C2B-C1B-NB	2.67	113.78	109.82
22	b	610	CLA	CMB-C2B-C3B	2.68	129.86	124.89
22	b	603	CLA	C3B-C4B-NB	2.68	112.67	109.21
25	1	609	CHL	C3B-C4B-NB	2.68	108.22	103.55
25	5	609	CHL	C3B-C4B-NB	2.68	108.22	103.55
22	B	606	CLA	C3B-C4B-NB	2.69	112.69	109.21
25	6	608	CHL	CHB-C1B-C2B	2.69	124.44	116.99
25	2	608	CHL	CHB-C1B-C2B	2.69	124.44	116.99
22	s	309	CLA	CMC-C2C-C3C	2.69	133.54	126.09
22	S	309	CLA	CMC-C2C-C3C	2.69	133.54	126.09
22	C	504	CLA	C3B-C4B-NB	2.69	112.69	109.21
25	7	309	CHL	O2D-CGD-CBD	2.70	117.79	111.20
25	3	309	CHL	O2D-CGD-CBD	2.70	117.79	111.20
22	G	610	CLA	CMB-C2B-C3B	2.70	129.90	124.89
22	g	610	CLA	CMB-C2B-C3B	2.70	129.90	124.89
22	C	501	CLA	CMC-C2C-C3C	2.70	133.56	126.09
25	Y	601	CHL	OBD-CAD-C3D	2.70	131.47	126.75
25	y	601	CHL	OBD-CAD-C3D	2.70	131.47	126.75
22	y	611	CLA	CMB-C2B-C3B	2.71	129.92	124.89
22	Y	611	CLA	CMB-C2B-C3B	2.71	129.92	124.89
25	1	608	CHL	CHB-C1B-C2B	2.71	124.50	116.99
25	5	608	CHL	CHB-C1B-C2B	2.71	124.50	116.99
22	n	610	CLA	CMC-C2C-C1C	2.72	129.14	125.02
22	N	610	CLA	CMC-C2C-C1C	2.72	129.14	125.02
25	N	601	CHL	CHB-C1B-C2B	2.72	124.52	116.99
25	n	601	CHL	CHB-C1B-C2B	2.72	124.52	116.99
25	1	605	CHL	CHB-C1B-C2B	2.72	124.53	116.99
25	5	605	CHL	CHB-C1B-C2B	2.72	124.53	116.99
25	1	601	CHL	CHB-C4A-C3A	2.72	124.49	117.08
25	5	601	CHL	CHB-C4A-C3A	2.72	124.49	117.08
22	B	602	CLA	CMB-C2B-C3B	2.72	129.94	124.89
25	N	608	CHL	CHB-C1B-C2B	2.72	124.53	116.99
25	n	608	CHL	CHB-C1B-C2B	2.72	124.53	116.99
22	d	403	CLA	C3B-C4B-NB	2.73	112.74	109.21
25	g	606	CHL	CHB-C4A-C3A	2.73	124.51	117.08
25	G	606	CHL	CHB-C4A-C3A	2.73	124.51	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	601	CHL	C3B-C4B-NB	2.73	108.31	103.55
25	y	601	CHL	C3B-C4B-NB	2.73	108.31	103.55
25	1	606	CHL	CHC-C4B-C3B	2.73	124.70	118.23
25	5	606	CHL	CHC-C4B-C3B	2.73	124.70	118.23
25	2	606	CHL	CHB-C4A-C3A	2.73	124.52	117.08
25	6	606	CHL	CHB-C4A-C3A	2.73	124.52	117.08
25	n	609	CHL	O2D-CGD-CBD	2.74	117.88	111.20
25	N	609	CHL	O2D-CGD-CBD	2.74	117.88	111.20
25	G	609	CHL	C3B-C4B-NB	2.74	108.32	103.55
25	g	609	CHL	C3B-C4B-NB	2.74	108.32	103.55
25	2	607	CHL	CHB-C1B-C2B	2.74	124.58	116.99
25	6	607	CHL	CHB-C1B-C2B	2.74	124.58	116.99
22	c	501	CLA	C3B-C4B-NB	2.74	112.75	109.21
22	S	311	CLA	CMB-C2B-C3B	2.74	129.98	124.89
22	s	311	CLA	CMB-C2B-C3B	2.74	129.98	124.89
25	s	307	CHL	CHC-C4B-C3B	2.74	124.73	118.23
25	S	307	CHL	CHC-C4B-C3B	2.74	124.73	118.23
25	Y	605	CHL	CHB-C4A-C3A	2.74	124.55	117.08
25	y	605	CHL	CHB-C4A-C3A	2.74	124.55	117.08
22	c	501	CLA	CMB-C2B-C3B	2.74	129.99	124.89
25	1	609	CHL	CHC-C4B-C3B	2.75	124.74	118.23
25	5	609	CHL	CHC-C4B-C3B	2.75	124.74	118.23
25	n	609	CHL	C3B-C4B-NB	2.75	108.34	103.55
25	N	609	CHL	C3B-C4B-NB	2.75	108.34	103.55
22	7	314	CLA	CMB-C2B-C3B	2.75	130.00	124.89
22	3	314	CLA	CMB-C2B-C3B	2.75	130.00	124.89
25	7	309	CHL	CHC-C4B-C3B	2.76	124.76	118.23
25	3	309	CHL	CHC-C4B-C3B	2.76	124.76	118.23
25	6	601	CHL	CHB-C1B-C2B	2.76	124.63	116.99
25	2	601	CHL	CHB-C1B-C2B	2.76	124.63	116.99
25	r	305	CHL	CHC-C4B-C3B	2.77	124.78	118.23
25	R	305	CHL	CHC-C4B-C3B	2.77	124.78	118.23
22	s	309	CLA	C3B-C4B-NB	2.77	112.79	109.21
22	S	309	CLA	C3B-C4B-NB	2.77	112.79	109.21
22	G	602	CLA	CMC-C2C-C1C	2.78	129.24	125.02
22	g	602	CLA	CMC-C2C-C1C	2.78	129.24	125.02
25	S	302	CHL	C3B-C4B-NB	2.78	108.40	103.55
25	s	302	CHL	C3B-C4B-NB	2.78	108.40	103.55
22	D	401	CLA	CMC-C2C-C3C	2.78	133.80	126.09
25	4	301	CHL	CHB-C1B-C2B	2.78	124.70	116.99
25	8	301	CHL	CHB-C1B-C2B	2.78	124.70	116.99
25	G	609	CHL	CHC-C4B-C3B	2.79	124.84	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	609	CHL	CHC-C4B-C3B	2.79	124.84	118.23
25	5	615	CHL	CHB-C1B-C2B	2.79	124.72	116.99
25	1	615	CHL	CHB-C1B-C2B	2.79	124.72	116.99
22	B	613	CLA	CMB-C2B-C3B	2.79	130.07	124.89
25	1	607	CHL	O2D-CGD-CBD	2.79	118.02	111.20
25	5	607	CHL	O2D-CGD-CBD	2.79	118.02	111.20
25	1	607	CHL	CHB-C1B-C2B	2.79	124.73	116.99
25	5	607	CHL	CHB-C1B-C2B	2.79	124.73	116.99
25	g	608	CHL	C3B-C4B-NB	2.80	108.42	103.55
25	G	608	CHL	C3B-C4B-NB	2.80	108.42	103.55
25	2	605	CHL	C3B-C4B-NB	2.80	108.42	103.55
25	6	605	CHL	C3B-C4B-NB	2.80	108.42	103.55
25	N	605	CHL	CHC-C4B-C3B	2.80	124.86	118.23
25	n	605	CHL	CHC-C4B-C3B	2.80	124.86	118.23
25	n	606	CHL	CHB-C4A-C3A	2.80	124.70	117.08
25	N	606	CHL	CHB-C4A-C3A	2.80	124.70	117.08
25	1	608	CHL	C3B-C4B-NB	2.80	108.43	103.55
25	5	608	CHL	C3B-C4B-NB	2.80	108.43	103.55
25	r	306	CHL	CHB-C1B-C2B	2.80	124.76	116.99
25	R	306	CHL	CHB-C1B-C2B	2.80	124.76	116.99
22	1	610	CLA	CMC-C2C-C1C	2.81	129.28	125.02
22	5	610	CLA	CMC-C2C-C1C	2.81	129.28	125.02
25	7	308	CHL	CHB-C1B-C2B	2.81	124.77	116.99
25	3	308	CHL	CHB-C1B-C2B	2.81	124.77	116.99
25	G	607	CHL	C3B-C4B-NB	2.81	108.44	103.55
25	g	607	CHL	C3B-C4B-NB	2.81	108.44	103.55
22	b	613	CLA	C3B-C4B-NB	2.81	112.84	109.21
22	b	604	CLA	CAC-C3C-C4C	2.81	128.79	124.83
22	5	614	CLA	C3B-C4B-NB	2.81	112.84	109.21
22	1	614	CLA	C3B-C4B-NB	2.81	112.84	109.21
22	b	604	CLA	C3C-C4C-NC	2.81	113.06	110.21
22	B	615	CLA	CED-O2D-CGD	2.82	122.57	115.97
25	n	609	CHL	CHD-C1D-C2D	2.82	124.79	116.99
25	N	609	CHL	CHD-C1D-C2D	2.82	124.79	116.99
25	1	605	CHL	CHC-C4B-C3B	2.82	124.90	118.23
25	5	605	CHL	CHC-C4B-C3B	2.82	124.90	118.23
25	3	301	CHL	C3B-C4B-NB	2.82	108.46	103.55
25	7	301	CHL	C3B-C4B-NB	2.82	108.46	103.55
25	N	605	CHL	CHB-C1B-C2B	2.82	124.79	116.99
25	n	605	CHL	CHB-C1B-C2B	2.82	124.79	116.99
22	y	612	CLA	C3C-C4C-NC	2.82	113.06	110.21
22	Y	612	CLA	C3C-C4C-NC	2.82	113.06	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	607	CHL	C3B-C4B-NB	2.82	108.46	103.55
25	N	607	CHL	C3B-C4B-NB	2.82	108.46	103.55
25	r	305	CHL	C3B-C4B-NB	2.82	108.47	103.55
25	R	305	CHL	C3B-C4B-NB	2.82	108.47	103.55
22	G	610	CLA	CMC-C2C-C1C	2.82	129.30	125.02
22	g	610	CLA	CMC-C2C-C1C	2.82	129.30	125.02
25	Y	601	CHL	CHB-C1B-C2B	2.83	124.83	116.99
25	y	601	CHL	CHB-C1B-C2B	2.83	124.83	116.99
25	4	306	CHL	CHB-C1B-C2B	2.83	124.83	116.99
25	8	306	CHL	CHB-C1B-C2B	2.83	124.83	116.99
25	N	601	CHL	CHC-C4B-C3B	2.83	124.94	118.23
25	n	601	CHL	CHC-C4B-C3B	2.83	124.94	118.23
25	G	607	CHL	CHB-C1B-C2B	2.84	124.85	116.99
25	g	607	CHL	CHB-C1B-C2B	2.84	124.85	116.99
25	3	306	CHL	C3B-C4B-NB	2.84	108.50	103.55
25	7	306	CHL	C3B-C4B-NB	2.84	108.50	103.55
25	r	305	CHL	CHB-C1B-C2B	2.84	124.85	116.99
25	R	305	CHL	CHB-C1B-C2B	2.84	124.85	116.99
25	s	306	CHL	CHC-C4B-C3B	2.84	124.96	118.23
25	S	306	CHL	CHC-C4B-C3B	2.84	124.96	118.23
22	a	405	CLA	CMB-C2B-C3B	2.84	130.17	124.89
25	1	601	CHL	C3B-C4B-NB	2.84	108.50	103.55
25	5	601	CHL	C3B-C4B-NB	2.84	108.50	103.55
25	1	607	CHL	CHC-C4B-C3B	2.84	124.96	118.23
25	5	607	CHL	CHC-C4B-C3B	2.84	124.96	118.23
25	n	607	CHL	CHB-C1B-C2B	2.84	124.87	116.99
25	N	607	CHL	CHB-C1B-C2B	2.84	124.87	116.99
25	G	609	CHL	CHD-C1D-C2D	2.86	124.90	116.99
25	g	609	CHL	CHD-C1D-C2D	2.86	124.90	116.99
25	4	307	CHL	CHB-C1B-C2B	2.86	124.91	116.99
25	8	307	CHL	CHB-C1B-C2B	2.86	124.91	116.99
25	7	307	CHL	CHC-C4B-C3B	2.86	125.00	118.23
25	3	307	CHL	CHC-C4B-C3B	2.86	125.00	118.23
22	4	309	CLA	CMC-C2C-C1C	2.86	129.36	125.02
22	8	309	CLA	CMC-C2C-C1C	2.86	129.36	125.02
22	C	509	CLA	CMB-C2B-C3B	2.86	130.21	124.89
25	8	308	CHL	CHB-C1B-C2B	2.87	124.93	116.99
25	4	308	CHL	CHB-C1B-C2B	2.87	124.93	116.99
25	8	308	CHL	CHC-C4B-C3B	2.87	125.02	118.23
25	4	308	CHL	CHC-C4B-C3B	2.87	125.02	118.23
25	g	601	CHL	CHC-C4B-C3B	2.87	125.03	118.23
25	4	306	CHL	CHC-C4B-C3B	2.87	125.03	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	306	CHL	CHC-C4B-C3B	2.87	125.03	118.23
25	G	601	CHL	CHC-C4B-C3B	2.87	125.03	118.23
23	d	402	PHO	C2B-C1B-NB	2.87	114.08	109.82
25	4	307	CHL	CHC-C4B-C3B	2.88	125.04	118.23
25	8	307	CHL	CHC-C4B-C3B	2.88	125.04	118.23
25	7	308	CHL	C3B-C4B-NB	2.88	108.57	103.55
25	3	308	CHL	C3B-C4B-NB	2.88	108.57	103.55
25	5	615	CHL	C3B-C4B-NB	2.89	108.58	103.55
25	1	615	CHL	C3B-C4B-NB	2.89	108.58	103.55
25	1	606	CHL	CHB-C1B-C2B	2.89	124.99	116.99
25	5	606	CHL	CHB-C1B-C2B	2.89	124.99	116.99
22	S	305	CLA	CMB-C2B-C3B	2.89	130.25	124.89
22	s	305	CLA	CMB-C2B-C3B	2.89	130.25	124.89
25	Y	607	CHL	CHB-C1B-C2B	2.89	125.00	116.99
25	y	607	CHL	CHB-C1B-C2B	2.89	125.00	116.99
22	B	608	CLA	C3B-C4B-NB	2.90	112.95	109.21
25	n	607	CHL	CHC-C4B-C3B	2.90	125.10	118.23
25	N	607	CHL	CHC-C4B-C3B	2.90	125.10	118.23
25	1	609	CHL	CHB-C1B-C2B	2.90	125.02	116.99
25	5	609	CHL	CHB-C1B-C2B	2.90	125.02	116.99
25	4	301	CHL	CHC-C4B-C3B	2.90	125.10	118.23
25	8	301	CHL	CHC-C4B-C3B	2.90	125.10	118.23
25	s	306	CHL	C3B-C4B-NB	2.90	108.61	103.55
25	S	306	CHL	C3B-C4B-NB	2.90	108.61	103.55
25	6	601	CHL	CHC-C4B-C3B	2.90	125.11	118.23
25	2	601	CHL	CHC-C4B-C3B	2.90	125.11	118.23
22	y	610	CLA	CMB-C2B-C3B	2.91	130.29	124.89
22	Y	610	CLA	CMB-C2B-C3B	2.91	130.29	124.89
25	3	301	CHL	CHB-C1B-C2B	2.91	125.05	116.99
25	7	301	CHL	CHB-C1B-C2B	2.91	125.05	116.99
25	7	307	CHL	CHB-C1B-C2B	2.91	125.05	116.99
25	3	307	CHL	CHB-C1B-C2B	2.91	125.05	116.99
22	c	504	CLA	CMB-C2B-C3B	2.91	130.30	124.89
22	b	611	CLA	C3B-C4B-NB	2.91	112.98	109.21
25	r	306	CHL	CHC-C4B-C3B	2.92	125.14	118.23
25	R	306	CHL	CHC-C4B-C3B	2.92	125.14	118.23
22	s	303	CLA	CED-O2D-CGD	2.92	122.81	115.97
22	S	303	CLA	CED-O2D-CGD	2.92	122.81	115.97
25	4	306	CHL	C3B-C4B-NB	2.92	108.64	103.55
25	8	306	CHL	C3B-C4B-NB	2.92	108.64	103.55
25	g	605	CHL	CHC-C4B-C3B	2.93	125.16	118.23
25	G	605	CHL	CHC-C4B-C3B	2.93	125.16	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	305	CHL	C3B-C4B-NB	2.93	108.65	103.55
25	4	305	CHL	C3B-C4B-NB	2.93	108.65	103.55
25	5	615	CHL	CHC-C4B-C3B	2.93	125.17	118.23
25	1	615	CHL	CHC-C4B-C3B	2.93	125.17	118.23
22	S	312	CLA	C3C-C4C-NC	2.93	113.18	110.21
22	s	312	CLA	C3C-C4C-NC	2.93	113.18	110.21
25	g	605	CHL	C3B-C4B-NB	2.93	108.66	103.55
25	G	605	CHL	C3B-C4B-NB	2.93	108.66	103.55
22	b	611	CLA	CMB-C2B-C3B	2.94	130.35	124.89
22	3	310	CLA	CMB-C2B-C3B	2.95	130.36	124.89
22	7	310	CLA	CMB-C2B-C3B	2.95	130.36	124.89
25	r	306	CHL	C3B-C4B-NB	2.95	108.69	103.55
25	R	306	CHL	C3B-C4B-NB	2.95	108.69	103.55
25	s	307	CHL	C3B-C4B-NB	2.95	108.69	103.55
25	S	307	CHL	C3B-C4B-NB	2.95	108.69	103.55
25	G	609	CHL	O2D-CGD-CBD	2.95	118.41	111.20
25	g	609	CHL	O2D-CGD-CBD	2.95	118.41	111.20
25	s	306	CHL	CHB-C1B-C2B	2.96	125.18	116.99
25	S	306	CHL	CHB-C1B-C2B	2.96	125.18	116.99
22	c	508	CLA	CMB-C2B-C3B	2.96	130.38	124.89
22	5	614	CLA	CED-O2D-CGD	2.96	122.90	115.97
22	1	614	CLA	CED-O2D-CGD	2.96	122.90	115.97
22	D	403	CLA	CMC-C2C-C1C	2.96	129.51	125.02
25	g	605	CHL	CHB-C1B-C2B	2.97	125.22	116.99
25	G	605	CHL	CHB-C1B-C2B	2.97	125.22	116.99
25	R	304	CHL	CHB-C1B-C2B	2.97	125.23	116.99
25	r	304	CHL	CHB-C1B-C2B	2.97	125.23	116.99
22	c	505	CLA	CMB-C2B-C3B	2.97	130.41	124.89
25	1	601	CHL	CHB-C1B-C2B	2.98	125.24	116.99
25	5	601	CHL	CHB-C1B-C2B	2.98	125.24	116.99
25	1	601	CHL	CHC-C4B-C3B	2.98	125.29	118.23
25	5	601	CHL	CHC-C4B-C3B	2.98	125.29	118.23
25	7	307	CHL	C3B-C4B-NB	2.99	108.76	103.55
25	3	307	CHL	C3B-C4B-NB	2.99	108.76	103.55
25	y	606	CHL	CHB-C1B-C2B	2.99	125.27	116.99
25	Y	606	CHL	CHB-C1B-C2B	2.99	125.27	116.99
23	d	402	PHO	O2D-CGD-CBD	2.99	116.65	111.30
25	1	607	CHL	C3B-C4B-NB	3.00	108.77	103.55
25	5	607	CHL	C3B-C4B-NB	3.00	108.77	103.55
25	3	306	CHL	CHC-C4B-C3B	3.00	125.33	118.23
25	7	306	CHL	CHC-C4B-C3B	3.00	125.33	118.23
25	3	301	CHL	CHC-C4B-C3B	3.00	125.33	118.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	301	CHL	CHC-C4B-C3B	3.00	125.33	118.23
25	N	608	CHL	C3B-C4B-NB	3.00	108.78	103.55
25	n	608	CHL	C3B-C4B-NB	3.00	108.78	103.55
23	a	404	PHO	C2B-C1B-NB	3.00	114.27	109.82
25	N	601	CHL	C3B-C4B-NB	3.00	108.78	103.55
25	n	601	CHL	C3B-C4B-NB	3.00	108.78	103.55
25	7	309	CHL	CHB-C1B-C2B	3.00	125.31	116.99
25	3	309	CHL	CHB-C1B-C2B	3.00	125.31	116.99
22	n	610	CLA	CMB-C2B-C3B	3.01	130.47	124.89
22	N	610	CLA	CMB-C2B-C3B	3.01	130.47	124.89
22	B	611	CLA	CMB-C2B-C3B	3.01	130.47	124.89
25	6	608	CHL	CHC-C4B-C3B	3.01	125.36	118.23
25	2	608	CHL	CHC-C4B-C3B	3.01	125.36	118.23
25	2	605	CHL	CHB-C1B-C2B	3.02	125.35	116.99
25	6	605	CHL	CHB-C1B-C2B	3.02	125.35	116.99
22	b	615	CLA	C3C-C4C-NC	3.02	113.27	110.21
25	4	307	CHL	C3B-C4B-NB	3.02	108.81	103.55
25	8	307	CHL	C3B-C4B-NB	3.02	108.81	103.55
25	3	302	CHL	CHC-C4B-C3B	3.02	125.39	118.23
25	7	302	CHL	CHC-C4B-C3B	3.02	125.39	118.23
22	Y	604	CLA	CMC-C2C-C1C	3.03	129.61	125.02
22	y	604	CLA	CMC-C2C-C1C	3.03	129.61	125.02
25	2	605	CHL	CHC-C4B-C3B	3.03	125.41	118.23
25	6	605	CHL	CHC-C4B-C3B	3.03	125.41	118.23
25	g	601	CHL	C3B-C4B-NB	3.03	108.83	103.55
25	G	601	CHL	C3B-C4B-NB	3.03	108.83	103.55
22	S	304	CLA	C3B-C4B-NB	3.03	113.13	109.21
22	s	304	CLA	C3B-C4B-NB	3.03	113.13	109.21
25	S	302	CHL	CHC-C4B-C3B	3.03	125.42	118.23
25	s	302	CHL	CHC-C4B-C3B	3.03	125.42	118.23
25	8	305	CHL	CHC-C4B-C3B	3.04	125.42	118.23
25	4	305	CHL	CHC-C4B-C3B	3.04	125.42	118.23
25	2	607	CHL	C3B-C4B-NB	3.04	108.84	103.55
25	1	606	CHL	C3B-C4B-NB	3.04	108.84	103.55
25	5	606	CHL	C3B-C4B-NB	3.04	108.84	103.55
25	6	607	CHL	C3B-C4B-NB	3.04	108.84	103.55
25	3	306	CHL	CHB-C1B-C2B	3.04	125.42	116.99
25	7	306	CHL	CHB-C1B-C2B	3.04	125.42	116.99
25	R	304	CHL	C3B-C4B-NB	3.04	108.85	103.55
25	r	304	CHL	C3B-C4B-NB	3.04	108.85	103.55
25	3	302	CHL	C3B-C4B-NB	3.05	108.87	103.55
25	7	302	CHL	C3B-C4B-NB	3.05	108.87	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	603	CLA	C3C-C4C-NC	3.06	113.31	110.21
22	N	603	CLA	C3C-C4C-NC	3.06	113.31	110.21
25	g	606	CHL	C3B-C4B-NB	3.06	108.88	103.55
25	G	606	CHL	C3B-C4B-NB	3.06	108.88	103.55
22	7	314	CLA	C3C-C4C-NC	3.06	113.31	110.21
22	3	314	CLA	C3C-C4C-NC	3.06	113.31	110.21
25	Y	601	CHL	CHD-C1D-C2D	3.07	125.49	116.99
25	y	601	CHL	CHD-C1D-C2D	3.07	125.49	116.99
22	C	501	CLA	CMB-C2B-C3B	3.07	130.59	124.89
25	7	309	CHL	CHD-C1D-C2D	3.07	125.50	116.99
25	3	309	CHL	CHD-C1D-C2D	3.07	125.50	116.99
25	G	607	CHL	CHC-C4B-C3B	3.08	125.52	118.23
25	g	607	CHL	CHC-C4B-C3B	3.08	125.52	118.23
25	2	606	CHL	C3B-C4B-NB	3.08	108.91	103.55
25	6	606	CHL	C3B-C4B-NB	3.08	108.91	103.55
22	a	403	CLA	CED-O2D-CGD	3.08	123.19	115.97
25	Y	607	CHL	C3B-C4B-NB	3.08	108.92	103.55
25	y	607	CHL	C3B-C4B-NB	3.08	108.92	103.55
22	a	402	CLA	O2D-CGD-CBD	3.08	116.81	111.30
25	S	308	CHL	C3B-C4B-NB	3.09	108.93	103.55
25	s	308	CHL	C3B-C4B-NB	3.09	108.93	103.55
25	N	608	CHL	CHC-C4B-C3B	3.09	125.54	118.23
25	n	608	CHL	CHC-C4B-C3B	3.09	125.54	118.23
22	C	508	CLA	CMC-C2C-C3C	3.09	134.65	126.09
22	R	308	CLA	CMC-C2C-C1C	3.09	129.71	125.02
22	r	308	CLA	CMC-C2C-C1C	3.09	129.71	125.02
25	Y	601	CHL	CHC-C4B-C3B	3.09	125.56	118.23
25	y	601	CHL	CHC-C4B-C3B	3.09	125.56	118.23
22	5	614	CLA	C3C-C4C-NC	3.10	113.35	110.21
22	1	614	CLA	C3C-C4C-NC	3.10	113.35	110.21
25	4	301	CHL	C3B-C4B-NB	3.10	108.96	103.55
25	8	301	CHL	C3B-C4B-NB	3.10	108.96	103.55
25	2	606	CHL	CHB-C1B-C2B	3.11	125.61	116.99
25	6	606	CHL	CHB-C1B-C2B	3.11	125.61	116.99
25	S	308	CHL	CHC-C4B-C3B	3.12	125.62	118.23
25	s	308	CHL	CHC-C4B-C3B	3.12	125.62	118.23
25	N	605	CHL	C3B-C4B-NB	3.12	108.98	103.55
25	n	605	CHL	C3B-C4B-NB	3.12	108.98	103.55
25	y	609	CHL	CHB-C1B-C2B	3.12	125.64	116.99
25	Y	609	CHL	CHB-C1B-C2B	3.12	125.64	116.99
23	D	402	PHO	C2B-C1B-NB	3.13	114.45	109.82
25	y	609	CHL	C3B-C4B-NB	3.13	109.00	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	609	CHL	C3B-C4B-NB	3.13	109.00	103.55
22	d	403	CLA	C3C-C4C-NC	3.13	113.38	110.21
22	G	603	CLA	C3C-C4C-NC	3.13	113.38	110.21
22	g	603	CLA	C3C-C4C-NC	3.13	113.38	110.21
25	G	609	CHL	CHB-C1B-C2B	3.13	125.66	116.99
25	g	609	CHL	CHB-C1B-C2B	3.13	125.66	116.99
22	b	616	CLA	C3C-C4C-NC	3.15	113.40	110.21
25	6	601	CHL	C3B-C4B-NB	3.15	109.04	103.55
25	2	601	CHL	C3B-C4B-NB	3.15	109.04	103.55
25	n	609	CHL	CHB-C1B-C2B	3.16	125.73	116.99
25	N	609	CHL	CHB-C1B-C2B	3.16	125.73	116.99
25	y	609	CHL	CHD-C1D-C2D	3.16	125.73	116.99
25	Y	609	CHL	CHD-C1D-C2D	3.16	125.73	116.99
22	C	510	CLA	CMB-C2B-C3B	3.16	130.75	124.89
22	b	615	CLA	CMB-C2B-C3B	3.16	130.76	124.89
22	N	614	CLA	C3C-C4C-NC	3.16	113.42	110.21
22	n	614	CLA	C3C-C4C-NC	3.16	113.42	110.21
25	y	606	CHL	C3B-C4B-NB	3.17	109.07	103.55
25	Y	606	CHL	C3B-C4B-NB	3.17	109.07	103.55
22	c	507	CLA	CMC-C2C-C3C	3.17	134.86	126.09
22	c	510	CLA	CMB-C2B-C3B	3.18	130.79	124.89
25	3	306	CHL	CHD-C1D-C2D	3.19	125.83	116.99
25	7	306	CHL	CHD-C1D-C2D	3.19	125.83	116.99
22	D	401	CLA	O2D-CGD-CBD	3.20	117.01	111.30
25	2	605	CHL	CHD-C1D-C2D	3.21	125.87	116.99
25	6	605	CHL	CHD-C1D-C2D	3.21	125.87	116.99
22	c	501	CLA	C3C-C4C-NC	3.21	113.46	110.21
25	n	607	CHL	CHD-C1D-C2D	3.21	125.88	116.99
25	N	607	CHL	CHD-C1D-C2D	3.21	125.88	116.99
25	S	308	CHL	CHD-C1D-C2D	3.21	125.89	116.99
25	s	308	CHL	CHD-C1D-C2D	3.21	125.89	116.99
22	Y	604	CLA	O2D-CGD-CBD	3.21	117.04	111.30
22	y	604	CLA	O2D-CGD-CBD	3.21	117.04	111.30
25	1	605	CHL	C3B-C4B-NB	3.21	109.15	103.55
25	5	605	CHL	C3B-C4B-NB	3.21	109.15	103.55
25	g	606	CHL	CHB-C1B-C2B	3.21	125.89	116.99
25	G	606	CHL	CHB-C1B-C2B	3.21	125.89	116.99
22	b	616	CLA	CMB-C2B-C3B	3.23	130.89	124.89
25	Y	605	CHL	CHD-C1D-C2D	3.24	125.97	116.99
25	y	605	CHL	CHD-C1D-C2D	3.24	125.97	116.99
22	B	604	CLA	C3B-C4B-NB	3.25	113.41	109.21
25	n	606	CHL	CHB-C1B-C2B	3.25	125.99	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	606	CHL	CHB-C1B-C2B	3.25	125.99	116.99
22	n	612	CLA	C3C-C4C-NC	3.25	113.51	110.21
22	N	612	CLA	C3C-C4C-NC	3.25	113.51	110.21
25	r	306	CHL	CHD-C1D-C2D	3.25	126.00	116.99
25	R	306	CHL	CHD-C1D-C2D	3.25	126.00	116.99
25	2	607	CHL	CHC-C4B-C3B	3.26	125.94	118.23
25	6	607	CHL	CHC-C4B-C3B	3.26	125.94	118.23
25	7	308	CHL	CHC-C4B-C3B	3.26	125.95	118.23
25	3	308	CHL	CHC-C4B-C3B	3.26	125.95	118.23
25	6	608	CHL	CHD-C1D-C2D	3.26	126.02	116.99
25	2	608	CHL	CHD-C1D-C2D	3.26	126.02	116.99
25	g	608	CHL	CHC-C4B-C3B	3.26	125.95	118.23
25	G	608	CHL	CHC-C4B-C3B	3.26	125.95	118.23
25	G	607	CHL	CHD-C1D-C2D	3.26	126.03	116.99
25	g	607	CHL	CHD-C1D-C2D	3.26	126.03	116.99
25	5	615	CHL	CHD-C1D-C2D	3.27	126.05	116.99
25	1	615	CHL	CHD-C1D-C2D	3.27	126.05	116.99
25	1	608	CHL	CHC-C4B-C3B	3.27	125.98	118.23
25	5	608	CHL	CHC-C4B-C3B	3.27	125.98	118.23
22	c	509	CLA	CAC-C3C-C4C	3.28	129.45	124.83
22	3	304	CLA	C3C-C4C-NC	3.29	113.54	110.21
22	7	304	CLA	C3C-C4C-NC	3.29	113.54	110.21
25	N	605	CHL	CHD-C1D-C2D	3.29	126.10	116.99
25	n	605	CHL	CHD-C1D-C2D	3.29	126.10	116.99
25	Y	607	CHL	CHD-C1D-C2D	3.29	126.11	116.99
25	y	607	CHL	CHD-C1D-C2D	3.29	126.11	116.99
25	Y	605	CHL	CHB-C1B-C2B	3.29	126.11	116.99
25	y	605	CHL	CHB-C1B-C2B	3.29	126.11	116.99
22	b	603	CLA	C3C-C4C-NC	3.30	113.55	110.21
25	S	302	CHL	CHD-C1D-C2D	3.30	126.12	116.99
25	s	302	CHL	CHD-C1D-C2D	3.30	126.12	116.99
25	g	605	CHL	CHD-C1D-C2D	3.31	126.15	116.99
25	G	605	CHL	CHD-C1D-C2D	3.31	126.15	116.99
25	8	308	CHL	C3B-C4B-NB	3.31	109.31	103.55
25	4	308	CHL	C3B-C4B-NB	3.31	109.31	103.55
22	A	403	CLA	CED-O2D-CGD	3.31	123.73	115.97
25	N	601	CHL	CHD-C1D-C2D	3.31	126.17	116.99
25	n	601	CHL	CHD-C1D-C2D	3.31	126.17	116.99
25	r	305	CHL	CHD-C1D-C2D	3.31	126.17	116.99
25	R	305	CHL	CHD-C1D-C2D	3.31	126.17	116.99
22	b	610	CLA	O2D-CGD-CBD	3.31	117.22	111.30
25	1	601	CHL	CHD-C1D-C2D	3.32	126.19	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	601	CHL	CHD-C1D-C2D	3.32	126.19	116.99
22	A	405	CLA	CMB-C2B-C3B	3.33	131.08	124.89
22	A	402	CLA	CMB-C2B-C3B	3.34	131.08	124.89
25	7	308	CHL	CHD-C1D-C2D	3.34	126.25	116.99
25	3	308	CHL	CHD-C1D-C2D	3.34	126.25	116.99
25	1	609	CHL	CHD-C1D-C2D	3.35	126.26	116.99
25	5	609	CHL	CHD-C1D-C2D	3.35	126.26	116.99
22	g	612	CLA	C3C-C4C-NC	3.35	113.61	110.21
22	G	612	CLA	C3C-C4C-NC	3.35	113.61	110.21
22	B	601	CLA	CMC-C2C-C1C	3.35	130.10	125.02
22	c	507	CLA	O2D-CGD-CBD	3.35	117.29	111.30
25	n	606	CHL	C3B-C4B-NB	3.35	109.39	103.55
25	N	606	CHL	C3B-C4B-NB	3.35	109.39	103.55
23	a	404	PHO	CAC-C3C-C4C	3.36	129.15	125.21
25	2	607	CHL	CHD-C1D-C2D	3.37	126.32	116.99
25	6	607	CHL	CHD-C1D-C2D	3.37	126.32	116.99
22	D	403	CLA	C3C-C4C-NC	3.37	113.63	110.21
22	b	616	CLA	C3B-C4B-NB	3.38	113.58	109.21
25	1	605	CHL	CHD-C1D-C2D	3.38	126.36	116.99
25	5	605	CHL	CHD-C1D-C2D	3.38	126.36	116.99
25	s	306	CHL	CHD-C1D-C2D	3.38	126.36	116.99
25	S	306	CHL	CHD-C1D-C2D	3.38	126.36	116.99
22	Y	614	CLA	C3C-C4C-NC	3.39	113.64	110.21
22	y	614	CLA	C3C-C4C-NC	3.39	113.64	110.21
23	a	404	PHO	C3C-C4C-NC	3.39	115.74	110.19
25	y	608	CHL	CHC-C4B-C3B	3.40	126.28	118.23
25	Y	608	CHL	CHC-C4B-C3B	3.40	126.28	118.23
25	Y	605	CHL	C3B-C4B-NB	3.40	109.47	103.55
25	y	605	CHL	C3B-C4B-NB	3.40	109.47	103.55
23	D	402	PHO	C3C-C4C-NC	3.40	115.75	110.19
22	B	616	CLA	O2D-CGD-CBD	3.41	117.38	111.30
25	8	308	CHL	CHD-C1D-C2D	3.41	126.44	116.99
25	4	308	CHL	CHD-C1D-C2D	3.41	126.44	116.99
25	2	606	CHL	CHD-C1D-C2D	3.41	126.45	116.99
25	6	606	CHL	CHD-C1D-C2D	3.41	126.45	116.99
25	4	307	CHL	CHD-C1D-C2D	3.41	126.45	116.99
25	8	307	CHL	CHD-C1D-C2D	3.41	126.45	116.99
22	7	305	CLA	C3C-C4C-NC	3.42	113.67	110.21
22	3	305	CLA	C3C-C4C-NC	3.42	113.67	110.21
22	c	511	CLA	C3C-C4C-NC	3.42	113.67	110.21
22	s	309	CLA	C3C-C4C-NC	3.42	113.68	110.21
22	S	309	CLA	C3C-C4C-NC	3.42	113.68	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	604	CLA	C3C-C4C-NC	3.43	113.68	110.21
22	N	604	CLA	C3C-C4C-NC	3.43	113.68	110.21
22	B	613	CLA	C3C-C4C-NC	3.43	113.69	110.21
22	b	604	CLA	CMC-C2C-C3C	3.44	135.60	126.09
25	s	307	CHL	CHD-C1D-C2D	3.44	126.50	116.99
25	S	307	CHL	CHD-C1D-C2D	3.44	126.50	116.99
23	d	402	PHO	C3C-C4C-NC	3.44	115.81	110.19
22	C	504	CLA	C3C-C4C-NC	3.44	113.69	110.21
25	4	306	CHL	CHD-C1D-C2D	3.44	126.52	116.99
25	8	306	CHL	CHD-C1D-C2D	3.44	126.52	116.99
22	R	303	CLA	C3C-C4C-NC	3.44	113.70	110.21
22	r	303	CLA	C3C-C4C-NC	3.44	113.70	110.21
22	B	610	CLA	O2D-CGD-CBD	3.45	117.46	111.30
22	B	612	CLA	O2D-CGD-CBD	3.45	117.46	111.30
22	c	509	CLA	CMB-C2B-C3B	3.46	131.31	124.89
25	1	607	CHL	CHD-C1D-C2D	3.46	126.58	116.99
25	5	607	CHL	CHD-C1D-C2D	3.46	126.58	116.99
25	6	601	CHL	CHD-C1D-C2D	3.46	126.58	116.99
25	2	601	CHL	CHD-C1D-C2D	3.46	126.58	116.99
22	6	603	CLA	C3C-C4C-NC	3.46	113.72	110.21
22	2	603	CLA	C3C-C4C-NC	3.46	113.72	110.21
22	b	605	CLA	C3C-C4C-NC	3.46	113.72	110.21
22	C	505	CLA	C3C-C4C-NC	3.47	113.72	110.21
22	G	614	CLA	C3C-C4C-NC	3.47	113.72	110.21
22	g	614	CLA	C3C-C4C-NC	3.47	113.72	110.21
25	7	307	CHL	CHD-C1D-C2D	3.47	126.60	116.99
25	3	307	CHL	CHD-C1D-C2D	3.47	126.60	116.99
22	6	609	CLA	CMC-C2C-C1C	3.47	130.28	125.02
22	2	609	CLA	CMC-C2C-C1C	3.47	130.28	125.02
22	Y	603	CLA	C3C-C4C-NC	3.48	113.73	110.21
22	y	603	CLA	C3C-C4C-NC	3.48	113.73	110.21
22	b	606	CLA	CMB-C2B-C3B	3.48	131.35	124.89
25	g	601	CHL	CHD-C1D-C2D	3.48	126.64	116.99
25	G	601	CHL	CHD-C1D-C2D	3.48	126.64	116.99
25	N	608	CHL	CHD-C1D-C2D	3.48	126.64	116.99
25	n	608	CHL	CHD-C1D-C2D	3.48	126.64	116.99
22	b	608	CLA	C3C-C4C-NC	3.49	113.74	110.21
22	d	404	CLA	C3C-C4C-NC	3.49	113.75	110.21
22	C	511	CLA	C3C-C4C-NC	3.49	113.75	110.21
22	A	405	CLA	O2D-CGD-CBD	3.50	117.54	111.30
22	C	502	CLA	C3C-C4C-NC	3.50	113.75	110.21
22	G	604	CLA	C3C-C4C-NC	3.50	113.75	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	g	604	CLA	C3C-C4C-NC	3.50	113.75	110.21
22	S	304	CLA	O2D-CGD-CBD	3.50	117.55	111.30
22	s	304	CLA	O2D-CGD-CBD	3.50	117.55	111.30
25	1	608	CHL	CHD-C1D-C2D	3.50	126.69	116.99
25	5	608	CHL	CHD-C1D-C2D	3.50	126.69	116.99
22	B	611	CLA	C3C-C4C-NC	3.51	113.77	110.21
22	D	403	CLA	CMB-C2B-C3B	3.52	131.42	124.89
22	s	313	CLA	C3C-C4C-NC	3.52	113.78	110.21
22	S	313	CLA	C3C-C4C-NC	3.52	113.78	110.21
25	1	606	CHL	CHD-C1D-C2D	3.52	126.75	116.99
25	5	606	CHL	CHD-C1D-C2D	3.52	126.75	116.99
22	3	310	CLA	CMC-C2C-C1C	3.53	130.37	125.02
22	7	310	CLA	CMC-C2C-C1C	3.53	130.37	125.02
25	R	304	CHL	CHD-C1D-C2D	3.53	126.77	116.99
25	r	304	CHL	CHD-C1D-C2D	3.53	126.77	116.99
22	2	613	CLA	C3C-C4C-NC	3.53	113.79	110.21
22	6	613	CLA	C3C-C4C-NC	3.53	113.79	110.21
22	a	402	CLA	CMB-C2B-C3B	3.53	131.45	124.89
22	n	611	CLA	C3C-C4C-NC	3.54	113.80	110.21
22	N	611	CLA	C3C-C4C-NC	3.54	113.80	110.21
22	C	501	CLA	C3C-C4C-NC	3.54	113.80	110.21
22	g	611	CLA	C3C-C4C-NC	3.54	113.80	110.21
22	G	611	CLA	C3C-C4C-NC	3.54	113.80	110.21
22	S	305	CLA	C3C-C4C-NC	3.55	113.80	110.21
22	s	305	CLA	C3C-C4C-NC	3.55	113.80	110.21
22	C	512	CLA	O2D-CGD-CBD	3.55	117.64	111.30
22	B	605	CLA	C3C-C4C-NC	3.55	113.81	110.21
22	5	604	CLA	C3C-C4C-NC	3.55	113.81	110.21
22	1	604	CLA	C3C-C4C-NC	3.55	113.81	110.21
22	b	614	CLA	CMC-C2C-C1C	3.56	130.42	125.02
22	1	612	CLA	C3C-C4C-NC	3.57	113.83	110.21
22	5	612	CLA	C3C-C4C-NC	3.57	113.83	110.21
25	y	608	CHL	CHD-C1D-C2D	3.57	126.87	116.99
25	Y	608	CHL	CHD-C1D-C2D	3.57	126.87	116.99
22	c	505	CLA	C3C-C4C-NC	3.58	113.84	110.21
25	y	606	CHL	CHD-C1D-C2D	3.58	126.90	116.99
25	Y	606	CHL	CHD-C1D-C2D	3.58	126.90	116.99
22	1	613	CLA	C3C-C4C-NC	3.58	113.84	110.21
22	5	613	CLA	C3C-C4C-NC	3.58	113.84	110.21
23	D	402	PHO	O2D-CGD-CBD	3.59	117.72	111.30
22	b	608	CLA	CMB-C2B-C3B	3.60	131.56	124.89
25	g	608	CHL	CHD-C1D-C2D	3.60	126.95	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	608	CHL	CHD-C1D-C2D	3.60	126.95	116.99
22	2	604	CLA	C3C-C4C-NC	3.60	113.86	110.21
22	s	301	CLA	C3C-C4C-NC	3.60	113.86	110.21
22	6	604	CLA	C3C-C4C-NC	3.60	113.86	110.21
25	8	305	CHL	CHD-C1D-C2D	3.60	126.97	116.99
25	4	305	CHL	CHD-C1D-C2D	3.60	126.97	116.99
22	1	603	CLA	C3C-C4C-NC	3.60	113.86	110.21
22	B	616	CLA	C3C-C4C-NC	3.60	113.86	110.21
22	5	603	CLA	C3C-C4C-NC	3.60	113.86	110.21
25	3	302	CHL	CHD-C1D-C2D	3.61	126.98	116.99
25	7	302	CHL	CHD-C1D-C2D	3.61	126.98	116.99
25	3	301	CHL	CHD-C1D-C2D	3.61	126.98	116.99
25	7	301	CHL	CHD-C1D-C2D	3.61	126.98	116.99
22	S	310	CLA	C3C-C4C-NC	3.61	113.87	110.21
22	s	310	CLA	C3C-C4C-NC	3.61	113.87	110.21
22	C	506	CLA	O2D-CGD-CBD	3.62	117.77	111.30
22	s	303	CLA	C3C-C4C-NC	3.62	113.88	110.21
22	S	303	CLA	C3C-C4C-NC	3.62	113.88	110.21
22	R	309	CLA	C3C-C4C-NC	3.62	113.88	110.21
22	r	309	CLA	C3C-C4C-NC	3.62	113.88	110.21
22	N	602	CLA	C3C-C4C-NC	3.63	113.89	110.21
22	n	602	CLA	C3C-C4C-NC	3.63	113.89	110.21
25	n	606	CHL	CHD-C1D-C2D	3.63	127.04	116.99
25	N	606	CHL	CHD-C1D-C2D	3.63	127.04	116.99
22	c	502	CLA	C3C-C4C-NC	3.63	113.89	110.21
22	r	310	CLA	C3C-C4C-NC	3.64	113.90	110.21
22	R	310	CLA	C3C-C4C-NC	3.64	113.90	110.21
22	B	602	CLA	O2D-CGD-CBD	3.64	117.81	111.30
22	d	403	CLA	CMB-C2B-C3B	3.65	131.66	124.89
22	b	612	CLA	C3C-C4C-NC	3.66	113.92	110.21
22	C	512	CLA	C3C-C4C-NC	3.68	113.94	110.21
22	4	304	CLA	C3C-C4C-NC	3.68	113.94	110.21
22	8	304	CLA	C3C-C4C-NC	3.68	113.94	110.21
22	c	504	CLA	C3C-C4C-NC	3.68	113.94	110.21
22	c	501	CLA	O2D-CGD-CBD	3.69	117.89	111.30
22	C	502	CLA	O2D-CGD-CBD	3.70	117.90	111.30
25	g	606	CHL	CHD-C1D-C2D	3.70	127.23	116.99
25	G	606	CHL	CHD-C1D-C2D	3.70	127.23	116.99
22	a	405	CLA	O2D-CGD-CBD	3.70	117.91	111.30
25	4	301	CHL	CHD-C1D-C2D	3.71	127.25	116.99
25	8	301	CHL	CHD-C1D-C2D	3.71	127.25	116.99
22	B	601	CLA	C3C-C4C-NC	3.71	113.97	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	O2D-CGD-CBD	3.72	117.94	111.30
22	8	310	CLA	C3C-C4C-NC	3.72	113.98	110.21
22	4	310	CLA	C3C-C4C-NC	3.72	113.98	110.21
22	C	508	CLA	C3C-C4C-NC	3.73	113.99	110.21
22	G	602	CLA	C3C-C4C-NC	3.74	114.00	110.21
22	g	602	CLA	C3C-C4C-NC	3.74	114.00	110.21
22	7	311	CLA	C3C-C4C-NC	3.74	114.00	110.21
22	3	311	CLA	C3C-C4C-NC	3.74	114.00	110.21
22	B	603	CLA	C3C-C4C-NC	3.74	114.00	110.21
22	n	613	CLA	C3C-C4C-NC	3.74	114.00	110.21
22	N	613	CLA	C3C-C4C-NC	3.74	114.00	110.21
22	b	614	CLA	C3C-C4C-NC	3.75	114.01	110.21
22	B	604	CLA	CAC-C3C-C4C	3.75	130.12	124.83
22	c	503	CLA	O2D-CGD-CBD	3.75	118.00	111.30
23	A	404	PHO	C3C-C4C-NC	3.75	116.32	110.19
22	C	509	CLA	C3C-C4C-NC	3.75	114.01	110.21
22	4	303	CLA	C3C-C4C-NC	3.75	114.01	110.21
22	8	303	CLA	C3C-C4C-NC	3.75	114.01	110.21
22	B	606	CLA	C3C-C4C-NC	3.76	114.02	110.21
22	D	404	CLA	C3C-C4C-NC	3.77	114.03	110.21
22	B	607	CLA	O2D-CGD-CBD	3.77	118.03	111.30
22	g	613	CLA	C3C-C4C-NC	3.77	114.03	110.21
22	G	613	CLA	C3C-C4C-NC	3.77	114.03	110.21
22	b	607	CLA	C3C-C4C-NC	3.77	114.03	110.21
22	R	308	CLA	O2D-CGD-CBD	3.77	118.04	111.30
22	r	308	CLA	O2D-CGD-CBD	3.77	118.04	111.30
22	Y	602	CLA	C3C-C4C-NC	3.77	114.03	110.21
22	y	602	CLA	C3C-C4C-NC	3.77	114.03	110.21
22	B	603	CLA	O2D-CGD-CBD	3.78	118.05	111.30
22	c	507	CLA	CAC-C3C-C4C	3.78	130.16	124.83
22	r	307	CLA	C3C-C4C-NC	3.78	114.04	110.21
22	R	307	CLA	C3C-C4C-NC	3.78	114.04	110.21
22	S	314	CLA	C3C-C4C-NC	3.79	114.05	110.21
22	s	314	CLA	C3C-C4C-NC	3.79	114.05	110.21
22	c	508	CLA	C3C-C4C-NC	3.79	114.05	110.21
22	b	612	CLA	CMB-C2B-C3B	3.79	131.93	124.89
22	6	611	CLA	C3C-C4C-NC	3.79	114.05	110.21
22	2	611	CLA	C3C-C4C-NC	3.79	114.05	110.21
22	b	611	CLA	C3C-C4C-NC	3.80	114.06	110.21
23	A	404	PHO	C2C-C1C-NC	3.80	115.45	109.82
22	c	502	CLA	O2D-CGD-CBD	3.81	118.10	111.30
22	y	611	CLA	C3C-C4C-NC	3.81	114.07	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	Y	611	CLA	C3C-C4C-NC	3.81	114.07	110.21
23	D	402	PHO	CAC-C3C-C4C	3.81	129.69	125.21
22	C	503	CLA	C3C-C4C-NC	3.82	114.08	110.21
22	2	610	CLA	C3C-C4C-NC	3.82	114.08	110.21
22	6	610	CLA	C3C-C4C-NC	3.82	114.08	110.21
22	B	605	CLA	O2D-CGD-CBD	3.82	118.13	111.30
22	S	301	CLA	O2D-CGD-CBD	3.83	118.14	111.30
22	5	611	CLA	C3C-C4C-NC	3.83	114.09	110.21
22	1	611	CLA	C3C-C4C-NC	3.83	114.09	110.21
22	C	501	CLA	O2D-CGD-CBD	3.83	118.15	111.30
22	a	402	CLA	C3C-C4C-NC	3.84	114.11	110.21
22	b	612	CLA	O2D-CGD-CBD	3.85	118.17	111.30
22	R	312	CLA	C3C-C4C-NC	3.85	114.11	110.21
22	r	312	CLA	C3C-C4C-NC	3.85	114.11	110.21
22	C	503	CLA	O2D-CGD-CBD	3.87	118.22	111.30
22	C	509	CLA	O2D-CGD-CBD	3.87	118.22	111.30
22	b	609	CLA	C3C-C4C-NC	3.88	114.14	110.21
22	A	403	CLA	C3C-C4C-NC	3.88	114.14	110.21
22	C	511	CLA	CMD-C2D-C3D	3.88	132.10	124.89
23	d	402	PHO	C2C-C1C-NC	3.89	115.58	109.82
22	r	307	CLA	O2D-CGD-CBD	3.89	118.25	111.30
22	R	307	CLA	O2D-CGD-CBD	3.89	118.25	111.30
22	c	512	CLA	O2D-CGD-CBD	3.90	118.27	111.30
22	B	609	CLA	C3C-C4C-NC	3.90	114.16	110.21
22	B	610	CLA	CMD-C2D-C3D	3.90	132.14	124.89
22	7	313	CLA	C3C-C4C-NC	3.90	114.17	110.21
22	3	313	CLA	C3C-C4C-NC	3.90	114.17	110.21
22	b	607	CLA	O2D-CGD-CBD	3.91	118.29	111.30
22	7	303	CLA	C3C-C4C-NC	3.91	114.17	110.21
22	3	303	CLA	C3C-C4C-NC	3.91	114.17	110.21
22	c	510	CLA	O2D-CGD-CBD	3.91	118.29	111.30
22	y	613	CLA	C3C-C4C-NC	3.92	114.18	110.21
22	Y	613	CLA	C3C-C4C-NC	3.92	114.18	110.21
22	8	310	CLA	O2D-CGD-CBD	3.92	118.31	111.30
22	4	310	CLA	O2D-CGD-CBD	3.92	118.31	111.30
22	C	507	CLA	O2D-CGD-CBD	3.92	118.31	111.30
22	C	504	CLA	O2D-CGD-CBD	3.93	118.32	111.30
22	2	602	CLA	C3C-C4C-NC	3.93	114.19	110.21
22	6	602	CLA	C3C-C4C-NC	3.93	114.19	110.21
22	b	614	CLA	O2D-CGD-CBD	3.94	118.34	111.30
22	B	608	CLA	C3C-C4C-NC	3.94	114.20	110.21
23	a	404	PHO	C2C-C1C-NC	3.94	115.66	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	401	CLA	C3C-C4C-NC	3.95	114.21	110.21
22	B	607	CLA	C3C-C4C-NC	3.95	114.21	110.21
22	c	510	CLA	C3C-C4C-NC	3.96	114.22	110.21
22	B	610	CLA	C3C-C4C-NC	3.96	114.23	110.21
22	D	401	CLA	C3C-C4C-NC	3.98	114.25	110.21
22	n	603	CLA	O2D-CGD-CBD	3.98	118.42	111.30
22	N	603	CLA	O2D-CGD-CBD	3.98	118.42	111.30
22	c	506	CLA	O2D-CGD-CBD	3.99	118.42	111.30
22	G	603	CLA	O2D-CGD-CBD	3.99	118.43	111.30
22	g	603	CLA	O2D-CGD-CBD	3.99	118.43	111.30
22	g	612	CLA	O2D-CGD-CBD	3.99	118.43	111.30
22	G	612	CLA	O2D-CGD-CBD	3.99	118.43	111.30
22	n	613	CLA	O2D-CGD-CBD	3.99	118.43	111.30
22	N	613	CLA	O2D-CGD-CBD	3.99	118.43	111.30
22	3	312	CLA	C3C-C4C-NC	4.00	114.26	110.21
22	7	312	CLA	C3C-C4C-NC	4.00	114.26	110.21
22	c	509	CLA	O2D-CGD-CBD	4.00	118.45	111.30
22	c	507	CLA	C3C-C4C-NC	4.01	114.27	110.21
22	1	603	CLA	O2D-CGD-CBD	4.01	118.47	111.30
22	5	603	CLA	O2D-CGD-CBD	4.01	118.47	111.30
22	D	403	CLA	O2D-CGD-CBD	4.02	118.48	111.30
22	C	506	CLA	C3C-C4C-NC	4.02	114.28	110.21
22	4	309	CLA	C3C-C4C-NC	4.02	114.28	110.21
22	8	309	CLA	C3C-C4C-NC	4.02	114.28	110.21
22	2	612	CLA	O2D-CGD-CBD	4.03	118.49	111.30
22	6	612	CLA	O2D-CGD-CBD	4.03	118.49	111.30
22	G	604	CLA	O2D-CGD-CBD	4.03	118.49	111.30
22	g	604	CLA	O2D-CGD-CBD	4.03	118.49	111.30
22	b	609	CLA	O2D-CGD-CBD	4.03	118.50	111.30
22	1	602	CLA	C3C-C4C-NC	4.03	114.30	110.21
22	5	602	CLA	C3C-C4C-NC	4.03	114.30	110.21
23	D	402	PHO	C2C-C1C-NC	4.03	115.79	109.82
22	y	610	CLA	C3C-C4C-NC	4.04	114.30	110.21
22	Y	610	CLA	C3C-C4C-NC	4.04	114.30	110.21
22	n	604	CLA	O2D-CGD-CBD	4.04	118.51	111.30
22	N	604	CLA	O2D-CGD-CBD	4.04	118.51	111.30
22	b	601	CLA	C3C-C4C-NC	4.04	114.30	110.21
22	R	308	CLA	C3C-C4C-NC	4.04	114.30	110.21
22	r	308	CLA	C3C-C4C-NC	4.04	114.30	110.21
23	d	402	PHO	CAC-C3C-C4C	4.04	129.96	125.21
22	C	510	CLA	O2D-CGD-CBD	4.05	118.53	111.30
23	A	404	PHO	CAC-C3C-C2C	4.05	134.52	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	504	CLA	O2D-CGD-CBD	4.06	118.55	111.30
22	B	616	CLA	CMD-C2D-C3D	4.07	132.44	124.89
22	R	301	CLA	C3C-C4C-NC	4.07	114.34	110.21
22	r	301	CLA	C3C-C4C-NC	4.07	114.34	110.21
22	b	613	CLA	C3C-C4C-NC	4.08	114.34	110.21
22	B	604	CLA	CMC-C2C-C3C	4.08	137.39	126.09
22	A	403	CLA	CMB-C2B-C3B	4.09	132.47	124.89
22	B	606	CLA	O2D-CGD-CBD	4.10	118.62	111.30
22	4	309	CLA	O2D-CGD-CBD	4.10	118.63	111.30
22	8	309	CLA	O2D-CGD-CBD	4.10	118.63	111.30
22	g	613	CLA	O2D-CGD-CBD	4.11	118.64	111.30
22	G	613	CLA	O2D-CGD-CBD	4.11	118.64	111.30
22	S	311	CLA	C3C-C4C-NC	4.12	114.38	110.21
22	s	311	CLA	C3C-C4C-NC	4.12	114.38	110.21
22	S	311	CLA	O2D-CGD-CBD	4.12	118.66	111.30
22	s	311	CLA	O2D-CGD-CBD	4.12	118.66	111.30
22	7	313	CLA	O2D-CGD-CBD	4.13	118.67	111.30
22	3	313	CLA	O2D-CGD-CBD	4.13	118.67	111.30
22	b	601	CLA	O2D-CGD-CBD	4.13	118.67	111.30
22	b	602	CLA	CAC-C3C-C4C	4.13	130.65	124.83
22	6	609	CLA	C3C-C4C-NC	4.14	114.41	110.21
22	2	609	CLA	C3C-C4C-NC	4.14	114.41	110.21
22	1	612	CLA	O2D-CGD-CBD	4.14	118.70	111.30
22	5	612	CLA	O2D-CGD-CBD	4.14	118.70	111.30
22	2	612	CLA	C3C-C4C-NC	4.15	114.41	110.21
22	6	612	CLA	C3C-C4C-NC	4.15	114.41	110.21
22	G	602	CLA	O2D-CGD-CBD	4.15	118.72	111.30
22	g	602	CLA	O2D-CGD-CBD	4.15	118.72	111.30
22	c	506	CLA	C3C-C4C-NC	4.15	114.42	110.21
22	n	612	CLA	O2D-CGD-CBD	4.16	118.73	111.30
22	N	612	CLA	O2D-CGD-CBD	4.16	118.73	111.30
22	c	503	CLA	C3C-C4C-NC	4.16	114.42	110.21
22	C	502	CLA	CAC-C3C-C4C	4.16	130.70	124.83
22	6	611	CLA	O2D-CGD-CBD	4.17	118.74	111.30
22	2	611	CLA	O2D-CGD-CBD	4.17	118.74	111.30
22	Y	604	CLA	C3C-C4C-NC	4.17	114.44	110.21
22	y	604	CLA	C3C-C4C-NC	4.17	114.44	110.21
22	B	601	CLA	O2D-CGD-CBD	4.19	118.78	111.30
22	N	614	CLA	O2D-CGD-CBD	4.19	118.79	111.30
22	n	614	CLA	O2D-CGD-CBD	4.19	118.79	111.30
22	3	310	CLA	C3C-C4C-NC	4.20	114.47	110.21
22	7	310	CLA	C3C-C4C-NC	4.20	114.47	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	510	CLA	C3C-C4C-NC	4.20	114.47	110.21
22	1	610	CLA	C3C-C4C-NC	4.21	114.47	110.21
22	5	610	CLA	C3C-C4C-NC	4.21	114.47	110.21
22	c	509	CLA	C3C-C4C-NC	4.21	114.48	110.21
22	A	405	CLA	C3C-C4C-NC	4.21	114.48	110.21
22	b	605	CLA	O2D-CGD-CBD	4.22	118.84	111.30
23	d	402	PHO	C2D-C1D-ND	4.22	116.07	109.82
22	4	303	CLA	O2D-CGD-CBD	4.22	118.84	111.30
22	8	303	CLA	O2D-CGD-CBD	4.22	118.84	111.30
22	R	311	CLA	O2D-CGD-CBD	4.22	118.85	111.30
22	r	311	CLA	O2D-CGD-CBD	4.22	118.85	111.30
22	y	613	CLA	O2D-CGD-CBD	4.24	118.88	111.30
22	Y	613	CLA	O2D-CGD-CBD	4.24	118.88	111.30
22	y	612	CLA	O2D-CGD-CBD	4.25	118.90	111.30
22	Y	612	CLA	O2D-CGD-CBD	4.25	118.90	111.30
22	r	302	CLA	CAC-C3C-C4C	4.25	130.83	124.83
22	R	302	CLA	CAC-C3C-C4C	4.25	130.83	124.83
22	s	309	CLA	CMD-C2D-C3D	4.26	132.79	124.89
22	S	309	CLA	CMD-C2D-C3D	4.26	132.79	124.89
22	G	610	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	g	610	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	6	603	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	2	603	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	3	312	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	7	312	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	3	304	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	7	304	CLA	O2D-CGD-CBD	4.26	118.91	111.30
22	r	302	CLA	C3C-C4C-NC	4.26	114.53	110.21
22	R	302	CLA	C3C-C4C-NC	4.26	114.53	110.21
22	R	309	CLA	O2D-CGD-CBD	4.27	118.93	111.30
22	r	309	CLA	O2D-CGD-CBD	4.27	118.93	111.30
22	G	610	CLA	C3C-C4C-NC	4.28	114.55	110.21
22	g	610	CLA	C3C-C4C-NC	4.28	114.55	110.21
22	c	508	CLA	O2D-CGD-CBD	4.29	118.96	111.30
23	D	402	PHO	C2D-C1D-ND	4.29	116.17	109.82
22	S	310	CLA	O2D-CGD-CBD	4.29	118.97	111.30
22	s	310	CLA	O2D-CGD-CBD	4.29	118.97	111.30
22	6	609	CLA	O2D-CGD-CBD	4.30	118.98	111.30
22	2	609	CLA	O2D-CGD-CBD	4.30	118.98	111.30
22	s	309	CLA	O2D-CGD-CBD	4.31	119.00	111.30
22	S	309	CLA	O2D-CGD-CBD	4.31	119.00	111.30
22	b	605	CLA	CED-O2D-CGD	4.31	126.07	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	403	CLA	O2D-CGD-CBD	4.31	119.00	111.30
22	n	610	CLA	O2D-CGD-CBD	4.32	119.02	111.30
22	N	610	CLA	O2D-CGD-CBD	4.32	119.02	111.30
22	R	311	CLA	C3C-C4C-NC	4.32	114.59	110.21
22	r	311	CLA	C3C-C4C-NC	4.32	114.59	110.21
22	8	302	CLA	C3C-C4C-NC	4.33	114.59	110.21
22	4	302	CLA	C3C-C4C-NC	4.33	114.59	110.21
22	s	301	CLA	O2D-CGD-CBD	4.33	119.03	111.30
22	5	604	CLA	O2D-CGD-CBD	4.33	119.04	111.30
22	1	604	CLA	O2D-CGD-CBD	4.33	119.04	111.30
22	r	302	CLA	O2D-CGD-CBD	4.33	119.04	111.30
22	R	302	CLA	O2D-CGD-CBD	4.33	119.04	111.30
22	A	402	CLA	O2D-CGD-CBD	4.34	119.05	111.30
22	A	403	CLA	O2D-CGD-CBD	4.34	119.05	111.30
22	b	616	CLA	O2D-CGD-CBD	4.34	119.05	111.30
22	5	614	CLA	CMD-C2D-C3D	4.34	132.95	124.89
22	1	614	CLA	CMD-C2D-C3D	4.34	132.95	124.89
22	y	610	CLA	O2D-CGD-CBD	4.34	119.06	111.30
22	Y	610	CLA	O2D-CGD-CBD	4.34	119.06	111.30
22	A	403	CLA	CMD-C2D-C3D	4.35	132.96	124.89
22	2	613	CLA	O2D-CGD-CBD	4.35	119.08	111.30
22	6	613	CLA	O2D-CGD-CBD	4.35	119.08	111.30
22	c	511	CLA	O2D-CGD-CBD	4.36	119.10	111.30
22	s	309	CLA	CAC-C3C-C4C	4.36	130.98	124.83
22	S	309	CLA	CAC-C3C-C4C	4.36	130.98	124.83
22	d	403	CLA	O2D-CGD-CBD	4.36	119.10	111.30
22	c	501	CLA	CAC-C3C-C4C	4.37	130.99	124.83
22	1	613	CLA	O2D-CGD-CBD	4.38	119.12	111.30
22	5	613	CLA	O2D-CGD-CBD	4.38	119.12	111.30
22	c	511	CLA	CMD-C2D-C3D	4.38	133.03	124.89
22	d	404	CLA	O2D-CGD-CBD	4.39	119.14	111.30
22	S	314	CLA	O2D-CGD-CBD	4.39	119.15	111.30
22	s	314	CLA	O2D-CGD-CBD	4.39	119.15	111.30
22	Y	603	CLA	O2D-CGD-CBD	4.40	119.16	111.30
22	y	603	CLA	O2D-CGD-CBD	4.40	119.16	111.30
22	B	603	CLA	CMB-C2B-C3B	4.40	133.06	124.89
22	7	314	CLA	O2D-CGD-CBD	4.40	119.17	111.30
22	3	314	CLA	O2D-CGD-CBD	4.40	119.17	111.30
22	b	613	CLA	O2D-CGD-CBD	4.41	119.17	111.30
22	B	613	CLA	O2D-CGD-CBD	4.41	119.18	111.30
22	4	304	CLA	O2D-CGD-CBD	4.41	119.18	111.30
22	8	304	CLA	O2D-CGD-CBD	4.41	119.18	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402	PHO	C4A-NA-C1A	4.42	111.73	108.16
22	n	610	CLA	C3C-C4C-NC	4.42	114.69	110.21
22	N	610	CLA	C3C-C4C-NC	4.42	114.69	110.21
23	D	402	PHO	C4A-NA-C1A	4.42	111.74	108.16
22	S	301	CLA	C3C-C4C-NC	4.42	114.69	110.21
22	1	602	CLA	O2D-CGD-CBD	4.43	119.21	111.30
22	5	602	CLA	O2D-CGD-CBD	4.43	119.21	111.30
22	a	403	CLA	C3C-C4C-NC	4.43	114.69	110.21
22	B	615	CLA	C3C-C4C-NC	4.44	114.70	110.21
23	a	404	PHO	C2D-C1D-ND	4.44	116.40	109.82
22	R	312	CLA	O2D-CGD-CBD	4.46	119.26	111.30
22	r	312	CLA	O2D-CGD-CBD	4.46	119.26	111.30
22	C	507	CLA	C3C-C4C-NC	4.47	114.73	110.21
22	a	405	CLA	C3C-C4C-NC	4.47	114.74	110.21
22	5	611	CLA	O2D-CGD-CBD	4.47	119.29	111.30
22	1	611	CLA	O2D-CGD-CBD	4.47	119.29	111.30
22	C	508	CLA	O2D-CGD-CBD	4.48	119.30	111.30
22	c	512	CLA	C3C-C4C-NC	4.48	114.75	110.21
22	B	609	CLA	O2D-CGD-CBD	4.48	119.30	111.30
22	B	604	CLA	O2D-CGD-CBD	4.48	119.31	111.30
22	Y	614	CLA	O2D-CGD-CBD	4.48	119.31	111.30
22	y	614	CLA	O2D-CGD-CBD	4.48	119.31	111.30
22	1	610	CLA	O2D-CGD-CBD	4.49	119.31	111.30
22	5	610	CLA	O2D-CGD-CBD	4.49	119.31	111.30
22	7	311	CLA	O2D-CGD-CBD	4.49	119.32	111.30
22	3	311	CLA	O2D-CGD-CBD	4.49	119.32	111.30
22	6	611	CLA	CAC-C3C-C4C	4.49	131.17	124.83
22	2	611	CLA	CAC-C3C-C4C	4.49	131.17	124.83
22	2	610	CLA	O2D-CGD-CBD	4.50	119.33	111.30
22	6	610	CLA	O2D-CGD-CBD	4.50	119.33	111.30
22	2	602	CLA	O2D-CGD-CBD	4.50	119.34	111.30
22	6	602	CLA	O2D-CGD-CBD	4.50	119.34	111.30
22	b	606	CLA	CMD-C2D-C3D	4.50	133.25	124.89
22	d	401	CLA	O2D-CGD-CBD	4.52	119.37	111.30
22	N	602	CLA	O2D-CGD-CBD	4.52	119.37	111.30
22	n	602	CLA	O2D-CGD-CBD	4.52	119.37	111.30
22	3	310	CLA	O2D-CGD-CBD	4.52	119.38	111.30
22	7	310	CLA	O2D-CGD-CBD	4.52	119.38	111.30
22	Y	614	CLA	CMD-C2D-C3D	4.53	133.30	124.89
22	y	614	CLA	CMD-C2D-C3D	4.53	133.30	124.89
22	G	614	CLA	O2D-CGD-CBD	4.53	119.40	111.30
22	g	614	CLA	O2D-CGD-CBD	4.53	119.40	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	CMD-C2D-C3D	4.54	133.31	124.89
22	B	614	CLA	C3C-C4C-NC	4.54	114.81	110.21
22	b	615	CLA	CMD-C2D-C3D	4.55	133.34	124.89
22	S	310	CLA	CMD-C2D-C3D	4.55	133.34	124.89
22	s	310	CLA	CMD-C2D-C3D	4.55	133.34	124.89
22	c	503	CLA	CMD-C2D-C3D	4.56	133.35	124.89
22	C	509	CLA	CAC-C3C-C4C	4.56	131.27	124.83
22	B	601	CLA	CAC-C3C-C4C	4.57	131.28	124.83
22	n	612	CLA	CAC-C3C-C4C	4.58	131.29	124.83
22	N	612	CLA	CAC-C3C-C4C	4.58	131.29	124.83
25	3	301	CHL	CMD-C2D-C3D	4.58	125.87	114.27
25	7	301	CHL	CMD-C2D-C3D	4.58	125.87	114.27
22	c	507	CLA	CMD-C2D-C3D	4.59	133.40	124.89
22	B	612	CLA	C3C-C4C-NC	4.59	114.86	110.21
22	b	601	CLA	CAC-C3C-C4C	4.60	131.31	124.83
22	b	608	CLA	O2D-CGD-CBD	4.60	119.51	111.30
22	B	603	CLA	CMD-C2D-C3D	4.61	133.44	124.89
22	C	507	CLA	CMD-C2D-C3D	4.61	133.45	124.89
22	C	512	CLA	CMD-C2D-C3D	4.62	133.46	124.89
22	B	606	CLA	CMD-C2D-C3D	4.62	133.46	124.89
22	b	610	CLA	C3C-C4C-NC	4.62	114.89	110.21
22	d	403	CLA	CMD-C2D-C3D	4.63	133.49	124.89
22	N	602	CLA	CMD-C2D-C3D	4.63	133.49	124.89
22	n	602	CLA	CMD-C2D-C3D	4.63	133.49	124.89
22	c	501	CLA	CMD-C2D-C3D	4.63	133.49	124.89
22	b	606	CLA	O2D-CGD-CBD	4.63	119.58	111.30
22	C	501	CLA	CAC-C3C-C4C	4.64	131.37	124.83
22	C	503	CLA	CMD-C2D-C3D	4.67	133.55	124.89
22	6	609	CLA	CMD-C2D-C3D	4.67	133.57	124.89
22	2	609	CLA	CMD-C2D-C3D	4.67	133.57	124.89
22	S	311	CLA	CAC-C3C-C4C	4.68	131.43	124.83
22	s	311	CLA	CAC-C3C-C4C	4.68	131.43	124.83
22	n	603	CLA	CMD-C2D-C3D	4.68	133.58	124.89
22	N	603	CLA	CMD-C2D-C3D	4.68	133.58	124.89
22	8	310	CLA	CAC-C3C-C4C	4.69	131.44	124.83
22	4	310	CLA	CAC-C3C-C4C	4.69	131.44	124.83
22	C	501	CLA	CMD-C2D-C3D	4.70	133.62	124.89
22	b	614	CLA	CMD-C2D-C3D	4.70	133.62	124.89
22	7	303	CLA	O2D-CGD-CBD	4.71	119.71	111.30
22	3	303	CLA	O2D-CGD-CBD	4.71	119.71	111.30
22	2	604	CLA	O2D-CGD-CBD	4.73	119.75	111.30
22	6	604	CLA	O2D-CGD-CBD	4.73	119.75	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	312	CLA	O2D-CGD-CBD	4.73	119.75	111.30
22	s	312	CLA	O2D-CGD-CBD	4.73	119.75	111.30
22	1	603	CLA	CMD-C2D-C3D	4.74	133.68	124.89
22	5	603	CLA	CMD-C2D-C3D	4.74	133.68	124.89
22	C	511	CLA	O2D-CGD-CBD	4.74	119.77	111.30
22	2	602	CLA	CMD-C2D-C3D	4.76	133.72	124.89
22	6	602	CLA	CMD-C2D-C3D	4.76	133.72	124.89
23	a	404	PHO	C4A-NA-C1A	4.76	112.01	108.16
22	r	310	CLA	CMD-C2D-C3D	4.76	133.72	124.89
22	R	310	CLA	CMD-C2D-C3D	4.76	133.72	124.89
23	A	404	PHO	C4A-NA-C1A	4.76	112.01	108.16
22	r	310	CLA	O2D-CGD-CBD	4.77	119.82	111.30
22	R	310	CLA	O2D-CGD-CBD	4.77	119.82	111.30
22	c	510	CLA	CMD-C2D-C3D	4.77	133.74	124.89
22	Y	602	CLA	O2D-CGD-CBD	4.78	119.84	111.30
22	y	602	CLA	O2D-CGD-CBD	4.78	119.84	111.30
22	7	305	CLA	O2D-CGD-CBD	4.78	119.85	111.30
22	3	305	CLA	O2D-CGD-CBD	4.78	119.85	111.30
22	6	603	CLA	CMD-C2D-C3D	4.79	133.77	124.89
22	2	603	CLA	CMD-C2D-C3D	4.79	133.77	124.89
22	b	609	CLA	CMD-C2D-C3D	4.79	133.78	124.89
22	g	611	CLA	CMD-C2D-C3D	4.79	133.79	124.89
22	G	611	CLA	CMD-C2D-C3D	4.79	133.79	124.89
22	B	608	CLA	O2D-CGD-CBD	4.79	119.87	111.30
22	S	305	CLA	CMD-C2D-C3D	4.80	133.79	124.89
22	s	305	CLA	CMD-C2D-C3D	4.80	133.79	124.89
22	B	605	CLA	CMD-C2D-C3D	4.80	133.79	124.89
22	G	614	CLA	CMD-C2D-C3D	4.80	133.80	124.89
22	g	614	CLA	CMD-C2D-C3D	4.80	133.80	124.89
22	D	401	CLA	CMD-C2D-C3D	4.81	133.81	124.89
22	c	504	CLA	CMD-C2D-C3D	4.81	133.82	124.89
22	b	602	CLA	C3C-C4C-NC	4.82	115.09	110.21
22	C	507	CLA	CAC-C3C-C4C	4.82	131.62	124.83
22	7	303	CLA	CMD-C2D-C3D	4.83	133.85	124.89
22	3	303	CLA	CMD-C2D-C3D	4.83	133.85	124.89
22	C	504	CLA	CMD-C2D-C3D	4.83	133.86	124.89
22	R	309	CLA	CMD-C2D-C3D	4.84	133.87	124.89
22	r	309	CLA	CMD-C2D-C3D	4.84	133.87	124.89
22	7	314	CLA	CMD-C2D-C3D	4.84	133.87	124.89
22	3	314	CLA	CMD-C2D-C3D	4.84	133.87	124.89
22	b	616	CLA	CMD-C2D-C3D	4.84	133.88	124.89
22	b	603	CLA	O2D-CGD-CBD	4.84	119.95	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	s	313	CLA	O2D-CGD-CBD	4.85	119.96	111.30
22	S	313	CLA	O2D-CGD-CBD	4.85	119.96	111.30
22	2	613	CLA	CMD-C2D-C3D	4.85	133.88	124.89
22	6	613	CLA	CMD-C2D-C3D	4.85	133.88	124.89
22	b	615	CLA	O2D-CGD-CBD	4.86	119.98	111.30
22	g	611	CLA	O2D-CGD-CBD	4.86	119.98	111.30
22	G	611	CLA	O2D-CGD-CBD	4.86	119.98	111.30
22	B	614	CLA	CMD-C2D-C3D	4.86	133.91	124.89
22	A	402	CLA	C3C-C4C-NC	4.86	115.14	110.21
22	c	502	CLA	CAC-C3C-C4C	4.86	131.69	124.83
22	s	301	CLA	CMD-C2D-C3D	4.86	133.92	124.89
22	8	302	CLA	O2D-CGD-CBD	4.87	120.00	111.30
22	4	302	CLA	O2D-CGD-CBD	4.87	120.00	111.30
22	8	310	CLA	CMD-C2D-C3D	4.87	133.94	124.89
22	4	310	CLA	CMD-C2D-C3D	4.87	133.94	124.89
22	r	310	CLA	CAC-C3C-C4C	4.88	131.71	124.83
22	R	310	CLA	CAC-C3C-C4C	4.88	131.71	124.83
22	1	602	CLA	CMD-C2D-C3D	4.89	133.96	124.89
22	5	602	CLA	CMD-C2D-C3D	4.89	133.96	124.89
22	G	603	CLA	CMD-C2D-C3D	4.89	133.96	124.89
22	g	603	CLA	CMD-C2D-C3D	4.89	133.96	124.89
22	b	607	CLA	CMD-C2D-C3D	4.89	133.97	124.89
22	n	611	CLA	CMD-C2D-C3D	4.91	134.00	124.89
22	N	611	CLA	CMD-C2D-C3D	4.91	134.00	124.89
22	b	615	CLA	CAC-C3C-C4C	4.91	131.76	124.83
22	4	309	CLA	CMD-C2D-C3D	4.92	134.03	124.89
22	8	309	CLA	CMD-C2D-C3D	4.92	134.03	124.89
22	R	301	CLA	CMD-C2D-C3D	4.92	134.03	124.89
22	r	301	CLA	CMD-C2D-C3D	4.92	134.03	124.89
22	2	604	CLA	CMD-C2D-C3D	4.93	134.04	124.89
22	6	604	CLA	CMD-C2D-C3D	4.93	134.04	124.89
22	y	611	CLA	O2D-CGD-CBD	4.94	120.12	111.30
22	Y	611	CLA	O2D-CGD-CBD	4.94	120.12	111.30
22	d	404	CLA	CMD-C2D-C3D	4.94	134.06	124.89
22	c	512	CLA	CAC-C3C-C4C	4.94	131.80	124.83
22	D	404	CLA	O2D-CGD-CBD	4.95	120.14	111.30
22	g	612	CLA	CAC-C3C-C4C	4.95	131.81	124.83
22	G	612	CLA	CAC-C3C-C4C	4.95	131.81	124.83
22	B	608	CLA	CMD-C2D-C3D	4.95	134.08	124.89
22	n	611	CLA	O2D-CGD-CBD	4.96	120.16	111.30
22	N	611	CLA	O2D-CGD-CBD	4.96	120.16	111.30
22	N	614	CLA	CMD-C2D-C3D	4.96	134.09	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	n	614	CLA	CMD-C2D-C3D	4.96	134.09	124.89
22	3	310	CLA	CMD-C2D-C3D	4.96	134.09	124.89
22	7	310	CLA	CMD-C2D-C3D	4.96	134.09	124.89
22	B	607	CLA	CMD-C2D-C3D	4.96	134.10	124.89
22	7	311	CLA	CMD-C2D-C3D	4.96	134.10	124.89
22	3	311	CLA	CMD-C2D-C3D	4.96	134.10	124.89
22	R	303	CLA	CAC-C3C-C4C	4.97	131.85	124.83
22	r	303	CLA	CAC-C3C-C4C	4.97	131.85	124.83
22	C	510	CLA	CMD-C2D-C3D	4.98	134.13	124.89
22	3	304	CLA	CMD-C2D-C3D	4.98	134.13	124.89
22	7	304	CLA	CMD-C2D-C3D	4.98	134.13	124.89
22	C	505	CLA	O2D-CGD-CBD	4.98	120.20	111.30
22	y	612	CLA	CAC-C3C-C4C	4.99	131.86	124.83
22	Y	612	CLA	CAC-C3C-C4C	4.99	131.86	124.83
22	y	613	CLA	CAC-C3C-C4C	4.99	131.86	124.83
22	Y	613	CLA	CAC-C3C-C4C	4.99	131.86	124.83
25	4	301	CHL	CMD-C2D-C3D	4.99	126.89	114.27
25	8	301	CHL	CMD-C2D-C3D	4.99	126.89	114.27
22	S	304	CLA	CMD-C2D-C3D	4.99	134.15	124.89
22	s	304	CLA	CMD-C2D-C3D	4.99	134.15	124.89
22	s	303	CLA	O2D-CGD-CBD	4.99	120.22	111.30
22	S	303	CLA	O2D-CGD-CBD	4.99	120.22	111.30
22	c	512	CLA	CMD-C2D-C3D	4.99	134.16	124.89
22	R	303	CLA	CMD-C2D-C3D	4.99	134.16	124.89
22	r	303	CLA	CMD-C2D-C3D	4.99	134.16	124.89
22	C	508	CLA	CMD-C2D-C3D	5.00	134.16	124.89
22	7	305	CLA	CMD-C2D-C3D	5.00	134.17	124.89
22	3	305	CLA	CMD-C2D-C3D	5.00	134.17	124.89
22	g	612	CLA	CMD-C2D-C3D	5.01	134.19	124.89
22	G	612	CLA	CMD-C2D-C3D	5.01	134.19	124.89
22	S	312	CLA	CMD-C2D-C3D	5.01	134.19	124.89
22	s	312	CLA	CMD-C2D-C3D	5.01	134.19	124.89
22	S	312	CLA	CAC-C3C-C4C	5.01	131.90	124.83
22	s	312	CLA	CAC-C3C-C4C	5.01	131.90	124.83
22	A	405	CLA	CMD-C2D-C3D	5.02	134.21	124.89
22	a	405	CLA	CMD-C2D-C3D	5.03	134.22	124.89
22	Y	602	CLA	CAC-C3C-C4C	5.03	131.92	124.83
22	y	602	CLA	CAC-C3C-C4C	5.03	131.92	124.83
22	c	505	CLA	O2D-CGD-CBD	5.03	120.29	111.30
22	2	610	CLA	CMD-C2D-C3D	5.03	134.23	124.89
22	6	610	CLA	CMD-C2D-C3D	5.03	134.23	124.89
22	g	613	CLA	CAC-C3C-C4C	5.04	131.94	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	613	CLA	CAC-C3C-C4C	5.04	131.94	124.83
22	1	613	CLA	CMD-C2D-C3D	5.05	134.26	124.89
22	5	613	CLA	CMD-C2D-C3D	5.05	134.26	124.89
22	a	403	CLA	CAC-C3C-C4C	5.05	131.95	124.83
22	D	404	CLA	CMD-C2D-C3D	5.05	134.26	124.89
22	n	612	CLA	CMD-C2D-C3D	5.05	134.26	124.89
22	N	612	CLA	CMD-C2D-C3D	5.05	134.26	124.89
22	S	301	CLA	CMD-C2D-C3D	5.05	134.27	124.89
22	R	312	CLA	CMD-C2D-C3D	5.05	134.27	124.89
22	r	312	CLA	CMD-C2D-C3D	5.05	134.27	124.89
22	B	613	CLA	CMD-C2D-C3D	5.07	134.30	124.89
22	B	611	CLA	O2D-CGD-CBD	5.07	120.37	111.30
22	B	604	CLA	CMD-C2D-C3D	5.08	134.31	124.89
22	G	602	CLA	CMD-C2D-C3D	5.08	134.32	124.89
22	g	602	CLA	CMD-C2D-C3D	5.08	134.32	124.89
22	c	510	CLA	CAC-C3C-C4C	5.09	132.01	124.83
22	7	313	CLA	CMD-C2D-C3D	5.09	134.34	124.89
22	3	313	CLA	CMD-C2D-C3D	5.09	134.34	124.89
22	G	610	CLA	CMD-C2D-C3D	5.09	134.34	124.89
22	g	610	CLA	CMD-C2D-C3D	5.09	134.34	124.89
22	b	610	CLA	CAC-C3C-C4C	5.10	132.02	124.83
22	B	602	CLA	CAC-C3C-C4C	5.10	132.02	124.83
22	4	304	CLA	CMD-C2D-C3D	5.10	134.36	124.89
22	8	304	CLA	CMD-C2D-C3D	5.10	134.36	124.89
22	a	402	CLA	CMD-C2D-C3D	5.10	134.36	124.89
22	S	305	CLA	CAC-C3C-C4C	5.11	132.03	124.83
22	s	305	CLA	CAC-C3C-C4C	5.11	132.03	124.83
22	S	310	CLA	CAC-C3C-C4C	5.11	132.03	124.83
22	s	310	CLA	CAC-C3C-C4C	5.11	132.03	124.83
22	b	610	CLA	CMD-C2D-C3D	5.11	134.38	124.89
22	1	612	CLA	CAC-C3C-C4C	5.11	132.04	124.83
22	5	612	CLA	CAC-C3C-C4C	5.11	132.04	124.83
22	c	502	CLA	CMD-C2D-C3D	5.11	134.38	124.89
22	6	611	CLA	CMD-C2D-C3D	5.11	134.38	124.89
22	2	611	CLA	CMD-C2D-C3D	5.11	134.38	124.89
22	g	613	CLA	CMD-C2D-C3D	5.12	134.39	124.89
22	G	613	CLA	CMD-C2D-C3D	5.12	134.39	124.89
22	R	301	CLA	O2D-CGD-CBD	5.12	120.45	111.30
22	r	301	CLA	O2D-CGD-CBD	5.12	120.45	111.30
22	c	511	CLA	CAC-C3C-C4C	5.12	132.05	124.83
22	3	312	CLA	CMD-C2D-C3D	5.12	134.39	124.89
22	y	610	CLA	CMD-C2D-C3D	5.12	134.39	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	7	312	CLA	CMD-C2D-C3D	5.12	134.39	124.89
22	Y	610	CLA	CMD-C2D-C3D	5.12	134.39	124.89
22	N	614	CLA	CAC-C3C-C4C	5.12	132.05	124.83
22	n	614	CLA	CAC-C3C-C4C	5.12	132.05	124.83
22	a	402	CLA	CAC-C3C-C4C	5.13	132.06	124.83
22	n	611	CLA	CAC-C3C-C4C	5.13	132.07	124.83
22	N	611	CLA	CAC-C3C-C4C	5.13	132.07	124.83
22	S	314	CLA	CMD-C2D-C3D	5.13	134.42	124.89
22	s	314	CLA	CMD-C2D-C3D	5.13	134.42	124.89
22	G	602	CLA	CAC-C3C-C4C	5.14	132.08	124.83
22	3	312	CLA	CAC-C3C-C4C	5.14	132.08	124.83
22	g	602	CLA	CAC-C3C-C4C	5.14	132.08	124.83
22	7	312	CLA	CAC-C3C-C4C	5.14	132.08	124.83
22	b	601	CLA	CMD-C2D-C3D	5.14	134.43	124.89
22	B	615	CLA	CMD-C2D-C3D	5.14	134.43	124.89
22	A	403	CLA	CAC-C3C-C4C	5.14	132.08	124.83
25	S	308	CHL	CBA-CAA-C2A	5.14	123.07	115.66
25	s	308	CHL	CBA-CAA-C2A	5.14	123.07	115.66
22	b	613	CLA	CMD-C2D-C3D	5.14	134.44	124.89
22	C	509	CLA	CMD-C2D-C3D	5.14	134.44	124.89
22	B	602	CLA	CMD-C2D-C3D	5.15	134.44	124.89
22	y	612	CLA	CMD-C2D-C3D	5.15	134.44	124.89
22	Y	612	CLA	CMD-C2D-C3D	5.15	134.44	124.89
22	1	610	CLA	CMD-C2D-C3D	5.15	134.44	124.89
22	5	610	CLA	CMD-C2D-C3D	5.15	134.44	124.89
22	B	608	CLA	CAC-C3C-C4C	5.15	132.09	124.83
22	Y	603	CLA	CAC-C3C-C4C	5.15	132.10	124.83
22	y	603	CLA	CAC-C3C-C4C	5.15	132.10	124.83
22	b	609	CLA	CAC-C3C-C4C	5.15	132.10	124.83
22	b	612	CLA	CAC-C3C-C4C	5.16	132.10	124.83
22	s	303	CLA	CMD-C2D-C3D	5.16	134.47	124.89
22	S	303	CLA	CMD-C2D-C3D	5.16	134.47	124.89
22	G	614	CLA	CAC-C3C-C4C	5.16	132.11	124.83
22	g	614	CLA	CAC-C3C-C4C	5.16	132.11	124.83
22	2	612	CLA	CMD-C2D-C3D	5.16	134.47	124.89
22	6	612	CLA	CMD-C2D-C3D	5.16	134.47	124.89
22	2	610	CLA	CAC-C3C-C4C	5.17	132.13	124.83
22	6	610	CLA	CAC-C3C-C4C	5.17	132.13	124.83
22	g	611	CLA	CAC-C3C-C4C	5.18	132.13	124.83
22	B	607	CLA	CAC-C3C-C4C	5.18	132.13	124.83
22	G	611	CLA	CAC-C3C-C4C	5.18	132.13	124.83
22	c	509	CLA	CMD-C2D-C3D	5.18	134.51	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	CAC-C3C-C4C	5.19	132.15	124.83
22	b	605	CLA	CMD-C2D-C3D	5.19	134.52	124.89
22	b	608	CLA	CMD-C2D-C3D	5.19	134.52	124.89
22	N	602	CLA	CAC-C3C-C4C	5.19	132.15	124.83
22	n	602	CLA	CAC-C3C-C4C	5.19	132.15	124.83
22	c	505	CLA	CMD-C2D-C3D	5.19	134.53	124.89
22	4	303	CLA	CMD-C2D-C3D	5.20	134.53	124.89
22	8	303	CLA	CMD-C2D-C3D	5.20	134.53	124.89
25	8	305	CHL	CMD-C2D-C3D	5.20	127.43	114.27
25	4	305	CHL	CMD-C2D-C3D	5.20	127.43	114.27
22	D	401	CLA	CAC-C3C-C4C	5.20	132.16	124.83
22	B	610	CLA	CAC-C3C-C4C	5.20	132.17	124.83
22	d	401	CLA	CMD-C2D-C3D	5.21	134.56	124.89
22	R	301	CLA	CAC-C3C-C4C	5.21	132.18	124.83
22	r	301	CLA	CAC-C3C-C4C	5.21	132.18	124.83
22	n	610	CLA	CMD-C2D-C3D	5.21	134.56	124.89
22	N	610	CLA	CMD-C2D-C3D	5.21	134.56	124.89
22	d	404	CLA	CAC-C3C-C4C	5.22	132.19	124.83
22	b	602	CLA	CMD-C2D-C3D	5.22	134.59	124.89
22	b	612	CLA	CMD-C2D-C3D	5.23	134.60	124.89
22	y	611	CLA	CAC-C3C-C4C	5.24	132.22	124.83
22	Y	611	CLA	CAC-C3C-C4C	5.24	132.22	124.83
22	G	604	CLA	CMD-C2D-C3D	5.24	134.61	124.89
22	g	604	CLA	CMD-C2D-C3D	5.24	134.61	124.89
22	S	311	CLA	CMD-C2D-C3D	5.24	134.61	124.89
22	s	311	CLA	CMD-C2D-C3D	5.24	134.61	124.89
22	C	502	CLA	CMD-C2D-C3D	5.24	134.62	124.89
22	B	602	CLA	C3C-C4C-NC	5.25	115.53	110.21
22	y	613	CLA	CMD-C2D-C3D	5.25	134.63	124.89
22	Y	613	CLA	CMD-C2D-C3D	5.25	134.63	124.89
22	n	613	CLA	CMD-C2D-C3D	5.25	134.63	124.89
22	N	613	CLA	CMD-C2D-C3D	5.25	134.63	124.89
22	2	613	CLA	CAC-C3C-C4C	5.25	132.24	124.83
22	6	613	CLA	CAC-C3C-C4C	5.25	132.24	124.83
22	7	314	CLA	CAC-C3C-C4C	5.26	132.24	124.83
22	3	314	CLA	CAC-C3C-C4C	5.26	132.24	124.83
22	B	601	CLA	CMD-C2D-C3D	5.26	134.65	124.89
23	A	404	PHO	CMD-C2D-C1D	5.26	133.24	125.04
22	1	613	CLA	CAC-C3C-C4C	5.26	132.25	124.83
22	5	613	CLA	CAC-C3C-C4C	5.26	132.25	124.83
25	N	608	CHL	CBA-CAA-C2A	5.26	123.24	115.66
25	n	608	CHL	CBA-CAA-C2A	5.26	123.24	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	309	CLA	CAC-C3C-C4C	5.27	132.26	124.83
22	r	309	CLA	CAC-C3C-C4C	5.27	132.26	124.83
22	7	303	CLA	CAC-C3C-C4C	5.28	132.28	124.83
22	3	303	CLA	CAC-C3C-C4C	5.28	132.28	124.83
22	a	403	CLA	CMD-C2D-C3D	5.28	134.69	124.89
22	b	611	CLA	CMD-C2D-C3D	5.28	134.69	124.89
22	n	604	CLA	CMD-C2D-C3D	5.28	134.69	124.89
22	N	604	CLA	CMD-C2D-C3D	5.28	134.69	124.89
22	d	401	CLA	CAC-C3C-C4C	5.28	132.28	124.83
22	C	510	CLA	CAC-C3C-C4C	5.30	132.30	124.83
22	R	312	CLA	CAC-C3C-C4C	5.30	132.30	124.83
22	r	312	CLA	CAC-C3C-C4C	5.30	132.30	124.83
22	5	611	CLA	CMD-C2D-C3D	5.30	134.73	124.89
22	1	611	CLA	CMD-C2D-C3D	5.30	134.73	124.89
22	1	612	CLA	CMD-C2D-C3D	5.31	134.74	124.89
22	5	612	CLA	CMD-C2D-C3D	5.31	134.74	124.89
22	B	615	CLA	O2D-CGD-CBD	5.31	120.78	111.30
22	A	402	CLA	CMD-C2D-C3D	5.31	134.74	124.89
22	Y	603	CLA	CMD-C2D-C3D	5.31	134.75	124.89
22	y	603	CLA	CMD-C2D-C3D	5.31	134.75	124.89
22	2	612	CLA	CAC-C3C-C4C	5.31	132.32	124.83
22	6	612	CLA	CAC-C3C-C4C	5.31	132.32	124.83
22	s	303	CLA	CAC-C3C-C4C	5.32	132.34	124.83
22	S	303	CLA	CAC-C3C-C4C	5.32	132.34	124.83
22	b	613	CLA	CAC-C3C-C4C	5.33	132.34	124.83
22	4	303	CLA	CAC-C3C-C4C	5.33	132.34	124.83
22	8	303	CLA	CAC-C3C-C4C	5.33	132.34	124.83
22	R	308	CLA	CAC-C3C-C4C	5.33	132.35	124.83
22	r	308	CLA	CAC-C3C-C4C	5.33	132.35	124.83
22	D	403	CLA	CMD-C2D-C3D	5.33	134.78	124.89
22	C	511	CLA	CAC-C3C-C4C	5.33	132.35	124.83
22	7	311	CLA	CAC-C3C-C4C	5.35	132.37	124.83
22	3	311	CLA	CAC-C3C-C4C	5.35	132.37	124.83
22	7	313	CLA	CAC-C3C-C4C	5.35	132.38	124.83
22	3	313	CLA	CAC-C3C-C4C	5.35	132.38	124.83
22	B	614	CLA	CAC-C3C-C4C	5.35	132.38	124.83
22	Y	614	CLA	CAC-C3C-C4C	5.36	132.38	124.83
22	y	614	CLA	CAC-C3C-C4C	5.36	132.38	124.83
22	5	604	CLA	CAC-C3C-C4C	5.36	132.39	124.83
22	1	604	CLA	CAC-C3C-C4C	5.36	132.39	124.83
22	n	613	CLA	CAC-C3C-C4C	5.37	132.40	124.83
22	N	613	CLA	CAC-C3C-C4C	5.37	132.40	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	CAC-C3C-C4C	5.37	132.40	124.83
22	D	404	CLA	CAC-C3C-C4C	5.37	132.40	124.83
22	5	611	CLA	CAC-C3C-C4C	5.39	132.43	124.83
22	1	611	CLA	CAC-C3C-C4C	5.39	132.43	124.83
22	1	610	CLA	CAC-C3C-C4C	5.39	132.43	124.83
22	5	610	CLA	CAC-C3C-C4C	5.39	132.43	124.83
22	2	602	CLA	CAC-C3C-C4C	5.39	132.44	124.83
22	6	602	CLA	CAC-C3C-C4C	5.39	132.44	124.83
22	y	610	CLA	CAC-C3C-C4C	5.40	132.44	124.83
22	Y	610	CLA	CAC-C3C-C4C	5.40	132.44	124.83
22	R	308	CLA	CMD-C2D-C3D	5.40	134.91	124.89
22	r	308	CLA	CMD-C2D-C3D	5.40	134.91	124.89
25	g	608	CHL	CMD-C2D-C3D	5.41	127.95	114.27
25	G	608	CHL	CMD-C2D-C3D	5.41	127.95	114.27
22	6	609	CLA	CAC-C3C-C4C	5.41	132.46	124.83
22	n	604	CLA	CAC-C3C-C4C	5.41	132.46	124.83
22	N	604	CLA	CAC-C3C-C4C	5.41	132.46	124.83
22	2	609	CLA	CAC-C3C-C4C	5.41	132.46	124.83
22	B	611	CLA	CMD-C2D-C3D	5.41	134.93	124.89
22	3	310	CLA	CAC-C3C-C4C	5.41	132.47	124.83
22	7	310	CLA	CAC-C3C-C4C	5.41	132.47	124.83
22	5	604	CLA	CMD-C2D-C3D	5.42	134.94	124.89
22	1	604	CLA	CMD-C2D-C3D	5.42	134.94	124.89
22	C	503	CLA	CAC-C3C-C4C	5.42	132.47	124.83
22	4	304	CLA	CAC-C3C-C4C	5.42	132.47	124.83
22	8	304	CLA	CAC-C3C-C4C	5.42	132.47	124.83
22	5	614	CLA	O2D-CGD-CBD	5.42	120.98	111.30
22	1	614	CLA	O2D-CGD-CBD	5.42	120.98	111.30
22	C	505	CLA	CMD-C2D-C3D	5.42	134.94	124.89
22	Y	604	CLA	CAC-C3C-C4C	5.44	132.50	124.83
22	y	604	CLA	CAC-C3C-C4C	5.44	132.50	124.83
22	b	604	CLA	CMD-C2D-C3D	5.44	134.99	124.89
22	6	603	CLA	CAC-C3C-C4C	5.45	132.51	124.83
22	2	603	CLA	CAC-C3C-C4C	5.45	132.51	124.83
22	1	602	CLA	CAC-C3C-C4C	5.46	132.53	124.83
22	5	602	CLA	CAC-C3C-C4C	5.46	132.53	124.83
22	b	608	CLA	CAC-C3C-C4C	5.46	132.53	124.83
22	B	613	CLA	CAC-C3C-C4C	5.46	132.53	124.83
22	7	305	CLA	CAC-C3C-C4C	5.46	132.53	124.83
22	3	305	CLA	CAC-C3C-C4C	5.46	132.53	124.83
22	c	506	CLA	CMD-C2D-C3D	5.47	135.03	124.89
23	A	404	PHO	C2D-C1D-ND	5.48	117.93	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	G	610	CLA	CAC-C3C-C4C	5.49	132.57	124.83
22	g	610	CLA	CAC-C3C-C4C	5.49	132.57	124.83
22	S	314	CLA	CAC-C3C-C4C	5.49	132.57	124.83
22	s	314	CLA	CAC-C3C-C4C	5.49	132.57	124.83
22	G	604	CLA	CAC-C3C-C4C	5.49	132.57	124.83
22	g	604	CLA	CAC-C3C-C4C	5.49	132.57	124.83
22	b	605	CLA	CAC-C3C-C4C	5.52	132.61	124.83
22	8	302	CLA	CAC-C3C-C4C	5.52	132.62	124.83
22	4	302	CLA	CAC-C3C-C4C	5.52	132.62	124.83
22	R	311	CLA	CMD-C2D-C3D	5.52	135.14	124.89
22	r	311	CLA	CMD-C2D-C3D	5.52	135.14	124.89
22	S	301	CLA	CAC-C3C-C4C	5.53	132.62	124.83
22	Y	602	CLA	CMD-C2D-C3D	5.53	135.15	124.89
22	y	602	CLA	CMD-C2D-C3D	5.53	135.15	124.89
22	2	604	CLA	CAC-C3C-C4C	5.54	132.65	124.83
22	6	604	CLA	CAC-C3C-C4C	5.54	132.65	124.83
22	1	603	CLA	CAC-C3C-C4C	5.55	132.66	124.83
22	5	603	CLA	CAC-C3C-C4C	5.55	132.66	124.83
25	1	609	CHL	CMD-C2D-C3D	5.55	128.32	114.27
25	5	609	CHL	CMD-C2D-C3D	5.55	128.32	114.27
25	1	608	CHL	CMD-C2D-C3D	5.56	128.34	114.27
25	5	608	CHL	CMD-C2D-C3D	5.56	128.34	114.27
22	B	612	CLA	CAC-C3C-C4C	5.57	132.68	124.83
22	s	301	CLA	CAC-C3C-C4C	5.58	132.69	124.83
22	s	313	CLA	CMD-C2D-C3D	5.58	135.24	124.89
22	S	313	CLA	CMD-C2D-C3D	5.58	135.24	124.89
25	y	606	CHL	CMD-C2D-C3D	5.58	128.40	114.27
25	Y	606	CHL	CMD-C2D-C3D	5.58	128.40	114.27
22	b	603	CLA	CAC-C3C-C4C	5.58	132.71	124.83
22	b	606	CLA	CAC-C3C-C4C	5.58	132.71	124.83
22	c	504	CLA	CAC-C3C-C4C	5.59	132.71	124.83
22	b	611	CLA	O2D-CGD-CBD	5.59	121.29	111.30
22	n	610	CLA	CAC-C3C-C4C	5.59	132.72	124.83
22	N	610	CLA	CAC-C3C-C4C	5.59	132.72	124.83
22	C	506	CLA	CMD-C2D-C3D	5.60	135.28	124.89
25	1	606	CHL	CMD-C2D-C3D	5.61	128.46	114.27
25	5	606	CHL	CMD-C2D-C3D	5.61	128.46	114.27
25	g	606	CHL	CMD-C2D-C3D	5.61	128.47	114.27
25	G	606	CHL	CMD-C2D-C3D	5.61	128.47	114.27
22	R	311	CLA	CAC-C3C-C4C	5.63	132.77	124.83
22	r	311	CLA	CAC-C3C-C4C	5.63	132.77	124.83
25	6	608	CHL	CMD-C2D-C3D	5.63	128.51	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	608	CHL	CMD-C2D-C3D	5.63	128.51	114.27
22	8	302	CLA	CMD-C2D-C3D	5.64	135.36	124.89
22	4	302	CLA	CMD-C2D-C3D	5.64	135.36	124.89
25	n	606	CHL	CMD-C2D-C3D	5.65	128.56	114.27
25	N	606	CHL	CMD-C2D-C3D	5.65	128.56	114.27
22	c	503	CLA	CAC-C3C-C4C	5.65	132.80	124.83
25	y	608	CHL	CBA-CAA-C2A	5.65	123.80	115.66
25	Y	608	CHL	CBA-CAA-C2A	5.65	123.80	115.66
22	B	603	CLA	CAC-C3C-C4C	5.66	132.81	124.83
25	G	607	CHL	CMD-C2D-C3D	5.66	128.59	114.27
25	g	607	CHL	CMD-C2D-C3D	5.66	128.59	114.27
22	3	304	CLA	CAC-C3C-C4C	5.66	132.81	124.83
22	7	304	CLA	CAC-C3C-C4C	5.66	132.81	124.83
22	B	614	CLA	O2D-CGD-CBD	5.66	121.42	111.30
22	a	405	CLA	CAC-C3C-C4C	5.68	132.84	124.83
22	C	504	CLA	CAC-C3C-C4C	5.68	132.84	124.83
22	B	609	CLA	CMD-C2D-C3D	5.69	135.44	124.89
25	y	608	CHL	CMD-C2D-C3D	5.69	128.67	114.27
25	Y	608	CHL	CMD-C2D-C3D	5.69	128.67	114.27
25	g	606	CHL	CMB-C2B-C3B	5.69	126.94	113.69
25	G	606	CHL	CMB-C2B-C3B	5.69	126.94	113.69
22	c	508	CLA	CMD-C2D-C3D	5.70	135.47	124.89
22	4	309	CLA	CAC-C3C-C4C	5.70	132.87	124.83
22	8	309	CLA	CAC-C3C-C4C	5.70	132.87	124.83
22	y	611	CLA	CMD-C2D-C3D	5.72	135.50	124.89
22	Y	611	CLA	CMD-C2D-C3D	5.72	135.50	124.89
25	4	307	CHL	CMD-C2D-C3D	5.72	128.75	114.27
25	8	307	CHL	CMD-C2D-C3D	5.72	128.75	114.27
25	Y	601	CHL	CBA-CAA-C2A	5.72	123.90	115.66
25	y	601	CHL	CBA-CAA-C2A	5.72	123.90	115.66
22	r	307	CLA	CMD-C2D-C3D	5.73	135.52	124.89
22	R	307	CLA	CMD-C2D-C3D	5.73	135.52	124.89
22	A	405	CLA	CAC-C3C-C4C	5.74	132.92	124.83
25	N	608	CHL	CMD-C2D-C3D	5.75	128.81	114.27
25	n	608	CHL	CMD-C2D-C3D	5.75	128.81	114.27
25	7	309	CHL	CMD-C2D-C3D	5.75	128.82	114.27
25	3	309	CHL	CMD-C2D-C3D	5.75	128.82	114.27
22	n	603	CLA	CAC-C3C-C4C	5.76	132.95	124.83
22	N	603	CLA	CAC-C3C-C4C	5.76	132.95	124.83
22	B	609	CLA	CAC-C3C-C4C	5.77	132.96	124.83
25	R	304	CHL	CMD-C2D-C3D	5.78	128.90	114.27
25	r	304	CHL	CMD-C2D-C3D	5.78	128.90	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	609	CHL	CMD-C2D-C3D	5.79	128.91	114.27
25	g	609	CHL	CMD-C2D-C3D	5.79	128.91	114.27
25	4	306	CHL	CMD-C2D-C3D	5.79	128.92	114.27
25	8	306	CHL	CMD-C2D-C3D	5.79	128.92	114.27
22	G	603	CLA	CAC-C3C-C4C	5.79	133.00	124.83
22	S	304	CLA	CAC-C3C-C4C	5.79	133.00	124.83
22	s	304	CLA	CAC-C3C-C4C	5.79	133.00	124.83
22	g	603	CLA	CAC-C3C-C4C	5.79	133.00	124.83
22	Y	604	CLA	CMD-C2D-C3D	5.79	135.64	124.89
22	y	604	CLA	CMD-C2D-C3D	5.79	135.64	124.89
22	S	305	CLA	O2D-CGD-CBD	5.79	121.65	111.30
22	s	305	CLA	O2D-CGD-CBD	5.79	121.65	111.30
25	7	308	CHL	CMD-C2D-C3D	5.80	128.94	114.27
25	3	308	CHL	CMD-C2D-C3D	5.80	128.94	114.27
25	1	607	CHL	CMD-C2D-C3D	5.80	128.96	114.27
25	5	607	CHL	CMD-C2D-C3D	5.80	128.96	114.27
25	2	606	CHL	CMD-C2D-C3D	5.81	128.97	114.27
25	6	606	CHL	CMD-C2D-C3D	5.81	128.97	114.27
25	2	607	CHL	CMD-C2D-C3D	5.81	128.97	114.27
25	6	607	CHL	CMD-C2D-C3D	5.81	128.97	114.27
25	Y	605	CHL	CMB-C2B-C3B	5.81	127.20	113.69
25	y	605	CHL	CMB-C2B-C3B	5.81	127.20	113.69
22	b	616	CLA	CAC-C3C-C4C	5.81	133.02	124.83
22	C	506	CLA	CAC-C3C-C4C	5.81	133.03	124.83
22	B	611	CLA	CAC-C3C-C4C	5.82	133.04	124.83
25	7	307	CHL	CMD-C2D-C3D	5.82	129.01	114.27
25	3	307	CHL	CMD-C2D-C3D	5.82	129.01	114.27
25	3	302	CHL	CMD-C2D-C3D	5.84	129.06	114.27
25	7	302	CHL	CMD-C2D-C3D	5.84	129.06	114.27
25	g	605	CHL	CMD-C2D-C3D	5.85	129.08	114.27
25	G	605	CHL	CMD-C2D-C3D	5.85	129.08	114.27
25	n	606	CHL	CMB-C2B-C3B	5.87	127.33	113.69
25	N	606	CHL	CMB-C2B-C3B	5.87	127.33	113.69
25	Y	607	CHL	CMD-C2D-C3D	5.87	129.12	114.27
25	y	607	CHL	CMD-C2D-C3D	5.87	129.12	114.27
25	s	306	CHL	CMD-C2D-C3D	5.88	129.15	114.27
25	S	306	CHL	CMD-C2D-C3D	5.88	129.15	114.27
25	4	307	CHL	CBA-CAA-C2A	5.88	124.13	115.66
25	8	307	CHL	CBA-CAA-C2A	5.88	124.13	115.66
25	s	307	CHL	CMD-C2D-C3D	5.90	129.20	114.27
25	S	307	CHL	CMD-C2D-C3D	5.90	129.20	114.27
22	C	505	CLA	CAC-C3C-C4C	5.90	133.15	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	CAC-C3C-C4C	5.90	133.16	124.83
25	n	607	CHL	CMD-C2D-C3D	5.90	129.21	114.27
25	N	607	CHL	CMD-C2D-C3D	5.90	129.21	114.27
25	n	609	CHL	CMD-C2D-C3D	5.91	129.22	114.27
25	N	609	CHL	CMD-C2D-C3D	5.91	129.22	114.27
22	c	508	CLA	CAC-C3C-C4C	5.92	133.19	124.83
22	C	508	CLA	CAC-C3C-C4C	5.93	133.19	124.83
25	2	605	CHL	CMD-C2D-C3D	5.93	129.28	114.27
25	6	605	CHL	CMD-C2D-C3D	5.93	129.28	114.27
25	1	601	CHL	CMD-C2D-C3D	5.93	129.29	114.27
25	5	601	CHL	CMD-C2D-C3D	5.93	129.29	114.27
25	y	609	CHL	CMD-C2D-C3D	5.95	129.32	114.27
25	Y	609	CHL	CMD-C2D-C3D	5.95	129.32	114.27
25	6	601	CHL	CMD-C2D-C3D	5.95	129.34	114.27
25	2	601	CHL	CMD-C2D-C3D	5.95	129.34	114.27
25	3	306	CHL	CMD-C2D-C3D	5.96	129.34	114.27
25	7	306	CHL	CMD-C2D-C3D	5.96	129.34	114.27
22	b	607	CLA	CAC-C3C-C4C	5.96	133.23	124.83
25	g	601	CHL	CMD-C2D-C3D	5.96	129.37	114.27
25	G	601	CHL	CMD-C2D-C3D	5.96	129.37	114.27
22	R	303	CLA	O2D-CGD-CBD	5.99	122.00	111.30
22	r	303	CLA	O2D-CGD-CBD	5.99	122.00	111.30
22	c	505	CLA	CAC-C3C-C4C	5.99	133.28	124.83
25	N	605	CHL	CMD-C2D-C3D	6.00	129.46	114.27
25	n	605	CHL	CMD-C2D-C3D	6.00	129.46	114.27
25	S	302	CHL	CMD-C2D-C3D	6.01	129.47	114.27
25	s	302	CHL	CMD-C2D-C3D	6.01	129.47	114.27
25	8	308	CHL	CMD-C2D-C3D	6.01	129.49	114.27
25	4	308	CHL	CMD-C2D-C3D	6.01	129.49	114.27
22	A	402	CLA	CAC-C3C-C4C	6.01	133.31	124.83
25	Y	605	CHL	C1D-CHD-C4C	6.02	125.19	112.37
25	y	605	CHL	C1D-CHD-C4C	6.02	125.19	112.37
25	r	305	CHL	CMD-C2D-C3D	6.03	129.53	114.27
25	R	305	CHL	CMD-C2D-C3D	6.03	129.53	114.27
25	r	306	CHL	CMD-C2D-C3D	6.03	129.54	114.27
25	R	306	CHL	CMD-C2D-C3D	6.03	129.54	114.27
22	c	506	CLA	CAC-C3C-C4C	6.04	133.35	124.83
25	4	301	CHL	CBA-CAA-C2A	6.06	124.39	115.66
25	8	301	CHL	CBA-CAA-C2A	6.06	124.39	115.66
22	B	615	CLA	CAC-C3C-C4C	6.08	133.41	124.83
25	Y	605	CHL	CMD-C2D-C3D	6.09	129.67	114.27
25	y	605	CHL	CMD-C2D-C3D	6.09	129.67	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	605	CHL	CMD-C2D-C3D	6.09	129.68	114.27
25	5	605	CHL	CMD-C2D-C3D	6.09	129.68	114.27
22	b	604	CLA	O2D-CGD-CBD	6.09	122.18	111.30
25	Y	601	CHL	C1D-CHD-C4C	6.09	125.34	112.37
25	y	601	CHL	C1D-CHD-C4C	6.09	125.34	112.37
22	B	605	CLA	CAC-C3C-C4C	6.09	133.43	124.83
25	5	615	CHL	CMD-C2D-C3D	6.10	129.71	114.27
25	1	615	CHL	CMD-C2D-C3D	6.10	129.71	114.27
25	S	308	CHL	CMD-C2D-C3D	6.12	129.77	114.27
25	s	308	CHL	CMD-C2D-C3D	6.12	129.77	114.27
25	n	609	CHL	C1D-CHD-C4C	6.13	125.43	112.37
25	N	609	CHL	C1D-CHD-C4C	6.13	125.43	112.37
22	r	302	CLA	CMD-C2D-C3D	6.13	136.26	124.89
22	R	302	CLA	CMD-C2D-C3D	6.13	136.26	124.89
25	N	601	CHL	CMD-C2D-C3D	6.14	129.81	114.27
25	n	601	CHL	CMD-C2D-C3D	6.14	129.81	114.27
25	n	606	CHL	C4B-CHC-C1C	6.15	125.47	112.37
25	N	606	CHL	C4B-CHC-C1C	6.15	125.47	112.37
25	N	605	CHL	C1D-CHD-C4C	6.16	125.50	112.37
25	n	605	CHL	C1D-CHD-C4C	6.16	125.50	112.37
25	S	308	CHL	C1D-CHD-C4C	6.17	125.51	112.37
25	s	308	CHL	C1D-CHD-C4C	6.17	125.51	112.37
22	B	612	CLA	CMD-C2D-C3D	6.18	136.36	124.89
22	5	614	CLA	CAC-C3C-C4C	6.19	133.55	124.83
22	1	614	CLA	CAC-C3C-C4C	6.19	133.55	124.83
25	Y	601	CHL	CMD-C2D-C3D	6.19	129.95	114.27
25	y	601	CHL	CMD-C2D-C3D	6.19	129.95	114.27
25	g	608	CHL	CMB-C2B-C3B	6.21	128.15	113.69
25	G	608	CHL	CMB-C2B-C3B	6.21	128.15	113.69
22	s	313	CLA	CAC-C3C-C4C	6.23	133.62	124.83
22	S	313	CLA	CAC-C3C-C4C	6.23	133.62	124.83
25	2	606	CHL	CMB-C2B-C3B	6.24	128.21	113.69
25	6	606	CHL	CMB-C2B-C3B	6.24	128.21	113.69
25	N	601	CHL	C1D-CHD-C4C	6.24	125.67	112.37
25	n	601	CHL	C1D-CHD-C4C	6.24	125.67	112.37
25	y	609	CHL	C4B-CHC-C1C	6.26	125.72	112.37
25	Y	609	CHL	C4B-CHC-C1C	6.26	125.72	112.37
22	r	307	CLA	CAC-C3C-C4C	6.29	133.70	124.83
22	R	307	CLA	CAC-C3C-C4C	6.29	133.70	124.83
25	g	606	CHL	C4B-CHC-C1C	6.30	125.79	112.37
25	G	606	CHL	C4B-CHC-C1C	6.30	125.79	112.37
25	1	608	CHL	CBA-CAA-C2A	6.31	124.75	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	608	CHL	CBA-CAA-C2A	6.31	124.75	115.66
22	b	614	CLA	CAC-C3C-C4C	6.32	133.75	124.83
25	S	302	CHL	C1D-CHD-C4C	6.32	125.84	112.37
25	s	302	CHL	C1D-CHD-C4C	6.32	125.84	112.37
25	s	307	CHL	C1D-CHD-C4C	6.33	125.85	112.37
25	S	307	CHL	C1D-CHD-C4C	6.33	125.85	112.37
25	g	601	CHL	C1D-CHD-C4C	6.36	125.91	112.37
25	G	601	CHL	C1D-CHD-C4C	6.36	125.91	112.37
25	G	607	CHL	C1D-CHD-C4C	6.36	125.92	112.37
25	g	607	CHL	C1D-CHD-C4C	6.36	125.92	112.37
25	8	308	CHL	C1D-CHD-C4C	6.37	125.95	112.37
25	4	308	CHL	C1D-CHD-C4C	6.37	125.95	112.37
25	1	605	CHL	C1D-CHD-C4C	6.39	125.98	112.37
25	5	605	CHL	C1D-CHD-C4C	6.39	125.98	112.37
25	7	309	CHL	C1D-CHD-C4C	6.39	125.99	112.37
25	3	309	CHL	C1D-CHD-C4C	6.39	125.99	112.37
25	7	308	CHL	C1D-CHD-C4C	6.40	126.00	112.37
25	3	308	CHL	C1D-CHD-C4C	6.40	126.00	112.37
25	y	608	CHL	C1D-CHD-C4C	6.40	126.00	112.37
25	Y	608	CHL	C1D-CHD-C4C	6.40	126.00	112.37
25	3	301	CHL	C1D-CHD-C4C	6.41	126.02	112.37
25	7	301	CHL	C1D-CHD-C4C	6.41	126.02	112.37
25	R	304	CHL	C4B-CHC-C1C	6.41	126.03	112.37
25	r	304	CHL	C4B-CHC-C1C	6.41	126.03	112.37
25	G	609	CHL	C1D-CHD-C4C	6.42	126.05	112.37
25	g	609	CHL	C1D-CHD-C4C	6.42	126.05	112.37
25	6	608	CHL	C1D-CHD-C4C	6.42	126.05	112.37
25	2	608	CHL	C1D-CHD-C4C	6.42	126.05	112.37
25	3	306	CHL	C1D-CHD-C4C	6.42	126.06	112.37
25	7	306	CHL	C1D-CHD-C4C	6.42	126.06	112.37
25	r	306	CHL	C1D-CHD-C4C	6.44	126.10	112.37
25	R	306	CHL	C1D-CHD-C4C	6.44	126.10	112.37
25	r	306	CHL	CBA-CAA-C2A	6.45	124.94	115.66
25	R	306	CHL	CBA-CAA-C2A	6.45	124.94	115.66
25	y	609	CHL	C1D-CHD-C4C	6.46	126.13	112.37
25	Y	609	CHL	C1D-CHD-C4C	6.46	126.13	112.37
25	Y	607	CHL	C4B-CHC-C1C	6.46	126.13	112.37
25	y	607	CHL	C4B-CHC-C1C	6.46	126.13	112.37
25	n	607	CHL	C4B-CHC-C1C	6.46	126.14	112.37
25	N	607	CHL	C4B-CHC-C1C	6.46	126.14	112.37
25	2	605	CHL	C1D-CHD-C4C	6.46	126.14	112.37
25	6	605	CHL	C1D-CHD-C4C	6.46	126.14	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	607	CHL	C1D-CHD-C4C	6.47	126.15	112.37
25	N	607	CHL	C1D-CHD-C4C	6.47	126.15	112.37
22	B	606	CLA	CAC-C3C-C4C	6.48	133.96	124.83
25	n	609	CHL	C4B-CHC-C1C	6.48	126.18	112.37
25	g	608	CHL	C1D-CHD-C4C	6.48	126.18	112.37
25	G	608	CHL	C1D-CHD-C4C	6.48	126.18	112.37
25	N	609	CHL	C4B-CHC-C1C	6.48	126.18	112.37
25	1	601	CHL	C1D-CHD-C4C	6.48	126.18	112.37
25	5	601	CHL	C1D-CHD-C4C	6.48	126.18	112.37
25	Y	605	CHL	C4B-CHC-C1C	6.48	126.19	112.37
25	y	605	CHL	C4B-CHC-C1C	6.48	126.19	112.37
25	N	608	CHL	C1D-CHD-C4C	6.48	126.19	112.37
25	n	608	CHL	C1D-CHD-C4C	6.48	126.19	112.37
25	4	301	CHL	C1D-CHD-C4C	6.49	126.21	112.37
25	8	301	CHL	C1D-CHD-C4C	6.49	126.21	112.37
25	s	306	CHL	C4B-CHC-C1C	6.50	126.21	112.37
25	S	306	CHL	C4B-CHC-C1C	6.50	126.21	112.37
25	1	609	CHL	C1D-CHD-C4C	6.50	126.22	112.37
25	5	609	CHL	C1D-CHD-C4C	6.50	126.22	112.37
25	5	615	CHL	C1D-CHD-C4C	6.50	126.22	112.37
25	1	615	CHL	C1D-CHD-C4C	6.50	126.22	112.37
23	a	404	PHO	CMD-C2D-C1D	6.50	135.17	125.04
25	g	605	CHL	C1D-CHD-C4C	6.51	126.24	112.37
25	G	605	CHL	C1D-CHD-C4C	6.51	126.24	112.37
25	2	607	CHL	C1D-CHD-C4C	6.51	126.25	112.37
25	6	607	CHL	C1D-CHD-C4C	6.51	126.25	112.37
25	2	606	CHL	C1D-CHD-C4C	6.54	126.30	112.37
25	6	606	CHL	C1D-CHD-C4C	6.54	126.30	112.37
25	7	309	CHL	C4B-CHC-C1C	6.54	126.31	112.37
25	3	309	CHL	C4B-CHC-C1C	6.54	126.31	112.37
25	Y	607	CHL	C1D-CHD-C4C	6.55	126.33	112.37
25	y	607	CHL	C1D-CHD-C4C	6.55	126.33	112.37
25	G	609	CHL	C4B-CHC-C1C	6.55	126.33	112.37
25	g	609	CHL	C4B-CHC-C1C	6.55	126.33	112.37
25	1	607	CHL	C1D-CHD-C4C	6.56	126.35	112.37
25	5	607	CHL	C1D-CHD-C4C	6.56	126.35	112.37
25	g	608	CHL	CBA-CAA-C2A	6.56	125.11	115.66
25	G	608	CHL	CBA-CAA-C2A	6.56	125.11	115.66
25	6	608	CHL	C4B-CHC-C1C	6.56	126.36	112.37
25	2	608	CHL	C4B-CHC-C1C	6.56	126.36	112.37
25	n	606	CHL	C1D-CHD-C4C	6.57	126.38	112.37
25	N	606	CHL	C1D-CHD-C4C	6.57	126.38	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	601	CHL	CBA-CAA-C2A	6.59	125.15	115.66
25	G	601	CHL	CBA-CAA-C2A	6.59	125.15	115.66
25	8	308	CHL	CMB-C2B-C3B	6.59	129.02	113.69
25	4	308	CHL	CMB-C2B-C3B	6.59	129.02	113.69
25	N	608	CHL	CMB-C2B-C3B	6.60	129.04	113.69
25	n	608	CHL	CMB-C2B-C3B	6.60	129.04	113.69
25	r	305	CHL	C1D-CHD-C4C	6.60	126.44	112.37
25	R	305	CHL	C1D-CHD-C4C	6.60	126.44	112.37
25	2	606	CHL	C4B-CHC-C1C	6.60	126.44	112.37
25	6	606	CHL	C4B-CHC-C1C	6.60	126.44	112.37
25	s	307	CHL	C4B-CHC-C1C	6.61	126.47	112.37
25	S	307	CHL	C4B-CHC-C1C	6.61	126.47	112.37
25	1	609	CHL	C4B-CHC-C1C	6.62	126.47	112.37
25	5	609	CHL	C4B-CHC-C1C	6.62	126.47	112.37
25	s	306	CHL	CMB-C2B-C3B	6.62	129.09	113.69
25	S	306	CHL	CMB-C2B-C3B	6.62	129.09	113.69
25	4	307	CHL	C1D-CHD-C4C	6.62	126.48	112.37
25	8	307	CHL	C1D-CHD-C4C	6.62	126.48	112.37
25	7	307	CHL	C1D-CHD-C4C	6.63	126.49	112.37
25	3	307	CHL	C1D-CHD-C4C	6.63	126.49	112.37
25	1	606	CHL	C1D-CHD-C4C	6.63	126.49	112.37
25	5	606	CHL	C1D-CHD-C4C	6.63	126.49	112.37
25	8	305	CHL	C1D-CHD-C4C	6.63	126.50	112.37
25	4	305	CHL	C1D-CHD-C4C	6.63	126.50	112.37
25	N	605	CHL	C4B-CHC-C1C	6.63	126.50	112.37
25	n	605	CHL	C4B-CHC-C1C	6.63	126.50	112.37
25	r	305	CHL	C4B-CHC-C1C	6.63	126.50	112.37
25	R	305	CHL	C4B-CHC-C1C	6.63	126.50	112.37
25	1	608	CHL	C1D-CHD-C4C	6.64	126.51	112.37
25	5	608	CHL	C1D-CHD-C4C	6.64	126.51	112.37
25	3	302	CHL	C1D-CHD-C4C	6.65	126.55	112.37
25	7	302	CHL	C1D-CHD-C4C	6.65	126.55	112.37
25	1	606	CHL	C4B-CHC-C1C	6.65	126.55	112.37
25	5	606	CHL	C4B-CHC-C1C	6.65	126.55	112.37
25	1	605	CHL	C4B-CHC-C1C	6.65	126.55	112.37
25	5	605	CHL	C4B-CHC-C1C	6.65	126.55	112.37
25	1	608	CHL	CMB-C2B-C3B	6.66	129.18	113.69
25	5	608	CHL	CMB-C2B-C3B	6.66	129.18	113.69
25	6	601	CHL	C1D-CHD-C4C	6.66	126.57	112.37
25	2	601	CHL	C1D-CHD-C4C	6.66	126.57	112.37
25	4	306	CHL	C1D-CHD-C4C	6.67	126.58	112.37
25	8	306	CHL	C1D-CHD-C4C	6.67	126.58	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	606	CHL	C1D-CHD-C4C	6.67	126.58	112.37
25	Y	606	CHL	C1D-CHD-C4C	6.67	126.58	112.37
25	R	304	CHL	CMB-C2B-C3B	6.67	129.21	113.69
25	r	304	CHL	CMB-C2B-C3B	6.67	129.21	113.69
25	3	306	CHL	CMB-C2B-C3B	6.68	129.22	113.69
25	7	306	CHL	CMB-C2B-C3B	6.68	129.22	113.69
25	N	601	CHL	C4B-CHC-C1C	6.68	126.60	112.37
25	n	601	CHL	C4B-CHC-C1C	6.68	126.60	112.37
25	Y	607	CHL	CMB-C2B-C3B	6.69	129.25	113.69
25	y	607	CHL	CMB-C2B-C3B	6.69	129.25	113.69
25	7	308	CHL	CMB-C2B-C3B	6.69	129.26	113.69
25	3	308	CHL	CMB-C2B-C3B	6.69	129.26	113.69
25	2	607	CHL	CMB-C2B-C3B	6.69	129.26	113.69
25	6	607	CHL	CMB-C2B-C3B	6.69	129.26	113.69
25	8	305	CHL	C4B-CHC-C1C	6.70	126.65	112.37
25	4	305	CHL	C4B-CHC-C1C	6.70	126.65	112.37
25	r	305	CHL	CMB-C2B-C3B	6.71	129.29	113.69
25	R	305	CHL	CMB-C2B-C3B	6.71	129.29	113.69
25	8	308	CHL	CBA-CAA-C2A	6.71	125.32	115.66
25	4	308	CHL	CBA-CAA-C2A	6.71	125.32	115.66
25	y	606	CHL	C4B-CHC-C1C	6.72	126.68	112.37
25	Y	606	CHL	C4B-CHC-C1C	6.72	126.68	112.37
25	1	601	CHL	CMB-C2B-C3B	6.72	129.31	113.69
25	5	601	CHL	CMB-C2B-C3B	6.72	129.31	113.69
25	6	601	CHL	C4B-CHC-C1C	6.72	126.69	112.37
25	2	601	CHL	C4B-CHC-C1C	6.72	126.69	112.37
25	n	609	CHL	CBA-CAA-C2A	6.72	125.34	115.66
25	N	609	CHL	CBA-CAA-C2A	6.72	125.34	115.66
25	2	605	CHL	C4B-CHC-C1C	6.72	126.69	112.37
25	6	605	CHL	C4B-CHC-C1C	6.72	126.69	112.37
25	3	306	CHL	C4B-CHC-C1C	6.73	126.71	112.37
25	7	306	CHL	C4B-CHC-C1C	6.73	126.71	112.37
25	g	605	CHL	C4B-CHC-C1C	6.73	126.71	112.37
25	G	605	CHL	C4B-CHC-C1C	6.73	126.71	112.37
25	1	607	CHL	C4B-CHC-C1C	6.74	126.73	112.37
25	5	607	CHL	C4B-CHC-C1C	6.74	126.73	112.37
25	7	307	CHL	C4B-CHC-C1C	6.75	126.75	112.37
25	3	307	CHL	C4B-CHC-C1C	6.75	126.75	112.37
25	S	302	CHL	CBA-CAA-C2A	6.76	125.39	115.66
25	s	302	CHL	CBA-CAA-C2A	6.76	125.39	115.66
25	r	306	CHL	CMB-C2B-C3B	6.76	129.43	113.69
25	R	306	CHL	CMB-C2B-C3B	6.76	129.43	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	307	CHL	C4B-CHC-C1C	6.76	126.79	112.37
25	8	307	CHL	C4B-CHC-C1C	6.76	126.79	112.37
25	R	304	CHL	C1D-CHD-C4C	6.78	126.82	112.37
25	r	304	CHL	C1D-CHD-C4C	6.78	126.82	112.37
25	4	306	CHL	CMB-C2B-C3B	6.78	129.47	113.69
25	8	306	CHL	CMB-C2B-C3B	6.78	129.47	113.69
25	G	607	CHL	C4B-CHC-C1C	6.79	126.83	112.37
25	g	607	CHL	C4B-CHC-C1C	6.79	126.83	112.37
25	g	601	CHL	C4B-CHC-C1C	6.79	126.84	112.37
25	G	601	CHL	C4B-CHC-C1C	6.79	126.84	112.37
25	4	307	CHL	CMB-C2B-C3B	6.79	129.48	113.69
25	8	307	CHL	CMB-C2B-C3B	6.79	129.48	113.69
25	2	605	CHL	CMB-C2B-C3B	6.79	129.49	113.69
25	6	605	CHL	CMB-C2B-C3B	6.79	129.49	113.69
25	3	302	CHL	C4B-CHC-C1C	6.79	126.84	112.37
25	7	302	CHL	C4B-CHC-C1C	6.79	126.84	112.37
25	6	601	CHL	CMB-C2B-C3B	6.79	129.49	113.69
25	2	601	CHL	CMB-C2B-C3B	6.79	129.49	113.69
25	8	308	CHL	C4B-CHC-C1C	6.80	126.86	112.37
25	4	308	CHL	C4B-CHC-C1C	6.80	126.86	112.37
25	N	605	CHL	CMB-C2B-C3B	6.80	129.51	113.69
25	n	605	CHL	CMB-C2B-C3B	6.80	129.51	113.69
25	5	615	CHL	C4B-CHC-C1C	6.80	126.87	112.37
25	1	615	CHL	C4B-CHC-C1C	6.80	126.87	112.37
25	3	301	CHL	C4B-CHC-C1C	6.80	126.87	112.37
25	7	301	CHL	C4B-CHC-C1C	6.80	126.87	112.37
25	1	606	CHL	CMB-C2B-C3B	6.81	129.52	113.69
25	5	606	CHL	CMB-C2B-C3B	6.81	129.52	113.69
25	g	605	CHL	CMB-C2B-C3B	6.81	129.52	113.69
25	G	605	CHL	CMB-C2B-C3B	6.81	129.52	113.69
25	7	307	CHL	CMB-C2B-C3B	6.82	129.55	113.69
25	3	307	CHL	CMB-C2B-C3B	6.82	129.55	113.69
25	4	301	CHL	CMB-C2B-C3B	6.83	129.58	113.69
25	8	301	CHL	CMB-C2B-C3B	6.83	129.58	113.69
25	2	607	CHL	CBA-CAA-C2A	6.84	125.52	115.66
25	6	607	CHL	CBA-CAA-C2A	6.84	125.52	115.66
25	1	607	CHL	CMB-C2B-C3B	6.84	129.61	113.69
25	5	607	CHL	CMB-C2B-C3B	6.84	129.61	113.69
25	s	306	CHL	C1D-CHD-C4C	6.85	126.97	112.37
25	S	306	CHL	C1D-CHD-C4C	6.85	126.97	112.37
25	4	306	CHL	C4B-CHC-C1C	6.85	126.97	112.37
25	8	306	CHL	C4B-CHC-C1C	6.85	126.97	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	301	CHL	CMB-C2B-C3B	6.85	129.63	113.69
25	7	301	CHL	CMB-C2B-C3B	6.85	129.63	113.69
25	N	601	CHL	CBA-CAA-C2A	6.86	125.53	115.66
25	n	601	CHL	CBA-CAA-C2A	6.86	125.53	115.66
25	1	605	CHL	CMB-C2B-C3B	6.86	129.66	113.69
25	5	605	CHL	CMB-C2B-C3B	6.86	129.66	113.69
25	4	301	CHL	C4B-CHC-C1C	6.87	127.01	112.37
25	8	301	CHL	C4B-CHC-C1C	6.87	127.01	112.37
25	N	601	CHL	CMB-C2B-C3B	6.87	129.68	113.69
25	n	601	CHL	CMB-C2B-C3B	6.87	129.68	113.69
25	y	608	CHL	CMB-C2B-C3B	6.88	129.69	113.69
25	Y	608	CHL	CMB-C2B-C3B	6.88	129.69	113.69
25	5	615	CHL	CMB-C2B-C3B	6.88	129.70	113.69
25	1	615	CHL	CMB-C2B-C3B	6.88	129.70	113.69
25	1	601	CHL	C4B-CHC-C1C	6.88	127.04	112.37
25	5	601	CHL	C4B-CHC-C1C	6.88	127.04	112.37
25	n	607	CHL	CMB-C2B-C3B	6.89	129.71	113.69
25	N	607	CHL	CMB-C2B-C3B	6.89	129.71	113.69
25	7	309	CHL	CMB-C2B-C3B	6.92	129.78	113.69
25	3	309	CHL	CMB-C2B-C3B	6.92	129.78	113.69
25	g	606	CHL	C1D-CHD-C4C	6.92	127.12	112.37
25	G	606	CHL	C1D-CHD-C4C	6.92	127.12	112.37
23	D	402	PHO	CMD-C2D-C1D	6.93	135.84	125.04
25	y	609	CHL	CMB-C2B-C3B	6.93	129.81	113.69
25	Y	609	CHL	CMB-C2B-C3B	6.93	129.81	113.69
25	y	606	CHL	CMB-C2B-C3B	6.94	129.82	113.69
25	Y	606	CHL	CMB-C2B-C3B	6.94	129.82	113.69
25	Y	601	CHL	CMB-C2B-C3B	6.94	129.83	113.69
25	y	601	CHL	CMB-C2B-C3B	6.94	129.83	113.69
25	1	609	CHL	CMB-C2B-C3B	6.95	129.85	113.69
25	5	609	CHL	CMB-C2B-C3B	6.95	129.85	113.69
25	s	307	CHL	CMB-C2B-C3B	6.96	129.87	113.69
25	S	307	CHL	CMB-C2B-C3B	6.96	129.87	113.69
25	n	609	CHL	CMB-C2B-C3B	6.96	129.87	113.69
25	N	609	CHL	CMB-C2B-C3B	6.96	129.87	113.69
25	3	302	CHL	CMB-C2B-C3B	6.96	129.88	113.69
25	7	302	CHL	CMB-C2B-C3B	6.96	129.88	113.69
25	S	308	CHL	CMB-C2B-C3B	6.96	129.89	113.69
25	s	308	CHL	CMB-C2B-C3B	6.96	129.89	113.69
25	Y	601	CHL	C4B-CHC-C1C	6.97	127.22	112.37
25	y	601	CHL	C4B-CHC-C1C	6.97	127.22	112.37
25	G	607	CHL	CMB-C2B-C3B	6.97	129.91	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	607	CHL	CMB-C2B-C3B	6.97	129.91	113.69
25	S	302	CHL	C4B-CHC-C1C	6.97	127.23	112.37
25	s	302	CHL	C4B-CHC-C1C	6.97	127.23	112.37
23	d	402	PHO	CMD-C2D-C1D	6.98	135.92	125.04
25	G	609	CHL	CMB-C2B-C3B	6.99	129.96	113.69
25	g	609	CHL	CMB-C2B-C3B	6.99	129.96	113.69
25	S	302	CHL	CMB-C2B-C3B	7.00	129.97	113.69
25	s	302	CHL	CMB-C2B-C3B	7.00	129.97	113.69
25	7	308	CHL	C4B-CHC-C1C	7.02	127.33	112.37
25	3	308	CHL	C4B-CHC-C1C	7.02	127.33	112.37
25	7	308	CHL	CBA-CAA-C2A	7.04	125.79	115.66
25	3	308	CHL	CBA-CAA-C2A	7.04	125.79	115.66
25	r	306	CHL	C4B-CHC-C1C	7.04	127.36	112.37
25	R	306	CHL	C4B-CHC-C1C	7.04	127.36	112.37
25	1	608	CHL	C4B-CHC-C1C	7.08	127.46	112.37
25	5	608	CHL	C4B-CHC-C1C	7.08	127.46	112.37
25	g	601	CHL	CMB-C2B-C3B	7.09	130.19	113.69
25	G	601	CHL	CMB-C2B-C3B	7.09	130.19	113.69
25	y	608	CHL	C4B-CHC-C1C	7.12	127.55	112.37
25	Y	608	CHL	C4B-CHC-C1C	7.12	127.55	112.37
25	G	607	CHL	CBA-CAA-C2A	7.15	125.96	115.66
25	g	607	CHL	CBA-CAA-C2A	7.15	125.96	115.66
25	Y	607	CHL	CBA-CAA-C2A	7.17	125.98	115.66
25	y	607	CHL	CBA-CAA-C2A	7.17	125.98	115.66
22	d	403	CLA	CAC-C3C-C4C	7.18	134.95	124.83
25	2	607	CHL	C4B-CHC-C1C	7.18	127.67	112.37
25	6	607	CHL	C4B-CHC-C1C	7.18	127.67	112.37
25	n	607	CHL	CBA-CAA-C2A	7.25	126.09	115.66
25	N	607	CHL	CBA-CAA-C2A	7.25	126.09	115.66
25	5	615	CHL	CBA-CAA-C2A	7.27	126.12	115.66
25	1	615	CHL	CBA-CAA-C2A	7.27	126.12	115.66
25	S	308	CHL	C4B-CHC-C1C	7.27	127.87	112.37
25	s	308	CHL	C4B-CHC-C1C	7.27	127.87	112.37
25	1	601	CHL	CBA-CAA-C2A	7.29	126.16	115.66
25	5	601	CHL	CBA-CAA-C2A	7.29	126.16	115.66
25	3	301	CHL	CBA-CAA-C2A	7.29	126.16	115.66
25	7	301	CHL	CBA-CAA-C2A	7.29	126.16	115.66
25	N	608	CHL	C4B-CHC-C1C	7.31	127.94	112.37
25	n	608	CHL	C4B-CHC-C1C	7.31	127.94	112.37
25	6	601	CHL	CBA-CAA-C2A	7.32	126.20	115.66
25	2	601	CHL	CBA-CAA-C2A	7.32	126.20	115.66
25	8	305	CHL	CMB-C2B-C3B	7.35	130.79	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	305	CHL	CMB-C2B-C3B	7.35	130.79	113.69
22	D	403	CLA	CAC-C3C-C4C	7.36	135.21	124.83
25	g	608	CHL	C4B-CHC-C1C	7.38	128.09	112.37
25	G	608	CHL	C4B-CHC-C1C	7.38	128.09	112.37
25	6	608	CHL	CBA-CAA-C2A	7.38	126.29	115.66
25	2	608	CHL	CBA-CAA-C2A	7.38	126.29	115.66
25	G	609	CHL	CBA-CAA-C2A	7.38	126.29	115.66
25	g	609	CHL	CBA-CAA-C2A	7.38	126.29	115.66
25	4	306	CHL	CBA-CAA-C2A	7.50	126.47	115.66
25	8	306	CHL	CBA-CAA-C2A	7.50	126.47	115.66
25	1	607	CHL	CBA-CAA-C2A	7.54	126.52	115.66
25	5	607	CHL	CBA-CAA-C2A	7.54	126.52	115.66
25	g	606	CHL	CBA-CAA-C2A	7.56	126.54	115.66
25	G	606	CHL	CBA-CAA-C2A	7.56	126.54	115.66
25	6	608	CHL	CMB-C2B-C3B	7.56	131.28	113.69
25	2	608	CHL	CMB-C2B-C3B	7.56	131.28	113.69
25	1	606	CHL	CBA-CAA-C2A	7.66	126.70	115.66
25	5	606	CHL	CBA-CAA-C2A	7.66	126.70	115.66
25	s	307	CHL	CBA-CAA-C2A	7.67	126.70	115.66
25	S	307	CHL	CBA-CAA-C2A	7.67	126.70	115.66
25	3	302	CHL	CBA-CAA-C2A	7.74	126.80	115.66
25	7	302	CHL	CBA-CAA-C2A	7.74	126.80	115.66
25	7	309	CHL	CBA-CAA-C2A	7.77	126.85	115.66
25	3	309	CHL	CBA-CAA-C2A	7.77	126.85	115.66
25	1	609	CHL	CBA-CAA-C2A	7.90	127.03	115.66
25	5	609	CHL	CBA-CAA-C2A	7.90	127.03	115.66
25	7	307	CHL	CBA-CAA-C2A	7.91	127.05	115.66
25	3	307	CHL	CBA-CAA-C2A	7.91	127.05	115.66
25	y	609	CHL	CBA-CAA-C2A	8.09	127.31	115.66
25	Y	609	CHL	CBA-CAA-C2A	8.09	127.31	115.66
25	2	606	CHL	CBA-CAA-C2A	8.17	127.43	115.66
25	6	606	CHL	CBA-CAA-C2A	8.17	127.43	115.66
25	n	606	CHL	CBA-CAA-C2A	8.23	127.52	115.66
25	N	606	CHL	CBA-CAA-C2A	8.23	127.52	115.66
25	R	304	CHL	CBA-CAA-C2A	8.28	127.59	115.66
25	r	304	CHL	CBA-CAA-C2A	8.28	127.59	115.66
22	b	606	CLA	C2C-C1C-NC	8.64	116.16	110.22
25	r	305	CHL	CBA-CAA-C2A	8.81	128.35	115.66
25	R	305	CHL	CBA-CAA-C2A	8.81	128.35	115.66
25	s	306	CHL	CBA-CAA-C2A	8.85	128.41	115.66
25	S	306	CHL	CBA-CAA-C2A	8.85	128.41	115.66
25	y	606	CHL	CBA-CAA-C2A	8.99	128.61	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	606	CHL	CBA-CAA-C2A	8.99	128.61	115.66
22	S	304	CLA	C2C-C1C-NC	9.23	116.57	110.22
22	s	304	CLA	C2C-C1C-NC	9.23	116.57	110.22
22	6	609	CLA	C2C-C1C-NC	9.23	116.57	110.22
22	2	609	CLA	C2C-C1C-NC	9.23	116.57	110.22
22	B	611	CLA	C2C-C1C-NC	9.30	116.62	110.22
22	B	601	CLA	C2C-C1C-NC	9.34	116.64	110.22
22	C	502	CLA	C2C-C1C-NC	9.35	116.65	110.22
22	4	309	CLA	C2C-C1C-NC	9.41	116.70	110.22
22	8	309	CLA	C2C-C1C-NC	9.41	116.70	110.22
22	b	612	CLA	C2C-C1C-NC	9.42	116.70	110.22
22	3	310	CLA	C2C-C1C-NC	9.42	116.70	110.22
22	7	310	CLA	C2C-C1C-NC	9.42	116.70	110.22
22	R	308	CLA	C2C-C1C-NC	9.48	116.74	110.22
22	r	308	CLA	C2C-C1C-NC	9.48	116.74	110.22
22	G	610	CLA	C2C-C1C-NC	9.50	116.75	110.22
22	g	610	CLA	C2C-C1C-NC	9.50	116.75	110.22
22	n	610	CLA	C2C-C1C-NC	9.52	116.77	110.22
22	N	610	CLA	C2C-C1C-NC	9.52	116.77	110.22
22	b	615	CLA	C2C-C1C-NC	9.53	116.77	110.22
25	8	305	CHL	CBA-CAA-C2A	9.54	129.40	115.66
25	4	305	CHL	CBA-CAA-C2A	9.54	129.40	115.66
22	b	601	CLA	C2C-C1C-NC	9.65	116.86	110.22
22	B	606	CLA	C2C-C1C-NC	9.74	116.92	110.22
22	7	314	CLA	C2C-C1C-NC	9.76	116.93	110.22
22	3	314	CLA	C2C-C1C-NC	9.76	116.93	110.22
22	b	605	CLA	C2C-C1C-NC	9.80	116.96	110.22
22	c	509	CLA	C2C-C1C-NC	9.85	116.99	110.22
22	r	302	CLA	C2C-C1C-NC	9.87	117.01	110.22
22	R	302	CLA	C2C-C1C-NC	9.87	117.01	110.22
22	b	608	CLA	C2C-C1C-NC	10.02	117.11	110.22
22	B	613	CLA	C2C-C1C-NC	10.05	117.13	110.22
22	s	301	CLA	C2C-C1C-NC	10.08	117.16	110.22
22	1	610	CLA	C2C-C1C-NC	10.09	117.16	110.22
22	5	610	CLA	C2C-C1C-NC	10.09	117.16	110.22
22	A	402	CLA	C2C-C1C-NC	10.10	117.17	110.22
22	G	614	CLA	C2C-C1C-NC	10.12	117.18	110.22
22	g	614	CLA	C2C-C1C-NC	10.12	117.18	110.22
22	b	611	CLA	C2C-C1C-NC	10.13	117.19	110.22
22	6	611	CLA	C2C-C1C-NC	10.14	117.19	110.22
22	2	611	CLA	C2C-C1C-NC	10.14	117.19	110.22
22	r	310	CLA	C2C-C1C-NC	10.17	117.22	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	310	CLA	C2C-C1C-NC	10.17	117.22	110.22
22	s	313	CLA	C2C-C1C-NC	10.20	117.24	110.22
22	S	313	CLA	C2C-C1C-NC	10.20	117.24	110.22
22	s	303	CLA	C2C-C1C-NC	10.24	117.26	110.22
22	S	303	CLA	C2C-C1C-NC	10.24	117.26	110.22
22	2	613	CLA	C2C-C1C-NC	10.24	117.26	110.22
22	6	613	CLA	C2C-C1C-NC	10.24	117.26	110.22
22	R	301	CLA	C2C-C1C-NC	10.27	117.28	110.22
22	r	301	CLA	C2C-C1C-NC	10.27	117.28	110.22
22	A	403	CLA	C2C-C1C-NC	10.28	117.29	110.22
22	B	614	CLA	C2C-C1C-NC	10.34	117.33	110.22
22	N	614	CLA	C2C-C1C-NC	10.34	117.33	110.22
22	n	614	CLA	C2C-C1C-NC	10.34	117.33	110.22
22	C	503	CLA	C2C-C1C-NC	10.35	117.34	110.22
22	d	404	CLA	C2C-C1C-NC	10.35	117.34	110.22
22	1	612	CLA	C2C-C1C-NC	10.42	117.39	110.22
22	5	612	CLA	C2C-C1C-NC	10.42	117.39	110.22
22	6	603	CLA	C2C-C1C-NC	10.44	117.40	110.22
22	C	512	CLA	C2C-C1C-NC	10.44	117.40	110.22
22	2	603	CLA	C2C-C1C-NC	10.44	117.40	110.22
22	3	304	CLA	C2C-C1C-NC	10.45	117.41	110.22
22	7	304	CLA	C2C-C1C-NC	10.45	117.41	110.22
22	R	312	CLA	C2C-C1C-NC	10.46	117.41	110.22
22	r	312	CLA	C2C-C1C-NC	10.46	117.41	110.22
22	7	303	CLA	C2C-C1C-NC	10.46	117.42	110.22
22	3	303	CLA	C2C-C1C-NC	10.46	117.42	110.22
22	2	610	CLA	C2C-C1C-NC	10.46	117.42	110.22
22	6	610	CLA	C2C-C1C-NC	10.46	117.42	110.22
22	S	310	CLA	C2C-C1C-NC	10.49	117.44	110.22
22	s	310	CLA	C2C-C1C-NC	10.49	117.44	110.22
22	a	402	CLA	C2C-C1C-NC	10.51	117.45	110.22
22	c	505	CLA	C2C-C1C-NC	10.51	117.45	110.22
22	y	610	CLA	C2C-C1C-NC	10.53	117.46	110.22
22	Y	610	CLA	C2C-C1C-NC	10.53	117.46	110.22
22	b	614	CLA	C2C-C1C-NC	10.53	117.47	110.22
22	b	602	CLA	C2C-C1C-NC	10.55	117.47	110.22
22	d	401	CLA	C2C-C1C-NC	10.55	117.47	110.22
22	R	303	CLA	C2C-C1C-NC	10.56	117.48	110.22
22	r	303	CLA	C2C-C1C-NC	10.56	117.48	110.22
22	n	603	CLA	C2C-C1C-NC	10.57	117.49	110.22
22	N	603	CLA	C2C-C1C-NC	10.57	117.49	110.22
22	C	509	CLA	C2C-C1C-NC	10.58	117.50	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	305	CLA	C2C-C1C-NC	10.59	117.50	110.22
22	s	305	CLA	C2C-C1C-NC	10.59	117.50	110.22
22	4	303	CLA	C2C-C1C-NC	10.60	117.51	110.22
22	8	303	CLA	C2C-C1C-NC	10.60	117.51	110.22
22	Y	603	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	y	603	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	n	604	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	N	604	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	r	307	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	R	307	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	S	311	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	s	311	CLA	C2C-C1C-NC	10.61	117.52	110.22
22	7	311	CLA	C2C-C1C-NC	10.62	117.52	110.22
22	3	311	CLA	C2C-C1C-NC	10.62	117.52	110.22
22	2	604	CLA	C2C-C1C-NC	10.64	117.54	110.22
22	6	604	CLA	C2C-C1C-NC	10.64	117.54	110.22
22	8	310	CLA	C2C-C1C-NC	10.65	117.54	110.22
22	4	310	CLA	C2C-C1C-NC	10.65	117.54	110.22
22	g	611	CLA	C2C-C1C-NC	10.65	117.55	110.22
22	G	611	CLA	C2C-C1C-NC	10.65	117.55	110.22
22	a	403	CLA	C2C-C1C-NC	10.66	117.56	110.22
22	7	305	CLA	C2C-C1C-NC	10.67	117.56	110.22
22	3	305	CLA	C2C-C1C-NC	10.67	117.56	110.22
22	4	304	CLA	C2C-C1C-NC	10.67	117.56	110.22
22	8	304	CLA	C2C-C1C-NC	10.67	117.56	110.22
22	y	612	CLA	C2C-C1C-NC	10.69	117.57	110.22
22	Y	612	CLA	C2C-C1C-NC	10.69	117.57	110.22
22	y	611	CLA	C2C-C1C-NC	10.70	117.58	110.22
22	2	602	CLA	C2C-C1C-NC	10.70	117.58	110.22
22	Y	611	CLA	C2C-C1C-NC	10.70	117.58	110.22
22	6	602	CLA	C2C-C1C-NC	10.70	117.58	110.22
22	1	603	CLA	C2C-C1C-NC	10.70	117.58	110.22
22	5	603	CLA	C2C-C1C-NC	10.70	117.58	110.22
22	R	311	CLA	C2C-C1C-NC	10.71	117.59	110.22
22	r	311	CLA	C2C-C1C-NC	10.71	117.59	110.22
22	1	613	CLA	C2C-C1C-NC	10.72	117.59	110.22
22	5	613	CLA	C2C-C1C-NC	10.72	117.59	110.22
22	G	603	CLA	C2C-C1C-NC	10.72	117.59	110.22
22	g	603	CLA	C2C-C1C-NC	10.72	117.59	110.22
22	g	612	CLA	C2C-C1C-NC	10.73	117.60	110.22
22	G	612	CLA	C2C-C1C-NC	10.73	117.60	110.22
22	R	309	CLA	C2C-C1C-NC	10.73	117.60	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r	309	CLA	C2C-C1C-NC	10.73	117.60	110.22
22	1	602	CLA	C2C-C1C-NC	10.74	117.61	110.22
22	5	602	CLA	C2C-C1C-NC	10.74	117.61	110.22
22	3	312	CLA	C2C-C1C-NC	10.75	117.62	110.22
22	7	312	CLA	C2C-C1C-NC	10.75	117.62	110.22
22	5	604	CLA	C2C-C1C-NC	10.75	117.62	110.22
22	1	604	CLA	C2C-C1C-NC	10.75	117.62	110.22
22	B	602	CLA	C2C-C1C-NC	10.77	117.63	110.22
22	c	504	CLA	C2C-C1C-NC	10.78	117.64	110.22
22	c	511	CLA	C2C-C1C-NC	10.80	117.65	110.22
22	Y	614	CLA	C2C-C1C-NC	10.82	117.66	110.22
22	y	614	CLA	C2C-C1C-NC	10.82	117.66	110.22
22	G	602	CLA	C2C-C1C-NC	10.85	117.68	110.22
22	g	602	CLA	C2C-C1C-NC	10.85	117.68	110.22
22	b	603	CLA	C2C-C1C-NC	10.85	117.68	110.22
22	D	404	CLA	C2C-C1C-NC	10.87	117.69	110.22
22	n	612	CLA	C2C-C1C-NC	10.89	117.71	110.22
22	N	612	CLA	C2C-C1C-NC	10.89	117.71	110.22
22	B	603	CLA	C2C-C1C-NC	10.89	117.71	110.22
22	5	611	CLA	C2C-C1C-NC	10.90	117.72	110.22
22	1	611	CLA	C2C-C1C-NC	10.90	117.72	110.22
22	n	611	CLA	C2C-C1C-NC	10.91	117.72	110.22
22	N	611	CLA	C2C-C1C-NC	10.91	117.72	110.22
22	B	605	CLA	C2C-C1C-NC	10.92	117.73	110.22
22	7	313	CLA	C2C-C1C-NC	10.94	117.74	110.22
22	3	313	CLA	C2C-C1C-NC	10.94	117.74	110.22
22	D	403	CLA	C2C-C1C-NC	10.96	117.75	110.22
22	c	503	CLA	C2C-C1C-NC	10.96	117.76	110.22
22	C	505	CLA	C2C-C1C-NC	10.97	117.77	110.22
22	A	405	CLA	C2C-C1C-NC	10.99	117.78	110.22
22	B	609	CLA	C2C-C1C-NC	11.00	117.78	110.22
22	c	502	CLA	C2C-C1C-NC	11.01	117.79	110.22
22	c	510	CLA	C2C-C1C-NC	11.04	117.81	110.22
22	Y	602	CLA	C2C-C1C-NC	11.05	117.82	110.22
22	y	602	CLA	C2C-C1C-NC	11.05	117.82	110.22
22	S	301	CLA	C2C-C1C-NC	11.08	117.84	110.22
22	2	612	CLA	C2C-C1C-NC	11.11	117.86	110.22
22	6	612	CLA	C2C-C1C-NC	11.11	117.86	110.22
22	B	610	CLA	C2C-C1C-NC	11.12	117.87	110.22
22	g	613	CLA	C2C-C1C-NC	11.14	117.89	110.22
22	G	613	CLA	C2C-C1C-NC	11.14	117.89	110.22
22	s	309	CLA	C2C-C1C-NC	11.15	117.89	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	309	CLA	C2C-C1C-NC	11.15	117.89	110.22
22	b	607	CLA	C2C-C1C-NC	11.15	117.89	110.22
22	N	602	CLA	C2C-C1C-NC	11.16	117.89	110.22
22	n	602	CLA	C2C-C1C-NC	11.16	117.89	110.22
22	B	612	CLA	C2C-C1C-NC	11.20	117.92	110.22
22	G	604	CLA	C2C-C1C-NC	11.22	117.94	110.22
22	g	604	CLA	C2C-C1C-NC	11.22	117.94	110.22
22	n	613	CLA	C2C-C1C-NC	11.23	117.94	110.22
22	N	613	CLA	C2C-C1C-NC	11.23	117.94	110.22
22	d	403	CLA	C2C-C1C-NC	11.23	117.94	110.22
22	S	314	CLA	C2C-C1C-NC	11.30	117.99	110.22
22	s	314	CLA	C2C-C1C-NC	11.30	117.99	110.22
22	C	507	CLA	C2C-C1C-NC	11.32	118.00	110.22
22	D	401	CLA	C2C-C1C-NC	11.32	118.00	110.22
22	B	615	CLA	C2C-C1C-NC	11.33	118.01	110.22
22	5	614	CLA	C2C-C1C-NC	11.35	118.03	110.22
22	1	614	CLA	C2C-C1C-NC	11.35	118.03	110.22
22	a	405	CLA	C2C-C1C-NC	11.36	118.03	110.22
22	b	604	CLA	C2C-C1C-NC	11.37	118.04	110.22
22	S	312	CLA	C2C-C1C-NC	11.44	118.09	110.22
22	s	312	CLA	C2C-C1C-NC	11.44	118.09	110.22
22	Y	604	CLA	C2C-C1C-NC	11.48	118.11	110.22
22	y	604	CLA	C2C-C1C-NC	11.48	118.11	110.22
22	C	511	CLA	C2C-C1C-NC	11.52	118.14	110.22
22	b	610	CLA	C2C-C1C-NC	11.63	118.22	110.22
22	8	302	CLA	C2C-C1C-NC	11.67	118.25	110.22
22	4	302	CLA	C2C-C1C-NC	11.67	118.25	110.22
22	B	607	CLA	C2C-C1C-NC	11.69	118.26	110.22
22	C	504	CLA	C2C-C1C-NC	11.69	118.26	110.22
22	b	613	CLA	C2C-C1C-NC	11.72	118.28	110.22
22	b	616	CLA	C2C-C1C-NC	11.77	118.31	110.22
22	c	512	CLA	C2C-C1C-NC	11.79	118.33	110.22
22	y	613	CLA	C2C-C1C-NC	11.80	118.34	110.22
22	Y	613	CLA	C2C-C1C-NC	11.80	118.34	110.22
22	B	608	CLA	C2C-C1C-NC	11.94	118.43	110.22
22	C	510	CLA	C2C-C1C-NC	11.95	118.44	110.22
22	c	501	CLA	C2C-C1C-NC	11.95	118.44	110.22
22	c	508	CLA	C2C-C1C-NC	11.96	118.44	110.22
22	C	501	CLA	C2C-C1C-NC	11.97	118.45	110.22
22	b	609	CLA	C2C-C1C-NC	12.01	118.48	110.22
22	c	506	CLA	C2C-C1C-NC	12.15	118.58	110.22
22	c	507	CLA	C2C-C1C-NC	12.16	118.58	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	C2C-C1C-NC	12.24	118.64	110.22
22	C	506	CLA	C2C-C1C-NC	12.62	118.90	110.22
22	C	508	CLA	C2C-C1C-NC	12.68	118.94	110.22
22	B	604	CLA	C2C-C1C-NC	13.55	119.54	110.22
25	4	307	CHL	O2D-CGD-CBD	20.37	160.89	111.20
25	8	307	CHL	O2D-CGD-CBD	20.37	160.89	111.20
25	s	307	CHL	O2D-CGD-CBD	20.46	161.12	111.20
25	S	307	CHL	O2D-CGD-CBD	20.46	161.12	111.20

All (613) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	5	604	CLA	NA
22	5	604	CLA	NC
22	5	604	CLA	ND
22	s	309	CLA	NC
22	s	309	CLA	ND
22	s	309	CLA	NA
22	G	610	CLA	NC
22	G	610	CLA	ND
22	G	610	CLA	NA
22	R	309	CLA	NC
22	R	309	CLA	ND
22	R	309	CLA	NA
22	3	304	CLA	NC
22	3	304	CLA	ND
22	3	304	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	5	611	CLA	NC
22	5	611	CLA	ND
22	5	611	CLA	NA
22	R	308	CLA	NC
22	R	308	CLA	ND
22	R	308	CLA	NA
22	4	309	CLA	NC
22	4	309	CLA	ND
22	4	309	CLA	NA
22	C	505	CLA	ND
22	C	505	CLA	NA
22	6	603	CLA	NC

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Mol	Chain	Res	Type	Atom
22	6	603	CLA	ND
22	6	603	CLA	NA
22	r	302	CLA	NC
22	r	302	CLA	ND
22	r	302	CLA	NA
22	2	604	CLA	NA
22	2	604	CLA	NC
22	2	604	CLA	ND
22	B	608	CLA	NA
22	S	301	CLA	NC
22	S	301	CLA	ND
22	S	301	CLA	NA
22	n	610	CLA	NC
22	n	610	CLA	ND
22	n	610	CLA	NA
22	2	612	CLA	NC
22	2	612	CLA	ND
22	2	612	CLA	NA
22	s	313	CLA	NA
22	s	313	CLA	NC
22	s	313	CLA	ND
22	g	613	CLA	NC
22	g	613	CLA	ND
22	g	613	CLA	NA
22	1	603	CLA	NC
22	1	603	CLA	ND
22	1	603	CLA	NA
22	8	302	CLA	NC
22	8	302	CLA	ND
22	n	613	CLA	NC
22	n	613	CLA	ND
22	n	613	CLA	NA
22	1	602	CLA	NC
22	1	602	CLA	ND
22	1	602	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	C	508	CLA	NC
22	C	508	CLA	ND

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Mol	Chain	Res	Type	Atom
22	C	508	CLA	NA
22	7	304	CLA	NC
22	7	304	CLA	ND
22	7	304	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	7	314	CLA	NC
22	7	314	CLA	ND
22	7	314	CLA	NA
22	3	310	CLA	NC
22	3	310	CLA	ND
22	3	310	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	A	405	CLA	NA
22	Y	603	CLA	NC
22	Y	603	CLA	ND
22	Y	603	CLA	NA
22	7	311	CLA	NC
22	7	311	CLA	ND
22	7	311	CLA	NA
22	8	310	CLA	NC
22	8	310	CLA	ND
22	8	310	CLA	NA
22	y	612	CLA	NC
22	y	612	CLA	ND
22	y	612	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	S	312	CLA	NC
22	S	312	CLA	ND
22	S	312	CLA	NA
22	G	604	CLA	NA
22	G	604	CLA	NC
22	G	604	CLA	ND
22	c	502	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	b	610	CLA	NC
22	b	610	CLA	ND

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Mol	Chain	Res	Type	Atom
22	b	610	CLA	NA
22	C	511	CLA	NA
22	7	303	CLA	NC
22	7	303	CLA	ND
22	7	303	CLA	NA
22	S	310	CLA	NC
22	S	310	CLA	ND
22	S	310	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	NA
22	c	507	CLA	ND
22	y	603	CLA	NC
22	y	603	CLA	ND
22	y	603	CLA	NA
22	a	403	CLA	NC
22	a	403	CLA	ND
22	a	403	CLA	NA
22	5	614	CLA	NC
22	5	614	CLA	ND
22	5	614	CLA	NA
22	R	303	CLA	NA
22	R	303	CLA	NC
22	R	303	CLA	ND
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	1	613	CLA	NC
22	1	613	CLA	ND
22	1	613	CLA	NA
22	g	604	CLA	NA
22	g	604	CLA	NC
22	g	604	CLA	ND
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	6	609	CLA	NC
22	6	609	CLA	ND
22	6	609	CLA	NA
22	B	604	CLA	ND
22	B	604	CLA	NA
22	Y	602	CLA	NC
22	Y	602	CLA	ND

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Mol	Chain	Res	Type	Atom
22	Y	602	CLA	NA
22	G	602	CLA	NC
22	G	602	CLA	ND
22	G	602	CLA	NA
22	3	303	CLA	NC
22	3	303	CLA	ND
22	3	303	CLA	NA
22	C	504	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	N	613	CLA	NC
22	N	613	CLA	ND
22	N	613	CLA	NA
22	n	603	CLA	NC
22	n	603	CLA	ND
22	n	603	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	7	313	CLA	NC
22	7	313	CLA	ND
22	7	313	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	d	401	CLA	NC
22	d	401	CLA	ND
22	d	401	CLA	NA
22	G	603	CLA	NC
22	G	603	CLA	ND
22	G	603	CLA	NA
22	Y	604	CLA	NA
22	Y	604	CLA	NC
22	Y	604	CLA	ND
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	G	614	CLA	NC
22	G	614	CLA	ND
22	G	614	CLA	NA
22	y	611	CLA	NC
22	y	611	CLA	ND

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Mol	Chain	Res	Type	Atom
22	y	611	CLA	NA
22	7	310	CLA	NC
22	7	310	CLA	ND
22	7	310	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND
22	C	512	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	B	616	CLA	NC
22	B	616	CLA	ND
22	B	616	CLA	NA
22	2	602	CLA	NC
22	2	602	CLA	ND
22	2	602	CLA	NA
22	R	311	CLA	NC
22	R	311	CLA	ND
22	R	311	CLA	NA
22	b	601	CLA	NC
22	b	601	CLA	ND
22	b	601	CLA	NA
22	Y	612	CLA	NC
22	Y	612	CLA	ND
22	Y	612	CLA	NA
22	g	611	CLA	NC
22	g	611	CLA	ND
22	g	611	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	3	312	CLA	NC
22	3	312	CLA	ND
22	3	312	CLA	NA
22	S	314	CLA	NC
22	S	314	CLA	ND
22	S	314	CLA	NA
22	y	604	CLA	NA
22	y	604	CLA	NC
22	y	604	CLA	ND
22	g	614	CLA	NC
22	g	614	CLA	ND

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Mol	Chain	Res	Type	Atom
22	g	614	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	s	314	CLA	NC
22	s	314	CLA	ND
22	s	314	CLA	NA
22	Y	614	CLA	NC
22	Y	614	CLA	ND
22	Y	614	CLA	NA
22	b	602	CLA	NC
22	b	602	CLA	NA
22	s	303	CLA	NC
22	s	303	CLA	ND
22	s	303	CLA	NA
22	R	312	CLA	NC
22	R	312	CLA	ND
22	R	312	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	2	610	CLA	NC
22	2	610	CLA	ND
22	2	610	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	S	305	CLA	NA
22	S	305	CLA	NC
22	S	305	CLA	ND
22	r	310	CLA	NC
22	r	310	CLA	ND
22	r	310	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	2	613	CLA	NC
22	2	613	CLA	ND
22	2	613	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	NA
22	B	615	CLA	NA

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Mol	Chain	Res	Type	Atom
22	B	615	CLA	NC
22	B	615	CLA	ND
22	4	304	CLA	NC
22	4	304	CLA	ND
22	4	304	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	NA
22	1	611	CLA	NC
22	1	611	CLA	ND
22	1	611	CLA	NA
22	y	610	CLA	NC
22	y	610	CLA	ND
22	y	610	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	NA
22	S	311	CLA	NC
22	S	311	CLA	ND
22	S	311	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	g	612	CLA	NC
22	g	612	CLA	ND
22	g	612	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	r	307	CLA	NC
22	r	307	CLA	ND
22	r	307	CLA	NA
22	4	303	CLA	NC
22	4	303	CLA	ND
22	4	303	CLA	NA
22	n	611	CLA	NC
22	n	611	CLA	ND
22	n	611	CLA	NA
22	8	309	CLA	NC
22	8	309	CLA	ND
22	8	309	CLA	NA
22	1	612	CLA	NC
22	1	612	CLA	ND
22	1	612	CLA	NA

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Mol	Chain	Res	Type	Atom
22	C	501	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	ND
22	5	602	CLA	NC
22	5	602	CLA	ND
22	5	602	CLA	NA
22	3	314	CLA	NC
22	3	314	CLA	ND
22	3	314	CLA	NA
22	N	603	CLA	NC
22	N	603	CLA	ND
22	N	603	CLA	NA
22	s	310	CLA	NC
22	s	310	CLA	ND
22	s	310	CLA	NA
22	r	309	CLA	NC
22	r	309	CLA	ND
22	r	309	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	NA
22	r	303	CLA	NA
22	r	303	CLA	NC
22	r	303	CLA	ND
22	G	611	CLA	NC
22	G	611	CLA	ND
22	G	611	CLA	NA
22	7	305	CLA	NA
22	7	305	CLA	NC
22	7	305	CLA	ND
22	N	602	CLA	NC
22	N	602	CLA	ND
22	N	602	CLA	NA
22	6	612	CLA	NC
22	6	612	CLA	ND
22	6	612	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	S	304	CLA	NC
22	S	304	CLA	ND
22	S	304	CLA	NA
22	c	508	CLA	NC

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Mol	Chain	Res	Type	Atom
22	c	508	CLA	ND
22	c	508	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	n	604	CLA	NA
22	n	604	CLA	NC
22	n	604	CLA	ND
22	S	303	CLA	NC
22	S	303	CLA	ND
22	S	303	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	b	604	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	6	610	CLA	NC
22	6	610	CLA	ND
22	6	610	CLA	NA
22	1	614	CLA	NC
22	1	614	CLA	ND
22	1	614	CLA	NA
22	3	305	CLA	NA
22	3	305	CLA	NC
22	3	305	CLA	ND
22	8	304	CLA	NC
22	8	304	CLA	ND
22	8	304	CLA	NA
22	4	310	CLA	NC
22	4	310	CLA	ND
22	4	310	CLA	NA
22	s	301	CLA	NC
22	s	301	CLA	ND
22	s	301	CLA	NA
22	s	304	CLA	NC
22	s	304	CLA	ND
22	s	304	CLA	NA
22	6	611	CLA	NC
22	6	611	CLA	ND
22	6	611	CLA	NA
22	g	602	CLA	NC

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Mol	Chain	Res	Type	Atom
22	g	602	CLA	ND
22	g	602	CLA	NA
22	D	403	CLA	ND
22	D	403	CLA	NA
22	5	603	CLA	NC
22	5	603	CLA	ND
22	5	603	CLA	NA
22	b	616	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	G	612	CLA	NC
22	G	612	CLA	ND
22	G	612	CLA	NA
22	7	312	CLA	NC
22	7	312	CLA	ND
22	7	312	CLA	NA
22	y	613	CLA	NC
22	y	613	CLA	ND
22	y	613	CLA	NA
22	1	610	CLA	NC
22	1	610	CLA	ND
22	1	610	CLA	NA
22	N	610	CLA	NC
22	N	610	CLA	ND
22	N	610	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	g	603	CLA	NC
22	g	603	CLA	ND
22	g	603	CLA	NA
22	3	313	CLA	NC
22	3	313	CLA	ND
22	3	313	CLA	NA
22	n	612	CLA	NC
22	n	612	CLA	ND
22	n	612	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	r	312	CLA	NC
22	r	312	CLA	ND

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Mol	Chain	Res	Type	Atom
22	r	312	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	5	612	CLA	NC
22	5	612	CLA	ND
22	5	612	CLA	NA
22	R	302	CLA	NC
22	R	302	CLA	ND
22	R	302	CLA	NA
22	s	305	CLA	NA
22	s	305	CLA	NC
22	s	305	CLA	ND
22	N	614	CLA	NC
22	N	614	CLA	ND
22	N	614	CLA	NA
22	s	312	CLA	NC
22	s	312	CLA	ND
22	s	312	CLA	NA
22	n	614	CLA	NC
22	n	614	CLA	ND
22	n	614	CLA	NA
22	C	502	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	Y	611	CLA	NC
22	Y	611	CLA	ND
22	Y	611	CLA	NA
22	S	313	CLA	NA
22	S	313	CLA	NC
22	S	313	CLA	ND
22	G	613	CLA	NC
22	G	613	CLA	ND
22	G	613	CLA	NA
22	6	613	CLA	NC
22	6	613	CLA	ND
22	6	613	CLA	NA
22	N	604	CLA	NA
22	N	604	CLA	NC
22	N	604	CLA	ND
22	6	602	CLA	NC
22	6	602	CLA	ND

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Mol	Chain	Res	Type	Atom
22	6	602	CLA	NA
22	R	301	CLA	NC
22	R	301	CLA	ND
22	R	301	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	NA
22	s	311	CLA	NC
22	s	311	CLA	ND
22	s	311	CLA	NA
22	A	403	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	1	604	CLA	NA
22	1	604	CLA	NC
22	1	604	CLA	ND
22	8	303	CLA	NC
22	8	303	CLA	ND
22	8	303	CLA	NA
22	n	602	CLA	NC
22	n	602	CLA	ND
22	n	602	CLA	NA
22	5	613	CLA	NC
22	5	613	CLA	ND
22	5	613	CLA	NA
22	6	604	CLA	NA
22	6	604	CLA	NC
22	6	604	CLA	ND
22	d	404	CLA	NC
22	d	404	CLA	ND
22	d	404	CLA	NA
22	y	602	CLA	NC
22	y	602	CLA	ND
22	y	602	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	r	308	CLA	NC
22	r	308	CLA	ND
22	r	308	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA

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Mol	Chain	Res	Type	Atom
22	d	403	CLA	ND
22	d	403	CLA	NA
22	r	301	CLA	NC
22	r	301	CLA	ND
22	r	301	CLA	NA
22	Y	613	CLA	NC
22	Y	613	CLA	ND
22	Y	613	CLA	NA
22	R	310	CLA	NC
22	R	310	CLA	ND
22	R	310	CLA	NA
22	2	603	CLA	NC
22	2	603	CLA	ND
22	2	603	CLA	NA
22	D	401	CLA	NA
22	D	401	CLA	NC
22	D	401	CLA	ND
22	g	610	CLA	NC
22	g	610	CLA	ND
22	g	610	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	NA
22	b	613	CLA	ND
22	2	609	CLA	NC
22	2	609	CLA	ND
22	2	609	CLA	NA
22	D	404	CLA	NC
22	D	404	CLA	ND
22	D	404	CLA	NA
22	c	511	CLA	NA
22	N	612	CLA	NC
22	N	612	CLA	ND
22	N	612	CLA	NA
22	b	603	CLA	NC
22	b	603	CLA	ND
22	Y	610	CLA	NC
22	Y	610	CLA	ND
22	Y	610	CLA	NA
22	4	302	CLA	NC
22	4	302	CLA	ND
22	3	311	CLA	NC
22	3	311	CLA	ND

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Mol	Chain	Res	Type	Atom
22	3	311	CLA	NA
22	a	402	CLA	NC
22	a	402	CLA	ND
22	a	402	CLA	NA
22	5	610	CLA	NC
22	5	610	CLA	ND
22	5	610	CLA	NA
22	S	309	CLA	NC
22	S	309	CLA	ND
22	S	309	CLA	NA
22	R	307	CLA	NC
22	R	307	CLA	ND
22	R	307	CLA	NA
22	r	311	CLA	NC
22	r	311	CLA	ND
22	r	311	CLA	NA
22	2	611	CLA	NC
22	2	611	CLA	ND
22	2	611	CLA	NA
22	N	611	CLA	NC
22	N	611	CLA	ND
22	N	611	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	b	605	CLA	NA
22	y	614	CLA	NC
22	y	614	CLA	ND
22	y	614	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	c	504	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	2	606	CHL	CED-O2D-CGD-CBD

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Mol	Chain	Res	Type	Atoms
25	6	606	CHL	CED-O2D-CGD-CBD
22	2	613	CLA	CED-O2D-CGD-CBD
22	6	613	CLA	CED-O2D-CGD-CBD
22	R	312	CLA	CED-O2D-CGD-CBD
22	r	312	CLA	CED-O2D-CGD-CBD
25	y	606	CHL	CED-O2D-CGD-CBD
25	Y	606	CHL	CED-O2D-CGD-CBD
22	c	511	CLA	CED-O2D-CGD-CBD
25	7	307	CHL	CED-O2D-CGD-CBD
25	3	307	CHL	CED-O2D-CGD-CBD
25	1	606	CHL	CED-O2D-CGD-CBD
25	5	606	CHL	CED-O2D-CGD-CBD
25	n	606	CHL	CED-O2D-CGD-CBD
25	N	606	CHL	CED-O2D-CGD-CBD
22	S	310	CLA	CED-O2D-CGD-CBD
22	s	310	CLA	CED-O2D-CGD-CBD
22	G	614	CLA	CED-O2D-CGD-CBD
22	g	614	CLA	CED-O2D-CGD-CBD
25	g	606	CHL	CED-O2D-CGD-CBD
25	G	606	CHL	CED-O2D-CGD-CBD
22	b	613	CLA	CED-O2D-CGD-CBD
22	4	309	CLA	CED-O2D-CGD-CBD
22	8	309	CLA	CED-O2D-CGD-CBD
22	s	313	CLA	CED-O2D-CGD-CBD
22	S	313	CLA	CED-O2D-CGD-CBD
22	C	511	CLA	CED-O2D-CGD-CBD
22	B	613	CLA	CED-O2D-CGD-CBD
22	5	614	CLA	CED-O2D-CGD-CBD
22	1	614	CLA	CED-O2D-CGD-CBD
25	r	305	CHL	CED-O2D-CGD-CBD
25	R	305	CHL	CED-O2D-CGD-CBD

There are no ring outliers.

154 monomers are involved in 438 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	1	601	CHL	2	0
25	1	605	CHL	1	0
25	1	606	CHL	1	0
25	1	608	CHL	4	0
25	1	609	CHL	2	0
22	1	611	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	612	CLA	1	0
22	1	613	CLA	1	0
22	1	614	CLA	2	0
25	1	615	CHL	2	0
25	2	601	CHL	3	0
22	2	602	CLA	1	0
25	2	605	CHL	2	0
25	2	606	CHL	2	0
25	2	607	CHL	5	0
25	2	608	CHL	3	0
22	2	609	CLA	1	0
22	2	610	CLA	2	0
22	2	611	CLA	1	0
22	2	612	CLA	1	0
22	2	613	CLA	15	0
25	3	301	CHL	1	0
25	3	306	CHL	1	0
25	3	308	CHL	4	0
25	3	309	CHL	3	0
22	3	311	CLA	1	0
22	3	313	CLA	1	0
25	4	301	CHL	10	0
22	4	302	CLA	2	0
22	4	303	CLA	1	0
22	4	304	CLA	1	0
25	4	305	CHL	1	0
25	4	306	CHL	2	0
25	4	308	CHL	1	0
22	4	309	CLA	3	0
25	5	601	CHL	2	0
25	5	605	CHL	1	0
25	5	606	CHL	1	0
25	5	608	CHL	4	0
25	5	609	CHL	2	0
22	5	610	CLA	1	0
22	5	612	CLA	1	0
22	5	613	CLA	1	0
22	5	614	CLA	2	0
25	6	601	CHL	3	0
22	6	602	CLA	1	0
25	6	605	CHL	2	0
25	6	606	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	6	607	CHL	5	0
25	6	608	CHL	3	0
22	6	610	CLA	2	0
22	6	611	CLA	1	0
22	6	612	CLA	1	0
22	6	613	CLA	16	0
25	7	301	CHL	1	0
25	7	306	CHL	1	0
25	7	307	CHL	1	0
25	7	308	CHL	4	0
25	7	309	CHL	3	0
22	7	311	CLA	1	0
22	7	313	CLA	1	0
25	8	301	CHL	12	0
22	8	302	CLA	2	0
22	8	303	CLA	1	0
22	8	304	CLA	1	0
25	8	305	CHL	1	0
25	8	306	CHL	2	0
25	8	307	CHL	1	0
25	8	308	CHL	1	0
22	8	309	CLA	4	0
22	A	402	CLA	2	0
22	A	403	CLA	1	0
23	A	404	PHO	3	0
22	A	405	CLA	1	0
22	B	601	CLA	2	0
22	B	602	CLA	7	0
22	B	603	CLA	3	0
22	B	604	CLA	3	0
22	B	606	CLA	3	0
22	B	607	CLA	2	0
22	B	608	CLA	1	0
22	B	609	CLA	4	0
22	B	610	CLA	1	0
22	B	611	CLA	3	0
22	B	612	CLA	2	0
22	B	613	CLA	1	0
22	B	614	CLA	5	0
22	B	615	CLA	1	0
22	B	616	CLA	3	0
22	C	501	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	502	CLA	3	0
22	C	504	CLA	1	0
22	C	505	CLA	1	0
22	C	506	CLA	3	0
22	C	507	CLA	1	0
22	C	508	CLA	5	0
22	C	509	CLA	3	0
22	C	510	CLA	1	0
22	C	511	CLA	3	0
22	C	512	CLA	1	0
23	D	402	PHO	2	0
22	D	403	CLA	4	0
24	E	101	HEM	4	0
25	G	601	CHL	2	0
22	G	602	CLA	1	0
25	G	605	CHL	1	0
25	G	606	CHL	2	0
25	G	607	CHL	1	0
25	G	608	CHL	5	0
25	G	609	CHL	3	0
22	G	610	CLA	1	0
22	G	611	CLA	6	0
22	G	612	CLA	2	0
22	G	613	CLA	2	0
22	G	614	CLA	1	0
25	N	601	CHL	1	0
22	N	602	CLA	1	0
25	N	605	CHL	1	0
25	N	606	CHL	3	0
25	N	607	CHL	2	0
25	N	608	CHL	3	0
25	N	609	CHL	2	0
22	N	610	CLA	2	0
22	N	611	CLA	1	0
22	N	613	CLA	1	0
22	R	302	CLA	22	0
22	R	303	CLA	1	0
25	R	304	CHL	1	0
25	R	305	CHL	3	0
25	R	306	CHL	2	0
22	R	307	CLA	2	0
22	R	308	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	R	311	CLA	2	0
22	R	312	CLA	72	0
22	S	301	CLA	24	0
25	S	302	CHL	1	0
22	S	303	CLA	3	0
22	S	304	CLA	1	0
25	S	306	CHL	1	0
25	S	308	CHL	2	0
22	S	309	CLA	1	0
22	S	310	CLA	1	0
22	S	313	CLA	3	0
25	Y	601	CHL	2	0
22	Y	602	CLA	1	0
25	Y	605	CHL	3	0
25	Y	606	CHL	3	0
25	Y	607	CHL	1	0
25	Y	608	CHL	2	0
25	Y	609	CHL	3	0
22	Y	610	CLA	1	0
22	Y	611	CLA	1	0
22	Y	613	CLA	2	0
22	Y	614	CLA	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.