



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2017 – 04:49 PM EST

PDB ID : 5GTI
Title : Native XFEL structure of photosystem II (two flash dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-08-20
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029077

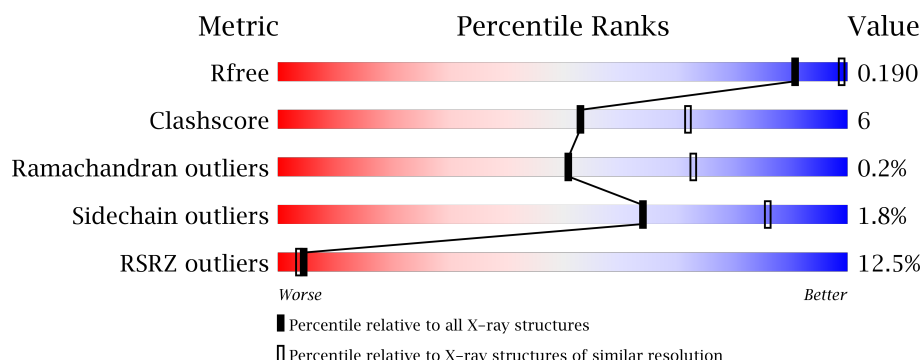
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>.</div> </div>
1	a	344	<div> <div>4%</div> <div>97%</div> <div>.</div> <div>..</div> </div>
2	B	505	<div> <div>12%</div> <div>81%</div> <div>19%</div> <div>.</div> </div>
2	b	505	<div> <div>14%</div> <div>97%</div> <div>.</div> </div>
3	C	455	<div> <div>16%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	40	
17	x	40	
18	Y	30	
18	y	30	
19	Z	62	
19	z	62	
20	R	34	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404	X	-	-	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	X
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	B	627	-	-	-	X
27	GOL	B	628	-	-	-	X
27	GOL	a	412	-	-	-	X
27	GOL	d	401	-	-	-	X
29	PL9	A	413	-	-	-	X
29	PL9	a	415	-	-	-	X
30	UNL	D	410	-	-	-	X
30	UNL	D	411	-	-	-	X
30	UNL	I	101	-	-	-	X
30	UNL	K	101	-	-	-	X
30	UNL	X	101	-	-	-	X
30	UNL	b	629	-	-	-	X
30	UNL	d	409	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	102	-	-	-	X
30	UNL	x	101	-	-	-	X
31	LHG	e	101	-	-	-	X
34	LMG	C	521	-	-	-	X
34	LMG	c	520	-	-	-	X
35	LMT	B	632	-	-	-	X
35	LMT	B	633	-	-	-	X
35	LMT	B	634	-	-	-	X
35	LMT	C	522	-	-	-	X
35	LMT	D	403	-	-	-	X
35	LMT	E	102	-	-	-	X
35	LMT	M	103	-	-	-	X
35	LMT	a	418	-	-	-	X
35	LMT	b	628	-	-	-	X
35	LMT	e	102	-	-	-	X
35	LMT	m	103	-	-	-	X
36	HTG	B	624	-	-	-	X
36	HTG	B	625	-	-	-	X
36	HTG	C	524	-	-	-	X
36	HTG	D	412	-	-	-	X
36	HTG	V	203	-	-	-	X
36	HTG	b	621	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	HTG	b	622	-	-	-	X
36	HTG	c	522	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 52752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			
1	a	334	Total	C	N	O	S	0	0	0
			2620	1716	431	458	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			
2	b	504	Total	C	N	O	S	0	0	0
			3969	2605	661	690	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	455	Total	C	N	O	S	0	0	0
			3519	2303	589	614	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

- Molecule 10 is a protein called Photosystem II PsbK protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

- Molecule 12 is a protein called Photosystem II PsbM protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	0	0
			260	173	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

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

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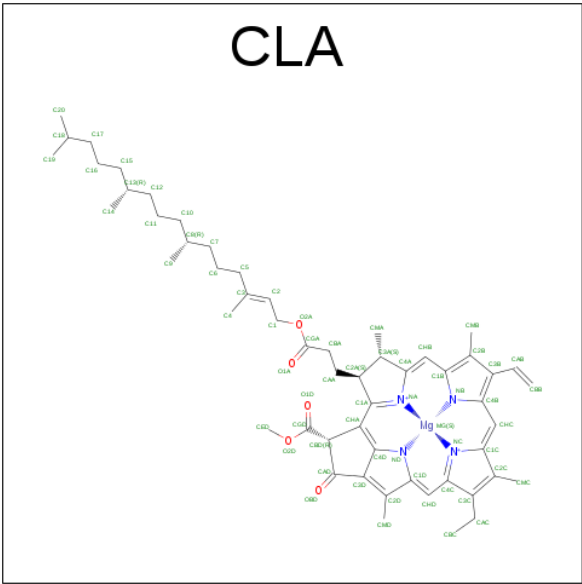
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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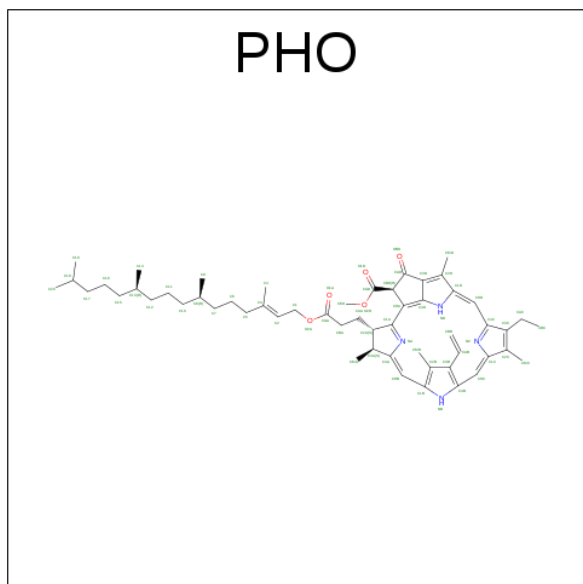
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23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	d	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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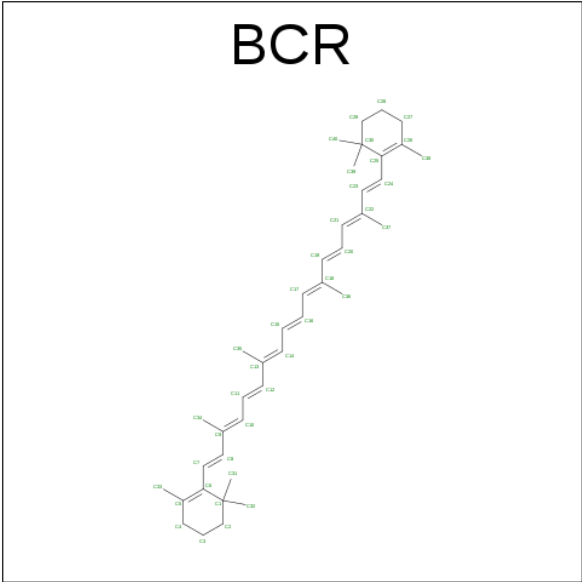
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



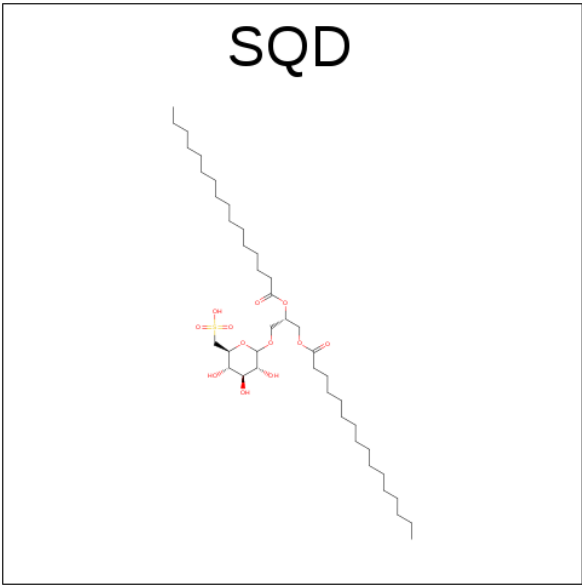
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



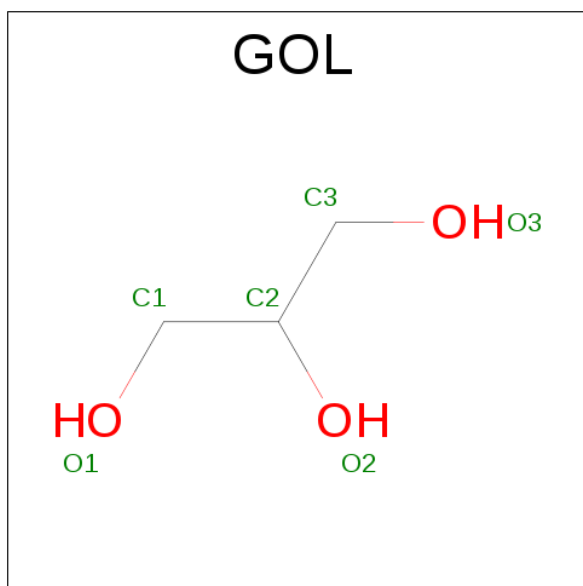
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	D	1	Total	C	O	S	0	0
			43	30	12	1		
26	L	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



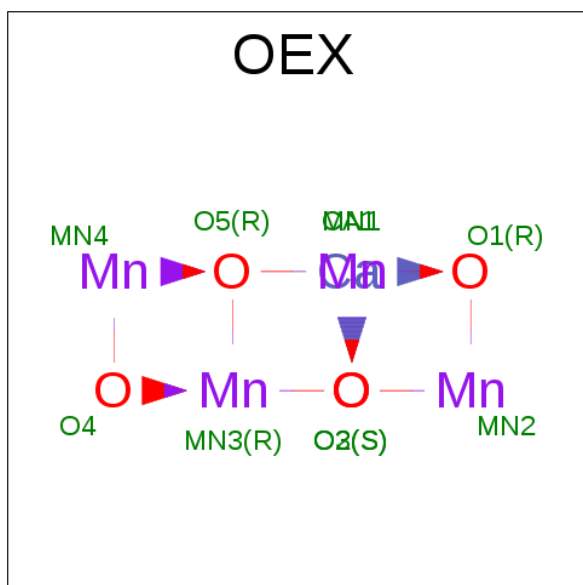
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		

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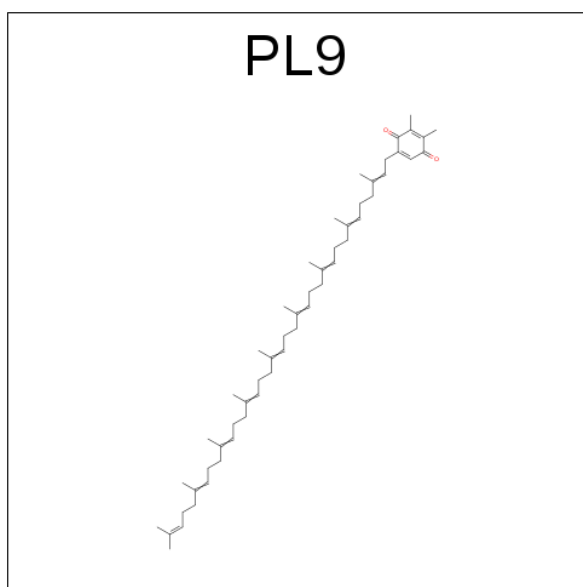
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	b	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		

- Molecule 28 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$).



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

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

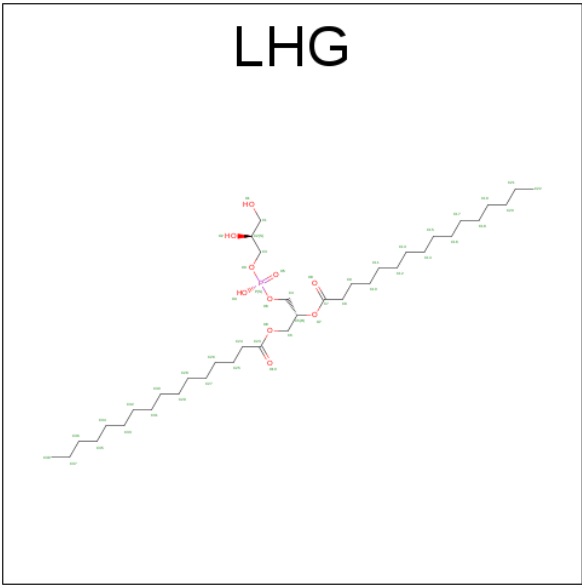
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	J	1	Total	C		0	0
			10	10			
30	i	1	Total	C	O	0	0
			40	35	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	K	1	Total	C	O	0	0
			34	29	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	I	1	Total	C	O	0	0
			40	35	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	a	1	Total	C	O	0	0
			30	25	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	x	1	Total	C	O	0	0
			18	16	2		
30	A	1	Total	C	O	0	0
			28	23	5		
30	j	1	Total	C		0	0
			10	10			
30	X	1	Total	C	O	0	0
			18	16	2		
30	d	1	Total	C	O	0	0
			17	16	1		
30	m	1	Total	C		0	0
			10	10			
30	b	2	Total	C	O	0	0
			69	59	10		
30	M	1	Total	C		0	0
			10	10			

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



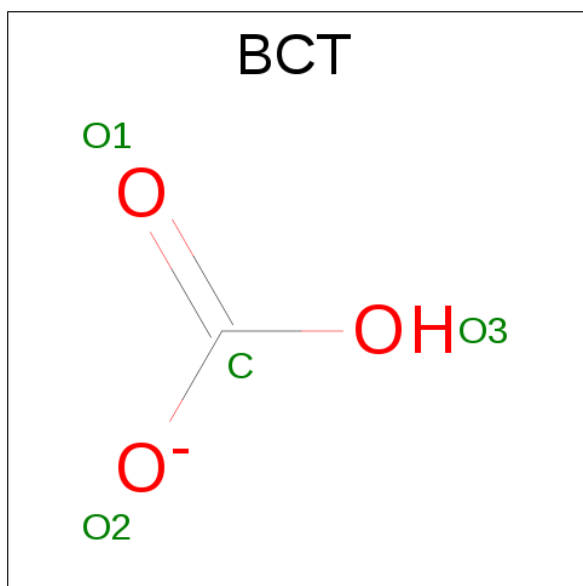
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	D	1	Total	C	O	P	0	0
			49	38	10	1		

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

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

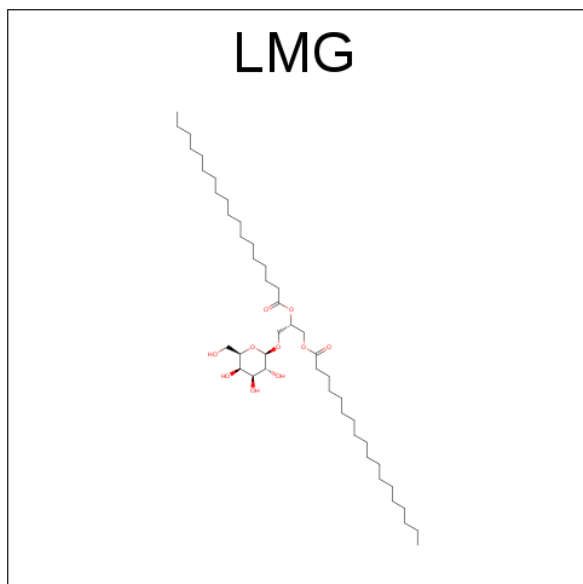


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Ca 1 1	0	0
33	C	1	Total Ca 1 1	0	0
33	V	1	Total Ca 1 1	0	0
33	c	2	Total Ca 2 2	0	0
33	O	1	Total Ca 1 1	0	0
33	o	1	Total Ca 1 1	0	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



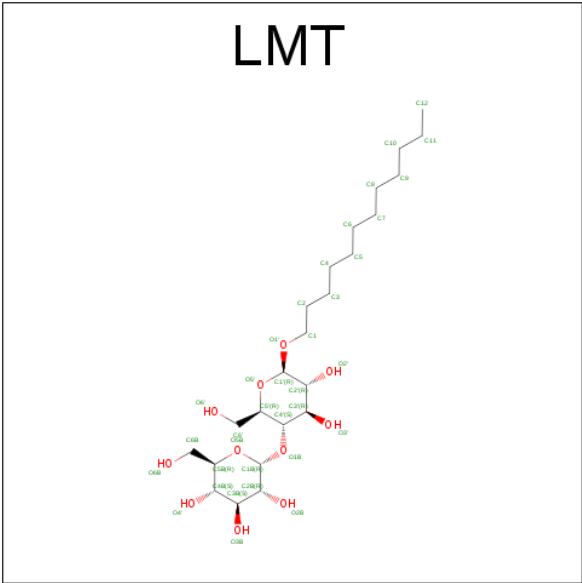
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	J	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		
34	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 35 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



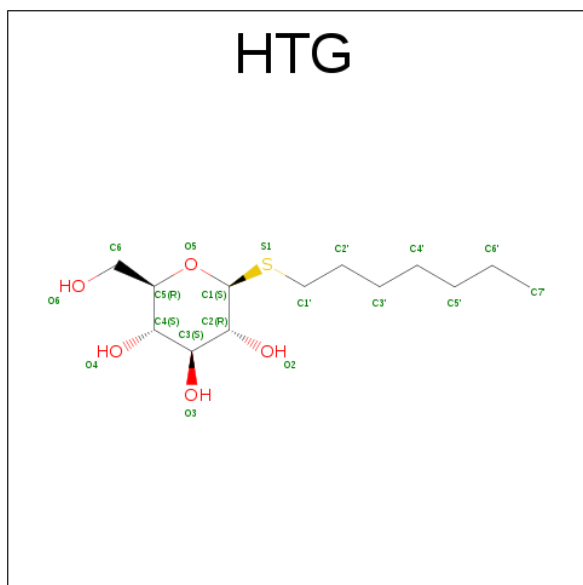
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			25	19	6		
35	B	1	Total	C	O	0	0
			35	24	11		
35	B	1	Total	C	O	0	0
			26	19	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			35	24	11		
35	D	1	Total	C	O	0	0
			35	24	11		
35	E	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	M	1	Total	C	O	0	0
			35	24	11		
35	a	1	Total	C	O	0	0
			35	24	11		
35	b	1	Total	C	O	0	0
			25	19	6		
35	b	1	Total	C	O	0	0
			25	19	6		
35	e	1	Total	C	O	0	0
			35	24	11		
35	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 36 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



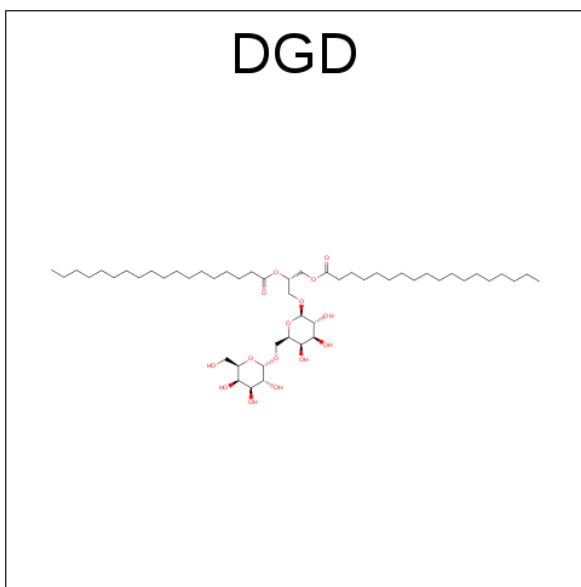
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		

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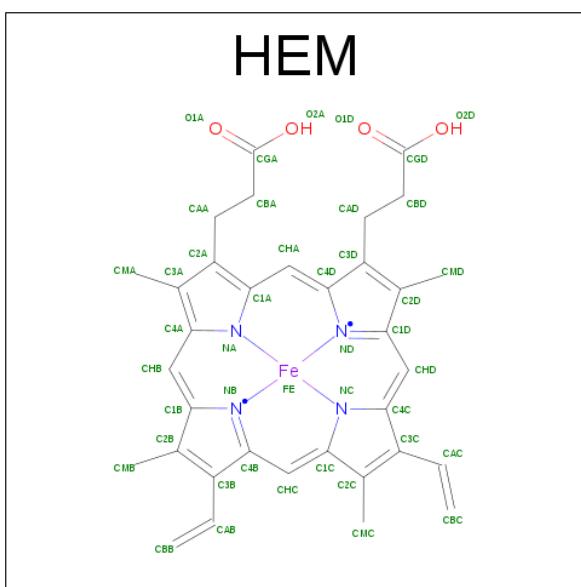
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	S		0	0
			9	8	1			
36	D	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O		0	0
			11	6	5			
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	h	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 37 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	E	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
38	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
38	e	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
38	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	135	Total	O		
			135	135	0	0
40	B	195	Total	O		
			195	195	0	0
40	C	151	Total	O		
			151	151	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	D	118	Total O 118 118	0	0
40	E	25	Total O 25 25	0	0
40	F	5	Total O 5 5	0	0
40	H	22	Total O 22 22	0	0
40	I	6	Total O 6 6	0	0
40	J	4	Total O 4 4	0	0
40	K	6	Total O 6 6	0	0
40	L	6	Total O 6 6	0	0
40	M	15	Total O 15 15	0	0
40	O	105	Total O 105 105	0	0
40	T	13	Total O 13 13	0	0
40	U	51	Total O 51 51	0	0
40	V	81	Total O 81 81	0	0
40	X	4	Total O 4 4	0	0
40	Y	1	Total O 1 1	0	0
40	Z	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	132	Total O 132 132	0	0
40	b	206	Total O 206 206	0	0
40	c	153	Total O 153 153	0	0
40	d	115	Total O 115 115	0	0

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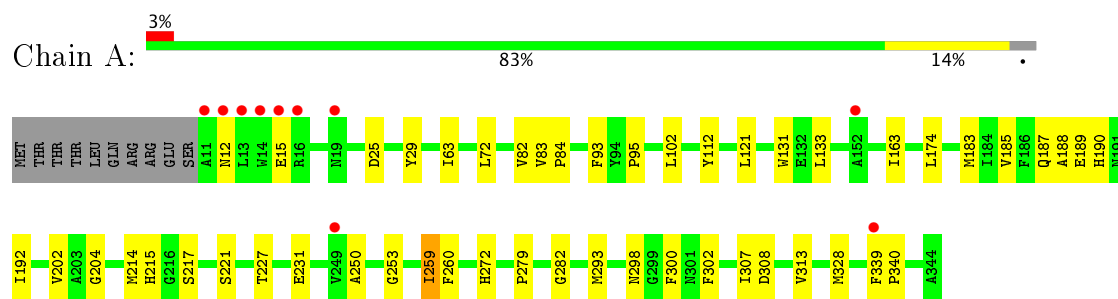
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	e	16	Total 16	O 16	0	0
40	f	5	Total 5	O 5	0	0
40	h	27	Total 27	O 27	0	0
40	i	3	Total 3	O 3	0	0
40	j	3	Total 3	O 3	0	0
40	k	6	Total 6	O 6	0	0
40	l	9	Total 9	O 9	0	0
40	m	18	Total 18	O 18	0	0
40	o	115	Total 115	O 115	0	0
40	t	9	Total 9	O 9	0	0
40	u	62	Total 62	O 62	0	0
40	v	78	Total 78	O 78	0	0
40	x	8	Total 8	O 8	0	0
40	z	1	Total 1	O 1	0	0

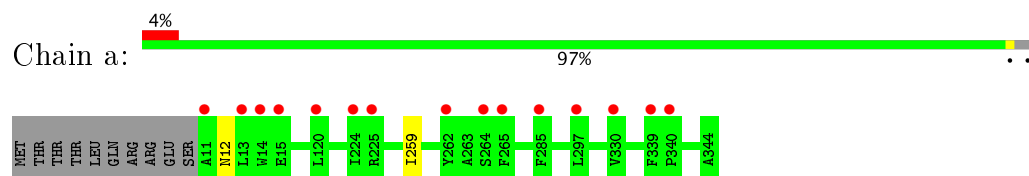
3 Residue-property plots [i](#)

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

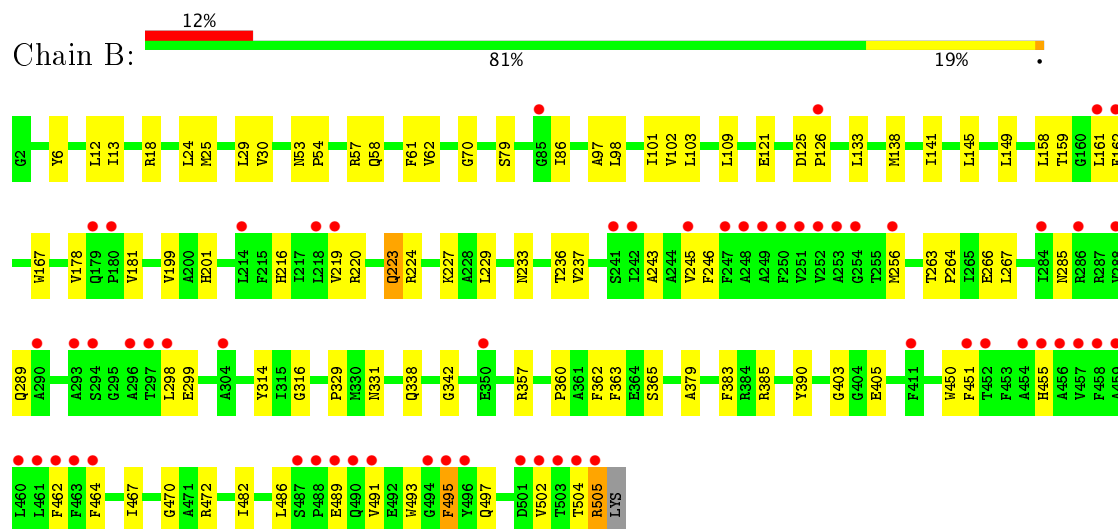
- Molecule 1: Photosystem II D1 protein



- Molecule 1: Photosystem II D1 protein

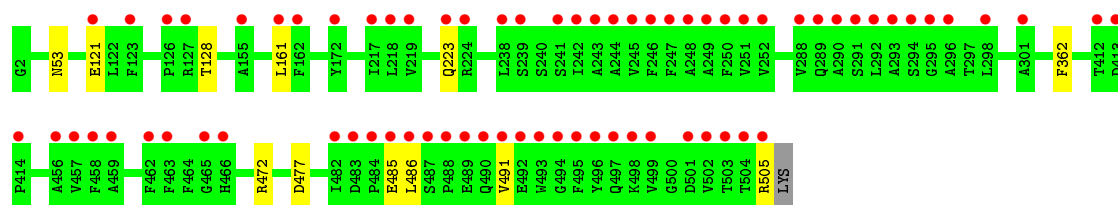


- Molecule 2: Photosystem II CP47 reaction center protein

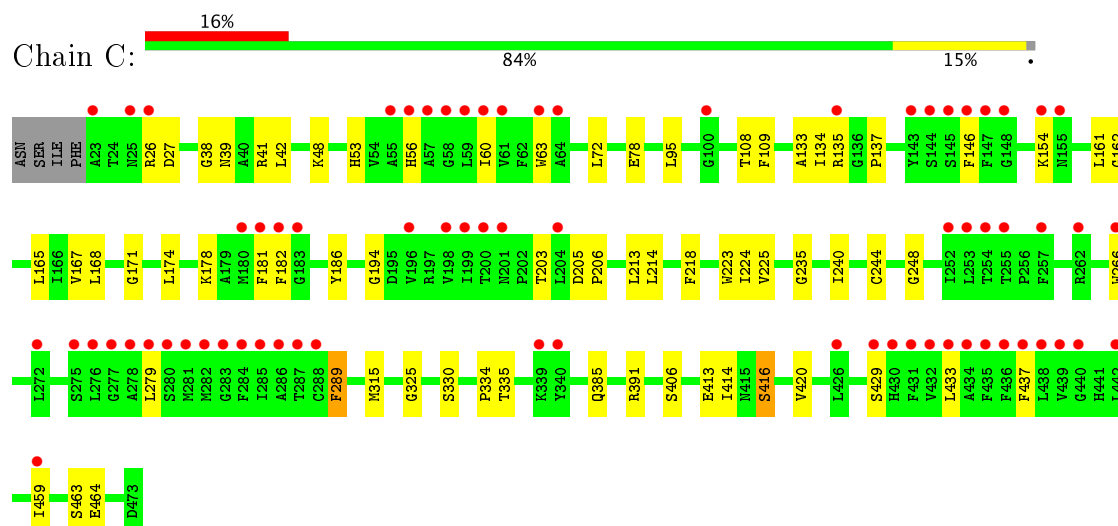


- Molecule 2: Photosystem II CP47 reaction center protein

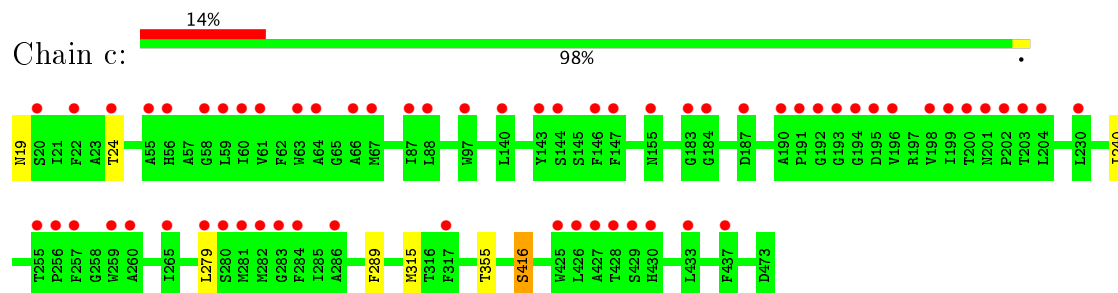




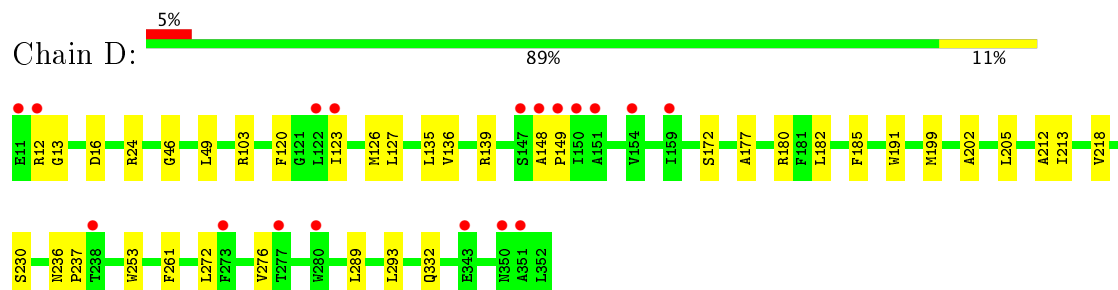
• Molecule 3: Photosystem II CP43 protein



• Molecule 3: Photosystem II CP43 protein

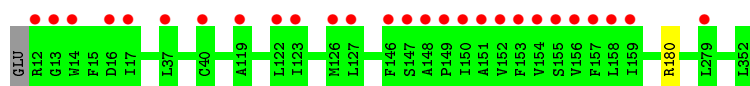


• Molecule 4: Photosystem II D2 protein



• Molecule 4: Photosystem II D2 protein

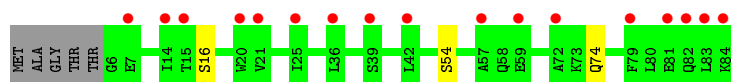
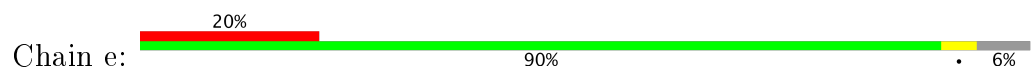




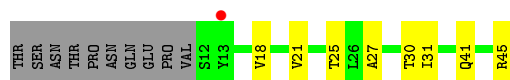
- Molecule 5: Cytochrome b559 subunit alpha



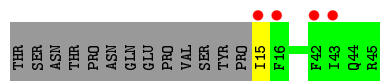
- Molecule 5: Cytochrome b559 subunit alpha



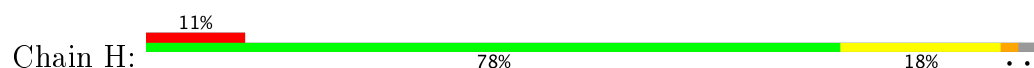
- Molecule 6: Cytochrome b559 subunit beta



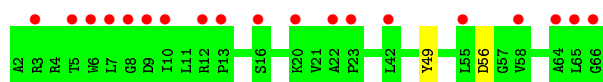
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

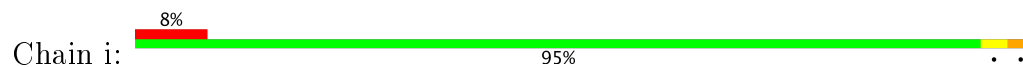


- Molecule 8: Photosystem II reaction center protein I

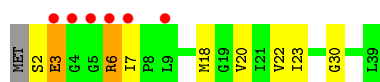
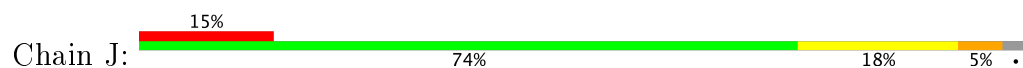




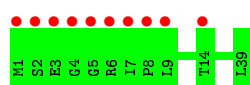
- Molecule 8: Photosystem II reaction center protein I



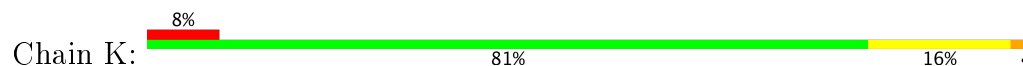
- Molecule 9: Photosystem II reaction center protein J



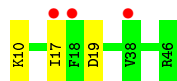
- Molecule 9: Photosystem II reaction center protein J



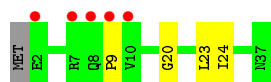
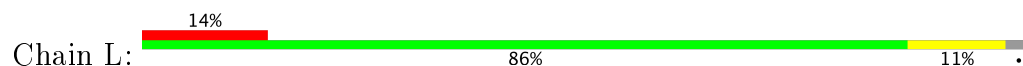
- Molecule 10: Photosystem II PsbK protein



- Molecule 10: Photosystem II PsbK protein

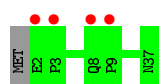


- Molecule 11: Photosystem II reaction center protein L

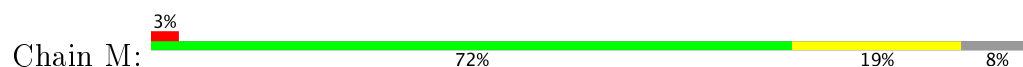


- Molecule 11: Photosystem II reaction center protein L

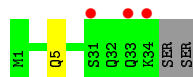




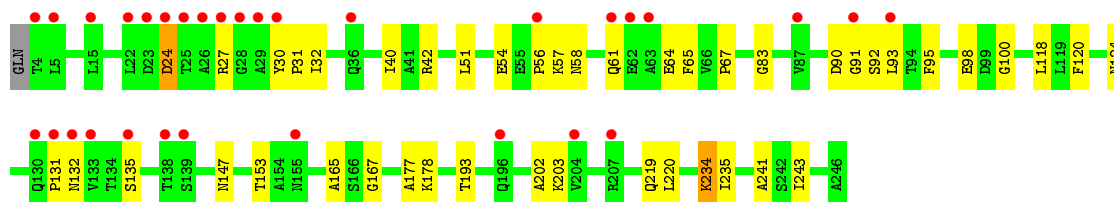
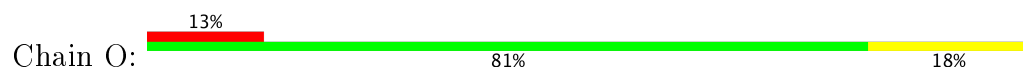
- Molecule 12: Photosystem II PsbM protein



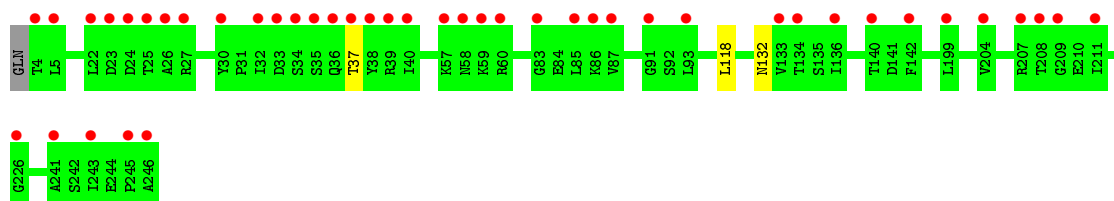
- Molecule 12: Photosystem II PsbM protein



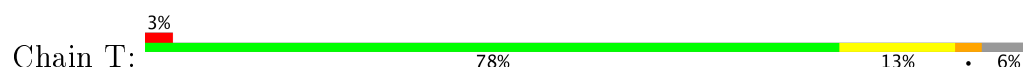
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

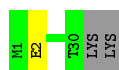


- Molecule 14: Photosystem II reaction center protein T

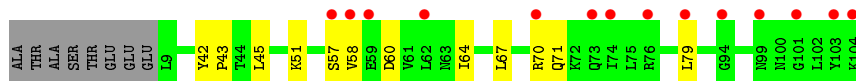
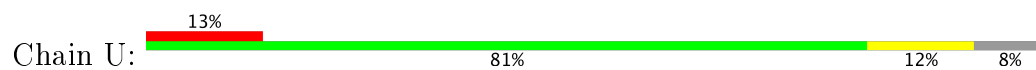


- Molecule 14: Photosystem II reaction center protein T





- Molecule 15: Photosystem II 12 kDa extrinsic protein



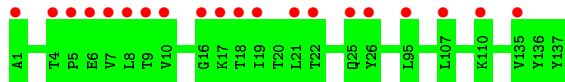
- Molecule 15: Photosystem II 12 kDa extrinsic protein



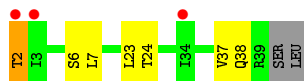
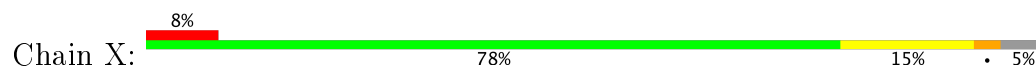
- Molecule 16: Cytochrome c-550



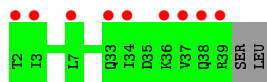
- Molecule 16: Cytochrome c-550



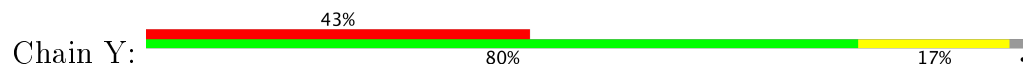
- Molecule 17: Photosystem II reaction center protein X



- Molecule 17: Photosystem II reaction center protein X

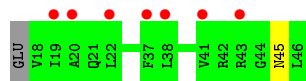


- Molecule 18: Photosystem II reaction center protein Ycf12

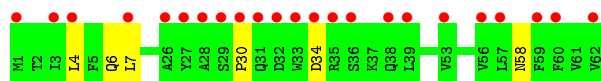
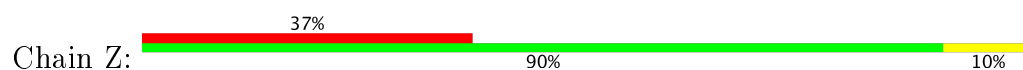




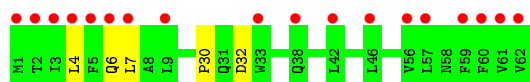
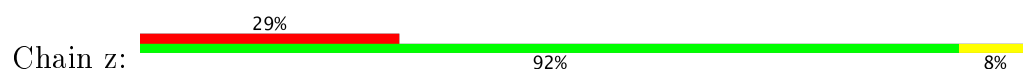
- Molecule 18: Photosystem II reaction center protein Ycf12



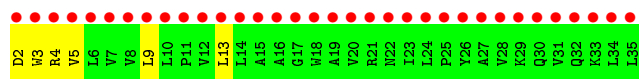
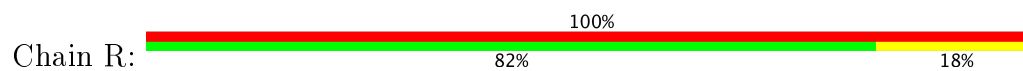
- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.52Å 231.23Å 287.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 46.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.50) 100.0 (46.51-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.187 0.146 , 0.190	Depositor DCC
R_{free} test set	14584 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52752	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, SQD, BCT, HEM, FME, UNL, HTG, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/2705	0.56	0/3689
1	a	0.43	0/2705	0.54	0/3689
2	B	0.42	0/4109	0.54	0/5600
2	b	0.41	0/4109	0.54	0/5600
3	C	0.39	0/3599	0.51	0/4900
3	c	0.39	0/3633	0.53	0/4946
4	D	0.43	0/2821	0.54	0/3844
4	d	0.43	0/2812	0.54	0/3832
5	E	0.35	0/681	0.53	0/928
5	e	0.37	0/667	0.49	0/908
6	F	0.34	0/284	0.48	0/387
6	f	0.40	0/257	0.49	0/349
7	H	0.36	0/519	0.53	0/708
7	h	0.35	0/524	0.49	0/713
8	I	0.37	0/311	0.51	0/419
8	i	0.36	0/311	0.54	0/419
9	J	0.36	0/278	0.46	0/376
9	j	0.35	0/283	0.47	0/383
10	K	0.35	0/303	0.53	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.42	0/303	0.51	0/412
11	l	0.38	0/303	0.53	0/412
12	M	0.44	0/253	0.58	0/346
12	m	0.42	0/262	0.58	0/357
13	O	0.38	0/1896	0.58	0/2571
13	o	0.39	0/1896	0.58	0/2571
14	T	0.54	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.57	0/1052
15	u	0.41	0/785	0.57	0/1064
16	V	0.37	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.37	0/1085	0.53	0/1473
17	X	0.33	0/284	0.49	0/384
17	x	0.31	0/284	0.46	0/384
18	Y	0.30	0/216	0.44	0/289
18	y	0.31	0/216	0.50	0/289
19	Z	0.32	0/490	0.46	0/669
19	z	0.32	0/490	0.43	0/669
20	R	0.27	0/279	0.43	0/383
All	All	0.40	0/42631	0.53	0/58018

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2620	0	2517	42	0
1	a	2620	0	2517	0	0
2	B	3969	0	3828	96	0
2	b	3969	0	3828	0	0
3	C	3486	0	3407	75	0
3	c	3519	0	3437	0	0
4	D	2726	0	2627	36	0
4	d	2717	0	2621	0	0
5	E	662	0	648	20	0
5	e	648	0	634	0	0
6	F	275	0	282	8	0
6	f	250	0	261	0	0
7	H	506	0	529	12	0
7	h	511	0	532	0	0
8	I	314	0	328	6	0
8	i	314	0	328	0	0
9	J	272	0	279	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	296	0	304	4	0
11	l	296	0	304	0	0
12	M	260	0	275	6	0
12	m	269	0	288	0	0
13	O	1865	0	1838	33	0
13	o	1865	0	1838	0	0
14	T	258	0	261	6	0
14	t	258	0	261	0	0
15	U	765	0	767	7	0
15	u	774	0	773	0	0
16	V	1064	0	1073	6	0
16	v	1064	0	1073	0	0
17	X	281	0	312	9	0
17	x	281	0	312	0	0
18	Y	215	0	246	4	0
18	y	215	0	246	0	0
19	Z	479	0	516	2	0
19	z	479	0	516	0	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	195	0	216	21	0
23	B	1040	0	1152	104	0
23	C	845	0	936	96	0
23	D	195	0	216	10	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	2	0
24	D	64	0	74	5	0
24	a	128	0	148	0	0
25	A	40	0	56	2	0
25	B	120	0	168	12	0
25	C	120	0	168	7	0
25	D	40	0	56	2	0
25	H	40	0	56	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	6	0
25	Y	40	0	56	3	0
25	a	40	0	56	0	0
25	b	120	0	168	0	0
25	c	80	0	112	0	0
25	d	40	0	56	0	0
25	h	40	0	56	0	0
25	k	40	0	56	0	0
25	t	40	0	56	0	0
25	y	40	0	56	0	0
26	A	108	0	156	5	0
26	B	54	0	78	2	0
26	D	43	0	53	2	0
26	L	54	0	78	4	0
26	a	108	0	156	0	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	12	0	16	4	0
27	C	6	0	8	0	0
27	O	6	0	8	0	0
27	a	6	0	8	0	0
27	b	6	0	8	0	0
27	d	6	0	8	0	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	5	0
29	D	55	0	80	2	0
29	a	55	0	80	0	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	1	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	M	10	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	69	0	0	0	0
30	c	32	0	0	0	0
30	d	17	0	0	0	0
30	i	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	49	0	74	4	0
31	D	98	0	148	11	0
31	E	42	0	57	2	0
31	L	49	0	74	0	0
31	b	49	0	74	0	0
31	d	147	0	222	0	0
31	e	42	0	57	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	C	1	0	0	0	0
33	O	1	0	0	0	0
33	V	1	0	0	0	0
33	c	2	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	7	0
34	J	51	0	72	4	0
34	Z	37	0	44	3	0
34	a	51	0	72	0	0
34	c	102	0	144	0	0
34	j	51	0	71	0	0
34	m	51	0	72	0	0
34	z	39	0	48	0	0
35	B	121	0	162	9	0
35	C	35	0	46	1	0
35	D	35	0	46	0	0
35	E	35	0	46	1	0
35	M	70	0	92	4	0
35	a	35	0	46	0	0
35	b	50	0	70	0	0
35	e	35	0	46	0	0
35	m	35	0	46	0	0
36	B	95	0	130	6	0
36	C	28	0	41	2	0
36	D	16	0	17	1	0
36	V	11	0	10	0	0
36	b	95	0	130	0	0
36	c	38	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	h	16	0	17	0	0
37	C	186	0	246	10	0
37	H	62	0	82	0	0
37	c	186	0	246	0	0
37	h	62	0	82	0	0
38	E	43	0	30	6	0
38	V	43	0	30	0	0
38	e	43	0	30	0	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	135	0	0	2	0
40	B	195	0	0	18	0
40	C	151	0	0	11	0
40	D	118	0	0	8	0
40	E	25	0	0	3	0
40	F	5	0	0	0	0
40	H	22	0	0	3	0
40	I	6	0	0	1	0
40	J	4	0	0	0	0
40	K	6	0	0	0	0
40	L	6	0	0	0	0
40	M	15	0	0	2	0
40	O	105	0	0	0	0
40	R	1	0	0	0	0
40	T	13	0	0	0	0
40	U	51	0	0	0	0
40	V	81	0	0	3	0
40	X	4	0	0	0	0
40	Y	1	0	0	0	0
40	Z	1	0	0	1	0
40	a	132	0	0	0	0
40	b	206	0	0	0	0
40	c	153	0	0	0	0
40	d	115	0	0	0	0
40	e	16	0	0	0	0
40	f	5	0	0	0	0
40	h	27	0	0	0	0
40	i	3	0	0	0	0
40	j	3	0	0	0	0
40	k	6	0	0	0	0
40	l	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	m	18	0	0	0	0
40	o	115	0	0	0	0
40	t	9	0	0	0	0
40	u	62	0	0	0	0
40	v	78	0	0	0	0
40	x	8	0	0	0	0
40	z	1	0	0	0	0
All	All	52752	0	51821	559	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (559) 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)
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.54	0.94
23:B:605:CLA:H42	23:B:606:CLA:H2	1.48	0.93
4:D:199:MET:O	40:D:501:HOH:O	1.96	0.83
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.38	0.81
25:B:618:BCR:H363	25:T:101:BCR:H19C	31.54	0.80
25:H:101:BCR:H331	25:H:101:BCR:HC8	1.65	0.79
5:E:67:THR:H	5:E:75:GLN:HE22	2.65	0.78
25:T:101:BCR:HC8	25:T:101:BCR:H321	1.95	0.76
31:D:408:LHG:H122	31:D:408:LHG:H382	15.58	0.76
4:D:24:ARG:HD3	17:X:37:VAL:HG22	2.12	0.76
7:H:37:LEU:O	40:H:201:HOH:O	2.03	0.75
4:D:202:ALA:HB3	40:D:501:HOH:O	1.86	0.75
25:B:619:BCR:H363	25:T:101:BCR:H19C	35.52	0.75
3:C:63:TRP:HB3	40:C:604:HOH:O	1.88	0.74
23:C:502:CLA:H151	23:C:508:CLA:HMB3	1.70	0.73
2:B:497:GLN:HB2	2:B:504:THR:HB	2.49	0.73
23:A:405:CLA:H152	29:A:413:PL9:H252	1.71	0.73
23:C:512:CLA:HBB1	23:C:512:CLA:HHC	4.65	0.72
13:O:54:GLU:HG2	13:O:64:GLU:H	1.54	0.72
5:E:9:PRO:HA	31:E:101:LHG:HC31	2.12	0.72
23:C:503:CLA:HBB1	34:C:520:LMG:H231	13.24	0.72
1:A:25:ASP:OD1	40:A:501:HOH:O	2.07	0.71
23:B:604:CLA:H42	23:B:605:CLA:H2	14.99	0.70
3:C:279:LEU:HD22	23:C:509:CLA:HED2	17.15	0.70
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.73	0.70
23:C:502:CLA:H61	23:C:512:CLA:H42	38.86	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:165:LEU:HD23	23:C:507:CLA:HED1	13.08	0.70
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	4.51	0.69
3:C:168:LEU:HD21	23:C:509:CLA:H61	24.54	0.69
26:A:409:SQD:H251	31:D:409:LHG:H131	1.76	0.68
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.27	0.68
26:A:411:SQD:H301	23:C:508:CLA:H71	44.00	0.67
8:I:35:LYS:O	8:I:37:LEU:N	2.72	0.67
1:A:253:GLY:HA3	2:B:491:VAL:HG12	4.15	0.67
23:B:610:CLA:HHC	23:B:610:CLA:HBB1	1.75	0.67
1:A:214:MET:HG2	29:A:413:PL9:H103	1.76	0.67
5:E:40:THR:HB	20:R:4:ARG:HD2	1.77	0.67
23:B:615:CLA:H92	35:M:103:LMT:H92	21.40	0.67
8:I:37:LEU:O	40:I:201:HOH:O	2.13	0.66
2:B:405:GLU:OE1	40:B:701:HOH:O	32.95	0.66
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.77	0.66
31:D:408:LHG:H142	31:D:408:LHG:H372	13.14	0.65
23:B:615:CLA:H2	23:B:616:CLA:HBB2	31.12	0.65
23:C:507:CLA:HMC2	23:C:508:CLA:H102	1.79	0.65
2:B:145:LEU:HD11	23:B:616:CLA:HMB2	1.77	0.65
2:B:61:PHE:O	40:B:701:HOH:O	2.14	0.65
2:B:103:LEU:HD21	23:B:605:CLA:HMC3	18.63	0.64
29:D:407:PL9:H28	40:D:501:HOH:O	1.96	0.64
3:C:174:LEU:HD22	23:C:502:CLA:H203	24.25	0.64
23:B:607:CLA:HBB1	23:B:607:CLA:HHC	1.79	0.64
23:C:507:CLA:H71	35:C:522:LMT:H111	1.79	0.64
2:B:314:TYR:O	40:B:702:HOH:O	52.92	0.64
23:B:602:CLA:H12	23:B:602:CLA:H71	1.78	0.63
5:E:27:ILE:HD11	38:E:103:HEM:HBC2	1.79	0.63
1:A:72:LEU:HD11	35:B:633:LMT:H52	43.01	0.63
2:B:103:LEU:HD21	23:B:606:CLA:HMC3	1.81	0.63
2:B:121:GLU:HG2	7:H:4:ARG:HG2	2.47	0.63
23:C:508:CLA:HBC3	23:C:510:CLA:H71	13.89	0.63
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.68	0.62
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.80	0.62
38:E:103:HEM:HAC	6:F:27:ALA:HB1	2.01	0.62
23:A:405:CLA:HMD3	4:D:182:LEU:HD11	1.81	0.62
13:O:58:ASN:HD21	13:O:61:GLN:HB2	3.81	0.62
36:B:624:HTG:H1	35:B:633:LMT:H21	1.82	0.62
3:C:95:LEU:HD13	23:C:502:CLA:H142	21.74	0.61
3:C:165:LEU:HD22	40:C:704:HOH:O	44.74	0.61
23:C:508:CLA:HBB1	23:C:508:CLA:HMB1	4.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ARG:NH2	26:L:102:SQD:O9	38.09	0.60
2:B:54:PRO:HB3	27:B:628:GOL:H11	1.84	0.60
5:E:60:GLN:HE21	5:E:62:SER:H	1.81	0.60
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.82	0.60
34:C:501:LMG:H211	37:C:517:DGD:HA82	1.83	0.60
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.85	0.59
2:B:497:GLN:NE2	17:X:38:GLN:O	2.34	0.59
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.33	0.59
23:A:404:CLA:HBB1	23:A:404:CLA:HMB1	1.85	0.59
23:C:506:CLA:HMC2	23:C:507:CLA:H102	10.21	0.59
31:D:409:LHG:H372	31:D:409:LHG:H132	1.85	0.59
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.85	0.58
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.14	0.58
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.83	0.58
4:D:46:GLY:HA2	40:D:526:HOH:O	2.02	0.58
2:B:167:TRP:NE1	40:B:706:HOH:O	2.32	0.58
7:H:56:ASP:OD1	17:X:2:THR:OG1	2.65	0.58
3:C:56:HIS:HB2	23:C:510:CLA:HMB2	1.84	0.57
23:B:615:CLA:H43	26:B:621:SQD:H111	1.85	0.57
3:C:60:ILE:HG22	23:C:504:CLA:HHD	1.86	0.57
26:A:409:SQD:H171	31:D:409:LHG:H182	1.86	0.57
23:B:604:CLA:HMD2	23:B:612:CLA:H203	20.30	0.57
23:C:505:CLA:CMD	23:C:507:CLA:HAB	33.95	0.57
1:A:183:MET:HA	23:A:404:CLA:HMD2	1.88	0.57
36:B:624:HTG:H61	35:B:633:LMT:H6E	1.86	0.57
23:A:407:CLA:H152	37:C:517:DGD:HAW1	1.86	0.57
13:O:92:SER:HB3	13:O:131:PRO:HA	1.87	0.57
2:B:30:VAL:HG12	23:B:605:CLA:HHD	11.90	0.56
23:B:615:CLA:H191	35:B:634:LMT:H102	1.85	0.56
5:E:60:GLN:HE21	5:E:62:SER:N	2.47	0.56
34:Z:101:LMG:O5	34:Z:101:LMG:O4	2.23	0.56
5:E:27:ILE:CD1	38:E:103:HEM:HBC2	2.35	0.56
23:A:407:CLA:H151	23:C:507:CLA:H13	1.86	0.56
13:O:83:GLY:HA2	13:O:98:GLU:HG3	2.21	0.56
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.00	0.56
2:B:264:PRO:HB2	40:B:706:HOH:O	2.06	0.56
1:A:227:THR:HB	1:A:231:GLU:HG3	1.94	0.56
2:B:216:HIS:HE1	23:B:610:CLA:C1A	2.19	0.56
2:B:98:LEU:HD13	36:B:624:HTG:H7'1	1.88	0.56
3:C:325:GLY:O	15:U:51:LYS:NZ	2.39	0.56
3:C:433:LEU:HD22	23:C:503:CLA:HMC3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:20:GLY:O	11:L:24:ILE:HG12	2.06	0.55
26:D:413:SQD:H241	6:F:18:VAL:HG22	1.87	0.55
2:B:462:PHE:CE1	23:B:614:CLA:HMB3	2.42	0.55
2:B:227:LYS:NZ	40:B:704:HOH:O	2.28	0.55
23:D:401:CLA:HHC	23:D:401:CLA:HBB1	1.88	0.55
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.38	0.55
3:C:26:ARG:HE	10:K:46:ARG:NH1	2.05	0.54
5:E:60:GLN:HG3	5:E:62:SER:H	1.91	0.54
2:B:216:HIS:HE1	23:B:609:CLA:C1A	16.10	0.54
3:C:167:VAL:HG11	23:C:512:CLA:HBA2	26.02	0.54
23:B:608:CLA:HAB	4:D:123:ILE:HG12	26.11	0.54
4:D:49:LEU:HD12	40:D:526:HOH:O	2.06	0.54
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.40	0.54
3:C:27:ASP:HB3	10:K:46:ARG:HG3	2.58	0.54
3:C:161:LEU:HD11	23:C:507:CLA:HBB1	1.90	0.54
8:I:17:LEU:HD22	8:I:21:PHE:HE2	1.79	0.54
23:B:611:CLA:HBB1	23:B:611:CLA:HMB1	4.46	0.54
3:C:41:ARG:NH1	23:C:511:CLA:HMD1	17.19	0.54
12:M:8:LEU:HD11	35:M:103:LMT:H91	1.90	0.54
13:O:56:PRO:HB3	13:O:61:GLN:HG2	1.89	0.53
2:B:462:PHE:CE1	23:B:613:CLA:HMB3	10.34	0.53
3:C:181:PHE:HE2	36:C:524:HTG:H7'3	1.73	0.53
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.91	0.53
25:H:101:BCR:H363	40:H:201:HOH:O	2.08	0.53
2:B:219:VAL:O	40:B:703:HOH:O	48.99	0.53
2:B:299:GLU:HG3	40:B:862:HOH:O	27.95	0.53
35:B:634:LMT:H123	12:M:12:ALA:HA	12.03	0.53
2:B:267:LEU:HG	40:B:706:HOH:O	2.08	0.53
23:B:605:CLA:HMA1	23:B:606:CLA:H3A	10.48	0.53
2:B:24:LEU:HD21	23:B:617:CLA:HAB	1.89	0.53
16:V:12:LEU:HD12	16:V:69:ILE:HB	2.23	0.53
23:C:513:CLA:H152	34:C:520:LMG:H422	30.51	0.52
24:A:406:PHO:HAB	4:D:205:LEU:HD13	1.90	0.52
23:C:504:CLA:H151	23:C:508:CLA:H143	19.90	0.52
31:A:415:LHG:H142	23:B:608:CLA:H201	1.91	0.52
2:B:285:ASN:O	2:B:289:GLN:HG2	2.09	0.52
40:E:203:HOH:O	9:J:2:SER:N	2.42	0.52
3:C:42:LEU:HD21	23:C:511:CLA:H2A	12.77	0.52
2:B:223:GLN:HA	2:B:223:GLN:HE21	3.81	0.52
23:B:607:CLA:H192	23:B:617:CLA:H101	1.92	0.52
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:A:415:LHG:H252	2:B:464:PHE:CZ	2.44	0.52
23:B:616:CLA:HHC	23:B:616:CLA:HBB1	1.92	0.52
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.92	0.52
23:C:505:CLA:HMD2	23:C:507:CLA:HAB	34.03	0.51
6:F:30:THR:HG21	34:J:101:LMG:H412	1.91	0.51
2:B:482:ILE:HD12	2:B:486:LEU:HD12	5.62	0.51
3:C:182:PHE:HA	36:C:523:HTG:H61	1.92	0.51
12:M:5:GLN:NE2	12:M:5:GLN:H	5.22	0.51
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.91	0.51
23:A:404:CLA:H191	31:D:408:LHG:H332	1.93	0.51
23:B:602:CLA:H101	23:B:609:CLA:H193	22.75	0.51
3:C:218:PHE:HE2	34:C:501:LMG:H111	1.75	0.51
40:M:203:HOH:O	14:T:1:FME:SD	2.59	0.51
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.61	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.10	0.51
26:A:411:SQD:H261	2:B:109:LEU:HD13	59.19	0.51
3:C:244:CYS:HA	40:C:704:HOH:O	47.67	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.11	0.51
7:H:41:PHE:N	40:H:201:HOH:O	2.43	0.51
3:C:413:GLU:OE2	40:C:601:HOH:O	2.19	0.51
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.40	0.51
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.92	0.51
13:O:27:ARG:NH1	13:O:202:ALA:O	2.43	0.51
1:A:102:LEU:HD12	36:B:629:HTG:H61	72.52	0.50
23:C:512:CLA:H143	23:C:513:CLA:H142	29.49	0.50
38:E:103:HEM:HMC2	6:F:31:ILE:HG13	1.93	0.50
2:B:450:TRP:HB3	23:B:608:CLA:HMB2	1.93	0.50
2:B:149:LEU:HG	23:B:606:CLA:HBB2	8.53	0.50
23:B:613:CLA:CMB	23:B:615:CLA:HBB1	2.41	0.50
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.92	0.50
14:T:14:ILE:HG22	25:T:101:BCR:H10C	1.93	0.50
23:A:407:CLA:H171	23:C:507:CLA:H112	1.92	0.50
23:B:604:CLA:HBB2	23:B:606:CLA:H193	1.93	0.50
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.14	0.50
1:A:63:ILE:HB	3:C:335:THR:HG21	1.94	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.50
4:D:332:GLN:OE1	4:D:332:GLN:N	2.68	0.50
2:B:141:ILE:HD11	7:H:14:LEU:HD22	2.38	0.50
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.47	0.50
23:B:609:CLA:HMD1	23:B:611:CLA:CBB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:510:CLA:H51	31:D:408:LHG:H371	39.93	0.50
2:B:54:PRO:HB2	27:B:628:GOL:H31	1.94	0.49
8:I:36:ASP:OD1	8:I:36:ASP:N	3.99	0.49
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.06	0.49
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.95	0.49
25:B:618:BCR:H291	40:B:861:HOH:O	2.11	0.49
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.93	0.49
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.56	0.49
2:B:57:ARG:HH21	2:B:331:ASN:HD22	1.60	0.49
3:C:174:LEU:HB3	23:C:503:CLA:H151	1.94	0.49
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.94	0.49
2:B:266:GLU:HB2	40:B:706:HOH:O	2.11	0.49
8:I:2:GLU:O	8:I:6:ILE:HG12	2.21	0.49
26:L:102:SQD:H462	26:L:102:SQD:H1	1.95	0.49
13:O:51:LEU:HD12	13:O:234:LYS:HG2	1.95	0.49
2:B:219:VAL:O	40:B:702:HOH:O	2.19	0.49
37:C:517:DGD:HG11	40:C:616:HOH:O	2.12	0.49
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.48	0.49
5:E:60:GLN:HB3	40:E:207:HOH:O	38.63	0.49
40:D:556:HOH:O	17:X:6:SER:HA	32.64	0.49
23:C:514:CLA:HAB	25:C:515:BCR:H24C	1.95	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.02	0.48
37:C:518:DGD:HAH1	34:J:101:LMG:H201	8.64	0.48
13:O:32:ILE:HG21	13:O:93:LEU:HD21	2.20	0.48
24:A:406:PHO:HBB1	24:A:406:PHO:HMB1	1.95	0.48
23:C:505:CLA:HAA1	23:C:505:CLA:HBD	2.12	0.48
1:A:221:SER:HA	4:D:139:ARG:HB2	1.96	0.48
26:B:621:SQD:H381	35:M:103:LMT:H123	16.25	0.48
13:O:124:ASN:HD22	13:O:147:ASN:ND2	2.07	0.48
2:B:145:LEU:HD11	23:B:615:CLA:HMB2	21.90	0.48
23:B:615:CLA:H152	23:B:615:CLA:H111	2.10	0.48
3:C:391:ARG:HD3	40:C:742:HOH:O	2.14	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.49	0.48
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.94	0.47
23:B:602:CLA:C4D	23:B:602:CLA:H72	2.44	0.47
5:E:26:THR:HB	38:E:103:HEM:HAB	2.32	0.47
19:Z:34:ASP:HB3	40:Z:201:HOH:O	2.14	0.47
3:C:406:SER:HA	3:C:420:VAL:HG23	1.97	0.47
3:C:60:ILE:HA	40:C:604:HOH:O	2.13	0.47
25:D:406:BCR:H381	34:J:101:LMG:H231	1.97	0.47
23:B:615:CLA:H41	23:B:615:CLA:H62	1.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:407:CLA:H171	23:C:507:CLA:H142	1.95	0.47
23:C:513:CLA:C4A	23:C:513:CLA:HBA1	4.89	0.47
3:C:429:SER:HA	37:C:517:DGD:HBW1	13.29	0.47
23:B:611:CLA:H122	23:B:616:CLA:HAA1	1.97	0.47
23:C:506:CLA:HMD2	23:C:508:CLA:HAB	1.96	0.47
24:D:402:PHO:H3A	23:D:404:CLA:H142	1.95	0.47
23:B:615:CLA:H61	23:B:615:CLA:H92	1.75	0.47
3:C:165:LEU:CD2	23:C:507:CLA:HED1	12.18	0.47
34:J:101:LMG:H292	34:J:101:LMG:H151	2.51	0.47
1:A:307:ILE:HD13	1:A:313:VAL:HA	2.13	0.47
23:C:509:CLA:H142	23:C:509:CLA:H111	1.74	0.47
31:D:408:LHG:H122	31:D:408:LHG:C38	15.29	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.51	0.46
23:B:605:CLA:HAB	23:B:612:CLA:H191	1.97	0.46
3:C:38:GLY:HA3	23:C:511:CLA:HMD3	15.15	0.46
13:O:132:ASN:O	13:O:132:ASN:ND2	4.77	0.46
2:B:497:GLN:HE22	17:X:38:GLN:HB2	2.17	0.46
25:A:408:BCR:H371	25:A:408:BCR:H24C	1.72	0.46
23:B:606:CLA:H162	23:B:606:CLA:H122	4.39	0.46
23:C:512:CLA:HBB1	23:C:512:CLA:HMB1	1.97	0.46
1:A:217:SER:HA	4:D:272:LEU:HD12	1.97	0.46
16:V:103:LYS:HB3	40:V:324:HOH:O	2.16	0.46
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.96	0.46
2:B:357:ARG:NE	40:B:708:HOH:O	2.37	0.46
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.97	0.46
23:C:507:CLA:HBD	23:C:507:CLA:HAA2	3.33	0.46
23:C:509:CLA:H192	23:C:512:CLA:HHD	13.76	0.46
2:B:462:PHE:HE1	23:B:613:CLA:HMB3	9.82	0.46
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.50	0.46
1:A:163:ILE:HD11	37:C:517:DGD:HA22	1.98	0.46
2:B:29:LEU:HD23	26:L:102:SQD:H201	37.76	0.46
23:C:512:CLA:O2D	23:C:513:CLA:HBB2	25.46	0.46
4:D:230:SER:HB2	40:D:577:HOH:O	2.16	0.46
23:C:506:CLA:HMC3	40:C:704:HOH:O	34.74	0.46
23:B:603:CLA:H3A	23:B:603:CLA:CGA	4.23	0.46
23:B:605:CLA:HBD	23:B:605:CLA:HAA1	2.18	0.46
25:B:620:BCR:C8	25:B:620:BCR:H331	2.45	0.46
3:C:214:LEU:HA	3:C:214:LEU:HD23	1.85	0.46
4:D:49:LEU:HB2	40:D:526:HOH:O	2.16	0.46
1:A:12:ASN:ND2	1:A:15:GLU:HB2	2.31	0.46
23:B:615:CLA:H203	34:B:622:LMG:H421	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:186:TYR:OH	3:C:194:GLY:HA3	2.16	0.46
23:D:401:CLA:C4A	23:D:401:CLA:HBA1	2.46	0.46
23:B:605:CLA:H111	23:B:605:CLA:H91	2.37	0.46
3:C:334:PRO:HA	13:O:153:THR:OG1	2.16	0.46
2:B:133:LEU:HB3	2:B:138:MET:SD	2.56	0.45
23:B:603:CLA:H101	23:B:610:CLA:H193	1.99	0.45
23:B:603:CLA:H143	23:B:608:CLA:HAC1	26.68	0.45
35:E:102:LMT:O2B	35:E:102:LMT:O3'	2.27	0.45
5:E:68:ASP:HB3	5:E:71:GLU:HB3	2.50	0.45
13:O:124:ASN:ND2	13:O:147:ASN:HD22	2.13	0.45
23:A:405:CLA:HBB1	23:A:405:CLA:HMB1	4.14	0.45
2:B:229:LEU:HD22	23:B:608:CLA:HED2	41.85	0.45
23:B:603:CLA:H141	23:B:603:CLA:H161	1.81	0.45
31:D:409:LHG:H141	31:D:409:LHG:H352	1.99	0.45
1:A:308:ASP:O	6:F:45:ARG:HD2	2.16	0.45
1:A:183:MET:HB3	23:A:404:CLA:HBC2	2.21	0.45
23:B:605:CLA:H41	23:B:605:CLA:H62	1.76	0.45
23:B:606:CLA:HAA1	23:B:606:CLA:HBD	1.99	0.45
3:C:433:LEU:HD22	23:C:502:CLA:HMC3	19.87	0.45
2:B:462:PHE:HE1	23:B:614:CLA:HMB3	1.81	0.45
29:A:413:PL9:H253	23:D:404:CLA:H141	1.99	0.45
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.47	0.45
2:B:24:LEU:HD21	23:B:616:CLA:CAB	12.99	0.45
2:B:360:PRO:HB3	27:B:627:GOL:H32	1.98	0.45
23:C:506:CLA:HBD	23:C:506:CLA:HAA1	1.99	0.45
3:C:78:GLU:HB3	40:V:325:HOH:O	30.58	0.45
7:H:43:LEU:HD12	7:H:43:LEU:HA	1.87	0.45
13:O:40:ILE:HG12	13:O:243:ILE:HD13	2.30	0.45
2:B:54:PRO:CB	27:B:628:GOL:H11	2.47	0.45
3:C:38:GLY:HA3	23:C:512:CLA:HMD3	1.99	0.45
23:C:507:CLA:H62	23:C:507:CLA:H41	1.70	0.45
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.57	0.45
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.45
23:B:611:CLA:H172	23:B:613:CLA:ND	4.42	0.45
5:E:33:ALA:HB3	40:E:219:HOH:O	2.16	0.45
13:O:30:TYR:HA	13:O:31:PRO:HD3	1.68	0.45
2:B:79:SER:HA	40:B:713:HOH:O	27.92	0.45
5:E:15:THR:HB	9:J:7:ILE:O	2.17	0.45
9:J:20:VAL:HA	9:J:23:ILE:HG22	2.25	0.45
23:A:404:CLA:CBD	23:D:401:CLA:HAC2	2.47	0.44
23:B:606:CLA:H161	23:B:606:CLA:H141	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:614:CLA:H41	23:B:614:CLA:H62	2.45	0.44
1:A:121:LEU:HD13	34:C:501:LMG:H182	1.99	0.44
23:C:506:CLA:H122	23:C:506:CLA:H162	4.42	0.44
3:C:109:PHE:CE2	34:C:520:LMG:HC72	26.04	0.44
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.63	0.44
2:B:363:PHE:HB3	2:B:365:SER:O	2.17	0.44
23:B:610:CLA:H152	23:B:610:CLA:OBD	18.91	0.44
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.99	0.44
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.05	0.44
3:C:146:PHE:HZ	23:C:512:CLA:HBB2	25.09	0.44
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.47	0.44
23:C:506:CLA:HMD3	23:C:508:CLA:HAB	1.99	0.44
3:C:56:HIS:HB2	23:C:509:CLA:HMB2	7.50	0.44
31:D:408:LHG:H192	14:T:17:PHE:HZ	1.82	0.44
11:L:9:PRO:HA	35:M:101:LMT:H6D	17.16	0.44
12:M:28:GLN:O	12:M:32:GLN:HG3	2.17	0.44
10:K:16:ALA:O	10:K:19:ASP:HB2	2.22	0.44
23:C:508:CLA:H92	23:C:508:CLA:H61	1.71	0.44
20:R:9:LEU:O	20:R:13:LEU:HG	2.17	0.44
1:A:131:TRP:CH2	23:C:505:CLA:HAA2	41.09	0.44
23:C:507:CLA:H142	23:C:507:CLA:H112	1.95	0.44
2:B:470:GLY:HA2	40:B:707:HOH:O	32.75	0.44
34:B:622:LMG:O10	12:M:4:ASN:ND2	2.51	0.44
2:B:245:VAL:HG22	23:B:613:CLA:H202	2.00	0.44
23:B:610:CLA:HBA1	23:B:610:CLA:H3A	1.82	0.44
3:C:171:GLY:O	3:C:174:LEU:HB2	2.18	0.44
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	15.40	0.44
3:C:213:LEU:HD21	25:C:516:BCR:C20	2.47	0.44
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.72	0.44
23:C:511:CLA:H191	34:Z:101:LMG:H242	21.46	0.44
24:D:402:PHO:HMB1	24:D:402:PHO:HBB1	2.00	0.44
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.28	0.44
25:A:408:BCR:H15C	25:A:408:BCR:H351	1.80	0.43
2:B:256:MET:HA	2:B:263:THR:HG21	2.19	0.43
23:B:604:CLA:H62	23:B:604:CLA:H41	2.14	0.43
2:B:13:ILE:HG12	23:B:613:CLA:HAC2	1.99	0.43
23:B:614:CLA:H162	23:B:614:CLA:H122	3.48	0.43
25:B:620:BCR:H351	25:B:620:BCR:H15C	1.86	0.43
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.00	0.43
23:C:507:CLA:H3A	23:C:507:CLA:HBA1	1.69	0.43
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:21:VAL:O	6:F:25:THR:HG23	2.26	0.43
13:O:51:LEU:HD23	13:O:67:PRO:HA	2.19	0.43
26:L:102:SQD:H211	25:T:101:BCR:H351	1.99	0.43
16:V:30:LYS:NZ	40:V:302:HOH:O	24.55	0.43
23:A:404:CLA:H193	23:A:404:CLA:H161	3.22	0.43
23:C:507:CLA:H111	23:C:507:CLA:H91	1.85	0.43
23:C:514:CLA:H161	34:C:521:LMG:H421	2.00	0.43
2:B:159:THR:HA	2:B:181:VAL:O	2.27	0.43
2:B:24:LEU:HD21	23:B:617:CLA:CAB	2.48	0.43
3:C:48:LYS:HG2	3:C:133:ALA:O	2.47	0.43
23:C:511:CLA:H112	23:C:511:CLA:H152	1.75	0.43
23:D:401:CLA:H203	23:D:401:CLA:H162	1.68	0.43
25:H:101:BCR:H331	25:H:101:BCR:C8	2.38	0.43
7:H:4:ARG:HH11	7:H:9:ASP:CG	2.71	0.43
9:J:3:GLU:O	9:J:6:ARG:HG2	2.75	0.43
23:B:609:CLA:HMD1	7:H:27:THR:HB	16.31	0.43
23:C:512:CLA:HBB1	23:C:512:CLA:CHC	4.89	0.43
37:C:518:DGD:HAE2	37:C:518:DGD:HA81	1.59	0.43
3:C:60:ILE:HG22	23:C:503:CLA:HHD	11.60	0.43
1:A:231:GLU:HB3	40:B:849:HOH:O	2.18	0.43
1:A:190:HIS:O	1:A:298:ASN:HB3	2.17	0.43
25:B:619:BCR:H351	25:B:619:BCR:H15C	1.76	0.43
3:C:385:GLN:HG3	40:C:709:HOH:O	18.16	0.43
3:C:463:SER:OG	8:I:33:LYS:NZ	2.49	0.43
31:E:101:LHG:HC61	31:E:101:LHG:H241	2.08	0.43
25:H:101:BCR:H393	17:X:7:LEU:HD21	2.00	0.43
14:T:2:GLU:CD	14:T:2:GLU:H	2.22	0.43
2:B:299:GLU:HG3	40:B:821:HOH:O	2.17	0.43
3:C:437:PHE:CE1	23:C:510:CLA:HMB3	9.83	0.43
31:A:415:LHG:H151	11:L:23:LEU:HD21	2.01	0.43
2:B:162:PHE:O	23:B:607:CLA:HHD	2.19	0.43
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.84	0.43
40:B:875:HOH:O	13:O:178:LYS:HD2	66.30	0.43
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.17	0.43
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.05	0.43
25:B:618:BCR:H351	25:B:618:BCR:H15C	1.93	0.43
25:C:527:BCR:H371	25:C:527:BCR:H24C	1.70	0.43
13:O:234:LYS:HE2	13:O:234:LYS:HB2	1.86	0.43
13:O:90:ASP:O	13:O:132:ASN:N	2.45	0.43
1:A:131:TRP:CH2	23:C:506:CLA:HAA2	2.54	0.42
25:C:516:BCR:H24C	25:C:516:BCR:H371	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:HIS:CB	23:C:513:CLA:HMD1	2.49	0.42
23:D:405:CLA:HHC	23:D:405:CLA:HBB1	2.01	0.42
5:E:25:ILE:O	5:E:28:PRO:HD2	2.19	0.42
23:B:606:CLA:H92	23:B:606:CLA:H61	1.75	0.42
23:B:612:CLA:H72	23:B:612:CLA:H112	1.78	0.42
23:B:612:CLA:H192	23:B:612:CLA:H162	2.64	0.42
23:B:615:CLA:HBB1	23:B:615:CLA:HHC	4.18	0.42
4:D:120:PHE:HA	4:D:123:ILE:HD12	2.00	0.42
4:D:261:PHE:HB2	29:D:407:PL9:H522	2.02	0.42
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.67	0.42
2:B:467:ILE:HA	2:B:467:ILE:HD13	1.97	0.42
23:B:602:CLA:H41	7:H:46:LEU:HA	21.15	0.42
5:E:60:GLN:HE21	5:E:62:SER:HB3	1.83	0.42
36:B:625:HTG:O6	13:O:177:ALA:O	2.24	0.42
1:A:187:GLN:HB2	23:A:404:CLA:HAC2	2.01	0.42
23:B:602:CLA:H111	23:B:602:CLA:H91	2.28	0.42
25:B:618:BCR:H371	25:B:618:BCR:H24C	1.92	0.42
3:C:154:LYS:NZ	40:C:617:HOH:O	2.52	0.42
3:C:203:THR:O	3:C:235:GLY:HA3	2.23	0.42
37:C:519:DGD:HBT2	37:C:519:DGD:HBH1	1.77	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.13	0.42
2:B:220:ARG:HG3	7:H:20:LYS:HG2	2.22	0.42
23:B:607:CLA:H161	23:B:607:CLA:H122	1.84	0.42
23:B:612:CLA:H102	23:B:612:CLA:H61	4.59	0.42
23:B:613:CLA:HMB1	23:B:615:CLA:HBB1	2.01	0.42
23:C:513:CLA:H203	23:C:513:CLA:H161	2.08	0.42
23:C:504:CLA:H43	37:C:518:DGD:HB32	19.42	0.42
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.54	0.42
3:C:433:LEU:HD13	23:C:503:CLA:CHC	2.49	0.42
3:C:165:LEU:HD21	23:C:507:CLA:CBB	2.50	0.42
23:C:509:CLA:H171	23:C:512:CLA:HMD2	16.92	0.42
1:A:221:SER:HB2	4:D:139:ARG:O	2.20	0.42
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.55	0.42
23:B:607:CLA:H192	23:B:607:CLA:H162	1.94	0.42
35:B:623:LMT:H62	35:B:623:LMT:H91	1.65	0.42
3:C:137:PRO:HG3	23:C:514:CLA:HED3	2.02	0.42
23:C:505:CLA:H41	23:C:505:CLA:H62	1.76	0.42
23:C:509:CLA:H62	23:C:509:CLA:H92	2.64	0.42
4:D:135:LEU:HD23	4:D:135:LEU:HA	1.82	0.42
4:D:13:GLY:HA3	36:D:412:HTG:H62	2.01	0.42
4:D:185:PHE:CG	23:D:404:CLA:HMD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:413:SQD:H342	17:X:24:THR:OG1	2.20	0.42
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.91	0.42
23:B:604:CLA:H2	23:B:606:CLA:H91	2.01	0.42
23:D:404:CLA:HBC3	23:D:404:CLA:HHD	2.02	0.42
17:X:23:LEU:HA	17:X:23:LEU:HD23	1.92	0.42
23:A:404:CLA:CB D	23:A:405:CLA:HAC2	15.75	0.42
2:B:102:VAL:HA	25:B:619:BCR:C40	2.50	0.42
2:B:12:LEU:HB2	23:B:613:CLA:HMC2	2.01	0.42
2:B:149:LEU:HA	2:B:149:LEU:HD12	1.85	0.42
23:B:613:CLA:H111	23:B:613:CLA:H72	4.45	0.42
23:B:616:CLA:H2	25:B:619:BCR:H362	18.07	0.42
23:C:506:CLA:H203	23:C:506:CLA:H162	4.61	0.42
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.20	0.42
18:Y:30:ILE:HA	18:Y:30:ILE:HD12	1.85	0.42
2:B:385:ARG:HG2	13:O:165:ALA:O	2.19	0.42
23:B:606:CLA:H192	23:B:606:CLA:H161	3.42	0.42
23:B:617:CLA:H91	23:B:617:CLA:H112	1.82	0.42
4:D:236:ASN:HA	4:D:237:PRO:HD3	2.02	0.42
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.76	0.42
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.89	0.41
35:B:623:LMT:H5'	30:D:411:UNL:O9	2.20	0.41
1:A:259:ILE:HG22	1:A:260:PHE:CD1	2.75	0.41
2:B:201:HIS:HB2	23:B:603:CLA:CHB	2.50	0.41
2:B:342:GLY:HA3	2:B:403:GLY:O	2.19	0.41
3:C:161:LEU:O	3:C:165:LEU:HG	2.63	0.41
3:C:433:LEU:HD13	23:C:502:CLA:CHC	17.32	0.41
23:C:502:CLA:H42	23:C:503:CLA:HMD1	2.01	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.56	0.41
38:E:103:HEM:CAC	6:F:27:ALA:HB1	2.57	0.41
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.02	0.41
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	9.39	0.41
3:C:178:LYS:HB2	23:C:502:CLA:H161	24.32	0.41
23:C:511:CLA:HMC1	40:C:604:HOH:O	2.19	0.41
15:U:42:TYR:HA	15:U:43:PRO:HA	1.86	0.41
3:C:42:LEU:HD23	23:C:511:CLA:HED3	15.69	0.41
13:O:120:PHE:CD1	13:O:235:ILE:HD13	2.62	0.41
15:U:64:ILE:HB	15:U:67:LEU:HD11	2.02	0.41
1:A:185:VAL:O	1:A:189:GLU:HG3	2.48	0.41
3:C:39:ASN:HD21	23:C:511:CLA:C1C	12.58	0.41
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.08	0.41
4:D:293:LEU:HA	4:D:293:LEU:HD12	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:HG11	23:A:405:CLA:C3D	2.51	0.41
23:B:603:CLA:HBB2	23:B:605:CLA:H193	20.93	0.41
23:B:614:CLA:OBD	23:B:615:CLA:HHC	2.20	0.41
35:B:632:LMT:H122	14:T:7:VAL:HG12	34.21	0.41
23:C:510:CLA:HBD	23:C:510:CLA:HAA2	2.02	0.41
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.87	0.41
23:A:407:CLA:HBA1	23:A:407:CLA:H3A	1.81	0.41
31:A:415:LHG:HC2	2:B:6:TYR:OH	2.21	0.41
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.55	0.41
13:O:91:GLY:HA3	13:O:132:ASN:HA	2.03	0.41
2:B:338:GLN:HA	13:O:57:LYS:HE3	40.52	0.41
23:A:404:CLA:HBD	23:D:401:CLA:HAC2	2.02	0.41
2:B:233:ASN:O	2:B:236:THR:HG22	2.25	0.41
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.55	0.41
2:B:502:VAL:O	2:B:505:ARG:HG3	2.20	0.41
23:B:602:CLA:HAA2	23:B:602:CLA:HBD	3.45	0.41
23:B:604:CLA:C2D	23:B:612:CLA:H172	21.55	0.41
25:B:618:BCR:H11C	25:B:618:BCR:H341	1.90	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.55	0.41
40:A:622:HOH:O	3:C:414:ILE:HD13	2.21	0.41
4:D:12:ARG:HD3	4:D:12:ARG:HA	1.91	0.41
15:U:45:LEU:HA	15:U:45:LEU:HD23	1.88	0.41
34:Z:101:LMG:H141	34:Z:101:LMG:H111	1.81	0.41
1:A:187:GLN:HB2	23:A:404:CLA:CAC	2.51	0.41
1:A:253:GLY:HA2	2:B:493:TRP:CH2	2.81	0.41
1:A:204:GLY:HA3	1:A:282:GLY:HA3	2.18	0.41
23:A:405:CLA:H61	23:A:405:CLA:H102	1.92	0.41
23:A:405:CLA:HMB3	24:D:402:PHO:H172	2.01	0.41
23:B:608:CLA:C4A	23:B:608:CLA:HBA2	2.51	0.41
23:B:616:CLA:H112	23:B:616:CLA:H152	1.47	0.41
2:B:62:VAL:HB	23:B:606:CLA:HED3	2.02	0.41
3:C:72:LEU:HD11	3:C:108:THR:HB	2.08	0.41
25:C:516:BCR:H11C	25:C:516:BCR:H341	1.79	0.41
31:D:408:LHG:HC82	31:D:408:LHG:H112	1.88	0.41
15:U:57:SER:O	15:U:60:ASP:HB2	2.32	0.41
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.15	0.41
29:A:413:PL9:H503	17:X:24:THR:OG1	2.21	0.41
23:B:610:CLA:H122	23:B:615:CLA:HAA1	35.53	0.41
2:B:97:ALA:O	2:B:101:ILE:HG12	2.21	0.41
3:C:41:ARG:NH1	23:C:512:CLA:HMD1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:516:BCR:H351	25:C:516:BCR:H15C	1.90	0.41
3:C:330:SER:HB3	13:O:100:GLY:O	2.25	0.41
1:A:215:HIS:HA	29:A:413:PL9:O1	2.21	0.41
23:B:612:CLA:HAA1	23:B:612:CLA:HBD	2.21	0.41
2:B:25:MET:HG2	25:B:618:BCR:H23C	2.03	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.74	0.41
23:C:510:CLA:C1D	23:C:510:CLA:H171	5.13	0.41
5:E:60:GLN:NE2	5:E:61:ARG:H	2.65	0.41
23:B:611:CLA:H162	23:B:611:CLA:H193	4.68	0.40
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.96	0.40
4:D:127:LEU:HA	4:D:127:LEU:HD23	1.95	0.40
25:Y:101:BCR:H341	25:Y:101:BCR:H11C	1.93	0.40
26:A:411:SQD:H341	23:C:508:CLA:H192	38.50	0.40
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.09	0.40
3:C:223:TRP:CG	3:C:224:ILE:N	2.87	0.40
23:C:508:CLA:H122	23:C:508:CLA:H162	4.32	0.40
23:C:509:CLA:H142	23:C:509:CLA:H112	2.99	0.40
9:J:18:MET:O	9:J:22:VAL:HG23	2.21	0.40
18:Y:32:GLY:HA3	25:Y:101:BCR:C15	2.51	0.40
23:B:613:CLA:H61	23:B:613:CLA:H102	1.82	0.40
23:B:617:CLA:H51	23:B:617:CLA:H11	1.86	0.40
3:C:135:ARG:HA	3:C:135:ARG:HD2	1.99	0.40
35:B:623:LMT:H6E	4:D:16:ASP:OD2	2.20	0.40
24:D:402:PHO:HHD	24:D:402:PHO:HBC2	2.04	0.40
5:E:60:GLN:NE2	5:E:62:SER:HB3	2.55	0.40
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.96	0.40
23:B:608:CLA:HMB1	4:D:126:MET:HB3	28.73	0.40
23:B:615:CLA:H3A	23:B:615:CLA:HBA1	3.22	0.40
36:B:625:HTG:O2	36:B:626:HTG:S1	54.58	0.40
3:C:134:ILE:HD13	23:C:511:CLA:H92	25.28	0.40
3:C:459:ILE:HG21	3:C:464:GLU:HG3	2.07	0.40
23:C:509:CLA:H2A	23:C:509:CLA:O2D	2.22	0.40
24:D:402:PHO:ND	24:D:402:PHO:NC	2.70	0.40
4:D:49:LEU:HD13	25:D:406:BCR:C15	2.51	0.40
20:R:3:TRP:CE2	20:R:4:ARG:HG2	2.57	0.40
2:B:237:VAL:HG12	23:B:613:CLA:HMD1	2.03	0.40
2:B:30:VAL:HG12	23:B:606:CLA:HHD	2.02	0.40
23:B:604:CLA:H143	23:B:609:CLA:HAC1	2.03	0.40
23:B:605:CLA:H61	23:B:605:CLA:H92	4.05	0.40
37:C:517:DGD:HB31	37:C:517:DGD:HB61	3.25	0.40
11:L:9:PRO:HB2	40:M:203:HOH:O	40.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	44	66
1	a	332/344 (96%)	327 (98%)	4 (1%)	1 (0%)	44	66
2	B	502/505 (99%)	498 (99%)	4 (1%)	0	100	100
2	b	502/505 (99%)	494 (98%)	8 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	51	73
3	c	453/455 (100%)	442 (98%)	10 (2%)	1 (0%)	51	73
4	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	i	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	6	8
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	O	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
13	o	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	89 (95%)	5 (5%)	0	100	100
15	u	95/104 (91%)	91 (96%)	4 (4%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	36/40 (90%)	36 (100%)	0	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	4	5
19	Z	60/62 (97%)	59 (98%)	0	1 (2%)	11	18
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	11	18
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5212/5384 (97%)	5097 (98%)	107 (2%)	8 (0%)	51	73

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416	SER
3	c	416	SER
19	Z	30	PRO
1	a	259	ILE
19	z	30	PRO
18	y	45	ASN
1	A	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/279 (96%)	269 (100%)	0	100	100
1	a	269/279 (96%)	268 (100%)	1 (0%)	93	98
2	B	402/403 (100%)	395 (98%)	7 (2%)	66	87
2	b	402/403 (100%)	390 (97%)	12 (3%)	46	74
3	C	352/356 (99%)	349 (99%)	3 (1%)	82	94
3	c	356/356 (100%)	348 (98%)	8 (2%)	57	82
4	D	277/277 (100%)	276 (100%)	1 (0%)	93	98
4	d	276/277 (100%)	275 (100%)	1 (0%)	93	98
5	E	72/73 (99%)	71 (99%)	1 (1%)	71	90
5	e	70/73 (96%)	67 (96%)	3 (4%)	33	58
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	36	62
7	H	54/54 (100%)	51 (94%)	3 (6%)	25	45
7	h	54/54 (100%)	52 (96%)	2 (4%)	39	66
8	I	34/34 (100%)	33 (97%)	1 (3%)	48	75
8	i	34/34 (100%)	32 (94%)	2 (6%)	23	42
9	J	26/27 (96%)	24 (92%)	2 (8%)	15	28
9	j	26/27 (96%)	26 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	9	17
10	k	30/30 (100%)	27 (90%)	3 (10%)	9	17
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	29/32 (91%)	29 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	43	70
13	O	206/207 (100%)	201 (98%)	5 (2%)	54	80
13	o	206/207 (100%)	203 (98%)	3 (2%)	70	89
14	T	26/28 (93%)	25 (96%)	1 (4%)	38	64
14	t	26/28 (93%)	25 (96%)	1 (4%)	38	64
15	U	83/89 (93%)	82 (99%)	1 (1%)	75	91
15	u	84/89 (94%)	82 (98%)	2 (2%)	54	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	117/117 (100%)	117 (100%)	0	100	100
16	v	117/117 (100%)	117 (100%)	0	100	100
17	X	31/33 (94%)	30 (97%)	1 (3%)	44	71
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	22 (100%)	0	100	100
19	Z	52/52 (100%)	49 (94%)	3 (6%)	23	43
19	z	52/52 (100%)	48 (92%)	4 (8%)	15	28
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4317/4403 (98%)	4241 (98%)	76 (2%)	64	86

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	161	LEU
2	B	223	GLN
2	B	362	PHE
2	B	472	ARG
2	B	495	PHE
2	B	505	ARG
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	180	ARG
5	E	54	SER
7	H	12	ARG
7	H	49	TYR
7	H	56	ASP
8	I	33	LYS
9	J	3	GLU
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
13	O	24	ASP
13	O	118	LEU
13	O	135	SER
13	O	219	GLN

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Mol	Chain	Res	Type
13	O	234	LYS
14	T	2	GLU
15	U	70	ARG
17	X	2	THR
19	Z	4	LEU
19	Z	6	GLN
19	Z	7	LEU
1	a	12	ASN
2	b	53	ASN
2	b	121	GLU
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
2	b	362	PHE
2	b	472	ARG
2	b	477	ASP
2	b	485	GLU
2	b	486	LEU
2	b	491	VAL
2	b	505	ARG
3	c	19	ASN
3	c	24	THR
3	c	240	ILE
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	416	SER
4	d	180	ARG
5	e	16	SER
5	e	54	SER
5	e	74	GLN
6	f	15	ILE
7	h	49	TYR
7	h	56	ASP
8	i	33	LYS
8	i	36	ASP
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
13	o	37	THR

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Mol	Chain	Res	Type
13	o	118	LEU
13	o	132	ASN
14	t	2	GLU
15	u	15	GLU
15	u	61	VAL
19	z	4	LEU
19	z	6	GLN
19	z	7	LEU
19	z	32	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	331	ASN
3	C	201	ASN
4	D	61	HIS
4	D	83	ASN
4	D	142	ASN
5	E	60	GLN
6	F	44	GLN
13	O	124	ASN
13	O	130	GLN
15	U	73	GLN
19	Z	58	ASN
2	b	53	ASN
2	b	223	GLN
2	b	331	ASN
3	c	201	ASN
4	d	83	ASN
4	d	142	ASN
5	e	60	GLN
5	e	75	GLN
6	f	44	GLN
12	m	5	GLN
13	o	124	ASN
13	o	130	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
8	FME	I	1	8	9,9,10	0.58	0	7,9,11	1.25	1 (14%)
12	FME	M	1	12	9,9,10	0.53	0	7,9,11	1.50	1 (14%)
14	FME	T	1	14	9,9,10	0.73	0	7,9,11	1.14	1 (14%)
8	FME	i	1	8	9,9,10	0.56	0	7,9,11	1.53	2 (28%)
12	FME	m	1	12	9,9,10	0.70	0	7,9,11	1.45	2 (28%)
14	FME	t	1	14	9,9,10	0.65	0	7,9,11	1.74	2 (28%)

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
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-3.17	117.76	125.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	O-C-CA	-2.99	118.17	125.15
8	i	1	FME	O-C-CA	-2.75	118.75	125.15
14	t	1	FME	CA-N-CN	-2.74	118.61	122.82
8	I	1	FME	O-C-CA	-2.42	119.51	125.15
12	m	1	FME	CA-N-CN	-2.39	119.15	122.82
14	T	1	FME	O-C-CA	-2.13	120.19	125.15
12	m	1	FME	O1-CN-N	-2.10	119.33	125.20
8	i	1	FME	CB-CA-C	-2.04	108.28	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 218 ligands modelled in this entry, 18 are unknown and 15 are monoatomic - leaving 185 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$
23	CLA	A	404	1	56,73,73	1.97	12 (21%)	65,113,113	2.31	23 (35%)
23	CLA	A	405	40	56,73,73	1.94	12 (21%)	65,113,113	2.10	20 (30%)
24	PHO	A	406	-	67,69,69	2.17	17 (25%)	87,99,99	1.99	23 (26%)
23	CLA	A	407	1	56,73,73	1.94	11 (19%)	65,113,113	2.09	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	A	408	-	41,41,41	0.97	1 (2%)	56,56,56	1.65	16 (28%)
26	SQD	A	409	-	53,54,54	0.96	3 (5%)	63,65,65	1.98	13 (20%)
27	GOL	A	410	-	5,5,5	0.36	0	5,5,5	0.22	0
26	SQD	A	411	-	53,54,54	1.01	3 (5%)	63,65,65	1.22	6 (9%)
28	OEX	A	412	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	PL9	A	413	-	55,55,55	0.61	1 (1%)	69,69,69	1.90	21 (30%)
31	LHG	A	415	-	48,48,48	0.84	2 (4%)	49,54,54	1.24	6 (12%)
32	BCT	A	416	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	602	40	56,73,73	1.98	12 (21%)	65,113,113	2.16	21 (32%)
23	CLA	B	603	2	56,73,73	1.99	12 (21%)	65,113,113	2.25	20 (30%)
23	CLA	B	604	2	56,73,73	1.95	12 (21%)	65,113,113	2.27	21 (32%)
23	CLA	B	605	2	56,73,73	1.92	10 (17%)	65,113,113	2.33	19 (29%)
23	CLA	B	606	2	56,73,73	1.90	13 (23%)	65,113,113	2.19	22 (33%)
23	CLA	B	607	2	56,73,73	1.86	11 (19%)	65,113,113	2.19	21 (32%)
23	CLA	B	608	40	56,73,73	1.96	12 (21%)	65,113,113	2.17	23 (35%)
23	CLA	B	609	2	56,73,73	1.87	11 (19%)	65,113,113	2.25	20 (30%)
23	CLA	B	610	2	56,73,73	1.91	11 (19%)	65,113,113	2.18	16 (24%)
23	CLA	B	611	40	56,73,73	1.99	12 (21%)	65,113,113	2.27	23 (35%)
23	CLA	B	612	2	56,73,73	1.97	11 (19%)	65,113,113	2.32	22 (33%)
23	CLA	B	613	2	56,73,73	1.94	12 (21%)	65,113,113	2.38	21 (32%)
23	CLA	B	614	2	56,73,73	1.99	12 (21%)	65,113,113	2.22	19 (29%)
23	CLA	B	615	2	56,73,73	1.89	12 (21%)	65,113,113	2.29	18 (27%)
23	CLA	B	616	2	56,73,73	1.90	11 (19%)	65,113,113	2.21	22 (33%)
23	CLA	B	617	2	56,73,73	1.95	11 (19%)	65,113,113	2.24	20 (30%)
25	BCR	B	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.63	10 (17%)
25	BCR	B	619	-	41,41,41	0.95	1 (2%)	56,56,56	1.55	12 (21%)
25	BCR	B	620	-	41,41,41	1.04	1 (2%)	56,56,56	1.49	12 (21%)
26	SQD	B	621	-	53,54,54	1.02	3 (5%)	63,65,65	1.62	10 (15%)
34	LMG	B	622	-	51,51,55	0.89	2 (3%)	59,59,63	1.19	5 (8%)
35	LMT	B	623	-	36,36,36	0.42	0	47,47,47	1.19	4 (8%)
36	HTG	B	624	-	19,19,19	0.96	1 (5%)	23,24,24	1.43	4 (17%)
36	HTG	B	625	-	19,19,19	0.81	1 (5%)	23,24,24	1.86	1 (4%)
36	HTG	B	626	-	19,19,19	0.94	1 (5%)	23,24,24	1.83	2 (8%)
27	GOL	B	627	-	5,5,5	0.33	0	5,5,5	0.36	0
27	GOL	B	628	-	5,5,5	0.52	0	5,5,5	0.47	0
36	HTG	B	629	-	19,19,19	0.95	2 (10%)	23,24,24	1.47	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	HTG	B	630	-	19,19,19	0.99	2 (10%)	23,24,24	1.57	1 (4%)
35	LMT	B	632	-	25,25,36	0.44	0	30,30,47	0.72	0
35	LMT	B	633	-	36,36,36	0.55	1 (2%)	47,47,47	1.03	1 (2%)
35	LMT	B	634	-	26,26,36	0.49	0	31,31,47	0.92	1 (3%)
34	LMG	C	501	-	51,51,55	0.94	2 (3%)	59,59,63	1.28	6 (10%)
23	CLA	C	502	3	56,73,73	1.92	12 (21%)	65,113,113	2.36	23 (35%)
23	CLA	C	503	3	56,73,73	1.90	11 (19%)	65,113,113	2.12	18 (27%)
23	CLA	C	504	3	56,73,73	1.89	12 (21%)	65,113,113	2.12	18 (27%)
23	CLA	C	505	40	56,73,73	2.00	12 (21%)	65,113,113	2.33	22 (33%)
23	CLA	C	506	3	56,73,73	1.89	12 (21%)	65,113,113	2.28	19 (29%)
23	CLA	C	507	3	56,73,73	1.92	12 (21%)	65,113,113	2.18	23 (35%)
23	CLA	C	508	40	56,73,73	1.90	12 (21%)	65,113,113	2.23	21 (32%)
23	CLA	C	509	3	56,73,73	2.04	11 (19%)	65,113,113	2.40	20 (30%)
23	CLA	C	510	3	56,73,73	1.97	12 (21%)	65,113,113	2.21	20 (30%)
23	CLA	C	511	3	56,73,73	1.92	11 (19%)	65,113,113	2.27	19 (29%)
23	CLA	C	512	3	56,73,73	1.99	12 (21%)	65,113,113	2.09	18 (27%)
23	CLA	C	513	3	56,73,73	1.94	11 (19%)	65,113,113	2.18	22 (33%)
23	CLA	C	514	3	56,73,73	1.92	11 (19%)	65,113,113	2.15	20 (30%)
25	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.54	7 (12%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	9 (16%)
37	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.23	8 (10%)
37	DGD	C	518	-	63,63,67	0.85	2 (3%)	77,77,81	1.00	4 (5%)
37	DGD	C	519	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	5 (6%)
34	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	3 (5%)
34	LMG	C	521	-	51,51,55	0.97	3 (5%)	59,59,63	1.23	4 (6%)
35	LMT	C	522	-	36,36,36	0.53	1 (2%)	47,47,47	1.07	5 (10%)
36	HTG	C	523	-	19,19,19	0.94	1 (5%)	23,24,24	1.69	3 (13%)
36	HTG	C	524	-	8,8,19	0.38	0	7,7,24	1.11	1 (14%)
27	GOL	C	525	-	5,5,5	0.37	0	5,5,5	0.19	0
25	BCR	C	527	-	41,41,41	0.99	1 (2%)	56,56,56	1.56	11 (19%)
23	CLA	D	401	40	56,73,73	1.94	11 (19%)	65,113,113	2.12	22 (33%)
24	PHO	D	402	-	67,69,69	2.13	17 (25%)	87,99,99	2.01	24 (27%)
35	LMT	D	403	-	36,36,36	0.57	1 (2%)	47,47,47	1.25	4 (8%)
23	CLA	D	404	4	56,73,73	1.99	12 (21%)	65,113,113	2.34	20 (30%)
23	CLA	D	405	4	56,73,73	1.95	11 (19%)	65,113,113	2.14	21 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	D	406	-	41,41,41	1.01	1 (2%)	56,56,56	1.77	13 (23%)
29	PL9	D	407	-	55,55,55	0.65	1 (1%)	69,69,69	1.61	18 (26%)
31	LHG	D	408	-	48,48,48	0.89	2 (4%)	49,54,54	1.04	3 (6%)
31	LHG	D	409	-	48,48,48	0.92	2 (4%)	49,54,54	1.10	3 (6%)
36	HTG	D	412	-	16,16,19	1.01	2 (12%)	20,21,24	1.69	1 (5%)
26	SQD	D	413	-	42,43,54	1.12	3 (7%)	52,54,65	1.77	14 (26%)
31	LHG	E	101	-	41,41,48	1.01	2 (4%)	42,47,54	1.15	3 (7%)
35	LMT	E	102	-	36,36,36	0.51	1 (2%)	47,47,47	0.91	2 (4%)
38	HEM	E	103	5,6	28,50,50	0.88	2 (7%)	17,82,82	2.25	4 (23%)
25	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.59	11 (19%)
37	DGD	H	102	-	63,63,67	0.87	2 (3%)	77,77,81	1.01	3 (3%)
34	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.10	5 (8%)
31	LHG	L	101	-	48,48,48	0.89	2 (4%)	49,54,54	1.20	4 (8%)
26	SQD	L	102	-	53,54,54	1.01	3 (5%)	63,65,65	1.69	12 (19%)
35	LMT	M	101	-	36,36,36	0.56	0	47,47,47	1.13	4 (8%)
35	LMT	M	103	-	36,36,36	0.46	0	47,47,47	0.84	2 (4%)
27	GOL	O	302	-	5,5,5	0.31	0	5,5,5	0.32	0
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.84	12 (21%)
38	HEM	V	202	16	28,50,50	0.98	3 (10%)	17,82,82	1.41	2 (11%)
36	HTG	V	203	-	11,11,19	0.28	0	13,15,24	1.40	1 (7%)
25	BCR	Y	101	-	41,41,41	0.95	1 (2%)	56,56,56	1.81	18 (32%)
34	LMG	Z	101	-	37,37,55	0.97	3 (8%)	45,45,63	1.59	8 (17%)
23	CLA	a	404	1	56,73,73	1.93	11 (19%)	65,113,113	2.27	25 (38%)
23	CLA	a	405	40	56,73,73	1.98	11 (19%)	65,113,113	2.29	22 (33%)
23	CLA	a	406	40	56,73,73	1.92	11 (19%)	65,113,113	2.15	21 (32%)
24	PHO	a	407	-	67,69,69	2.12	16 (23%)	87,99,99	2.02	26 (29%)
24	PHO	a	408	-	67,69,69	2.22	15 (22%)	87,99,99	1.87	24 (27%)
23	CLA	a	409	1	56,73,73	1.93	12 (21%)	65,113,113	2.19	26 (40%)
25	BCR	a	410	-	41,41,41	0.97	1 (2%)	56,56,56	1.56	11 (19%)
26	SQD	a	411	-	53,54,54	0.95	3 (5%)	63,65,65	1.75	15 (23%)
27	GOL	a	412	-	5,5,5	0.42	0	5,5,5	0.26	0
26	SQD	a	413	-	53,54,54	1.06	4 (7%)	63,65,65	1.37	8 (12%)
28	OEX	a	414	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	PL9	a	415	-	55,55,55	0.63	1 (1%)	69,69,69	1.94	19 (27%)
34	LMG	a	417	-	51,51,55	0.94	3 (5%)	59,59,63	1.13	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	a	418	-	36,36,36	0.49	0	47,47,47	0.78	1 (2%)
32	BCT	a	419	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	601	40	56,73,73	1.98	11 (19%)	65,113,113	2.13	19 (29%)
23	CLA	b	602	2	56,73,73	1.98	12 (21%)	65,113,113	2.28	27 (41%)
23	CLA	b	603	2	56,73,73	1.91	12 (21%)	65,113,113	2.29	20 (30%)
23	CLA	b	604	2	56,73,73	1.86	11 (19%)	65,113,113	2.30	20 (30%)
23	CLA	b	605	2	56,73,73	1.92	12 (21%)	65,113,113	2.30	21 (32%)
23	CLA	b	606	2	56,73,73	1.85	11 (19%)	65,113,113	2.19	20 (30%)
23	CLA	b	607	40	56,73,73	1.87	12 (21%)	65,113,113	2.35	20 (30%)
23	CLA	b	608	2	56,73,73	1.97	11 (19%)	65,113,113	2.15	20 (30%)
23	CLA	b	609	2	56,73,73	1.95	11 (19%)	65,113,113	2.15	19 (29%)
23	CLA	b	610	40	56,73,73	2.00	12 (21%)	65,113,113	2.25	22 (33%)
23	CLA	b	611	2	56,73,73	1.95	12 (21%)	65,113,113	2.48	19 (29%)
23	CLA	b	612	2	56,73,73	1.98	12 (21%)	65,113,113	2.24	19 (29%)
23	CLA	b	613	2	56,73,73	2.02	11 (19%)	65,113,113	2.18	19 (29%)
23	CLA	b	614	2	56,73,73	1.98	12 (21%)	65,113,113	2.21	20 (30%)
23	CLA	b	615	2	56,73,73	1.88	11 (19%)	65,113,113	2.20	20 (30%)
23	CLA	b	616	2	56,73,73	1.95	12 (21%)	65,113,113	2.32	21 (32%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.39	6 (10%)
25	BCR	b	618	-	41,41,41	0.96	1 (2%)	56,56,56	1.53	13 (23%)
25	BCR	b	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.81	12 (21%)
35	LMT	b	620	-	25,25,36	0.46	0	30,30,47	0.69	0
36	HTG	b	621	-	19,19,19	1.22	2 (10%)	23,24,24	1.96	5 (21%)
36	HTG	b	622	-	19,19,19	0.99	2 (10%)	23,24,24	1.53	2 (8%)
36	HTG	b	623	-	19,19,19	1.06	2 (10%)	23,24,24	1.85	3 (13%)
27	GOL	b	624	-	5,5,5	0.33	0	5,5,5	0.38	0
36	HTG	b	625	-	19,19,19	0.97	2 (10%)	23,24,24	1.61	3 (13%)
36	HTG	b	626	-	19,19,19	1.06	2 (10%)	23,24,24	1.41	2 (8%)
35	LMT	b	628	-	25,25,36	0.53	1 (4%)	30,30,47	1.29	4 (13%)
31	LHG	b	630	-	48,48,48	0.92	2 (4%)	49,54,54	1.10	2 (4%)
23	CLA	c	501	3	56,73,73	1.91	12 (21%)	65,113,113	2.20	20 (30%)
23	CLA	c	502	3	56,73,73	2.00	11 (19%)	65,113,113	2.22	18 (27%)
23	CLA	c	503	3	56,73,73	1.91	12 (21%)	65,113,113	2.23	21 (32%)
23	CLA	c	504	40	56,73,73	1.98	12 (21%)	65,113,113	2.26	21 (32%)
23	CLA	c	505	3	56,73,73	1.92	12 (21%)	65,113,113	2.21	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	506	3	56,73,73	1.88	11 (19%)	65,113,113	2.22	21 (32%)
23	CLA	c	507	40	56,73,73	1.92	12 (21%)	65,113,113	2.16	21 (32%)
23	CLA	c	508	3	56,73,73	2.00	12 (21%)	65,113,113	2.32	18 (27%)
23	CLA	c	509	3	56,73,73	1.96	12 (21%)	65,113,113	2.25	21 (32%)
23	CLA	c	510	3	56,73,73	1.91	12 (21%)	65,113,113	2.23	23 (35%)
23	CLA	c	511	3	56,73,73	1.96	12 (21%)	65,113,113	2.15	19 (29%)
23	CLA	c	512	3	56,73,73	1.92	12 (21%)	65,113,113	2.31	21 (32%)
23	CLA	c	513	3	56,73,73	1.95	12 (21%)	65,113,113	2.18	22 (33%)
25	BCR	c	514	-	41,41,41	0.99	1 (2%)	56,56,56	1.86	13 (23%)
25	BCR	c	515	-	41,41,41	0.96	1 (2%)	56,56,56	1.67	15 (26%)
37	DGD	c	516	-	63,63,67	0.84	2 (3%)	77,77,81	1.11	6 (7%)
37	DGD	c	517	-	63,63,67	0.90	3 (4%)	77,77,81	1.01	4 (5%)
37	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.12	5 (6%)
34	LMG	c	519	-	51,51,55	0.95	3 (5%)	59,59,63	1.09	5 (8%)
34	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.23	7 (11%)
36	HTG	c	521	-	19,19,19	0.91	1 (5%)	23,24,24	1.71	1 (4%)
36	HTG	c	522	-	19,19,19	0.98	2 (10%)	23,24,24	1.61	3 (13%)
27	GOL	d	401	-	5,5,5	0.29	0	5,5,5	0.52	0
23	CLA	d	402	4	56,73,73	1.91	12 (21%)	65,113,113	2.31	20 (30%)
23	CLA	d	403	4	56,73,73	1.94	11 (19%)	65,113,113	2.14	19 (29%)
25	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	1.67	14 (25%)
29	PL9	d	405	-	55,55,55	0.62	1 (1%)	69,69,69	1.79	22 (31%)
31	LHG	d	406	-	48,48,48	0.85	2 (4%)	49,54,54	1.13	5 (10%)
31	LHG	d	407	-	48,48,48	0.90	2 (4%)	49,54,54	0.97	4 (8%)
31	LHG	d	408	-	48,48,48	0.94	2 (4%)	49,54,54	1.03	4 (8%)
31	LHG	e	101	-	41,41,48	1.01	2 (4%)	42,47,54	0.98	2 (4%)
35	LMT	e	102	-	36,36,36	0.47	0	47,47,47	0.90	3 (6%)
38	HEM	e	103	5,6	28,50,50	0.93	2 (7%)	17,82,82	1.90	3 (17%)
26	SQD	f	101	-	42,43,54	1.16	3 (7%)	52,54,65	1.69	8 (15%)
36	HTG	h	101	-	16,16,19	1.07	2 (12%)	20,21,24	1.50	1 (5%)
25	BCR	h	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.46	10 (17%)
37	DGD	h	103	-	63,63,67	0.88	3 (4%)	77,77,81	0.99	3 (3%)
34	LMG	j	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.11	5 (8%)
25	BCR	k	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.60	13 (23%)
34	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	LMT	m	103	-	36,36,36	0.50	0	47,47,47	0.97	2 (4%)
25	BCR	t	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.83	14 (25%)
38	HEM	v	201	16	28,50,50	0.91	3 (10%)	17,82,82	1.61	3 (17%)
25	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.66	12 (21%)
34	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.15	4 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	404	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	405	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	A	406	-	-	0/53/103/103	0/1/6/6
23	CLA	A	407	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
26	SQD	A	409	-	-	0/49/69/69	0/1/1/1
27	GOL	A	410	-	-	0/4/4/4	0/0/0/0
26	SQD	A	411	-	-	0/49/69/69	0/1/1/1
28	OEX	A	412	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	A	413	-	-	0/53/73/73	0/1/1/1
31	LHG	A	415	-	-	0/53/53/53	0/0/0/0
32	BCT	A	416	21	-	0/0/0/0	0/0/0/0
23	CLA	B	602	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	2	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	616	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	2	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	B	621	-	-	0/49/69/69	0/1/1/1
34	LMG	B	622	-	-	0/46/66/70	0/1/1/1
35	LMT	B	623	-	-	0/21/61/61	0/2/2/2
36	HTG	B	624	-	-	0/10/30/30	0/1/1/1
36	HTG	B	625	-	-	0/10/30/30	0/1/1/1
36	HTG	B	626	-	-	0/10/30/30	0/1/1/1
27	GOL	B	627	-	-	0/4/4/4	0/0/0/0
27	GOL	B	628	-	-	0/4/4/4	0/0/0/0
36	HTG	B	629	-	-	0/10/30/30	0/1/1/1
36	HTG	B	630	-	-	0/10/30/30	0/1/1/1
35	LMT	B	632	-	-	0/17/37/61	0/1/1/2
35	LMT	B	633	-	-	0/21/61/61	0/2/2/2
35	LMT	B	634	-	-	0/17/38/61	0/1/1/2
34	LMG	C	501	-	-	1/46/66/70	0/1/1/1
23	CLA	C	502	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	3	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	514	3	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
37	DGD	C	517	-	-	0/51/91/95	0/2/2/2
37	DGD	C	518	-	-	0/51/91/95	0/2/2/2
37	DGD	C	519	-	-	0/51/91/95	0/2/2/2
34	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	LMG	C	521	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMT	C	522	-	-	1/21/61/61	0/2/2/2
36	HTG	C	523	-	-	0/10/30/30	0/1/1/1
36	HTG	C	524	-	-	0/6/6/30	0/0/0/1
27	GOL	C	525	-	-	0/4/4/4	0/0/0/0
25	BCR	C	527	-	-	0/29/63/63	0/2/2/2
23	CLA	D	401	40	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
35	LMT	D	403	-	-	0/21/61/61	0/2/2/2
23	CLA	D	404	4	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	D	405	4	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	D	406	-	-	0/29/63/63	0/2/2/2
29	PL9	D	407	-	-	0/53/73/73	0/1/1/1
31	LHG	D	408	-	-	0/53/53/53	0/0/0/0
31	LHG	D	409	-	-	0/53/53/53	0/0/0/0
36	HTG	D	412	-	-	0/7/27/30	0/1/1/1
26	SQD	D	413	-	-	2/38/58/69	0/1/1/1
31	LHG	E	101	-	-	0/46/46/53	0/0/0/0
35	LMT	E	102	-	-	0/21/61/61	0/2/2/2
38	HEM	E	103	5,6	-	0/6/54/54	0/0/8/8
25	BCR	H	101	-	-	0/29/63/63	0/2/2/2
37	DGD	H	102	-	-	0/51/91/95	0/2/2/2
34	LMG	J	101	39	-	0/46/66/70	0/1/1/1
31	LHG	L	101	-	-	0/53/53/53	0/0/0/0
26	SQD	L	102	-	-	0/49/69/69	0/1/1/1
35	LMT	M	101	-	-	0/21/61/61	0/2/2/2
35	LMT	M	103	-	-	0/21/61/61	0/2/2/2
27	GOL	O	302	-	-	0/4/4/4	0/0/0/0
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
38	HEM	V	202	16	-	0/6/54/54	0/0/8/8
36	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
34	LMG	Z	101	-	-	2/31/51/70	0/1/1/1
23	CLA	a	404	1	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	405	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	406	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6
23	CLA	a	409	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
26	SQD	a	411	-	-	0/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	a	412	-	-	0/4/4/4	0/0/0/0
26	SQD	a	413	-	-	0/49/69/69	0/1/1/1
28	OEX	a	414	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	a	415	-	-	0/53/73/73	0/1/1/1
34	LMG	a	417	-	-	0/46/66/70	0/1/1/1
35	LMT	a	418	-	-	0/21/61/61	0/2/2/2
32	BCT	a	419	21	-	0/0/0/0	0/0/0/0
23	CLA	b	601	40	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	602	2	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	603	2	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	604	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	2	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	2	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	2	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	617	-	-	0/29/63/63	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
35	LMT	b	620	-	-	0/17/37/61	0/1/1/2
36	HTG	b	621	-	-	0/10/30/30	0/1/1/1
36	HTG	b	622	-	-	0/10/30/30	0/1/1/1
36	HTG	b	623	-	-	0/10/30/30	0/1/1/1
27	GOL	b	624	-	-	0/4/4/4	0/0/0/0
36	HTG	b	625	-	-	0/10/30/30	0/1/1/1
36	HTG	b	626	-	-	0/10/30/30	0/1/1/1
35	LMT	b	628	-	-	0/17/37/61	0/1/1/2
31	LHG	b	630	-	-	0/53/53/53	0/0/0/0
23	CLA	c	501	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	502	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	3	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	504	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	505	3	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	512	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	3	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
37	DGD	c	516	-	-	0/51/91/95	0/2/2/2
37	DGD	c	517	-	-	0/51/91/95	0/2/2/2
37	DGD	c	518	-	-	0/51/91/95	0/2/2/2
34	LMG	c	519	-	-	0/46/66/70	0/1/1/1
34	LMG	c	520	-	-	0/46/66/70	0/1/1/1
36	HTG	c	521	-	-	0/10/30/30	0/1/1/1
36	HTG	c	522	-	-	0/10/30/30	0/1/1/1
27	GOL	d	401	-	-	0/4/4/4	0/0/0/0
23	CLA	d	402	4	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	4	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	d	404	-	-	0/29/63/63	0/2/2/2
29	PL9	d	405	-	-	0/53/73/73	0/1/1/1
31	LHG	d	406	-	-	0/53/53/53	0/0/0/0
31	LHG	d	407	-	-	0/53/53/53	0/0/0/0
31	LHG	d	408	-	-	0/53/53/53	0/0/0/0
31	LHG	e	101	-	-	0/46/46/53	0/0/0/0
35	LMT	e	102	-	-	0/21/61/61	0/2/2/2
38	HEM	e	103	5,6	-	0/6/54/54	0/0/8/8
26	SQD	f	101	-	-	2/38/58/69	0/1/1/1
36	HTG	h	101	-	-	0/7/27/30	0/1/1/1
25	BCR	h	102	-	-	0/29/63/63	0/2/2/2
37	DGD	h	103	-	-	0/51/91/95	0/2/2/2
34	LMG	j	101	39	-	0/46/66/70	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
34	LMG	m	101	-	-	0/46/66/70	0/1/1/1
35	LMT	m	103	-	-	0/21/61/61	0/2/2/2
25	BCR	t	101	-	-	0/29/63/63	0/2/2/2
38	HEM	v	201	16	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	y	101	-	-	0/29/63/63	0/2/2/2
34	LMG	z	101	-	-	0/34/54/70	0/1/1/1

All (1036) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	BCR	C23-C22	-5.44	1.34	1.45
25	y	101	BCR	C23-C22	-5.17	1.34	1.45
25	b	619	BCR	C23-C22	-5.09	1.34	1.45
25	k	101	BCR	C23-C22	-5.09	1.34	1.45
25	B	620	BCR	C23-C22	-4.97	1.35	1.45
25	T	101	BCR	C23-C22	-4.96	1.35	1.45
25	H	101	BCR	C23-C22	-4.95	1.35	1.45
25	C	527	BCR	C23-C22	-4.94	1.35	1.45
25	C	516	BCR	C23-C22	-4.92	1.35	1.45
25	C	515	BCR	C23-C22	-4.82	1.35	1.45
25	D	406	BCR	C23-C22	-4.79	1.35	1.45
25	c	514	BCR	C23-C22	-4.76	1.35	1.45
25	B	618	BCR	C23-C22	-4.75	1.35	1.45
25	A	408	BCR	C23-C22	-4.72	1.35	1.45
25	h	102	BCR	C23-C22	-4.72	1.35	1.45
25	t	101	BCR	C23-C22	-4.70	1.35	1.45
25	b	617	BCR	C23-C22	-4.65	1.35	1.45
25	a	410	BCR	C23-C22	-4.60	1.35	1.45
25	b	618	BCR	C23-C22	-4.54	1.36	1.45
36	b	621	HTG	C1'-S1	-4.49	1.75	1.81
25	c	515	BCR	C23-C22	-4.48	1.36	1.45
25	Y	101	BCR	C23-C22	-4.30	1.36	1.45
25	B	619	BCR	C23-C22	-4.12	1.37	1.45
36	b	623	HTG	C1'-S1	-3.76	1.76	1.81
36	b	626	HTG	C1'-S1	-3.72	1.76	1.81
36	B	624	HTG	C1'-S1	-3.70	1.76	1.81
24	D	402	PHO	C4A-NA	-3.63	1.26	1.35
36	b	622	HTG	C1'-S1	-3.52	1.76	1.81
36	B	630	HTG	C1'-S1	-3.47	1.76	1.81
24	A	406	PHO	C4A-NA	-3.47	1.26	1.35
36	h	101	HTG	C1'-S1	-3.43	1.77	1.81
36	c	522	HTG	C1'-S1	-3.41	1.77	1.81
36	b	625	HTG	C1'-S1	-3.38	1.77	1.81
36	C	523	HTG	C1'-S1	-3.28	1.77	1.81
36	B	626	HTG	C1'-S1	-3.26	1.77	1.81
36	B	629	HTG	C1'-S1	-3.23	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	C4A-NA	-3.22	1.27	1.35
36	D	412	HTG	C1'-S1	-3.06	1.77	1.81
36	c	521	HTG	C1'-S1	-3.04	1.77	1.81
24	a	407	PHO	C4A-NA	-2.94	1.28	1.35
38	e	103	HEM	C3B-C2B	-2.91	1.36	1.40
36	B	625	HTG	C1'-S1	-2.91	1.77	1.81
26	f	101	SQD	C6-S	-2.58	1.67	1.77
38	V	202	HEM	C1B-NB	-2.57	1.33	1.36
26	D	413	SQD	C6-S	-2.56	1.67	1.77
26	A	411	SQD	C6-S	-2.55	1.67	1.77
26	L	102	SQD	C6-S	-2.49	1.67	1.77
38	V	202	HEM	C4D-ND	-2.46	1.33	1.36
26	A	409	SQD	C6-S	-2.45	1.67	1.77
26	B	621	SQD	C6-S	-2.43	1.67	1.77
38	v	201	HEM	C3B-C2B	-2.42	1.37	1.40
24	a	408	PHO	C1A-NA	-2.41	1.32	1.37
26	a	413	SQD	C6-S	-2.40	1.67	1.77
26	a	411	SQD	C6-S	-2.37	1.67	1.77
37	c	518	DGD	O2G-C2G	-2.34	1.40	1.46
36	b	621	HTG	C1-S1	-2.32	1.77	1.80
38	E	103	HEM	C3B-C2B	-2.29	1.37	1.40
24	D	402	PHO	C1A-NA	-2.28	1.32	1.37
36	B	629	HTG	C1-S1	-2.28	1.77	1.80
36	b	626	HTG	C1-S1	-2.27	1.77	1.80
36	D	412	HTG	C1-S1	-2.25	1.77	1.80
38	V	202	HEM	C3B-C2B	-2.23	1.37	1.40
38	v	201	HEM	C1B-NB	-2.22	1.34	1.36
36	c	522	HTG	C1-S1	-2.19	1.77	1.80
24	A	406	PHO	C1A-NA	-2.18	1.32	1.37
23	B	609	CLA	C1C-NC	-2.17	1.34	1.37
36	b	623	HTG	C1-S1	-2.16	1.77	1.80
36	B	630	HTG	C1-S1	-2.13	1.77	1.80
36	b	625	HTG	C1-S1	-2.11	1.77	1.80
23	B	606	CLA	C1C-NC	-2.10	1.34	1.37
38	v	201	HEM	C4D-ND	-2.09	1.34	1.36
38	e	103	HEM	C4D-ND	-2.08	1.34	1.36
25	b	619	BCR	C30-C25	-2.07	1.51	1.53
23	a	406	CLA	C1C-NC	-2.07	1.34	1.37
36	h	101	HTG	C1-S1	-2.05	1.77	1.80
38	E	103	HEM	C1B-NB	-2.05	1.34	1.36
36	b	622	HTG	C1-S1	-2.01	1.77	1.80
35	b	628	LMT	O1'-C1'	2.00	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	PHO	C4D-CHA	2.01	1.49	1.44
34	C	521	LMG	O1-C1	2.01	1.43	1.40
23	B	611	CLA	C4C-C3C	2.01	1.48	1.45
23	b	611	CLA	C1C-C2C	2.02	1.48	1.44
35	E	102	LMT	O1'-C1'	2.03	1.43	1.40
34	c	519	LMG	O1-C1	2.04	1.43	1.40
26	a	413	SQD	O6-C1	2.04	1.43	1.40
23	B	606	CLA	C4C-C3C	2.04	1.48	1.45
23	b	616	CLA	C1C-C2C	2.05	1.48	1.44
23	C	510	CLA	C4C-C3C	2.05	1.48	1.45
23	C	508	CLA	C4C-C3C	2.05	1.48	1.45
37	c	517	DGD	O3G-C1D	2.07	1.43	1.40
23	C	504	CLA	C1C-C2C	2.08	1.48	1.44
23	b	602	CLA	C4C-C3C	2.08	1.48	1.45
34	a	417	LMG	O1-C1	2.09	1.43	1.40
23	B	613	CLA	CHD-C4C	2.10	1.47	1.41
23	B	617	CLA	CHD-C4C	2.10	1.47	1.41
23	c	512	CLA	C4C-C3C	2.10	1.48	1.45
23	B	611	CLA	CHD-C4C	2.12	1.47	1.41
24	A	406	PHO	C4D-CHA	2.12	1.49	1.44
23	c	511	CLA	C4C-C3C	2.13	1.48	1.45
34	Z	101	LMG	O1-C1	2.13	1.43	1.40
23	B	614	CLA	CHD-C4C	2.13	1.47	1.41
23	B	612	CLA	CHD-C4C	2.14	1.47	1.41
23	b	604	CLA	CHD-C4C	2.14	1.47	1.41
23	c	508	CLA	C4C-C3C	2.15	1.48	1.45
24	D	402	PHO	C4C-C3C	2.15	1.49	1.45
23	c	508	CLA	CHD-C4C	2.15	1.47	1.41
23	c	507	CLA	C4C-C3C	2.16	1.48	1.45
23	B	602	CLA	C4C-C3C	2.17	1.48	1.45
24	a	407	PHO	C4D-CHA	2.17	1.50	1.44
23	B	616	CLA	CHD-C4C	2.17	1.47	1.41
23	B	615	CLA	C1C-C2C	2.17	1.48	1.44
37	h	103	DGD	O5D-C1E	2.18	1.44	1.40
23	b	616	CLA	CHD-C4C	2.19	1.47	1.41
23	b	607	CLA	CHD-C4C	2.19	1.47	1.41
23	b	612	CLA	CHD-C4C	2.19	1.47	1.41
23	B	602	CLA	CHD-C4C	2.20	1.47	1.41
23	B	606	CLA	CHD-C4C	2.20	1.47	1.41
23	c	506	CLA	C4C-C3C	2.20	1.48	1.45
24	a	407	PHO	C4C-C3C	2.20	1.49	1.45
23	c	513	CLA	C4C-C3C	2.20	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405	CLA	CHD-C4C	2.21	1.47	1.41
23	b	615	CLA	C4C-C3C	2.21	1.48	1.45
23	b	613	CLA	CHD-C4C	2.21	1.47	1.41
23	b	614	CLA	C4C-C3C	2.22	1.49	1.45
23	b	605	CLA	C4C-C3C	2.22	1.49	1.45
23	c	502	CLA	CHD-C4C	2.22	1.47	1.41
23	d	402	CLA	CHD-C4C	2.22	1.47	1.41
23	b	611	CLA	CHD-C4C	2.23	1.47	1.41
23	a	405	CLA	C1C-C2C	2.23	1.48	1.44
23	c	505	CLA	C4C-C3C	2.24	1.49	1.45
23	b	614	CLA	CHD-C4C	2.24	1.47	1.41
23	C	507	CLA	C4C-C3C	2.24	1.49	1.45
23	D	401	CLA	CHD-C4C	2.24	1.47	1.41
23	c	505	CLA	CHD-C4C	2.25	1.47	1.41
23	b	605	CLA	CHD-C4C	2.25	1.47	1.41
23	B	604	CLA	CHD-C4C	2.25	1.47	1.41
23	c	504	CLA	CHD-C4C	2.25	1.47	1.41
23	a	405	CLA	CHD-C4C	2.26	1.47	1.41
23	C	502	CLA	C4C-C3C	2.27	1.49	1.45
23	B	610	CLA	CHD-C4C	2.27	1.48	1.41
23	C	503	CLA	C1C-C2C	2.27	1.48	1.44
23	b	603	CLA	CHD-C4C	2.27	1.48	1.41
23	a	406	CLA	CHD-C4C	2.28	1.48	1.41
35	C	522	LMT	O1'-C1'	2.28	1.44	1.40
23	C	505	CLA	C4C-C3C	2.28	1.49	1.45
23	A	405	CLA	CHD-C4C	2.28	1.48	1.41
23	a	406	CLA	C1B-CHB	2.28	1.46	1.40
23	c	512	CLA	CHD-C4C	2.28	1.48	1.41
23	c	501	CLA	C1C-C2C	2.28	1.49	1.44
23	b	608	CLA	CHD-C4C	2.29	1.48	1.41
23	A	404	CLA	C1B-CHB	2.29	1.46	1.40
23	c	509	CLA	C4C-C3C	2.29	1.49	1.45
23	b	607	CLA	C4C-C3C	2.29	1.49	1.45
23	c	511	CLA	CHD-C4C	2.29	1.48	1.41
23	c	509	CLA	CHD-C4C	2.29	1.48	1.41
23	b	601	CLA	C1C-C2C	2.30	1.49	1.44
23	b	606	CLA	CHD-C4C	2.30	1.48	1.41
23	A	407	CLA	C1C-C2C	2.30	1.49	1.44
24	A	406	PHO	C3B-C4B	2.30	1.48	1.43
23	C	511	CLA	C4B-CHC	2.30	1.46	1.40
23	B	613	CLA	C4C-C3C	2.30	1.49	1.45
23	C	512	CLA	C4C-C3C	2.30	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C4C-C3C	2.30	1.49	1.45
23	b	615	CLA	CHD-C4C	2.32	1.48	1.41
23	c	502	CLA	C1C-C2C	2.32	1.49	1.44
23	b	605	CLA	C1C-C2C	2.32	1.49	1.44
23	B	609	CLA	C1C-C2C	2.32	1.49	1.44
23	d	403	CLA	CHD-C4C	2.32	1.48	1.41
35	B	633	LMT	O1'-C1'	2.33	1.44	1.40
23	C	513	CLA	CHD-C4C	2.33	1.48	1.41
23	C	502	CLA	CHD-C4C	2.33	1.48	1.41
23	c	510	CLA	C4C-C3C	2.33	1.49	1.45
23	C	506	CLA	C4C-C3C	2.33	1.49	1.45
23	B	607	CLA	CHD-C4C	2.33	1.48	1.41
23	b	612	CLA	C4C-C3C	2.34	1.49	1.45
23	C	505	CLA	CHD-C4C	2.34	1.48	1.41
23	B	608	CLA	CHD-C4C	2.34	1.48	1.41
23	A	405	CLA	C4C-C3C	2.34	1.49	1.45
23	d	402	CLA	C4C-C3C	2.35	1.49	1.45
23	c	503	CLA	C1C-C2C	2.35	1.49	1.44
23	A	405	CLA	C1C-C2C	2.36	1.49	1.44
23	b	610	CLA	CHD-C4C	2.36	1.48	1.41
23	C	506	CLA	CHD-C4C	2.36	1.48	1.41
23	B	616	CLA	C1C-C2C	2.36	1.49	1.44
23	a	404	CLA	CHD-C4C	2.36	1.48	1.41
23	b	602	CLA	CHD-C4C	2.36	1.48	1.41
23	C	514	CLA	CHD-C4C	2.37	1.48	1.41
23	D	404	CLA	CHD-C4C	2.37	1.48	1.41
23	b	616	CLA	C4C-C3C	2.37	1.49	1.45
23	A	407	CLA	CHD-C4C	2.38	1.48	1.41
23	c	510	CLA	C1C-C2C	2.38	1.49	1.44
23	C	512	CLA	CHD-C4C	2.38	1.48	1.41
23	B	616	CLA	C4B-CHC	2.38	1.46	1.40
23	c	506	CLA	CHD-C4C	2.39	1.48	1.41
23	b	603	CLA	C1B-CHB	2.39	1.46	1.40
23	A	404	CLA	CHD-C4C	2.39	1.48	1.41
24	A	406	PHO	C4C-C3C	2.39	1.49	1.45
23	C	503	CLA	CHD-C4C	2.40	1.48	1.41
23	a	405	CLA	C1B-CHB	2.40	1.46	1.40
23	C	508	CLA	C1B-CHB	2.40	1.46	1.40
23	B	604	CLA	C1C-C2C	2.41	1.49	1.44
23	a	406	CLA	C4B-CHC	2.41	1.46	1.40
23	B	611	CLA	C1C-C2C	2.42	1.49	1.44
23	B	617	CLA	C1C-C2C	2.42	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C1C-C2C	2.42	1.49	1.44
23	C	507	CLA	CHD-C4C	2.42	1.48	1.41
23	A	404	CLA	C4C-C3C	2.43	1.49	1.45
23	c	503	CLA	CHD-C4C	2.43	1.48	1.41
23	b	608	CLA	C1C-C2C	2.44	1.49	1.44
23	C	509	CLA	C4C-C3C	2.44	1.49	1.45
23	b	611	CLA	C4C-C3C	2.44	1.49	1.45
23	b	611	CLA	C4B-CHC	2.44	1.46	1.40
23	c	501	CLA	CHD-C4C	2.45	1.48	1.41
23	C	504	CLA	CHD-C4C	2.45	1.48	1.41
23	c	504	CLA	C1C-C2C	2.46	1.49	1.44
23	C	507	CLA	C1C-C2C	2.46	1.49	1.44
23	c	512	CLA	C1C-C2C	2.46	1.49	1.44
23	B	609	CLA	C4B-CHC	2.47	1.46	1.40
23	C	510	CLA	CHD-C4C	2.47	1.48	1.41
23	B	615	CLA	CHD-C4C	2.47	1.48	1.41
23	a	405	CLA	C4B-CHC	2.47	1.46	1.40
23	B	603	CLA	CHD-C4C	2.48	1.48	1.41
23	b	609	CLA	C1C-C2C	2.48	1.49	1.44
23	b	615	CLA	C4B-CHC	2.48	1.46	1.40
23	b	614	CLA	C1C-C2C	2.49	1.49	1.44
23	B	604	CLA	C4C-C3C	2.49	1.49	1.45
23	B	607	CLA	C1C-C2C	2.49	1.49	1.44
29	d	405	PL9	C6-C5	2.49	1.48	1.35
23	c	501	CLA	C4C-C3C	2.50	1.49	1.45
23	C	502	CLA	C1C-C2C	2.50	1.49	1.44
23	B	614	CLA	C4C-C3C	2.50	1.49	1.45
35	D	403	LMT	O1'-C1'	2.50	1.44	1.40
23	C	508	CLA	CHD-C4C	2.51	1.48	1.41
29	D	407	PL9	C6-C5	2.51	1.48	1.35
23	d	403	CLA	C1C-C2C	2.52	1.49	1.44
24	a	407	PHO	C3B-C4B	2.52	1.48	1.43
24	D	402	PHO	CHB-C4A	2.52	1.46	1.40
23	C	509	CLA	C1C-C2C	2.52	1.49	1.44
23	B	608	CLA	C4C-C3C	2.53	1.49	1.45
23	d	402	CLA	C1C-C2C	2.53	1.49	1.44
23	c	510	CLA	CHD-C4C	2.53	1.48	1.41
23	b	606	CLA	C1C-C2C	2.53	1.49	1.44
23	C	512	CLA	C4B-CHC	2.54	1.46	1.40
23	B	616	CLA	C1B-CHB	2.54	1.46	1.40
23	b	612	CLA	C1C-C2C	2.54	1.49	1.44
23	c	506	CLA	C4B-CHC	2.54	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CHD-C4C	2.54	1.48	1.41
23	b	601	CLA	CHD-C4C	2.54	1.48	1.41
23	C	506	CLA	C4B-CHC	2.54	1.46	1.40
23	B	610	CLA	C1C-C2C	2.55	1.49	1.44
23	c	511	CLA	C1C-C2C	2.55	1.49	1.44
23	B	607	CLA	C1B-CHB	2.55	1.46	1.40
23	b	609	CLA	CHD-C4C	2.56	1.48	1.41
34	Z	101	LMG	O8-C28	2.56	1.46	1.33
23	c	507	CLA	C1B-CHB	2.56	1.46	1.40
23	C	513	CLA	C1B-CHB	2.56	1.47	1.40
23	C	511	CLA	CHD-C4C	2.56	1.48	1.41
23	B	603	CLA	C4C-C3C	2.57	1.49	1.45
23	C	507	CLA	C1B-CHB	2.57	1.47	1.40
23	b	607	CLA	C4B-CHC	2.57	1.47	1.40
23	A	407	CLA	C1B-CHB	2.59	1.47	1.40
23	B	602	CLA	C1C-C2C	2.60	1.49	1.44
23	b	616	CLA	C4B-CHC	2.60	1.47	1.40
23	c	509	CLA	C1C-C2C	2.60	1.49	1.44
23	b	610	CLA	C1C-C2C	2.60	1.49	1.44
23	b	608	CLA	C1B-CHB	2.61	1.47	1.40
23	c	504	CLA	C4B-CHC	2.61	1.47	1.40
23	a	409	CLA	C1C-C2C	2.62	1.49	1.44
23	c	513	CLA	C1C-C2C	2.64	1.49	1.44
23	c	513	CLA	CHD-C4C	2.64	1.49	1.41
23	b	612	CLA	C1B-CHB	2.64	1.47	1.40
23	c	502	CLA	C4B-CHC	2.64	1.47	1.40
23	b	602	CLA	C1C-C2C	2.64	1.49	1.44
23	B	614	CLA	C1C-C2C	2.64	1.49	1.44
23	C	504	CLA	C4C-C3C	2.65	1.49	1.45
23	B	602	CLA	C1B-CHB	2.65	1.47	1.40
23	a	409	CLA	C1B-CHB	2.66	1.47	1.40
23	B	613	CLA	C4B-CHC	2.66	1.47	1.40
23	C	509	CLA	C4B-CHC	2.66	1.47	1.40
23	a	404	CLA	C1C-C2C	2.66	1.49	1.44
23	B	608	CLA	C1B-CHB	2.66	1.47	1.40
23	b	610	CLA	C4C-C3C	2.66	1.49	1.45
23	c	509	CLA	C4B-CHC	2.67	1.47	1.40
23	C	505	CLA	C1C-C2C	2.67	1.49	1.44
23	D	404	CLA	C4B-CHC	2.67	1.47	1.40
23	c	512	CLA	C1B-CHB	2.68	1.47	1.40
23	b	605	CLA	C4B-CHC	2.68	1.47	1.40
23	b	604	CLA	C1B-CHB	2.69	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C1B-CHB	2.69	1.47	1.40
23	a	409	CLA	C4C-C3C	2.69	1.49	1.45
23	B	614	CLA	C4B-CHC	2.70	1.47	1.40
23	B	614	CLA	C1B-CHB	2.70	1.47	1.40
23	b	604	CLA	C4B-CHC	2.70	1.47	1.40
23	b	601	CLA	C1B-CHB	2.70	1.47	1.40
23	D	404	CLA	C4C-C3C	2.70	1.49	1.45
23	B	615	CLA	C4C-C3C	2.71	1.49	1.45
23	a	409	CLA	CHD-C4C	2.71	1.49	1.41
23	A	405	CLA	C1B-CHB	2.72	1.47	1.40
29	A	413	PL9	C6-C5	2.72	1.49	1.35
23	C	508	CLA	C1C-C2C	2.72	1.49	1.44
23	c	506	CLA	C1B-CHB	2.72	1.47	1.40
23	D	401	CLA	C1B-CHB	2.73	1.47	1.40
23	B	603	CLA	C4B-CHC	2.73	1.47	1.40
23	C	506	CLA	C1C-C2C	2.73	1.49	1.44
23	c	504	CLA	C4C-C3C	2.73	1.49	1.45
23	b	602	CLA	C1B-CHB	2.73	1.47	1.40
23	B	606	CLA	C1C-C2C	2.73	1.49	1.44
23	b	603	CLA	C4B-CHC	2.74	1.47	1.40
23	b	607	CLA	C1C-C2C	2.74	1.49	1.44
23	a	404	CLA	C4B-CHC	2.74	1.47	1.40
23	B	605	CLA	C1C-C2C	2.74	1.49	1.44
23	C	504	CLA	C1B-CHB	2.74	1.47	1.40
23	A	405	CLA	C4B-CHC	2.75	1.47	1.40
23	c	513	CLA	C1B-CHB	2.75	1.47	1.40
23	C	510	CLA	C4B-CHC	2.75	1.47	1.40
23	C	505	CLA	C4B-CHC	2.75	1.47	1.40
23	c	501	CLA	C4B-CHC	2.75	1.47	1.40
23	A	404	CLA	C1C-C2C	2.75	1.49	1.44
23	B	607	CLA	C4B-CHC	2.76	1.47	1.40
23	B	603	CLA	C1B-CHB	2.76	1.47	1.40
23	C	512	CLA	C1C-C2C	2.76	1.49	1.44
23	B	602	CLA	C4B-CHC	2.76	1.47	1.40
23	c	504	CLA	C1B-CHB	2.76	1.47	1.40
23	B	605	CLA	C4B-CHC	2.77	1.47	1.40
23	c	508	CLA	C4B-CHC	2.77	1.47	1.40
23	C	511	CLA	C1B-CHB	2.77	1.47	1.40
23	C	514	CLA	C4B-CHC	2.77	1.47	1.40
23	c	505	CLA	C1C-C2C	2.77	1.49	1.44
23	c	511	CLA	C4B-CHC	2.77	1.47	1.40
23	c	503	CLA	C4C-C3C	2.78	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C4B-CHC	2.78	1.47	1.40
23	c	507	CLA	C1C-C2C	2.79	1.49	1.44
23	b	606	CLA	C4B-CHC	2.79	1.47	1.40
23	d	402	CLA	C1B-CHB	2.79	1.47	1.40
23	c	503	CLA	C1B-CHB	2.79	1.47	1.40
23	d	402	CLA	C4B-CHC	2.80	1.47	1.40
29	a	415	PL9	C6-C5	2.80	1.50	1.35
23	B	610	CLA	C1B-CHB	2.80	1.47	1.40
23	B	612	CLA	C1C-C2C	2.80	1.49	1.44
23	B	612	CLA	C4B-CHC	2.81	1.47	1.40
23	B	613	CLA	C1C-C2C	2.81	1.50	1.44
23	b	608	CLA	C4B-CHC	2.81	1.47	1.40
23	b	603	CLA	C1C-C2C	2.82	1.50	1.44
23	b	616	CLA	C1B-CHB	2.82	1.47	1.40
23	C	510	CLA	C1B-CHB	2.82	1.47	1.40
23	b	601	CLA	C4B-CHC	2.82	1.47	1.40
23	b	604	CLA	C1C-C2C	2.82	1.50	1.44
23	a	409	CLA	C4B-CHC	2.83	1.47	1.40
23	b	606	CLA	C1B-CHB	2.83	1.47	1.40
23	a	404	CLA	C1B-CHB	2.83	1.47	1.40
23	C	502	CLA	C1B-CHB	2.83	1.47	1.40
23	c	513	CLA	C4B-CHC	2.83	1.47	1.40
23	B	613	CLA	C1B-CHB	2.84	1.47	1.40
23	B	615	CLA	C4B-CHC	2.84	1.47	1.40
23	C	512	CLA	C1B-CHB	2.84	1.47	1.40
23	B	604	CLA	C1B-CHB	2.84	1.47	1.40
23	b	614	CLA	C4B-CHC	2.85	1.47	1.40
23	C	513	CLA	C1C-C2C	2.85	1.50	1.44
23	b	612	CLA	C4B-CHC	2.85	1.47	1.40
23	B	605	CLA	C1B-CHB	2.86	1.47	1.40
23	C	507	CLA	C4B-CHC	2.86	1.47	1.40
23	C	508	CLA	C4B-CHC	2.86	1.47	1.40
23	C	502	CLA	C4B-CHC	2.86	1.47	1.40
23	b	613	CLA	C1C-C2C	2.87	1.50	1.44
23	b	609	CLA	C4B-CHC	2.87	1.47	1.40
23	B	617	CLA	C1B-CHB	2.87	1.47	1.40
23	C	504	CLA	C4B-CHC	2.87	1.47	1.40
23	b	615	CLA	C1B-CHB	2.87	1.47	1.40
23	B	615	CLA	C1B-CHB	2.87	1.47	1.40
23	B	617	CLA	C4B-CHC	2.87	1.47	1.40
23	c	501	CLA	C1B-CHB	2.88	1.47	1.40
23	C	514	CLA	C1B-CHB	2.88	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C4C-C3C	2.90	1.50	1.45
23	C	503	CLA	C4B-CHC	2.90	1.47	1.40
23	c	508	CLA	C1C-C2C	2.91	1.50	1.44
23	B	606	CLA	C4B-CHC	2.91	1.47	1.40
23	c	503	CLA	C4B-CHC	2.92	1.47	1.40
23	b	614	CLA	C1B-CHB	2.92	1.47	1.40
23	B	610	CLA	C4B-CHC	2.92	1.47	1.40
23	D	405	CLA	C1B-CHB	2.93	1.47	1.40
23	B	609	CLA	C1B-CHB	2.93	1.47	1.40
23	c	505	CLA	C4B-CHC	2.94	1.47	1.40
23	A	407	CLA	C4B-CHC	2.94	1.48	1.40
24	A	406	PHO	CHB-C4A	2.94	1.47	1.40
24	a	408	PHO	C3B-C4B	2.95	1.49	1.43
23	b	605	CLA	C1B-CHB	2.95	1.48	1.40
24	a	407	PHO	CHD-C4C	2.95	1.47	1.40
23	B	611	CLA	C1B-CHB	2.96	1.48	1.40
23	B	604	CLA	C4B-CHC	2.96	1.48	1.40
23	c	502	CLA	C1B-CHB	2.97	1.48	1.40
23	B	606	CLA	C1B-CHB	2.97	1.48	1.40
23	D	404	CLA	C1B-CHB	2.98	1.48	1.40
23	b	602	CLA	C4B-CHC	2.99	1.48	1.40
23	c	508	CLA	C1B-CHB	2.99	1.48	1.40
23	C	514	CLA	C1C-C2C	2.99	1.50	1.44
23	b	607	CLA	C1B-CHB	3.00	1.48	1.40
23	b	610	CLA	C1B-CHB	3.00	1.48	1.40
23	D	405	CLA	C1C-C2C	3.00	1.50	1.44
23	c	507	CLA	C4B-CHC	3.01	1.48	1.40
23	C	503	CLA	C1B-CHB	3.01	1.48	1.40
23	b	609	CLA	C1B-CHB	3.01	1.48	1.40
23	c	510	CLA	C1B-CHB	3.01	1.48	1.40
23	b	613	CLA	C1B-CHB	3.02	1.48	1.40
23	c	509	CLA	C1B-CHB	3.02	1.48	1.40
23	C	513	CLA	C4B-CHC	3.03	1.48	1.40
23	B	612	CLA	C1B-CHB	3.05	1.48	1.40
23	C	509	CLA	C1B-CHB	3.06	1.48	1.40
23	B	608	CLA	C1C-C2C	3.07	1.50	1.44
23	D	404	CLA	C1C-C2C	3.08	1.50	1.44
24	D	402	PHO	C3B-C4B	3.10	1.50	1.43
23	C	506	CLA	C1B-CHB	3.10	1.48	1.40
23	c	512	CLA	C4B-CHC	3.11	1.48	1.40
23	C	505	CLA	C1B-CHB	3.11	1.48	1.40
23	B	611	CLA	C4B-CHC	3.17	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	CHB-C4A	3.17	1.48	1.40
23	A	404	CLA	C4B-CHC	3.18	1.48	1.40
23	C	510	CLA	C1C-C2C	3.18	1.50	1.44
23	b	610	CLA	C4B-CHC	3.20	1.48	1.40
23	B	608	CLA	C4B-CHC	3.23	1.48	1.40
23	b	613	CLA	C4B-CHC	3.23	1.48	1.40
23	D	401	CLA	C1C-C2C	3.24	1.50	1.44
23	d	403	CLA	C4B-CHC	3.24	1.48	1.40
24	a	408	PHO	CHD-C4C	3.24	1.48	1.40
23	D	401	CLA	C4B-CHC	3.25	1.48	1.40
24	A	406	PHO	CHC-C4B	3.28	1.48	1.40
24	a	407	PHO	CHB-C4A	3.28	1.48	1.40
23	D	405	CLA	C4B-CHC	3.29	1.48	1.40
24	a	407	PHO	CHC-C4B	3.32	1.48	1.40
23	b	611	CLA	C1B-CHB	3.33	1.49	1.40
23	c	511	CLA	C1B-CHB	3.33	1.49	1.40
23	A	404	CLA	O2A-CGA	3.33	1.43	1.33
24	A	406	PHO	OBD-CAD	3.36	1.28	1.22
31	d	406	LHG	O7-C7	3.38	1.44	1.34
34	J	101	LMG	O7-C10	3.40	1.44	1.34
23	c	505	CLA	C1B-CHB	3.45	1.49	1.40
24	D	402	PHO	CHD-C4C	3.47	1.48	1.40
23	a	404	CLA	O2A-CGA	3.50	1.43	1.33
24	D	402	PHO	O2A-CGA	3.54	1.43	1.33
31	A	415	LHG	O8-C23	3.56	1.43	1.33
31	A	415	LHG	O7-C7	3.59	1.44	1.34
31	D	408	LHG	O8-C23	3.59	1.43	1.33
34	j	101	LMG	O7-C10	3.59	1.44	1.34
24	a	407	PHO	O2A-CGA	3.63	1.44	1.33
24	D	402	PHO	CHC-C4B	3.63	1.49	1.40
31	L	101	LHG	O7-C7	3.63	1.44	1.34
23	b	610	CLA	O2A-CGA	3.64	1.44	1.33
37	C	517	DGD	O1G-C1A	3.64	1.44	1.33
26	A	409	SQD	O47-C7	3.68	1.45	1.34
23	C	506	CLA	C3D-C2D	3.68	1.47	1.39
24	a	407	PHO	OBD-CAD	3.69	1.28	1.22
31	d	406	LHG	O8-C23	3.70	1.44	1.33
37	c	517	DGD	O2G-C1B	3.73	1.45	1.34
37	C	518	DGD	O2G-C1B	3.75	1.45	1.34
37	c	518	DGD	O2G-C1B	3.75	1.45	1.34
24	A	406	PHO	CHD-C4C	3.75	1.49	1.40
34	m	101	LMG	O7-C10	3.75	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	O2A-CGA	3.77	1.44	1.33
23	b	611	CLA	CHC-C1C	3.78	1.46	1.35
34	B	622	LMG	O7-C10	3.78	1.45	1.34
31	d	407	LHG	O8-C23	3.80	1.44	1.33
37	C	519	DGD	O2G-C1B	3.80	1.45	1.34
37	c	516	DGD	O2G-C1B	3.82	1.45	1.34
37	h	103	DGD	O1G-C1A	3.82	1.44	1.33
23	b	604	CLA	O2A-CGA	3.83	1.44	1.33
23	D	404	CLA	O2A-CGA	3.85	1.44	1.33
23	c	501	CLA	OBD-CAD	3.87	1.27	1.22
23	B	604	CLA	O2A-CGA	3.88	1.44	1.33
23	B	605	CLA	C3D-C2D	3.89	1.48	1.39
24	D	402	PHO	C3D-C2D	3.90	1.49	1.38
23	c	501	CLA	O2A-CGA	3.90	1.44	1.33
23	b	604	CLA	C3D-C2D	3.91	1.48	1.39
34	z	101	LMG	O7-C10	3.91	1.45	1.34
37	h	103	DGD	O2G-C1B	3.91	1.45	1.34
23	c	510	CLA	O2A-CGA	3.92	1.44	1.33
23	c	510	CLA	C3D-C2D	3.93	1.48	1.39
26	D	413	SQD	O48-C23	3.93	1.44	1.33
24	a	408	PHO	C3D-C2D	3.93	1.49	1.38
24	a	407	PHO	C3D-C2D	3.93	1.49	1.38
31	d	407	LHG	O7-C7	3.94	1.45	1.34
24	A	406	PHO	C3D-C2D	3.94	1.49	1.38
23	C	502	CLA	OBD-CAD	3.94	1.28	1.22
31	D	408	LHG	O7-C7	3.94	1.45	1.34
24	a	408	PHO	OBD-CAD	3.94	1.29	1.22
23	a	406	CLA	O2A-CGA	3.95	1.45	1.33
37	H	102	DGD	O2G-C1B	3.95	1.45	1.34
23	B	607	CLA	OBD-CAD	3.96	1.28	1.22
23	B	615	CLA	OBD-CAD	3.96	1.28	1.22
26	a	411	SQD	O47-C7	3.96	1.45	1.34
23	B	613	CLA	O2A-CGA	3.97	1.45	1.33
24	a	408	PHO	CHC-C4B	3.97	1.50	1.40
37	C	519	DGD	O1G-C1A	3.97	1.45	1.33
34	c	519	LMG	O7-C10	3.97	1.45	1.34
23	B	606	CLA	OBD-CAD	3.98	1.28	1.22
23	b	605	CLA	O2A-CGA	3.98	1.45	1.33
31	b	630	LHG	O7-C7	3.98	1.45	1.34
34	C	520	LMG	O7-C10	3.99	1.45	1.34
23	c	504	CLA	O2A-CGA	3.99	1.45	1.33
23	b	606	CLA	OBD-CAD	3.99	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	O2A-CGA	4.00	1.45	1.33
23	c	505	CLA	C3D-C2D	4.00	1.48	1.39
23	C	514	CLA	OBD-CAD	4.01	1.28	1.22
23	B	609	CLA	O2A-CGA	4.01	1.45	1.33
23	C	510	CLA	O2A-CGA	4.01	1.45	1.33
23	b	616	CLA	O2A-CGA	4.01	1.45	1.33
31	E	101	LHG	O7-C7	4.01	1.45	1.34
37	c	518	DGD	O1G-C1A	4.01	1.45	1.33
34	Z	101	LMG	O7-C10	4.02	1.46	1.34
23	C	506	CLA	O2A-CGA	4.02	1.45	1.33
23	c	504	CLA	CHC-C1C	4.02	1.47	1.35
23	B	611	CLA	O2A-CGA	4.02	1.45	1.33
23	b	607	CLA	O2A-CGA	4.03	1.45	1.33
23	B	615	CLA	O2A-CGA	4.03	1.45	1.33
24	D	402	PHO	OBD-CAD	4.04	1.29	1.22
23	A	407	CLA	O2A-CGA	4.04	1.45	1.33
23	B	609	CLA	CHC-C1C	4.04	1.47	1.35
23	B	614	CLA	CHC-C1C	4.04	1.47	1.35
23	b	605	CLA	CHC-C1C	4.04	1.47	1.35
37	C	518	DGD	O1G-C1A	4.04	1.45	1.33
31	D	409	LHG	O7-C7	4.05	1.46	1.34
23	c	506	CLA	CHC-C1C	4.05	1.47	1.35
23	b	607	CLA	OBD-CAD	4.05	1.28	1.22
31	e	101	LHG	O7-C7	4.05	1.46	1.34
23	b	606	CLA	O2A-CGA	4.05	1.45	1.33
23	B	609	CLA	OBD-CAD	4.06	1.28	1.22
23	a	409	CLA	OBD-CAD	4.08	1.28	1.22
23	b	602	CLA	O2A-CGA	4.08	1.45	1.33
31	D	409	LHG	O8-C23	4.08	1.45	1.33
23	c	505	CLA	O2A-CGA	4.09	1.45	1.33
23	B	617	CLA	O2A-CGA	4.09	1.45	1.33
31	d	408	LHG	O8-C23	4.09	1.45	1.33
23	b	613	CLA	O2A-CGA	4.09	1.45	1.33
23	d	403	CLA	OBD-CAD	4.10	1.28	1.22
23	b	609	CLA	O2A-CGA	4.10	1.45	1.33
26	A	411	SQD	O47-C7	4.10	1.46	1.34
23	D	405	CLA	O2A-CGA	4.10	1.45	1.33
24	A	406	PHO	O2A-CGA	4.11	1.45	1.33
23	B	606	CLA	O2A-CGA	4.11	1.45	1.33
23	B	612	CLA	O2A-CGA	4.11	1.45	1.33
23	c	511	CLA	C3D-C2D	4.11	1.48	1.39
23	C	502	CLA	O2A-CGA	4.11	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	417	LMG	O7-C10	4.11	1.46	1.34
37	C	517	DGD	O2G-C1B	4.11	1.46	1.34
23	C	508	CLA	OBD-CAD	4.11	1.28	1.22
23	b	607	CLA	CHC-C1C	4.12	1.47	1.35
26	a	411	SQD	O48-C23	4.12	1.45	1.33
34	a	417	LMG	O8-C28	4.13	1.45	1.33
34	J	101	LMG	O8-C28	4.13	1.45	1.33
23	B	616	CLA	O2A-CGA	4.13	1.45	1.33
34	C	501	LMG	O7-C10	4.14	1.46	1.34
31	b	630	LHG	O8-C23	4.15	1.45	1.33
23	c	510	CLA	CHC-C1C	4.15	1.47	1.35
37	c	516	DGD	O1G-C1A	4.15	1.45	1.33
23	C	509	CLA	CHC-C1C	4.15	1.47	1.35
23	C	511	CLA	O2A-CGA	4.15	1.45	1.33
23	b	611	CLA	OBD-CAD	4.16	1.28	1.22
23	B	605	CLA	O2A-CGA	4.16	1.45	1.33
23	a	409	CLA	O2A-CGA	4.16	1.45	1.33
23	D	405	CLA	C3D-C2D	4.16	1.48	1.39
23	b	614	CLA	O2A-CGA	4.16	1.45	1.33
23	c	503	CLA	O2A-CGA	4.16	1.45	1.33
23	b	615	CLA	CHC-C1C	4.16	1.47	1.35
23	C	507	CLA	O2A-CGA	4.17	1.45	1.33
34	B	622	LMG	O8-C28	4.17	1.45	1.33
23	C	505	CLA	CHC-C1C	4.18	1.47	1.35
34	m	101	LMG	O8-C28	4.18	1.45	1.33
23	c	506	CLA	O2A-CGA	4.18	1.45	1.33
23	b	616	CLA	CHC-C1C	4.19	1.47	1.35
23	b	612	CLA	OBD-CAD	4.19	1.28	1.22
23	D	404	CLA	CHC-C1C	4.19	1.47	1.35
23	b	614	CLA	C3D-C2D	4.19	1.49	1.39
34	C	520	LMG	O8-C28	4.19	1.45	1.33
26	L	102	SQD	O47-C7	4.19	1.46	1.34
23	c	511	CLA	O2A-CGA	4.20	1.45	1.33
26	A	409	SQD	O48-C23	4.20	1.45	1.33
23	b	606	CLA	C3D-C2D	4.20	1.49	1.39
23	B	616	CLA	CHC-C1C	4.20	1.47	1.35
23	C	513	CLA	O2A-CGA	4.21	1.45	1.33
23	B	613	CLA	CHC-C1C	4.21	1.47	1.35
23	B	615	CLA	CHC-C1C	4.21	1.47	1.35
23	B	604	CLA	OBD-CAD	4.21	1.28	1.22
34	C	521	LMG	O7-C10	4.21	1.46	1.34
34	c	520	LMG	O8-C28	4.21	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	f	101	SQD	O48-C23	4.22	1.45	1.33
23	c	502	CLA	O2A-CGA	4.22	1.45	1.33
26	L	102	SQD	O48-C23	4.22	1.45	1.33
34	C	501	LMG	O8-C28	4.22	1.45	1.33
23	D	401	CLA	O2A-CGA	4.22	1.45	1.33
34	c	520	LMG	O7-C10	4.22	1.46	1.34
23	b	603	CLA	C3D-C2D	4.23	1.49	1.39
31	L	101	LHG	O8-C23	4.23	1.45	1.33
23	C	504	CLA	OBD-CAD	4.23	1.28	1.22
34	j	101	LMG	O8-C28	4.23	1.45	1.33
23	B	614	CLA	O2A-CGA	4.23	1.45	1.33
23	C	507	CLA	OBD-CAD	4.23	1.28	1.22
23	b	612	CLA	O2A-CGA	4.24	1.45	1.33
23	b	615	CLA	OBD-CAD	4.24	1.28	1.22
23	D	404	CLA	C3D-C2D	4.24	1.49	1.39
23	C	511	CLA	CHC-C1C	4.24	1.47	1.35
23	B	612	CLA	CHC-C1C	4.24	1.47	1.35
26	a	413	SQD	O47-C7	4.24	1.46	1.34
23	c	502	CLA	OBD-CAD	4.24	1.28	1.22
23	B	613	CLA	OBD-CAD	4.25	1.28	1.22
23	B	610	CLA	OBD-CAD	4.25	1.28	1.22
23	B	603	CLA	O2A-CGA	4.25	1.45	1.33
23	b	606	CLA	CHC-C1C	4.26	1.47	1.35
23	a	405	CLA	CHC-C1C	4.26	1.47	1.35
23	C	514	CLA	O2A-CGA	4.26	1.45	1.33
26	B	621	SQD	O47-C7	4.26	1.46	1.34
23	c	505	CLA	OBD-CAD	4.26	1.28	1.22
37	c	517	DGD	O1G-C1A	4.26	1.45	1.33
23	B	607	CLA	CHC-C1C	4.26	1.47	1.35
23	C	505	CLA	O2A-CGA	4.27	1.45	1.33
23	d	403	CLA	O2A-CGA	4.27	1.45	1.33
23	b	608	CLA	CHC-C1C	4.27	1.47	1.35
23	C	512	CLA	O2A-CGA	4.27	1.45	1.33
31	d	408	LHG	O7-C7	4.27	1.46	1.34
23	b	606	CLA	O2D-CGD	4.27	1.44	1.33
34	c	519	LMG	O8-C28	4.28	1.45	1.33
23	C	504	CLA	C3D-C2D	4.28	1.49	1.39
23	b	604	CLA	OBD-CAD	4.28	1.28	1.22
23	c	509	CLA	CHC-C1C	4.28	1.47	1.35
23	B	602	CLA	CHC-C1C	4.28	1.47	1.35
23	b	613	CLA	CHC-C1C	4.28	1.47	1.35
26	f	101	SQD	O47-C7	4.28	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	O2D-CGD	4.28	1.44	1.33
26	B	621	SQD	O48-C23	4.29	1.46	1.33
23	B	607	CLA	O2A-CGA	4.29	1.46	1.33
23	d	403	CLA	O2D-CGD	4.29	1.44	1.33
23	C	504	CLA	O2A-CGA	4.29	1.46	1.33
31	e	101	LHG	O8-C23	4.29	1.46	1.33
23	B	608	CLA	OBD-CAD	4.29	1.28	1.22
23	a	406	CLA	CHC-C1C	4.29	1.47	1.35
23	A	404	CLA	OBD-CAD	4.29	1.28	1.22
23	c	508	CLA	O2A-CGA	4.30	1.46	1.33
23	c	501	CLA	CHC-C1C	4.30	1.47	1.35
23	a	406	CLA	OBD-CAD	4.30	1.28	1.22
23	b	602	CLA	OBD-CAD	4.30	1.28	1.22
23	C	510	CLA	CHC-C1C	4.30	1.47	1.35
37	H	102	DGD	O1G-C1A	4.30	1.46	1.33
31	E	101	LHG	O8-C23	4.30	1.46	1.33
23	C	507	CLA	CHC-C1C	4.30	1.47	1.35
23	c	509	CLA	O2A-CGA	4.31	1.46	1.33
23	b	613	CLA	OBD-CAD	4.31	1.28	1.22
23	c	509	CLA	C3D-C2D	4.31	1.49	1.39
24	a	408	PHO	O2A-CGA	4.31	1.46	1.33
23	A	405	CLA	O2A-CGA	4.31	1.46	1.33
23	b	615	CLA	O2A-CGA	4.32	1.46	1.33
23	c	512	CLA	O2A-CGA	4.32	1.46	1.33
23	B	608	CLA	C3D-C2D	4.32	1.49	1.39
23	c	513	CLA	O2A-CGA	4.32	1.46	1.33
26	D	413	SQD	O47-C7	4.33	1.46	1.34
23	B	617	CLA	CHC-C1C	4.33	1.48	1.35
23	b	615	CLA	C3D-C2D	4.33	1.49	1.39
34	C	521	LMG	O8-C28	4.33	1.46	1.33
23	B	610	CLA	O2A-CGA	4.33	1.46	1.33
23	c	503	CLA	CHC-C1C	4.33	1.48	1.35
23	c	512	CLA	OBD-CAD	4.34	1.28	1.22
23	c	502	CLA	C3D-C2D	4.34	1.49	1.39
23	a	405	CLA	O2A-CGA	4.34	1.46	1.33
23	b	603	CLA	CHC-C1C	4.34	1.48	1.35
23	a	404	CLA	CHC-C1C	4.34	1.48	1.35
23	C	504	CLA	CHC-C1C	4.34	1.48	1.35
23	C	508	CLA	O2A-CGA	4.34	1.46	1.33
23	c	510	CLA	OBD-CAD	4.34	1.28	1.22
23	B	617	CLA	OBD-CAD	4.35	1.28	1.22
23	B	610	CLA	CHC-C1C	4.35	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	O2A-CGA	4.35	1.46	1.33
23	c	507	CLA	O2A-CGA	4.35	1.46	1.33
23	c	513	CLA	CHC-C1C	4.35	1.48	1.35
23	d	402	CLA	CHC-C1C	4.36	1.48	1.35
23	B	609	CLA	C3D-C2D	4.36	1.49	1.39
26	A	411	SQD	O48-C23	4.36	1.46	1.33
23	c	511	CLA	O2D-CGD	4.37	1.44	1.33
23	b	611	CLA	O2A-CGA	4.37	1.46	1.33
23	c	503	CLA	O2D-CGD	4.37	1.44	1.33
23	c	508	CLA	OBD-CAD	4.37	1.28	1.22
23	c	502	CLA	CHC-C1C	4.37	1.48	1.35
23	D	404	CLA	OBD-CAD	4.37	1.28	1.22
23	C	514	CLA	O2D-CGD	4.37	1.44	1.33
23	c	511	CLA	CHC-C1C	4.38	1.48	1.35
23	b	607	CLA	C3D-C2D	4.38	1.49	1.39
23	C	508	CLA	CHC-C1C	4.38	1.48	1.35
23	C	502	CLA	CHC-C1C	4.39	1.48	1.35
23	C	510	CLA	C3D-C2D	4.39	1.49	1.39
23	b	614	CLA	CHC-C1C	4.39	1.48	1.35
23	d	402	CLA	C3D-C2D	4.39	1.49	1.39
23	C	503	CLA	C3D-C2D	4.40	1.49	1.39
23	b	612	CLA	C3D-C2D	4.40	1.49	1.39
23	b	604	CLA	CHC-C1C	4.40	1.48	1.35
23	A	407	CLA	OBD-CAD	4.40	1.28	1.22
23	B	612	CLA	C3D-C2D	4.41	1.49	1.39
23	c	513	CLA	OBD-CAD	4.41	1.28	1.22
23	b	612	CLA	CHC-C1C	4.41	1.48	1.35
23	d	402	CLA	OBD-CAD	4.41	1.28	1.22
23	C	513	CLA	OBD-CAD	4.41	1.28	1.22
23	C	513	CLA	C3D-C2D	4.41	1.49	1.39
23	B	608	CLA	O2A-CGA	4.41	1.46	1.33
23	d	402	CLA	O2A-CGA	4.41	1.46	1.33
23	C	502	CLA	C3D-C2D	4.42	1.49	1.39
23	a	404	CLA	C3D-C2D	4.42	1.49	1.39
23	D	401	CLA	OBD-CAD	4.43	1.28	1.22
23	b	616	CLA	OBD-CAD	4.43	1.28	1.22
23	A	405	CLA	OBD-CAD	4.43	1.28	1.22
23	A	407	CLA	C3D-C2D	4.44	1.49	1.39
23	C	502	CLA	O2D-CGD	4.44	1.44	1.33
23	C	506	CLA	CHC-C1C	4.44	1.48	1.35
23	b	608	CLA	O2A-CGA	4.44	1.46	1.33
23	c	506	CLA	OBD-CAD	4.44	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	CLA	O2D-CGD	4.44	1.44	1.33
23	C	505	CLA	C3D-C2D	4.44	1.49	1.39
23	b	610	CLA	C3D-C2D	4.44	1.49	1.39
23	B	604	CLA	CHC-C1C	4.44	1.48	1.35
23	c	508	CLA	CHC-C1C	4.44	1.48	1.35
23	c	512	CLA	CHC-C1C	4.44	1.48	1.35
23	B	607	CLA	O2D-CGD	4.44	1.44	1.33
23	D	401	CLA	C3D-C2D	4.44	1.49	1.39
23	C	505	CLA	OBD-CAD	4.44	1.28	1.22
23	b	610	CLA	CHC-C1C	4.45	1.48	1.35
23	b	601	CLA	CHC-C1C	4.45	1.48	1.35
23	B	602	CLA	O2A-CGA	4.45	1.46	1.33
23	a	409	CLA	C3D-C2D	4.45	1.49	1.39
23	A	405	CLA	C3D-C2D	4.45	1.49	1.39
23	b	609	CLA	C3D-C2D	4.45	1.49	1.39
23	a	404	CLA	OBD-CAD	4.46	1.28	1.22
23	c	507	CLA	OBD-CAD	4.46	1.28	1.22
23	c	513	CLA	C3D-C2D	4.46	1.49	1.39
23	b	611	CLA	O2D-CGD	4.46	1.44	1.33
23	c	507	CLA	C3D-C2D	4.46	1.49	1.39
23	b	601	CLA	O2A-CGA	4.47	1.46	1.33
24	D	402	PHO	CHD-C1D	4.47	1.47	1.38
23	c	505	CLA	CHC-C1C	4.47	1.48	1.35
23	b	608	CLA	C3D-C2D	4.48	1.49	1.39
23	B	603	CLA	CHC-C1C	4.48	1.48	1.35
23	C	507	CLA	C3D-C2D	4.48	1.49	1.39
23	C	503	CLA	OBD-CAD	4.48	1.28	1.22
23	A	404	CLA	C3D-C2D	4.48	1.49	1.39
23	b	602	CLA	CHC-C1C	4.48	1.48	1.35
23	c	504	CLA	OBD-CAD	4.48	1.28	1.22
23	C	506	CLA	OBD-CAD	4.49	1.28	1.22
23	c	503	CLA	OBD-CAD	4.49	1.28	1.22
23	B	606	CLA	CHC-C1C	4.49	1.48	1.35
23	c	506	CLA	C3D-C2D	4.49	1.49	1.39
23	d	402	CLA	O2D-CGD	4.49	1.44	1.33
23	B	608	CLA	CHC-C1C	4.50	1.48	1.35
23	c	503	CLA	C3D-C2D	4.50	1.49	1.39
23	C	511	CLA	C3D-C2D	4.50	1.49	1.39
23	C	503	CLA	CHC-C1C	4.50	1.48	1.35
23	b	610	CLA	OBD-CAD	4.50	1.28	1.22
23	B	604	CLA	C3D-C2D	4.50	1.49	1.39
34	z	101	LMG	O8-C28	4.50	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	OBD-CAD	4.50	1.28	1.22
23	B	614	CLA	OBD-CAD	4.51	1.28	1.22
23	C	513	CLA	O2D-CGD	4.51	1.44	1.33
23	b	602	CLA	C3D-C2D	4.51	1.49	1.39
23	b	611	CLA	C3D-C2D	4.52	1.49	1.39
23	B	602	CLA	C3D-C2D	4.53	1.49	1.39
23	D	401	CLA	CHC-C1C	4.54	1.48	1.35
23	C	512	CLA	CHC-C1C	4.54	1.48	1.35
23	c	509	CLA	OBD-CAD	4.54	1.28	1.22
23	c	508	CLA	O2D-CGD	4.54	1.44	1.33
23	b	605	CLA	C3D-C2D	4.54	1.49	1.39
23	C	508	CLA	O2D-CGD	4.54	1.44	1.33
23	a	409	CLA	CHC-C1C	4.54	1.48	1.35
23	C	506	CLA	O2D-CGD	4.54	1.44	1.33
23	B	615	CLA	C3D-C2D	4.55	1.49	1.39
23	B	611	CLA	CHC-C1C	4.55	1.48	1.35
23	A	407	CLA	CHC-C1C	4.55	1.48	1.35
23	c	501	CLA	O2D-CGD	4.57	1.44	1.33
23	C	514	CLA	CHC-C1C	4.57	1.48	1.35
23	B	607	CLA	C3D-C2D	4.57	1.49	1.39
23	B	605	CLA	CHC-C1C	4.57	1.48	1.35
23	b	608	CLA	OBD-CAD	4.58	1.29	1.22
23	c	507	CLA	CHC-C1C	4.58	1.48	1.35
23	B	611	CLA	C3D-C2D	4.58	1.49	1.39
23	b	609	CLA	CHC-C1C	4.58	1.48	1.35
23	a	406	CLA	O2D-CGD	4.58	1.44	1.33
23	c	504	CLA	C3D-C2D	4.58	1.49	1.39
23	B	614	CLA	C3D-C2D	4.59	1.49	1.39
23	c	507	CLA	O2D-CGD	4.59	1.44	1.33
23	b	601	CLA	C3D-C2D	4.59	1.49	1.39
23	C	511	CLA	O2D-CGD	4.60	1.44	1.33
23	C	510	CLA	OBD-CAD	4.60	1.29	1.22
23	C	512	CLA	OBD-CAD	4.60	1.29	1.22
26	a	413	SQD	O48-C23	4.60	1.46	1.33
23	b	605	CLA	OBD-CAD	4.61	1.29	1.22
23	D	405	CLA	OBD-CAD	4.61	1.29	1.22
23	D	405	CLA	CHC-C1C	4.61	1.48	1.35
24	a	407	PHO	CHD-C1D	4.62	1.47	1.38
23	b	609	CLA	OBD-CAD	4.62	1.29	1.22
23	a	404	CLA	O2D-CGD	4.62	1.44	1.33
24	D	402	PHO	O2D-CGD	4.62	1.44	1.33
23	B	604	CLA	O2D-CGD	4.62	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	O2D-CGD	4.63	1.44	1.33
23	C	513	CLA	CHC-C1C	4.63	1.48	1.35
23	c	512	CLA	O2D-CGD	4.63	1.44	1.33
23	B	603	CLA	OBD-CAD	4.63	1.29	1.22
23	B	617	CLA	O2D-CGD	4.64	1.45	1.33
23	b	608	CLA	O2D-CGD	4.64	1.45	1.33
23	C	514	CLA	C3D-C2D	4.64	1.50	1.39
23	C	512	CLA	C3D-C2D	4.64	1.50	1.39
23	c	501	CLA	C3D-C2D	4.65	1.50	1.39
23	B	602	CLA	OBD-CAD	4.65	1.29	1.22
23	B	610	CLA	C3D-C2D	4.65	1.50	1.39
23	C	509	CLA	O2D-CGD	4.65	1.45	1.33
23	B	609	CLA	O2D-CGD	4.65	1.45	1.33
23	a	406	CLA	C3D-C2D	4.65	1.50	1.39
23	A	405	CLA	O2D-CGD	4.65	1.45	1.33
23	c	513	CLA	O2D-CGD	4.65	1.45	1.33
23	B	606	CLA	C3D-C2D	4.65	1.50	1.39
23	C	508	CLA	C3D-C2D	4.66	1.50	1.39
23	A	404	CLA	CHC-C1C	4.66	1.48	1.35
23	b	610	CLA	O2D-CGD	4.66	1.45	1.33
23	d	403	CLA	C3D-C2D	4.66	1.50	1.39
24	a	407	PHO	O2D-CGD	4.66	1.45	1.33
23	d	403	CLA	CHC-C1C	4.67	1.49	1.35
23	b	605	CLA	O2D-CGD	4.67	1.45	1.33
23	C	509	CLA	C3D-C2D	4.67	1.50	1.39
23	B	612	CLA	OBD-CAD	4.68	1.29	1.22
23	B	617	CLA	C3D-C2D	4.68	1.50	1.39
23	b	615	CLA	O2D-CGD	4.68	1.45	1.33
23	B	613	CLA	C3D-C2D	4.68	1.50	1.39
23	b	607	CLA	O2D-CGD	4.69	1.45	1.33
23	C	503	CLA	O2D-CGD	4.69	1.45	1.33
23	b	604	CLA	O2D-CGD	4.69	1.45	1.33
23	b	612	CLA	O2D-CGD	4.70	1.45	1.33
23	a	409	CLA	O2D-CGD	4.70	1.45	1.33
23	B	603	CLA	C3D-C2D	4.71	1.50	1.39
23	b	614	CLA	OBD-CAD	4.71	1.29	1.22
23	B	615	CLA	O2D-CGD	4.72	1.45	1.33
23	B	613	CLA	O2D-CGD	4.72	1.45	1.33
23	b	613	CLA	O2D-CGD	4.72	1.45	1.33
23	b	601	CLA	OBD-CAD	4.72	1.29	1.22
23	b	603	CLA	OBD-CAD	4.72	1.29	1.22
23	c	508	CLA	C3D-C2D	4.72	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	O2D-CGD	4.72	1.45	1.33
24	a	407	PHO	CHC-C1C	4.73	1.48	1.38
23	c	505	CLA	O2D-CGD	4.73	1.45	1.33
23	c	512	CLA	C3D-C2D	4.73	1.50	1.39
24	A	406	PHO	O2D-CGD	4.74	1.45	1.33
23	a	405	CLA	O2D-CGD	4.74	1.45	1.33
23	B	603	CLA	O2D-CGD	4.76	1.45	1.33
23	c	502	CLA	O2D-CGD	4.77	1.45	1.33
23	d	402	CLA	C3C-C2C	4.77	1.47	1.36
23	C	511	CLA	OBD-CAD	4.77	1.29	1.22
24	a	408	PHO	CHD-C1D	4.78	1.48	1.38
23	C	510	CLA	O2D-CGD	4.79	1.45	1.33
23	B	605	CLA	OBD-CAD	4.79	1.29	1.22
23	b	613	CLA	C3D-C2D	4.79	1.50	1.39
23	b	607	CLA	C3C-C2C	4.80	1.47	1.36
23	C	505	CLA	O2D-CGD	4.80	1.45	1.33
23	D	405	CLA	O2D-CGD	4.80	1.45	1.33
23	C	509	CLA	OBD-CAD	4.80	1.29	1.22
23	c	511	CLA	OBD-CAD	4.80	1.29	1.22
23	B	608	CLA	O2D-CGD	4.81	1.45	1.33
23	b	603	CLA	O2D-CGD	4.81	1.45	1.33
23	B	606	CLA	O2D-CGD	4.82	1.45	1.33
23	D	404	CLA	O2D-CGD	4.82	1.45	1.33
23	b	609	CLA	O2D-CGD	4.82	1.45	1.33
23	B	602	CLA	O2D-CGD	4.83	1.45	1.33
23	B	612	CLA	C3C-C2C	4.83	1.47	1.36
23	b	614	CLA	O2D-CGD	4.83	1.45	1.33
23	A	405	CLA	CHC-C1C	4.84	1.49	1.35
23	C	512	CLA	C3C-C2C	4.85	1.47	1.36
23	A	407	CLA	O2D-CGD	4.88	1.45	1.33
23	b	616	CLA	O2D-CGD	4.88	1.45	1.33
23	b	616	CLA	C3D-C2D	4.88	1.50	1.39
23	c	506	CLA	C3C-C2C	4.89	1.47	1.36
23	B	611	CLA	OBD-CAD	4.90	1.29	1.22
23	B	616	CLA	O2D-CGD	4.90	1.45	1.33
23	C	512	CLA	O2D-CGD	4.91	1.45	1.33
23	a	405	CLA	C3D-C2D	4.92	1.50	1.39
23	B	610	CLA	O2D-CGD	4.93	1.45	1.33
23	B	614	CLA	O2D-CGD	4.93	1.45	1.33
23	b	601	CLA	O2D-CGD	4.93	1.45	1.33
23	D	401	CLA	O2D-CGD	4.94	1.45	1.33
23	c	506	CLA	O2D-CGD	4.94	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	O2D-CGD	4.94	1.45	1.33
23	b	609	CLA	C3C-C2C	4.94	1.47	1.36
23	b	602	CLA	O2D-CGD	4.95	1.45	1.33
23	B	616	CLA	OBD-CAD	4.96	1.29	1.22
23	c	510	CLA	C3C-C2C	4.96	1.47	1.36
23	B	616	CLA	C3D-C2D	4.98	1.50	1.39
23	B	616	CLA	C3C-C2C	4.98	1.47	1.36
23	B	614	CLA	C3C-C2C	5.01	1.47	1.36
23	c	504	CLA	C3C-C2C	5.01	1.47	1.36
23	C	507	CLA	O2D-CGD	5.01	1.45	1.33
23	c	504	CLA	O2D-CGD	5.01	1.45	1.33
23	c	503	CLA	C3C-C2C	5.02	1.47	1.36
23	b	604	CLA	C3C-C2C	5.03	1.47	1.36
24	D	402	PHO	CHB-C1B	5.04	1.48	1.38
23	B	605	CLA	C3C-C2C	5.04	1.47	1.36
24	a	408	PHO	O2D-CGD	5.06	1.46	1.33
23	C	514	CLA	C3C-C2C	5.06	1.47	1.36
23	C	503	CLA	C3C-C2C	5.06	1.47	1.36
23	c	510	CLA	O2D-CGD	5.08	1.46	1.33
23	B	610	CLA	C3C-C2C	5.08	1.47	1.36
23	B	613	CLA	C3C-C2C	5.09	1.47	1.36
23	a	404	CLA	C3C-C2C	5.09	1.47	1.36
23	C	510	CLA	C3C-C2C	5.10	1.47	1.36
24	A	406	PHO	CHD-C1D	5.10	1.48	1.38
23	B	612	CLA	O2D-CGD	5.11	1.46	1.33
23	C	507	CLA	C3C-C2C	5.12	1.47	1.36
24	A	406	PHO	C3C-C2C	5.13	1.47	1.36
23	C	506	CLA	C3C-C2C	5.13	1.47	1.36
23	A	405	CLA	C3C-C2C	5.13	1.47	1.36
24	D	402	PHO	CHC-C1C	5.14	1.48	1.38
24	a	407	PHO	CHB-C1B	5.14	1.48	1.38
23	A	404	CLA	C3C-C2C	5.14	1.47	1.36
23	C	502	CLA	C3C-C2C	5.15	1.47	1.36
23	c	507	CLA	C3C-C2C	5.17	1.47	1.36
23	B	606	CLA	C3C-C2C	5.18	1.47	1.36
23	b	608	CLA	C3C-C2C	5.18	1.47	1.36
23	B	615	CLA	C3C-C2C	5.18	1.47	1.36
23	b	602	CLA	C3C-C2C	5.18	1.47	1.36
23	c	509	CLA	C3C-C2C	5.18	1.47	1.36
23	a	409	CLA	C3C-C2C	5.18	1.47	1.36
23	b	605	CLA	C3C-C2C	5.20	1.47	1.36
23	B	606	CLA	C3B-C2B	5.21	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	401	CLA	C3C-C2C	5.21	1.47	1.36
23	C	511	CLA	C3C-C2C	5.21	1.47	1.36
23	B	609	CLA	C3C-C2C	5.22	1.47	1.36
23	b	601	CLA	C3C-C2C	5.23	1.48	1.36
23	C	513	CLA	C3C-C2C	5.23	1.48	1.36
23	b	614	CLA	C3C-C2C	5.23	1.48	1.36
23	B	608	CLA	C3C-C2C	5.23	1.48	1.36
23	d	403	CLA	C3C-C2C	5.24	1.48	1.36
23	B	607	CLA	C3C-C2C	5.25	1.48	1.36
23	B	604	CLA	C3C-C2C	5.26	1.48	1.36
23	c	502	CLA	C3C-C2C	5.29	1.48	1.36
23	c	513	CLA	C3C-C2C	5.31	1.48	1.36
23	C	505	CLA	C3C-C2C	5.32	1.48	1.36
23	c	505	CLA	C3C-C2C	5.32	1.48	1.36
23	b	606	CLA	C3C-C2C	5.33	1.48	1.36
24	a	408	PHO	CHC-C1C	5.33	1.49	1.38
23	b	603	CLA	C3C-C2C	5.34	1.48	1.36
24	D	402	PHO	C3C-C2C	5.34	1.48	1.36
23	b	611	CLA	C3C-C2C	5.35	1.48	1.36
23	c	501	CLA	C3C-C2C	5.35	1.48	1.36
23	C	508	CLA	C3B-C2B	5.35	1.47	1.40
23	b	612	CLA	C3C-C2C	5.35	1.48	1.36
23	C	504	CLA	C3C-C2C	5.37	1.48	1.36
23	b	616	CLA	C3C-C2C	5.37	1.48	1.36
24	A	406	PHO	CHB-C1B	5.38	1.49	1.38
23	D	405	CLA	C3C-C2C	5.38	1.48	1.36
23	c	511	CLA	C3C-C2C	5.38	1.48	1.36
23	B	611	CLA	C3C-C2C	5.39	1.48	1.36
23	D	401	CLA	C3B-C2B	5.40	1.47	1.40
24	a	408	PHO	CHB-C1B	5.41	1.49	1.38
23	B	610	CLA	C3B-C2B	5.41	1.47	1.40
23	B	616	CLA	C3B-C2B	5.42	1.47	1.40
23	a	405	CLA	C3C-C2C	5.43	1.48	1.36
24	A	406	PHO	CHC-C1C	5.43	1.49	1.38
23	a	406	CLA	C3C-C2C	5.44	1.48	1.36
23	A	407	CLA	C3C-C2C	5.45	1.48	1.36
23	c	512	CLA	C3C-C2C	5.45	1.48	1.36
23	b	607	CLA	C3B-C2B	5.46	1.47	1.40
23	B	607	CLA	C3B-C2B	5.47	1.47	1.40
23	B	603	CLA	C3C-C2C	5.47	1.48	1.36
23	c	508	CLA	C3C-C2C	5.48	1.48	1.36
23	b	615	CLA	C3C-C2C	5.48	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C3C-C2C	5.48	1.48	1.36
23	C	508	CLA	C3C-C2C	5.48	1.48	1.36
23	B	602	CLA	C3C-C2C	5.52	1.48	1.36
23	c	512	CLA	C3B-C2B	5.53	1.47	1.40
23	C	503	CLA	C3B-C2B	5.54	1.47	1.40
23	B	617	CLA	C3C-C2C	5.54	1.48	1.36
23	D	405	CLA	C3B-C2B	5.54	1.47	1.40
23	b	615	CLA	C3B-C2B	5.59	1.47	1.40
23	b	610	CLA	C3C-C2C	5.59	1.48	1.36
23	c	505	CLA	C3B-C2B	5.60	1.47	1.40
23	b	603	CLA	C3B-C2B	5.61	1.47	1.40
23	A	405	CLA	C3B-C2B	5.63	1.47	1.40
23	c	506	CLA	C3B-C2B	5.63	1.47	1.40
23	D	404	CLA	C3C-C2C	5.63	1.48	1.36
23	c	507	CLA	C3B-C2B	5.64	1.47	1.40
23	C	504	CLA	C3B-C2B	5.69	1.47	1.40
23	B	615	CLA	C3B-C2B	5.70	1.47	1.40
23	B	609	CLA	C3B-C2B	5.70	1.47	1.40
23	C	509	CLA	C3C-C2C	5.74	1.49	1.36
23	a	409	CLA	C3B-C2B	5.75	1.47	1.40
24	a	408	PHO	C3C-C2C	5.77	1.49	1.36
24	a	407	PHO	C3C-C2C	5.78	1.49	1.36
23	b	606	CLA	C3B-C2B	5.79	1.48	1.40
23	C	511	CLA	C3B-C2B	5.83	1.48	1.40
23	B	608	CLA	C3B-C2B	5.83	1.48	1.40
23	C	507	CLA	C3B-C2B	5.88	1.48	1.40
23	c	503	CLA	C3B-C2B	5.88	1.48	1.40
23	b	604	CLA	C3B-C2B	5.95	1.48	1.40
23	d	402	CLA	C3B-C2B	5.97	1.48	1.40
23	C	506	CLA	C3B-C2B	5.97	1.48	1.40
24	D	402	PHO	C3B-C2B	6.01	1.48	1.37
23	B	605	CLA	C3B-C2B	6.04	1.48	1.40
23	c	513	CLA	C3B-C2B	6.06	1.48	1.40
23	b	605	CLA	C3B-C2B	6.07	1.48	1.40
23	C	514	CLA	C3B-C2B	6.08	1.48	1.40
23	c	510	CLA	C3B-C2B	6.08	1.48	1.40
23	A	407	CLA	C3B-C2B	6.13	1.48	1.40
23	B	603	CLA	C3B-C2B	6.15	1.48	1.40
23	b	609	CLA	C3B-C2B	6.17	1.48	1.40
23	C	513	CLA	C3B-C2B	6.19	1.48	1.40
23	d	403	CLA	C3B-C2B	6.21	1.48	1.40
23	B	611	CLA	C3B-C2B	6.21	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	501	CLA	C3B-C2B	6.24	1.48	1.40
23	b	601	CLA	C3B-C2B	6.24	1.48	1.40
23	B	602	CLA	C3B-C2B	6.25	1.48	1.40
23	b	616	CLA	C3B-C2B	6.36	1.48	1.40
23	c	509	CLA	C3B-C2B	6.37	1.48	1.40
23	B	617	CLA	C3B-C2B	6.38	1.48	1.40
23	a	406	CLA	C3B-C2B	6.39	1.48	1.40
23	B	604	CLA	C3B-C2B	6.41	1.48	1.40
23	c	511	CLA	C3B-C2B	6.44	1.48	1.40
23	C	510	CLA	C3B-C2B	6.47	1.48	1.40
23	a	405	CLA	C3B-C2B	6.47	1.48	1.40
23	c	508	CLA	C3B-C2B	6.55	1.49	1.40
23	B	612	CLA	C3B-C2B	6.55	1.49	1.40
23	b	610	CLA	C3B-C2B	6.56	1.49	1.40
24	a	408	PHO	C3B-C2B	6.57	1.49	1.37
23	b	608	CLA	C3B-C2B	6.59	1.49	1.40
24	A	406	PHO	C3B-C2B	6.61	1.49	1.37
23	a	404	CLA	C3B-C2B	6.61	1.49	1.40
23	b	602	CLA	C3B-C2B	6.62	1.49	1.40
24	a	407	PHO	C3B-C2B	6.63	1.49	1.37
23	C	502	CLA	C3B-C2B	6.64	1.49	1.40
23	B	613	CLA	C3B-C2B	6.64	1.49	1.40
23	C	512	CLA	C3B-C2B	6.69	1.49	1.40
23	b	614	CLA	C3B-C2B	6.70	1.49	1.40
23	C	505	CLA	C3B-C2B	6.74	1.49	1.40
23	b	611	CLA	C3B-C2B	6.78	1.49	1.40
23	b	612	CLA	C3B-C2B	6.79	1.49	1.40
23	c	504	CLA	C3B-C2B	6.82	1.49	1.40
23	D	404	CLA	C3B-C2B	6.83	1.49	1.40
23	b	613	CLA	C3B-C2B	6.89	1.49	1.40
23	C	509	CLA	C3B-C2B	6.90	1.49	1.40
23	A	404	CLA	C3B-C2B	7.00	1.49	1.40
23	B	614	CLA	C3B-C2B	7.09	1.49	1.40
23	c	502	CLA	C3B-C2B	7.33	1.50	1.40

All (2182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	CHD-C4C-C3C	-6.86	114.58	124.92
23	B	609	CLA	CHD-C4C-C3C	-6.81	114.66	124.92
23	b	607	CLA	C1C-NC-C4C	-6.63	103.24	107.06
23	B	617	CLA	CHD-C4C-C3C	-6.56	115.03	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	CHD-C4C-C3C	-6.56	115.04	124.92
23	D	405	CLA	CHD-C4C-C3C	-6.51	115.11	124.92
23	d	402	CLA	C1C-NC-C4C	-6.51	103.31	107.06
23	b	611	CLA	C1C-NC-C4C	-6.47	103.33	107.06
23	b	613	CLA	CHD-C4C-C3C	-6.38	115.31	124.92
25	D	406	BCR	C7-C8-C9	-6.36	116.66	126.21
23	B	606	CLA	CHD-C4C-C3C	-6.33	115.39	124.92
23	D	401	CLA	CHD-C4C-C3C	-6.27	115.47	124.92
23	B	610	CLA	CHD-C4C-C3C	-6.17	115.62	124.92
23	C	510	CLA	CHD-C4C-C3C	-6.14	115.66	124.92
23	c	502	CLA	CHD-C4C-C3C	-6.12	115.69	124.92
23	c	505	CLA	CHD-C4C-C3C	-6.12	115.70	124.92
23	C	513	CLA	CHD-C4C-C3C	-6.10	115.73	124.92
23	d	403	CLA	CHD-C4C-C3C	-6.09	115.74	124.92
23	a	406	CLA	CHD-C4C-C3C	-6.05	115.80	124.92
23	b	608	CLA	CHD-C4C-C3C	-6.05	115.80	124.92
23	C	509	CLA	CHD-C4C-C3C	-6.00	115.87	124.92
23	c	512	CLA	CHD-C4C-C3C	-5.98	115.91	124.92
23	B	613	CLA	C1C-NC-C4C	-5.98	103.62	107.06
23	b	606	CLA	CHD-C4C-C3C	-5.97	115.92	124.92
23	A	407	CLA	CHD-C4C-C3C	-5.97	115.92	124.92
23	C	506	CLA	CHD-C4C-C3C	-5.97	115.92	124.92
23	c	508	CLA	CHD-C4C-C3C	-5.97	115.93	124.92
23	c	511	CLA	CHD-C4C-C3C	-5.96	115.94	124.92
23	C	514	CLA	CHD-C4C-C3C	-5.96	115.94	124.92
23	b	604	CLA	CHD-C4C-C3C	-5.96	115.94	124.92
23	b	602	CLA	CHD-C4C-C3C	-5.94	115.96	124.92
23	B	605	CLA	CHD-C4C-C3C	-5.93	115.98	124.92
23	C	509	CLA	C1C-NC-C4C	-5.92	103.65	107.06
23	b	605	CLA	CHD-C4C-C3C	-5.91	116.01	124.92
23	B	613	CLA	CHD-C4C-C3C	-5.90	116.03	124.92
23	B	607	CLA	CHD-C4C-C3C	-5.84	116.11	124.92
23	D	404	CLA	C1C-NC-C4C	-5.84	103.70	107.06
23	b	610	CLA	CHD-C4C-C3C	-5.82	116.15	124.92
23	B	605	CLA	C1C-NC-C4C	-5.81	103.71	107.06
23	C	505	CLA	C1C-NC-C4C	-5.81	103.71	107.06
23	B	616	CLA	CHD-C4C-C3C	-5.79	116.19	124.92
23	c	505	CLA	C1C-NC-C4C	-5.78	103.73	107.06
23	C	508	CLA	CHD-C4C-C3C	-5.78	116.21	124.92
23	b	603	CLA	CHD-C4C-C3C	-5.78	116.21	124.92
23	B	602	CLA	CHD-C4C-C3C	-5.75	116.25	124.92
23	B	604	CLA	CHD-C4C-C3C	-5.74	116.28	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CHD-C4C-C3C	-5.73	116.28	124.92
23	b	609	CLA	CHD-C4C-C3C	-5.73	116.29	124.92
23	b	601	CLA	CHD-C4C-C3C	-5.72	116.30	124.92
23	D	404	CLA	CHD-C4C-C3C	-5.72	116.30	124.92
23	B	614	CLA	C1C-NC-C4C	-5.70	103.78	107.06
23	b	607	CLA	CHD-C4C-C3C	-5.69	116.35	124.92
23	C	506	CLA	C1C-NC-C4C	-5.67	103.80	107.06
23	b	612	CLA	CHD-C4C-C3C	-5.63	116.44	124.92
23	b	614	CLA	CHD-C4C-C3C	-5.63	116.44	124.92
23	c	508	CLA	C1C-NC-C4C	-5.63	103.82	107.06
23	b	616	CLA	CHD-C4C-C3C	-5.62	116.44	124.92
23	c	509	CLA	CHD-C4C-C3C	-5.62	116.45	124.92
23	A	404	CLA	CHD-C4C-C3C	-5.59	116.49	124.92
23	B	608	CLA	CHD-C4C-C3C	-5.58	116.51	124.92
23	C	502	CLA	C1C-NC-C4C	-5.58	103.84	107.06
23	C	503	CLA	CHD-C4C-C3C	-5.56	116.54	124.92
23	a	405	CLA	CHD-C4C-C3C	-5.56	116.54	124.92
25	Y	101	BCR	C33-C5-C6	-5.54	118.30	124.51
23	c	503	CLA	C1C-NC-C4C	-5.53	103.87	107.06
23	B	612	CLA	C1C-NC-C4C	-5.51	103.89	107.06
23	a	404	CLA	CHD-C4C-C3C	-5.50	116.62	124.92
23	B	610	CLA	C1C-NC-C4C	-5.50	103.89	107.06
24	A	406	PHO	C3D-C2D-C1D	-5.49	97.68	105.82
25	T	101	BCR	C15-C16-C17	-5.49	111.75	123.46
23	B	614	CLA	CHD-C4C-C3C	-5.48	116.66	124.92
23	b	611	CLA	CHD-C4C-C3C	-5.48	116.66	124.92
23	C	512	CLA	CHD-C4C-C3C	-5.45	116.70	124.92
23	b	604	CLA	C1C-NC-C4C	-5.45	103.92	107.06
23	c	507	CLA	CHD-C4C-C3C	-5.44	116.71	124.92
23	b	616	CLA	C1C-NC-C4C	-5.44	103.93	107.06
24	a	407	PHO	C3D-C2D-C1D	-5.44	97.76	105.82
23	C	504	CLA	CHD-C4C-C3C	-5.42	116.75	124.92
23	c	506	CLA	CHD-C4C-C3C	-5.41	116.76	124.92
23	c	513	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
23	C	507	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
25	y	101	BCR	C33-C5-C6	-5.35	118.52	124.51
23	C	505	CLA	CHD-C4C-C3C	-5.33	116.89	124.92
23	c	504	CLA	C1C-NC-C4C	-5.30	104.01	107.06
25	c	514	BCR	C15-C14-C13	-5.28	119.77	127.31
23	c	504	CLA	CHD-C4C-C3C	-5.27	116.97	124.92
23	B	615	CLA	CHD-C4C-C3C	-5.27	116.98	124.92
24	D	402	PHO	C3D-C2D-C1D	-5.26	98.02	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C1C-NC-C4C	-5.22	104.05	107.06
23	c	506	CLA	C1C-NC-C4C	-5.20	104.07	107.06
23	c	510	CLA	CHD-C4C-C3C	-5.19	117.09	124.92
23	c	510	CLA	C1-C2-C3	-5.15	116.46	125.96
23	B	603	CLA	CHD-C4C-C3C	-5.13	117.18	124.92
25	b	619	BCR	C3-C4-C5	-5.12	104.97	113.78
23	d	402	CLA	CHD-C4C-C3C	-5.11	117.22	124.92
23	c	509	CLA	C1C-NC-C4C	-5.08	104.13	107.06
23	c	501	CLA	CHD-C4C-C3C	-5.07	117.28	124.92
23	A	404	CLA	C1C-NC-C4C	-5.07	104.14	107.06
23	a	409	CLA	CHD-C4C-C3C	-5.04	117.32	124.92
23	b	615	CLA	CHD-C4C-C3C	-5.01	117.37	124.92
23	c	503	CLA	CHD-C4C-C3C	-5.00	117.38	124.92
23	B	609	CLA	C1C-NC-C4C	-4.99	104.18	107.06
23	A	405	CLA	CHD-C4C-C3C	-4.99	117.40	124.92
25	B	618	BCR	C33-C5-C6	-4.97	118.94	124.51
23	B	608	CLA	C1C-NC-C4C	-4.97	104.19	107.06
23	B	616	CLA	C1C-NC-C4C	-4.91	104.23	107.06
23	b	605	CLA	C1C-NC-C4C	-4.88	104.25	107.06
23	C	504	CLA	C1C-NC-C4C	-4.86	104.26	107.06
23	a	404	CLA	C1C-NC-C4C	-4.83	104.27	107.06
25	T	101	BCR	C7-C8-C9	-4.81	118.98	126.21
23	C	508	CLA	C1C-NC-C4C	-4.81	104.29	107.06
23	b	615	CLA	C1C-NC-C4C	-4.81	104.29	107.06
23	b	614	CLA	C1C-NC-C4C	-4.80	104.29	107.06
29	d	405	PL9	C42-C43-C44	-4.78	115.66	127.68
24	a	408	PHO	C3D-C2D-C1D	-4.77	98.74	105.82
26	A	409	SQD	C1-C2-C3	-4.75	101.15	109.98
23	C	503	CLA	C1C-NC-C4C	-4.73	104.33	107.06
23	a	405	CLA	C1C-C2C-C3C	-4.72	101.68	106.92
25	c	515	BCR	C7-C8-C9	-4.71	119.14	126.21
23	B	615	CLA	C1C-NC-C4C	-4.70	104.35	107.06
23	c	512	CLA	C1C-NC-C4C	-4.68	104.36	107.06
23	C	511	CLA	CHD-C4C-C3C	-4.67	117.88	124.92
23	c	511	CLA	C1C-NC-C4C	-4.67	104.37	107.06
25	Y	101	BCR	C16-C17-C18	-4.66	120.66	127.31
23	B	611	CLA	C1C-NC-C4C	-4.65	104.38	107.06
23	b	606	CLA	C1C-NC-C4C	-4.63	104.39	107.06
25	C	515	BCR	C15-C14-C13	-4.61	120.73	127.31
23	C	511	CLA	C1C-NC-C4C	-4.60	104.41	107.06
25	t	101	BCR	C33-C5-C6	-4.60	119.36	124.51
23	B	606	CLA	C1C-NC-C4C	-4.59	104.41	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	C1C-NC-C4C	-4.59	104.42	107.06
23	c	513	CLA	C1C-NC-C4C	-4.56	104.43	107.06
24	a	408	PHO	C1-C2-C3	-4.54	117.59	125.96
23	C	510	CLA	C1C-NC-C4C	-4.52	104.45	107.06
23	a	405	CLA	C1C-NC-C4C	-4.52	104.46	107.06
23	b	610	CLA	C1C-NC-C4C	-4.50	104.46	107.06
23	b	602	CLA	C1C-NC-C4C	-4.48	104.48	107.06
23	c	502	CLA	C1C-NC-C4C	-4.46	104.49	107.06
25	c	514	BCR	C20-C21-C22	-4.45	120.96	127.31
23	c	501	CLA	C1C-NC-C4C	-4.45	104.50	107.06
23	C	513	CLA	C1C-NC-C4C	-4.44	104.50	107.06
23	B	607	CLA	C1C-NC-C4C	-4.43	104.50	107.06
23	b	603	CLA	C1C-NC-C4C	-4.42	104.51	107.06
25	T	101	BCR	C33-C5-C6	-4.42	119.56	124.51
23	b	611	CLA	O2D-CGD-O1D	-4.42	114.93	123.82
26	A	409	SQD	C1-O5-C5	-4.41	105.41	113.72
25	b	617	BCR	C7-C8-C9	-4.40	119.60	126.21
23	b	612	CLA	C1C-NC-C4C	-4.38	104.54	107.06
23	C	502	CLA	C1D-CHD-C4C	-4.37	116.51	122.48
23	c	510	CLA	C1C-NC-C4C	-4.37	104.54	107.06
23	B	604	CLA	C1C-NC-C4C	-4.35	104.55	107.06
23	C	512	CLA	C1C-NC-C4C	-4.35	104.55	107.06
23	B	603	CLA	C1C-NC-C4C	-4.34	104.56	107.06
23	b	601	CLA	C1C-NC-C4C	-4.34	104.56	107.06
25	d	404	BCR	C7-C8-C9	-4.34	119.70	126.21
23	C	507	CLA	C1C-NC-C4C	-4.31	104.58	107.06
25	B	619	BCR	C15-C14-C13	-4.30	121.17	127.31
25	B	618	BCR	C7-C8-C9	-4.28	119.78	126.21
23	B	617	CLA	C1C-NC-C4C	-4.28	104.59	107.06
23	C	505	CLA	C1C-C2C-C3C	-4.27	102.18	106.92
23	b	603	CLA	C1D-CHD-C4C	-4.27	116.65	122.48
23	c	507	CLA	C1C-NC-C4C	-4.27	104.60	107.06
23	C	510	CLA	C1-C2-C3	-4.24	118.15	125.96
23	b	609	CLA	C1C-NC-C4C	-4.23	104.62	107.06
23	C	511	CLA	C1-C2-C3	-4.23	118.17	125.96
23	A	407	CLA	C1C-NC-C4C	-4.23	104.62	107.06
38	E	103	HEM	CBD-CAD-C3D	-4.22	104.42	112.47
23	a	404	CLA	C1C-C2C-C3C	-4.20	102.26	106.92
23	B	605	CLA	C1-C2-C3	-4.20	118.22	125.96
23	d	402	CLA	C1C-C2C-C3C	-4.18	102.28	106.92
23	B	616	CLA	C1D-CHD-C4C	-4.18	116.78	122.48
23	c	509	CLA	C1-C2-C3	-4.17	118.27	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	O2D-CGD-O1D	-4.12	115.52	123.82
23	b	616	CLA	C1D-CHD-C4C	-4.12	116.86	122.48
23	B	606	CLA	C1D-CHD-C4C	-4.11	116.86	122.48
25	t	101	BCR	C15-C16-C17	-4.11	114.69	123.46
25	T	101	BCR	C11-C10-C9	-4.11	121.44	127.31
23	D	405	CLA	C1C-NC-C4C	-4.10	104.70	107.06
23	B	602	CLA	C1C-NC-C4C	-4.09	104.70	107.06
25	b	619	BCR	C7-C8-C9	-4.09	120.07	126.21
23	a	404	CLA	C1D-CHD-C4C	-4.08	116.90	122.48
23	a	409	CLA	C1C-NC-C4C	-4.08	104.71	107.06
23	c	502	CLA	C1C-C2C-C3C	-4.07	102.41	106.92
26	a	411	SQD	C1-C2-C3	-4.03	102.49	109.98
23	D	404	CLA	C1C-C2C-C3C	-3.99	102.49	106.92
23	C	502	CLA	O2D-CGD-O1D	-3.98	115.81	123.82
23	c	508	CLA	C1C-C2C-C3C	-3.96	102.53	106.92
29	a	415	PL9	C7-C3-C2	-3.96	117.60	123.23
29	a	415	PL9	C32-C33-C34	-3.96	117.73	127.68
23	b	611	CLA	C1C-C2C-C3C	-3.96	102.53	106.92
23	B	614	CLA	C1C-C2C-C3C	-3.95	102.54	106.92
25	b	619	BCR	C15-C14-C13	-3.94	121.69	127.31
29	A	413	PL9	C7-C3-C2	-3.94	117.63	123.23
23	B	609	CLA	C1D-CHD-C4C	-3.94	117.10	122.48
25	C	515	BCR	C16-C17-C18	-3.93	121.70	127.31
23	b	608	CLA	C1C-NC-C4C	-3.92	104.80	107.06
23	B	612	CLA	C1C-C2C-C3C	-3.92	102.58	106.92
24	a	407	PHO	C4C-C3C-C2C	-3.91	102.42	106.81
25	c	514	BCR	C16-C17-C18	-3.90	121.74	127.31
25	d	404	BCR	C38-C26-C25	-3.90	120.14	124.51
25	k	101	BCR	C11-C10-C9	-3.89	121.75	127.31
25	k	101	BCR	C24-C23-C22	-3.89	120.37	126.21
23	D	401	CLA	C1C-C2C-C3C	-3.88	102.62	106.92
23	d	403	CLA	O2D-CGD-O1D	-3.87	116.03	123.82
25	C	527	BCR	C7-C8-C9	-3.87	120.40	126.21
23	d	403	CLA	C1C-NC-C4C	-3.87	104.83	107.06
25	H	101	BCR	C7-C8-C9	-3.87	120.40	126.21
23	B	617	CLA	C1D-CHD-C4C	-3.85	117.22	122.48
23	B	608	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	B	615	CLA	C1C-C2C-C3C	-3.82	102.68	106.92
25	H	101	BCR	C16-C17-C18	-3.82	121.86	127.31
23	C	505	CLA	C1D-CHD-C4C	-3.81	117.28	122.48
25	d	404	BCR	C33-C5-C6	-3.80	120.25	124.51
25	D	406	BCR	C38-C26-C25	-3.79	120.27	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C1D-CHD-C4C	-3.79	117.31	122.48
25	k	101	BCR	C15-C14-C13	-3.79	121.91	127.31
23	A	404	CLA	C1D-CHD-C4C	-3.78	117.32	122.48
25	b	617	BCR	C33-C5-C6	-3.77	120.29	124.51
23	b	606	CLA	C1D-CHD-C4C	-3.76	117.34	122.48
25	A	408	BCR	C15-C14-C13	-3.75	121.95	127.31
23	C	509	CLA	C4C-C3C-C2C	-3.74	101.17	106.91
24	D	402	PHO	C1-C2-C3	-3.74	119.06	125.96
25	C	516	BCR	C11-C10-C9	-3.74	121.98	127.31
25	H	101	BCR	C24-C23-C22	-3.74	120.60	126.21
29	D	407	PL9	C42-C43-C44	-3.73	118.30	127.68
23	b	603	CLA	C1C-C2C-C3C	-3.73	102.78	106.92
23	C	513	CLA	C1D-CHD-C4C	-3.73	117.38	122.48
23	b	615	CLA	C1C-C2C-C3C	-3.73	102.78	106.92
23	a	406	CLA	C1D-CHD-C4C	-3.73	117.39	122.48
29	a	415	PL9	C27-C28-C29	-3.73	118.32	127.68
23	C	509	CLA	O2D-CGD-O1D	-3.71	116.35	123.82
23	B	613	CLA	C1-C2-C3	-3.71	119.12	125.96
23	b	605	CLA	C1D-CHD-C4C	-3.70	117.42	122.48
23	C	502	CLA	C1C-C2C-C3C	-3.70	102.81	106.92
23	B	604	CLA	C1D-CHD-C4C	-3.70	117.43	122.48
23	B	615	CLA	O2D-CGD-O1D	-3.70	116.38	123.82
23	D	404	CLA	C1-C2-C3	-3.70	119.15	125.96
25	t	101	BCR	C11-C10-C9	-3.69	122.04	127.31
23	A	405	CLA	C1C-C2C-C3C	-3.69	102.83	106.92
23	c	502	CLA	O2D-CGD-O1D	-3.69	116.41	123.82
23	D	405	CLA	C1D-CHD-C4C	-3.68	117.46	122.48
23	B	616	CLA	C1C-C2C-C3C	-3.67	102.84	106.92
25	D	406	BCR	C33-C5-C6	-3.65	120.42	124.51
23	c	511	CLA	C1-C2-C3	-3.65	119.24	125.96
23	c	510	CLA	C1C-C2C-C3C	-3.63	102.89	106.92
23	a	405	CLA	CBC-CAC-C3C	-3.63	102.10	112.41
23	b	602	CLA	C1D-CHD-C4C	-3.62	117.53	122.48
26	a	411	SQD	C5-C6-S	-3.62	109.29	114.34
23	c	504	CLA	C1C-C2C-C3C	-3.62	102.91	106.92
23	c	501	CLA	O2D-CGD-O1D	-3.62	116.54	123.82
23	b	609	CLA	C1-C2-C3	-3.60	119.33	125.96
25	c	514	BCR	C11-C10-C9	-3.59	122.19	127.31
23	b	602	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
23	B	606	CLA	O2D-CGD-O1D	-3.59	116.60	123.82
23	C	507	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
23	A	404	CLA	CAA-C2A-C3A	-3.59	102.98	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	PHO	C4C-C3C-C2C	-3.58	102.78	106.81
23	c	512	CLA	C1D-CHD-C4C	-3.58	117.59	122.48
23	b	607	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
23	a	404	CLA	CAA-C2A-C3A	-3.58	102.99	112.81
25	Y	101	BCR	C15-C14-C13	-3.58	122.20	127.31
25	C	515	BCR	C33-C5-C6	-3.58	120.50	124.51
23	C	508	CLA	C1D-CHD-C4C	-3.58	117.60	122.48
23	b	612	CLA	C1-C2-C3	-3.57	119.37	125.96
23	b	611	CLA	C1-C2-C3	-3.57	119.38	125.96
23	C	504	CLA	C1D-CHD-C4C	-3.56	117.61	122.48
23	B	612	CLA	C1D-CHD-C4C	-3.56	117.62	122.48
23	B	603	CLA	CAA-C2A-C3A	-3.56	103.05	112.81
23	C	511	CLA	C1C-C2C-C3C	-3.55	102.98	106.92
23	C	506	CLA	C1D-CHD-C4C	-3.55	117.63	122.48
23	b	609	CLA	O2D-CGD-O1D	-3.55	116.67	123.82
23	b	610	CLA	C1-C2-C3	-3.55	119.42	125.96
23	A	404	CLA	C1C-C2C-C3C	-3.55	102.99	106.92
23	b	610	CLA	C1D-CHD-C4C	-3.54	117.64	122.48
26	A	409	SQD	C44-O6-C1	-3.54	106.49	113.76
23	C	508	CLA	O2D-CGD-O1D	-3.54	116.69	123.82
25	b	619	BCR	C10-C11-C12	-3.54	112.39	123.23
23	B	611	CLA	C1D-CHD-C4C	-3.53	117.65	122.48
25	b	619	BCR	C24-C23-C22	-3.53	120.90	126.21
23	b	605	CLA	C1C-C2C-C3C	-3.53	103.01	106.92
25	B	618	BCR	C16-C17-C18	-3.53	122.27	127.31
23	b	604	CLA	C1C-C2C-C3C	-3.52	103.01	106.92
23	b	611	CLA	CHC-C1C-C2C	-3.51	117.07	126.65
25	T	101	BCR	C12-C13-C14	-3.51	113.55	118.94
23	B	603	CLA	C1C-C2C-C3C	-3.51	103.03	106.92
23	b	615	CLA	CHC-C1C-C2C	-3.51	117.09	126.65
26	A	409	SQD	C45-O47-C7	-3.50	109.60	117.88
23	c	512	CLA	C1C-C2C-C3C	-3.50	103.04	106.92
23	B	605	CLA	C1C-C2C-C3C	-3.50	103.04	106.92
23	c	513	CLA	C1C-C2C-C3C	-3.50	103.04	106.92
25	t	101	BCR	C12-C13-C14	-3.50	113.58	118.94
23	B	607	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
23	b	608	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
23	a	405	CLA	C1D-CHD-C4C	-3.49	117.72	122.48
23	b	614	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
23	B	610	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
23	A	407	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
23	A	405	CLA	C1C-NC-C4C	-3.46	105.06	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C1D-CHD-C4C	-3.46	117.75	122.48
25	D	406	BCR	C24-C23-C22	-3.46	121.01	126.21
23	B	611	CLA	C1-C2-C3	-3.46	119.58	125.96
25	b	618	BCR	C7-C8-C9	-3.46	121.02	126.21
23	B	613	CLA	O2D-CGD-O1D	-3.45	116.87	123.82
23	b	614	CLA	O2D-CGD-O1D	-3.45	116.87	123.82
23	C	508	CLA	C1C-C2C-C3C	-3.45	103.09	106.92
23	C	503	CLA	C1C-C2C-C3C	-3.45	103.09	106.92
25	a	410	BCR	C15-C14-C13	-3.45	122.39	127.31
23	B	614	CLA	C1-C2-C3	-3.44	119.61	125.96
34	C	501	LMG	C7-O1-C1	-3.44	106.69	113.76
23	b	605	CLA	O2D-CGD-O1D	-3.44	116.89	123.82
23	c	508	CLA	O2D-CGD-O1D	-3.44	116.90	123.82
23	a	405	CLA	CAA-C2A-C3A	-3.44	103.38	112.81
25	h	102	BCR	C16-C17-C18	-3.44	122.40	127.31
23	b	601	CLA	C1D-CHD-C4C	-3.43	117.79	122.48
25	b	619	BCR	C38-C26-C25	-3.43	120.67	124.51
23	B	607	CLA	O2D-CGD-O1D	-3.43	116.93	123.82
23	C	511	CLA	CHC-C1C-C2C	-3.42	117.32	126.65
24	a	408	PHO	C4C-C3C-C2C	-3.42	102.97	106.81
23	B	617	CLA	C4C-C3C-C2C	-3.42	101.67	106.91
23	b	603	CLA	CAA-C2A-C3A	-3.42	103.45	112.81
23	B	604	CLA	O2A-CGA-O1A	-3.41	115.09	123.55
25	B	618	BCR	C28-C27-C26	-3.40	107.93	113.78
25	y	101	BCR	C15-C14-C13	-3.40	122.45	127.31
23	b	601	CLA	C1C-C2C-C3C	-3.40	103.15	106.92
23	D	405	CLA	O2D-CGD-O1D	-3.40	116.98	123.82
23	A	404	CLA	O2A-CGA-O1A	-3.40	115.11	123.55
23	B	615	CLA	CHC-C1C-C2C	-3.40	117.39	126.65
23	b	606	CLA	C1C-C2C-C3C	-3.40	103.15	106.92
23	C	502	CLA	C1-C2-C3	-3.39	119.70	125.96
23	B	602	CLA	C1C-C2C-C3C	-3.39	103.16	106.92
23	C	506	CLA	C1C-C2C-C3C	-3.39	103.16	106.92
24	a	407	PHO	O2D-CGD-O1D	-3.39	117.01	123.82
25	a	410	BCR	C20-C21-C22	-3.39	122.48	127.31
25	C	527	BCR	C11-C10-C9	-3.39	122.48	127.31
23	B	609	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
23	B	613	CLA	C1D-CHD-C4C	-3.38	117.86	122.48
23	c	512	CLA	C1-C2-C3	-3.38	119.73	125.96
23	b	607	CLA	C1D-CHD-C4C	-3.37	117.87	122.48
29	A	413	PL9	C37-C38-C39	-3.37	119.21	127.68
23	C	514	CLA	O2D-CGD-O1D	-3.36	117.05	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C1D-CHD-C4C	-3.36	117.89	122.48
23	c	509	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
23	b	604	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
23	c	501	CLA	C1C-C2C-C3C	-3.35	103.21	106.92
23	b	613	CLA	C1C-C2C-C3C	-3.35	103.21	106.92
23	b	614	CLA	C1-C2-C3	-3.34	119.80	125.96
23	c	510	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
25	b	618	BCR	C37-C22-C21	-3.34	118.24	122.92
23	b	611	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
23	c	507	CLA	C1C-C2C-C3C	-3.34	103.22	106.92
23	B	611	CLA	C4C-C3C-C2C	-3.34	101.79	106.91
23	c	509	CLA	C1C-C2C-C3C	-3.34	103.22	106.92
29	A	413	PL9	C32-C33-C34	-3.33	119.31	127.68
23	b	612	CLA	C1C-C2C-C3C	-3.33	103.23	106.92
23	B	607	CLA	C1D-CHD-C4C	-3.33	117.94	122.48
29	a	415	PL9	C42-C43-C44	-3.32	119.33	127.68
23	b	613	CLA	C1D-CHD-C4C	-3.32	117.94	122.48
25	h	102	BCR	C38-C26-C25	-3.32	120.79	124.51
23	c	512	CLA	CMA-C3A-C4A	-3.32	102.86	111.77
23	a	406	CLA	C1C-NC-C4C	-3.31	105.15	107.06
25	A	408	BCR	C38-C26-C25	-3.31	120.80	124.51
29	d	405	PL9	C22-C23-C24	-3.30	119.39	127.68
23	a	409	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
23	b	607	CLA	CAA-C2A-C3A	-3.29	103.78	112.81
23	C	513	CLA	C1C-C2C-C3C	-3.29	103.27	106.92
23	c	513	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
23	C	507	CLA	C1-C2-C3	-3.29	119.90	125.96
23	c	505	CLA	C4C-C3C-C2C	-3.28	101.87	106.91
26	a	411	SQD	C45-O47-C7	-3.28	110.11	117.88
23	b	615	CLA	C11-C10-C8	-3.28	104.97	115.73
23	B	615	CLA	C1D-CHD-C4C	-3.27	118.01	122.48
23	B	612	CLA	OBD-CAD-C3D	-3.27	122.00	128.03
23	C	503	CLA	O2D-CGD-O1D	-3.26	117.25	123.82
23	C	514	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
23	B	606	CLA	C4C-C3C-C2C	-3.26	101.91	106.91
23	c	511	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
25	B	619	BCR	C37-C22-C21	-3.25	118.36	122.92
23	c	511	CLA	C1C-C2C-C3C	-3.25	103.31	106.92
23	C	504	CLA	C1C-C2C-C3C	-3.25	103.31	106.92
25	b	618	BCR	C38-C26-C25	-3.25	120.87	124.51
23	C	504	CLA	CHC-C1C-C2C	-3.25	117.79	126.65
25	A	408	BCR	C24-C23-C22	-3.25	121.33	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
25	B	620	BCR	C38-C26-C25	-3.24	120.88	124.51
26	L	102	SQD	C5-C6-S	-3.24	109.82	114.34
29	a	415	PL9	C22-C23-C24	-3.24	119.54	127.68
23	b	610	CLA	C1C-C2C-C3C	-3.23	103.33	106.92
23	c	503	CLA	C1C-C2C-C3C	-3.23	103.33	106.92
23	c	502	CLA	C1D-CHD-C4C	-3.23	118.07	122.48
23	c	506	CLA	C1C-C2C-C3C	-3.23	103.34	106.92
23	c	510	CLA	CBC-CAC-C3C	-3.23	103.25	112.41
23	B	613	CLA	C4C-C3C-C2C	-3.22	101.96	106.91
23	a	405	CLA	CHC-C1C-C2C	-3.22	117.86	126.65
23	b	616	CLA	C4C-C3C-C2C	-3.22	101.97	106.91
23	B	615	CLA	O2A-CGA-O1A	-3.21	115.57	123.55
23	b	616	CLA	CHC-C1C-C2C	-3.21	117.90	126.65
23	c	502	CLA	C1-C2-C3	-3.21	120.05	125.96
23	C	509	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
23	a	406	CLA	C1C-C2C-C3C	-3.21	103.36	106.92
23	C	512	CLA	C1C-C2C-C3C	-3.20	103.37	106.92
23	D	401	CLA	C1D-CHD-C4C	-3.20	118.12	122.48
23	a	406	CLA	C1-C2-C3	-3.20	120.07	125.96
38	E	103	HEM	CBA-CAA-C2A	-3.19	106.39	112.48
23	B	604	CLA	C1C-C2C-C3C	-3.19	103.38	106.92
23	a	409	CLA	C1C-C2C-C3C	-3.19	103.39	106.92
23	b	609	CLA	C1C-C2C-C3C	-3.18	103.40	106.92
23	B	615	CLA	CBC-CAC-C3C	-3.18	103.39	112.41
23	D	401	CLA	CAA-C2A-C3A	-3.17	104.12	112.81
23	d	402	CLA	C1-C2-C3	-3.16	120.14	125.96
23	B	603	CLA	O2D-CGD-O1D	-3.16	117.47	123.82
26	D	413	SQD	C5-C6-S	-3.15	109.94	114.34
23	c	501	CLA	CHC-C1C-C2C	-3.15	118.05	126.65
23	d	403	CLA	C1D-CHD-C4C	-3.15	118.18	122.48
23	C	502	CLA	CBC-CAC-C3C	-3.15	103.47	112.41
23	c	506	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
38	e	103	HEM	CBD-CAD-C3D	-3.14	106.47	112.47
23	B	609	CLA	C4C-C3C-C2C	-3.14	102.09	106.91
23	c	501	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
23	C	514	CLA	C2A-C1A-CHA	-3.14	118.36	123.92
25	t	101	BCR	C3-C4-C5	-3.14	108.39	113.78
24	a	407	PHO	C4D-CHA-C1A	-3.13	118.10	125.06
23	c	512	CLA	O2D-CGD-O1D	-3.13	117.53	123.82
31	A	415	LHG	O8-C23-O10	-3.13	115.79	123.55
23	a	409	CLA	CAA-C2A-C3A	-3.12	104.25	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C40-C30-C25	-3.12	105.25	110.31
23	c	503	CLA	O2D-CGD-O1D	-3.12	117.54	123.82
23	b	609	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
23	D	405	CLA	C4C-C3C-C2C	-3.12	102.12	106.91
23	b	612	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
23	c	505	CLA	C1D-CHD-C4C	-3.12	118.22	122.48
23	C	511	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
23	c	507	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
23	c	513	CLA	CAA-C2A-C3A	-3.11	104.27	112.81
23	C	509	CLA	C1C-C2C-C3C	-3.11	103.47	106.92
23	c	506	CLA	CHC-C1C-C2C	-3.11	118.17	126.65
25	H	101	BCR	C38-C26-C25	-3.11	121.03	124.51
23	b	608	CLA	C1D-CHD-C4C	-3.11	118.24	122.48
23	C	502	CLA	CHC-C1C-C2C	-3.10	118.19	126.65
23	a	409	CLA	O2D-CGD-O1D	-3.10	117.58	123.82
25	C	527	BCR	C24-C23-C22	-3.10	121.55	126.21
26	B	621	SQD	C5-C6-S	-3.10	110.02	114.34
23	c	505	CLA	O2D-CGD-O1D	-3.10	117.59	123.82
23	C	514	CLA	C1C-C2C-C3C	-3.09	103.49	106.92
23	C	510	CLA	C1D-CHD-C4C	-3.09	118.27	122.48
23	b	603	CLA	O2D-CGD-O1D	-3.09	117.61	123.82
24	D	402	PHO	C4D-ND-C1D	-3.08	101.42	106.98
25	c	515	BCR	C11-C10-C9	-3.08	122.92	127.31
24	D	402	PHO	CHC-C1C-C2C	-3.08	118.56	125.62
24	D	402	PHO	C6-C5-C3	-3.07	105.69	112.66
23	B	617	CLA	O2D-CGD-O1D	-3.07	117.64	123.82
29	A	413	PL9	C27-C28-C29	-3.07	119.97	127.68
23	c	504	CLA	C1D-CHD-C4C	-3.07	118.29	122.48
23	B	603	CLA	CHC-C1C-C2C	-3.06	118.29	126.65
23	c	502	CLA	CBC-CAC-C3C	-3.06	103.71	112.41
23	C	510	CLA	C1C-C2C-C3C	-3.06	103.52	106.92
23	D	404	CLA	C2A-C1A-CHA	-3.06	118.50	123.92
25	a	410	BCR	C24-C23-C22	-3.06	121.62	126.21
23	C	506	CLA	C1-C2-C3	-3.06	120.33	125.96
23	D	401	CLA	C1C-NC-C4C	-3.05	105.30	107.06
29	A	413	PL9	C22-C23-C24	-3.05	120.01	127.68
23	B	613	CLA	C1C-C2C-C3C	-3.05	103.53	106.92
23	b	608	CLA	O2D-CGD-O1D	-3.05	117.68	123.82
23	b	604	CLA	C1-C2-C3	-3.05	120.34	125.96
23	a	404	CLA	O2A-CGA-O1A	-3.05	115.99	123.55
23	B	602	CLA	C1D-CHD-C4C	-3.04	118.33	122.48
25	c	515	BCR	C38-C26-C25	-3.04	121.10	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	415	PL9	C37-C38-C39	-3.04	120.04	127.68
23	b	602	CLA	CAA-C2A-C3A	-3.04	104.47	112.81
23	b	616	CLA	C1C-C2C-C3C	-3.04	103.55	106.92
23	c	505	CLA	C1C-C2C-C3C	-3.04	103.55	106.92
23	c	507	CLA	O1D-CGD-CBD	-3.04	119.15	124.60
37	c	516	DGD	C2G-O2G-C1B	-3.03	110.70	117.88
23	c	504	CLA	CHC-C1C-C2C	-3.03	118.38	126.65
23	c	506	CLA	C1-C2-C3	-3.03	120.37	125.96
23	A	404	CLA	CAA-C2A-C1A	-3.03	102.05	111.97
23	C	509	CLA	CHC-C1C-C2C	-3.03	118.39	126.65
23	b	609	CLA	CBC-CAC-C3C	-3.03	103.82	112.41
31	A	415	LHG	C5-O7-C7	-3.02	110.73	117.88
23	c	501	CLA	C1-C2-C3	-3.02	120.40	125.96
25	d	404	BCR	C15-C14-C13	-3.02	123.01	127.31
23	b	607	CLA	C4C-C3C-C2C	-3.02	102.28	106.91
23	a	406	CLA	CHC-C1C-C2C	-3.02	118.43	126.65
23	B	608	CLA	CAA-C2A-C3A	-3.01	104.55	112.81
23	B	610	CLA	C4C-C3C-C2C	-3.01	102.28	106.91
31	D	408	LHG	O8-C23-O10	-3.01	116.07	123.55
25	b	618	BCR	C20-C21-C22	-3.01	123.01	127.31
25	B	620	BCR	C15-C14-C13	-3.00	123.02	127.31
23	B	604	CLA	CAA-C2A-C3A	-3.00	104.57	112.81
23	C	510	CLA	C4C-C3C-C2C	-3.00	102.30	106.91
38	V	202	HEM	CBA-CAA-C2A	-3.00	106.74	112.48
23	B	605	CLA	O2A-CGA-O1A	-3.00	116.10	123.55
23	d	403	CLA	C1C-C2C-C3C	-3.00	103.59	106.92
25	B	620	BCR	C7-C8-C9	-3.00	121.70	126.21
25	Y	101	BCR	C16-C15-C14	-3.00	117.06	123.46
23	B	616	CLA	CHC-C1C-C2C	-2.99	118.49	126.65
37	C	517	DGD	O6D-C1D-O3G	-2.99	102.92	110.02
23	c	508	CLA	C1D-CHD-C4C	-2.99	118.40	122.48
23	c	503	CLA	C1-C2-C3	-2.99	120.45	125.96
23	B	611	CLA	CAA-C2A-C3A	-2.99	104.62	112.81
23	a	406	CLA	C4C-C3C-C2C	-2.99	102.33	106.91
23	B	602	CLA	C1-C2-C3	-2.99	120.46	125.96
23	b	604	CLA	O1D-CGD-CBD	-2.98	119.25	124.60
23	C	506	CLA	C4C-C3C-C2C	-2.98	102.34	106.91
23	C	513	CLA	O1D-CGD-CBD	-2.98	119.26	124.60
23	b	613	CLA	C4C-C3C-C2C	-2.97	102.35	106.91
23	C	508	CLA	C4C-C3C-C2C	-2.97	102.35	106.91
25	A	408	BCR	C11-C10-C9	-2.97	123.07	127.31
23	B	605	CLA	O2D-CGD-O1D	-2.97	117.84	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	O2A-CGA-O1A	-2.97	116.18	123.55
23	c	510	CLA	O1D-CGD-CBD	-2.97	119.27	124.60
23	A	405	CLA	O2A-CGA-O1A	-2.97	116.19	123.55
23	B	609	CLA	C1-C2-C3	-2.96	120.50	125.96
23	c	511	CLA	O2D-CGD-O1D	-2.96	117.86	123.82
23	C	503	CLA	C1D-CHD-C4C	-2.96	118.44	122.48
23	b	610	CLA	C4C-C3C-C2C	-2.96	102.36	106.91
23	D	404	CLA	O2A-CGA-O1A	-2.96	116.20	123.55
23	C	507	CLA	CBC-CAC-C3C	-2.96	104.00	112.41
25	h	102	BCR	C7-C8-C9	-2.96	121.77	126.21
23	b	605	CLA	CHC-C1C-C2C	-2.96	118.58	126.65
23	a	406	CLA	CAA-C2A-C3A	-2.95	104.71	112.81
23	b	607	CLA	CHC-C1C-C2C	-2.95	118.60	126.65
23	b	610	CLA	CAA-C2A-C3A	-2.95	104.72	112.81
37	h	103	DGD	O1G-C1A-O1A	-2.95	116.22	123.55
23	b	614	CLA	C1C-C2C-C3C	-2.95	103.65	106.92
23	C	505	CLA	O2D-CGD-O1D	-2.95	117.89	123.82
23	C	505	CLA	CHC-C1C-C2C	-2.94	118.62	126.65
25	a	410	BCR	C37-C22-C21	-2.94	118.80	122.92
29	A	413	PL9	C42-C43-C44	-2.94	120.30	127.68
23	B	605	CLA	C4C-C3C-C2C	-2.94	102.40	106.91
25	C	527	BCR	C20-C21-C22	-2.94	123.12	127.31
23	b	614	CLA	C4C-C3C-C2C	-2.94	102.41	106.91
23	B	604	CLA	O2D-CGD-O1D	-2.93	117.92	123.82
23	b	614	CLA	O2A-CGA-O1A	-2.93	116.27	123.55
23	A	405	CLA	CHC-C1C-C2C	-2.93	118.66	126.65
23	d	402	CLA	O2D-CGD-O1D	-2.93	117.92	123.82
25	y	101	BCR	C23-C24-C25	-2.92	119.06	127.25
23	c	510	CLA	CHC-C1C-C2C	-2.92	118.68	126.65
25	c	515	BCR	C3-C4-C5	-2.92	108.75	113.78
23	B	611	CLA	C1C-C2C-C3C	-2.92	103.68	106.92
23	b	605	CLA	C2A-C1A-CHA	-2.92	118.75	123.92
23	C	504	CLA	C4C-C3C-C2C	-2.92	102.44	106.91
23	c	503	CLA	CHC-C1C-C2C	-2.92	118.70	126.65
23	c	509	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
23	c	506	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
25	C	516	BCR	C33-C5-C6	-2.90	121.26	124.51
23	b	612	CLA	C4C-C3C-C2C	-2.90	102.45	106.91
37	c	516	DGD	O3G-C3G-C2G	-2.90	104.10	110.99
24	A	406	PHO	CHC-C1C-C2C	-2.89	118.98	125.62
23	C	512	CLA	C1D-CHD-C4C	-2.89	118.53	122.48
23	c	506	CLA	O2D-CGD-O1D	-2.89	118.01	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	616	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
23	C	514	CLA	C4C-C3C-C2C	-2.89	102.48	106.91
24	D	402	PHO	O2D-CGD-O1D	-2.89	118.02	123.82
25	t	101	BCR	C21-C20-C19	-2.88	114.38	123.23
35	M	101	LMT	C1-O1'-C1'	-2.88	108.92	113.87
24	A	406	PHO	C4C-C3C-C2C	-2.88	103.57	106.81
23	C	512	CLA	CHC-C1C-C2C	-2.88	118.79	126.65
23	b	601	CLA	O2D-CGD-O1D	-2.87	118.04	123.82
23	B	606	CLA	C1C-C2C-C3C	-2.87	103.73	106.92
23	C	507	CLA	C2A-C1A-CHA	-2.87	118.83	123.92
24	A	406	PHO	O1D-CGD-CBD	-2.87	119.45	124.60
25	b	619	BCR	C39-C30-C25	-2.87	105.66	110.31
23	c	512	CLA	CHC-C1C-C2C	-2.87	118.84	126.65
23	B	602	CLA	CHC-C1C-C2C	-2.86	118.84	126.65
23	b	612	CLA	C2A-C1A-CHA	-2.86	118.85	123.92
23	a	404	CLA	CHC-C1C-C2C	-2.85	118.86	126.65
25	D	406	BCR	C40-C30-C25	-2.85	105.68	110.31
23	C	514	CLA	C1-C2-C3	-2.85	120.70	125.96
23	D	404	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
23	D	404	CLA	C4C-C3C-C2C	-2.85	102.54	106.91
23	B	605	CLA	C1D-CHD-C4C	-2.85	118.59	122.48
23	B	616	CLA	CBC-CAC-C3C	-2.85	104.33	112.41
25	B	620	BCR	C20-C21-C22	-2.85	123.25	127.31
26	B	621	SQD	C1-C2-C3	-2.84	104.69	109.98
23	B	609	CLA	O2A-CGA-O1A	-2.84	116.50	123.55
25	H	101	BCR	C11-C10-C9	-2.84	123.26	127.31
23	b	601	CLA	CHC-C1C-C2C	-2.84	118.91	126.65
23	b	611	CLA	C4C-C3C-C2C	-2.84	102.56	106.91
23	B	617	CLA	O1D-CGD-CBD	-2.83	119.51	124.60
25	A	408	BCR	C20-C21-C22	-2.83	123.26	127.31
23	B	614	CLA	C1D-CHD-C4C	-2.83	118.61	122.48
34	m	101	LMG	C7-O1-C1	-2.83	107.95	113.76
23	d	403	CLA	O2A-CGA-O1A	-2.83	116.52	123.55
25	c	514	BCR	C37-C22-C21	-2.83	118.96	122.92
23	b	605	CLA	O2A-CGA-O1A	-2.83	116.53	123.55
23	B	603	CLA	C4C-C3C-C2C	-2.83	102.57	106.91
23	C	503	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
25	C	527	BCR	C3-C4-C5	-2.82	108.93	113.78
24	a	407	PHO	CHD-C1D-C2D	-2.82	119.14	125.62
23	c	502	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
23	d	403	CLA	C4C-C3C-C2C	-2.82	102.58	106.91
23	B	614	CLA	CHC-C1C-C2C	-2.82	118.96	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C4C-C3C-C2C	-2.82	102.58	106.91
23	c	501	CLA	C4C-C3C-C2C	-2.81	102.59	106.91
31	d	406	LHG	O8-C23-O10	-2.81	116.56	123.55
23	b	612	CLA	O2A-CGA-O1A	-2.81	116.56	123.55
23	A	404	CLA	CAA-CBA-CGA	-2.81	104.88	113.35
23	c	508	CLA	C4C-C3C-C2C	-2.81	102.60	106.91
23	C	512	CLA	C4C-C3C-C2C	-2.81	102.60	106.91
25	A	408	BCR	C8-C7-C6	-2.81	119.39	127.25
23	c	504	CLA	C4C-C3C-C2C	-2.81	102.60	106.91
23	C	507	CLA	CHC-C1C-C2C	-2.81	119.00	126.65
23	b	616	CLA	OBD-CAD-C3D	-2.81	122.86	128.03
23	B	602	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
25	c	514	BCR	C38-C26-C25	-2.80	121.37	124.51
23	A	405	CLA	C1D-CHD-C4C	-2.80	118.66	122.48
23	B	607	CLA	CHC-C1C-C2C	-2.80	119.01	126.65
23	B	612	CLA	C1-C2-C3	-2.80	120.80	125.96
23	A	407	CLA	C4C-C3C-C2C	-2.80	102.62	106.91
23	b	615	CLA	C4C-C3C-C2C	-2.80	102.62	106.91
23	C	503	CLA	CBC-CAC-C3C	-2.80	104.47	112.41
29	d	405	PL9	C36-C37-C38	-2.79	102.38	111.97
23	C	503	CLA	C1-C2-C3	-2.79	120.81	125.96
25	A	408	BCR	C7-C8-C9	-2.79	122.02	126.21
24	A	406	PHO	C1C-C2C-C3C	-2.79	103.27	106.51
23	A	405	CLA	O2D-CGD-O1D	-2.79	118.21	123.82
26	a	411	SQD	C1-O5-C5	-2.79	108.46	113.72
23	B	607	CLA	C4C-C3C-C2C	-2.79	102.63	106.91
23	b	604	CLA	O2A-CGA-O1A	-2.78	116.64	123.55
23	a	405	CLA	C1-C2-C3	-2.78	120.83	125.96
23	d	402	CLA	CHC-C1C-C2C	-2.78	119.06	126.65
25	C	515	BCR	C7-C8-C9	-2.78	122.04	126.21
23	D	405	CLA	C1C-C2C-C3C	-2.78	103.84	106.92
29	D	407	PL9	C12-C13-C14	-2.78	120.70	127.68
23	B	604	CLA	C4C-C3C-C2C	-2.78	102.65	106.91
23	B	603	CLA	C1D-CHD-C4C	-2.78	118.69	122.48
23	B	608	CLA	C1D-CHD-C4C	-2.77	118.69	122.48
23	c	512	CLA	C4C-C3C-C2C	-2.77	102.66	106.91
23	B	604	CLA	CHC-C1C-C2C	-2.77	119.09	126.65
25	t	101	BCR	C20-C21-C22	-2.77	123.36	127.31
23	B	611	CLA	O1D-CGD-CBD	-2.77	119.63	124.60
23	b	608	CLA	C4C-C3C-C2C	-2.77	102.66	106.91
23	b	604	CLA	C4C-C3C-C2C	-2.77	102.66	106.91
23	c	511	CLA	C4C-C3C-C2C	-2.77	102.67	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	605	CLA	C4C-C3C-C2C	-2.77	102.67	106.91
23	d	402	CLA	C1D-CHD-C4C	-2.76	118.71	122.48
23	D	405	CLA	C2A-C1A-CHA	-2.76	119.02	123.92
25	t	101	BCR	C7-C6-C5	-2.76	114.95	121.54
38	v	201	HEM	CBA-CAA-C2A	-2.76	107.20	112.48
24	a	407	PHO	CHC-C1C-C2C	-2.76	119.28	125.62
25	D	406	BCR	C28-C27-C26	-2.76	109.04	113.78
37	C	518	DGD	C2G-O2G-C1B	-2.76	111.36	117.88
23	B	609	CLA	CHC-C1C-C2C	-2.76	119.13	126.65
23	b	604	CLA	O2D-CGD-O1D	-2.76	118.28	123.82
23	B	604	CLA	CBC-CAC-C3C	-2.75	104.59	112.41
23	B	606	CLA	C2A-C1A-CHA	-2.75	119.04	123.92
25	d	404	BCR	C23-C24-C25	-2.75	119.55	127.25
23	A	407	CLA	C1D-CHD-C4C	-2.75	118.72	122.48
23	c	511	CLA	CHC-C1C-C2C	-2.75	119.15	126.65
23	b	611	CLA	O2A-CGA-O1A	-2.75	116.72	123.55
23	b	603	CLA	CHC-C1C-C2C	-2.75	119.16	126.65
24	D	402	PHO	C1C-C2C-C3C	-2.74	103.33	106.51
24	a	407	PHO	C4D-ND-C1D	-2.74	102.03	106.98
25	c	514	BCR	C35-C13-C14	-2.74	119.08	122.92
23	A	405	CLA	CBC-CAC-C3C	-2.74	104.62	112.41
23	d	403	CLA	C2A-C1A-CHA	-2.74	119.06	123.92
25	A	408	BCR	C37-C22-C21	-2.74	119.08	122.92
29	A	413	PL9	C17-C18-C19	-2.74	120.80	127.68
23	b	607	CLA	O2A-CGA-O1A	-2.74	116.75	123.55
23	B	606	CLA	O2A-CGA-O1A	-2.74	116.76	123.55
25	y	101	BCR	C28-C27-C26	-2.73	109.08	113.78
25	k	101	BCR	C3-C4-C5	-2.73	109.08	113.78
23	B	612	CLA	CBC-CAC-C3C	-2.73	104.65	112.41
31	A	415	LHG	O8-C6-C5	-2.73	101.79	108.66
23	a	409	CLA	CHC-C1C-C2C	-2.73	119.20	126.65
29	D	407	PL9	C37-C38-C39	-2.73	120.83	127.68
25	b	619	BCR	C4-C5-C6	-2.72	118.74	122.74
26	f	101	SQD	C4-C3-C2	-2.72	106.03	110.84
23	D	404	CLA	CHC-C1C-C2C	-2.72	119.23	126.65
23	c	506	CLA	CGD-CBD-CAD	-2.72	101.60	110.71
23	C	507	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
24	D	402	PHO	C4D-CHA-C1A	-2.72	119.02	125.06
23	b	610	CLA	O2A-CGA-O1A	-2.72	116.81	123.55
25	y	101	BCR	C10-C11-C12	-2.72	114.90	123.23
34	J	101	LMG	C8-O7-C10	-2.72	111.46	117.88
25	c	514	BCR	C28-C27-C26	-2.71	109.11	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CHC-C1C-C2C	-2.71	119.25	126.65
25	A	408	BCR	C33-C5-C6	-2.71	121.47	124.51
23	C	506	CLA	CHC-C1C-C2C	-2.71	119.27	126.65
24	a	408	PHO	CHC-C1C-C2C	-2.71	119.41	125.62
23	A	405	CLA	CAA-C2A-C3A	-2.70	105.39	112.81
23	c	513	CLA	C4C-C3C-C2C	-2.70	102.76	106.91
23	a	409	CLA	C4C-C3C-C2C	-2.70	102.76	106.91
23	b	602	CLA	C1-C2-C3	-2.70	120.98	125.96
23	c	506	CLA	CAA-C2A-C3A	-2.70	105.40	112.81
23	b	602	CLA	C11-C10-C8	-2.70	106.86	115.73
23	c	508	CLA	C2A-C1A-CHA	-2.70	119.14	123.92
25	a	410	BCR	C38-C26-C25	-2.70	121.49	124.51
23	C	511	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
23	b	613	CLA	O2A-CGA-O1A	-2.69	116.86	123.55
23	A	407	CLA	CAA-C2A-C3A	-2.69	105.43	112.81
23	b	610	CLA	C2A-C1A-CHA	-2.69	119.15	123.92
23	B	607	CLA	C2A-C1A-CHA	-2.69	119.15	123.92
23	b	606	CLA	C4C-C3C-C2C	-2.68	102.79	106.91
37	C	517	DGD	C4E-C3E-C2E	-2.68	106.10	110.84
23	b	614	CLA	CHC-C1C-C2C	-2.68	119.33	126.65
26	D	413	SQD	C1-C2-C3	-2.68	104.99	109.98
23	c	507	CLA	C1-C2-C3	-2.68	121.01	125.96
23	a	409	CLA	C2A-C1A-CHA	-2.68	119.16	123.92
23	B	610	CLA	CHC-C1C-C2C	-2.68	119.34	126.65
23	B	604	CLA	C2A-C1A-CHA	-2.68	119.17	123.92
25	t	101	BCR	C37-C22-C21	-2.68	119.17	122.92
26	D	413	SQD	O47-C7-O49	-2.67	117.01	123.68
23	D	401	CLA	O2A-CGA-O1A	-2.67	116.91	123.55
29	d	405	PL9	C7-C8-C9	-2.67	122.24	126.71
23	B	617	CLA	C1C-C2C-C3C	-2.67	103.96	106.92
23	b	608	CLA	CHC-C1C-C2C	-2.67	119.37	126.65
23	a	404	CLA	C2A-C1A-CHA	-2.67	119.19	123.92
23	b	612	CLA	CHC-C1C-C2C	-2.67	119.37	126.65
23	b	609	CLA	CHC-C1C-C2C	-2.67	119.38	126.65
25	B	620	BCR	C24-C23-C22	-2.67	122.21	126.21
23	c	507	CLA	C4C-C3C-C2C	-2.66	102.82	106.91
23	B	617	CLA	CHC-C1C-C2C	-2.66	119.39	126.65
23	C	507	CLA	C1D-CHD-C4C	-2.66	118.84	122.48
23	D	401	CLA	C2A-C1A-CHA	-2.66	119.20	123.92
23	D	401	CLA	C1-C2-C3	-2.66	121.06	125.96
25	B	620	BCR	C37-C22-C21	-2.66	119.20	122.92
23	b	610	CLA	CHC-C1C-C2C	-2.66	119.40	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	408	PHO	C4D-ND-C1D	-2.66	102.19	106.98
23	b	610	CLA	O2D-CGD-O1D	-2.65	118.48	123.82
23	b	602	CLA	CHC-C1C-C2C	-2.65	119.44	126.65
23	B	602	CLA	C2A-C1A-CHA	-2.64	119.23	123.92
23	C	513	CLA	C4C-C3C-C2C	-2.64	102.85	106.91
23	D	405	CLA	CAA-C2A-C3A	-2.64	105.56	112.81
23	C	503	CLA	C4C-C3C-C2C	-2.64	102.86	106.91
25	C	516	BCR	C15-C14-C13	-2.64	123.54	127.31
23	B	608	CLA	C2A-C1A-CHA	-2.64	119.24	123.92
34	j	101	LMG	C8-O7-C10	-2.64	111.65	117.88
23	D	401	CLA	CBC-CAC-C3C	-2.64	104.93	112.41
23	b	604	CLA	CHC-C1C-C2C	-2.63	119.46	126.65
23	c	508	CLA	CHC-C1C-C2C	-2.63	119.48	126.65
23	B	613	CLA	CHC-C1C-C2C	-2.63	119.48	126.65
23	c	509	CLA	CHC-C1C-C2C	-2.63	119.48	126.65
23	C	506	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
23	d	402	CLA	CBC-CAC-C3C	-2.63	104.95	112.41
23	C	504	CLA	O2A-CGA-O1A	-2.63	117.03	123.55
25	A	408	BCR	C16-C17-C18	-2.62	123.56	127.31
23	B	608	CLA	CBC-CAC-C3C	-2.62	104.96	112.41
23	C	509	CLA	C1-C2-C3	-2.62	121.12	125.96
23	c	505	CLA	CHC-C1C-C2C	-2.62	119.50	126.65
23	b	609	CLA	C4C-C3C-C2C	-2.62	102.89	106.91
23	b	602	CLA	C2A-C1A-CHA	-2.62	119.27	123.92
23	B	605	CLA	O1D-CGD-CBD	-2.62	119.90	124.60
31	d	408	LHG	O8-C23-O10	-2.62	117.05	123.55
23	A	407	CLA	CHC-C1C-C2C	-2.62	119.51	126.65
29	d	405	PL9	C37-C38-C39	-2.62	121.11	127.68
37	C	519	DGD	C3G-C2G-C1G	-2.62	105.96	111.86
23	c	505	CLA	C1-C2-C3	-2.61	121.14	125.96
23	c	504	CLA	O1D-CGD-CBD	-2.61	119.91	124.60
23	a	404	CLA	O2D-CGD-O1D	-2.61	118.57	123.82
23	B	602	CLA	O2D-CGD-O1D	-2.61	118.57	123.82
23	C	513	CLA	CHC-C1C-C2C	-2.61	119.54	126.65
23	c	510	CLA	O2A-CGA-O1A	-2.61	117.08	123.55
23	C	508	CLA	C1-C2-C3	-2.61	121.16	125.96
23	B	617	CLA	CBC-CAC-C3C	-2.61	105.01	112.41
25	C	527	BCR	C10-C11-C12	-2.60	115.25	123.23
23	D	401	CLA	CMA-C3A-C2A	-2.60	103.21	113.77
23	B	603	CLA	C2A-C1A-CHA	-2.60	119.31	123.92
23	B	610	CLA	C1D-CHD-C4C	-2.60	118.94	122.48
31	d	406	LHG	C5-O7-C7	-2.60	111.74	117.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	CBC-CAC-C3C	-2.60	105.04	112.41
23	b	605	CLA	C1-C2-C3	-2.60	121.17	125.96
37	C	517	DGD	C3G-C2G-C1G	-2.60	106.00	111.86
23	A	405	CLA	C2A-C1A-CHA	-2.59	119.32	123.92
25	B	620	BCR	C21-C20-C19	-2.59	115.28	123.23
23	a	409	CLA	CMA-C3A-C2A	-2.59	103.26	113.77
26	L	102	SQD	C1-C2-C3	-2.59	105.17	109.98
25	B	619	BCR	C38-C26-C25	-2.59	121.61	124.51
23	c	501	CLA	O2A-CGA-O1A	-2.59	117.13	123.55
23	B	611	CLA	CHC-C1C-C2C	-2.58	119.60	126.65
23	C	514	CLA	CAA-C2A-C3A	-2.58	105.73	112.81
23	C	509	CLA	O2A-CGA-O1A	-2.58	117.14	123.55
23	b	602	CLA	C4C-C3C-C2C	-2.58	102.95	106.91
23	b	601	CLA	C4C-C3C-C2C	-2.58	102.95	106.91
23	b	608	CLA	C1-C2-C3	-2.58	121.21	125.96
25	T	101	BCR	C16-C17-C18	-2.58	123.63	127.31
25	b	618	BCR	C28-C27-C26	-2.58	109.35	113.78
24	D	402	PHO	CHD-C1D-C2D	-2.57	119.71	125.62
23	A	404	CLA	C2A-C1A-CHA	-2.57	119.36	123.92
23	b	603	CLA	C4C-C3C-C2C	-2.57	102.97	106.91
23	c	513	CLA	CHC-C1C-C2C	-2.57	119.64	126.65
24	A	406	PHO	C4D-CHA-C1A	-2.57	119.35	125.06
23	B	612	CLA	C2A-C1A-CHA	-2.57	119.37	123.92
25	k	101	BCR	C10-C11-C12	-2.56	115.36	123.23
23	B	610	CLA	C1-C2-C3	-2.56	121.24	125.96
23	c	513	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
24	a	407	PHO	O2A-CGA-O1A	-2.56	117.19	123.55
25	c	515	BCR	C33-C5-C6	-2.56	121.64	124.51
23	a	406	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
23	c	512	CLA	O1D-CGD-CBD	-2.56	120.01	124.60
23	B	605	CLA	CHC-C1C-C2C	-2.56	119.68	126.65
23	B	607	CLA	O2A-CGA-O1A	-2.56	117.20	123.55
23	C	502	CLA	C4C-C3C-C2C	-2.56	102.99	106.91
23	C	510	CLA	O2D-CGD-O1D	-2.55	118.68	123.82
34	m	101	LMG	C8-O7-C10	-2.55	111.84	117.88
23	b	601	CLA	C2A-C1A-CHA	-2.55	119.39	123.92
23	C	508	CLA	CHC-C1C-C2C	-2.55	119.69	126.65
25	b	618	BCR	C24-C23-C22	-2.55	122.38	126.21
29	d	405	PL9	C17-C18-C19	-2.55	121.27	127.68
29	d	405	PL9	C31-C32-C33	-2.55	103.22	111.97
23	C	507	CLA	CAA-C2A-C3A	-2.55	105.82	112.81
23	c	512	CLA	CBC-CAC-C3C	-2.55	105.17	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	615	CLA	C2A-C1A-CHA	-2.55	119.40	123.92
23	D	401	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
25	C	527	BCR	C38-C26-C25	-2.55	121.66	124.51
24	a	408	PHO	C1C-C2C-C3C	-2.55	103.56	106.51
23	C	505	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
25	d	404	BCR	C28-C27-C26	-2.54	109.41	113.78
26	a	411	SQD	C44-O6-C1	-2.54	108.55	113.76
23	A	404	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
23	c	513	CLA	C2A-C1A-CHA	-2.54	119.42	123.92
24	a	407	PHO	C1C-C2C-C3C	-2.53	103.57	106.51
23	b	615	CLA	CBC-CAC-C3C	-2.53	105.22	112.41
23	C	511	CLA	CBC-CAC-C3C	-2.53	105.22	112.41
23	b	616	CLA	O2A-CGA-O1A	-2.53	117.26	123.55
23	B	602	CLA	O1D-CGD-CBD	-2.53	120.06	124.60
25	y	101	BCR	C16-C17-C18	-2.52	123.71	127.31
23	C	507	CLA	C4C-C3C-C2C	-2.52	103.04	106.91
23	a	409	CLA	C1-C2-C3	-2.52	121.31	125.96
25	C	516	BCR	C7-C8-C9	-2.52	122.43	126.21
23	c	502	CLA	C2A-C1A-CHA	-2.52	119.45	123.92
25	B	618	BCR	C15-C14-C13	-2.52	123.72	127.31
23	C	513	CLA	CBC-CAC-C3C	-2.52	105.26	112.41
23	c	507	CLA	CHC-C1C-C2C	-2.52	119.78	126.65
23	a	405	CLA	O2D-CGD-O1D	-2.51	118.76	123.82
23	b	608	CLA	C2A-C1A-CHA	-2.51	119.46	123.92
23	D	401	CLA	CHC-C1C-C2C	-2.51	119.80	126.65
23	B	606	CLA	OBD-CAD-C3D	-2.51	123.40	128.03
23	B	608	CLA	CHC-C1C-C2C	-2.51	119.81	126.65
23	b	603	CLA	C2A-C1A-CHA	-2.51	119.47	123.92
23	A	404	CLA	CHC-C1C-C2C	-2.51	119.81	126.65
25	C	527	BCR	C15-C14-C13	-2.50	123.73	127.31
23	B	613	CLA	O2A-CGA-O1A	-2.50	117.33	123.55
25	d	404	BCR	C16-C17-C18	-2.50	123.74	127.31
26	A	409	SQD	O47-C7-O49	-2.50	117.44	123.68
26	a	411	SQD	O5-C1-C2	-2.50	105.47	110.30
25	y	101	BCR	C21-C20-C19	-2.50	115.56	123.23
25	D	406	BCR	C3-C4-C5	-2.50	109.48	113.78
23	B	612	CLA	CHC-C1C-C2C	-2.50	119.83	126.65
25	B	618	BCR	C11-C10-C9	-2.49	123.75	127.31
25	C	516	BCR	C34-C9-C10	-2.49	119.43	122.92
23	b	605	CLA	CBC-CAC-C3C	-2.49	105.34	112.41
34	z	101	LMG	C8-O7-C10	-2.49	111.99	117.88
37	c	518	DGD	C3G-C2G-C1G	-2.49	106.25	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C11-C12-C13	-2.48	107.58	115.73
29	A	413	PL9	C12-C13-C14	-2.48	121.46	127.68
24	A	406	PHO	C1-C2-C3	-2.47	121.40	125.96
23	C	513	CLA	O2A-CGA-O1A	-2.47	117.41	123.55
23	B	606	CLA	CHC-C1C-C2C	-2.47	119.91	126.65
23	A	405	CLA	C4C-C3C-C2C	-2.47	103.12	106.91
25	c	514	BCR	C34-C9-C10	-2.47	119.46	122.92
23	a	406	CLA	O2A-CGA-O1A	-2.47	117.42	123.55
23	B	611	CLA	O2D-CGD-O1D	-2.47	118.85	123.82
23	C	506	CLA	O1D-CGD-CBD	-2.47	120.17	124.60
26	A	409	SQD	O9-S-O7	-2.47	105.30	113.86
37	c	516	DGD	C3G-C2G-C1G	-2.47	106.29	111.86
24	A	406	PHO	C4D-ND-C1D	-2.47	102.53	106.98
37	C	517	DGD	C2G-O2G-C1B	-2.46	112.05	117.88
29	D	407	PL9	C22-C23-C24	-2.46	121.49	127.68
25	b	618	BCR	C3-C4-C5	-2.46	109.54	113.78
34	Z	101	LMG	C9-C8-C7	-2.46	106.30	111.86
25	a	410	BCR	C33-C5-C6	-2.46	121.75	124.51
24	a	408	PHO	CBA-CAA-C2A	-2.46	106.43	113.80
23	C	505	CLA	C1-C2-C3	-2.46	121.42	125.96
25	C	516	BCR	C21-C20-C19	-2.46	115.69	123.23
23	b	607	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
23	b	606	CLA	C2A-C1A-CHA	-2.46	119.56	123.92
25	c	515	BCR	C15-C14-C13	-2.46	123.80	127.31
25	C	515	BCR	C38-C26-C25	-2.46	121.76	124.51
23	B	608	CLA	C4C-C3C-C2C	-2.46	103.14	106.91
25	b	618	BCR	C15-C14-C13	-2.46	123.80	127.31
23	c	506	CLA	O2A-CGA-O1A	-2.46	117.45	123.55
23	b	615	CLA	C11-C12-C13	-2.45	107.68	115.73
23	b	611	CLA	CBC-CAC-C3C	-2.45	105.45	112.41
23	c	507	CLA	C1D-CHD-C4C	-2.45	119.14	122.48
23	B	615	CLA	C4C-C3C-C2C	-2.45	103.15	106.91
23	B	608	CLA	C4A-NA-C1A	-2.45	103.41	106.45
23	c	502	CLA	C4C-C3C-C2C	-2.45	103.16	106.91
23	C	507	CLA	O2A-CGA-O1A	-2.45	117.48	123.55
23	B	616	CLA	C4C-C3C-C2C	-2.45	103.16	106.91
23	d	403	CLA	CHC-C1C-C2C	-2.45	119.98	126.65
23	a	404	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
29	D	407	PL9	C7-C8-C9	-2.44	122.63	126.71
23	B	616	CLA	C1-C2-C3	-2.44	121.46	125.96
23	c	513	CLA	C1-C2-C3	-2.44	121.47	125.96
23	b	613	CLA	CHC-C1C-C2C	-2.43	120.01	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CMA-C3A-C4A	-2.43	105.24	111.77
23	d	403	CLA	CBC-CAC-C3C	-2.43	105.51	112.41
23	B	614	CLA	C4C-C3C-C2C	-2.42	103.19	106.91
23	c	507	CLA	C6-C7-C8	-2.42	107.78	115.73
29	a	415	PL9	C17-C18-C19	-2.42	121.60	127.68
23	B	613	CLA	C2A-C1A-CHA	-2.42	119.63	123.92
25	H	101	BCR	C15-C14-C13	-2.42	123.86	127.31
25	B	620	BCR	C10-C11-C12	-2.42	115.82	123.23
23	d	402	CLA	O2A-CGA-O1A	-2.41	117.56	123.55
23	a	409	CLA	OBD-CAD-C3D	-2.41	123.58	128.03
29	d	405	PL9	C12-C13-C14	-2.41	121.62	127.68
23	d	402	CLA	C2A-C1A-CHA	-2.41	119.65	123.92
25	a	410	BCR	C11-C10-C9	-2.41	123.88	127.31
23	c	508	CLA	CAA-C2A-C3A	-2.41	106.21	112.81
26	a	411	SQD	O47-C7-O49	-2.41	117.68	123.68
25	b	619	BCR	C21-C20-C19	-2.40	115.86	123.23
23	c	509	CLA	C2A-C1A-CHA	-2.40	119.66	123.92
25	C	515	BCR	C23-C24-C25	-2.40	120.53	127.25
24	A	406	PHO	C4A-NA-C1A	-2.40	106.22	108.16
23	D	404	CLA	OBD-CAD-C3D	-2.40	123.61	128.03
23	B	612	CLA	C4C-C3C-C2C	-2.40	103.23	106.91
25	D	406	BCR	C21-C20-C19	-2.40	115.88	123.23
34	J	101	LMG	O7-C10-O9	-2.40	117.70	123.68
34	J	101	LMG	O8-C28-O10	-2.40	117.60	123.55
24	a	407	PHO	C3B-C2B-C1B	-2.39	101.46	106.30
23	B	607	CLA	CBC-CAC-C3C	-2.39	105.62	112.41
23	c	504	CLA	CBC-CAC-C3C	-2.39	105.62	112.41
23	a	405	CLA	O2A-CGA-O1A	-2.39	117.61	123.55
36	B	624	HTG	O2-C2-C3	-2.39	105.16	110.36
23	C	513	CLA	CBA-CAA-C2A	-2.39	106.65	113.80
34	m	101	LMG	C1-C2-C3	-2.39	105.54	109.98
34	m	101	LMG	O8-C28-O10	-2.39	117.63	123.55
23	b	614	CLA	CAA-C2A-C3A	-2.39	106.27	112.81
23	C	510	CLA	CHC-C1C-C2C	-2.39	120.14	126.65
23	c	506	CLA	C2A-C1A-CHA	-2.38	119.69	123.92
23	a	404	CLA	CAA-C2A-C1A	-2.38	104.18	111.97
23	b	614	CLA	C2A-C1A-CHA	-2.38	119.70	123.92
25	h	102	BCR	C10-C11-C12	-2.38	115.94	123.23
25	d	404	BCR	C23-C22-C21	-2.38	115.29	118.94
23	C	511	CLA	C4-C3-C2	-2.37	117.36	123.69
25	h	102	BCR	C37-C22-C21	-2.37	119.61	122.92
24	a	408	PHO	C4D-CHA-C1A	-2.37	119.80	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	102	SQD	C1-O5-C5	-2.37	109.26	113.72
25	B	618	BCR	C36-C18-C17	-2.37	119.61	122.92
26	f	101	SQD	O47-C7-O49	-2.36	117.78	123.68
25	A	408	BCR	C31-C1-C6	-2.36	106.48	110.31
23	C	504	CLA	C1-C2-C3	-2.36	121.61	125.96
25	Y	101	BCR	C37-C22-C21	-2.36	119.62	122.92
25	Y	101	BCR	C21-C20-C19	-2.36	116.00	123.23
23	d	402	CLA	C4C-C3C-C2C	-2.36	103.29	106.91
23	B	616	CLA	O2D-CGD-O1D	-2.36	119.08	123.82
23	A	407	CLA	C1-C2-C3	-2.35	121.62	125.96
23	B	612	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
23	d	403	CLA	CAA-C2A-C3A	-2.35	106.38	112.81
25	A	408	BCR	C3-C4-C5	-2.34	109.75	113.78
23	b	602	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
23	C	511	CLA	O2A-CGA-O1A	-2.34	117.73	123.55
23	d	402	CLA	CAA-C2A-C3A	-2.34	106.39	112.81
34	j	101	LMG	O8-C28-O10	-2.34	117.73	123.55
23	D	404	CLA	C1D-CHD-C4C	-2.34	119.29	122.48
23	B	603	CLA	O1D-CGD-CBD	-2.34	120.40	124.60
23	D	405	CLA	CHC-C1C-C2C	-2.34	120.28	126.65
23	C	514	CLA	CHC-C1C-C2C	-2.34	120.28	126.65
23	c	509	CLA	O2D-CGD-O1D	-2.33	119.12	123.82
25	b	618	BCR	C21-C20-C19	-2.33	116.07	123.23
23	A	407	CLA	CMA-C3A-C2A	-2.33	104.30	113.77
25	D	406	BCR	C16-C17-C18	-2.33	123.98	127.31
26	D	413	SQD	C44-O6-C1	-2.33	108.97	113.76
25	h	102	BCR	C16-C15-C14	-2.33	118.49	123.46
24	a	408	PHO	O2D-CGD-O1D	-2.33	119.14	123.82
25	b	617	BCR	C3-C4-C5	-2.33	109.78	113.78
23	B	606	CLA	C1-C2-C3	-2.33	121.67	125.96
23	c	504	CLA	C2A-C1A-CHA	-2.33	119.79	123.92
23	b	603	CLA	CBC-CAC-C3C	-2.33	105.81	112.41
23	B	607	CLA	C11-C10-C8	-2.32	108.10	115.73
23	c	508	CLA	O2A-CGA-O1A	-2.32	117.78	123.55
23	B	604	CLA	O1D-CGD-CBD	-2.32	120.43	124.60
34	C	520	LMG	O8-C28-O10	-2.32	117.78	123.55
25	a	410	BCR	C32-C1-C6	-2.32	106.54	110.31
25	Y	101	BCR	C10-C11-C12	-2.32	116.11	123.23
23	a	409	CLA	O2A-CGA-O1A	-2.32	117.79	123.55
23	b	606	CLA	CBC-CAC-C3C	-2.32	105.82	112.41
23	b	602	CLA	O1D-CGD-CBD	-2.32	120.44	124.60
23	b	616	CLA	C1-C2-C3	-2.31	121.70	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C2A-C1A-CHA	-2.31	119.82	123.92
26	L	102	SQD	C44-O6-C1	-2.31	109.02	113.76
23	b	601	CLA	O1D-CGD-CBD	-2.31	120.46	124.60
34	B	622	LMG	O1-C1-C2	-2.31	104.47	108.23
25	h	102	BCR	C36-C18-C17	-2.31	119.69	122.92
23	C	511	CLA	C2A-C1A-CHA	-2.30	119.83	123.92
23	C	506	CLA	O2A-CGA-O1A	-2.30	117.83	123.55
29	D	407	PL9	C36-C37-C38	-2.30	104.07	111.97
26	A	409	SQD	O48-C23-O10	-2.30	117.84	123.55
23	c	507	CLA	C2A-C1A-CHA	-2.30	119.84	123.92
23	b	608	CLA	OBD-CAD-C3D	-2.29	123.80	128.03
23	B	612	CLA	O2D-CGD-O1D	-2.29	119.20	123.82
23	C	502	CLA	OBD-CAD-C3D	-2.29	123.81	128.03
38	v	201	HEM	CBD-CAD-C3D	-2.29	108.10	112.47
23	B	607	CLA	CAA-C2A-C3A	-2.29	106.54	112.81
23	a	406	CLA	CBC-CAC-C3C	-2.28	105.92	112.41
29	d	405	PL9	C27-C28-C29	-2.28	121.94	127.68
24	a	408	PHO	CHD-C1D-C2D	-2.28	120.40	125.62
25	b	619	BCR	C16-C17-C18	-2.27	124.06	127.31
23	A	405	CLA	CMA-C3A-C4A	-2.27	105.66	111.77
23	b	609	CLA	C2A-C1A-CHA	-2.27	119.89	123.92
31	L	101	LHG	C5-O7-C7	-2.27	112.51	117.88
23	B	617	CLA	C2A-C1A-CHA	-2.27	119.89	123.92
23	a	404	CLA	C1-C2-C3	-2.27	121.77	125.96
25	Y	101	BCR	C29-C28-C27	-2.27	105.93	111.34
23	C	510	CLA	C2A-C1A-CHA	-2.27	119.89	123.92
37	c	516	DGD	O2G-C1B-O1B	-2.27	118.02	123.68
37	c	517	DGD	O1G-C1A-O1A	-2.27	117.92	123.55
25	c	514	BCR	C7-C8-C9	-2.26	122.82	126.21
23	A	404	CLA	C16-C15-C13	-2.25	108.33	115.73
25	k	101	BCR	C20-C21-C22	-2.25	124.10	127.31
23	C	512	CLA	C11-C10-C8	-2.25	108.34	115.73
25	c	515	BCR	C37-C22-C21	-2.25	119.77	122.92
35	b	628	LMT	C3'-C4'-C5'	-2.25	106.10	110.88
23	b	610	CLA	O1D-CGD-CBD	-2.25	120.56	124.60
23	C	507	CLA	C4A-NA-C1A	-2.25	103.66	106.45
23	b	609	CLA	C4A-NA-C1A	-2.25	103.66	106.45
23	C	508	CLA	C11-C10-C8	-2.24	108.36	115.73
23	b	601	CLA	CBC-CAC-C3C	-2.24	106.04	112.41
23	b	615	CLA	O2D-CGD-O1D	-2.24	119.31	123.82
31	A	415	LHG	O7-C7-O9	-2.24	118.09	123.68
23	c	506	CLA	CBC-CAC-C3C	-2.24	106.05	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d	406	LHG	O7-C7-O9	-2.24	118.09	123.68
23	A	407	CLA	CMA-C3A-C4A	-2.24	105.76	111.77
26	D	413	SQD	O48-C23-O10	-2.24	117.99	123.55
23	B	610	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
25	B	619	BCR	C16-C17-C18	-2.24	124.12	127.31
24	a	408	PHO	C4-C3-C2	-2.24	117.72	123.69
23	C	508	CLA	O2A-CGA-O1A	-2.24	118.00	123.55
25	B	619	BCR	C33-C5-C6	-2.23	122.01	124.51
25	t	101	BCR	C16-C17-C18	-2.23	124.13	127.31
29	D	407	PL9	C7-C3-C2	-2.23	120.06	123.23
34	c	520	LMG	C9-C8-C7	-2.23	106.83	111.86
23	C	509	CLA	C2A-C1A-CHA	-2.23	119.97	123.92
23	C	514	CLA	CBC-CAC-C3C	-2.22	106.10	112.41
23	B	602	CLA	CMA-C3A-C4A	-2.22	105.80	111.77
25	Y	101	BCR	C40-C30-C25	-2.22	106.70	110.31
23	c	510	CLA	C4-C3-C2	-2.22	117.76	123.69
26	D	413	SQD	C46-C45-C44	-2.22	106.85	111.86
31	D	409	LHG	O8-C23-O10	-2.22	118.05	123.55
23	c	505	CLA	C2A-C1A-CHA	-2.22	119.99	123.92
25	d	404	BCR	C11-C10-C9	-2.22	124.15	127.31
24	D	402	PHO	C3B-C2B-C1B	-2.22	101.83	106.30
24	a	407	PHO	C3A-C4A-CHB	-2.21	118.01	121.75
23	C	510	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
23	B	616	CLA	C6-C7-C8	-2.21	108.47	115.73
25	B	620	BCR	C3-C4-C5	-2.21	109.98	113.78
25	c	515	BCR	C21-C20-C19	-2.21	116.45	123.23
23	b	609	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
23	B	611	CLA	C6-C7-C8	-2.21	108.49	115.73
25	d	404	BCR	C21-C20-C19	-2.20	116.47	123.23
23	b	616	CLA	O1D-CGD-CBD	-2.20	120.64	124.60
23	C	506	CLA	CBC-CAC-C3C	-2.20	106.16	112.41
23	B	602	CLA	CBC-CAC-C3C	-2.20	106.16	112.41
25	c	514	BCR	C3-C4-C5	-2.20	110.00	113.78
23	b	613	CLA	O2D-CGD-O1D	-2.20	119.40	123.82
25	B	618	BCR	C31-C1-C6	-2.20	106.75	110.31
25	Y	101	BCR	C28-C27-C26	-2.20	110.00	113.78
23	c	511	CLA	CAA-CBA-CGA	-2.19	106.74	113.35
23	B	608	CLA	O2D-CGD-O1D	-2.19	119.41	123.82
29	d	405	PL9	C16-C17-C18	-2.19	104.44	111.97
24	a	407	PHO	CBA-CAA-C2A	-2.19	107.24	113.80
34	B	622	LMG	C8-O7-C10	-2.18	112.72	117.88
23	D	405	CLA	CBC-CAC-C3C	-2.18	106.23	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	CBC-CAC-C3C	-2.18	106.23	112.41
37	C	518	DGD	O1G-C1A-O1A	-2.18	118.14	123.55
23	b	610	CLA	CMA-C3A-C2A	-2.17	104.95	113.77
23	B	609	CLA	CBC-CAC-C3C	-2.17	106.24	112.41
29	d	405	PL9	C36-C34-C33	-2.17	116.66	121.10
23	c	510	CLA	C4C-C3C-C2C	-2.17	103.58	106.91
25	C	527	BCR	C37-C22-C21	-2.17	119.88	122.92
24	A	406	PHO	O2D-CGD-O1D	-2.17	119.45	123.82
23	c	513	CLA	O2A-CGA-O1A	-2.17	118.17	123.55
23	b	613	CLA	C2A-C1A-CHA	-2.17	120.08	123.92
24	a	408	PHO	C3B-C2B-C1B	-2.17	101.93	106.30
23	C	502	CLA	C2A-C1A-CHA	-2.16	120.08	123.92
25	C	516	BCR	C24-C23-C22	-2.16	122.96	126.21
25	d	404	BCR	C40-C30-C25	-2.16	106.80	110.31
23	b	602	CLA	C4A-NA-C1A	-2.16	103.77	106.45
23	b	616	CLA	C2A-C1A-CHA	-2.16	120.09	123.92
25	k	101	BCR	C7-C8-C9	-2.16	122.97	126.21
23	B	609	CLA	C2A-C1A-CHA	-2.16	120.09	123.92
34	c	519	LMG	C8-O7-C10	-2.16	112.78	117.88
23	b	601	CLA	CAA-C2A-C3A	-2.15	106.90	112.81
23	b	616	CLA	C4A-NA-C1A	-2.15	103.78	106.45
38	e	103	HEM	C3C-C4C-NC	-2.15	106.88	110.94
23	C	505	CLA	CBC-CAC-C3C	-2.15	106.31	112.41
25	H	101	BCR	C31-C1-C6	-2.15	106.82	110.31
23	c	503	CLA	CBC-CAC-C3C	-2.15	106.31	112.41
34	C	501	LMG	O7-C10-O9	-2.15	118.32	123.68
25	k	101	BCR	C34-C9-C10	-2.15	119.92	122.92
31	E	101	LHG	O8-C23-O10	-2.15	118.22	123.55
29	d	405	PL9	C25-C24-C23	-2.15	117.97	123.69
23	A	407	CLA	CBC-CAC-C3C	-2.14	106.32	112.41
29	d	405	PL9	C45-C44-C43	-2.14	117.97	123.69
23	C	505	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
25	T	101	BCR	C7-C6-C5	-2.14	116.43	121.54
23	c	502	CLA	O2A-CGA-O1A	-2.14	118.23	123.55
23	b	611	CLA	C2A-C1A-CHA	-2.14	120.12	123.92
23	c	513	CLA	C4A-NA-C1A	-2.14	103.80	106.45
23	B	603	CLA	O2A-CGA-O1A	-2.14	118.24	123.55
25	b	617	BCR	C16-C17-C18	-2.14	124.26	127.31
29	A	413	PL9	C47-C48-C49	-2.14	120.17	127.80
23	c	507	CLA	C4A-NA-C1A	-2.13	103.80	106.45
37	c	516	DGD	C6D-O5D-C1E	-2.13	109.38	113.76
23	B	611	CLA	C2A-C1A-CHA	-2.13	120.14	123.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C7-C6-C5	-2.13	116.46	121.54
23	b	602	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
23	D	401	CLA	C4C-C3C-C2C	-2.13	103.64	106.91
23	B	616	CLA	O2A-CGA-O1A	-2.13	118.27	123.55
23	D	405	CLA	OBD-CAD-C3D	-2.13	124.11	128.03
23	C	502	CLA	CAA-C2A-C3A	-2.13	106.98	112.81
25	k	101	BCR	C28-C27-C26	-2.13	110.13	113.78
23	C	505	CLA	CAA-C2A-C3A	-2.12	106.98	112.81
24	A	406	PHO	CHD-C1D-C2D	-2.12	120.75	125.62
23	B	611	CLA	CAA-CBA-CGA	-2.12	106.95	113.35
25	B	620	BCR	C2-C3-C4	-2.12	106.29	111.34
23	c	501	CLA	C2A-C1A-CHA	-2.12	120.16	123.92
23	c	501	CLA	CBC-CAC-C3C	-2.12	106.39	112.41
23	b	606	CLA	O2A-CGA-O1A	-2.12	118.29	123.55
34	j	101	LMG	O7-C10-O9	-2.12	118.40	123.68
29	a	415	PL9	C47-C48-C49	-2.12	120.25	127.80
34	C	501	LMG	C9-C8-C7	-2.11	107.09	111.86
34	c	519	LMG	O8-C28-O10	-2.11	118.30	123.55
25	b	617	BCR	C37-C22-C21	-2.11	119.96	122.92
31	d	407	LHG	O8-C23-O10	-2.11	118.31	123.55
23	B	616	CLA	C2A-C1A-CHA	-2.11	120.18	123.92
29	A	413	PL9	C37-C36-C34	-2.11	105.80	112.93
26	A	411	SQD	O48-C23-O10	-2.11	118.31	123.55
23	A	404	CLA	C4A-NA-C1A	-2.11	103.84	106.45
23	B	617	CLA	O2A-CGA-O1A	-2.11	118.32	123.55
25	Y	101	BCR	C36-C18-C17	-2.11	119.97	122.92
23	B	612	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
24	a	408	PHO	O1D-CGD-CBD	-2.10	120.82	124.60
23	B	613	CLA	O1D-CGD-CBD	-2.10	120.83	124.60
34	c	520	LMG	O8-C28-O10	-2.10	118.33	123.55
26	A	411	SQD	C46-C45-C44	-2.10	107.12	111.86
23	b	611	CLA	OBD-CAD-C3D	-2.10	124.16	128.03
23	c	510	CLA	C2A-C1A-CHA	-2.10	120.20	123.92
23	c	511	CLA	CBC-CAC-C3C	-2.10	106.45	112.41
23	a	404	CLA	CMA-C3A-C4A	-2.10	106.14	111.77
25	Y	101	BCR	C11-C10-C9	-2.10	124.32	127.31
26	B	621	SQD	O48-C23-O10	-2.09	118.35	123.55
23	B	613	CLA	C11-C12-C13	-2.09	108.86	115.73
23	c	509	CLA	O1D-CGD-CBD	-2.09	120.84	124.60
23	C	508	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
26	L	102	SQD	O47-C7-O49	-2.09	118.46	123.68
23	a	404	CLA	CBC-CAC-C3C	-2.09	106.48	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	BCR	C10-C11-C12	-2.09	116.82	123.23
23	c	513	CLA	CBC-CAC-C3C	-2.09	106.48	112.41
31	d	407	LHG	C5-O7-C7	-2.09	112.94	117.88
25	Y	101	BCR	C38-C26-C25	-2.09	122.17	124.51
23	B	614	CLA	O2D-CGD-O1D	-2.09	119.62	123.82
25	c	515	BCR	C15-C16-C17	-2.09	119.01	123.46
35	a	418	LMT	C1B-O1B-C4'	-2.09	112.92	118.00
23	b	607	CLA	CBC-CAC-C3C	-2.08	106.49	112.41
34	z	101	LMG	C7-O1-C1	-2.08	109.48	113.76
23	c	512	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
25	h	102	BCR	C20-C21-C22	-2.08	124.34	127.31
25	c	515	BCR	C16-C17-C18	-2.08	124.34	127.31
23	C	512	CLA	C2A-C1A-CHA	-2.08	120.22	123.92
25	D	406	BCR	C10-C11-C12	-2.08	116.84	123.23
23	B	603	CLA	C4A-NA-C1A	-2.08	103.87	106.45
37	H	102	DGD	C2G-O2G-C1B	-2.08	112.97	117.88
23	b	615	CLA	C2A-C1A-CHA	-2.08	120.24	123.92
23	a	405	CLA	C2A-C1A-CHA	-2.08	120.24	123.92
23	a	409	CLA	CBC-CAC-C3C	-2.08	106.52	112.41
23	C	510	CLA	O1D-CGD-CBD	-2.08	120.87	124.60
23	b	602	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
23	C	504	CLA	CBC-CAC-C3C	-2.07	106.53	112.41
25	D	406	BCR	C32-C1-C6	-2.07	106.95	110.31
23	b	604	CLA	CHA-C1A-NA	-2.07	121.37	126.18
23	C	508	CLA	C6-C7-C8	-2.07	108.93	115.73
23	B	614	CLA	CBC-CAC-C3C	-2.07	106.54	112.41
37	C	517	DGD	O1G-C1A-O1A	-2.07	118.42	123.55
25	B	619	BCR	C10-C11-C12	-2.07	116.89	123.23
29	d	405	PL9	C42-C41-C39	-2.07	105.94	112.93
23	b	614	CLA	CBC-CAC-C3C	-2.07	106.55	112.41
23	B	609	CLA	O2D-CGD-O1D	-2.07	119.66	123.82
23	D	401	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
23	a	406	CLA	C2A-C1A-CHA	-2.06	120.26	123.92
23	a	406	CLA	OBD-CAD-C3D	-2.06	124.23	128.03
26	a	411	SQD	O4-C4-C3	-2.06	105.87	110.36
23	c	507	CLA	O2A-CGA-O1A	-2.06	118.43	123.55
23	a	409	CLA	C4A-NA-C1A	-2.06	103.90	106.45
38	E	103	HEM	C3C-C4C-NC	-2.06	107.06	110.94
23	C	509	CLA	CAA-C2A-C3A	-2.06	107.17	112.81
23	B	604	CLA	C5-C3-C2	-2.06	116.89	121.10
24	A	406	PHO	CBA-CAA-C2A	-2.06	107.64	113.80
37	C	519	DGD	O3G-C3G-C2G	-2.06	106.10	110.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	BCR	C35-C13-C14	-2.05	120.05	122.92
23	B	603	CLA	CBC-CAC-C3C	-2.05	106.59	112.41
23	c	512	CLA	OBD-CAD-C3D	-2.05	124.25	128.03
23	b	608	CLA	C11-C10-C8	-2.05	109.01	115.73
23	B	611	CLA	O2A-CGA-O1A	-2.05	118.47	123.55
23	B	617	CLA	C4A-NA-C1A	-2.05	103.91	106.45
31	d	408	LHG	C6-C5-C4	-2.05	107.24	111.86
23	B	608	CLA	O2A-CGA-O1A	-2.04	118.47	123.55
25	C	515	BCR	C21-C20-C19	-2.04	116.96	123.23
23	b	607	CLA	C1B-CHB-C4A	-2.04	126.07	130.12
37	C	519	DGD	O1G-C1A-O1A	-2.04	118.48	123.55
37	c	518	DGD	O5D-C6D-C5D	-2.04	105.53	108.94
34	c	519	LMG	O7-C10-O9	-2.04	118.58	123.68
23	C	508	CLA	OBD-CAD-C3D	-2.04	124.27	128.03
25	C	516	BCR	C38-C26-C25	-2.04	122.22	124.51
23	C	504	CLA	OBD-CAD-C3D	-2.04	124.27	128.03
23	a	405	CLA	C4C-C3C-C2C	-2.03	103.79	106.91
37	c	518	DGD	O6E-C1E-O5D	-2.03	105.19	110.02
23	c	503	CLA	O2A-CGA-O1A	-2.03	118.50	123.55
25	b	618	BCR	C8-C7-C6	-2.03	121.57	127.25
23	b	615	CLA	C6-C7-C8	-2.03	109.08	115.73
24	a	407	PHO	OBD-CAD-C3D	-2.03	123.45	128.43
25	T	101	BCR	C10-C11-C12	-2.03	117.02	123.23
23	C	513	CLA	C4A-NA-C1A	-2.02	103.94	106.45
23	B	608	CLA	O1D-CGD-CBD	-2.02	120.97	124.60
23	a	409	CLA	CMA-C3A-C4A	-2.02	106.33	111.77
25	T	101	BCR	C21-C20-C19	-2.02	117.03	123.23
25	B	619	BCR	C35-C13-C14	-2.02	120.09	122.92
23	a	404	CLA	C4C-C3C-C2C	-2.02	103.81	106.91
23	C	512	CLA	CBC-CAC-C3C	-2.02	106.67	112.41
25	B	619	BCR	C36-C18-C17	-2.02	120.09	122.92
25	H	101	BCR	C39-C30-C25	-2.02	107.03	110.31
25	b	618	BCR	C10-C11-C12	-2.02	117.04	123.23
37	C	517	DGD	O2G-C1B-O1B	-2.02	118.64	123.68
23	c	510	CLA	C6-C7-C8	-2.02	109.11	115.73
25	c	514	BCR	C15-C16-C17	-2.02	119.16	123.46
23	c	510	CLA	CAA-C2A-C3A	-2.02	107.28	112.81
23	B	610	CLA	C2A-C1A-CHA	-2.02	120.34	123.92
23	C	513	CLA	C1-C2-C3	-2.02	122.24	125.96
23	b	604	CLA	CBC-CAC-C3C	-2.01	106.69	112.41
23	C	507	CLA	OBD-CAD-C3D	-2.01	124.31	128.03
23	b	602	CLA	CMA-C3A-C2A	-2.01	105.60	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	OBD-CAD-C3D	-2.01	124.32	128.03
25	Y	101	BCR	C8-C7-C6	-2.01	121.62	127.25
23	B	606	CLA	CAA-C2A-C3A	-2.01	107.30	112.81
23	c	503	CLA	C2A-C1A-CHA	-2.01	120.35	123.92
23	B	612	CLA	O1D-CGD-CBD	-2.01	120.99	124.60
23	C	502	CLA	O2A-CGA-O1A	-2.01	118.56	123.55
23	A	404	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
34	B	622	LMG	C12-C11-C10	-2.01	106.25	113.58
23	c	503	CLA	C4A-NA-C1A	-2.01	103.96	106.45
23	B	617	CLA	C1-C2-C3	-2.01	122.25	125.96
26	a	411	SQD	O48-C23-O10	-2.01	118.56	123.55
23	b	606	CLA	C4A-NA-C1A	-2.01	103.96	106.45
29	D	407	PL9	C42-C41-C39	-2.00	106.15	112.93
25	b	617	BCR	C38-C26-C25	-2.00	122.27	124.51
23	C	514	CLA	CMA-C3A-C2A	-2.00	105.64	113.77
25	d	404	BCR	C29-C30-C25	2.00	113.61	110.48
23	d	402	CLA	CHB-C4A-NA	2.00	127.28	124.51
23	B	614	CLA	CED-O2D-CGD	2.01	120.67	115.97
25	y	101	BCR	C33-C5-C4	2.02	117.28	113.45
23	a	406	CLA	CMB-C2B-C3B	2.02	128.64	124.89
23	a	409	CLA	CHB-C4A-NA	2.02	127.31	124.51
25	D	406	BCR	C37-C22-C23	2.02	121.32	118.10
23	B	607	CLA	CAC-C3C-C4C	2.03	127.69	124.83
23	D	401	CLA	CAA-CBA-CGA	2.03	119.46	113.35
23	B	607	CLA	CMB-C2B-C3B	2.03	128.66	124.89
23	b	606	CLA	C1-O2A-CGA	2.03	121.65	116.77
24	a	408	PHO	C2A-C1A-NA	2.04	114.38	111.91
23	B	606	CLA	C4-C3-C5	2.04	118.83	115.29
35	M	101	LMT	O5B-C5B-C6B	2.04	111.30	106.41
23	B	616	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	b	608	CLA	C4-C3-C5	2.04	118.83	115.29
23	D	405	CLA	CMB-C2B-C1B	2.04	131.60	128.46
24	A	406	PHO	CBD-CHA-C1A	2.05	131.18	126.36
23	B	605	CLA	CMB-C2B-C3B	2.05	128.69	124.89
23	c	509	CLA	CMB-C2B-C3B	2.05	128.69	124.89
23	a	405	CLA	CMC-C2C-C1C	2.05	128.13	125.02
35	E	102	LMT	C2'-C3'-C4'	2.05	113.86	109.61
23	B	611	CLA	CMB-C2B-C3B	2.05	128.70	124.89
37	C	517	DGD	O1G-C1A-C2A	2.05	117.87	111.90
25	d	404	BCR	C38-C26-C27	2.05	117.35	113.45
23	B	617	CLA	CMB-C2B-C3B	2.06	128.71	124.89
25	c	515	BCR	C29-C30-C25	2.06	113.69	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	PHO	C4D-C3D-CAD	2.06	109.23	105.41
24	D	402	PHO	CBD-CHA-C1A	2.06	131.21	126.36
25	A	408	BCR	C37-C22-C23	2.06	121.38	118.10
35	E	102	LMT	O1B-C1B-C2B	2.06	112.76	108.11
23	D	404	CLA	CMB-C2B-C3B	2.06	128.72	124.89
23	c	508	CLA	C1-O2A-CGA	2.06	121.72	116.77
29	D	407	PL9	C2-C1-C6	2.07	121.29	117.82
24	D	402	PHO	CMB-C2B-C1B	2.07	128.26	125.04
29	d	405	PL9	C7-C3-C4	2.07	118.56	116.88
23	c	504	CLA	CED-O2D-CGD	2.07	120.82	115.97
26	a	411	SQD	O7-S-C6	2.07	108.60	106.83
23	B	608	CLA	C4-C3-C5	2.07	118.88	115.29
23	C	502	CLA	C3D-CAD-CBD	2.07	110.52	107.60
25	k	101	BCR	C36-C18-C19	2.07	121.40	118.10
25	c	515	BCR	C33-C5-C4	2.07	117.38	113.45
23	B	610	CLA	C1-O2A-CGA	2.07	121.75	116.77
36	b	621	HTG	C3-C4-C5	2.08	113.88	110.22
35	m	103	LMT	O1B-C1B-C2B	2.08	112.80	108.11
23	C	504	CLA	CMB-C2B-C3B	2.08	128.75	124.89
23	a	404	CLA	CED-O2D-CGD	2.08	120.85	115.97
23	B	608	CLA	CAC-C3C-C4C	2.08	127.77	124.83
23	b	606	CLA	CAC-C3C-C4C	2.08	127.77	124.83
24	a	407	PHO	C4-C3-C5	2.09	118.91	115.29
35	C	522	LMT	O5'-C1'-C2'	2.10	114.34	110.30
25	B	619	BCR	C37-C22-C23	2.10	121.44	118.10
23	b	612	CLA	CAC-C3C-C4C	2.10	127.79	124.83
35	e	102	LMT	O5'-C5'-C4'	2.10	114.04	109.75
35	M	103	LMT	C2'-C3'-C4'	2.10	113.96	109.61
24	a	408	PHO	C2C-C1C-NC	2.10	112.93	109.82
23	a	405	CLA	C4-C3-C5	2.10	118.93	115.29
25	t	101	BCR	C33-C5-C4	2.10	117.44	113.45
25	A	408	BCR	C36-C18-C19	2.10	121.45	118.10
26	B	621	SQD	O8-S-C6	2.10	108.58	106.01
35	M	103	LMT	O5'-C5'-C4'	2.11	114.06	109.75
36	B	624	HTG	O5-C1-C2	2.11	113.17	110.28
35	C	522	LMT	O5'-C5'-C4'	2.11	114.06	109.75
31	L	101	LHG	O4-P-O5	2.11	123.19	112.28
23	C	508	CLA	CAC-C3C-C4C	2.11	127.81	124.83
23	a	409	CLA	CMB-C2B-C3B	2.11	128.81	124.89
23	A	405	CLA	CMC-C2C-C1C	2.11	128.22	125.02
23	c	505	CLA	C1-O2A-CGA	2.12	121.85	116.77
23	c	503	CLA	C1-O2A-CGA	2.12	121.85	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	602	CLA	CMC-C2C-C1C	2.12	128.23	125.02
25	h	102	BCR	C35-C13-C12	2.12	121.48	118.10
25	a	410	BCR	C36-C18-C19	2.12	121.48	118.10
23	c	512	CLA	CMC-C2C-C1C	2.12	128.24	125.02
25	C	527	BCR	C36-C18-C19	2.12	121.48	118.10
23	B	609	CLA	CAC-C3C-C2C	2.13	131.18	127.49
23	C	509	CLA	CAC-C3C-C2C	2.13	131.19	127.49
25	B	620	BCR	C29-C30-C25	2.14	113.82	110.48
23	D	405	CLA	O2A-CGA-CBA	2.14	118.12	111.90
23	c	510	CLA	CMB-C2B-C3B	2.14	128.87	124.89
23	D	405	CLA	CHB-C4A-NA	2.14	127.48	124.51
23	D	404	CLA	CAC-C3C-C4C	2.14	127.85	124.83
24	a	408	PHO	CBD-CHA-C1A	2.15	131.41	126.36
23	B	612	CLA	C1-O2A-CGA	2.15	121.93	116.77
29	A	413	PL9	C51-C49-C50	2.15	119.63	114.60
23	B	605	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	b	611	CLA	CMB-C2B-C3B	2.16	128.90	124.89
23	b	615	CLA	C1-O2A-CGA	2.16	121.95	116.77
23	b	602	CLA	CAC-C3C-C4C	2.16	127.87	124.83
25	c	515	BCR	C37-C22-C23	2.16	121.54	118.10
25	D	406	BCR	C29-C30-C25	2.16	113.86	110.48
23	b	603	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	C	508	CLA	C4-C3-C5	2.18	119.07	115.29
23	b	616	CLA	CMB-C2B-C3B	2.18	128.94	124.89
25	Y	101	BCR	C33-C5-C4	2.18	117.59	113.45
34	C	501	LMG	O8-C28-C29	2.18	118.25	111.90
25	H	101	BCR	C2-C1-C6	2.18	113.89	110.48
23	c	501	CLA	CMC-C2C-C1C	2.19	128.34	125.02
25	b	619	BCR	C37-C22-C23	2.19	121.59	118.10
25	B	618	BCR	C33-C5-C4	2.20	117.62	113.45
23	B	606	CLA	CHB-C4A-NA	2.20	127.55	124.51
23	a	404	CLA	C4-C3-C5	2.20	119.10	115.29
23	B	609	CLA	C4-C3-C5	2.20	119.10	115.29
23	C	513	CLA	CHB-C4A-NA	2.20	127.55	124.51
25	B	620	BCR	C37-C22-C23	2.21	121.61	118.10
35	C	522	LMT	O1'-C1'-C2'	2.21	111.83	108.23
23	B	612	CLA	CMB-C2B-C3B	2.21	129.00	124.89
23	a	406	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	b	603	CLA	CAC-C3C-C4C	2.22	127.95	124.83
23	C	505	CLA	CMB-C2B-C3B	2.22	129.00	124.89
23	b	613	CLA	CHB-C4A-NA	2.22	127.58	124.51
25	C	516	BCR	C2-C1-C6	2.22	113.95	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C37-C22-C23	2.23	121.65	118.10
24	a	407	PHO	C4D-C3D-CAD	2.23	109.54	105.41
24	a	408	PHO	O2A-CGA-CBA	2.23	118.39	111.90
23	c	511	CLA	CAC-C3C-C4C	2.23	127.98	124.83
25	A	408	BCR	C35-C13-C12	2.23	121.66	118.10
23	C	510	CLA	CMB-C2B-C3B	2.23	129.04	124.89
36	C	523	HTG	O5-C1-C2	2.24	113.34	110.28
34	Z	101	LMG	O6-C5-C4	2.24	113.78	109.66
23	a	405	CLA	CHB-C4A-NA	2.24	127.61	124.51
36	b	621	HTG	O5-C5-C4	2.24	113.79	109.66
23	B	609	CLA	CHB-C4A-NA	2.25	127.62	124.51
34	C	501	LMG	O1-C1-C2	2.25	111.90	108.23
36	b	623	HTG	C1-O5-C5	2.25	117.02	112.69
23	C	505	CLA	O2A-CGA-CBA	2.26	118.47	111.90
35	B	623	LMT	O1B-C4'-C3'	2.26	112.64	107.19
25	y	101	BCR	C1-C6-C7	2.26	122.09	115.73
23	C	503	CLA	C4-C3-C5	2.27	119.22	115.29
23	d	403	CLA	C4-C3-C5	2.27	119.22	115.29
23	b	613	CLA	C4-C3-C5	2.27	119.23	115.29
26	A	411	SQD	O9-S-C6	2.27	108.77	106.83
29	a	415	PL9	C45-C44-C46	2.28	119.24	115.29
23	c	504	CLA	CHB-C4A-NA	2.28	127.66	124.51
35	m	103	LMT	O5B-C5B-C4B	2.28	113.85	109.66
25	k	101	BCR	C2-C1-C6	2.28	114.04	110.48
23	c	503	CLA	CMC-C2C-C1C	2.28	128.48	125.02
36	B	624	HTG	C1-O5-C5	2.28	117.09	112.69
23	b	610	CLA	CAC-C3C-C4C	2.28	128.05	124.83
23	b	605	CLA	C1-O2A-CGA	2.29	122.26	116.77
23	c	505	CLA	CMC-C2C-C1C	2.29	128.49	125.02
23	B	602	CLA	CAC-C3C-C4C	2.29	128.06	124.83
29	A	413	PL9	C45-C44-C46	2.29	119.27	115.29
23	C	509	CLA	CHB-C4A-NA	2.29	127.68	124.51
25	Y	101	BCR	C34-C9-C8	2.30	121.76	118.10
23	C	505	CLA	CAC-C3C-C4C	2.30	128.07	124.83
23	B	609	CLA	CMC-C2C-C1C	2.30	128.51	125.02
24	a	408	PHO	C4D-C3D-CAD	2.30	109.68	105.41
23	b	614	CLA	CMB-C2B-C3B	2.30	129.16	124.89
38	V	202	HEM	CAD-CBD-CGD	2.30	116.60	112.66
35	B	634	LMT	O1'-C1'-C2'	2.31	112.00	108.23
23	c	509	CLA	CED-O2D-CGD	2.31	121.38	115.97
23	C	513	CLA	CMB-C2B-C3B	2.31	129.18	124.89
23	b	613	CLA	CED-O2D-CGD	2.31	121.39	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	CLA	CMC-C2C-C1C	2.31	128.53	125.02
23	c	509	CLA	C4-C3-C5	2.31	119.30	115.29
23	C	514	CLA	C4-C3-C5	2.31	119.30	115.29
25	C	527	BCR	C2-C1-C6	2.32	114.10	110.48
23	A	405	CLA	C4-C3-C5	2.32	119.31	115.29
29	D	407	PL9	C40-C39-C41	2.32	119.31	115.29
23	c	506	CLA	CMC-C2C-C1C	2.32	128.54	125.02
25	k	101	BCR	C34-C9-C8	2.32	121.80	118.10
35	D	403	LMT	O1B-C1B-C2B	2.32	113.34	108.11
23	a	405	CLA	CMB-C2B-C3B	2.33	129.21	124.89
23	b	615	CLA	O2A-CGA-CBA	2.33	118.68	111.90
24	D	402	PHO	O2A-CGA-CBA	2.33	118.68	111.90
23	C	505	CLA	CHB-C4A-NA	2.33	127.74	124.51
23	b	607	CLA	C1-O2A-CGA	2.33	122.37	116.77
23	C	507	CLA	CMB-C2B-C3B	2.33	129.22	124.89
23	b	601	CLA	CMC-C2C-C1C	2.34	128.56	125.02
29	d	405	PL9	C51-C49-C50	2.34	120.05	114.60
26	B	621	SQD	C3-C4-C5	2.34	114.33	110.22
23	c	509	CLA	CAC-C3C-C4C	2.34	128.13	124.83
29	D	407	PL9	C25-C24-C26	2.34	119.35	115.29
23	a	405	CLA	CAA-CBA-CGA	2.34	120.40	113.35
36	c	522	HTG	O5-C5-C4	2.34	113.97	109.66
36	B	629	HTG	O5-C5-C4	2.34	113.98	109.66
25	B	619	BCR	C2-C1-C6	2.35	114.14	110.48
35	e	102	LMT	C1B-C2B-C3B	2.35	114.34	109.98
23	B	602	CLA	CHB-C4A-NA	2.35	127.75	124.51
25	h	102	BCR	C29-C30-C25	2.35	114.14	110.48
34	Z	101	LMG	C1-O6-C5	2.35	118.13	113.72
26	D	413	SQD	O8-S-C6	2.35	108.88	106.01
24	A	406	PHO	C2B-C1B-NB	2.36	113.31	109.82
23	B	612	CLA	O2A-CGA-CBA	2.37	118.79	111.90
29	a	415	PL9	C40-C39-C41	2.37	119.40	115.29
36	b	626	HTG	C1-O5-C5	2.37	117.26	112.69
29	a	415	PL9	C51-C49-C50	2.37	120.14	114.60
24	a	408	PHO	CAC-C3C-C4C	2.38	128.00	125.21
25	Y	101	BCR	C36-C18-C19	2.38	121.89	118.10
35	M	101	LMT	O1B-C1B-C2B	2.38	113.48	108.11
37	c	517	DGD	O5D-C1E-C2E	2.38	112.12	108.23
23	b	612	CLA	CMC-C2C-C1C	2.38	128.64	125.02
24	a	407	PHO	CAC-C3C-C4C	2.39	128.01	125.21
23	B	604	CLA	CAC-C3C-C4C	2.39	128.20	124.83
23	C	506	CLA	CAC-C3C-C4C	2.39	128.20	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	C4-C3-C5	2.39	119.44	115.29
23	B	607	CLA	C4-C3-C5	2.39	119.44	115.29
37	C	519	DGD	O2G-C1B-C2B	2.39	116.52	111.55
35	e	102	LMT	O1B-C1B-C2B	2.39	113.51	108.11
23	b	615	CLA	CAC-C3C-C4C	2.40	128.21	124.83
23	A	407	CLA	O2A-CGA-CBA	2.40	118.87	111.90
23	C	504	CLA	CAC-C3C-C4C	2.40	128.21	124.83
25	a	410	BCR	C2-C1-C6	2.40	114.23	110.48
29	D	407	PL9	C30-C29-C31	2.40	119.46	115.29
23	b	604	CLA	C4-C3-C5	2.40	119.46	115.29
24	a	407	PHO	C3C-C4C-NC	2.40	114.12	110.19
23	B	603	CLA	CMB-C2B-C3B	2.40	129.35	124.89
23	c	505	CLA	CAC-C3C-C4C	2.40	128.22	124.83
25	b	619	BCR	C33-C5-C4	2.41	118.02	113.45
23	C	502	CLA	CMB-C2B-C3B	2.41	129.37	124.89
23	B	602	CLA	C4-C3-C5	2.41	119.47	115.29
23	c	505	CLA	C4-C3-C5	2.42	119.48	115.29
23	C	503	CLA	O2A-CGA-CBA	2.42	118.93	111.90
24	a	407	PHO	CMC-C2C-C1C	2.42	128.81	125.04
23	d	402	CLA	C4-C3-C5	2.42	119.49	115.29
23	B	606	CLA	CAC-C3C-C4C	2.42	128.24	124.83
23	B	604	CLA	CMC-C2C-C1C	2.42	128.70	125.02
23	c	504	CLA	O2A-CGA-CBA	2.43	118.96	111.90
25	c	515	BCR	C36-C18-C19	2.43	121.97	118.10
23	d	402	CLA	CMC-C2C-C1C	2.44	128.71	125.02
23	c	503	CLA	C4-C3-C5	2.44	119.51	115.29
23	b	607	CLA	CMC-C2C-C1C	2.44	128.72	125.02
23	B	611	CLA	CAC-C3C-C4C	2.44	128.27	124.83
23	C	502	CLA	O2A-CGA-CBA	2.44	119.01	111.90
36	C	523	HTG	C1-O5-C5	2.45	117.41	112.69
37	H	102	DGD	O1G-C1A-C2A	2.45	119.04	111.90
23	D	405	CLA	CAC-C3C-C4C	2.45	128.29	124.83
23	a	404	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	b	602	CLA	C4-C3-C5	2.46	119.56	115.29
24	A	406	PHO	C2C-C1C-NC	2.46	113.47	109.82
23	C	513	CLA	C4-C3-C5	2.46	119.56	115.29
24	D	402	PHO	C4D-C3D-CAD	2.47	109.98	105.41
24	D	402	PHO	C4-C3-C5	2.47	119.58	115.29
23	c	513	CLA	CMB-C2B-C3B	2.48	129.49	124.89
23	C	505	CLA	C4-C3-C5	2.48	119.59	115.29
23	c	507	CLA	C4-C3-C5	2.49	119.60	115.29
23	b	611	CLA	CAC-C3C-C4C	2.49	128.34	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	f	101	SQD	O5-C5-C4	2.49	114.24	109.66
23	B	607	CLA	CMC-C2C-C1C	2.49	128.79	125.02
25	d	404	BCR	C37-C22-C23	2.49	122.06	118.10
25	H	101	BCR	C7-C6-C5	2.49	127.48	121.54
23	B	608	CLA	C1-O2A-CGA	2.49	122.75	116.77
23	D	401	CLA	C3B-C4B-NB	2.50	112.44	109.21
23	b	607	CLA	O2A-CGA-CBA	2.50	119.17	111.90
29	a	415	PL9	C53-C6-C1	2.50	120.15	114.84
23	b	610	CLA	CMC-C2C-C1C	2.50	128.81	125.02
23	c	501	CLA	CMB-C2B-C3B	2.51	129.54	124.89
23	b	606	CLA	O2A-CGA-CBA	2.51	119.21	111.90
23	A	405	CLA	CAC-C3C-C4C	2.51	128.38	124.83
23	B	616	CLA	CMB-C2B-C1B	2.51	132.33	128.46
26	a	413	SQD	O8-S-C6	2.52	109.08	106.01
29	A	413	PL9	C40-C39-C41	2.52	119.65	115.29
29	D	407	PL9	C20-C19-C21	2.52	119.66	115.29
23	C	503	CLA	CAC-C3C-C4C	2.52	128.38	124.83
23	c	509	CLA	CMC-C2C-C1C	2.53	128.85	125.02
23	C	502	CLA	CMC-C2C-C1C	2.53	128.86	125.02
23	b	602	CLA	CMB-C2B-C3B	2.53	129.59	124.89
23	b	601	CLA	CMB-C2B-C3B	2.54	129.60	124.89
23	C	511	CLA	CAC-C3C-C4C	2.54	128.41	124.83
23	B	617	CLA	C4-C3-C5	2.54	119.69	115.29
35	B	623	LMT	C1'-O5'-C5'	2.54	118.51	113.72
23	c	511	CLA	CMC-C2C-C1C	2.55	128.88	125.02
23	C	505	CLA	C1-O2A-CGA	2.55	122.89	116.77
35	D	403	LMT	O5B-C5B-C4B	2.55	114.36	109.66
23	b	615	CLA	C4-C3-C5	2.55	119.72	115.29
24	D	402	PHO	C2A-C1A-NA	2.55	115.00	111.91
34	C	521	LMG	O8-C28-C29	2.55	119.33	111.90
23	c	511	CLA	CMB-C2B-C3B	2.56	129.64	124.89
23	c	504	CLA	C1-O2A-CGA	2.56	122.92	116.77
23	B	606	CLA	CMB-C2B-C1B	2.56	132.41	128.46
26	a	413	SQD	O5-C5-C4	2.57	114.39	109.66
29	A	413	PL9	C10-C9-C11	2.57	119.74	115.29
31	D	408	LHG	O8-C23-C24	2.57	119.37	111.90
23	c	508	CLA	CMC-C2C-C1C	2.57	128.92	125.02
23	c	513	CLA	C4-C3-C5	2.57	119.75	115.29
34	a	417	LMG	O8-C28-C29	2.57	119.38	111.90
23	A	404	CLA	CAC-C3C-C4C	2.57	128.46	124.83
23	B	608	CLA	O2A-CGA-CBA	2.58	119.40	111.90
26	f	101	SQD	O5-C1-C2	2.58	115.27	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b	623	HTG	O5-C1-C2	2.58	113.81	110.28
35	B	623	LMT	C3'-C4'-C5'	2.58	116.34	110.88
23	B	615	CLA	CMC-C2C-C1C	2.58	128.93	125.02
29	D	407	PL9	C51-C49-C50	2.59	120.64	114.60
26	a	413	SQD	C1-O5-C5	2.59	118.59	113.72
23	C	512	CLA	O2A-CGA-CBA	2.59	119.44	111.90
26	a	411	SQD	O48-C23-C24	2.59	119.44	111.90
23	a	405	CLA	O2A-CGA-CBA	2.59	119.44	111.90
23	c	502	CLA	CMC-C2C-C1C	2.59	128.95	125.02
24	A	406	PHO	CMC-C2C-C1C	2.60	129.09	125.04
29	D	407	PL9	C15-C14-C16	2.60	119.79	115.29
29	a	415	PL9	C10-C9-C11	2.60	119.80	115.29
23	b	607	CLA	C4-C3-C5	2.60	119.80	115.29
23	b	614	CLA	CMC-C2C-C1C	2.60	128.96	125.02
23	a	406	CLA	C4-C3-C5	2.60	119.80	115.29
23	A	404	CLA	C4-C3-C5	2.61	119.81	115.29
24	a	408	PHO	C2B-C1B-NB	2.61	113.68	109.82
29	A	413	PL9	C53-C6-C1	2.61	120.38	114.84
29	A	413	PL9	C25-C24-C26	2.61	119.81	115.29
36	B	629	HTG	C1-O5-C5	2.61	117.72	112.69
23	C	502	CLA	CAC-C3C-C4C	2.61	128.52	124.83
29	a	415	PL9	C20-C19-C21	2.62	119.83	115.29
23	a	409	CLA	CMC-C2C-C1C	2.62	128.99	125.02
29	A	413	PL9	C35-C34-C36	2.62	119.83	115.29
24	D	402	PHO	C3C-C4C-NC	2.62	114.48	110.19
23	B	606	CLA	CMC-C2C-C1C	2.62	129.00	125.02
23	c	507	CLA	C3B-C4B-NB	2.62	112.60	109.21
29	a	415	PL9	C35-C34-C36	2.63	119.84	115.29
25	b	618	BCR	C37-C22-C23	2.63	122.28	118.10
23	b	614	CLA	CAC-C3C-C4C	2.63	128.54	124.83
23	b	604	CLA	CAC-C3C-C4C	2.63	128.54	124.83
23	B	611	CLA	CMC-C2C-C1C	2.63	129.01	125.02
24	a	407	PHO	CMB-C2B-C1B	2.63	129.14	125.04
34	c	520	LMG	C1-O6-C5	2.64	118.69	113.72
23	b	601	CLA	O2A-CGA-CBA	2.64	119.59	111.90
23	c	505	CLA	O2A-CGA-CBA	2.64	119.59	111.90
25	H	101	BCR	C29-C30-C25	2.64	114.61	110.48
35	b	628	LMT	C1'-C2'-C3'	2.64	114.89	109.98
23	b	603	CLA	C4-C3-C5	2.64	119.88	115.29
23	c	507	CLA	CAC-C3C-C4C	2.65	128.57	124.83
26	D	413	SQD	C3-C4-C5	2.65	114.89	110.22
29	d	405	PL9	C53-C6-C1	2.65	120.47	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C3B-C4B-NB	2.65	112.64	109.21
23	C	506	CLA	C4-C3-C5	2.65	119.89	115.29
23	C	503	CLA	CMC-C2C-C1C	2.66	129.05	125.02
26	f	101	SQD	O48-C23-C24	2.66	119.63	111.90
37	C	518	DGD	O1G-C1A-C2A	2.66	119.63	111.90
23	C	505	CLA	CMC-C2C-C1C	2.66	129.05	125.02
23	B	603	CLA	CAC-C3C-C4C	2.66	128.58	124.83
25	B	619	BCR	C36-C18-C19	2.66	122.33	118.10
23	b	609	CLA	CAC-C3C-C4C	2.66	128.58	124.83
29	d	405	PL9	C40-C39-C41	2.66	119.90	115.29
36	B	626	HTG	O5-C1-C2	2.66	113.92	110.28
26	A	409	SQD	O8-S-C6	2.66	109.26	106.01
24	D	402	PHO	C2C-C1C-NC	2.66	113.77	109.82
31	e	101	LHG	O8-C23-C24	2.67	119.66	111.90
23	B	608	CLA	CED-O2D-CGD	2.67	122.22	115.97
23	C	513	CLA	C3B-C4B-NB	2.67	112.66	109.21
23	C	506	CLA	O2A-CGA-CBA	2.67	119.67	111.90
36	b	621	HTG	O5-C1-C2	2.67	113.94	110.28
23	d	403	CLA	CAC-C3C-C4C	2.67	128.60	124.83
34	c	520	LMG	C3-C4-C5	2.68	114.93	110.22
26	D	413	SQD	O5-C5-C4	2.68	114.59	109.66
25	c	514	BCR	C2-C1-C6	2.68	114.67	110.48
23	c	507	CLA	O2A-CGA-CBA	2.68	119.70	111.90
23	C	514	CLA	CAC-C3C-C4C	2.68	128.61	124.83
23	b	610	CLA	C3B-C4B-NB	2.68	112.68	109.21
23	D	401	CLA	O2A-CGA-CBA	2.69	119.74	111.90
23	C	510	CLA	O2A-CGA-CBA	2.69	119.74	111.90
23	B	613	CLA	CMC-C2C-C1C	2.70	129.11	125.02
23	a	406	CLA	O2A-CGA-CBA	2.70	119.77	111.90
23	B	613	CLA	CMB-C2B-C3B	2.70	129.91	124.89
23	b	605	CLA	CED-O2D-CGD	2.71	122.32	115.97
23	b	610	CLA	CMB-C2B-C3B	2.71	129.92	124.89
23	a	409	CLA	O2A-CGA-CBA	2.71	119.78	111.90
25	B	618	BCR	C29-C30-C25	2.72	114.73	110.48
23	B	616	CLA	CAC-C3C-C4C	2.72	128.67	124.83
37	h	103	DGD	O2G-C1B-C2B	2.72	117.21	111.55
23	c	501	CLA	O2A-CGA-CBA	2.72	119.83	111.90
23	c	504	CLA	C4-C3-C5	2.73	120.02	115.29
23	C	506	CLA	CMC-C2C-C1C	2.73	129.16	125.02
23	c	501	CLA	C4-C3-C5	2.73	120.02	115.29
23	c	504	CLA	CMC-C2C-C1C	2.73	129.16	125.02
23	b	616	CLA	C4-C3-C5	2.73	120.03	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	517	DGD	O1G-C1A-C2A	2.73	119.86	111.90
23	d	403	CLA	C3B-C4B-NB	2.74	112.75	109.21
23	B	605	CLA	C4-C3-C5	2.74	120.04	115.29
25	b	618	BCR	C29-C30-C25	2.74	114.76	110.48
24	a	407	PHO	C2C-C1C-NC	2.74	113.88	109.82
23	B	611	CLA	C3B-C4B-NB	2.74	112.75	109.21
36	C	524	HTG	C1-S1-C1'	2.74	110.19	100.35
23	b	608	CLA	CMB-C2B-C3B	2.75	129.99	124.89
23	C	510	CLA	C1-O2A-CGA	2.75	123.36	116.77
23	B	608	CLA	C3B-C4B-NB	2.75	112.77	109.21
24	D	402	PHO	CAC-C3C-C4C	2.76	128.45	125.21
23	b	609	CLA	C3B-C4B-NB	2.76	112.78	109.21
23	B	614	CLA	O2A-CGA-CBA	2.77	119.95	111.90
31	d	406	LHG	O8-C23-C24	2.77	119.95	111.90
23	B	610	CLA	CMC-C2C-C1C	2.77	129.22	125.02
24	a	407	PHO	C2B-C1B-NB	2.77	113.92	109.82
23	B	616	CLA	O2A-CGA-CBA	2.78	119.98	111.90
23	C	514	CLA	C3B-C4B-NB	2.78	112.80	109.21
23	B	606	CLA	C3B-C4B-NB	2.79	112.82	109.21
26	L	102	SQD	O9-S-C6	2.79	109.21	106.83
23	c	513	CLA	CAC-C3C-C4C	2.79	128.77	124.83
23	b	612	CLA	C4-C3-C5	2.79	120.14	115.29
23	b	605	CLA	C4-C3-C5	2.80	120.15	115.29
23	b	606	CLA	CMC-C2C-C1C	2.80	129.27	125.02
34	a	417	LMG	O6-C5-C4	2.80	114.82	109.66
36	b	625	HTG	O5-C5-C4	2.80	114.82	109.66
34	j	101	LMG	O8-C28-C29	2.80	120.06	111.90
23	C	510	CLA	CAC-C3C-C4C	2.81	128.80	124.83
23	B	615	CLA	CAC-C3C-C4C	2.81	128.80	124.83
23	C	509	CLA	O2A-CGA-CBA	2.81	120.08	111.90
35	B	633	LMT	O5'-C5'-C4'	2.81	115.51	109.75
23	C	509	CLA	CMB-C2B-C3B	2.81	130.11	124.89
24	a	407	PHO	CBD-CHA-C1A	2.82	132.99	126.36
23	c	512	CLA	C3B-C4B-NB	2.82	112.85	109.21
23	C	514	CLA	O2A-CGA-CBA	2.82	120.11	111.90
26	D	413	SQD	O48-C23-C24	2.82	120.11	111.90
23	c	510	CLA	C4-C3-C5	2.83	120.19	115.29
23	b	616	CLA	CAC-C3C-C4C	2.83	128.82	124.83
23	c	503	CLA	O2A-CGA-CBA	2.83	120.14	111.90
26	L	102	SQD	O48-C23-C24	2.83	120.14	111.90
23	C	508	CLA	O2A-CGA-CBA	2.84	120.16	111.90
36	b	622	HTG	O5-C1-C2	2.84	114.17	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C3B-C4B-NB	2.84	112.88	109.21
23	B	613	CLA	CAC-C3C-C4C	2.85	128.84	124.83
23	b	608	CLA	CMC-C2C-C1C	2.85	129.34	125.02
23	B	614	CLA	C4-C3-C5	2.85	120.23	115.29
25	T	101	BCR	C16-C15-C14	2.85	129.54	123.46
23	b	602	CLA	O2A-CGA-CBA	2.85	120.19	111.90
23	B	605	CLA	CMC-C2C-C1C	2.85	129.34	125.02
23	B	613	CLA	C4-C3-C5	2.85	120.23	115.29
23	D	404	CLA	C4-C3-C5	2.85	120.24	115.29
31	D	408	LHG	O7-C7-C8	2.86	117.48	111.55
25	t	101	BCR	C1-C6-C7	2.86	123.76	115.73
36	b	621	HTG	C1-O5-C5	2.86	118.19	112.69
34	Z	101	LMG	O6-C1-C2	2.86	115.81	110.30
29	a	415	PL9	C25-C24-C26	2.87	120.26	115.29
23	b	610	CLA	C4-C3-C5	2.87	120.27	115.29
31	d	407	LHG	O8-C23-C24	2.87	120.25	111.90
23	B	606	CLA	O2A-CGA-CBA	2.87	120.25	111.90
23	c	512	CLA	CHB-C4A-NA	2.87	128.49	124.51
23	C	502	CLA	C4-C3-C5	2.87	120.27	115.29
23	C	507	CLA	CAC-C3C-C4C	2.87	128.88	124.83
23	B	614	CLA	CAC-C3C-C4C	2.88	128.89	124.83
37	C	519	DGD	O1G-C1A-C2A	2.88	120.28	111.90
37	c	518	DGD	O1G-C1A-C2A	2.88	120.28	111.90
29	D	407	PL9	C7-C3-C4	2.88	119.22	116.88
23	C	508	CLA	CMC-C2C-C1C	2.88	129.39	125.02
23	C	510	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	b	609	CLA	CMC-C2C-C1C	2.90	129.41	125.02
31	L	101	LHG	O8-C23-C24	2.90	120.33	111.90
23	c	513	CLA	O2A-CGA-CBA	2.90	120.33	111.90
23	c	506	CLA	C4-C3-C5	2.90	120.32	115.29
23	b	605	CLA	CAC-C3C-C4C	2.90	128.92	124.83
23	b	608	CLA	O2A-CGA-CBA	2.90	120.34	111.90
23	B	603	CLA	O2A-CGA-CBA	2.90	120.35	111.90
25	c	515	BCR	C2-C1-C6	2.91	115.02	110.48
23	c	502	CLA	O2A-CGA-CBA	2.91	120.37	111.90
23	c	502	CLA	CMB-C2B-C3B	2.91	130.30	124.89
23	b	603	CLA	CMC-C2C-C1C	2.93	129.46	125.02
23	b	607	CLA	CAC-C3C-C4C	2.93	128.96	124.83
23	A	407	CLA	CMB-C2B-C3B	2.93	130.33	124.89
23	c	510	CLA	CAC-C3C-C4C	2.93	128.97	124.83
23	b	613	CLA	CMC-C2C-C1C	2.93	129.47	125.02
37	c	518	DGD	O2G-C1B-C2B	2.93	117.65	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	CLA	C4-C3-C5	2.94	120.39	115.29
31	d	408	LHG	O8-C23-C24	2.94	120.46	111.90
23	b	606	CLA	C4-C3-C5	2.95	120.40	115.29
29	d	405	PL9	C35-C34-C36	2.95	120.40	115.29
23	c	512	CLA	O2A-CGA-CBA	2.95	120.48	111.90
23	a	409	CLA	CAC-C3C-C4C	2.95	128.99	124.83
31	E	101	LHG	O8-C23-C24	2.95	120.49	111.90
31	A	415	LHG	O8-C23-C24	2.95	120.49	111.90
23	C	512	CLA	CMB-C2B-C3B	2.96	130.38	124.89
23	b	605	CLA	CMC-C2C-C1C	2.96	129.51	125.02
23	C	509	CLA	C4-C3-C5	2.96	120.43	115.29
25	T	101	BCR	C35-C13-C12	2.97	122.83	118.10
23	b	612	CLA	CMB-C2B-C3B	2.97	130.41	124.89
23	c	513	CLA	C3B-C4B-NB	2.98	113.06	109.21
26	L	102	SQD	O8-S-C6	2.98	109.64	106.01
26	B	621	SQD	O9-S-C6	2.98	109.38	106.83
23	B	613	CLA	O2A-CGA-CBA	2.99	120.59	111.90
23	B	604	CLA	C3B-C4B-NB	2.99	113.08	109.21
23	b	604	CLA	C3B-C4B-NB	2.99	113.08	109.21
26	B	621	SQD	O48-C23-C24	3.00	120.62	111.90
23	D	404	CLA	CMC-C2C-C1C	3.00	129.56	125.02
23	c	504	CLA	CMB-C2B-C3B	3.00	130.46	124.89
29	A	413	PL9	C20-C19-C21	3.00	120.50	115.29
23	B	617	CLA	O2A-CGA-CBA	3.01	120.67	111.90
25	Y	101	BCR	C37-C22-C23	3.01	122.90	118.10
23	c	511	CLA	C4-C3-C5	3.01	120.52	115.29
23	c	506	CLA	O2A-CGA-CBA	3.02	120.67	111.90
23	B	609	CLA	O2A-CGA-CBA	3.02	120.68	111.90
23	b	601	CLA	C3B-C4B-NB	3.02	113.11	109.21
23	C	513	CLA	CMC-C2C-C1C	3.02	129.60	125.02
23	B	604	CLA	C4-C3-C5	3.03	120.54	115.29
23	b	602	CLA	CMC-C2C-C1C	3.03	129.62	125.02
23	b	613	CLA	C3B-C4B-NB	3.04	113.14	109.21
34	c	520	LMG	O8-C28-C29	3.06	120.80	111.90
26	A	411	SQD	O48-C23-C24	3.06	120.81	111.90
36	b	625	HTG	C1-O5-C5	3.06	118.59	112.69
23	B	610	CLA	C3B-C4B-NB	3.07	113.17	109.21
23	C	507	CLA	C4-C3-C5	3.07	120.61	115.29
34	B	622	LMG	O8-C28-C29	3.07	120.83	111.90
23	b	613	CLA	CMB-C2B-C3B	3.07	130.59	124.89
23	c	511	CLA	O2A-CGA-CBA	3.07	120.84	111.90
23	a	404	CLA	O2D-CGD-CBD	3.07	116.79	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	CMC-C2C-C1C	3.08	129.68	125.02
26	a	413	SQD	O7-S-C6	3.08	109.46	106.83
23	A	404	CLA	C3B-C4B-NB	3.08	113.19	109.21
23	b	602	CLA	C3B-C4B-NB	3.09	113.20	109.21
23	B	615	CLA	C4-C3-C5	3.09	120.64	115.29
23	C	514	CLA	CMC-C2C-C1C	3.09	129.70	125.02
23	C	507	CLA	CMC-C2C-C1C	3.09	129.71	125.02
23	b	608	CLA	C3B-C4B-NB	3.10	113.21	109.21
23	C	507	CLA	O2A-CGA-CBA	3.10	120.91	111.90
23	c	505	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	c	501	CLA	C3B-C4B-NB	3.10	113.22	109.21
23	c	512	CLA	C4-C3-C5	3.10	120.67	115.29
25	k	101	BCR	C29-C30-C25	3.10	115.33	110.48
23	D	405	CLA	C3B-C4B-NB	3.11	113.22	109.21
23	c	504	CLA	CAC-C3C-C4C	3.11	129.21	124.83
23	B	607	CLA	C3B-C4B-NB	3.11	113.23	109.21
34	J	101	LMG	O8-C28-C29	3.11	120.94	111.90
26	a	413	SQD	C3-C4-C5	3.11	115.69	110.22
23	b	601	CLA	C4-C3-C5	3.11	120.68	115.29
24	D	402	PHO	C2B-C1B-NB	3.11	114.43	109.82
23	c	507	CLA	CMC-C2C-C1C	3.11	129.74	125.02
26	L	102	SQD	C3-C4-C5	3.12	115.72	110.22
23	A	405	CLA	O2A-CGA-CBA	3.12	120.99	111.90
34	Z	101	LMG	C4-C3-C2	3.13	116.35	110.84
23	C	512	CLA	CMC-C2C-C1C	3.13	129.76	125.02
31	b	630	LHG	O8-C23-C24	3.13	121.01	111.90
23	B	616	CLA	CMC-C2C-C1C	3.14	129.78	125.02
34	z	101	LMG	O8-C28-C29	3.14	121.03	111.90
23	B	602	CLA	O2A-CGA-CBA	3.14	121.03	111.90
23	b	611	CLA	O2A-CGA-CBA	3.14	121.04	111.90
23	C	504	CLA	O2A-CGA-CBA	3.15	121.05	111.90
35	C	522	LMT	O1B-C4'-C3'	3.15	114.78	107.19
23	B	610	CLA	O2A-CGA-CBA	3.16	121.09	111.90
31	D	409	LHG	O8-C23-C24	3.16	121.10	111.90
29	A	413	PL9	C15-C14-C16	3.16	120.78	115.29
34	Z	101	LMG	C3-C4-C5	3.17	115.80	110.22
23	A	404	CLA	CMB-C2B-C3B	3.17	130.77	124.89
29	D	407	PL9	C53-C6-C1	3.17	121.57	114.84
23	c	510	CLA	O2A-CGA-CBA	3.17	121.13	111.90
23	c	508	CLA	O2A-CGA-CBA	3.18	121.16	111.90
23	C	503	CLA	C3B-C4B-NB	3.19	113.34	109.21
23	d	403	CLA	O2A-CGA-CBA	3.19	121.19	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	B	602	CLA	C3B-C4B-NB	3.20	113.34	109.21
23	B	603	CLA	C3B-C4B-NB	3.20	113.34	109.21
29	A	413	PL9	C30-C29-C31	3.20	120.84	115.29
23	c	503	CLA	C3B-C4B-NB	3.20	113.35	109.21
24	A	406	PHO	C2A-C1A-NA	3.20	115.79	111.91
23	C	504	CLA	C4-C3-C5	3.21	120.85	115.29
23	B	616	CLA	CED-O2D-CGD	3.21	123.49	115.97
24	A	406	PHO	C1-O2A-CGA	3.21	124.47	116.77
23	D	405	CLA	CMC-C2C-C1C	3.21	129.89	125.02
23	c	506	CLA	CAC-C3C-C4C	3.21	129.36	124.83
26	a	413	SQD	O47-C7-C8	3.22	118.23	111.55
23	B	607	CLA	O2A-CGA-CBA	3.22	121.26	111.90
23	b	605	CLA	O2A-CGA-CBA	3.22	121.27	111.90
23	C	512	CLA	C4-C3-C5	3.23	120.89	115.29
23	B	617	CLA	C3B-C4B-NB	3.24	113.39	109.21
34	c	519	LMG	O8-C28-C29	3.24	121.32	111.90
23	A	405	CLA	C3B-C4B-NB	3.24	113.40	109.21
23	C	511	CLA	O2A-CGA-CBA	3.25	121.36	111.90
23	b	606	CLA	C3B-C4B-NB	3.26	113.42	109.21
26	D	413	SQD	O9-S-C6	3.26	109.61	106.83
23	B	605	CLA	C3B-C4B-NB	3.26	113.43	109.21
23	a	404	CLA	O2A-CGA-CBA	3.27	121.41	111.90
23	b	616	CLA	O2A-CGA-CBA	3.27	121.41	111.90
23	C	504	CLA	C3B-C4B-NB	3.27	113.44	109.21
36	c	522	HTG	C1-O5-C5	3.27	118.99	112.69
34	C	520	LMG	O8-C28-C29	3.27	121.42	111.90
23	c	508	CLA	CMB-C2B-C3B	3.28	130.97	124.89
23	d	403	CLA	CMC-C2C-C1C	3.28	130.00	125.02
23	c	510	CLA	CMC-C2C-C1C	3.28	130.00	125.02
23	c	509	CLA	C3B-C4B-NB	3.28	113.45	109.21
23	c	510	CLA	C3B-C4B-NB	3.29	113.46	109.21
23	A	404	CLA	O2D-CGD-CBD	3.30	117.19	111.30
23	c	502	CLA	C3B-C4B-NB	3.31	113.49	109.21
23	c	509	CLA	O2A-CGA-CBA	3.31	121.53	111.90
23	C	502	CLA	C3B-C4B-NB	3.31	113.49	109.21
31	e	101	LHG	O7-C7-C8	3.31	118.43	111.55
31	d	407	LHG	O7-C7-C8	3.31	118.43	111.55
23	d	402	CLA	O2A-CGA-CBA	3.32	121.55	111.90
23	b	603	CLA	O2A-CGA-CBA	3.32	121.55	111.90
29	d	405	PL9	C20-C19-C21	3.32	121.05	115.29
29	a	415	PL9	C30-C29-C31	3.33	121.06	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	628	LMT	C1'-O5'-C5'	3.33	119.99	113.72
23	b	613	CLA	O2A-CGA-CBA	3.34	121.61	111.90
23	A	407	CLA	C3B-C4B-NB	3.35	113.54	109.21
23	b	612	CLA	C3B-C4B-NB	3.35	113.54	109.21
34	m	101	LMG	O8-C28-C29	3.36	121.68	111.90
25	t	101	BCR	C37-C22-C23	3.36	123.46	118.10
23	b	614	CLA	C3B-C4B-NB	3.36	113.56	109.21
23	B	615	CLA	O2A-CGA-CBA	3.37	121.71	111.90
23	c	508	CLA	C3B-C4B-NB	3.38	113.58	109.21
23	B	608	CLA	CMC-C2C-C1C	3.38	130.15	125.02
26	A	409	SQD	O48-C23-C24	3.39	121.75	111.90
23	B	614	CLA	O2D-CGD-CBD	3.39	117.36	111.30
23	b	604	CLA	CMC-C2C-C1C	3.39	130.16	125.02
23	b	613	CLA	O2D-CGD-CBD	3.39	117.36	111.30
23	B	604	CLA	O2A-CGA-CBA	3.40	121.80	111.90
23	B	609	CLA	C3B-C4B-NB	3.40	113.61	109.21
23	B	614	CLA	C3B-C4B-NB	3.40	113.61	109.21
23	c	501	CLA	CAC-C3C-C4C	3.41	129.64	124.83
36	V	203	HTG	C1-C2-C3	3.42	113.99	109.65
23	B	616	CLA	C3B-C4B-NB	3.42	113.63	109.21
26	a	411	SQD	O9-S-C6	3.42	109.75	106.83
23	c	503	CLA	CAC-C3C-C4C	3.42	129.66	124.83
34	C	521	LMG	O6-C5-C4	3.43	115.97	109.66
23	a	409	CLA	C4-C3-C5	3.43	121.24	115.29
23	c	511	CLA	C3B-C4B-NB	3.43	113.65	109.21
23	b	605	CLA	C3B-C4B-NB	3.44	113.66	109.21
23	b	614	CLA	O2A-CGA-CBA	3.44	121.91	111.90
23	a	406	CLA	C3B-C4B-NB	3.45	113.67	109.21
23	b	610	CLA	O2A-CGA-CBA	3.46	121.95	111.90
23	D	404	CLA	O2A-CGA-CBA	3.46	121.96	111.90
23	b	604	CLA	O2A-CGA-CBA	3.46	121.97	111.90
23	B	605	CLA	O2A-CGA-CBA	3.46	121.98	111.90
23	b	603	CLA	C3B-C4B-NB	3.47	113.69	109.21
34	m	101	LMG	O7-C10-C11	3.47	118.75	111.55
23	B	611	CLA	O2A-CGA-CBA	3.47	122.00	111.90
25	T	101	BCR	C15-C14-C13	3.48	132.27	127.31
23	C	506	CLA	C3B-C4B-NB	3.48	113.71	109.21
23	C	513	CLA	O2A-CGA-CBA	3.48	122.03	111.90
34	C	520	LMG	O7-C10-C11	3.48	118.78	111.55
23	B	614	CLA	CMB-C2B-C3B	3.49	131.37	124.89
25	B	619	BCR	C29-C30-C25	3.49	115.94	110.48
29	a	415	PL9	C15-C14-C16	3.50	121.35	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	CLA	CMC-C2C-C1C	3.50	130.32	125.02
23	B	612	CLA	C3B-C4B-NB	3.50	113.74	109.21
23	c	509	CLA	C1-O2A-CGA	3.50	125.18	116.77
23	B	615	CLA	C3B-C4B-NB	3.52	113.76	109.21
23	d	402	CLA	C3B-C4B-NB	3.53	113.77	109.21
35	M	101	LMT	O1'-C1'-C2'	3.53	113.99	108.23
29	d	405	PL9	C25-C24-C26	3.53	121.42	115.29
35	b	628	LMT	O5'-C1'-C2'	3.54	117.12	110.30
26	D	413	SQD	O7-S-C6	3.55	109.86	106.83
23	b	609	CLA	O2A-CGA-CBA	3.55	122.22	111.90
34	j	101	LMG	O7-C10-C11	3.55	118.92	111.55
23	C	511	CLA	C4-C3-C5	3.55	121.45	115.29
23	B	614	CLA	CMC-C2C-C1C	3.56	130.42	125.02
23	a	409	CLA	C3B-C4B-NB	3.58	113.83	109.21
29	D	407	PL9	C10-C9-C11	3.58	121.50	115.29
37	c	517	DGD	O2G-C1B-C2B	3.59	119.00	111.55
26	a	413	SQD	O48-C23-C24	3.59	122.36	111.90
34	z	101	LMG	O7-C10-C11	3.60	119.03	111.55
23	C	512	CLA	C3B-C4B-NB	3.60	113.86	109.21
24	a	408	PHO	C4-C3-C5	3.60	121.54	115.29
23	a	404	CLA	CMB-C2B-C3B	3.60	131.58	124.89
34	C	521	LMG	C3-C4-C5	3.60	116.57	110.22
23	b	612	CLA	O2A-CGA-CBA	3.62	122.42	111.90
23	b	616	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	a	404	CLA	C3B-C4B-NB	3.62	113.89	109.21
36	B	624	HTG	C1'-S1-C1	3.62	105.66	100.28
23	C	512	CLA	CAC-C3C-C4C	3.63	129.94	124.83
31	d	406	LHG	O7-C7-C8	3.63	119.08	111.55
23	B	612	CLA	CMC-C2C-C1C	3.64	130.53	125.02
38	v	201	HEM	CAD-CBD-CGD	3.64	118.89	112.66
23	B	613	CLA	C3B-C4B-NB	3.64	113.92	109.21
23	D	401	CLA	CMC-C2C-C1C	3.65	130.56	125.02
35	D	403	LMT	C1'-O5'-C5'	3.66	120.60	113.72
24	a	407	PHO	O2A-CGA-CBA	3.67	122.58	111.90
23	A	407	CLA	C4-C3-C5	3.72	121.74	115.29
37	H	102	DGD	O2G-C1B-C2B	3.72	119.28	111.55
31	d	408	LHG	O7-C7-C8	3.72	119.28	111.55
23	b	615	CLA	C3B-C4B-NB	3.72	114.02	109.21
37	h	103	DGD	O1G-C1A-C2A	3.72	122.73	111.90
26	A	411	SQD	O47-C7-C8	3.73	119.30	111.55
23	C	510	CLA	CMC-C2C-C1C	3.74	130.69	125.02
23	c	506	CLA	C3B-C4B-NB	3.74	114.04	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	623	LMT	O5'-C5'-C4'	3.74	117.40	109.75
37	C	518	DGD	O2G-C1B-C2B	3.76	119.36	111.55
35	C	522	LMT	C1'-O5'-C5'	3.76	120.80	113.72
34	c	520	LMG	O7-C10-C11	3.77	119.38	111.55
25	t	101	BCR	C35-C13-C12	3.78	124.12	118.10
34	B	622	LMG	O7-C10-C11	3.82	119.48	111.55
31	A	415	LHG	O7-C7-C8	3.83	119.51	111.55
23	A	407	CLA	O2D-CGD-CBD	3.84	118.16	111.30
24	A	406	PHO	CAC-C3C-C4C	3.86	129.74	125.21
35	D	403	LMT	O5'-C5'-C4'	3.88	117.70	109.75
34	a	417	LMG	O7-C10-C11	3.89	119.63	111.55
34	c	520	LMG	O6-C5-C4	3.90	116.84	109.66
23	C	509	CLA	C3B-C4B-NB	3.90	114.26	109.21
23	c	504	CLA	C3B-C4B-NB	3.91	114.26	109.21
23	C	504	CLA	O2D-CGD-CBD	3.91	118.29	111.30
23	c	510	CLA	O2D-CGD-CBD	3.91	118.29	111.30
26	D	413	SQD	O6-C1-C2	3.92	114.63	108.23
23	c	510	CLA	C3C-C4C-NC	3.93	114.19	110.21
23	b	607	CLA	C3B-C4B-NB	3.94	114.30	109.21
23	c	506	CLA	O2D-CGD-CBD	3.95	118.35	111.30
23	C	511	CLA	C3B-C4B-NB	3.95	114.32	109.21
23	C	512	CLA	O2D-CGD-CBD	3.96	118.37	111.30
23	a	405	CLA	O2D-CGD-CBD	3.96	118.38	111.30
31	b	630	LHG	O7-C7-C8	4.03	119.92	111.55
34	Z	101	LMG	C1-C2-C3	4.04	117.48	109.98
31	L	101	LHG	O7-C7-C8	4.04	119.95	111.55
23	B	610	CLA	O2D-CGD-CBD	4.05	118.53	111.30
23	C	505	CLA	C3B-C4B-NB	4.06	114.45	109.21
34	C	521	LMG	O7-C10-C11	4.06	119.98	111.55
26	A	409	SQD	O9-S-C6	4.06	110.30	106.83
23	C	511	CLA	C3C-C4C-NC	4.07	114.33	110.21
23	a	405	CLA	C3B-C4B-NB	4.13	114.55	109.21
34	c	519	LMG	O7-C10-C11	4.13	120.12	111.55
23	a	405	CLA	C3C-C4C-NC	4.14	114.40	110.21
23	B	616	CLA	O2D-CGD-CBD	4.17	118.76	111.30
23	B	615	CLA	C3C-C4C-NC	4.18	114.44	110.21
23	C	514	CLA	O2D-CGD-CBD	4.22	118.84	111.30
23	D	401	CLA	C3C-C4C-NC	4.23	114.50	110.21
26	a	411	SQD	O8-S-C6	4.24	111.19	106.01
23	A	405	CLA	C3C-C4C-NC	4.25	114.51	110.21
23	b	611	CLA	C3B-C4B-NB	4.25	114.70	109.21
29	d	405	PL9	C10-C9-C11	4.28	122.71	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C3C-C4C-NC	4.29	114.55	110.21
31	D	409	LHG	O7-C7-C8	4.29	120.45	111.55
23	c	511	CLA	O2D-CGD-CBD	4.29	118.97	111.30
37	c	516	DGD	O2G-C1B-C2B	4.29	120.47	111.55
23	A	404	CLA	O2A-CGA-CBA	4.31	124.43	111.90
23	b	615	CLA	O2D-CGD-CBD	4.31	119.00	111.30
23	a	404	CLA	C3C-C4C-NC	4.33	114.59	110.21
26	a	413	SQD	O9-S-C6	4.34	110.54	106.83
34	Z	101	LMG	O7-C10-C11	4.34	120.57	111.55
34	J	101	LMG	O7-C10-C11	4.35	120.58	111.55
23	C	507	CLA	C3C-C4C-NC	4.35	114.62	110.21
23	b	601	CLA	C3C-C4C-NC	4.37	114.64	110.21
23	b	615	CLA	C3C-C4C-NC	4.40	114.67	110.21
31	E	101	LHG	O7-C7-C8	4.40	120.70	111.55
23	B	609	CLA	O2D-CGD-CBD	4.41	119.18	111.30
23	a	406	CLA	C3C-C4C-NC	4.43	114.70	110.21
23	D	401	CLA	O2D-CGD-CBD	4.46	119.26	111.30
26	f	101	SQD	C1-O5-C5	4.47	122.13	113.72
23	c	501	CLA	C3C-C4C-NC	4.47	114.74	110.21
23	D	404	CLA	O2D-CGD-CBD	4.48	119.30	111.30
26	L	102	SQD	O6-C1-C2	4.51	115.59	108.23
23	B	616	CLA	C3C-C4C-NC	4.51	114.78	110.21
23	B	603	CLA	C3C-C4C-NC	4.54	114.81	110.21
23	C	507	CLA	O2D-CGD-CBD	4.54	119.41	111.30
23	d	402	CLA	O2D-CGD-CBD	4.54	119.42	111.30
23	b	609	CLA	C3C-C4C-NC	4.56	114.83	110.21
26	B	621	SQD	O47-C7-C8	4.56	121.03	111.55
23	B	604	CLA	C3C-C4C-NC	4.56	114.83	110.21
23	A	404	CLA	C3C-C4C-NC	4.59	114.86	110.21
23	b	608	CLA	O2D-CGD-CBD	4.60	119.52	111.30
23	C	504	CLA	C3C-C4C-NC	4.61	114.88	110.21
23	b	603	CLA	C3C-C4C-NC	4.61	114.88	110.21
23	c	502	CLA	C3C-C4C-NC	4.63	114.90	110.21
24	D	402	PHO	O2D-CGD-CBD	4.64	119.59	111.30
23	B	602	CLA	C3C-C4C-NC	4.64	114.92	110.21
23	b	605	CLA	C3C-C4C-NC	4.65	114.92	110.21
23	c	503	CLA	C3C-C4C-NC	4.65	114.92	110.21
23	B	608	CLA	O2D-CGD-CBD	4.66	119.63	111.30
26	a	411	SQD	O47-C7-C8	4.66	121.23	111.55
23	b	602	CLA	C3C-C4C-NC	4.67	114.94	110.21
23	c	513	CLA	C3C-C4C-NC	4.67	114.94	110.21
23	c	506	CLA	C3C-C4C-NC	4.67	114.95	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	512	CLA	C3C-C4C-NC	4.68	114.95	110.21
23	b	608	CLA	C3C-C4C-NC	4.69	114.97	110.21
23	C	503	CLA	C3C-C4C-NC	4.70	114.97	110.21
37	C	517	DGD	O2G-C1B-C2B	4.73	121.37	111.55
23	d	403	CLA	C3C-C4C-NC	4.74	115.01	110.21
23	b	606	CLA	C3C-C4C-NC	4.74	115.01	110.21
23	c	507	CLA	C3C-C4C-NC	4.74	115.02	110.21
23	B	606	CLA	O2D-CGD-CBD	4.74	119.78	111.30
23	b	607	CLA	O2D-CGD-CBD	4.75	119.78	111.30
23	c	504	CLA	C3C-C4C-NC	4.75	115.02	110.21
23	B	612	CLA	O2D-CGD-CBD	4.76	119.80	111.30
23	c	511	CLA	C3C-C4C-NC	4.76	115.04	110.21
24	a	408	PHO	C2D-C1D-ND	4.78	116.90	109.82
23	A	405	CLA	O2D-CGD-CBD	4.79	119.86	111.30
23	b	610	CLA	C3C-C4C-NC	4.81	115.08	110.21
23	c	504	CLA	O2D-CGD-CBD	4.81	119.89	111.30
23	B	608	CLA	C3C-C4C-NC	4.82	115.09	110.21
23	a	406	CLA	O2D-CGD-CBD	4.84	119.94	111.30
23	B	614	CLA	C3C-C4C-NC	4.86	115.13	110.21
23	b	612	CLA	C3C-C4C-NC	4.86	115.14	110.21
23	B	607	CLA	C3C-C4C-NC	4.87	115.15	110.21
23	a	409	CLA	O2D-CGD-CBD	4.88	120.02	111.30
23	C	513	CLA	C3C-C4C-NC	4.88	115.16	110.21
23	C	502	CLA	C3C-C4C-NC	4.88	115.16	110.21
23	c	509	CLA	O2D-CGD-CBD	4.89	120.03	111.30
24	a	408	PHO	O2D-CGD-CBD	4.89	120.04	111.30
23	A	407	CLA	C3C-C4C-NC	4.90	115.17	110.21
23	c	512	CLA	C3C-C4C-NC	4.90	115.17	110.21
24	A	406	PHO	C2D-C1D-ND	4.91	117.09	109.82
23	C	505	CLA	C3C-C4C-NC	4.93	115.21	110.21
23	b	614	CLA	C3C-C4C-NC	4.95	115.22	110.21
26	B	621	SQD	O6-C1-C2	4.95	116.31	108.23
23	c	513	CLA	O2D-CGD-CBD	4.97	120.18	111.30
23	c	509	CLA	C3C-C4C-NC	4.98	115.26	110.21
23	d	402	CLA	C3C-C4C-NC	5.00	115.28	110.21
23	b	609	CLA	O2D-CGD-CBD	5.02	120.28	111.30
36	B	629	HTG	C1'-S1-C1	5.03	107.74	100.28
23	b	616	CLA	C3C-C4C-NC	5.05	115.32	110.21
26	A	409	SQD	O47-C7-C8	5.06	122.06	111.55
23	C	514	CLA	C3C-C4C-NC	5.07	115.34	110.21
23	b	611	CLA	C3C-C4C-NC	5.08	115.35	110.21
34	C	501	LMG	O7-C10-C11	5.08	122.11	111.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	409	SQD	O7-S-C6	5.08	111.17	106.83
26	a	411	SQD	O6-C1-C2	5.11	116.56	108.23
23	C	510	CLA	O2D-CGD-CBD	5.11	120.43	111.30
36	b	626	HTG	C1'-S1-C1	5.12	107.87	100.28
23	D	405	CLA	O2D-CGD-CBD	5.12	120.44	111.30
23	b	602	CLA	O2D-CGD-CBD	5.12	120.45	111.30
23	C	513	CLA	O2D-CGD-CBD	5.13	120.46	111.30
23	C	505	CLA	O2D-CGD-CBD	5.16	120.52	111.30
23	D	405	CLA	C2C-C1C-NC	5.16	113.77	110.22
26	L	102	SQD	O47-C7-C8	5.17	122.29	111.55
23	d	403	CLA	O2D-CGD-CBD	5.17	120.55	111.30
26	L	102	SQD	O7-S-C6	5.18	111.26	106.83
23	b	612	CLA	O2D-CGD-CBD	5.20	120.59	111.30
23	C	508	CLA	C3C-C4C-NC	5.21	115.49	110.21
23	C	510	CLA	C3C-C4C-NC	5.21	115.49	110.21
23	B	606	CLA	C3C-C4C-NC	5.24	115.52	110.21
23	B	612	CLA	C3C-C4C-NC	5.26	115.54	110.21
23	D	405	CLA	C3C-C4C-NC	5.29	115.57	110.21
23	C	506	CLA	C3C-C4C-NC	5.29	115.57	110.21
23	B	617	CLA	C3C-C4C-NC	5.31	115.59	110.21
23	b	604	CLA	C3C-C4C-NC	5.31	115.59	110.21
23	B	607	CLA	O2D-CGD-CBD	5.33	120.82	111.30
23	c	502	CLA	O2D-CGD-CBD	5.33	120.83	111.30
26	A	411	SQD	O8-S-C6	5.35	112.54	106.01
23	b	606	CLA	O2D-CGD-CBD	5.37	120.89	111.30
23	b	610	CLA	O2D-CGD-CBD	5.40	120.95	111.30
23	D	401	CLA	C2C-C1C-NC	5.41	113.94	110.22
26	f	101	SQD	O47-C7-C8	5.41	122.78	111.55
23	b	605	CLA	O2D-CGD-CBD	5.41	120.97	111.30
23	c	503	CLA	O2D-CGD-CBD	5.42	120.98	111.30
36	b	625	HTG	C1'-S1-C1	5.43	108.33	100.28
23	b	613	CLA	C3C-C4C-NC	5.43	115.71	110.21
23	D	404	CLA	C3C-C4C-NC	5.45	115.74	110.21
24	a	407	PHO	C2D-C1D-ND	5.46	117.90	109.82
23	C	503	CLA	O2D-CGD-CBD	5.46	121.05	111.30
23	d	403	CLA	C2C-C1C-NC	5.46	113.98	110.22
23	c	505	CLA	O2D-CGD-CBD	5.47	121.07	111.30
24	D	402	PHO	C2D-C1D-ND	5.48	117.93	109.82
23	c	508	CLA	C3C-C4C-NC	5.48	115.76	110.21
24	A	406	PHO	O2D-CGD-CBD	5.48	121.10	111.30
23	b	603	CLA	O2D-CGD-CBD	5.49	121.11	111.30
23	B	609	CLA	C3C-C4C-NC	5.49	115.78	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	O2D-CGD-CBD	5.50	121.13	111.30
23	B	611	CLA	C3C-C4C-NC	5.52	115.81	110.21
26	B	621	SQD	O7-S-C6	5.55	111.57	106.83
26	A	409	SQD	O6-C1-C2	5.55	117.29	108.23
23	C	506	CLA	O2D-CGD-CBD	5.59	121.29	111.30
23	C	511	CLA	O2D-CGD-CBD	5.60	121.31	111.30
23	b	616	CLA	O2D-CGD-CBD	5.62	121.34	111.30
23	c	501	CLA	O2D-CGD-CBD	5.62	121.35	111.30
23	B	610	CLA	C3C-C4C-NC	5.63	115.92	110.21
23	B	602	CLA	O2D-CGD-CBD	5.64	121.37	111.30
38	e	103	HEM	CAD-CBD-CGD	5.65	122.32	112.66
23	C	502	CLA	O2D-CGD-CBD	5.67	121.43	111.30
23	b	607	CLA	C3C-C4C-NC	5.71	115.99	110.21
23	b	601	CLA	O2D-CGD-CBD	5.71	121.50	111.30
36	h	101	HTG	C1'-S1-C1	5.72	108.76	100.28
23	B	611	CLA	O2D-CGD-CBD	5.72	121.52	111.30
23	c	505	CLA	C3C-C4C-NC	5.75	116.04	110.21
36	b	622	HTG	C1'-S1-C1	5.76	108.83	100.28
23	B	617	CLA	C2C-C1C-NC	5.76	114.19	110.22
23	B	604	CLA	O2D-CGD-CBD	5.77	121.61	111.30
36	c	522	HTG	C1'-S1-C1	5.78	108.85	100.28
23	B	613	CLA	C3C-C4C-NC	5.79	116.07	110.21
23	c	508	CLA	O2D-CGD-CBD	5.79	121.65	111.30
23	B	605	CLA	C3C-C4C-NC	5.81	116.09	110.21
23	C	513	CLA	C2C-C1C-NC	5.81	114.22	110.22
23	C	510	CLA	C2C-C1C-NC	5.83	114.23	110.22
29	A	413	PL9	C7-C3-C4	5.83	121.62	116.88
24	a	407	PHO	O2D-CGD-CBD	5.86	121.77	111.30
23	C	514	CLA	C2C-C1C-NC	5.86	114.25	110.22
23	b	609	CLA	C2C-C1C-NC	5.88	114.26	110.22
23	b	614	CLA	O2D-CGD-CBD	5.92	121.87	111.30
26	D	413	SQD	O47-C7-C8	5.94	123.88	111.55
23	B	611	CLA	C2C-C1C-NC	5.98	114.33	110.22
23	c	507	CLA	C2C-C1C-NC	5.99	114.34	110.22
23	B	615	CLA	O2D-CGD-CBD	6.01	122.05	111.30
23	b	611	CLA	O2D-CGD-CBD	6.05	122.11	111.30
23	B	603	CLA	O2D-CGD-CBD	6.06	122.13	111.30
23	B	605	CLA	O2D-CGD-CBD	6.08	122.17	111.30
23	C	509	CLA	C3C-C4C-NC	6.11	116.40	110.21
23	B	606	CLA	C2C-C1C-NC	6.11	114.42	110.22
23	b	614	CLA	C2C-C1C-NC	6.11	114.42	110.22
23	C	508	CLA	O2D-CGD-CBD	6.12	122.24	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406	CLA	C2C-C1C-NC	6.15	114.45	110.22
23	B	613	CLA	O2D-CGD-CBD	6.16	122.31	111.30
23	A	405	CLA	C2C-C1C-NC	6.19	114.48	110.22
23	b	604	CLA	O2D-CGD-CBD	6.19	122.37	111.30
26	f	101	SQD	O7-S-C6	6.23	112.15	106.83
23	A	407	CLA	C2C-C1C-NC	6.23	114.51	110.22
23	c	512	CLA	O2D-CGD-CBD	6.25	122.47	111.30
23	b	608	CLA	C2C-C1C-NC	6.25	114.52	110.22
23	C	512	CLA	C2C-C1C-NC	6.27	114.53	110.22
29	a	415	PL9	C7-C3-C4	6.31	122.01	116.88
23	B	604	CLA	C2C-C1C-NC	6.33	114.58	110.22
23	a	409	CLA	C2C-C1C-NC	6.35	114.59	110.22
23	c	511	CLA	C2C-C1C-NC	6.37	114.60	110.22
23	B	602	CLA	C2C-C1C-NC	6.39	114.61	110.22
24	a	408	PHO	CMD-C2D-C1D	6.41	135.03	125.04
23	b	612	CLA	C2C-C1C-NC	6.42	114.64	110.22
23	b	606	CLA	C2C-C1C-NC	6.43	114.65	110.22
23	B	617	CLA	O2D-CGD-CBD	6.46	122.85	111.30
23	B	607	CLA	C2C-C1C-NC	6.46	114.67	110.22
23	b	613	CLA	C2C-C1C-NC	6.48	114.68	110.22
23	b	601	CLA	C2C-C1C-NC	6.50	114.69	110.22
23	b	602	CLA	C2C-C1C-NC	6.51	114.70	110.22
38	E	103	HEM	CAD-CBD-CGD	6.55	123.86	112.66
23	C	503	CLA	C2C-C1C-NC	6.58	114.75	110.22
23	B	612	CLA	C2C-C1C-NC	6.59	114.75	110.22
23	B	605	CLA	C2C-C1C-NC	6.59	114.75	110.22
23	b	610	CLA	C2C-C1C-NC	6.60	114.76	110.22
23	C	508	CLA	C2C-C1C-NC	6.61	114.77	110.22
23	c	512	CLA	C2C-C1C-NC	6.62	114.77	110.22
23	B	609	CLA	C2C-C1C-NC	6.62	114.78	110.22
23	c	513	CLA	C2C-C1C-NC	6.64	114.79	110.22
23	c	510	CLA	C2C-C1C-NC	6.64	114.79	110.22
23	b	604	CLA	C2C-C1C-NC	6.65	114.80	110.22
23	c	505	CLA	C2C-C1C-NC	6.67	114.81	110.22
23	B	613	CLA	C2C-C1C-NC	6.67	114.81	110.22
23	C	507	CLA	C2C-C1C-NC	6.69	114.82	110.22
23	B	610	CLA	C2C-C1C-NC	6.70	114.83	110.22
23	c	507	CLA	O2D-CGD-CBD	6.70	123.27	111.30
23	b	603	CLA	C2C-C1C-NC	6.75	114.86	110.22
36	C	523	HTG	C1'-S1-C1	6.76	110.31	100.28
36	B	630	HTG	C1'-S1-C1	6.77	110.32	100.28
24	D	402	PHO	CMD-C2D-C1D	6.81	135.66	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C2C-C1C-NC	6.84	114.92	110.22
24	a	407	PHO	CMD-C2D-C1D	6.84	135.70	125.04
23	c	509	CLA	C2C-C1C-NC	6.86	114.94	110.22
23	c	501	CLA	C2C-C1C-NC	6.88	114.95	110.22
23	B	616	CLA	C2C-C1C-NC	6.93	114.98	110.22
23	A	404	CLA	C2C-C1C-NC	6.94	114.99	110.22
23	B	603	CLA	C2C-C1C-NC	7.00	115.03	110.22
23	c	502	CLA	C2C-C1C-NC	7.02	115.05	110.22
23	a	404	CLA	C2C-C1C-NC	7.04	115.06	110.22
23	C	504	CLA	C2C-C1C-NC	7.10	115.10	110.22
23	C	506	CLA	C2C-C1C-NC	7.11	115.11	110.22
23	b	605	CLA	C2C-C1C-NC	7.18	115.16	110.22
36	D	412	HTG	C1'-S1-C1	7.21	110.98	100.28
23	C	502	CLA	C2C-C1C-NC	7.23	115.19	110.22
23	c	506	CLA	C2C-C1C-NC	7.24	115.20	110.22
36	b	621	HTG	C1'-S1-C1	7.28	111.08	100.28
23	b	616	CLA	C2C-C1C-NC	7.28	115.23	110.22
36	c	521	HTG	C1'-S1-C1	7.34	111.16	100.28
23	c	503	CLA	C2C-C1C-NC	7.36	115.28	110.22
23	c	508	CLA	C2C-C1C-NC	7.37	115.29	110.22
23	C	509	CLA	C2C-C1C-NC	7.40	115.31	110.22
23	B	614	CLA	C2C-C1C-NC	7.48	115.36	110.22
23	B	615	CLA	C2C-C1C-NC	7.49	115.37	110.22
36	b	623	HTG	C1'-S1-C1	7.54	111.47	100.28
23	c	504	CLA	C2C-C1C-NC	7.61	115.46	110.22
23	C	511	CLA	C2C-C1C-NC	7.68	115.50	110.22
36	B	626	HTG	C1'-S1-C1	7.68	111.68	100.28
23	D	404	CLA	C2C-C1C-NC	7.71	115.52	110.22
23	b	607	CLA	C2C-C1C-NC	7.72	115.53	110.22
36	B	625	HTG	C1'-S1-C1	7.76	111.79	100.28
23	b	615	CLA	C2C-C1C-NC	7.86	115.63	110.22
23	a	405	CLA	C2C-C1C-NC	7.92	115.67	110.22
24	A	406	PHO	CMD-C2D-C1D	7.94	137.41	125.04
23	d	402	CLA	C2C-C1C-NC	8.13	115.81	110.22
23	C	505	CLA	C2C-C1C-NC	8.23	115.88	110.22
23	b	611	CLA	C2C-C1C-NC	8.73	116.23	110.22

All (194) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	c	502	CLA	NC
23	c	502	CLA	ND

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Mol	Chain	Res	Type	Atom
23	c	502	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	D	404	CLA	ND
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	a	404	CLA	NC
23	a	404	CLA	ND
23	a	404	CLA	NA

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Mol	Chain	Res	Type	Atom
23	D	401	CLA	NC
23	D	401	CLA	ND
23	D	401	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	c	509	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	d	402	CLA	ND
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	503	CLA	NA
23	B	609	CLA	NC
23	B	609	CLA	ND
23	B	609	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	ND
23	A	407	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	C	514	CLA	NC
23	C	514	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	c	505	CLA	ND
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	b	602	CLA	NC
23	b	602	CLA	ND
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA

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Mol	Chain	Res	Type	Atom
23	b	612	CLA	NC
23	b	612	CLA	ND
23	b	612	CLA	NA
23	c	501	CLA	NC
23	c	501	CLA	ND
23	c	501	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	B	616	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	C	512	CLA	NC

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Mol	Chain	Res	Type	Atom
23	C	512	CLA	ND
23	C	512	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	b	603	CLA	NC
23	b	603	CLA	ND
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	609	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	NA
23	b	616	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA

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Mol	Chain	Res	Type	Atom
23	D	405	CLA	NC
23	D	405	CLA	ND
23	D	405	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	ND
23	a	405	CLA	NA
23	B	617	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	b	601	CLA	ND
23	b	601	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	C	506	CLA	ND
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	C	522	LMT	C1-O1'-C1'-O5'
34	C	501	LMG	C8-O7-C10-C11
34	Z	101	LMG	C8-O7-C10-O9
34	Z	101	LMG	C8-O7-C10-C11
26	D	413	SQD	C45-O47-C7-O49
26	D	413	SQD	C45-O47-C7-C8
26	f	101	SQD	C45-O47-C7-O49
26	f	101	SQD	C45-O47-C7-C8

There are no ring outliers.

86 monomers are involved in 334 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	404	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	405	CLA	7	0
24	A	406	PHO	2	0
23	A	407	CLA	5	0
25	A	408	BCR	2	0
26	A	409	SQD	2	0
26	A	411	SQD	3	0
29	A	413	PL9	5	0
31	A	415	LHG	4	0
23	B	602	CLA	6	0
23	B	603	CLA	6	0
23	B	604	CLA	8	0
23	B	605	CLA	12	0
23	B	606	CLA	14	0
23	B	607	CLA	5	0
23	B	608	CLA	7	0
23	B	609	CLA	5	0
23	B	610	CLA	6	0
23	B	611	CLA	5	0
23	B	612	CLA	8	0
23	B	613	CLA	12	0
23	B	614	CLA	6	0
23	B	615	CLA	15	0
23	B	616	CLA	7	0
23	B	617	CLA	5	0
25	B	618	BCR	6	0
25	B	619	BCR	4	0
25	B	620	BCR	2	0
26	B	621	SQD	2	0
34	B	622	LMG	2	0
35	B	623	LMT	3	0
36	B	624	HTG	3	0
36	B	625	HTG	2	0
36	B	626	HTG	1	0
27	B	627	GOL	1	0
27	B	628	GOL	3	0
36	B	629	HTG	1	0
35	B	632	LMT	1	0
35	B	633	LMT	3	0
35	B	634	LMT	2	0
34	C	501	LMG	3	0
23	C	502	CLA	11	0
23	C	503	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	504	CLA	6	0
23	C	505	CLA	5	0
23	C	506	CLA	9	0
23	C	507	CLA	17	0
23	C	508	CLA	12	0
23	C	509	CLA	9	0
23	C	510	CLA	8	0
23	C	511	CLA	9	0
23	C	512	CLA	13	0
23	C	513	CLA	7	0
23	C	514	CLA	3	0
25	C	515	BCR	2	0
25	C	516	BCR	4	0
37	C	517	DGD	6	0
37	C	518	DGD	3	0
37	C	519	DGD	1	0
34	C	520	LMG	3	0
34	C	521	LMG	1	0
35	C	522	LMT	1	0
36	C	523	HTG	1	0
36	C	524	HTG	1	0
25	C	527	BCR	1	0
23	D	401	CLA	5	0
24	D	402	PHO	5	0
23	D	404	CLA	4	0
23	D	405	CLA	1	0
25	D	406	BCR	2	0
29	D	407	PL9	2	0
31	D	408	LHG	7	0
31	D	409	LHG	4	0
36	D	412	HTG	1	0
26	D	413	SQD	2	0
31	E	101	LHG	2	0
35	E	102	LMT	1	0
38	E	103	HEM	6	0
25	H	101	BCR	5	0
34	J	101	LMG	4	0
26	L	102	SQD	4	0
35	M	101	LMT	1	0
35	M	103	LMT	3	0
25	T	101	BCR	6	0
25	Y	101	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	Z	101	LMG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	0.06	10 (2%) 51 53	22, 33, 58, 97	0
1	a	334/344 (97%)	0.21	15 (4%) 34 36	24, 36, 65, 113	0
2	B	504/505 (99%)	0.32	59 (11%) 5 4	24, 38, 68, 118	0
2	b	504/505 (99%)	0.48	72 (14%) 3 2	25, 40, 77, 122	0
3	C	451/455 (99%)	0.65	71 (15%) 2 2	27, 48, 70, 108	0
3	c	455/455 (100%)	0.46	62 (13%) 3 3	32, 52, 72, 118	0
4	D	342/342 (100%)	0.09	18 (5%) 27 28	22, 35, 58, 113	0
4	d	341/342 (99%)	0.29	27 (7%) 13 13	24, 39, 59, 124	0
5	E	81/84 (96%)	0.35	6 (7%) 15 15	40, 59, 90, 125	0
5	e	79/84 (94%)	0.96	17 (21%) 1 1	45, 62, 100, 125	0
6	F	34/44 (77%)	-0.08	1 (2%) 52 55	41, 51, 81, 96	0
6	f	31/44 (70%)	-0.07	4 (12%) 4 3	48, 53, 84, 128	0
7	H	64/65 (98%)	0.37	7 (10%) 6 6	37, 51, 72, 104	0
7	h	65/65 (100%)	1.15	19 (29%) 1 0	40, 54, 79, 152	0
8	I	37/38 (97%)	0.44	7 (18%) 1 1	36, 48, 98, 129	0
8	i	37/38 (97%)	0.24	3 (8%) 13 12	38, 49, 107, 137	0
9	J	38/39 (97%)	0.29	6 (15%) 2 2	37, 55, 113, 156	0
9	j	39/39 (100%)	0.88	10 (25%) 1 0	46, 56, 109, 137	0
10	K	37/37 (100%)	0.14	3 (8%) 13 12	49, 58, 81, 98	0
10	k	37/37 (100%)	0.41	3 (8%) 13 12	52, 60, 82, 99	0
11	L	36/37 (97%)	0.52	5 (13%) 3 3	23, 30, 98, 143	0
11	l	36/37 (97%)	0.21	4 (11%) 6 5	24, 31, 97, 143	0
12	M	32/36 (88%)	-0.19	1 (3%) 49 52	24, 31, 53, 125	0
12	m	33/36 (91%)	-0.28	3 (9%) 10 10	24, 32, 66, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.36	31 (12%) 4 3	22, 50, 103, 163	0
13	o	243/244 (99%)	0.57	44 (18%) 1 1	26, 50, 108, 151	0
14	T	29/32 (90%)	0.30	1 (3%) 46 48	26, 31, 68, 97	0
14	t	29/32 (90%)	-0.02	0 100 100	26, 31, 69, 98	0
15	U	96/104 (92%)	0.57	14 (14%) 3 2	32, 44, 72, 86	0
15	u	97/104 (93%)	-0.08	4 (4%) 38 40	37, 47, 72, 105	0
16	V	137/137 (100%)	0.18	5 (3%) 43 45	30, 46, 75, 111	0
16	v	137/137 (100%)	0.47	20 (14%) 3 2	37, 54, 79, 112	0
17	X	38/40 (95%)	0.41	3 (7%) 13 13	49, 58, 80, 121	0
17	x	38/40 (95%)	1.09	9 (23%) 1 0	50, 60, 84, 123	0
18	Y	29/30 (96%)	1.73	13 (44%) 0 0	60, 76, 112, 120	0
18	y	29/30 (96%)	1.06	7 (24%) 1 0	63, 76, 107, 118	0
19	Z	62/62 (100%)	1.46	23 (37%) 0 0	57, 77, 127, 161	0
19	z	62/62 (100%)	1.60	18 (29%) 1 0	61, 79, 127, 161	0
20	R	34/34 (100%)	6.41	34 (100%) 0 0	92, 116, 145, 149	0
All	All	5284/5384 (98%)	0.44	659 (12%) 4 4	22, 45, 88, 163	0

All (659) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	11.0
20	R	20	VAL	10.2
2	b	495	PHE	9.4
20	R	35	LEU	9.0
20	R	14	LEU	8.3
20	R	6	LEU	8.2
1	A	11	ALA	8.1
20	R	8	VAL	8.1
20	R	19	ALA	8.1
20	R	15	ALA	8.0
9	j	3	GLU	7.9
20	R	23	ILE	7.9
17	x	38	GLN	7.8
20	R	5	VAL	7.6
9	j	2	SER	7.2
20	R	3	TRP	7.1
20	R	4	ARG	6.8

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Mol	Chain	Res	Type	RSRZ
20	R	7	VAL	6.8
20	R	31	VAL	6.8
8	I	38	GLU	6.7
2	b	486	LEU	6.6
7	h	66	GLY	6.5
19	z	4	LEU	6.4
20	R	24	LEU	6.4
2	b	494	GLY	6.4
3	C	437	PHE	6.4
2	b	218	LEU	6.2
3	C	253	LEU	6.2
1	A	13	LEU	6.2
20	R	12	VAL	6.2
13	o	27	ARG	6.1
2	b	488	PRO	6.0
2	b	493	TRP	5.9
20	R	13	LEU	5.9
9	J	5	GLY	5.9
20	R	34	LEU	5.9
19	Z	32	ASP	5.9
3	C	181	PHE	5.9
20	R	16	ALA	5.9
2	b	487	SER	5.8
2	B	496	TYR	5.8
3	C	276	LEU	5.8
20	R	27	ALA	5.7
5	E	84	LYS	5.7
8	i	37	LEU	5.7
20	R	17	GLY	5.6
20	R	10	LEU	5.6
19	Z	33	TRP	5.6
13	o	22	LEU	5.6
18	Y	18	VAL	5.5
20	R	26	TYR	5.5
4	D	238	THR	5.4
20	R	11	PRO	5.4
7	h	6	TRP	5.4
3	C	60	ILE	5.4
8	I	37	LEU	5.4
20	R	21	ARG	5.4
19	z	60	PHE	5.4
3	c	143	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
20	R	33	LYS	5.4
19	z	7	LEU	5.4
20	R	2	ASP	5.3
17	x	33	GLN	5.3
18	Y	19	ILE	5.3
7	h	65	LEU	5.2
19	z	61	VAL	5.2
19	z	1	MET	5.2
20	R	32	GLN	5.2
19	z	3	ILE	5.2
3	C	433	LEU	5.2
19	z	5	PHE	5.1
18	y	19	ILE	5.1
9	j	5	GLY	5.1
19	Z	31	GLN	5.0
20	R	22	ASN	4.9
19	z	2	THR	4.9
3	c	60	ILE	4.9
11	l	3	PRO	4.8
17	x	37	VAL	4.8
17	X	2	THR	4.8
4	d	12	ARG	4.8
3	C	279	LEU	4.8
19	z	57	LEU	4.8
2	B	495	PHE	4.8
3	c	426	LEU	4.8
13	o	25	THR	4.7
20	R	28	VAL	4.7
2	b	249	ALA	4.7
3	C	143	TYR	4.6
2	b	161	LEU	4.6
2	B	494	GLY	4.6
1	A	12	ASN	4.6
13	o	243	ILE	4.6
17	x	2	THR	4.6
2	b	504	THR	4.6
2	b	496	TYR	4.6
4	d	17	ILE	4.6
9	j	7	ILE	4.6
2	b	484	PRO	4.6
19	Z	30	PRO	4.6
2	B	461	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
3	C	281	MET	4.5
2	b	491	VAL	4.5
13	o	36	GLN	4.5
17	x	34	ILE	4.5
17	x	3	ILE	4.4
3	C	23	ALA	4.4
13	o	142	PHE	4.4
15	U	58	VAL	4.4
3	c	200	THR	4.4
19	Z	34	ASP	4.4
2	b	497	GLN	4.4
13	o	38	TYR	4.4
3	C	438	LEU	4.4
13	O	25	THR	4.3
2	b	489	GLU	4.3
11	L	2	GLU	4.3
3	C	280	SER	4.3
2	b	503	THR	4.3
2	B	253	ALA	4.3
13	o	32	ILE	4.3
3	C	282	MET	4.3
10	k	18	PHE	4.3
3	c	279	LEU	4.3
3	C	283	GLY	4.2
11	l	2	GLU	4.2
19	z	56	VAL	4.2
2	b	245	VAL	4.2
3	c	63	TRP	4.2
20	R	30	GLN	4.2
2	B	251	VAL	4.1
2	b	502	VAL	4.1
18	Y	21	GLN	4.1
16	v	21	LEU	4.1
3	C	61	VAL	4.1
1	A	15	GLU	4.1
2	b	492	GLU	4.1
2	b	246	PHE	4.1
2	B	488	PRO	4.0
13	o	35	SER	4.0
15	U	73	GLN	4.0
2	B	458	PHE	4.0
3	C	204	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	C	155	ASN	4.0
3	c	430	HIS	4.0
5	E	15	THR	4.0
17	x	36	LYS	4.0
2	b	248	ALA	3.9
3	C	198	VAL	3.9
3	c	198	VAL	3.9
3	C	436	PHE	3.9
3	c	201	ASN	3.9
2	b	499	VAL	3.9
4	d	154	VAL	3.9
18	Y	43	ARG	3.9
20	R	9	LEU	3.9
2	B	462	PHE	3.8
15	U	104	LYS	3.8
3	C	286	ALA	3.8
7	h	22	ALA	3.8
13	O	27	ARG	3.8
13	o	87	VAL	3.8
9	j	1	MET	3.8
3	c	140	LEU	3.8
9	j	9	LEU	3.8
16	v	107	LEU	3.8
20	R	25	PRO	3.8
3	C	430	HIS	3.8
3	C	285	ILE	3.8
11	L	7	ARG	3.8
3	c	433	LEU	3.7
15	U	70	ARG	3.7
3	c	191	PRO	3.7
13	o	246	ALA	3.7
3	c	87	ILE	3.7
9	J	7	ILE	3.7
2	b	296	ALA	3.7
19	Z	35	ARG	3.7
3	C	429	SER	3.7
16	v	10	VAL	3.7
8	I	36	ASP	3.7
10	k	17	ILE	3.6
3	C	262	ARG	3.6
5	E	17	VAL	3.6
13	o	133	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	a	11	ALA	3.6
2	b	462	PHE	3.6
3	C	277	GLY	3.6
2	b	498	LYS	3.6
15	U	62	LEU	3.6
3	c	203	THR	3.6
2	b	250	PHE	3.6
13	O	26	ALA	3.6
3	C	435	PHE	3.6
2	B	489	GLU	3.6
13	o	134	THR	3.6
2	B	252	VAL	3.6
3	C	147	PHE	3.5
3	c	202	PRO	3.5
3	C	59	LEU	3.5
5	E	83	LEU	3.5
5	e	20	TRP	3.5
2	b	295	GLY	3.5
2	B	505	ARG	3.5
2	b	252	VAL	3.5
7	h	23	PRO	3.5
3	c	146	PHE	3.5
20	R	29	LYS	3.5
3	C	148	GLY	3.5
3	C	434	ALA	3.5
16	v	4	THR	3.5
2	b	251	VAL	3.5
2	b	294	SER	3.5
13	O	135	SER	3.5
3	C	278	ALA	3.5
13	o	26	ALA	3.5
19	Z	3	ILE	3.5
15	U	79	LEU	3.5
3	C	284	PHE	3.5
5	e	79	PHE	3.5
2	b	247	PHE	3.4
13	o	37	THR	3.4
3	C	440	GLY	3.4
3	C	432	VAL	3.4
19	z	62	VAL	3.4
13	o	211	ILE	3.4
19	Z	29	SER	3.4

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Mol	Chain	Res	Type	RSRZ
13	O	24	ASP	3.4
4	d	148	ALA	3.4
17	x	39	ARG	3.4
3	C	439	VAL	3.4
2	b	217	ILE	3.4
3	C	252	ILE	3.4
16	v	19	ILE	3.4
3	C	145	SER	3.4
16	v	17	LYS	3.4
3	c	195	ASP	3.4
2	b	298	LEU	3.4
2	b	485	GLU	3.4
3	c	283	GLY	3.4
6	f	42	PHE	3.4
12	m	33	GLN	3.4
13	o	4	THR	3.4
3	C	431	PHE	3.3
4	d	157	PHE	3.3
7	H	6	TRP	3.3
13	o	33	ASP	3.3
13	o	204	VAL	3.3
2	B	248	ALA	3.3
2	B	249	ALA	3.3
2	b	288	VAL	3.3
17	X	3	ILE	3.3
3	c	282	MET	3.3
2	B	502	VAL	3.3
4	D	12	ARG	3.3
2	b	244	ALA	3.3
18	Y	25	ILE	3.3
3	c	155	ASN	3.3
19	Z	36	SER	3.3
2	b	293	ALA	3.3
13	o	245	PRO	3.2
19	z	9	LEU	3.2
2	B	296	ALA	3.2
2	B	454	ALA	3.2
13	o	136	ILE	3.2
18	y	37	PHE	3.2
4	d	152	VAL	3.2
3	C	63	TRP	3.2
3	c	427	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
4	d	153	PHE	3.2
13	o	24	ASP	3.2
19	z	59	PHE	3.2
1	A	16	ARG	3.2
7	h	58	VAL	3.2
2	B	504	THR	3.2
19	Z	39	LEU	3.2
9	j	4	GLY	3.2
18	Y	46	LEU	3.2
3	c	20	SER	3.2
18	Y	20	ALA	3.1
3	C	146	PHE	3.1
4	d	155	SER	3.1
2	B	459	ALA	3.1
12	m	34	LYS	3.1
3	c	437	PHE	3.1
13	O	56	PRO	3.1
18	y	41	VAL	3.1
8	I	34	ARG	3.1
1	a	13	LEU	3.1
3	c	59	LEU	3.1
2	b	219	VAL	3.1
4	D	11	GLU	3.1
7	H	2	ALA	3.1
13	O	62	GLU	3.1
3	C	25	ASN	3.1
2	B	457	VAL	3.1
3	C	275	SER	3.1
13	o	59	LYS	3.1
4	d	159	ILE	3.1
4	d	13	GLY	3.1
5	E	11	SER	3.1
5	e	25	ILE	3.0
17	X	34	ILE	3.0
5	e	72	ALA	3.0
13	o	85	LEU	3.0
16	V	135	VAL	3.0
9	J	4	GLY	3.0
2	B	451	PHE	3.0
4	d	149	PRO	3.0
2	b	162	PHE	3.0
3	c	192	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
13	O	28	GLY	3.0
13	O	22	LEU	3.0
13	O	133	VAL	3.0
2	B	460	LEU	3.0
2	b	126	PRO	3.0
5	e	59	GLU	3.0
3	c	429	SER	3.0
19	Z	27	TYR	3.0
3	C	57	ALA	3.0
3	c	260	ALA	3.0
4	d	151	ALA	3.0
13	O	93	LEU	3.0
11	L	10	VAL	2.9
2	B	290	ALA	2.9
2	b	292	LEU	2.9
3	c	190	ALA	2.9
13	o	5	LEU	2.9
15	U	103	TYR	2.9
15	U	59	GLU	2.9
2	b	291	SER	2.9
3	c	193	GLY	2.9
3	C	180	MET	2.9
1	a	224	ILE	2.9
8	i	38	GLU	2.9
2	B	161	LEU	2.9
2	b	290	ALA	2.9
7	h	10	ILE	2.9
15	U	74	ILE	2.9
2	B	242	ILE	2.9
2	b	458	PHE	2.9
2	b	483	ASP	2.9
19	z	42	LEU	2.9
1	a	265	PHE	2.9
2	b	238	LEU	2.9
3	C	200	THR	2.9
3	C	254	THR	2.9
13	O	5	LEU	2.9
13	O	29	ALA	2.9
3	C	135	ARG	2.8
7	h	12	ARG	2.8
16	v	5	PRO	2.8
5	e	57	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	487	SER	2.8
4	d	147	SER	2.8
3	c	196	VAL	2.8
13	o	60	ARG	2.8
2	b	459	ALA	2.8
7	h	7	LEU	2.8
13	o	93	LEU	2.8
18	Y	45	ASN	2.8
3	c	147	PHE	2.8
4	d	150	ILE	2.8
19	Z	26	ALA	2.8
16	v	16	GLY	2.8
3	c	280	SER	2.8
3	C	199	ILE	2.8
4	D	150	ILE	2.8
16	v	26	TYR	2.8
3	c	64	ALA	2.8
5	e	83	LEU	2.8
13	O	91	GLY	2.8
15	U	99	ASN	2.8
13	O	139	SER	2.8
2	b	127	ARG	2.8
11	L	9	PRO	2.8
9	J	3	GLU	2.8
16	v	22	THR	2.8
4	D	122	LEU	2.8
5	e	84	LYS	2.7
13	o	57	LYS	2.7
19	z	46	LEU	2.7
2	B	293	ALA	2.7
2	B	297	THR	2.7
2	b	242	ILE	2.7
2	b	412	THR	2.7
3	c	257	PHE	2.7
7	H	46	LEU	2.7
18	Y	38	LEU	2.7
4	d	123	ILE	2.7
5	e	36	LEU	2.7
19	Z	7	LEU	2.7
18	Y	42	ARG	2.7
13	O	130	GLN	2.7
3	c	88	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
10	K	29	PRO	2.7
19	z	38	GLN	2.7
13	O	204	VAL	2.7
10	K	14	ALA	2.7
6	f	43	ILE	2.7
2	B	294	SER	2.6
3	c	61	VAL	2.6
2	B	85	GLY	2.6
3	C	201	ASN	2.6
19	Z	60	PHE	2.6
2	B	490	GLN	2.6
1	A	14	TRP	2.6
1	a	264	SER	2.6
7	h	64	ALA	2.6
2	B	250	PHE	2.6
2	b	123	PHE	2.6
3	C	257	PHE	2.6
3	c	199	ILE	2.6
7	h	13	PRO	2.6
13	O	23	ASP	2.6
13	o	207	ARG	2.6
13	o	58	ASN	2.6
19	Z	56	VAL	2.6
1	a	15	GLU	2.6
11	L	8	GLN	2.6
13	o	83	GLY	2.6
12	m	31	SER	2.6
13	O	132	ASN	2.6
2	b	457	VAL	2.6
4	d	14	TRP	2.6
16	V	12	LEU	2.6
2	B	247	PHE	2.6
2	b	482	ILE	2.6
2	b	121	GLU	2.6
7	h	8	GLY	2.6
1	a	225	ARG	2.6
3	c	255	THR	2.6
3	c	284	PHE	2.6
4	D	159	ILE	2.6
15	u	103	TYR	2.6
4	d	156	VAL	2.6
2	B	284	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	182	PHE	2.6
3	c	22	PHE	2.6
10	K	28	ILE	2.6
2	B	241	SER	2.6
3	C	56	HIS	2.6
13	O	207	ARG	2.6
1	a	262	TYR	2.6
3	C	340	TYR	2.6
16	V	136	TYR	2.6
4	D	148	ALA	2.5
2	B	126	PRO	2.5
3	c	265	ILE	2.5
3	c	317	PHE	2.5
18	y	43	ARG	2.5
4	d	126	MET	2.5
2	b	172	TYR	2.5
4	D	351	ALA	2.5
2	B	245	VAL	2.5
13	o	199	LEU	2.5
16	v	8	LEU	2.5
16	v	25	GLN	2.5
3	C	272	LEU	2.5
16	v	7	VAL	2.5
3	c	56	HIS	2.5
19	Z	59	PHE	2.5
19	z	6	GLN	2.5
2	B	350	GLU	2.5
3	C	287	THR	2.5
15	U	101	GLY	2.5
4	d	146	PHE	2.5
15	U	76	ARG	2.5
2	B	304	ALA	2.5
5	e	21	VAL	2.5
1	a	285	PHE	2.5
2	B	463	PHE	2.5
7	H	42	LEU	2.5
10	k	38	VAL	2.5
19	Z	53	VAL	2.5
2	b	505	ARG	2.5
3	c	144	SER	2.5
7	h	3	ARG	2.5
14	T	29	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
7	h	9	ASP	2.5
1	A	19	ASN	2.5
3	C	55	ALA	2.5
3	C	255	THR	2.5
13	O	4	THR	2.5
9	J	6	ARG	2.4
2	B	452	THR	2.4
4	d	119	ALA	2.4
13	o	208	THR	2.4
4	D	147	SER	2.4
3	c	259	TRP	2.4
8	I	6	ILE	2.4
1	a	340	PRO	2.4
2	b	414	PRO	2.4
3	C	154	LYS	2.4
1	a	14	TRP	2.4
2	b	223	GLN	2.4
16	V	50	PRO	2.4
2	b	301	ALA	2.4
19	Z	62	VAL	2.4
2	b	490	GLN	2.4
4	D	123	ILE	2.4
8	I	26	GLY	2.4
19	z	33	TRP	2.4
8	I	29	ALA	2.4
5	e	14	ILE	2.4
2	b	501	ASP	2.4
3	C	288	CYS	2.4
3	c	425	TRP	2.4
13	o	39	ARG	2.4
5	e	42	LEU	2.4
2	B	219	VAL	2.4
3	C	196	VAL	2.4
3	C	26	ARG	2.4
2	B	162	PHE	2.3
9	j	6	ARG	2.3
5	e	39	SER	2.3
13	o	86	LYS	2.3
3	c	58	GLY	2.3
4	d	158	LEU	2.3
7	H	43	LEU	2.3
18	Y	22	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
18	y	22	LEU	2.3
4	D	154	VAL	2.3
13	O	87	VAL	2.3
1	A	152	ALA	2.3
3	C	442	LEU	2.3
13	O	15	LEU	2.3
2	B	501	ASP	2.3
5	e	15	THR	2.3
6	F	13	TYR	2.3
3	C	58	GLY	2.3
3	C	183	GLY	2.3
2	B	214	LEU	2.3
4	d	37	LEU	2.3
3	C	459	ILE	2.3
13	o	40	ILE	2.3
4	D	151	ALA	2.3
2	B	503	THR	2.3
13	o	209	GLY	2.3
16	V	132	GLY	2.3
2	B	298	LEU	2.3
9	J	9	LEU	2.3
2	B	455	HIS	2.3
3	c	256	PRO	2.3
3	c	97	TRP	2.3
4	D	280	TRP	2.3
6	f	15	ILE	2.3
2	B	411	PHE	2.3
2	b	243	ALA	2.3
13	O	63	ALA	2.3
13	O	138	THR	2.3
19	Z	38	GLN	2.3
3	C	426	LEU	2.3
3	c	204	LEU	2.3
4	d	127	LEU	2.3
7	h	42	LEU	2.3
16	v	95	LEU	2.3
3	c	184	GLY	2.3
2	b	289	GLN	2.3
7	h	16	SER	2.3
2	B	180	PRO	2.2
4	D	149	PRO	2.2
2	b	241	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	64	ALA	2.2
16	v	1	ALA	2.2
4	d	279	LEU	2.2
7	h	20	LYS	2.2
11	l	8	GLN	2.2
1	A	249	VAL	2.2
2	b	463	PHE	2.2
6	f	16	PHE	2.2
3	C	266	TRP	2.2
13	O	131	PRO	2.2
3	c	183	GLY	2.2
5	e	81	GLU	2.2
3	c	67	MET	2.2
2	b	155	ALA	2.2
3	c	55	ALA	2.2
13	O	155	ASN	2.2
16	v	110	LYS	2.2
1	a	330	VAL	2.2
7	H	10	ILE	2.2
18	y	20	ALA	2.2
2	B	464	PHE	2.2
13	o	140	THR	2.2
5	e	7	GLU	2.2
16	v	6	GLU	2.2
7	H	8	GLY	2.2
19	Z	28	ALA	2.2
4	D	273	PHE	2.2
15	u	101	GLY	2.2
13	o	30	TYR	2.2
12	M	33	GLN	2.2
9	j	14	THR	2.2
1	A	339	PHE	2.2
2	B	286	ARG	2.2
7	h	55	LEU	2.2
2	B	456	ALA	2.1
3	c	24	THR	2.1
16	v	9	THR	2.1
3	c	230	LEU	2.1
4	d	122	LEU	2.1
5	E	74	GLN	2.1
4	D	350	ASN	2.1
3	c	187	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	491	VAL	2.1
2	b	456	ALA	2.1
13	O	30	TYR	2.1
16	v	135	VAL	2.1
1	a	297	LEU	2.1
18	y	38	LEU	2.1
2	b	466	HIS	2.1
2	b	224	ARG	2.1
19	Z	4	LEU	2.1
3	C	339	LYS	2.1
13	o	34	SER	2.1
3	c	194	GLY	2.1
15	U	94	GLY	2.1
5	e	82	GLN	2.1
19	Z	1	MET	2.1
7	h	5	THR	2.1
1	a	120	LEU	2.1
19	Z	57	LEU	2.1
4	D	343	GLU	2.1
3	c	66	ALA	2.1
3	c	428	THR	2.1
4	D	277	THR	2.1
13	o	23	ASP	2.1
13	O	36	GLN	2.1
2	B	256	MET	2.0
16	v	18	THR	2.0
2	B	218	LEU	2.0
2	b	413	ASP	2.0
3	c	281	MET	2.0
9	j	8	PRO	2.0
2	B	288	VAL	2.0
8	i	2	GLU	2.0
2	b	239	SER	2.0
3	C	144	SER	2.0
13	O	196	GLN	2.0
2	B	254	GLY	2.0
3	C	100	GLY	2.0
13	o	91	GLY	2.0
15	u	66	GLY	2.0
1	a	339	PHE	2.0
2	B	179	GLN	2.0
3	c	286	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
4	d	40	CYS	2.0
13	O	61	GLN	2.0
13	o	241	ALA	2.0
18	Y	40	ALA	2.0
18	Y	23	THR	2.0
2	b	465	GLY	2.0
13	o	226	GLY	2.0
15	U	57	SER	2.0
15	u	102	LEU	2.0
17	x	7	LEU	2.0
4	d	16	ASP	2.0
11	l	9	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
8	FME	i	1	10/11	0.96	0.10	-	38,50,63,74	0
12	FME	M	1	10/11	0.97	0.16	-	33,41,72,72	0
12	FME	m	1	10/11	0.96	0.11	-	26,43,69,74	0
14	FME	T	1	10/11	0.98	0.09	-	19,37,45,52	0
8	FME	I	1	10/11	0.97	0.17	-	29,49,53,54	0
14	FME	t	1	10/11	0.97	0.10	-	22,34,47,66	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	GOL	d	401	6/6	0.76	0.68	29.98	36,51,76,77	0
30	UNL	i	101	40/-	0.74	0.38	26.06	56,91,147,151	0
36	HTG	b	622	19/19	0.76	0.83	16.83	77,105,127,134	0
30	UNL	j	102	10/-	0.73	0.31	12.64	57,81,94,94	0
30	UNL	K	101	34/-	0.73	0.32	10.65	62,102,116,137	0
36	HTG	B	625	19/19	0.72	0.44	10.00	43,101,109,111	0
35	LMT	M	103	35/35	0.68	0.34	9.83	37,128,152,157	0
36	HTG	V	203	11/19	0.86	0.60	9.71	88,101,107,108	0
27	GOL	B	627	6/6	0.95	0.36	9.70	60,77,93,95	0
35	LMT	D	403	35/35	0.61	0.39	8.48	40,112,125,126	0
36	HTG	C	524	9/19	0.56	1.22	8.27	70,90,106,139	0
35	LMT	B	633	35/35	0.58	0.44	8.16	39,117,133,139	0
35	LMT	E	102	35/35	0.72	0.56	7.32	91,129,157,163	0
35	LMT	e	102	35/35	0.65	0.80	6.25	75,139,161,171	0
30	UNL	I	101	40/-	0.70	0.32	5.73	39,89,141,148	0
27	GOL	a	412	6/6	0.88	0.25	5.61	56,70,85,86	0
30	UNL	D	410	17/-	0.87	0.37	5.55	46,64,94,102	0
29	PL9	A	413	55/55	0.78	0.35	5.24	44,83,100,110	0
36	HTG	c	522	19/19	0.70	0.82	5.07	83,139,149,158	0
30	UNL	D	411	40/-	0.84	0.28	4.94	49,76,125,128	0
36	HTG	D	412	16/19	0.47	0.41	4.58	43,118,136,138	0
30	UNL	X	101	18/-	0.89	0.20	4.55	39,66,83,87	0
35	LMT	a	418	35/35	0.85	0.54	3.91	97,118,139,139	0
36	HTG	b	621	19/19	0.78	0.26	3.74	33,91,127,144	0
30	UNL	b	629	36/-	0.81	0.33	3.59	46,85,130,141	0
34	LMG	C	521	51/55	0.52	0.51	3.39	50,107,149,153	0
30	UNL	x	101	18/-	0.84	0.31	3.27	47,66,104,105	0
31	LHG	e	101	42/49	0.73	0.43	3.03	63,119,140,150	0
35	LMT	B	634	26/35	0.88	0.18	3.01	48,90,109,115	0
35	LMT	b	628	25/35	0.78	0.28	2.84	37,63,135,142	0
30	UNL	d	409	17/-	0.94	0.38	2.76	48,58,94,99	0
35	LMT	C	522	35/35	0.60	0.64	2.74	83,119,141,151	0
27	GOL	B	628	6/6	0.86	0.26	2.67	47,58,65,72	0
29	PL9	a	415	55/55	0.75	0.34	2.61	56,82,108,115	0
34	LMG	c	520	51/55	0.64	0.43	2.59	62,104,135,147	0
35	LMT	m	103	35/35	0.64	0.49	2.40	40,85,113,117	0
35	LMT	B	632	25/35	0.82	0.27	2.20	41,68,135,136	0
36	HTG	B	624	19/19	0.88	0.21	2.08	33,71,128,130	0
31	LHG	D	408	49/49	0.96	0.26	1.96	25,37,56,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	LHG	d	407	49/49	0.91	0.25	1.92	24,38,58,65	0
31	LHG	A	415	49/49	0.90	0.34	1.90	29,46,67,82	0
34	LMG	Z	101	37/55	0.72	0.40	1.73	57,103,134,149	0
29	PL9	d	405	55/55	0.95	0.21	1.71	24,33,49,66	0
23	CLA	b	601	65/65	0.92	0.27	1.71	46,70,107,135	0
26	SQD	A	411	54/54	0.85	0.25	1.68	41,71,114,129	0
31	LHG	E	101	42/49	0.80	0.27	1.66	47,95,114,121	0
26	SQD	L	102	54/54	0.79	0.26	1.64	39,73,114,123	0
23	CLA	c	503	65/65	0.93	0.44	1.63	44,55,67,84	0
27	GOL	A	410	6/6	0.96	0.13	1.60	45,57,60,90	0
29	PL9	D	407	55/55	0.95	0.24	1.56	20,30,44,53	0
31	LHG	L	101	49/49	0.93	0.25	1.53	26,39,54,75	0
27	GOL	C	525	6/6	0.93	0.26	1.50	45,56,66,73	0
22	CL	a	403	1/1	0.98	0.27	1.50	41,41,41,41	0
34	LMG	z	101	39/55	0.85	0.24	1.49	69,117,144,151	0
23	CLA	B	602	65/65	0.94	0.21	1.48	39,61,93,123	0
35	LMT	M	101	35/35	0.68	0.34	1.47	40,85,105,107	0
25	BCR	T	101	40/40	0.97	0.24	1.42	21,37,55,60	0
31	LHG	d	406	49/49	0.94	0.23	1.37	27,48,81,84	0
23	CLA	c	502	65/65	0.91	0.43	1.37	40,55,70,74	0
25	BCR	t	101	40/40	0.96	0.24	1.34	23,43,64,68	0
34	LMG	J	101	51/55	0.91	0.20	1.31	33,54,96,105	0
26	SQD	a	413	54/54	0.89	0.22	1.31	37,73,134,146	0
26	SQD	f	101	43/54	0.79	0.32	1.26	86,117,154,157	0
34	LMG	c	519	51/55	0.87	0.28	1.22	47,78,122,143	0
23	CLA	b	605	65/65	0.95	0.26	1.13	26,34,51,76	0
31	LHG	D	409	49/49	0.94	0.21	1.13	32,50,107,117	0
31	LHG	d	408	49/49	0.94	0.21	1.12	40,55,105,111	0
36	HTG	B	629	19/19	0.90	0.19	1.10	47,59,78,83	0
23	CLA	C	511	65/65	0.95	0.48	1.09	36,48,61,67	0
37	DGD	c	516	62/66	0.94	0.24	1.06	35,47,74,93	0
31	LHG	b	630	49/49	0.91	0.17	1.04	26,43,59,64	0
23	CLA	B	611	65/65	0.96	0.23	1.02	29,41,55,70	0
26	SQD	B	621	54/54	0.81	0.24	0.98	44,82,109,118	0
24	PHO	a	408	64/64	0.96	0.28	0.97	30,40,53,60	0
24	PHO	a	407	64/64	0.98	0.20	0.96	24,31,45,50	0
34	LMG	C	501	51/55	0.83	0.29	0.96	40,81,110,113	0
25	BCR	B	618	40/40	0.96	0.18	0.90	24,37,48,49	0
37	DGD	H	102	62/66	0.90	0.29	0.90	29,42,64,68	0
37	DGD	h	103	62/66	0.88	0.29	0.89	34,46,67,76	0
24	PHO	A	406	64/64	0.97	0.20	0.87	22,29,39,46	0
23	CLA	a	409	65/65	0.96	0.18	0.87	30,44,124,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	DGD	C	518	62/66	0.88	0.23	0.86	35,51,111,119	0
23	CLA	B	606	65/65	0.95	0.21	0.84	24,33,46,51	0
23	CLA	c	501	65/65	0.94	0.23	0.82	43,53,67,72	0
25	BCR	C	516	40/40	0.92	0.22	0.81	38,50,63,68	0
23	CLA	A	407	65/65	0.97	0.15	0.80	28,38,98,117	0
37	DGD	c	518	62/66	0.95	0.20	0.80	39,50,74,97	0
23	CLA	B	604	65/65	0.96	0.27	0.78	30,43,56,67	0
37	DGD	C	517	62/66	0.92	0.26	0.77	30,41,77,88	0
35	LMT	B	623	35/35	0.84	0.26	0.77	50,95,120,122	0
36	HTG	h	101	16/19	0.79	0.38	0.77	71,110,125,143	0
24	PHO	D	402	64/64	0.97	0.24	0.75	25,31,44,55	0
37	DGD	C	519	62/66	0.93	0.17	0.72	30,44,80,109	0
39	MG	J	103	1/1	0.97	0.17	0.70	43,43,43,43	0
25	BCR	d	404	40/40	0.94	0.15	0.69	43,55,79,81	0
23	CLA	C	506	65/65	0.95	0.28	0.68	33,44,75,82	0
23	CLA	C	509	65/65	0.94	0.32	0.67	33,46,93,103	0
25	BCR	D	406	40/40	0.92	0.19	0.65	35,46,78,84	0
37	DGD	c	517	62/66	0.93	0.23	0.64	42,55,110,126	0
23	CLA	b	603	65/65	0.95	0.27	0.64	32,44,61,70	0
25	BCR	B	620	40/40	0.92	0.16	0.63	30,43,67,78	0
23	CLA	b	604	65/65	0.95	0.33	0.62	24,33,95,101	0
34	LMG	j	101	51/55	0.93	0.17	0.62	41,56,92,119	0
23	CLA	C	503	65/65	0.93	0.36	0.60	33,43,60,67	0
23	CLA	b	610	65/65	0.95	0.22	0.60	35,44,56,61	0
25	BCR	h	102	40/40	0.71	0.29	0.59	42,57,71,74	0
23	CLA	b	608	65/65	0.95	0.29	0.59	34,44,67,72	0
23	CLA	C	510	65/65	0.94	0.32	0.59	39,53,71,79	0
26	SQD	a	411	54/54	0.94	0.19	0.56	44,69,108,113	0
23	CLA	c	508	65/65	0.93	0.20	0.55	39,53,121,131	0
23	CLA	b	612	65/65	0.93	0.28	0.55	28,35,48,69	0
23	CLA	c	509	65/65	0.92	0.25	0.53	46,56,73,79	0
23	CLA	D	405	65/65	0.93	0.18	0.52	33,48,111,119	0
25	BCR	b	618	40/40	0.96	0.22	0.51	22,36,51,56	0
23	CLA	c	510	65/65	0.95	0.34	0.51	39,51,67,71	0
22	CL	A	403	1/1	0.99	0.25	0.50	27,27,27,27	0
34	LMG	a	417	51/55	0.87	0.22	0.50	42,79,99,115	0
23	CLA	B	613	65/65	0.94	0.25	0.49	26,33,45,65	0
23	CLA	B	608	65/65	0.96	0.23	0.49	20,28,59,67	0
27	GOL	b	624	6/6	0.92	0.15	0.48	75,92,97,104	0
25	BCR	B	619	40/40	0.96	0.23	0.47	21,36,52,60	0
25	BCR	A	408	40/40	0.97	0.17	0.47	23,34,48,56	0
23	CLA	B	612	65/65	0.92	0.26	0.46	24,32,49,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	LMG	B	622	51/55	0.87	0.23	0.45	35,53,83,101	0
23	CLA	B	605	65/65	0.94	0.31	0.44	22,31,101,111	0
23	CLA	C	514	65/65	0.89	0.26	0.43	50,65,100,107	0
25	BCR	H	101	40/40	0.82	0.23	0.43	35,46,66,73	0
23	CLA	B	614	65/65	0.97	0.32	0.37	23,31,72,87	0
23	CLA	c	511	65/65	0.92	0.19	0.35	47,56,78,89	0
34	LMG	m	101	51/55	0.90	0.20	0.35	33,52,85,99	0
23	CLA	c	504	65/65	0.95	0.30	0.34	41,52,94,117	0
23	CLA	b	602	65/65	0.89	0.25	0.34	36,48,68,77	0
34	LMG	C	520	51/55	0.83	0.28	0.32	43,75,125,134	0
26	SQD	D	413	43/54	0.90	0.30	0.31	58,106,117,124	0
23	CLA	D	401	65/65	0.97	0.16	0.29	21,28,43,47	0
25	BCR	Y	101	40/40	0.94	0.15	0.29	40,51,62,71	0
38	HEM	e	103	43/43	0.97	0.21	0.29	52,78,106,116	0
23	CLA	B	603	65/65	0.90	0.23	0.28	31,41,57,69	0
23	CLA	d	403	65/65	0.92	0.17	0.27	41,52,102,116	0
23	CLA	c	512	65/65	0.89	0.22	0.26	53,66,96,104	0
23	CLA	b	607	65/65	0.96	0.18	0.25	21,30,58,67	0
25	BCR	y	101	40/40	0.89	0.18	0.24	48,60,74,77	0
23	CLA	c	505	65/65	0.93	0.20	0.23	36,46,76,82	0
23	CLA	B	609	65/65	0.97	0.24	0.23	30,42,56,66	0
23	CLA	b	611	65/65	0.96	0.21	0.21	27,35,57,62	0
23	CLA	C	513	65/65	0.88	0.23	0.20	46,60,106,112	0
23	CLA	C	502	65/65	0.92	0.23	0.18	36,45,67,70	0
23	CLA	C	508	65/65	0.91	0.24	0.16	40,51,66,78	0
35	LMT	b	620	25/35	0.79	0.24	0.16	55,88,143,147	0
25	BCR	b	617	40/40	0.95	0.16	0.15	21,35,45,51	0
23	CLA	C	504	65/65	0.91	0.29	0.15	37,47,66,75	0
26	SQD	A	409	54/54	0.94	0.16	0.12	41,66,99,109	0
23	CLA	c	513	65/65	0.90	0.22	0.10	58,74,112,119	0
23	CLA	b	613	65/65	0.96	0.26	0.08	24,36,79,89	0
23	CLA	d	402	65/65	0.96	0.22	0.08	27,32,58,72	0
23	CLA	a	406	65/65	0.97	0.21	0.07	30,38,98,103	0
23	CLA	B	610	65/65	0.91	0.17	0.05	31,42,53,89	0
25	BCR	a	410	40/40	0.96	0.15	0.05	28,38,55,58	0
23	CLA	D	404	65/65	0.94	0.18	0.02	21,29,50,56	0
23	CLA	b	609	65/65	0.90	0.17	-0.00	39,48,63,74	0
25	BCR	b	619	40/40	0.94	0.15	-0.02	33,46,69,80	0
23	CLA	a	404	65/65	0.96	0.19	-0.03	27,33,52,66	0
23	CLA	C	505	65/65	0.93	0.23	-0.04	32,46,91,111	0
25	BCR	c	515	40/40	0.96	0.14	-0.04	41,54,66,70	0
23	CLA	B	617	65/65	0.94	0.21	-0.04	33,45,121,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	a	405	65/65	0.96	0.15	-0.05	23,29,52,60	0
25	BCR	C	527	40/40	0.93	0.17	-0.09	43,55,71,72	0
23	CLA	C	512	65/65	0.90	0.18	-0.11	39,54,77,85	0
23	CLA	b	614	65/65	0.95	0.15	-0.12	25,35,93,107	0
38	HEM	v	201	43/43	0.98	0.14	-0.13	44,53,63,82	0
23	CLA	c	507	65/65	0.90	0.19	-0.14	43,57,70,72	0
23	CLA	c	506	65/65	0.96	0.15	-0.15	47,65,98,117	0
23	CLA	A	405	65/65	0.96	0.15	-0.16	24,33,85,94	0
25	BCR	k	101	40/40	0.93	0.18	-0.16	50,60,84,87	0
23	CLA	B	615	65/65	0.93	0.18	-0.17	23,32,86,95	0
23	CLA	b	606	65/65	0.94	0.15	-0.18	29,42,91,110	0
23	CLA	B	607	65/65	0.94	0.14	-0.18	28,37,76,93	0
33	CA	c	523	1/1	0.96	0.18	-0.21	68,68,68,68	0
23	CLA	A	404	65/65	0.96	0.17	-0.24	22,25,39,58	0
23	CLA	b	615	65/65	0.91	0.18	-0.32	33,43,65,87	0
33	CA	C	526	1/1	0.98	0.26	-0.33	59,59,59,59	0
39	MG	j	103	1/1	0.96	0.14	-0.38	48,48,48,48	0
23	CLA	C	507	65/65	0.93	0.16	-0.46	42,57,106,115	0
25	BCR	C	515	40/40	0.94	0.17	-0.47	49,60,74,82	0
22	CL	a	402	1/1	1.00	0.13	-0.52	28,28,28,28	0
23	CLA	B	616	65/65	0.93	0.15	-0.53	29,38,60,67	0
38	HEM	V	202	43/43	0.98	0.12	-0.57	33,36,48,70	0
36	HTG	b	625	19/19	0.93	0.11	-0.59	40,60,90,94	0
23	CLA	b	616	65/65	0.90	0.20	-0.63	34,51,101,111	0
38	HEM	E	103	43/43	0.98	0.09	-0.75	43,56,69,83	0
25	BCR	c	514	40/40	0.94	0.14	-0.76	58,68,80,83	0
22	CL	A	402	1/1	0.99	0.11	-1.19	24,24,24,24	0
32	BCT	a	419	4/4	0.98	0.07	-1.36	41,45,48,58	0
32	BCT	A	416	4/4	0.98	0.08	-1.58	32,45,46,51	0
28	OEX	A	412	10/10	0.99	0.10	-1.66	23,32,46,47	0
28	OEX	a	414	10/10	0.99	0.09	-2.18	29,36,46,48	0
33	CA	O	301	1/1	0.86	0.13	-2.38	101,101,101,101	0
33	CA	c	524	1/1	0.98	0.08	-2.71	66,66,66,66	0
33	CA	o	301	1/1	0.93	0.12	-3.86	89,89,89,89	0
21	FE2	a	401	1/1	0.99	0.04	-3.93	47,47,47,47	0
21	FE2	A	401	1/1	0.99	0.05	-4.16	46,46,46,46	0
33	CA	V	201	1/1	0.93	0.11	-	94,94,94,94	0
36	HTG	C	523	19/19	0.80	0.43	-	95,107,121,133	0
36	HTG	c	521	19/19	0.81	0.37	-	71,125,137,163	0
36	HTG	B	630	19/19	0.82	0.27	-	67,116,145,154	0
30	UNL	B	631	33/-	0.68	0.26	-	36,92,134,151	0
30	UNL	m	102	10/-	0.75	0.32	-	36,47,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	UNL	c	525	32/-	0.72	0.33	-	74,104,124,132	0
30	UNL	M	102	10/-	0.85	0.28	-	38,51,60,60	0
30	UNL	a	416	30/-	0.55	0.50	-	86,102,121,129	0
30	UNL	A	414	28/-	0.27	0.57	-	66,93,121,126	0
30	UNL	J	102	10/-	0.66	0.45	-	59,66,85,90	0
36	HTG	B	626	19/19	0.48	0.70	-	51,135,163,189	0
33	CA	B	601	1/1	0.77	0.12	-	144,144,144,144	0
36	HTG	b	623	19/19	0.58	0.63	-	73,116,140,180	0
30	UNL	b	627	33/-	0.59	0.45	-	53,80,145,147	0
27	GOL	O	302	6/6	0.83	0.27	-	63,68,72,78	0
36	HTG	b	626	19/19	0.82	0.25	-	66,114,151,181	0

6.5 Other polymers [i](#)

There are no such residues in this entry.