



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2017 – 04:47 PM EST

PDB ID : 5GTH
Title : Native XFEL structure of photosystem II (dark 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

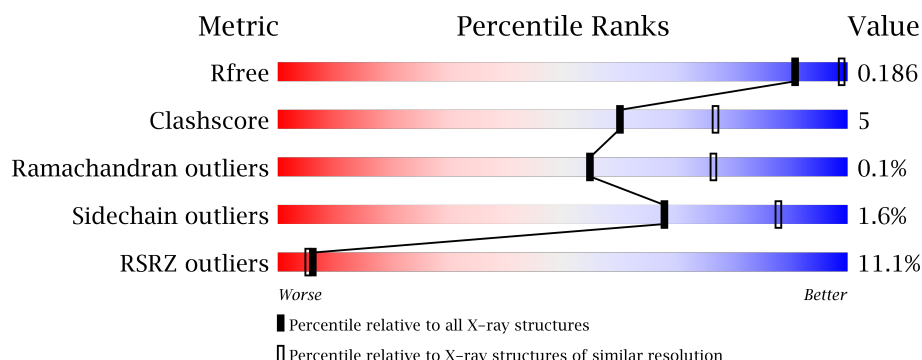
1 Overall quality at a glance

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>85%</div> <div>12%</div> <div>.</div> </div>
1	a	344	<div> <div>3%</div> <div>97%</div> <div>.</div> <div>..</div> </div>
2	B	505	<div> <div>10%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	b	505	<div> <div>11%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>14%</div> <div>86%</div> <div>13%</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	406	X	-	-	-
23	CLA	A	408	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	502	X	-	-	-
23	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	404	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	408	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	-	-	-
23	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	401	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
27	GOL	A	411	-	-	-	X
27	GOL	B	625	-	-	-	X
27	GOL	B	626	-	-	-	X
27	GOL	a	411	-	-	-	X
27	GOL	d	402	-	-	-	X
29	PL9	A	414	-	-	-	X
29	PL9	a	414	-	-	-	X
30	UNL	D	410	-	-	-	X
30	UNL	D	411	-	-	-	X
30	UNL	I	102	-	-	-	X
30	UNL	J	102	-	-	-	X
30	UNL	K	101	-	-	-	X
30	UNL	X	101	-	-	-	X
30	UNL	b	629	-	-	-	X
30	UNL	i	101	-	-	-	X
30	UNL	j	102	-	-	-	X
30	UNL	x	101	-	-	-	X
31	LHG	E	101	-	-	-	X
31	LHG	e	101	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	z	101	-	-	-	X
34	HTG	B	622	-	-	-	X
34	HTG	B	623	-	-	-	X
34	HTG	C	522	-	-	-	X
34	HTG	D	412	-	-	-	X
34	HTG	V	203	-	-	-	X
34	HTG	b	622	-	-	-	X
34	HTG	b	623	-	-	-	X
34	HTG	b	628	-	-	-	X
34	HTG	c	522	-	-	-	X
35	LMT	B	630	-	-	-	X
35	LMT	B	631	-	-	-	X
35	LMT	D	402	-	-	-	X
35	LMT	E	102	-	-	-	X
35	LMT	I	101	-	-	-	X
35	LMT	M	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	LMT	a	417	-	-	-	X
35	LMT	b	627	-	-	-	X
35	LMT	e	102	-	-	-	X
35	LMT	m	102	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 52773 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 protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2634	1728	432	459	15			
1	a	334	Total	C	N	O	S	0	5	0
			2639	1732	431	461	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	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3501	2291	584	613	13			
3	c	455	Total	C	N	O	S	0	5	0
			3537	2317	589	618	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	1	0
			2729	1807	445	465	12			
4	d	341	Total	C	N	O	S	0	1	0
			2720	1802	444	462	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	1	0
			665	434	107	124			
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	1	0
			514	344	84	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 reaction center protein K.

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	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	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	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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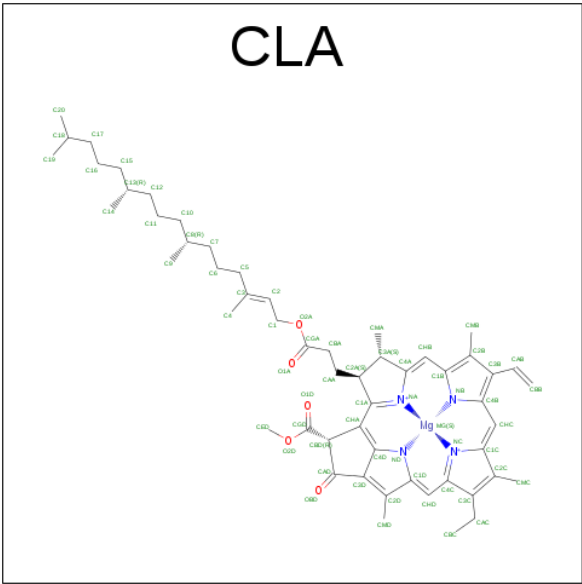
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	0
			1	1		

- 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	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

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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	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

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

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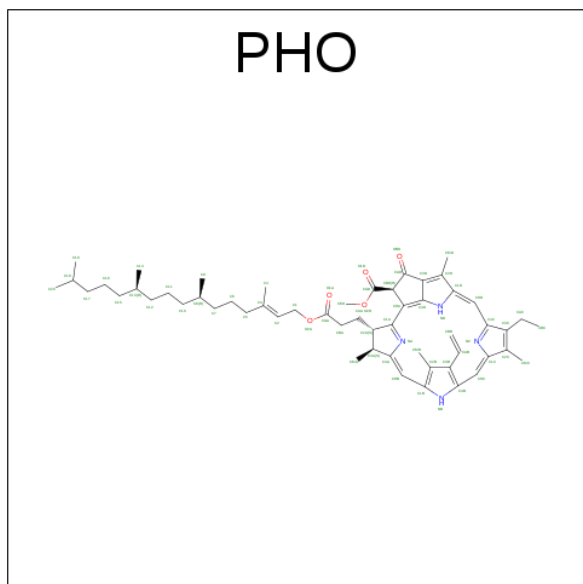
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N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

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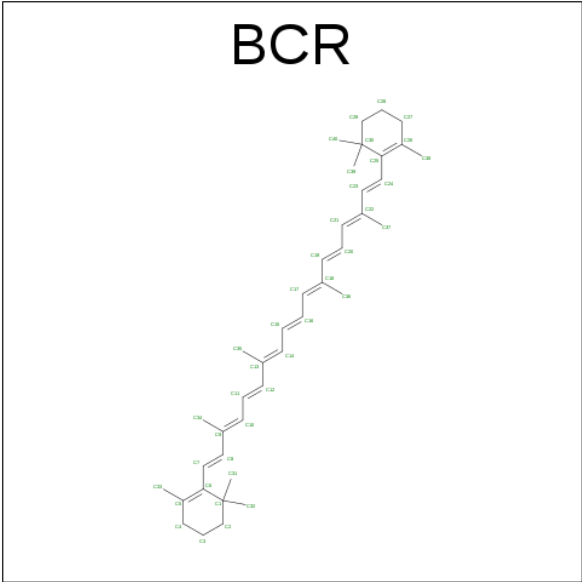
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- 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: $C_{40}H_{56}$).



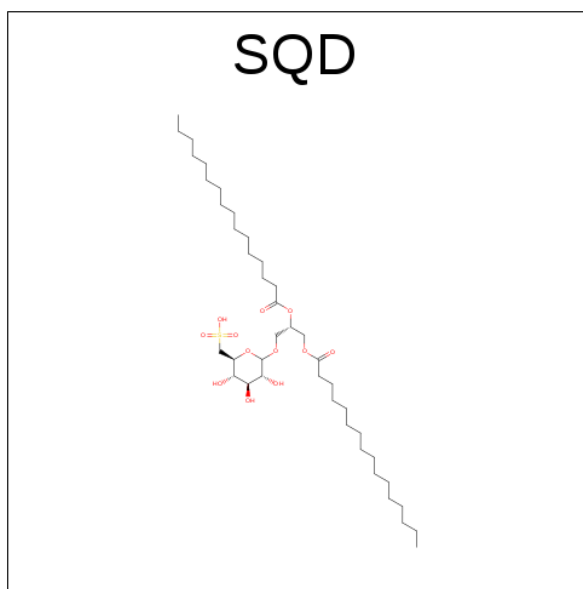
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
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-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



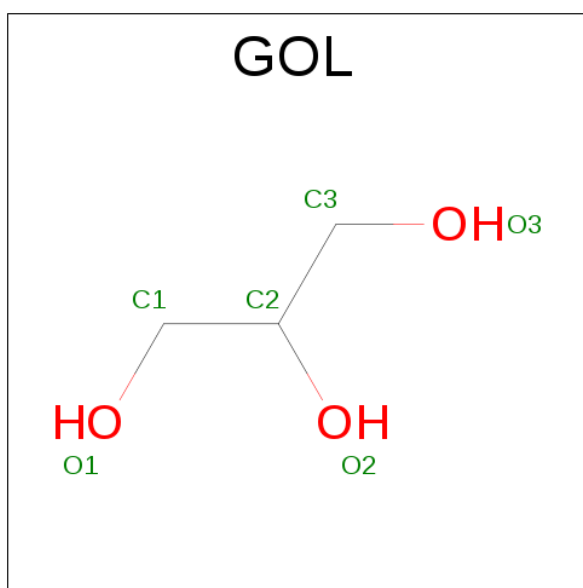
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0

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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: $C_3H_8O_3$).



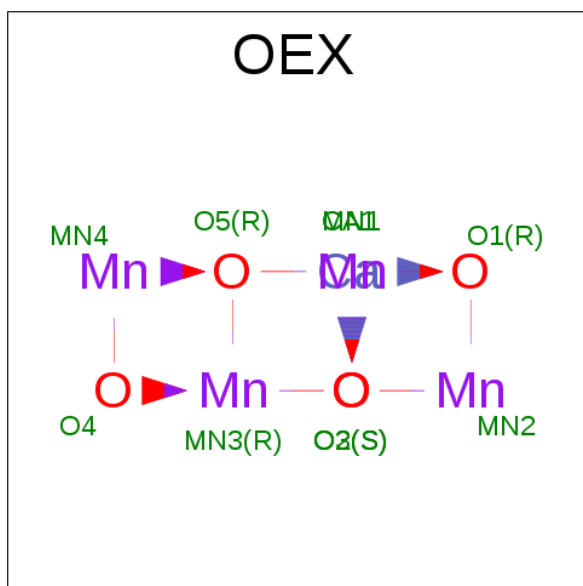
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

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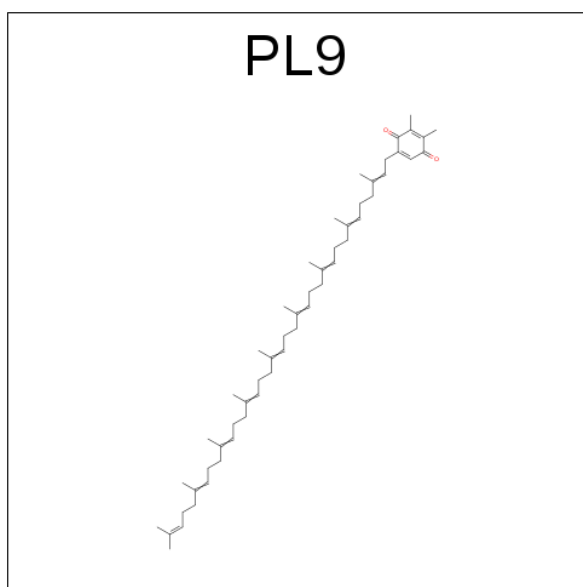
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	d	1	Total	C	O	0	0
			6	3	3		

- 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:).

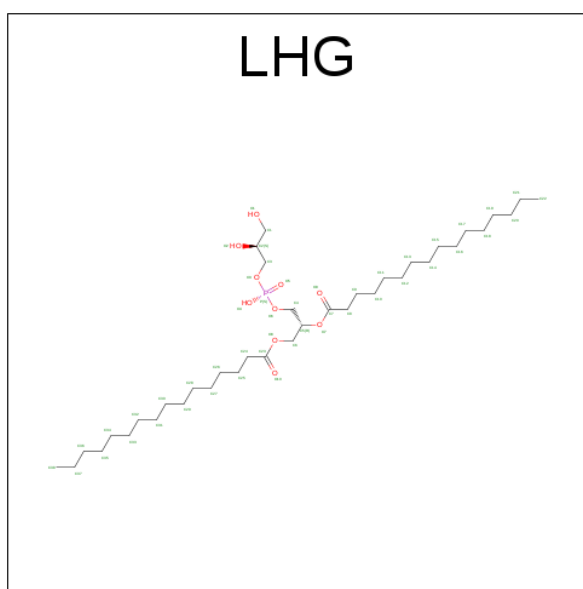
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	J	1	Total	C		0	0
			10	10			
30	i	1	Total	C	O	0	0
			40	35	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	K	1	Total	C	O	0	0
			34	29	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	I	1	Total	C	O	0	0
			40	35	5		
30	c	1	Total	C	O	0	0
			32	27	5		
30	a	1	Total	C	O	0	0
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

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

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



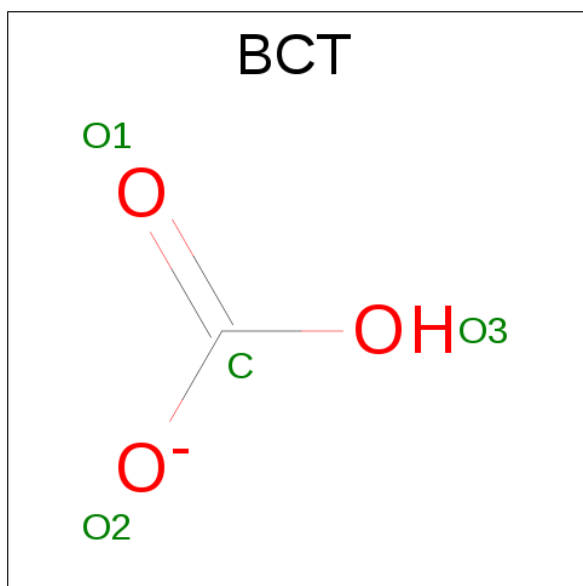
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O P 49 38 10 1	0	0
31	A	1	Total C O P 49 38 10 1	0	0
31	D	1	Total C O P 49 38 10 1	0	0

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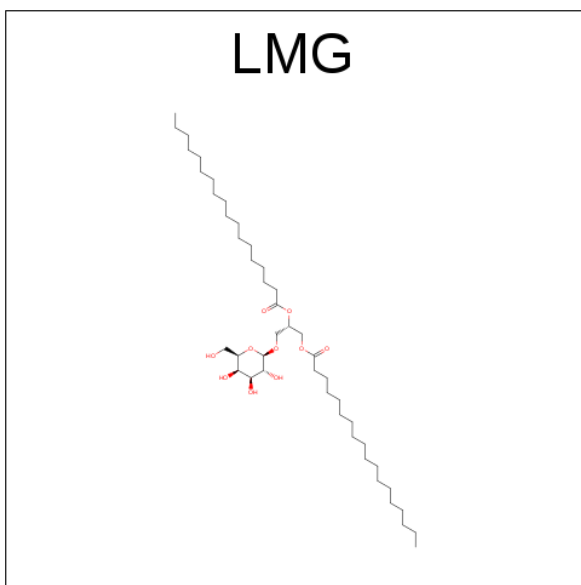
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total	C	O	P	0	0
			49	38	10	1		
31	E	1	Total	C	O	P	0	0
			42	31	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	d	1	Total	C	O	P	0	0
			49	38	10	1		
31	e	1	Total	C	O	P	0	0
			42	31	10	1		
31	l	1	Total	C	O	P	0	0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

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



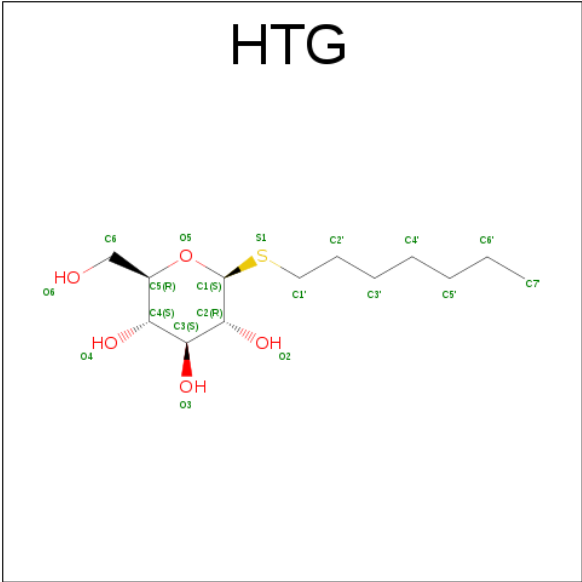
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $\text{C}_{45}\text{H}_{86}\text{O}_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



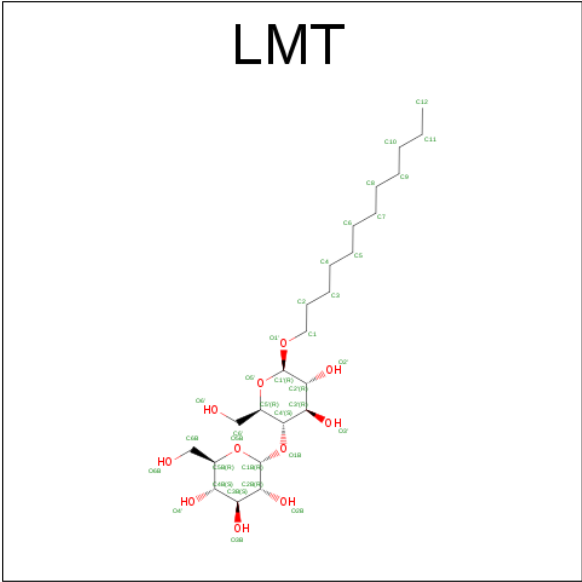
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			16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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	d	1	Total	C	O	S	0	0
			16	10	5	1		

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



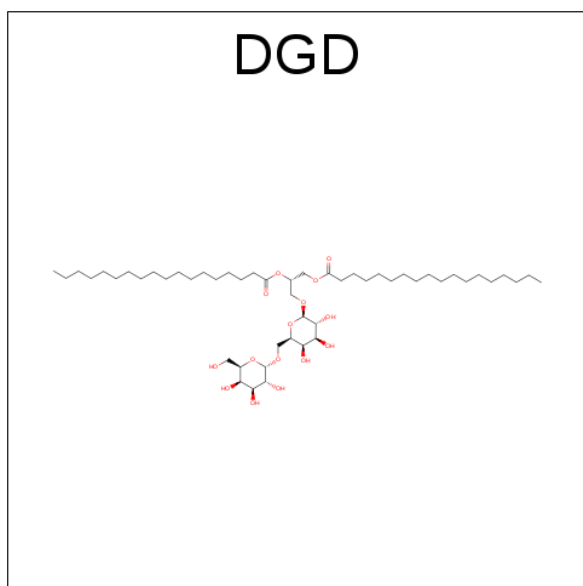
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O		0	0
			25	19	6			
35	B	1	Total	C	O		0	0
			35	24	11			
35	B	1	Total	C	O		0	0
			26	19	7			
35	D	1	Total	C	O		0	0
			35	24	11			
35	D	1	Total	C	O		0	0
			35	24	11			
35	E	1	Total	C	O		0	0
			35	24	11			
35	I	1	Total	C	O		0	0
			35	24	11			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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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 DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



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

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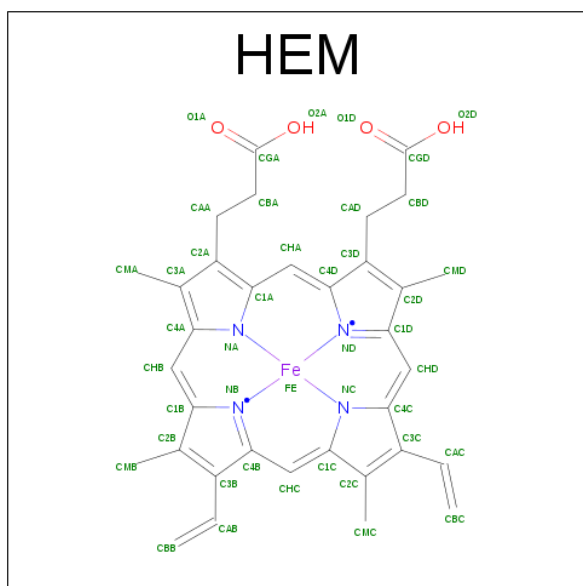
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- 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 43	C 34	Fe 1	N 4	O 4	0	0
38	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
38	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	127	Total	O	0	0
			127	127		
40	B	175	Total	O	0	0
			175	175		
40	C	148	Total	O	0	0
			148	148		
40	D	111	Total	O	0	0
			111	111		
40	E	18	Total	O	0	0
			18	18		
40	F	5	Total	O	0	0
			5	5		
40	H	19	Total	O	0	0
			19	19		
40	I	6	Total	O	0	0
			6	6		
40	J	5	Total	O	0	0
			5	5		
40	K	6	Total	O	0	0
			6	6		
40	L	9	Total	O	0	0
			9	9		
40	M	14	Total	O	0	0
			14	14		
40	O	100	Total	O	0	0
			100	100		
40	T	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	46	Total 46	O 46	0	0
40	V	78	Total 79	O 79	0	1
40	X	3	Total 3	O 3	0	0
40	Y	1	Total 1	O 1	0	0
40	a	130	Total 130	O 130	0	0
40	b	192	Total 192	O 192	0	0
40	c	136	Total 136	O 136	0	0
40	d	108	Total 108	O 108	0	0
40	e	15	Total 15	O 15	0	0
40	f	5	Total 5	O 5	0	0
40	h	28	Total 28	O 28	0	0
40	i	4	Total 4	O 4	0	0
40	j	3	Total 3	O 3	0	0
40	k	4	Total 4	O 4	0	0
40	l	7	Total 7	O 7	0	0
40	m	11	Total 11	O 11	0	0
40	o	109	Total 109	O 109	0	0
40	t	7	Total 7	O 7	0	0
40	u	64	Total 64	O 64	0	0
40	v	71	Total 71	O 71	0	0
40	x	4	Total 4	O 4	0	0

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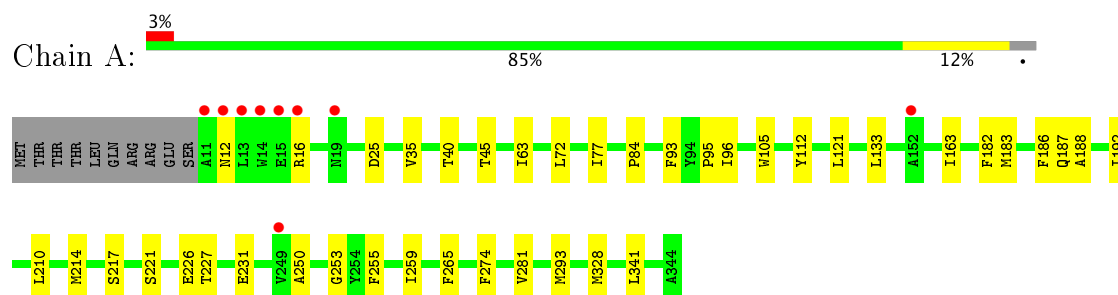
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	y	2	Total	O	0	0
			2	2		

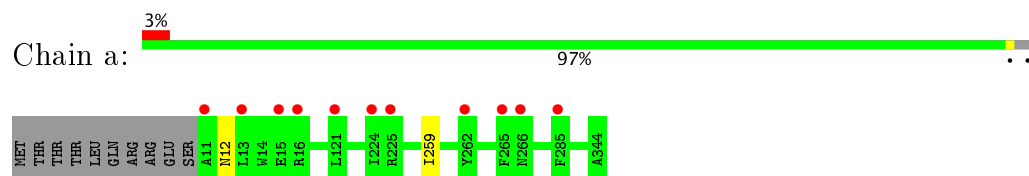
3 Residue-property plots [i](#)

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.

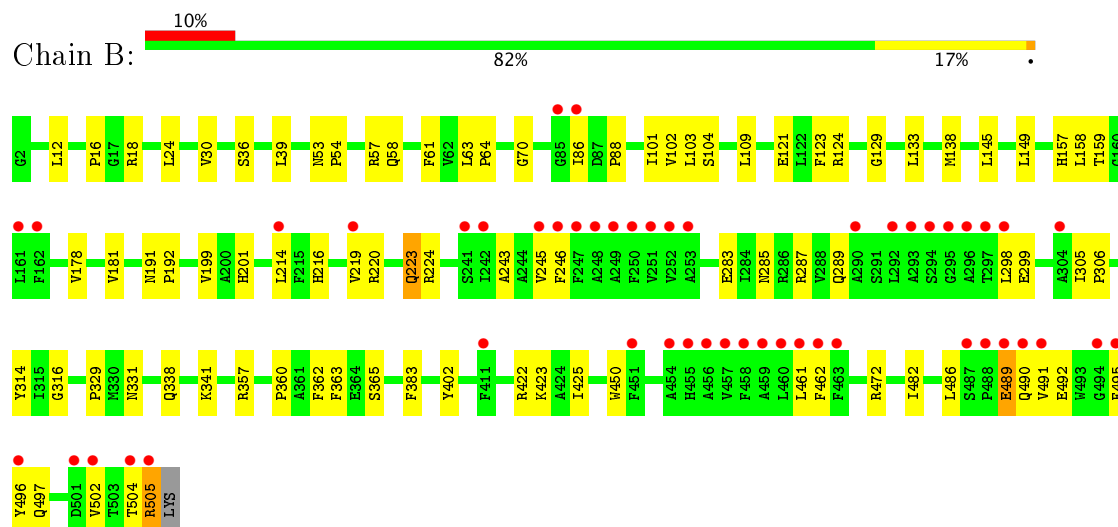
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1

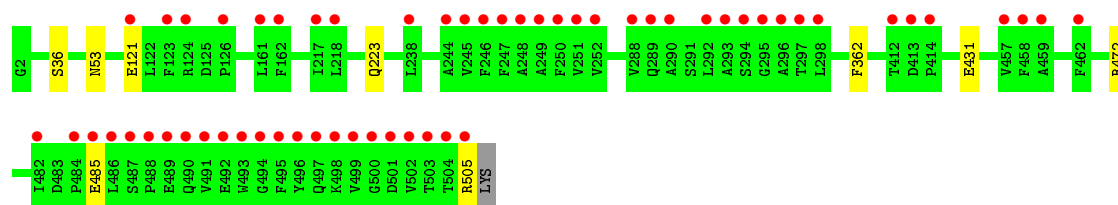


- Molecule 2: Photosystem II CP47 reaction center protein

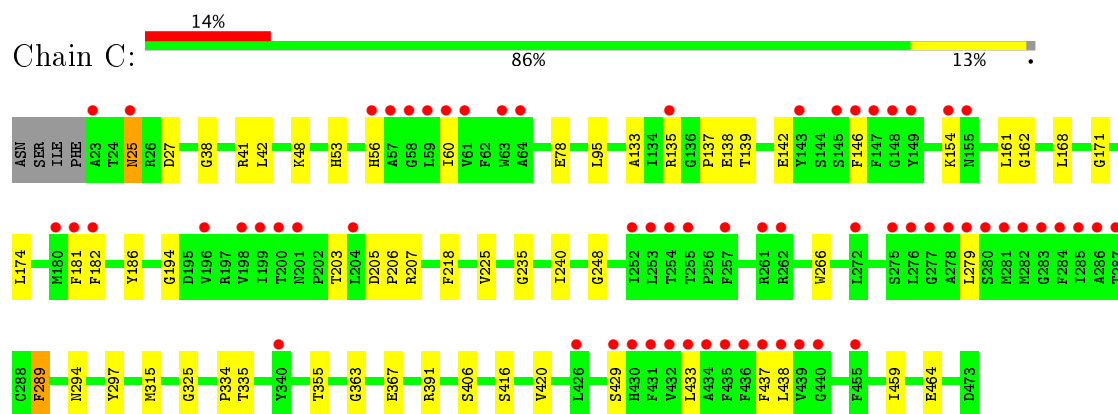


- Molecule 2: Photosystem II CP47 reaction center protein

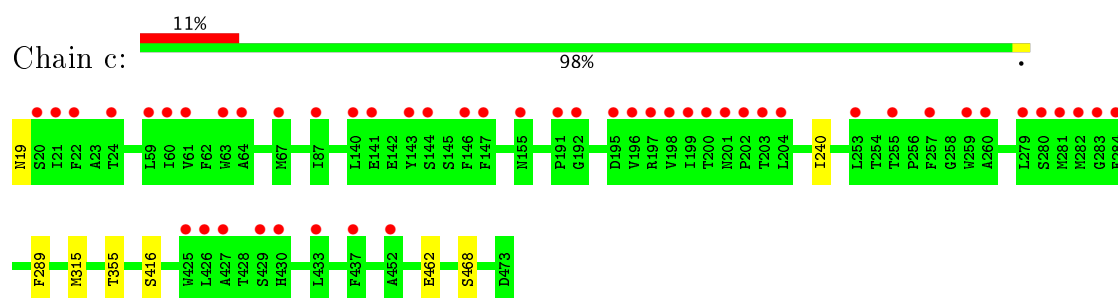




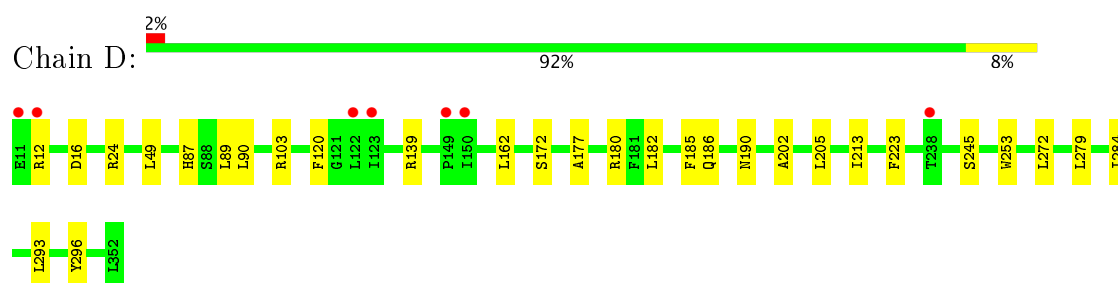
• Molecule 3: Photosystem II CP43 reaction center protein



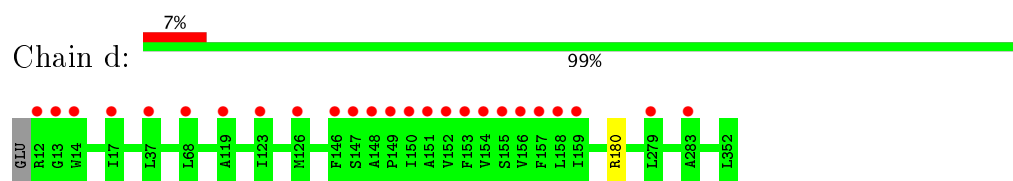
• Molecule 3: Photosystem II CP43 reaction center protein



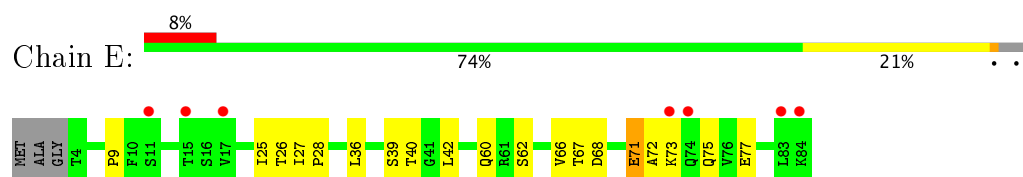
• Molecule 4: Photosystem II D2 protein



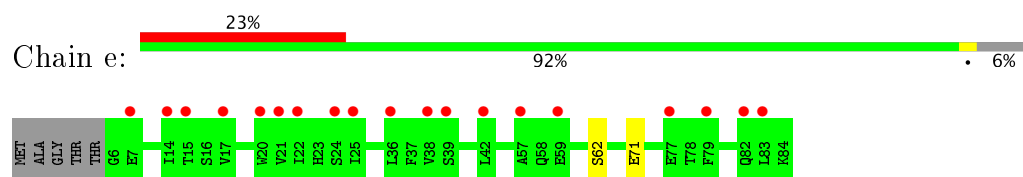
• Molecule 4: Photosystem II D2 protein



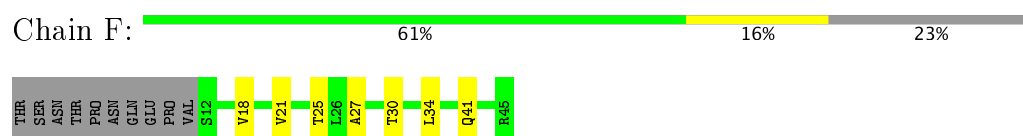
• Molecule 5: Cytochrome b559 subunit alpha



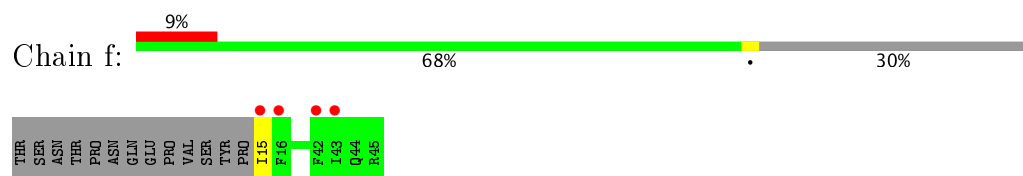
- Molecule 5: Cytochrome b559 subunit alpha



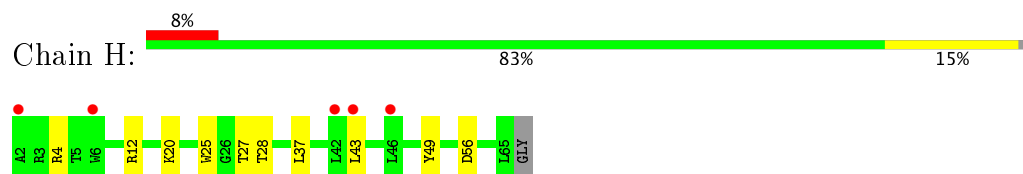
- Molecule 6: Cytochrome b559 subunit beta



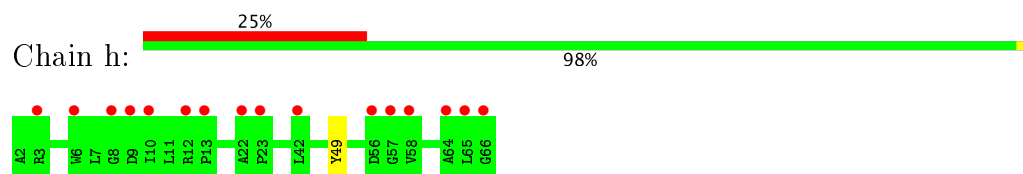
- Molecule 6: Cytochrome b559 subunit beta



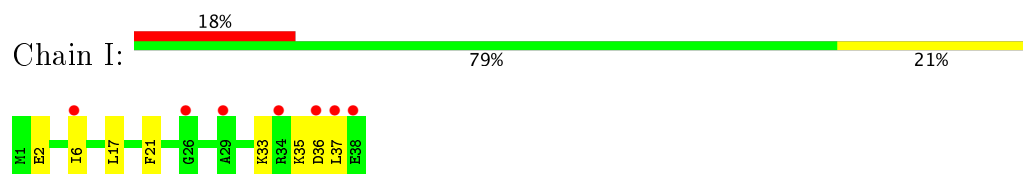
- Molecule 7: Photosystem II reaction center protein H



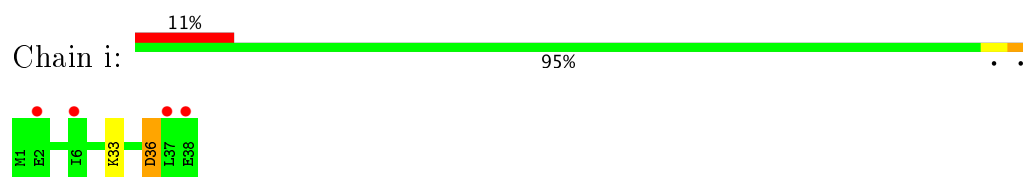
- Molecule 7: Photosystem II reaction center protein H



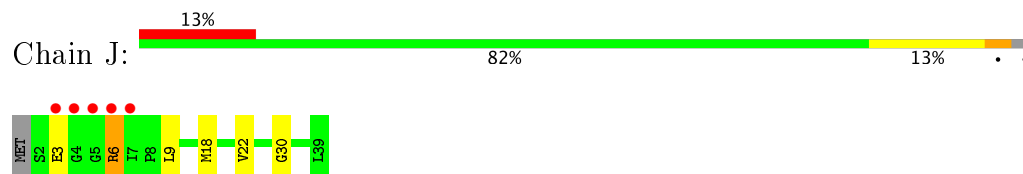
- Molecule 8: Photosystem II reaction center protein I



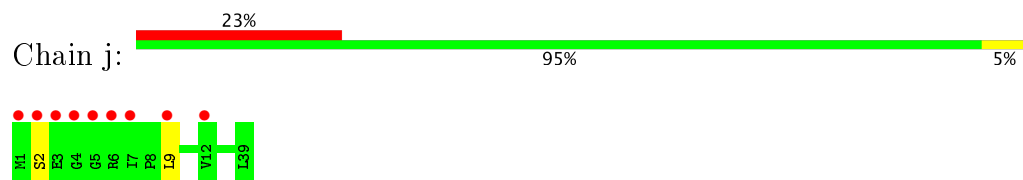
- Molecule 8: Photosystem II reaction center protein I



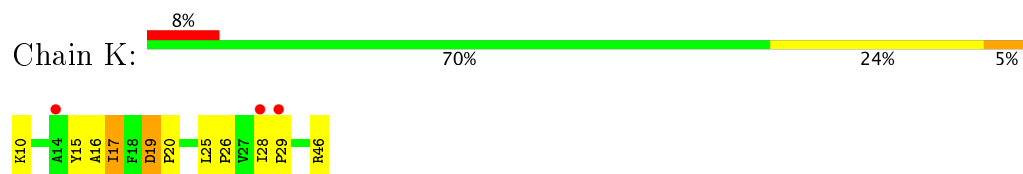
- Molecule 9: Photosystem II reaction center protein J



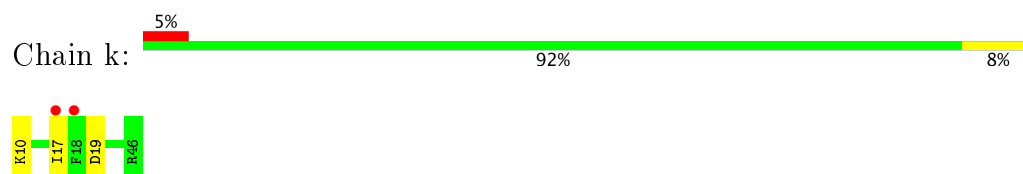
- Molecule 9: Photosystem II reaction center protein J



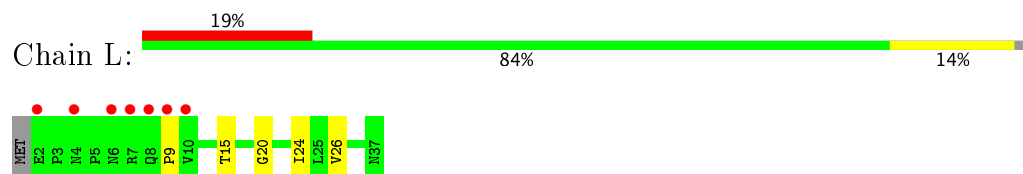
- Molecule 10: Photosystem II reaction center protein K



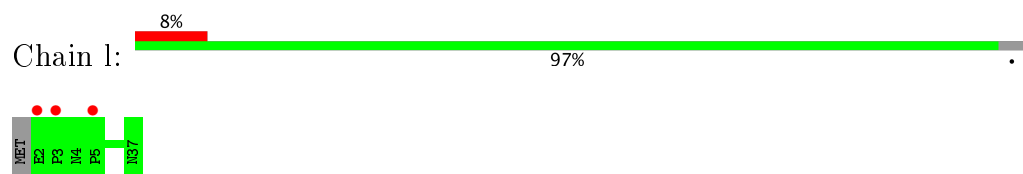
- Molecule 10: Photosystem II reaction center protein K



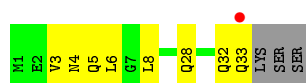
- Molecule 11: Photosystem II reaction center protein L



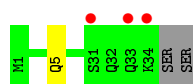
- Molecule 11: Photosystem II reaction center protein L



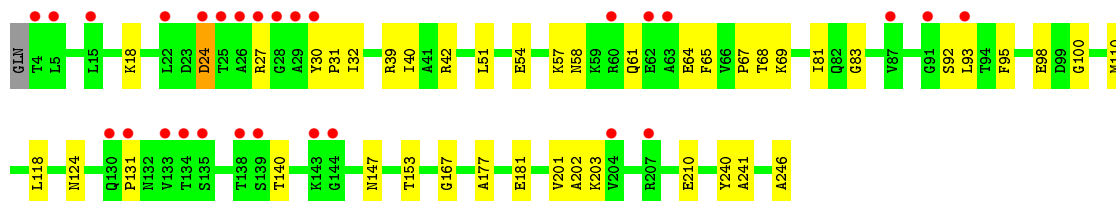
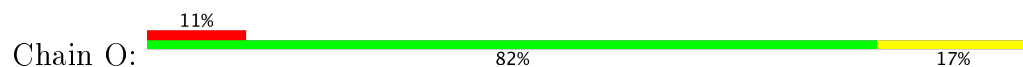
- Molecule 12: Photosystem II reaction center protein M



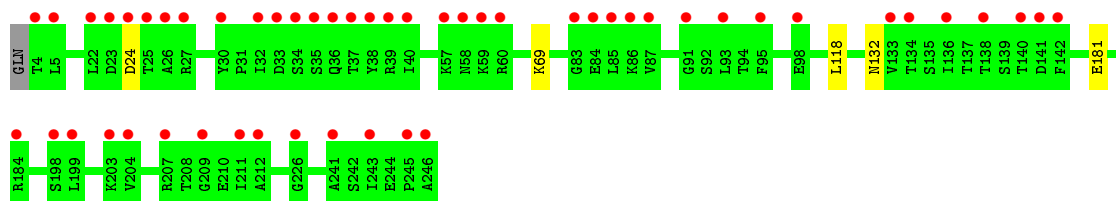
- Molecule 12: Photosystem II reaction center protein M



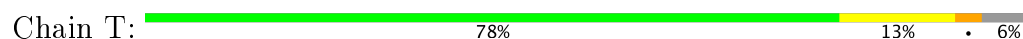
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



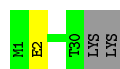
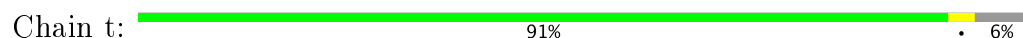
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



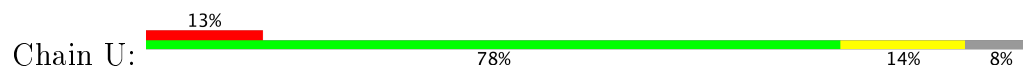
- Molecule 14: Photosystem II reaction center protein T

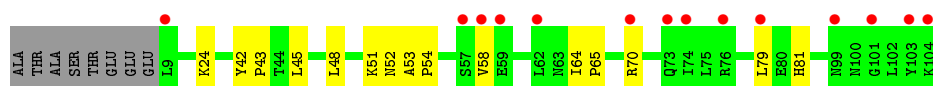


- Molecule 14: Photosystem II reaction center protein T

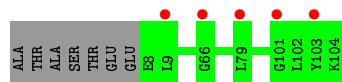


- Molecule 15: Photosystem II 12 kDa extrinsic protein





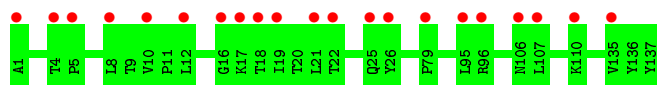
- Molecule 15: Photosystem II 12 kDa extrinsic protein



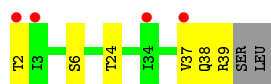
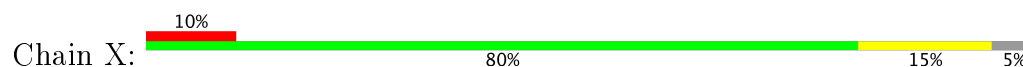
- Molecule 16: Cytochrome c-550



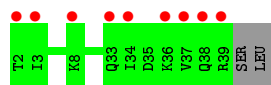
- Molecule 16: Cytochrome c-550



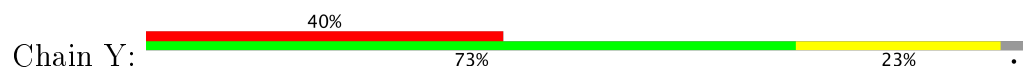
- Molecule 17: Photosystem II reaction center protein X



- Molecule 17: Photosystem II reaction center protein X

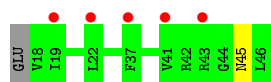


- Molecule 18: Photosystem II reaction center protein Ycf12

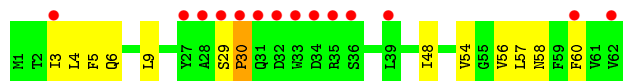
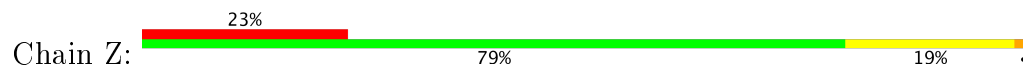


- Molecule 18: Photosystem II reaction center protein Ycf12

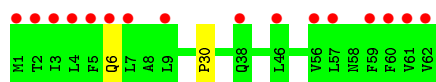




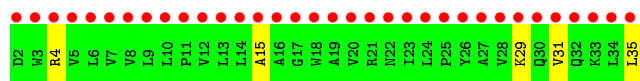
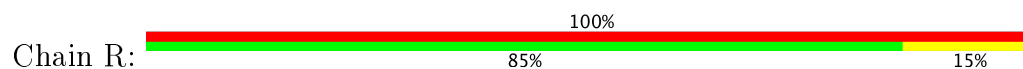
- Molecule 19: Photosystem II reaction center protein Z



- 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	1.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.139 , 0.186 0.147 , 0.186	Depositor DCC
R_{free} test set	14584 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	71.5	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	52773	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 [i](#)

5.1 Standard geometry [i](#)

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	0/2728	0.56	0/3719
1	a	0.45	0/2739	0.56	0/3735
2	B	0.42	0/4171	0.55	0/5683
2	b	0.42	0/4138	0.55	0/5640
3	C	0.40	0/3626	0.53	0/4936
3	c	0.41	0/3670	0.53	0/4996
4	D	0.45	0/2827	0.55	0/3852
4	d	0.45	0/2818	0.53	0/3840
5	E	0.34	0/687	0.53	0/936
5	e	0.34	0/667	0.50	0/908
6	F	0.34	0/284	0.47	0/387
6	f	0.38	0/257	0.48	0/349
7	H	0.35	0/530	0.51	0/723
7	h	0.34	0/524	0.50	0/713
8	I	0.37	0/311	0.49	0/419
8	i	0.37	0/311	0.52	0/419
9	J	0.36	0/278	0.48	0/376
9	j	0.37	0/283	0.50	0/383
10	K	0.36	0/303	0.54	0/416
10	k	0.32	0/303	0.51	0/416
11	L	0.43	0/311	0.48	0/423
11	l	0.39	0/311	0.50	0/423
12	M	0.44	0/261	0.55	0/357
12	m	0.44	0/262	0.60	0/357
13	O	0.37	0/1935	0.57	0/2623
13	o	0.37	0/1910	0.56	0/2589
14	T	0.51	0/257	0.56	0/349
14	t	0.52	0/257	0.52	0/349
15	U	0.40	0/776	0.58	0/1052
15	u	0.40	0/785	0.57	0/1064
16	V	0.38	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.37	0/1085	0.52	0/1473
17	X	0.35	0/284	0.48	0/384
17	x	0.31	0/284	0.49	0/384
18	Y	0.30	0/216	0.45	0/289
18	y	0.32	0/216	0.52	0/289
19	Z	0.32	0/490	0.45	0/669
19	z	0.34	0/490	0.45	0/669
20	R	0.28	0/279	0.43	0/383
All	All	0.41	0/42949	0.54	0/58445

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	2634	0	2546	32	0
1	a	2639	0	2554	0	0
2	B	4007	0	3879	73	0
2	b	3986	0	3855	0	0
3	C	3501	0	3428	52	0
3	c	3537	0	3471	0	0
4	D	2729	0	2632	25	0
4	d	2720	0	2626	0	0
5	E	665	0	653	19	0
5	e	648	0	634	0	0
6	F	275	0	282	7	0
6	f	250	0	261	0	0
7	H	514	0	542	9	0
7	h	511	0	532	0	0
8	I	314	0	328	5	0
8	i	314	0	328	0	0
9	J	272	0	279	4	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	9	0
10	k	293	0	305	0	0
11	L	301	0	315	4	0
11	l	301	0	315	0	0
12	M	265	0	286	8	0
12	m	269	0	288	0	0
13	O	1889	0	1871	27	0
13	o	1873	0	1852	0	0
14	T	258	0	261	6	0
14	t	258	0	261	0	0
15	U	765	0	767	8	0
15	u	774	0	773	0	0
16	V	1064	0	1073	8	0
16	v	1064	0	1073	0	0
17	X	281	0	312	7	0
17	x	281	0	312	0	0
18	Y	215	0	246	5	0
18	y	215	0	246	0	0
19	Z	479	0	516	7	0
19	z	479	0	516	0	0
20	R	273	0	305	5	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	260	0	288	22	0
23	B	1040	0	1152	77	0
23	C	845	0	936	86	0
23	D	130	0	144	8	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	195	0	216	0	0
24	A	64	0	74	6	0
24	D	64	0	74	1	0
24	a	128	0	148	0	0
25	A	40	0	56	2	0
25	B	120	0	168	12	0
25	C	80	0	112	8	0
25	D	40	0	56	2	0
25	H	40	0	56	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	K	40	0	56	1	0
25	T	40	0	56	6	0
25	Y	40	0	56	2	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	10	0
26	B	54	0	78	2	0
26	D	43	0	53	1	0
26	L	54	0	78	5	0
26	a	108	0	156	0	0
26	f	43	0	53	0	0
27	A	6	0	8	1	0
27	B	12	0	16	2	0
27	C	6	0	8	1	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	9	0
29	D	55	0	80	3	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	98	0	148	4	0
31	D	98	0	148	14	0
31	E	42	0	57	3	0
31	d	147	0	222	0	0
31	e	42	0	57	0	0
31	l	49	0	74	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	51	0	72	1	0
33	C	102	0	144	8	0
33	J	51	0	72	4	0
33	Z	88	0	116	4	0
33	a	51	0	72	0	0
33	b	51	0	72	0	0
33	c	102	0	144	0	0
33	j	51	0	72	0	0
33	z	39	0	48	0	0
34	B	76	0	104	6	0
34	C	38	0	52	2	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	76	0	104	0	0
34	c	38	0	52	0	0
34	d	16	0	17	0	0
35	B	86	0	116	4	0
35	D	70	0	92	3	0
35	E	35	0	46	1	0
35	I	35	0	46	1	0
35	M	70	0	92	3	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	C	186	0	246	13	0
36	H	62	0	82	1	0
36	c	186	0	246	0	0
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	V	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
38	E	43	0	30	5	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	127	0	0	2	0
40	B	175	0	0	4	0
40	C	148	0	0	2	0
40	D	111	0	0	1	0
40	E	18	0	0	1	0
40	F	5	0	0	0	0
40	H	19	0	0	0	0
40	I	6	0	0	1	0
40	J	5	0	0	1	0
40	K	6	0	0	0	0
40	L	9	0	0	0	0
40	M	14	0	0	1	0
40	O	100	0	0	1	0
40	T	10	0	0	1	0
40	U	46	0	0	0	0
40	V	79	0	0	3	0
40	X	3	0	0	0	0
40	Y	1	0	0	0	0
40	a	130	0	0	0	0
40	b	192	0	0	0	0
40	c	136	0	0	0	0
40	d	108	0	0	0	0
40	e	15	0	0	0	0
40	f	5	0	0	0	0
40	h	28	0	0	0	0
40	i	4	0	0	0	0
40	j	3	0	0	0	0
40	k	4	0	0	0	0
40	l	7	0	0	0	0
40	m	11	0	0	0	0
40	o	109	0	0	0	0
40	t	7	0	0	0	0
40	u	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	v	71	0	0	0	0
40	x	4	0	0	0	0
40	y	2	0	0	0	0
All	All	52773	0	52080	492	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 5.

All (492) 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)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.46	0.95
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.57	0.91
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.27	0.81
34:B:622:HTG:H1	35:B:630:LMT:H21	1.60	0.81
26:A:410:SQD:H251	31:D:409:LHG:H131	1.66	0.75
5:E:67:THR:H	5:E:75:GLN:HE22	2.81	0.75
1:A:25:ASP:OD1	40:A:501:HOH:O	2.05	0.75
5:E:9:PRO:HA	31:E:101:LHG:HC31	2.37	0.74
40:M:205:HOH:O	14:T:1:FME:SD	2.45	0.74
13:O:54:GLU:HG2	13:O:64:GLU:H	1.53	0.73
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.70	0.72
2:B:121:GLU:HG2	7:H:4:ARG:HG2	2.55	0.72
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.20	0.72
23:C:503:CLA:HBB1	23:C:512:CLA:H41	25.99	0.71
23:C:508:CLA:HBC3	23:C:510:CLA:H71	13.55	0.70
3:C:279:LEU:HD22	23:C:509:CLA:HED2	16.99	0.70
5:E:40:THR:HB	20:R:4:ARG:HG2	1.72	0.70
16:V:30:LYS:NZ	40:V:301:HOH:O	5.38	0.69
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.26	0.69
6:F:30:THR:HG21	33:J:101:LMG:H412	1.74	0.69
23:C:508:CLA:HBB1	23:C:508:CLA:HMB1	3.70	0.68
3:C:168:LEU:HD21	23:C:509:CLA:H61	24.42	0.68
25:B:618:BCR:H363	25:T:101:BCR:H19C	35.53	0.67
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.77	0.66
8:I:37:LEU:O	40:I:201:HOH:O	2.14	0.66
12:M:5:GLN:HE21	12:M:5:GLN:H	4.17	0.66
29:A:414:PL9:H253	23:D:404:CLA:H141	1.78	0.66
31:D:409:LHG:H372	31:D:409:LHG:H132	1.78	0.66
23:C:510:CLA:H192	23:C:510:CLA:HBC3	8.16	0.65
8:I:36:ASP:OD1	8:I:36:ASP:N	4.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:GLN:HB2	2:B:504:THR:HB	2.15	0.65
4:D:205:LEU:HD13	24:D:401:PHO:HAB	1.79	0.65
23:B:601:CLA:H12	23:B:601:CLA:H71	1.79	0.64
23:B:612:CLA:HMB1	23:B:612:CLA:HBB1	1.80	0.63
24:A:407:PHO:H3A	23:D:404:CLA:H142	1.80	0.63
23:A:408:CLA:H172	36:C:517:DGD:HAF1	1.79	0.63
13:O:124:ASN:ND2	13:O:147:ASN:HD22	1.97	0.63
23:A:408:CLA:H171	23:C:507:CLA:H142	1.81	0.63
8:I:35:LYS:O	8:I:37:LEU:N	2.73	0.63
31:D:409:LHG:H372	31:D:409:LHG:H142	3.85	0.63
2:B:145:LEU:HD11	23:B:615:CLA:HMB2	1.80	0.63
2:B:103:LEU:HD21	23:B:605:CLA:HMC3	1.81	0.62
13:O:27:ARG:NH1	13:O:202:ALA:O	2.32	0.62
33:C:501:LMG:H211	36:C:517:DGD:HA82	1.81	0.62
1:A:253:GLY:HA3	2:B:491:VAL:HG12	4.12	0.61
1:A:40:THR:HG23	23:A:408:CLA:HBB1	2.16	0.61
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.82	0.61
23:C:505:CLA:CMD	23:C:507:CLA:HAB	34.12	0.61
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.82	0.61
3:C:182:PHE:HA	34:C:521:HTG:H61	1.87	0.61
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.83	0.61
2:B:462:PHE:CE1	23:B:613:CLA:HMB3	2.37	0.61
16:V:118:HIS:ND1	40:V:301:HOH:O	2.31	0.61
23:A:406:CLA:H152	29:A:414:PL9:H252	1.82	0.60
3:C:218:PHE:HE2	33:C:501:LMG:H111	1.67	0.60
23:C:507:CLA:HMC2	23:C:508:CLA:H102	1.84	0.60
2:B:285:ASN:O	2:B:289:GLN:HG2	2.01	0.60
23:D:404:CLA:H162	7:H:37:LEU:HD21	38.01	0.59
31:D:408:LHG:HC62	11:L:15:THR:HG23	1.85	0.59
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.38	0.59
34:B:623:HTG:O6	13:O:177:ALA:O	2.21	0.59
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.84	0.59
23:C:505:CLA:HMD2	23:C:507:CLA:HAB	34.21	0.59
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.84	0.58
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.15	0.58
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.32	0.58
8:I:17:LEU:HD22	8:I:21:PHE:HE2	1.75	0.58
5:E:27:ILE:HD11	38:E:103:HEM:HBC2	1.88	0.57
25:T:101:BCR:HC8	25:T:101:BCR:H321	1.86	0.57
33:Z:102:LMG:O4	33:Z:102:LMG:O5	2.23	0.57
12:M:8:LEU:HD11	35:M:103:LMT:H91	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:438:LEU:HD11	23:C:505:CLA:HBB1	19.87	0.57
2:B:18:ARG:NH2	26:L:101:SQD:O9	38.11	0.57
23:A:406:CLA:HMD3	4:D:182:LEU:HD11	1.87	0.57
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.85	0.57
31:A:417:LHG:H201	11:L:26:VAL:HG11	1.87	0.56
13:O:92:SER:HB3	13:O:131:PRO:HA	1.88	0.56
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	9.44	0.56
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.70	0.56
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.88	0.56
26:A:410:SQD:H301	23:C:508:CLA:H71	36.79	0.56
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.03	0.56
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.88	0.56
7:H:56:ASP:OD1	17:X:2:THR:OG1	3.89	0.56
31:A:417:LHG:H191	29:D:407:PL9:H201	1.88	0.55
8:I:2:GLU:O	8:I:6:ILE:HG12	2.19	0.55
23:A:405:CLA:HMD3	4:D:182:LEU:HD11	10.79	0.55
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.89	0.55
23:C:509:CLA:H192	23:C:512:CLA:HHD	13.39	0.55
1:A:187:GLN:HB2	23:A:404:CLA:HAC2	1.88	0.55
23:B:601:CLA:HAC1	25:H:101:BCR:H383	2.16	0.55
4:D:24:ARG:HD3	17:X:37:VAL:HG22	2.26	0.55
23:B:609:CLA:HMD1	7:H:27:THR:HB	2.00	0.54
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.54
16:V:6:GLU:OE2	16:V:6:GLU:N	2.40	0.54
23:B:602:CLA:H101	23:B:609:CLA:H193	1.95	0.54
23:C:513:CLA:O2D	23:C:514:CLA:HBB2	2.08	0.54
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.70	0.54
2:B:57:ARG:HH21	2:B:331:ASN:HD22	1.56	0.54
3:C:174:LEU:HB3	23:C:502:CLA:H152	21.90	0.53
23:C:507:CLA:H71	35:I:101:LMT:H111	1.89	0.53
23:C:506:CLA:H71	25:C:515:BCR:H10C	42.99	0.53
23:B:612:CLA:H171	23:B:613:CLA:HBB2	2.20	0.53
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.39	0.53
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.91	0.53
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.99	0.53
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.91	0.53
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.53	0.52
23:A:408:CLA:H152	36:C:517:DGD:HAW2	1.91	0.52
25:D:406:BCR:H383	33:J:101:LMG:H171	1.90	0.52
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.43	0.52
3:C:181:PHE:HE2	34:C:522:HTG:H7'3	1.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:614:CLA:H43	26:B:620:SQD:H111	1.91	0.52
1:A:183:MET:HA	23:A:404:CLA:HMD2	1.94	0.52
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.14	0.52
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.93	0.52
3:C:41:ARG:NH1	23:C:511:CLA:HMD1	17.19	0.52
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.80	0.52
23:C:504:CLA:H42	36:C:517:DGD:HB42	17.45	0.51
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.25	0.51
5:E:27:ILE:CD1	38:E:103:HEM:HBC2	2.40	0.51
5:E:36:LEU:HA	5:E:39:SER:OG	2.09	0.51
1:A:227:THR:HB	1:A:231:GLU:HG3	1.96	0.51
26:A:410:SQD:H192	31:D:409:LHG:H201	1.92	0.51
23:C:512:CLA:H143	23:C:513:CLA:H142	28.41	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.51
4:D:49:LEU:HD13	25:D:406:BCR:C15	2.41	0.51
12:M:5:GLN:NE2	12:M:5:GLN:H	4.39	0.51
23:B:601:CLA:H2	23:B:601:CLA:H72	4.47	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.51
13:O:58:ASN:HD21	13:O:61:GLN:HB2	4.37	0.51
23:A:406:CLA:HED1	36:C:519:DGD:HAE2	1.92	0.51
3:C:429:SER:HA	36:C:517:DGD:HBW1	13.34	0.51
23:B:609:CLA:HBB1	23:B:609:CLA:HHC	1.91	0.51
2:B:341:LYS:NZ	34:B:622:HTG:S1	35.79	0.51
3:C:38:GLY:HA3	23:C:511:CLA:HMD3	15.12	0.51
3:C:56:HIS:HB2	23:C:509:CLA:HMB2	7.54	0.51
31:D:409:LHG:H122	31:D:409:LHG:C38	4.96	0.51
3:C:363:GLY:O	3:C:367:GLU:HG2	2.18	0.50
23:C:512:CLA:O2D	23:C:513:CLA:HBB2	25.24	0.50
13:O:81:ILE:HA	13:O:100:GLY:HA3	1.93	0.50
23:A:408:CLA:H151	23:C:507:CLA:H13	1.93	0.50
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.93	0.50
23:B:605:CLA:HBD	23:B:605:CLA:HAA1	1.93	0.50
3:C:325:GLY:O	15:U:51:LYS:NZ	2.44	0.50
9:J:18:MET:O	9:J:22:VAL:HG23	2.12	0.49
1:A:226:GLU:OE2	40:A:501:HOH:O	30.54	0.49
3:C:186:TYR:OH	3:C:194:GLY:HA3	2.13	0.49
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.49
10:K:17:ILE:H	10:K:17:ILE:HD13	1.77	0.49
23:B:614:CLA:H162	23:B:614:CLA:H122	4.63	0.49
23:B:614:CLA:H41	23:B:614:CLA:H62	1.56	0.49
29:A:414:PL9:H262	31:E:101:LHG:H201	4.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:D:413:SQD:H241	6:F:18:VAL:HG22	1.94	0.49
31:D:409:LHG:H122	31:D:409:LHG:H382	4.47	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.13	0.48
23:B:605:CLA:HMA1	23:B:606:CLA:H3A	2.04	0.48
33:B:621:LMG:O10	12:M:4:ASN:ND2	2.45	0.48
3:C:433:LEU:HD22	23:C:503:CLA:HMC3	1.94	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.48	0.48
23:B:605:CLA:H41	23:B:605:CLA:H62	2.44	0.48
3:C:78:GLU:HB3	40:V:321:HOH:O	31.40	0.48
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.42	0.48
2:B:462:PHE:HE1	23:B:613:CLA:HMB3	1.78	0.48
3:C:406:SER:HA	3:C:420:VAL:HG23	1.95	0.48
23:C:504:CLA:H151	23:C:508:CLA:H143	20.29	0.48
23:D:404:CLA:H112	23:D:404:CLA:H142	2.14	0.48
13:O:210:GLU:OE2	13:O:240:TYR:OH	2.61	0.48
23:B:610:CLA:HHC	23:B:610:CLA:HBB1	2.17	0.48
14:T:2:GLU:CD	14:T:2:GLU:H	2.17	0.48
2:B:245:VAL:HG22	23:B:612:CLA:H202	1.95	0.48
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.96	0.48
2:B:497:GLN:HE22	17:X:38:GLN:HB2	2.23	0.48
23:A:408:CLA:H171	23:C:507:CLA:H112	1.95	0.48
34:B:622:HTG:H61	35:B:630:LMT:H6E	1.95	0.48
33:C:520:LMG:H232	33:C:520:LMG:H391	9.48	0.48
2:B:299:GLU:HG2	2:B:402:TYR:HD1	1.79	0.47
23:C:512:CLA:HHC	23:C:512:CLA:HBB1	4.60	0.47
23:C:506:CLA:HMD2	23:C:508:CLA:HAB	1.93	0.47
26:L:101:SQD:H1	26:L:101:SQD:H462	1.97	0.47
3:C:174:LEU:HD22	23:C:502:CLA:H203	24.14	0.47
5:E:26:THR:HB	38:E:103:HEM:HAB	2.53	0.47
1:A:214:MET:HG2	29:A:414:PL9:H103	2.00	0.47
5:E:67:THR:N	5:E:75:GLN:HE22	3.43	0.47
12:M:5:GLN:HE21	12:M:5:GLN:N	4.68	0.47
4:D:12:ARG:HH12	17:X:39:ARG:NH1	2.13	0.47
23:C:507:CLA:H2	25:C:516:BCR:H10C	1.95	0.47
1:A:217:SER:HA	4:D:272:LEU:HD12	1.97	0.47
5:E:68:ASP:OD1	5:E:71:GLU:HB2	2.32	0.47
23:A:406:CLA:HMB3	24:A:407:PHO:H172	1.95	0.47
31:A:416:LHG:H361	23:B:613:CLA:H51	1.96	0.47
3:C:391:ARG:HD3	40:C:715:HOH:O	2.14	0.47
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.95	0.47
2:B:283:GLU:OE2	2:B:287:ARG:NH1	4.81	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:408:LHG:H192	14:T:17:PHE:HZ	1.80	0.47
13:O:83:GLY:HA2	13:O:98:GLU:HG3	2.23	0.47
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.49	0.47
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.50	0.47
26:A:410:SQD:H271	31:D:409:LHG:H141	4.57	0.47
29:A:414:PL9:H171	29:A:414:PL9:H151	1.57	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.51	0.46
3:C:146:PHE:HZ	23:C:512:CLA:HBB2	25.04	0.46
23:C:505:CLA:HAA1	23:C:505:CLA:HBD	2.17	0.46
2:B:216:HIS:CE1	23:B:609:CLA:NA	2.82	0.46
2:B:357:ARG:HB3	40:B:746:HOH:O	18.29	0.46
25:C:515:BCR:H15C	25:C:515:BCR:H351	1.79	0.46
3:C:53:HIS:CB	23:C:513:CLA:HMD1	2.46	0.46
23:D:404:CLA:H61	23:D:404:CLA:H41	3.54	0.46
23:B:608:CLA:H191	4:D:89:LEU:HD13	1.98	0.46
6:F:21:VAL:O	6:F:25:THR:HG23	2.16	0.46
11:L:9:PRO:HA	35:M:101:LMT:H6D	17.24	0.46
23:A:404:CLA:HBB1	23:A:404:CLA:HMB1	1.96	0.46
23:B:608:CLA:H102	4:D:120:PHE:CE1	3.06	0.46
23:B:615:CLA:H152	23:B:615:CLA:H112	1.56	0.46
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.97	0.46
23:C:514:CLA:H152	33:Z:101:LMG:H412	1.96	0.46
23:C:505:CLA:H62	23:C:505:CLA:H41	1.68	0.46
2:B:36[A]:SER:OG	25:B:618:BCR:H362	2.16	0.46
23:B:615:CLA:HBB1	23:B:615:CLA:HHC	1.97	0.46
25:B:619:BCR:C8	25:B:619:BCR:H331	2.46	0.46
23:C:506:CLA:HMD3	23:C:508:CLA:HAB	1.95	0.46
7:H:25:TRP:O	7:H:28:THR:OG1	2.28	0.46
24:A:407:PHO:HBC3	4:D:279:LEU:HD22	2.09	0.46
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.81	0.46
23:A:408:CLA:H152	23:C:506:CLA:H101	8.12	0.46
23:C:507:CLA:H91	23:C:507:CLA:H111	1.80	0.46
12:M:28:GLN:O	12:M:32:GLN:HG3	2.16	0.46
25:B:617:BCR:H371	25:B:617:BCR:H24C	1.86	0.45
3:C:27:ASP:HB3	10:K:46:ARG:HG3	2.63	0.45
26:A:410:SQD:H141	31:D:409:LHG:H152	3.53	0.45
36:C:518:DGD:HBH2	31:D:409:LHG:H211	12.15	0.45
13:O:32:ILE:HG21	13:O:93:LEU:HD21	1.99	0.45
2:B:363:PHE:HB3	2:B:365:SER:O	2.16	0.45
2:B:489:GLU:HB3	2:B:495:PHE:CG	2.51	0.45
23:B:614:CLA:H92	35:M:101:LMT:H101	15.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.99	0.45
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.75	0.45
11:L:20:GLY:O	11:L:24[A]:ILE:HG12	2.16	0.45
3:C:38:GLY:HA3	23:C:512:CLA:HMD3	1.98	0.45
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.51	0.45
2:B:220:ARG:HG3	7:H:20:LYS:HG2	2.23	0.45
1:A:163:ILE:HD11	36:C:517:DGD:HA22	1.99	0.45
23:B:603:CLA:C4D	23:B:605:CLA:H43	2.47	0.45
2:B:86:ILE:HD12	2:B:88:PRO:HD3	2.19	0.45
3:C:437:PHE:CZ	23:C:511:CLA:HMB3	2.51	0.45
33:C:501:LMG:H152	36:C:517:DGD:HA91	1.99	0.45
13:O:39:ARG:NH2	13:O:98:GLU:OE1	3.53	0.45
23:C:514:CLA:H172	33:Z:101:LMG:H402	1.98	0.45
1:A:12:ASN:O	1:A:16:ARG:HG3	2.17	0.45
2:B:490:GLN:HG3	2:B:496:TYR:HE2	2.36	0.45
23:B:604:CLA:HMB1	23:B:604:CLA:HBB1	1.97	0.45
2:B:54:PRO:HB3	27:B:626:GOL:H11	1.99	0.45
23:C:506:CLA:HBD	23:C:506:CLA:HAA1	1.99	0.45
26:L:101:SQD:H332	26:L:101:SQD:H302	1.80	0.45
40:D:576:HOH:O	17:X:6:SER:HA	49.61	0.45
26:B:620:SQD:H383	26:B:620:SQD:H351	1.84	0.45
3:C:56:HIS:HB2	23:C:510:CLA:HMB2	1.98	0.45
4:D:186:GLN:HB2	23:D:404:CLA:HBC1	1.99	0.45
25:H:101:BCR:C8	25:H:101:BCR:H331	2.47	0.45
25:K:102:BCR:H371	25:K:102:BCR:H24C	1.68	0.45
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.04	0.45
23:B:616:CLA:H92	23:B:616:CLA:H62	2.21	0.45
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.44
2:B:299:GLU:HG3	40:B:800:HOH:O	2.17	0.44
2:B:497:GLN:NE2	17:X:38:GLN:O	2.46	0.44
25:B:618:BCR:H351	25:B:618:BCR:H15C	1.78	0.44
23:A:408:CLA:H143	23:C:506:CLA:H192	2.00	0.44
23:C:508:CLA:H93	31:D:409:LHG:H162	35.39	0.44
38:E:103:HEM:HAC	6:F:27:ALA:HB1	1.98	0.44
26:A:412:SQD:H262	26:A:412:SQD:H292	1.72	0.44
31:A:416:LHG:H312	31:A:416:LHG:H282	1.74	0.44
23:B:614:CLA:H101	25:B:617:BCR:H362	2.50	0.44
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.02	0.44
23:C:509:CLA:H62	23:C:509:CLA:H92	2.66	0.44
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.99	0.44
5:E:66:VAL:HA	5:E:75:GLN:NE2	4.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.99	0.44
23:A:404:CLA:H191	31:D:408:LHG:H321	2.79	0.44
27:A:411:GOL:H11	34:B:622:HTG:O5	59.21	0.44
3:C:203:THR:O	3:C:235:GLY:HA3	2.18	0.44
23:C:510:CLA:H61	23:C:510:CLA:H102	4.09	0.44
23:B:615:CLA:H61	23:B:615:CLA:H92	3.14	0.44
23:A:408:CLA:H152	23:C:506:CLA:H142	5.64	0.44
23:B:603:CLA:H141	23:B:603:CLA:H161	2.55	0.44
23:B:604:CLA:H62	23:B:604:CLA:H41	1.74	0.44
23:B:616:CLA:H11	23:B:616:CLA:H51	1.81	0.44
3:C:154:LYS:HG2	3:C:266:TRP:CE3	2.53	0.44
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.99	0.44
23:C:504:CLA:HBB2	23:C:513:CLA:H92	2.00	0.44
23:C:508:CLA:H62	23:C:508:CLA:H41	1.75	0.44
1:A:72:LEU:HD11	35:B:630:LMT:H52	43.41	0.44
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.09	0.44
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.99	0.44
23:C:514:CLA:HAB	25:C:515:BCR:H24C	1.99	0.44
35:E:102:LMT:O6'	40:E:201:HOH:O	2.21	0.44
1:A:214:MET:HG2	29:A:414:PL9:C10	2.48	0.44
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.88	0.44
4:D:185:PHE:CG	23:D:404:CLA:HMD3	2.53	0.44
9:J:6:ARG:HG3	40:J:201:HOH:O	2.17	0.44
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	2.00	0.44
2:B:54:PRO:HD2	2:B:57:ARG:HG3	2.00	0.44
3:C:171:GLY:O	3:C:174:LEU:HB2	2.32	0.44
13:O:124:ASN:HD22	13:O:147:ASN:ND2	2.05	0.44
15:U:48:LEU:O	15:U:52:ASN:ND2	2.41	0.44
29:A:414:PL9:H503	17:X:24:THR:OG1	2.37	0.43
23:C:507:CLA:H62	23:C:507:CLA:H41	1.83	0.43
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.88	0.43
25:A:409:BCR:H341	25:A:409:BCR:H11C	1.95	0.43
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.80	0.43
2:B:360:PRO:HB3	27:B:625:GOL:H32	1.99	0.43
33:C:501:LMG:H161	33:C:501:LMG:H191	1.80	0.43
23:C:513:CLA:H161	23:C:513:CLA:H203	2.21	0.43
23:A:405:CLA:HED1	36:C:518:DGD:HAE2	37.67	0.43
23:B:603:CLA:H3A	23:B:603:CLA:CGA	2.54	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	2.00	0.43
1:A:341:LEU:HD13	27:C:523:GOL:H31	1.99	0.43
7:H:43:LEU:HD12	7:H:43:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:VAL:O	40:B:702:HOH:O	62.19	0.43
38:E:103:HEM:CAC	6:F:27:ALA:HB1	2.59	0.43
5:E:26:THR:HA	20:R:15:ALA:HB1	2.00	0.43
13:O:18:LYS:HD3	40:O:460:HOH:O	2.17	0.43
34:B:622:HTG:H3'1	34:B:622:HTG:H6'2	1.94	0.43
25:H:101:BCR:H11C	25:H:101:BCR:H341	1.79	0.43
26:L:101:SQD:H211	25:T:101:BCR:H351	1.99	0.43
23:C:514:CLA:H162	23:C:514:CLA:H141	1.82	0.43
2:B:39:LEU:HD22	35:D:402:LMT:H51	47.73	0.43
33:C:501:LMG:H232	23:C:506:CLA:H92	2.00	0.43
23:C:509:CLA:H142	23:C:509:CLA:H111	1.71	0.43
25:H:101:BCR:HC8	25:H:101:BCR:H331	2.00	0.43
24:A:407:PHO:H72	24:A:407:PHO:H112	1.91	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.19	0.43
23:B:611:CLA:HBB1	23:B:611:CLA:HMB1	2.25	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.43
2:B:102:VAL:HA	25:B:618:BCR:C40	2.49	0.43
3:C:294:ASN:HA	3:C:297:TYR:O	2.30	0.43
23:C:505:CLA:HBB1	23:C:505:CLA:HMB1	2.01	0.43
23:C:508:CLA:H122	23:C:508:CLA:H162	4.23	0.43
36:C:518:DGD:HAF2	36:C:518:DGD:HAE2	1.86	0.43
3:C:60:ILE:HG22	23:C:504:CLA:HHH	1.99	0.43
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.64	0.43
33:J:101:LMG:H242	33:J:101:LMG:H341	7.32	0.43
25:Y:101:BCR:H351	25:Y:101:BCR:H15C	1.88	0.43
2:B:101:ILE:O	2:B:104:SER:HB3	2.24	0.42
2:B:58:GLN:C	2:B:329:PRO:HB3	2.39	0.42
2:B:61:PHE:CZ	23:B:607:CLA:HBB1	2.54	0.42
23:B:609:CLA:C3B	25:H:101:BCR:H323	2.53	0.42
23:B:606:CLA:H192	23:B:616:CLA:H101	2.01	0.42
23:C:505:CLA:H112	23:C:505:CLA:H72	4.45	0.42
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.97	0.42
2:B:338:GLN:HA	13:O:57:LYS:HE3	40.31	0.42
23:B:602:CLA:H162	23:B:602:CLA:H203	1.75	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.62	0.42
3:C:48:LYS:HG2	3:C:133:ALA:O	2.46	0.42
20:R:29:LYS:HE2	20:R:29:LYS:HB3	1.79	0.42
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.21	0.42
23:B:603:CLA:HBB2	23:B:605:CLA:H193	2.35	0.42
35:B:629:LMT:H2'	40:T:203:HOH:O	46.62	0.42
3:C:42:LEU:HD11	23:C:511:CLA:HMA3	12.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:E:101:LHG:H261	31:E:101:LHG:H291	1.71	0.42
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.56	0.42
23:A:404:CLA:H193	23:A:404:CLA:H161	3.31	0.42
23:A:405:CLA:HED1	29:D:407:PL9:H362	2.01	0.42
2:B:124:ARG:HD2	2:B:129:GLY:O	2.43	0.42
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	2.07	0.42
2:B:133:LEU:HB3	2:B:138:MET:SD	2.59	0.42
35:D:403:LMT:O2B	30:D:411:UNL:O6	2.37	0.42
23:B:616:CLA:H111	23:B:616:CLA:H152	1.68	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.90	0.42
23:C:506:CLA:H122	23:C:506:CLA:H162	4.29	0.42
23:B:614:CLA:H61	23:B:614:CLA:H92	1.67	0.42
35:D:403:LMT:H62	35:D:403:LMT:H91	1.81	0.42
23:B:602:CLA:H92	36:H:102:DGD:HB71	2.00	0.42
18:Y:38:LEU:O	18:Y:42:ARG:HG2	3.96	0.42
19:Z:56:VAL:HG12	19:Z:60:PHE:HE1	2.31	0.42
1:A:133:LEU:HD12	1:A:133:LEU:HA	1.89	0.42
23:B:610:CLA:H122	23:B:615:CLA:HAA1	2.00	0.42
18:Y:30:ILE:HA	18:Y:30:ILE:HD12	1.86	0.42
10:K:16:ALA:O	10:K:19:ASP:HB2	2.28	0.42
1:A:274:PHE:HD1	26:A:410:SQD:H101	1.85	0.42
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.42
23:B:602:CLA:H111	23:B:602:CLA:H91	1.84	0.42
25:B:618:BCR:H361	25:B:618:BCR:H20C	2.12	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.02	0.42
25:A:409:BCR:H351	25:A:409:BCR:H15C	1.85	0.41
2:B:214:LEU:HD23	2:B:214:LEU:HA	1.88	0.41
3:C:161:LEU:HD11	23:C:507:CLA:HBB1	2.02	0.41
23:C:508:CLA:H92	23:C:508:CLA:H61	1.88	0.41
25:C:515:BCR:H24C	25:C:515:BCR:H371	1.88	0.41
6:F:34:LEU:HD23	6:F:34:LEU:HA	1.93	0.41
2:B:502:VAL:O	2:B:505:ARG:HG3	2.20	0.41
25:B:619:BCR:H351	25:B:619:BCR:H15C	1.88	0.41
36:C:517:DGD:HA91	36:C:518:DGD:HBF2	27.02	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
4:D:293:LEU:HA	4:D:293:LEU:HD12	2.06	0.41
26:L:101:SQD:H212	26:L:101:SQD:H181	1.86	0.41
13:O:51:LEU:HD23	13:O:67:PRO:HA	2.09	0.41
15:U:45:LEU:HA	15:U:45:LEU:HD23	1.87	0.41
1:A:281:VAL:HG12	26:A:410:SQD:H201	5.23	0.41
23:B:601:CLA:H42	23:B:601:CLA:OBD	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:605:CLA:H92	23:B:605:CLA:H61	1.75	0.41
2:B:149:LEU:HG	23:B:606:CLA:HBB2	2.02	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CD2	2.55	0.41
3:C:433:LEU:HD13	23:C:503:CLA:CHC	2.51	0.41
23:C:502:CLA:H151	23:C:508:CLA:HMB3	2.02	0.41
23:C:513:CLA:HBA1	23:C:513:CLA:C4A	4.80	0.41
1:A:265:PHE:HE2	29:A:414:PL9:H111	1.96	0.41
23:B:614:CLA:HBD	23:B:614:CLA:HAA1	2.01	0.41
23:C:509:CLA:H112	23:C:509:CLA:H91	1.82	0.41
31:D:409:LHG:H372	31:D:409:LHG:C13	2.50	0.41
23:B:604:CLA:H91	23:B:604:CLA:H111	2.10	0.41
23:C:506:CLA:H101	23:C:506:CLA:H61	1.79	0.41
25:C:515:BCR:H20C	25:C:515:BCR:H361	1.85	0.41
15:U:24:LYS:HB3	15:U:81:HIS:O	2.21	0.41
23:B:604:CLA:HAB	23:B:611:CLA:H191	2.02	0.41
23:B:611:CLA:H92	23:B:611:CLA:H62	1.91	0.41
33:C:501:LMG:H121	23:C:506:CLA:H201	2.02	0.41
9:J:3:GLU:O	9:J:6:ARG:HG2	2.86	0.41
20:R:31:VAL:O	20:R:35:LEU:HG	2.21	0.41
15:U:64:ILE:HA	15:U:65:PRO:HD3	1.85	0.41
1:A:182:PHE:O	1:A:186:PHE:HB2	2.31	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD3	2.02	0.41
5:E:25:ILE:O	5:E:28:PRO:HD2	2.21	0.41
10:K:26:PRO:O	10:K:29:PRO:HD2	2.24	0.41
5:E:42:LEU:HA	20:R:4:ARG:HH21	1.85	0.41
16:V:93:PRO:HA	16:V:101:PHE:CD2	2.56	0.41
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.28	0.41
23:B:608:CLA:H3A	23:B:608:CLA:HBA2	1.99	0.41
23:C:507:CLA:H112	23:C:507:CLA:H142	1.94	0.41
25:C:516:BCR:H371	25:C:516:BCR:H24C	1.82	0.41
13:O:140:THR:O	13:O:201:VAL:HB	2.46	0.41
1:A:121[A]:LEU:HG	33:C:501:LMG:H182	2.02	0.41
23:B:605:CLA:H91	23:B:605:CLA:H111	2.38	0.41
23:B:613:CLA:H203	23:B:613:CLA:H161	4.46	0.41
23:B:616:CLA:H112	23:B:616:CLA:H91	1.80	0.41
25:B:619:BCR:H24C	25:B:619:BCR:H371	1.80	0.41
23:C:506:CLA:H93	23:C:506:CLA:H111	1.87	0.41
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.21	0.41
40:C:609:HOH:O	10:K:25:LEU:HB2	32.06	0.41
13:O:30:TYR:HA	13:O:31:PRO:HD3	1.89	0.41
16:V:80:THR:HA	16:V:86:GLN:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:611:CLA:H172	23:B:613:CLA:ND	4.05	0.41
23:C:502:CLA:HMD2	23:C:503:CLA:H101	2.02	0.41
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.66	0.41
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.86	0.41
1:A:45:THR:HG21	26:A:412:SQD:H202	2.03	0.41
2:B:157:HIS:HE1	23:B:606:CLA:NA	2.19	0.41
2:B:223:GLN:HA	2:B:223:GLN:HE21	3.79	0.41
23:B:615:CLA:HBA1	23:B:615:CLA:H3A	2.07	0.41
3:C:154:LYS:HE3	3:C:266:TRP:CE2	2.55	0.41
23:C:506:CLA:HMC2	23:C:507:CLA:H102	9.97	0.41
4:D:223:PHE:CZ	4:D:245:SER:HB2	2.56	0.41
33:J:101:LMG:H231	33:J:101:LMG:H191	2.03	0.41
12:M:6:LEU:HA	12:M:6:LEU:HD23	2.11	0.41
10:K:15:TYR:CE1	19:Z:5:PHE:HZ	2.39	0.41
1:A:210:LEU:HG	24:A:407:PHO:NC	2.47	0.40
2:B:191:ASN:HA	2:B:192:PRO:HD2	1.96	0.40
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.03	0.40
23:D:404:CLA:H62	23:D:404:CLA:H92	2.51	0.40
5:E:66:VAL:HA	5:E:75:GLN:HE22	4.35	0.40
23:B:609:CLA:C2B	25:H:101:BCR:H323	2.73	0.40
14:T:14:ILE:HG22	25:T:101:BCR:H10C	2.18	0.40
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.03	0.40
24:A:407:PHO:HHD	24:A:407:PHO:HBC2	2.04	0.40
2:B:159:THR:HA	2:B:181:VAL:O	2.27	0.40
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.93	0.40
23:B:604:CLA:HBD	23:B:604:CLA:HAA1	2.15	0.40
23:B:607:CLA:HMC2	25:B:618:BCR:H321	2.69	0.40
3:C:135:ARG:HD2	3:C:135:ARG:HA	2.05	0.40
3:C:137:PRO:HG3	23:C:514:CLA:HED3	2.02	0.40
23:A:405:CLA:H92	23:A:405:CLA:H62	1.89	0.40
2:B:423:LYS:NZ	40:B:709:HOH:O	34.49	0.40
2:B:201:HIS:HB2	23:B:602:CLA:CHB	2.51	0.40
2:B:450:TRP:HB3	23:B:607:CLA:HMB2	2.02	0.40
2:B:63:LEU:N	2:B:64:PRO:HD2	2.46	0.40
36:C:518:DGD:HAE2	36:C:518:DGD:HA81	1.80	0.40
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.57	0.40
10:K:28:ILE:HD11	18:Y:28:ILE:HD13	2.20	0.40
19:Z:48:ILE:HD11	33:Z:101:LMG:H192	19.67	0.40
29:A:414:PL9:H251	29:A:414:PL9:H272	1.91	0.40
26:A:412:SQD:H261	2:B:109:LEU:HD13	59.40	0.40
2:B:24:LEU:HD21	23:B:616:CLA:CAB	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:612:CLA:H162	23:B:612:CLA:H122	1.91	0.40
3:C:139:THR:OG1	3:C:142:GLU:OE2	2.38	0.40
4:D:202:ALA:HB2	29:D:407:PL9:H353	2.04	0.40
5:E:68:ASP:O	5:E:72:ALA:HB2	2.31	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.87	0.40
16:V:41:HIS:HA	16:V:45:ILE:O	2.21	0.40
2:B:482:ILE:HD12	2:B:486:LEU:HD22	2.04	0.40
23:B:612:CLA:HAA1	23:B:612:CLA:HBD	2.15	0.40
3:C:25:ASN:O	3:C:41:ARG:HD3	2.20	0.40
23:C:513:CLA:H101	23:C:514:CLA:H141	2.02	0.40
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.84	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	335/344 (97%)	328 (98%)	6 (2%)	1 (0%)	44	66
1	a	337/344 (98%)	330 (98%)	6 (2%)	1 (0%)	44	66
2	B	510/505 (101%)	504 (99%)	6 (1%)	0	100	100
2	b	506/505 (100%)	499 (99%)	7 (1%)	0	100	100
3	C	453/455 (100%)	441 (97%)	10 (2%)	2 (0%)	38	59
3	c	458/455 (101%)	445 (97%)	11 (2%)	2 (0%)	38	59
4	D	341/342 (100%)	332 (97%)	9 (3%)	0	100	100
4	d	340/342 (99%)	334 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	75 (97%)	2 (3%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	60 (95%)	3 (5%)	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	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	238 (97%)	8 (3%)	0	100	100
13	o	243/244 (100%)	234 (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%)	91 (97%)	3 (3%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	128 (95%)	7 (5%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	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%)	24 (89%)	3 (11%)	0	100	100
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	5255/5384 (98%)	5126 (98%)	120 (2%)	9 (0%)	55	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	Z	30	PRO
19	z	30	PRO
1	A	259	ILE
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	272/279 (98%)	271 (100%)	1 (0%)	93	98
1	a	274/279 (98%)	273 (100%)	1 (0%)	93	98
2	B	410/403 (102%)	403 (98%)	7 (2%)	66	87
2	b	406/403 (101%)	397 (98%)	9 (2%)	57	82
3	C	356/356 (100%)	351 (99%)	5 (1%)	71	90
3	c	361/356 (101%)	353 (98%)	8 (2%)	57	82
4	D	278/277 (100%)	277 (100%)	1 (0%)	93	98
4	d	277/277 (100%)	276 (100%)	1 (0%)	93	98
5	E	73/73 (100%)	72 (99%)	1 (1%)	71	90
5	e	70/73 (96%)	68 (97%)	2 (3%)	48	75
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	36	62
7	H	55/54 (102%)	52 (94%)	3 (6%)	25	46
7	h	54/54 (100%)	53 (98%)	1 (2%)	62	85
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	26/27 (96%)	24 (92%)	2 (8%)	15	28
10	K	30/30 (100%)	27 (90%)	3 (10%)	9	17
10	k	30/30 (100%)	27 (90%)	3 (10%)	9	17
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	35/35 (100%)	35 (100%)	0	100	100
12	M	30/32 (94%)	29 (97%)	1 (3%)	43	70
12	m	30/32 (94%)	29 (97%)	1 (3%)	43	70
13	O	211/207 (102%)	207 (98%)	4 (2%)	62	85
13	o	208/207 (100%)	203 (98%)	5 (2%)	54	80
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%)	84 (100%)	0	100	100
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%)	31 (100%)	0	100	100
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%)	21 (96%)	1 (4%)	32	56
19	Z	52/52 (100%)	50 (96%)	2 (4%)	38	64
19	z	52/52 (100%)	51 (98%)	1 (2%)	62	85
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4360/4403 (99%)	4288 (98%)	72 (2%)	68	87

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
2	B	53	ASN
2	B	223	GLN
2	B	362	PHE
2	B	472	ARG
2	B	489	GLU
2	B	492	GLU

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Mol	Chain	Res	Type
2	B	505	ARG
3	C	25	ASN
3	C	207	ARG
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	180	ARG
5	E	71	GLU
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
8	I	33	LYS
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
12	M	33	GLN
13	O	24	ASP
13	O	69	LYS
13	O	118	LEU
13	O	181	GLU
14	T	2	GLU
15	U	70	ARG
19	Z	3	ILE
19	Z	6	GLN
1	a	12	ASN
2	b	36	SER
2	b	53	ASN
2	b	121	GLU
2	b	223	GLN
2	b	362	PHE
2	b	431	GLU
2	b	472	ARG
2	b	485	GLU
2	b	505	ARG
3	c	19	ASN
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	462[A]	GLU

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Mol	Chain	Res	Type
3	c	462[B]	GLU
3	c	468	SER
4	d	180	ARG
5	e	62	SER
5	e	71	GLU
6	f	15	ILE
7	h	49	TYR
8	i	33	LYS
8	i	36	ASP
9	j	2	SER
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	19	ASP
12	m	5	GLN
13	o	24	ASP
13	o	69	LYS
13	o	118	LEU
13	o	132	ASN
13	o	181	GLU
14	t	2	GLU
18	y	45	ASN
19	z	6	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) 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
12	M	5	GLN
13	O	124	ASN
13	O	130	GLN
15	U	73	GLN
15	U	78	ASN
15	U	81	HIS
17	X	33	GLN

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Mol	Chain	Res	Type
19	Z	58	ASN
2	b	14	ASN
2	b	53	ASN
2	b	223	GLN
2	b	331	ASN
3	c	201	ASN
4	d	83	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	0.54	0	7,9,11	1.33	1 (14%)
12	FME	M	1	12	9,9,10	0.55	0	7,9,11	1.60	2 (28%)
14	FME	T	1	14	9,9,10	0.66	0	7,9,11	1.43	1 (14%)
8	FME	i	1	8	9,9,10	0.57	0	7,9,11	1.54	1 (14%)
12	FME	m	1	12	9,9,10	0.61	0	7,9,11	1.33	1 (14%)
14	FME	t	1	14	9,9,10	0.58	0	7,9,11	1.83	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 (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-3.23	117.62	125.15
8	I	1	FME	O-C-CA	-2.74	118.77	125.15
14	T	1	FME	O-C-CA	-2.69	118.88	125.15
12	M	1	FME	O-C-CA	-2.66	118.95	125.15
14	t	1	FME	CA-N-CN	-2.63	118.77	122.82
8	i	1	FME	O-C-CA	-2.56	119.18	125.15
12	M	1	FME	CA-N-CN	-2.31	119.27	122.82
12	m	1	FME	CA-N-CN	-2.19	119.45	122.82

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 214 ligands modelled in this entry, 18 are unknown and 14 are monoatomic - leaving 182 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	2.29	25 (38%)
23	CLA	A	405	40	56,73,73	1.99	11 (19%)	65,113,113	2.14	22 (33%)
23	CLA	A	406	40	56,73,73	1.93	12 (21%)	65,113,113	2.05	20 (30%)
24	PHO	A	407	-	67,69,69	2.13	17 (25%)	87,99,99	2.04	26 (29%)
23	CLA	A	408	1	56,73,73	1.89	12 (21%)	65,113,113	2.18	21 (32%)
25	BCR	A	409	-	41,41,41	0.99	1 (2%)	56,56,56	1.58	12 (21%)
26	SQD	A	410	-	53,54,54	0.95	3 (5%)	63,65,65	2.01	13 (20%)
27	GOL	A	411	-	5,5,5	0.38	0	5,5,5	0.25	0
26	SQD	A	412	-	53,54,54	1.02	3 (5%)	63,65,65	1.24	7 (11%)
28	OEX	A	413	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	PL9	A	414	-	55,55,55	0.63	1 (1%)	69,69,69	1.89	21 (30%)
31	LHG	A	416	-	48,48,48	0.88	2 (4%)	49,54,54	1.15	4 (8%)
31	LHG	A	417	-	48,48,48	0.92	2 (4%)	49,54,54	1.12	2 (4%)
32	BCT	A	418	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	B	601	40	56,73,73	2.00	12 (21%)	65,113,113	2.19	21 (32%)
23	CLA	B	602	2	56,73,73	1.96	12 (21%)	65,113,113	2.23	23 (35%)
23	CLA	B	603	2	56,73,73	1.92	11 (19%)	65,113,113	2.28	19 (29%)
23	CLA	B	604	2	56,73,73	1.90	11 (19%)	65,113,113	2.38	19 (29%)
23	CLA	B	605	2	56,73,73	1.90	12 (21%)	65,113,113	2.14	20 (30%)
23	CLA	B	606	2	56,73,73	1.88	11 (19%)	65,113,113	2.21	21 (32%)
23	CLA	B	607	40	56,73,73	1.93	12 (21%)	65,113,113	2.20	22 (33%)
23	CLA	B	608	2	56,73,73	1.90	11 (19%)	65,113,113	2.20	21 (32%)
23	CLA	B	609	2	56,73,73	1.89	11 (19%)	65,113,113	2.17	17 (26%)
23	CLA	B	610	40	56,73,73	2.00	12 (21%)	65,113,113	2.32	21 (32%)
23	CLA	B	611	2	56,73,73	1.95	11 (19%)	65,113,113	2.25	21 (32%)
23	CLA	B	612	2	56,73,73	1.90	11 (19%)	65,113,113	2.40	21 (32%)
23	CLA	B	613	2	56,73,73	1.99	12 (21%)	65,113,113	2.35	21 (32%)
23	CLA	B	614	2	56,73,73	1.90	13 (23%)	65,113,113	2.38	21 (32%)
23	CLA	B	615	2	56,73,73	1.89	11 (19%)	65,113,113	2.18	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	616	2	56,73,73	1.98	12 (21%)	65,113,113	2.17	18 (27%)
25	BCR	B	617	-	41,41,41	1.01	1 (2%)	56,56,56	1.52	10 (17%)
25	BCR	B	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.66	13 (23%)
25	BCR	B	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.38	10 (17%)
26	SQD	B	620	-	53,54,54	1.04	4 (7%)	63,65,65	1.64	12 (19%)
33	LMG	B	621	-	51,51,55	0.89	2 (3%)	59,59,63	1.15	5 (8%)
34	HTG	B	622	-	19,19,19	1.00	1 (5%)	23,24,24	1.48	4 (17%)
34	HTG	B	623	-	19,19,19	0.82	1 (5%)	23,24,24	1.94	1 (4%)
34	HTG	B	624	-	19,19,19	0.98	1 (5%)	23,24,24	2.01	2 (8%)
27	GOL	B	625	-	5,5,5	0.35	0	5,5,5	0.35	0
27	GOL	B	626	-	5,5,5	0.49	0	5,5,5	0.41	0
34	HTG	B	627	-	19,19,19	0.95	2 (10%)	23,24,24	1.59	1 (4%)
35	LMT	B	629	-	25,25,36	0.45	0	30,30,47	0.71	0
35	LMT	B	630	-	36,36,36	0.52	1 (2%)	47,47,47	0.98	2 (4%)
35	LMT	B	631	-	26,26,36	0.49	0	31,31,47	0.82	1 (3%)
33	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.20	4 (6%)
23	CLA	C	502	3	56,73,73	1.90	12 (21%)	65,113,113	2.37	22 (33%)
23	CLA	C	503	3	56,73,73	1.92	11 (19%)	65,113,113	2.12	18 (27%)
23	CLA	C	504	3	56,73,73	1.88	11 (19%)	65,113,113	2.00	18 (27%)
23	CLA	C	505	40	56,73,73	2.03	12 (21%)	65,113,113	2.37	23 (35%)
23	CLA	C	506	3	56,73,73	1.91	12 (21%)	65,113,113	2.35	20 (30%)
23	CLA	C	507	3	56,73,73	1.93	12 (21%)	65,113,113	2.23	23 (35%)
23	CLA	C	508	40	56,73,73	1.92	12 (21%)	65,113,113	2.26	20 (30%)
23	CLA	C	509	3	56,73,73	2.05	12 (21%)	65,113,113	2.44	20 (30%)
23	CLA	C	510	3	56,73,73	2.02	12 (21%)	65,113,113	2.18	21 (32%)
23	CLA	C	511	3	56,73,73	1.92	12 (21%)	65,113,113	2.18	23 (35%)
23	CLA	C	512	3	56,73,73	1.96	12 (21%)	65,113,113	2.20	21 (32%)
23	CLA	C	513	3	56,73,73	1.95	11 (19%)	65,113,113	2.20	24 (36%)
23	CLA	C	514	3	56,73,73	1.93	12 (21%)	65,113,113	2.10	19 (29%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.58	10 (17%)
25	BCR	C	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.56	10 (17%)
36	DGD	C	517	-	63,63,67	0.81	2 (3%)	77,77,81	1.10	7 (9%)
36	DGD	C	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	5 (6%)
36	DGD	C	519	-	63,63,67	0.80	2 (3%)	77,77,81	1.02	6 (7%)
33	LMG	C	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.04	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	C	521	-	19,19,19	0.90	1 (5%)	23,24,24	1.59	3 (13%)
34	HTG	C	522	-	19,19,19	1.03	2 (10%)	23,24,24	2.01	5 (21%)
27	GOL	C	523	-	5,5,5	0.37	0	5,5,5	0.23	0
24	PHO	D	401	-	67,69,69	2.12	16 (23%)	87,99,99	2.08	26 (29%)
35	LMT	D	402	-	36,36,36	0.64	1 (2%)	47,47,47	1.31	5 (10%)
35	LMT	D	403	-	36,36,36	0.44	0	47,47,47	1.39	9 (19%)
23	CLA	D	404	4	56,73,73	1.95	12 (21%)	65,113,113	2.46	23 (35%)
23	CLA	D	405	4	56,73,73	1.92	11 (19%)	65,113,113	2.23	20 (30%)
25	BCR	D	406	-	41,41,41	1.02	1 (2%)	56,56,56	1.81	14 (25%)
29	PL9	D	407	-	55,55,55	0.63	1 (1%)	69,69,69	1.69	21 (30%)
31	LHG	D	408	-	48,48,48	0.86	2 (4%)	49,54,54	0.99	3 (6%)
31	LHG	D	409	-	48,48,48	0.91	2 (4%)	49,54,54	1.15	5 (10%)
34	HTG	D	412	-	16,16,19	1.02	2 (12%)	20,21,24	1.73	1 (5%)
26	SQD	D	413	-	42,43,54	1.12	3 (7%)	52,54,65	1.92	13 (25%)
31	LHG	E	101	-	41,41,48	1.02	2 (4%)	42,47,54	1.17	4 (9%)
35	LMT	E	102	-	36,36,36	0.53	1 (2%)	47,47,47	0.90	1 (2%)
38	HEM	E	103	5,6	28,50,50	0.85	0	17,82,82	2.16	4 (23%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.72	13 (23%)
36	DGD	H	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.03	6 (7%)
35	LMT	I	101	-	36,36,36	0.51	1 (2%)	47,47,47	1.14	5 (10%)
33	LMG	J	101	39	51,51,55	0.90	2 (3%)	59,59,63	1.01	5 (8%)
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	9 (16%)
26	SQD	L	101	-	53,54,54	1.00	3 (5%)	63,65,65	1.67	9 (14%)
35	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.05	2 (4%)
35	LMT	M	103	-	36,36,36	0.47	0	47,47,47	0.82	1 (2%)
25	BCR	T	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.73	14 (25%)
38	HEM	V	202	16	28,50,50	0.99	3 (10%)	17,82,82	1.59	3 (17%)
34	HTG	V	203	-	11,11,19	0.25	0	13,15,24	1.13	2 (15%)
25	BCR	Y	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.67	10 (17%)
33	LMG	Z	101	-	51,51,55	0.97	2 (3%)	59,59,63	1.29	5 (8%)
33	LMG	Z	102	-	37,37,55	0.99	3 (8%)	45,45,63	1.68	8 (17%)
23	CLA	a	404	1	56,73,73	1.91	11 (19%)	65,113,113	2.42	24 (36%)
23	CLA	a	405	40	56,73,73	1.98	12 (21%)	65,113,113	2.12	23 (35%)
24	PHO	a	406	-	67,69,69	2.09	17 (25%)	87,99,99	1.94	26 (29%)
24	PHO	a	407	-	67,69,69	2.17	15 (22%)	87,99,99	1.98	24 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	a	408	1	56,73,73	1.93	12 (21%)	65,113,113	2.25	24 (36%)
25	BCR	a	409	-	41,41,41	0.93	1 (2%)	56,56,56	1.50	11 (19%)
26	SQD	a	410	-	53,54,54	0.94	3 (5%)	63,65,65	1.88	14 (22%)
27	GOL	a	411	-	5,5,5	0.36	0	5,5,5	0.39	0
26	SQD	a	412	-	53,54,54	1.04	3 (5%)	63,65,65	1.39	8 (12%)
28	OEX	a	413	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
29	PL9	a	414	-	55,55,55	0.63	1 (1%)	69,69,69	1.93	18 (26%)
33	LMG	a	416	-	51,51,55	0.93	2 (3%)	59,59,63	1.09	3 (5%)
35	LMT	a	417	-	36,36,36	0.46	0	47,47,47	0.81	1 (2%)
32	BCT	a	418	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	601	40	56,73,73	1.98	12 (21%)	65,113,113	2.15	21 (32%)
23	CLA	b	602	2	56,73,73	1.98	12 (21%)	65,113,113	2.29	25 (38%)
23	CLA	b	603	2	56,73,73	1.96	12 (21%)	65,113,113	2.15	20 (30%)
23	CLA	b	604	2	56,73,73	1.93	11 (19%)	65,113,113	2.34	18 (27%)
23	CLA	b	605	2	56,73,73	1.94	12 (21%)	65,113,113	2.24	17 (26%)
23	CLA	b	606	2	56,73,73	1.87	11 (19%)	65,113,113	2.20	23 (35%)
23	CLA	b	607	40	56,73,73	1.87	12 (21%)	65,113,113	2.24	19 (29%)
23	CLA	b	608	2	56,73,73	2.00	12 (21%)	65,113,113	2.20	19 (29%)
23	CLA	b	609	2	56,73,73	1.91	12 (21%)	65,113,113	2.25	20 (30%)
23	CLA	b	610	40	56,73,73	2.03	12 (21%)	65,113,113	2.31	24 (36%)
23	CLA	b	611	2	56,73,73	1.98	12 (21%)	65,113,113	2.30	20 (30%)
23	CLA	b	612	2	56,73,73	2.01	12 (21%)	65,113,113	2.21	19 (29%)
23	CLA	b	613	2	56,73,73	1.97	12 (21%)	65,113,113	2.29	20 (30%)
23	CLA	b	614	2	56,73,73	1.94	12 (21%)	65,113,113	2.29	22 (33%)
23	CLA	b	615	2	56,73,73	1.85	11 (19%)	65,113,113	2.19	17 (26%)
23	CLA	b	616	2	56,73,73	1.93	11 (19%)	65,113,113	2.18	22 (33%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.51	10 (17%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.38	8 (14%)
25	BCR	b	619	-	41,41,41	1.05	1 (2%)	56,56,56	1.68	12 (21%)
33	LMG	b	620	-	51,51,55	0.85	2 (3%)	59,59,63	1.29	8 (13%)
35	LMT	b	621	-	25,25,36	0.45	0	30,30,47	0.69	0
34	HTG	b	622	-	19,19,19	0.94	1 (5%)	23,24,24	1.67	2 (8%)
34	HTG	b	623	-	19,19,19	1.05	1 (5%)	23,24,24	2.06	2 (8%)
27	GOL	b	624	-	5,5,5	0.29	0	5,5,5	0.43	0
34	HTG	b	625	-	19,19,19	0.90	2 (10%)	23,24,24	1.91	3 (13%)
35	LMT	b	627	-	25,25,36	0.55	1 (4%)	30,30,47	1.14	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	HTG	b	628	-	19,19,19	0.99	1 (5%)	23,24,24	1.96	4 (17%)
23	CLA	c	501	3	56,73,73	1.88	12 (21%)	65,113,113	2.16	20 (30%)
23	CLA	c	502	3	56,73,73	1.96	12 (21%)	65,113,113	2.30	19 (29%)
23	CLA	c	503	3	56,73,73	1.92	12 (21%)	65,113,113	2.24	20 (30%)
23	CLA	c	504	40	56,73,73	1.98	12 (21%)	65,113,113	2.20	24 (36%)
23	CLA	c	505	3	56,73,73	1.92	11 (19%)	65,113,113	2.24	19 (29%)
23	CLA	c	506	3	56,73,73	1.93	11 (19%)	65,113,113	2.28	22 (33%)
23	CLA	c	507	40	56,73,73	1.91	11 (19%)	65,113,113	2.18	19 (29%)
23	CLA	c	508	3	56,73,73	2.02	12 (21%)	65,113,113	2.31	19 (29%)
23	CLA	c	509	3	56,73,73	1.99	12 (21%)	65,113,113	2.24	19 (29%)
23	CLA	c	510	3	56,73,73	1.86	12 (21%)	65,113,113	2.26	23 (35%)
23	CLA	c	511	3	56,73,73	1.98	12 (21%)	65,113,113	2.15	19 (29%)
23	CLA	c	512	3	56,73,73	1.93	12 (21%)	65,113,113	2.28	19 (29%)
23	CLA	c	513	3	56,73,73	1.95	12 (21%)	65,113,113	2.22	22 (33%)
25	BCR	c	514	-	41,41,41	1.03	1 (2%)	56,56,56	1.79	13 (23%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.70	17 (30%)
36	DGD	c	516	-	63,63,67	0.82	2 (3%)	77,77,81	1.19	7 (9%)
36	DGD	c	517	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
36	DGD	c	518	-	63,63,67	0.85	3 (4%)	77,77,81	1.12	6 (7%)
33	LMG	c	519	-	51,51,55	0.93	2 (3%)	59,59,63	1.06	3 (5%)
33	LMG	c	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.26	6 (10%)
34	HTG	c	521	-	19,19,19	0.89	1 (5%)	23,24,24	1.75	1 (4%)
34	HTG	c	522	-	19,19,19	0.94	2 (10%)	23,24,24	1.63	3 (13%)
23	CLA	d	401	40	56,73,73	1.95	11 (19%)	65,113,113	2.26	22 (33%)
27	GOL	d	402	-	5,5,5	0.26	0	5,5,5	0.55	0
23	CLA	d	403	4	56,73,73	1.92	12 (21%)	65,113,113	2.26	22 (33%)
23	CLA	d	404	4	56,73,73	1.96	11 (19%)	65,113,113	2.09	24 (36%)
25	BCR	d	405	-	41,41,41	1.07	1 (2%)	56,56,56	1.86	14 (25%)
29	PL9	d	406	-	55,55,55	0.61	1 (1%)	69,69,69	1.76	19 (27%)
31	LHG	d	407	-	48,48,48	0.87	2 (4%)	49,54,54	1.08	5 (10%)
31	LHG	d	408	-	48,48,48	0.87	2 (4%)	49,54,54	0.94	3 (6%)
31	LHG	d	409	-	48,48,48	0.95	2 (4%)	49,54,54	1.04	3 (6%)
34	HTG	d	411	-	16,16,19	1.09	2 (12%)	20,21,24	1.76	1 (5%)
31	LHG	e	101	-	41,41,48	1.01	2 (4%)	42,47,54	0.99	2 (4%)
35	LMT	e	102	-	36,36,36	0.50	0	47,47,47	0.87	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HEM	e	103	5,6	28,50,50	0.84	1 (3%)	17,82,82	1.87	3 (17%)
26	SQD	f	101	-	42,43,54	1.16	3 (7%)	52,54,65	1.57	9 (17%)
25	BCR	h	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.47	9 (16%)
36	DGD	h	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.05	5 (6%)
33	LMG	j	101	39	51,51,55	0.87	2 (3%)	59,59,63	1.10	5 (8%)
25	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	13 (23%)
31	LHG	l	101	-	48,48,48	0.93	2 (4%)	49,54,54	1.09	4 (8%)
35	LMT	m	102	-	36,36,36	0.51	0	47,47,47	0.97	2 (4%)
25	BCR	t	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.72	16 (28%)
38	HEM	v	201	16	28,50,50	0.98	3 (10%)	17,82,82	1.61	4 (23%)
25	BCR	y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.63	11 (19%)
33	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.13	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	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	406	40	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	407	-	-	0/53/103/103	0/1/6/6
23	CLA	A	408	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410	-	-	0/49/69/69	0/1/1/1
27	GOL	A	411	-	-	0/4/4/4	0/0/0/0
26	SQD	A	412	-	-	0/49/69/69	0/1/1/1
28	OEX	A	413	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	A	414	-	-	0/53/73/73	0/1/1/1
31	LHG	A	416	-	-	0/53/53/53	0/0/0/0
31	LHG	A	417	-	-	0/53/53/53	0/0/0/0
32	BCT	A	418	21	-	0/0/0/0	0/0/0/0
23	CLA	B	601	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	602	2	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	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	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
26	SQD	B	620	-	-	0/49/69/69	0/1/1/1
33	LMG	B	621	-	-	0/46/66/70	0/1/1/1
34	HTG	B	622	-	-	0/10/30/30	0/1/1/1
34	HTG	B	623	-	-	0/10/30/30	0/1/1/1
34	HTG	B	624	-	-	0/10/30/30	0/1/1/1
27	GOL	B	625	-	-	0/4/4/4	0/0/0/0
27	GOL	B	626	-	-	0/4/4/4	0/0/0/0
34	HTG	B	627	-	-	0/10/30/30	0/1/1/1
35	LMT	B	629	-	-	0/17/37/61	0/1/1/2
35	LMT	B	630	-	-	0/21/61/61	0/2/2/2
35	LMT	B	631	-	-	0/17/38/61	0/1/1/2
33	LMG	C	501	-	-	0/46/66/70	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	2/2/20/25	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2
36	DGD	C	518	-	-	0/51/91/95	0/2/2/2
36	DGD	C	519	-	-	0/51/91/95	0/2/2/2
33	LMG	C	520	-	-	0/46/66/70	0/1/1/1
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
27	GOL	C	523	-	-	0/4/4/4	0/0/0/0
24	PHO	D	401	-	-	0/53/103/103	0/1/6/6
35	LMT	D	402	-	-	0/21/61/61	0/2/2/2
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
34	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
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
35	LMT	I	101	-	-	0/21/61/61	0/2/2/2
33	LMG	J	101	39	-	0/46/66/70	0/1/1/1
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
26	SQD	L	101	-	-	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
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
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
25	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
33	LMG	Z	102	-	-	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	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	a	406	-	-	0/53/103/103	0/1/6/6
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
23	CLA	a	408	1	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	a	409	-	-	0/29/63/63	0/2/2/2
26	SQD	a	410	-	-	0/49/69/69	0/1/1/1
27	GOL	a	411	-	-	0/4/4/4	0/0/0/0
26	SQD	a	412	-	-	0/49/69/69	0/1/1/1
28	OEX	a	413	1,3,40	-	0/0/68/68	0/0/6/6
29	PL9	a	414	-	-	0/53/73/73	0/1/1/1
33	LMG	a	416	-	-	0/46/66/70	0/1/1/1
35	LMT	a	417	-	-	0/21/61/61	0/2/2/2
32	BCT	a	418	21	-	0/0/0/0	0/0/0/0
23	CLA	b	601	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	602	2	3/3/20/25	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
33	LMG	b	620	-	-	0/46/66/70	0/1/1/1
35	LMT	b	621	-	-	0/17/37/61	0/1/1/2
34	HTG	b	622	-	-	0/10/30/30	0/1/1/1
34	HTG	b	623	-	-	0/10/30/30	0/1/1/1
27	GOL	b	624	-	-	0/4/4/4	0/0/0/0
34	HTG	b	625	-	-	0/10/30/30	0/1/1/1
35	LMT	b	627	-	-	0/17/37/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HTG	b	628	-	-	0/10/30/30	0/1/1/1
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
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	2/2/20/25	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	3/3/20/25	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
36	DGD	c	516	-	-	0/51/91/95	0/2/2/2
36	DGD	c	517	-	-	0/51/91/95	0/2/2/2
36	DGD	c	518	-	-	0/51/91/95	0/2/2/2
33	LMG	c	519	-	-	0/46/66/70	0/1/1/1
33	LMG	c	520	-	-	0/46/66/70	0/1/1/1
34	HTG	c	521	-	-	0/10/30/30	0/1/1/1
34	HTG	c	522	-	-	0/10/30/30	0/1/1/1
23	CLA	d	401	40	3/3/20/25	0/37/135/135	0/0/9/9
27	GOL	d	402	-	-	0/4/4/4	0/0/0/0
23	CLA	d	403	4	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	d	404	4	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	d	405	-	-	0/29/63/63	0/2/2/2
29	PL9	d	406	-	-	0/53/73/73	0/1/1/1
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	d	409	-	-	0/53/53/53	0/0/0/0
34	HTG	d	411	-	-	0/7/27/30	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
26	SQD	f	101	-	-	2/38/58/69	0/1/1/1
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
36	DGD	h	102	-	-	0/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	j	101	39	-	0/46/66/70	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LHG	l	101	-	-	0/53/53/53	0/0/0/0
35	LMT	m	102	-	-	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
25	BCR	y	101	-	-	0/29/63/63	0/2/2/2
33	LMG	z	101	-	-	0/34/54/70	0/1/1/1

All (1031) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	K	102	BCR	C23-C22	-5.18	1.34	1.45
25	C	515	BCR	C23-C22	-5.16	1.34	1.45
25	k	101	BCR	C23-C22	-5.07	1.34	1.45
25	b	619	BCR	C23-C22	-5.06	1.34	1.45
25	d	405	BCR	C23-C22	-4.98	1.35	1.45
25	D	406	BCR	C23-C22	-4.95	1.35	1.45
25	c	514	BCR	C23-C22	-4.89	1.35	1.45
25	t	101	BCR	C23-C22	-4.87	1.35	1.45
25	C	516	BCR	C23-C22	-4.85	1.35	1.45
25	b	618	BCR	C23-C22	-4.81	1.35	1.45
25	B	619	BCR	C23-C22	-4.80	1.35	1.45
25	A	409	BCR	C23-C22	-4.80	1.35	1.45
25	H	101	BCR	C23-C22	-4.77	1.35	1.45
25	y	101	BCR	C23-C22	-4.74	1.35	1.45
25	b	617	BCR	C23-C22	-4.74	1.35	1.45
25	T	101	BCR	C23-C22	-4.73	1.35	1.45
25	c	515	BCR	C23-C22	-4.65	1.35	1.45
25	h	101	BCR	C23-C22	-4.62	1.35	1.45
25	Y	101	BCR	C23-C22	-4.52	1.36	1.45
25	B	617	BCR	C23-C22	-4.47	1.36	1.45
25	a	409	BCR	C23-C22	-4.33	1.36	1.45
25	B	618	BCR	C23-C22	-3.96	1.37	1.45
24	A	407	PHO	C4A-NA	-3.83	1.25	1.35
34	B	622	HTG	C1'-S1	-3.81	1.76	1.81
34	b	628	HTG	C1'-S1	-3.76	1.76	1.81
34	b	623	HTG	C1'-S1	-3.73	1.76	1.81
34	C	522	HTG	C1'-S1	-3.55	1.76	1.81
34	d	411	HTG	C1'-S1	-3.54	1.76	1.81
34	B	624	HTG	C1'-S1	-3.49	1.76	1.81
34	B	627	HTG	C1'-S1	-3.28	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	622	HTG	C1'-S1	-3.28	1.77	1.81
24	D	401	PHO	C4A-NA	-3.27	1.27	1.35
24	a	407	PHO	C4A-NA	-3.25	1.27	1.35
34	c	522	HTG	C1'-S1	-3.24	1.77	1.81
24	a	406	PHO	C4A-NA	-3.13	1.27	1.35
34	C	521	HTG	C1'-S1	-3.12	1.77	1.81
34	D	412	HTG	C1'-S1	-3.05	1.77	1.81
34	c	521	HTG	C1'-S1	-2.99	1.77	1.81
34	B	623	HTG	C1'-S1	-2.88	1.77	1.81
34	b	625	HTG	C1'-S1	-2.84	1.77	1.81
38	V	202	HEM	C4D-ND	-2.63	1.33	1.36
26	f	101	SQD	C6-S	-2.61	1.66	1.77
38	v	201	HEM	C1B-NB	-2.59	1.33	1.36
26	A	412	SQD	C6-S	-2.58	1.67	1.77
38	e	103	HEM	C3B-C2B	-2.53	1.37	1.40
26	B	620	SQD	C6-S	-2.51	1.67	1.77
26	a	412	SQD	C6-S	-2.51	1.67	1.77
26	D	413	SQD	C6-S	-2.49	1.67	1.77
26	A	410	SQD	C6-S	-2.45	1.67	1.77
26	L	101	SQD	C6-S	-2.41	1.67	1.77
26	a	410	SQD	C6-S	-2.37	1.67	1.77
38	V	202	HEM	C3B-C2B	-2.36	1.37	1.40
38	V	202	HEM	C1B-NB	-2.35	1.34	1.36
34	b	625	HTG	C1-S1	-2.28	1.77	1.80
24	A	407	PHO	C1A-NA	-2.26	1.32	1.37
38	v	201	HEM	C3B-C2B	-2.26	1.37	1.40
34	B	627	HTG	C1-S1	-2.25	1.77	1.80
36	c	518	DGD	O2G-C2G	-2.23	1.40	1.46
34	D	412	HTG	C1-S1	-2.22	1.77	1.80
24	a	407	PHO	C1A-NA	-2.17	1.32	1.37
38	v	201	HEM	C4D-ND	-2.12	1.34	1.36
34	d	411	HTG	C1-S1	-2.10	1.77	1.80
34	C	522	HTG	C1-S1	-2.08	1.77	1.80
23	B	614	CLA	C1C-NC	-2.05	1.34	1.37
34	c	522	HTG	C1-S1	-2.04	1.77	1.80
24	a	406	PHO	C1A-NA	-2.02	1.33	1.37
23	b	608	CLA	C4C-C3C	2.00	1.48	1.45
36	H	102	DGD	O5D-C1E	2.01	1.43	1.40
24	A	407	PHO	C4D-CHA	2.01	1.49	1.44
24	D	401	PHO	C1D-C2D	2.02	1.50	1.45
23	A	406	CLA	CHD-C4C	2.02	1.47	1.41
23	C	505	CLA	C4C-C3C	2.03	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C4C-C3C	2.03	1.48	1.45
35	I	101	LMT	O1'-C1'	2.04	1.43	1.40
23	C	509	CLA	CHD-C4C	2.04	1.47	1.41
23	b	607	CLA	CHD-C4C	2.05	1.47	1.41
23	b	604	CLA	CHD-C4C	2.05	1.47	1.41
23	A	406	CLA	C4C-C3C	2.06	1.48	1.45
23	A	408	CLA	C4C-C3C	2.06	1.48	1.45
23	b	613	CLA	C4C-C3C	2.07	1.48	1.45
23	C	514	CLA	C4C-C3C	2.08	1.48	1.45
23	b	601	CLA	C4C-C3C	2.08	1.48	1.45
36	h	102	DGD	O5D-C1E	2.09	1.43	1.40
23	A	405	CLA	CHD-C4C	2.10	1.47	1.41
24	D	401	PHO	C3B-C4B	2.10	1.47	1.43
23	d	401	CLA	C1C-C2C	2.10	1.48	1.44
23	B	613	CLA	CHD-C4C	2.11	1.47	1.41
36	c	517	DGD	O3G-C1D	2.12	1.43	1.40
23	C	502	CLA	CHD-C4C	2.12	1.47	1.41
23	B	604	CLA	CHD-C4C	2.13	1.47	1.41
23	b	615	CLA	C4C-C3C	2.13	1.48	1.45
35	B	630	LMT	O1'-C1'	2.13	1.43	1.40
35	E	102	LMT	O1'-C1'	2.13	1.43	1.40
23	B	612	CLA	C4C-C3C	2.14	1.48	1.45
23	B	608	CLA	CHD-C4C	2.14	1.47	1.41
23	c	506	CLA	C4C-C3C	2.14	1.48	1.45
26	B	620	SQD	O6-C1	2.15	1.43	1.40
23	c	502	CLA	C4C-C3C	2.15	1.48	1.45
23	B	614	CLA	C1C-C2C	2.15	1.48	1.44
35	b	627	LMT	O1'-C1'	2.16	1.44	1.40
23	b	602	CLA	C4C-C3C	2.16	1.48	1.45
23	B	610	CLA	CHD-C4C	2.17	1.47	1.41
23	c	513	CLA	C4C-C3C	2.17	1.48	1.45
23	b	611	CLA	C1C-C2C	2.17	1.48	1.44
23	D	404	CLA	C4B-CHC	2.18	1.45	1.40
23	C	505	CLA	CHD-C4C	2.20	1.47	1.41
24	a	406	PHO	C4D-CHA	2.20	1.50	1.44
23	b	614	CLA	C1C-C2C	2.21	1.48	1.44
23	c	510	CLA	C1C-C2C	2.21	1.48	1.44
23	c	502	CLA	C1C-C2C	2.21	1.48	1.44
23	a	404	CLA	C1C-C2C	2.21	1.48	1.44
23	C	506	CLA	C4C-C3C	2.22	1.48	1.45
23	b	603	CLA	C4C-C3C	2.22	1.48	1.45
23	B	616	CLA	C4C-C3C	2.22	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C1C-C2C	2.22	1.48	1.44
23	b	615	CLA	CHD-C4C	2.23	1.47	1.41
23	c	511	CLA	C4C-C3C	2.23	1.49	1.45
23	C	506	CLA	CHD-C4C	2.23	1.47	1.41
23	c	504	CLA	CHD-C4C	2.24	1.47	1.41
23	B	614	CLA	C4C-C3C	2.25	1.49	1.45
33	Z	102	LMG	O1-C1	2.25	1.44	1.40
23	d	403	CLA	C1C-C2C	2.25	1.48	1.44
23	C	503	CLA	C1C-C2C	2.25	1.48	1.44
23	B	610	CLA	C1C-C2C	2.26	1.48	1.44
23	B	608	CLA	C1C-C2C	2.26	1.48	1.44
23	b	609	CLA	C4C-C3C	2.26	1.49	1.45
23	a	405	CLA	C1C-C2C	2.26	1.48	1.44
23	a	405	CLA	C4C-C3C	2.27	1.49	1.45
23	B	609	CLA	CHD-C4C	2.27	1.48	1.41
23	a	404	CLA	CHD-C4C	2.27	1.48	1.41
23	d	401	CLA	CHD-C4C	2.27	1.48	1.41
23	c	508	CLA	CHD-C4C	2.27	1.48	1.41
23	d	403	CLA	CHD-C4C	2.27	1.48	1.41
23	C	512	CLA	CHD-C4C	2.27	1.48	1.41
23	B	611	CLA	CHD-C4C	2.28	1.48	1.41
23	b	605	CLA	C4C-C3C	2.28	1.49	1.45
23	c	503	CLA	C4C-C3C	2.28	1.49	1.45
23	c	512	CLA	C4C-C3C	2.29	1.49	1.45
23	c	512	CLA	CHD-C4C	2.29	1.48	1.41
23	c	506	CLA	CHD-C4C	2.29	1.48	1.41
23	D	405	CLA	CHD-C4C	2.29	1.48	1.41
23	b	616	CLA	CHD-C4C	2.30	1.48	1.41
23	C	507	CLA	C1C-C2C	2.31	1.49	1.44
23	b	608	CLA	CHD-C4C	2.31	1.48	1.41
23	B	614	CLA	C4B-CHC	2.31	1.46	1.40
23	B	610	CLA	C4C-C3C	2.31	1.49	1.45
23	b	605	CLA	C1C-C2C	2.31	1.49	1.44
23	B	606	CLA	CHD-C4C	2.32	1.48	1.41
24	D	401	PHO	C4C-C3C	2.33	1.49	1.45
23	C	508	CLA	C4C-C3C	2.33	1.49	1.45
23	b	613	CLA	CHD-C4C	2.33	1.48	1.41
23	a	405	CLA	CHD-C4C	2.33	1.48	1.41
23	A	404	CLA	C1C-C2C	2.34	1.49	1.44
23	c	505	CLA	CHD-C4C	2.34	1.48	1.41
23	c	508	CLA	C4C-C3C	2.34	1.49	1.45
23	B	615	CLA	C4B-CHC	2.35	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C1C-C2C	2.35	1.49	1.44
23	b	611	CLA	CHD-C4C	2.35	1.48	1.41
23	c	507	CLA	CHD-C4C	2.35	1.48	1.41
23	b	612	CLA	CHD-C4C	2.35	1.48	1.41
23	b	607	CLA	C4C-C3C	2.35	1.49	1.45
23	b	606	CLA	CHD-C4C	2.36	1.48	1.41
23	c	502	CLA	CHD-C4C	2.36	1.48	1.41
23	C	502	CLA	C4C-C3C	2.36	1.49	1.45
23	B	601	CLA	C4C-C3C	2.36	1.49	1.45
23	c	510	CLA	C4C-C3C	2.37	1.49	1.45
23	c	501	CLA	C1C-C2C	2.37	1.49	1.44
23	B	616	CLA	CHD-C4C	2.37	1.48	1.41
23	b	610	CLA	CHD-C4C	2.37	1.48	1.41
23	B	614	CLA	CHD-C4C	2.37	1.48	1.41
23	c	503	CLA	CHD-C4C	2.38	1.48	1.41
23	B	605	CLA	CHD-C4C	2.38	1.48	1.41
23	B	601	CLA	CHD-C4C	2.38	1.48	1.41
23	d	404	CLA	CHD-C4C	2.38	1.48	1.41
23	C	502	CLA	C1C-C2C	2.38	1.49	1.44
23	A	408	CLA	CHD-C4C	2.39	1.48	1.41
23	b	605	CLA	CHD-C4C	2.39	1.48	1.41
23	B	615	CLA	CHD-C4C	2.39	1.48	1.41
23	C	503	CLA	CHD-C4C	2.39	1.48	1.41
23	c	502	CLA	C4B-CHC	2.39	1.46	1.40
23	C	508	CLA	CHD-C4C	2.39	1.48	1.41
23	C	508	CLA	C1B-CHB	2.40	1.46	1.40
23	b	609	CLA	CHD-C4C	2.40	1.48	1.41
23	d	404	CLA	C1C-C2C	2.40	1.49	1.44
23	c	501	CLA	C4C-C3C	2.40	1.49	1.45
23	a	408	CLA	CHD-C4C	2.41	1.48	1.41
23	B	601	CLA	C1C-C2C	2.41	1.49	1.44
23	B	603	CLA	CHD-C4C	2.41	1.48	1.41
23	b	603	CLA	CHD-C4C	2.41	1.48	1.41
23	B	605	CLA	C4C-C3C	2.42	1.49	1.45
23	b	603	CLA	C1B-CHB	2.42	1.46	1.40
23	C	511	CLA	C1C-C2C	2.42	1.49	1.44
23	C	510	CLA	C4C-C3C	2.42	1.49	1.45
23	d	404	CLA	C1B-CHB	2.42	1.46	1.40
23	B	602	CLA	C1C-C2C	2.42	1.49	1.44
23	D	404	CLA	CHD-C4C	2.42	1.48	1.41
23	C	514	CLA	CHD-C4C	2.42	1.48	1.41
23	b	614	CLA	CHD-C4C	2.43	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	C4C-C3C	2.43	1.49	1.45
23	b	609	CLA	C1C-C2C	2.43	1.49	1.44
23	A	408	CLA	C1C-C2C	2.43	1.49	1.44
23	c	501	CLA	CHD-C4C	2.43	1.48	1.41
23	B	604	CLA	C1C-C2C	2.43	1.49	1.44
23	c	510	CLA	CHD-C4C	2.44	1.48	1.41
23	c	509	CLA	CHD-C4C	2.44	1.48	1.41
23	C	510	CLA	CHD-C4C	2.45	1.48	1.41
29	D	407	PL9	C6-C5	2.45	1.48	1.35
23	A	404	CLA	CHD-C4C	2.45	1.48	1.41
24	a	406	PHO	C3B-C4B	2.45	1.48	1.43
23	c	513	CLA	CHD-C4C	2.45	1.48	1.41
23	A	404	CLA	C1B-CHB	2.46	1.46	1.40
23	C	512	CLA	C4C-C3C	2.46	1.49	1.45
23	b	612	CLA	C4C-C3C	2.46	1.49	1.45
23	B	607	CLA	C4C-C3C	2.46	1.49	1.45
24	a	406	PHO	C4C-C3C	2.47	1.49	1.45
23	C	508	CLA	C1C-C2C	2.47	1.49	1.44
23	C	504	CLA	C4C-C3C	2.47	1.49	1.45
23	C	513	CLA	C1B-CHB	2.48	1.46	1.40
23	C	507	CLA	C4C-C3C	2.48	1.49	1.45
23	b	602	CLA	CHD-C4C	2.48	1.48	1.41
23	c	511	CLA	C1C-C2C	2.49	1.49	1.44
23	C	513	CLA	CHD-C4C	2.49	1.48	1.41
23	b	608	CLA	C1C-C2C	2.49	1.49	1.44
23	B	602	CLA	C4B-CHC	2.49	1.46	1.40
23	b	613	CLA	C1C-C2C	2.49	1.49	1.44
23	B	603	CLA	C1B-CHB	2.50	1.46	1.40
23	A	406	CLA	C1B-CHB	2.50	1.46	1.40
23	B	607	CLA	CHD-C4C	2.50	1.48	1.41
23	C	509	CLA	C4B-CHC	2.51	1.46	1.40
23	b	606	CLA	C1C-C2C	2.51	1.49	1.44
23	C	509	CLA	C1C-C2C	2.51	1.49	1.44
23	C	507	CLA	CHD-C4C	2.51	1.48	1.41
23	A	408	CLA	C1B-CHB	2.52	1.46	1.40
23	C	511	CLA	CHD-C4C	2.52	1.48	1.41
23	B	615	CLA	C1C-C2C	2.52	1.49	1.44
23	b	612	CLA	C1C-C2C	2.52	1.49	1.44
23	c	504	CLA	C4C-C3C	2.52	1.49	1.45
29	d	406	PL9	C6-C5	2.52	1.48	1.35
23	B	613	CLA	C4C-C3C	2.52	1.49	1.45
23	A	406	CLA	C4B-CHC	2.54	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C1C-C2C	2.54	1.49	1.44
23	b	607	CLA	C4B-CHC	2.56	1.46	1.40
23	c	511	CLA	CHD-C4C	2.56	1.48	1.41
23	b	605	CLA	C4B-CHC	2.56	1.46	1.40
23	B	616	CLA	C1C-C2C	2.56	1.49	1.44
23	b	601	CLA	CHD-C4C	2.57	1.48	1.41
23	B	602	CLA	CHD-C4C	2.57	1.48	1.41
23	C	513	CLA	C1C-C2C	2.58	1.49	1.44
23	C	502	CLA	C4B-CHC	2.58	1.47	1.40
23	c	510	CLA	C4B-CHC	2.58	1.47	1.40
33	Z	102	LMG	O8-C28	2.58	1.46	1.33
23	C	504	CLA	CHD-C4C	2.59	1.48	1.41
23	B	605	CLA	C1C-C2C	2.59	1.49	1.44
23	d	401	CLA	C4B-CHC	2.59	1.47	1.40
23	B	609	CLA	C1C-C2C	2.59	1.49	1.44
23	B	603	CLA	C4C-C3C	2.59	1.49	1.45
23	C	507	CLA	C1B-CHB	2.60	1.47	1.40
23	a	408	CLA	C4C-C3C	2.60	1.49	1.45
23	B	615	CLA	C1B-CHB	2.61	1.47	1.40
23	C	511	CLA	C4B-CHC	2.61	1.47	1.40
23	a	408	CLA	C1C-C2C	2.61	1.49	1.44
23	d	403	CLA	C4C-C3C	2.61	1.49	1.45
23	c	506	CLA	C1B-CHB	2.62	1.47	1.40
23	B	602	CLA	C4C-C3C	2.62	1.49	1.45
23	a	405	CLA	C4B-CHC	2.62	1.47	1.40
23	d	401	CLA	C1B-CHB	2.63	1.47	1.40
23	b	601	CLA	C1B-CHB	2.63	1.47	1.40
23	C	503	CLA	C1B-CHB	2.63	1.47	1.40
23	B	607	CLA	C1B-CHB	2.63	1.47	1.40
23	c	509	CLA	C1C-C2C	2.63	1.49	1.44
23	b	607	CLA	C1C-C2C	2.63	1.49	1.44
23	c	506	CLA	C4B-CHC	2.63	1.47	1.40
23	B	608	CLA	C4B-CHC	2.64	1.47	1.40
23	b	615	CLA	C4B-CHC	2.64	1.47	1.40
23	B	601	CLA	C1B-CHB	2.64	1.47	1.40
23	C	514	CLA	C4B-CHC	2.64	1.47	1.40
23	B	603	CLA	C4B-CHC	2.65	1.47	1.40
23	a	405	CLA	C1B-CHB	2.65	1.47	1.40
23	C	511	CLA	C4C-C3C	2.66	1.49	1.45
23	c	507	CLA	C1B-CHB	2.66	1.47	1.40
23	b	614	CLA	C4B-CHC	2.66	1.47	1.40
23	B	611	CLA	C4B-CHC	2.66	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C1B-CHB	2.66	1.47	1.40
23	B	612	CLA	C1C-C2C	2.67	1.49	1.44
23	c	508	CLA	C4B-CHC	2.67	1.47	1.40
23	c	507	CLA	C1C-C2C	2.67	1.49	1.44
23	B	604	CLA	C4B-CHC	2.67	1.47	1.40
23	a	408	CLA	C4B-CHC	2.68	1.47	1.40
23	B	607	CLA	C4B-CHC	2.68	1.47	1.40
23	A	406	CLA	C1C-C2C	2.68	1.49	1.44
23	C	509	CLA	C4C-C3C	2.69	1.49	1.45
23	c	512	CLA	C1B-CHB	2.69	1.47	1.40
23	a	404	CLA	C4B-CHC	2.70	1.47	1.40
23	b	616	CLA	C1C-C2C	2.70	1.49	1.44
23	c	503	CLA	C1C-C2C	2.70	1.49	1.44
23	b	606	CLA	C4B-CHC	2.70	1.47	1.40
23	C	504	CLA	C4B-CHC	2.71	1.47	1.40
29	A	414	PL9	C6-C5	2.71	1.49	1.35
23	C	504	CLA	C1B-CHB	2.71	1.47	1.40
23	a	408	CLA	C1B-CHB	2.71	1.47	1.40
23	b	608	CLA	C1B-CHB	2.72	1.47	1.40
23	b	611	CLA	C4C-C3C	2.72	1.49	1.45
23	B	613	CLA	C1C-C2C	2.72	1.49	1.44
23	B	612	CLA	C4B-CHC	2.72	1.47	1.40
23	B	602	CLA	C1B-CHB	2.72	1.47	1.40
23	b	602	CLA	C1C-C2C	2.73	1.49	1.44
23	c	503	CLA	C1B-CHB	2.73	1.47	1.40
23	c	513	CLA	C1B-CHB	2.73	1.47	1.40
23	c	504	CLA	C4B-CHC	2.74	1.47	1.40
23	b	607	CLA	C1B-CHB	2.74	1.47	1.40
23	C	510	CLA	C1B-CHB	2.74	1.47	1.40
23	C	506	CLA	C4B-CHC	2.74	1.47	1.40
23	D	405	CLA	C1B-CHB	2.74	1.47	1.40
23	C	512	CLA	C4B-CHC	2.75	1.47	1.40
23	b	606	CLA	C1B-CHB	2.75	1.47	1.40
23	B	607	CLA	C1C-C2C	2.75	1.49	1.44
23	c	507	CLA	C4B-CHC	2.75	1.47	1.40
29	a	414	PL9	C6-C5	2.76	1.49	1.35
23	A	408	CLA	C4B-CHC	2.76	1.47	1.40
23	B	612	CLA	C1B-CHB	2.76	1.47	1.40
24	A	407	PHO	CHB-C4A	2.78	1.47	1.40
23	b	613	CLA	C4B-CHC	2.78	1.47	1.40
23	C	514	CLA	C1B-CHB	2.78	1.47	1.40
23	c	508	CLA	C1C-C2C	2.78	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C4B-CHC	2.78	1.47	1.40
23	B	616	CLA	C4B-CHC	2.79	1.47	1.40
23	C	502	CLA	C1B-CHB	2.80	1.47	1.40
23	B	611	CLA	C1C-C2C	2.80	1.50	1.44
23	a	404	CLA	C1B-CHB	2.81	1.47	1.40
23	c	504	CLA	C1C-C2C	2.82	1.50	1.44
23	c	509	CLA	C4B-CHC	2.82	1.47	1.40
23	c	511	CLA	C4B-CHC	2.82	1.47	1.40
23	C	508	CLA	C4B-CHC	2.82	1.47	1.40
23	c	512	CLA	C4B-CHC	2.83	1.47	1.40
23	D	404	CLA	C1B-CHB	2.83	1.47	1.40
23	b	602	CLA	C1B-CHB	2.83	1.47	1.40
23	D	405	CLA	C1C-C2C	2.83	1.50	1.44
23	c	504	CLA	C1B-CHB	2.83	1.47	1.40
23	B	601	CLA	C4B-CHC	2.83	1.47	1.40
23	B	608	CLA	C1B-CHB	2.83	1.47	1.40
35	D	402	LMT	O1'-C1'	2.83	1.45	1.40
23	B	616	CLA	C1B-CHB	2.84	1.47	1.40
23	C	513	CLA	C4B-CHC	2.84	1.47	1.40
23	C	511	CLA	C1B-CHB	2.84	1.47	1.40
23	C	507	CLA	C4B-CHC	2.85	1.47	1.40
23	b	615	CLA	C1B-CHB	2.85	1.47	1.40
23	C	505	CLA	C1C-C2C	2.85	1.50	1.44
23	c	509	CLA	C4C-C3C	2.85	1.50	1.45
23	b	612	CLA	C1B-CHB	2.85	1.47	1.40
23	d	403	CLA	C4B-CHC	2.86	1.47	1.40
23	B	606	CLA	C1B-CHB	2.86	1.47	1.40
23	C	503	CLA	C4B-CHC	2.86	1.47	1.40
23	b	604	CLA	C4B-CHC	2.86	1.47	1.40
23	C	514	CLA	C1C-C2C	2.87	1.50	1.44
23	c	513	CLA	C4B-CHC	2.87	1.47	1.40
23	C	512	CLA	C1C-C2C	2.87	1.50	1.44
23	C	510	CLA	C4B-CHC	2.87	1.47	1.40
23	c	508	CLA	C1B-CHB	2.87	1.47	1.40
23	c	509	CLA	C1B-CHB	2.88	1.47	1.40
23	A	404	CLA	C4B-CHC	2.88	1.47	1.40
23	b	604	CLA	C1C-C2C	2.89	1.50	1.44
23	b	610	CLA	C1C-C2C	2.89	1.50	1.44
23	b	604	CLA	C1B-CHB	2.90	1.47	1.40
23	b	614	CLA	C1B-CHB	2.90	1.47	1.40
23	d	403	CLA	C1B-CHB	2.90	1.47	1.40
23	A	404	CLA	C4C-C3C	2.90	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C1B-CHB	2.90	1.47	1.40
23	B	609	CLA	C1B-CHB	2.91	1.47	1.40
23	D	404	CLA	C1C-C2C	2.91	1.50	1.44
23	b	613	CLA	C1B-CHB	2.91	1.47	1.40
23	C	512	CLA	C1B-CHB	2.92	1.47	1.40
23	b	609	CLA	C1B-CHB	2.93	1.47	1.40
23	b	603	CLA	C1C-C2C	2.93	1.50	1.44
23	c	502	CLA	C1B-CHB	2.93	1.47	1.40
23	A	405	CLA	C1B-CHB	2.93	1.47	1.40
23	b	601	CLA	C4B-CHC	2.94	1.47	1.40
23	C	505	CLA	C4B-CHC	2.94	1.48	1.40
23	B	610	CLA	C1B-CHB	2.95	1.48	1.40
23	B	614	CLA	C1B-CHB	2.95	1.48	1.40
23	D	404	CLA	C4C-C3C	2.95	1.50	1.45
23	c	513	CLA	C1C-C2C	2.95	1.50	1.44
23	c	510	CLA	C1B-CHB	2.95	1.48	1.40
23	b	611	CLA	C4B-CHC	2.96	1.48	1.40
23	B	613	CLA	C4B-CHC	2.96	1.48	1.40
23	C	506	CLA	C1B-CHB	2.96	1.48	1.40
23	b	602	CLA	C4B-CHC	2.96	1.48	1.40
23	c	505	CLA	C1C-C2C	2.96	1.50	1.44
23	C	506	CLA	C1C-C2C	2.96	1.50	1.44
23	b	610	CLA	C1B-CHB	2.97	1.48	1.40
23	B	606	CLA	C4B-CHC	2.97	1.48	1.40
23	b	603	CLA	C4B-CHC	2.98	1.48	1.40
23	B	609	CLA	C4B-CHC	2.98	1.48	1.40
23	C	510	CLA	C1C-C2C	2.98	1.50	1.44
24	a	406	PHO	CHD-C4C	2.98	1.47	1.40
23	B	613	CLA	C1B-CHB	2.99	1.48	1.40
23	b	610	CLA	C4C-C3C	2.99	1.50	1.45
24	a	407	PHO	CHB-C4A	2.99	1.47	1.40
24	D	401	PHO	CHB-C4A	2.99	1.47	1.40
24	a	406	PHO	CHB-C4A	3.01	1.47	1.40
23	c	505	CLA	C4B-CHC	3.01	1.48	1.40
23	D	405	CLA	C4B-CHC	3.03	1.48	1.40
23	B	604	CLA	C1B-CHB	3.04	1.48	1.40
23	b	612	CLA	C4B-CHC	3.04	1.48	1.40
23	b	605	CLA	C1B-CHB	3.05	1.48	1.40
23	B	605	CLA	C1B-CHB	3.05	1.48	1.40
23	d	404	CLA	C4B-CHC	3.06	1.48	1.40
24	D	401	PHO	CHC-C4B	3.08	1.47	1.40
23	b	608	CLA	C4B-CHC	3.08	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	C3B-C4B	3.09	1.49	1.43
23	B	610	CLA	C4B-CHC	3.09	1.48	1.40
23	C	509	CLA	C1B-CHB	3.10	1.48	1.40
23	c	501	CLA	C4B-CHC	3.10	1.48	1.40
24	a	407	PHO	C3B-C4B	3.10	1.50	1.43
23	A	405	CLA	C1C-C2C	3.14	1.50	1.44
23	B	611	CLA	C1B-CHB	3.15	1.48	1.40
23	c	501	CLA	C1B-CHB	3.16	1.48	1.40
24	a	406	PHO	CHC-C4B	3.18	1.48	1.40
23	b	610	CLA	C4B-CHC	3.20	1.48	1.40
23	c	503	CLA	C4B-CHC	3.22	1.48	1.40
23	B	605	CLA	C4B-CHC	3.23	1.48	1.40
23	c	505	CLA	C1B-CHB	3.25	1.48	1.40
23	c	511	CLA	C1B-CHB	3.26	1.48	1.40
23	b	616	CLA	C4B-CHC	3.27	1.48	1.40
24	A	407	PHO	CHC-C4B	3.27	1.48	1.40
23	b	611	CLA	C1B-CHB	3.29	1.48	1.40
23	a	404	CLA	O2A-CGA	3.31	1.43	1.33
31	D	408	LHG	O8-C23	3.37	1.43	1.33
24	A	407	PHO	CHD-C4C	3.38	1.48	1.40
31	d	407	LHG	O7-C7	3.45	1.44	1.34
33	j	101	LMG	O7-C10	3.46	1.44	1.34
24	a	406	PHO	OBD-CAD	3.47	1.28	1.22
24	a	407	PHO	CHD-C4C	3.48	1.48	1.40
24	D	401	PHO	OBD-CAD	3.50	1.28	1.22
24	a	407	PHO	CHC-C4B	3.54	1.48	1.40
23	A	408	CLA	OBD-CAD	3.55	1.27	1.22
24	A	407	PHO	O2A-CGA	3.56	1.43	1.33
23	b	607	CLA	O2A-CGA	3.56	1.43	1.33
33	b	620	LMG	O7-C10	3.56	1.44	1.34
24	D	401	PHO	CHD-C4C	3.60	1.49	1.40
24	A	407	PHO	OBD-CAD	3.61	1.28	1.22
23	C	502	CLA	OBD-CAD	3.62	1.27	1.22
36	C	517	DGD	O1G-C1A	3.64	1.44	1.33
26	A	410	SQD	O47-C7	3.65	1.44	1.34
31	d	408	LHG	O8-C23	3.65	1.44	1.33
23	A	405	CLA	C4B-CHC	3.67	1.49	1.40
23	D	405	CLA	O2A-CGA	3.67	1.44	1.33
33	J	101	LMG	O7-C10	3.68	1.45	1.34
31	A	416	LHG	O7-C7	3.68	1.45	1.34
23	B	603	CLA	O2A-CGA	3.69	1.44	1.33
23	A	404	CLA	O2A-CGA	3.70	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	416	LHG	O8-C23	3.71	1.44	1.33
36	c	517	DGD	O2G-C1B	3.71	1.45	1.34
36	c	518	DGD	O2G-C1B	3.72	1.45	1.34
36	C	519	DGD	O2G-C1B	3.73	1.45	1.34
23	C	506	CLA	C3D-C2D	3.73	1.48	1.39
23	B	604	CLA	C3D-C2D	3.77	1.48	1.39
31	d	407	LHG	O8-C23	3.78	1.44	1.33
23	b	606	CLA	OBD-CAD	3.79	1.27	1.22
24	A	407	PHO	C3D-C2D	3.79	1.49	1.38
33	B	621	LMG	O7-C10	3.79	1.45	1.34
23	B	609	CLA	OBD-CAD	3.80	1.27	1.22
23	b	610	CLA	O2A-CGA	3.80	1.44	1.33
23	D	404	CLA	OBD-CAD	3.80	1.27	1.22
36	C	517	DGD	O2G-C1B	3.80	1.45	1.34
36	C	518	DGD	O1G-C1A	3.81	1.44	1.33
23	c	510	CLA	C3D-C2D	3.82	1.48	1.39
24	a	406	PHO	O2A-CGA	3.82	1.44	1.33
23	B	608	CLA	O2A-CGA	3.82	1.44	1.33
23	B	610	CLA	O2A-CGA	3.82	1.44	1.33
31	D	409	LHG	O8-C23	3.83	1.44	1.33
36	c	516	DGD	O2G-C1B	3.83	1.45	1.34
36	C	519	DGD	O1G-C1A	3.83	1.44	1.33
31	D	408	LHG	O7-C7	3.83	1.45	1.34
23	A	408	CLA	O2A-CGA	3.83	1.44	1.33
31	d	408	LHG	O7-C7	3.84	1.45	1.34
24	a	407	PHO	C3D-C2D	3.84	1.49	1.38
36	C	518	DGD	O2G-C1B	3.84	1.45	1.34
31	A	417	LHG	O7-C7	3.85	1.45	1.34
23	b	603	CLA	O2A-CGA	3.85	1.44	1.33
23	B	605	CLA	O2A-CGA	3.86	1.44	1.33
23	b	616	CLA	O2A-CGA	3.88	1.44	1.33
24	D	401	PHO	C3D-C2D	3.88	1.49	1.38
26	a	410	SQD	O47-C7	3.88	1.45	1.34
23	b	604	CLA	O2A-CGA	3.88	1.44	1.33
31	E	101	LHG	O7-C7	3.89	1.45	1.34
24	a	406	PHO	C3D-C2D	3.89	1.49	1.38
23	B	606	CLA	OBD-CAD	3.89	1.28	1.22
23	b	614	CLA	O2A-CGA	3.89	1.44	1.33
23	b	604	CLA	C3D-C2D	3.90	1.48	1.39
23	b	609	CLA	O2A-CGA	3.91	1.44	1.33
23	B	614	CLA	O2A-CGA	3.91	1.44	1.33
23	B	602	CLA	O2A-CGA	3.91	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	O2A-CGA	3.91	1.44	1.33
23	B	614	CLA	CHC-C1C	3.92	1.46	1.35
23	b	606	CLA	O2A-CGA	3.92	1.44	1.33
24	a	407	PHO	OBD-CAD	3.93	1.29	1.22
23	b	613	CLA	OBD-CAD	3.94	1.28	1.22
23	b	611	CLA	OBD-CAD	3.94	1.28	1.22
33	z	101	LMG	O7-C10	3.94	1.45	1.34
23	b	602	CLA	O2A-CGA	3.95	1.45	1.33
23	c	501	CLA	O2A-CGA	3.95	1.45	1.33
31	l	101	LHG	O7-C7	3.96	1.45	1.34
23	B	613	CLA	O2A-CGA	3.97	1.45	1.33
36	H	102	DGD	O2G-C1B	3.98	1.45	1.34
23	c	510	CLA	O2A-CGA	3.99	1.45	1.33
26	a	412	SQD	O47-C7	3.99	1.45	1.34
33	C	520	LMG	O7-C10	3.99	1.45	1.34
36	h	102	DGD	O2G-C1B	3.99	1.45	1.34
23	B	611	CLA	O2A-CGA	3.99	1.45	1.33
23	b	605	CLA	CHC-C1C	3.99	1.47	1.35
23	c	505	CLA	C3D-C2D	4.00	1.48	1.39
23	C	509	CLA	O2A-CGA	4.00	1.45	1.33
36	c	516	DGD	O1G-C1A	4.00	1.45	1.33
33	c	519	LMG	O7-C10	4.00	1.45	1.34
23	B	612	CLA	O2A-CGA	4.01	1.45	1.33
36	h	102	DGD	O1G-C1A	4.01	1.45	1.33
36	c	518	DGD	O1G-C1A	4.01	1.45	1.33
23	b	613	CLA	O2A-CGA	4.01	1.45	1.33
33	b	620	LMG	O8-C28	4.02	1.45	1.33
23	C	509	CLA	CHC-C1C	4.03	1.47	1.35
23	c	502	CLA	CHC-C1C	4.03	1.47	1.35
26	D	413	SQD	O48-C23	4.03	1.45	1.33
31	D	409	LHG	O7-C7	4.03	1.46	1.34
23	D	404	CLA	O2A-CGA	4.03	1.45	1.33
23	C	504	CLA	O2A-CGA	4.05	1.45	1.33
33	j	101	LMG	O8-C28	4.05	1.45	1.33
36	H	102	DGD	O1G-C1A	4.05	1.45	1.33
23	c	510	CLA	OBD-CAD	4.06	1.28	1.22
23	a	408	CLA	O2A-CGA	4.06	1.45	1.33
26	a	410	SQD	O48-C23	4.06	1.45	1.33
23	c	503	CLA	OBD-CAD	4.07	1.28	1.22
31	e	101	LHG	O7-C7	4.07	1.46	1.34
33	a	416	LMG	O8-C28	4.08	1.45	1.33
23	c	503	CLA	O2A-CGA	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	O2A-CGA	4.09	1.45	1.33
23	B	604	CLA	O2A-CGA	4.10	1.45	1.33
23	D	404	CLA	CHC-C1C	4.10	1.47	1.35
23	C	505	CLA	CHC-C1C	4.10	1.47	1.35
24	D	401	PHO	O2A-CGA	4.10	1.45	1.33
33	C	501	LMG	O7-C10	4.10	1.46	1.34
23	B	614	CLA	OBD-CAD	4.11	1.28	1.22
23	b	614	CLA	CHC-C1C	4.11	1.47	1.35
33	J	101	LMG	O8-C28	4.11	1.45	1.33
23	b	615	CLA	OBD-CAD	4.11	1.28	1.22
33	a	416	LMG	O7-C10	4.11	1.46	1.34
23	B	615	CLA	CHC-C1C	4.11	1.47	1.35
23	c	510	CLA	CHC-C1C	4.11	1.47	1.35
23	B	616	CLA	O2A-CGA	4.11	1.45	1.33
23	c	511	CLA	C3D-C2D	4.11	1.48	1.39
23	c	505	CLA	O2A-CGA	4.11	1.45	1.33
31	d	409	LHG	O8-C23	4.12	1.45	1.33
33	C	520	LMG	O8-C28	4.12	1.45	1.33
23	c	511	CLA	O2A-CGA	4.12	1.45	1.33
23	C	507	CLA	O2A-CGA	4.12	1.45	1.33
23	c	506	CLA	O2A-CGA	4.13	1.45	1.33
23	c	506	CLA	CHC-C1C	4.13	1.47	1.35
23	C	511	CLA	C3D-C2D	4.13	1.48	1.39
23	B	612	CLA	CHC-C1C	4.13	1.47	1.35
23	B	607	CLA	OBD-CAD	4.13	1.28	1.22
23	a	405	CLA	O2A-CGA	4.13	1.45	1.33
26	L	101	SQD	O47-C7	4.13	1.46	1.34
33	Z	102	LMG	O7-C10	4.14	1.46	1.34
23	B	603	CLA	OBD-CAD	4.14	1.28	1.22
24	a	407	PHO	O2A-CGA	4.14	1.45	1.33
23	c	501	CLA	OBD-CAD	4.15	1.28	1.22
23	A	406	CLA	O2A-CGA	4.15	1.45	1.33
23	a	404	CLA	CHC-C1C	4.16	1.47	1.35
33	c	520	LMG	O7-C10	4.16	1.46	1.34
23	b	615	CLA	C3D-C2D	4.17	1.48	1.39
23	C	513	CLA	O2A-CGA	4.17	1.45	1.33
23	d	401	CLA	OBD-CAD	4.17	1.28	1.22
23	b	611	CLA	CHC-C1C	4.18	1.47	1.35
23	c	503	CLA	C3D-C2D	4.18	1.48	1.39
23	A	405	CLA	OBD-CAD	4.18	1.28	1.22
23	C	502	CLA	O2A-CGA	4.19	1.45	1.33
23	b	603	CLA	C3D-C2D	4.19	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	CHC-C1C	4.20	1.47	1.35
23	A	408	CLA	C3D-C2D	4.20	1.49	1.39
26	f	101	SQD	O48-C23	4.20	1.45	1.33
23	B	606	CLA	O2A-CGA	4.20	1.45	1.33
23	B	608	CLA	OBD-CAD	4.20	1.28	1.22
23	B	611	CLA	CHC-C1C	4.20	1.47	1.35
23	C	511	CLA	O2A-CGA	4.21	1.45	1.33
23	B	603	CLA	CHC-C1C	4.21	1.47	1.35
23	c	504	CLA	CHC-C1C	4.21	1.47	1.35
33	c	519	LMG	O8-C28	4.21	1.45	1.33
23	b	615	CLA	O2A-CGA	4.21	1.45	1.33
33	B	621	LMG	O8-C28	4.22	1.45	1.33
23	b	606	CLA	CHC-C1C	4.22	1.47	1.35
23	b	612	CLA	OBD-CAD	4.22	1.28	1.22
23	c	513	CLA	O2A-CGA	4.22	1.45	1.33
23	c	504	CLA	O2A-CGA	4.22	1.45	1.33
23	C	502	CLA	CHC-C1C	4.23	1.47	1.35
23	C	502	CLA	C3D-C2D	4.23	1.49	1.39
31	A	417	LHG	O8-C23	4.23	1.45	1.33
23	C	508	CLA	CHC-C1C	4.23	1.47	1.35
23	c	502	CLA	O2A-CGA	4.24	1.45	1.33
26	A	410	SQD	O48-C23	4.24	1.45	1.33
23	d	403	CLA	C3D-C2D	4.24	1.49	1.39
23	C	508	CLA	OBD-CAD	4.24	1.28	1.22
33	c	520	LMG	O8-C28	4.25	1.45	1.33
23	B	615	CLA	O2A-CGA	4.25	1.45	1.33
23	B	608	CLA	CHC-C1C	4.25	1.47	1.35
23	B	613	CLA	CHC-C1C	4.25	1.47	1.35
23	c	509	CLA	O2A-CGA	4.25	1.45	1.33
23	b	615	CLA	CHC-C1C	4.26	1.47	1.35
23	C	512	CLA	CHC-C1C	4.26	1.47	1.35
23	C	510	CLA	CHC-C1C	4.26	1.47	1.35
23	C	504	CLA	OBD-CAD	4.26	1.28	1.22
23	C	503	CLA	OBD-CAD	4.26	1.28	1.22
23	B	607	CLA	O2A-CGA	4.26	1.45	1.33
23	B	602	CLA	CHC-C1C	4.26	1.47	1.35
31	d	409	LHG	O7-C7	4.26	1.46	1.34
26	L	101	SQD	O48-C23	4.26	1.45	1.33
23	b	602	CLA	OBD-CAD	4.26	1.28	1.22
23	C	504	CLA	O2D-CGD	4.27	1.44	1.33
23	c	501	CLA	O2D-CGD	4.27	1.44	1.33
23	C	514	CLA	O2A-CGA	4.27	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	O2A-CGA	4.27	1.45	1.33
31	e	101	LHG	O8-C23	4.27	1.45	1.33
33	Z	101	LMG	O7-C10	4.27	1.46	1.34
26	A	412	SQD	O47-C7	4.27	1.46	1.34
23	B	601	CLA	CHC-C1C	4.27	1.47	1.35
23	C	506	CLA	O2A-CGA	4.28	1.45	1.33
23	C	507	CLA	CHC-C1C	4.28	1.47	1.35
31	l	101	LHG	O8-C23	4.28	1.45	1.33
23	C	507	CLA	C3D-C2D	4.30	1.49	1.39
23	D	404	CLA	C3D-C2D	4.30	1.49	1.39
23	b	607	CLA	CHC-C1C	4.30	1.47	1.35
23	C	504	CLA	C3D-C2D	4.30	1.49	1.39
23	b	614	CLA	C3D-C2D	4.30	1.49	1.39
23	D	405	CLA	C3D-C2D	4.30	1.49	1.39
26	A	412	SQD	O48-C23	4.31	1.46	1.33
23	C	512	CLA	C3D-C2D	4.31	1.49	1.39
33	Z	101	LMG	O8-C28	4.31	1.46	1.33
23	b	608	CLA	CHC-C1C	4.31	1.47	1.35
23	c	501	CLA	CHC-C1C	4.31	1.47	1.35
23	c	509	CLA	CHC-C1C	4.31	1.47	1.35
33	C	501	LMG	O8-C28	4.31	1.46	1.33
26	B	620	SQD	O48-C23	4.31	1.46	1.33
23	c	512	CLA	O2A-CGA	4.32	1.46	1.33
23	b	608	CLA	O2A-CGA	4.32	1.46	1.33
23	C	505	CLA	O2A-CGA	4.32	1.46	1.33
23	C	512	CLA	O2A-CGA	4.32	1.46	1.33
23	c	507	CLA	O2A-CGA	4.32	1.46	1.33
26	B	620	SQD	O47-C7	4.32	1.46	1.34
23	B	602	CLA	OBD-CAD	4.33	1.28	1.22
23	B	607	CLA	CHC-C1C	4.33	1.48	1.35
23	B	608	CLA	C3D-C2D	4.33	1.49	1.39
23	C	506	CLA	OBD-CAD	4.34	1.28	1.22
23	c	512	CLA	CHC-C1C	4.34	1.48	1.35
23	a	405	CLA	CHC-C1C	4.34	1.48	1.35
26	f	101	SQD	O47-C7	4.35	1.46	1.34
23	C	504	CLA	CHC-C1C	4.35	1.48	1.35
23	d	401	CLA	CHC-C1C	4.36	1.48	1.35
23	C	503	CLA	O2D-CGD	4.36	1.44	1.33
23	B	612	CLA	OBD-CAD	4.36	1.28	1.22
23	B	605	CLA	C3D-C2D	4.36	1.49	1.39
23	B	607	CLA	C3D-C2D	4.36	1.49	1.39
23	b	601	CLA	CHC-C1C	4.36	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	O2A-CGA	4.36	1.46	1.33
23	d	403	CLA	CHC-C1C	4.36	1.48	1.35
23	b	616	CLA	OBD-CAD	4.36	1.28	1.22
23	d	403	CLA	O2A-CGA	4.37	1.46	1.33
23	b	602	CLA	CHC-C1C	4.37	1.48	1.35
23	c	513	CLA	OBD-CAD	4.37	1.28	1.22
36	c	517	DGD	O1G-C1A	4.37	1.46	1.33
23	A	408	CLA	CHC-C1C	4.38	1.48	1.35
23	d	403	CLA	OBD-CAD	4.38	1.28	1.22
23	b	611	CLA	O2A-CGA	4.38	1.46	1.33
26	D	413	SQD	O47-C7	4.38	1.47	1.34
23	C	508	CLA	O2A-CGA	4.38	1.46	1.33
23	d	404	CLA	O2A-CGA	4.38	1.46	1.33
23	C	505	CLA	OBD-CAD	4.38	1.28	1.22
23	a	408	CLA	C3D-C2D	4.39	1.49	1.39
23	C	502	CLA	O2D-CGD	4.39	1.44	1.33
23	c	503	CLA	CHC-C1C	4.39	1.48	1.35
23	B	606	CLA	C3D-C2D	4.40	1.49	1.39
23	b	606	CLA	C3D-C2D	4.40	1.49	1.39
23	b	601	CLA	O2A-CGA	4.40	1.46	1.33
23	c	502	CLA	OBD-CAD	4.40	1.28	1.22
23	C	514	CLA	OBD-CAD	4.40	1.28	1.22
23	c	501	CLA	C3D-C2D	4.40	1.49	1.39
23	C	512	CLA	OBD-CAD	4.41	1.28	1.22
23	b	607	CLA	OBD-CAD	4.41	1.28	1.22
23	C	510	CLA	C3D-C2D	4.41	1.49	1.39
23	c	504	CLA	OBD-CAD	4.41	1.28	1.22
23	c	512	CLA	C3D-C2D	4.41	1.49	1.39
24	a	406	PHO	CHC-C1C	4.41	1.47	1.38
23	c	508	CLA	CHC-C1C	4.41	1.48	1.35
23	c	511	CLA	CHC-C1C	4.42	1.48	1.35
23	B	605	CLA	CHC-C1C	4.42	1.48	1.35
23	C	511	CLA	CHC-C1C	4.42	1.48	1.35
23	C	503	CLA	CHC-C1C	4.42	1.48	1.35
23	d	401	CLA	O2A-CGA	4.42	1.46	1.33
23	a	408	CLA	OBD-CAD	4.42	1.28	1.22
23	b	612	CLA	C3D-C2D	4.42	1.49	1.39
24	a	406	PHO	O2D-CGD	4.42	1.44	1.33
23	A	406	CLA	C3D-C2D	4.42	1.49	1.39
23	b	604	CLA	CHC-C1C	4.43	1.48	1.35
23	B	611	CLA	OBD-CAD	4.43	1.28	1.22
23	B	612	CLA	C3D-C2D	4.43	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	O2A-CGA	4.43	1.46	1.33
23	B	611	CLA	C3D-C2D	4.43	1.49	1.39
23	B	607	CLA	O2D-CGD	4.44	1.44	1.33
23	a	408	CLA	CHC-C1C	4.44	1.48	1.35
23	d	404	CLA	O2D-CGD	4.45	1.44	1.33
23	b	610	CLA	C3D-C2D	4.45	1.49	1.39
31	E	101	LHG	O8-C23	4.45	1.46	1.33
23	b	609	CLA	C3D-C2D	4.45	1.49	1.39
23	b	609	CLA	CHC-C1C	4.45	1.48	1.35
23	a	404	CLA	C3D-C2D	4.45	1.49	1.39
23	c	505	CLA	OBD-CAD	4.45	1.28	1.22
23	B	606	CLA	CHC-C1C	4.45	1.48	1.35
23	b	610	CLA	O2D-CGD	4.46	1.44	1.33
26	a	412	SQD	O48-C23	4.46	1.46	1.33
23	b	612	CLA	CHC-C1C	4.46	1.48	1.35
23	C	503	CLA	O2A-CGA	4.46	1.46	1.33
23	b	606	CLA	O2D-CGD	4.47	1.44	1.33
23	C	503	CLA	C3D-C2D	4.48	1.49	1.39
23	c	507	CLA	CHC-C1C	4.48	1.48	1.35
23	A	404	CLA	CHC-C1C	4.48	1.48	1.35
23	C	514	CLA	C3D-C2D	4.48	1.49	1.39
23	C	513	CLA	CHC-C1C	4.49	1.48	1.35
23	c	509	CLA	OBD-CAD	4.49	1.28	1.22
23	C	507	CLA	OBD-CAD	4.49	1.28	1.22
23	A	404	CLA	OBD-CAD	4.49	1.28	1.22
23	B	604	CLA	CHC-C1C	4.49	1.48	1.35
23	c	506	CLA	C3D-C2D	4.49	1.49	1.39
23	c	513	CLA	CHC-C1C	4.49	1.48	1.35
23	A	405	CLA	O2D-CGD	4.49	1.44	1.33
23	A	404	CLA	C3D-C2D	4.49	1.49	1.39
23	c	513	CLA	C3D-C2D	4.50	1.49	1.39
23	C	513	CLA	O2D-CGD	4.50	1.44	1.33
23	B	614	CLA	C3D-C2D	4.50	1.49	1.39
23	B	603	CLA	O2D-CGD	4.50	1.44	1.33
23	B	603	CLA	C3D-C2D	4.50	1.49	1.39
23	b	610	CLA	CHC-C1C	4.51	1.48	1.35
23	a	405	CLA	C3D-C2D	4.51	1.49	1.39
23	B	601	CLA	O2A-CGA	4.51	1.46	1.33
23	c	505	CLA	CHC-C1C	4.51	1.48	1.35
23	A	405	CLA	CHC-C1C	4.51	1.48	1.35
23	c	504	CLA	C3D-C2D	4.52	1.49	1.39
23	B	610	CLA	CHC-C1C	4.52	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	O2D-CGD	4.52	1.44	1.33
23	B	605	CLA	OBD-CAD	4.53	1.28	1.22
33	z	101	LMG	O8-C28	4.53	1.46	1.33
23	d	404	CLA	OBD-CAD	4.53	1.28	1.22
23	C	513	CLA	OBD-CAD	4.53	1.28	1.22
23	c	508	CLA	O2D-CGD	4.53	1.44	1.33
23	A	406	CLA	OBD-CAD	4.53	1.28	1.22
23	B	616	CLA	OBD-CAD	4.53	1.28	1.22
23	c	507	CLA	C3D-C2D	4.54	1.49	1.39
23	C	505	CLA	C3D-C2D	4.54	1.49	1.39
23	c	505	CLA	O2D-CGD	4.55	1.44	1.33
23	B	612	CLA	O2D-CGD	4.55	1.44	1.33
23	B	616	CLA	O2D-CGD	4.56	1.44	1.33
23	C	514	CLA	CHC-C1C	4.56	1.48	1.35
23	B	609	CLA	C3D-C2D	4.56	1.49	1.39
23	C	514	CLA	O2D-CGD	4.57	1.44	1.33
23	C	506	CLA	CHC-C1C	4.57	1.48	1.35
23	c	512	CLA	OBD-CAD	4.57	1.29	1.22
23	b	602	CLA	C3D-C2D	4.57	1.49	1.39
24	A	407	PHO	CHB-C1B	4.58	1.47	1.38
23	b	608	CLA	OBD-CAD	4.58	1.29	1.22
23	C	511	CLA	O2D-CGD	4.58	1.44	1.33
23	a	405	CLA	O2D-CGD	4.58	1.44	1.33
23	B	613	CLA	OBD-CAD	4.58	1.29	1.22
23	C	513	CLA	C3D-C2D	4.59	1.49	1.39
23	B	609	CLA	CHC-C1C	4.59	1.48	1.35
23	A	404	CLA	O2D-CGD	4.60	1.44	1.33
23	B	601	CLA	OBD-CAD	4.60	1.29	1.22
23	b	601	CLA	OBD-CAD	4.60	1.29	1.22
23	d	404	CLA	CHC-C1C	4.61	1.48	1.35
23	c	503	CLA	O2D-CGD	4.61	1.44	1.33
23	a	405	CLA	OBD-CAD	4.61	1.29	1.22
23	b	605	CLA	OBD-CAD	4.61	1.29	1.22
23	b	615	CLA	O2D-CGD	4.61	1.44	1.33
23	d	401	CLA	O2D-CGD	4.62	1.44	1.33
23	c	509	CLA	C3D-C2D	4.62	1.49	1.39
23	B	610	CLA	C3D-C2D	4.62	1.49	1.39
23	a	404	CLA	O2D-CGD	4.63	1.44	1.33
23	b	611	CLA	C3D-C2D	4.63	1.49	1.39
23	B	616	CLA	CHC-C1C	4.63	1.48	1.35
24	a	406	PHO	CHD-C1D	4.63	1.47	1.38
23	b	603	CLA	CHC-C1C	4.63	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	OBD-CAD	4.63	1.29	1.22
23	b	607	CLA	C3D-C2D	4.64	1.49	1.39
23	b	616	CLA	C3D-C2D	4.65	1.50	1.39
23	c	506	CLA	OBD-CAD	4.65	1.29	1.22
23	B	616	CLA	C3D-C2D	4.66	1.50	1.39
23	A	405	CLA	C3D-C2D	4.66	1.50	1.39
23	C	509	CLA	O2D-CGD	4.66	1.45	1.33
23	b	605	CLA	O2D-CGD	4.66	1.45	1.33
23	B	606	CLA	O2D-CGD	4.66	1.45	1.33
23	B	610	CLA	O2D-CGD	4.67	1.45	1.33
23	a	408	CLA	O2D-CGD	4.68	1.45	1.33
23	b	604	CLA	O2D-CGD	4.68	1.45	1.33
24	a	407	PHO	CHB-C1B	4.68	1.47	1.38
23	b	614	CLA	OBD-CAD	4.68	1.29	1.22
23	D	405	CLA	O2D-CGD	4.68	1.45	1.33
23	B	604	CLA	O2D-CGD	4.68	1.45	1.33
23	C	508	CLA	O2D-CGD	4.69	1.45	1.33
23	c	507	CLA	O2D-CGD	4.70	1.45	1.33
23	b	610	CLA	OBD-CAD	4.70	1.29	1.22
23	b	603	CLA	OBD-CAD	4.70	1.29	1.22
23	B	609	CLA	O2A-CGA	4.70	1.47	1.33
23	D	405	CLA	CHC-C1C	4.71	1.49	1.35
23	C	506	CLA	O2D-CGD	4.71	1.45	1.33
23	a	404	CLA	OBD-CAD	4.72	1.29	1.22
24	A	407	PHO	CHC-C1C	4.72	1.47	1.38
23	c	507	CLA	OBD-CAD	4.72	1.29	1.22
23	b	604	CLA	OBD-CAD	4.73	1.29	1.22
24	D	401	PHO	O2D-CGD	4.73	1.45	1.33
23	b	612	CLA	O2D-CGD	4.73	1.45	1.33
23	B	601	CLA	C3D-C2D	4.73	1.50	1.39
23	D	404	CLA	O2D-CGD	4.74	1.45	1.33
23	B	604	CLA	OBD-CAD	4.74	1.29	1.22
23	b	605	CLA	C3D-C2D	4.74	1.50	1.39
23	B	605	CLA	O2D-CGD	4.75	1.45	1.33
23	c	502	CLA	C3D-C2D	4.75	1.50	1.39
23	B	602	CLA	C3D-C2D	4.75	1.50	1.39
23	b	607	CLA	O2D-CGD	4.75	1.45	1.33
23	b	609	CLA	C3C-C2C	4.75	1.46	1.36
23	A	406	CLA	CHC-C1C	4.76	1.49	1.35
23	c	512	CLA	O2D-CGD	4.76	1.45	1.33
23	b	613	CLA	C3D-C2D	4.76	1.50	1.39
23	b	616	CLA	CHC-C1C	4.76	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	OBD-CAD	4.76	1.29	1.22
23	d	404	CLA	C3D-C2D	4.76	1.50	1.39
23	C	510	CLA	OBD-CAD	4.76	1.29	1.22
23	b	601	CLA	C3D-C2D	4.77	1.50	1.39
23	b	616	CLA	O2D-CGD	4.78	1.45	1.33
23	b	608	CLA	C3D-C2D	4.79	1.50	1.39
23	B	613	CLA	C3D-C2D	4.79	1.50	1.39
23	d	403	CLA	O2D-CGD	4.79	1.45	1.33
23	b	609	CLA	OBD-CAD	4.79	1.29	1.22
23	B	615	CLA	C3D-C2D	4.80	1.50	1.39
23	b	614	CLA	O2D-CGD	4.80	1.45	1.33
23	b	608	CLA	O2D-CGD	4.80	1.45	1.33
23	C	509	CLA	C3D-C2D	4.80	1.50	1.39
23	b	614	CLA	C3C-C2C	4.81	1.47	1.36
23	D	405	CLA	OBD-CAD	4.81	1.29	1.22
23	c	502	CLA	O2D-CGD	4.82	1.45	1.33
24	a	407	PHO	CHD-C1D	4.82	1.48	1.38
23	c	508	CLA	C3D-C2D	4.82	1.50	1.39
23	C	510	CLA	O2D-CGD	4.83	1.45	1.33
23	B	613	CLA	O2D-CGD	4.83	1.45	1.33
24	A	407	PHO	O2D-CGD	4.83	1.45	1.33
23	B	608	CLA	O2D-CGD	4.84	1.45	1.33
24	A	407	PHO	CHD-C1D	4.84	1.48	1.38
23	C	509	CLA	OBD-CAD	4.84	1.29	1.22
23	C	508	CLA	C3D-C2D	4.85	1.50	1.39
23	c	511	CLA	OBD-CAD	4.86	1.29	1.22
23	B	614	CLA	O2D-CGD	4.87	1.45	1.33
24	D	401	PHO	CHD-C1D	4.87	1.48	1.38
23	c	510	CLA	O2D-CGD	4.88	1.45	1.33
23	B	609	CLA	C3C-C2C	4.88	1.47	1.36
23	b	609	CLA	O2D-CGD	4.88	1.45	1.33
23	C	507	CLA	C3C-C2C	4.88	1.47	1.36
23	A	406	CLA	O2D-CGD	4.89	1.45	1.33
23	B	611	CLA	C3C-C2C	4.89	1.47	1.36
23	b	613	CLA	O2D-CGD	4.89	1.45	1.33
23	c	504	CLA	C3C-C2C	4.91	1.47	1.36
23	d	401	CLA	C3D-C2D	4.91	1.50	1.39
23	B	615	CLA	OBD-CAD	4.91	1.29	1.22
23	c	504	CLA	O2D-CGD	4.92	1.45	1.33
23	B	611	CLA	O2D-CGD	4.92	1.45	1.33
23	B	609	CLA	O2D-CGD	4.92	1.45	1.33
23	c	510	CLA	C3C-C2C	4.92	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	O2D-CGD	4.92	1.45	1.33
23	B	602	CLA	O2D-CGD	4.93	1.45	1.33
23	A	408	CLA	O2D-CGD	4.93	1.45	1.33
23	B	615	CLA	O2D-CGD	4.94	1.45	1.33
23	B	601	CLA	O2D-CGD	4.95	1.45	1.33
23	c	509	CLA	O2D-CGD	4.95	1.45	1.33
23	b	611	CLA	O2D-CGD	4.95	1.45	1.33
23	B	604	CLA	C3C-C2C	4.97	1.47	1.36
23	C	512	CLA	C3C-C2C	4.98	1.47	1.36
23	a	404	CLA	C3C-C2C	4.98	1.47	1.36
24	D	401	PHO	CHC-C1C	4.98	1.48	1.38
23	b	607	CLA	C3C-C2C	4.99	1.47	1.36
23	C	506	CLA	C3C-C2C	4.99	1.47	1.36
23	B	613	CLA	C3C-C2C	4.99	1.47	1.36
24	a	407	PHO	O2D-CGD	4.99	1.45	1.33
23	b	602	CLA	O2D-CGD	5.01	1.45	1.33
23	c	506	CLA	O2D-CGD	5.02	1.45	1.33
23	B	609	CLA	C3B-C2B	5.03	1.47	1.40
23	C	505	CLA	O2D-CGD	5.04	1.46	1.33
23	B	615	CLA	C3C-C2C	5.04	1.47	1.36
23	b	603	CLA	O2D-CGD	5.05	1.46	1.33
23	C	512	CLA	O2D-CGD	5.06	1.46	1.33
24	a	406	PHO	CHB-C1B	5.06	1.48	1.38
23	B	605	CLA	C3B-C2B	5.07	1.47	1.40
23	d	403	CLA	C3C-C2C	5.07	1.47	1.36
23	b	601	CLA	O2D-CGD	5.08	1.46	1.33
24	D	401	PHO	CHB-C1B	5.09	1.48	1.38
23	c	506	CLA	C3C-C2C	5.09	1.47	1.36
24	D	401	PHO	C3C-C2C	5.10	1.47	1.36
23	c	502	CLA	C3C-C2C	5.13	1.47	1.36
23	c	507	CLA	C3C-C2C	5.13	1.47	1.36
23	B	605	CLA	C3C-C2C	5.13	1.47	1.36
23	c	503	CLA	C3C-C2C	5.14	1.47	1.36
23	C	502	CLA	C3C-C2C	5.15	1.47	1.36
23	c	511	CLA	C3C-C2C	5.15	1.47	1.36
23	c	513	CLA	C3C-C2C	5.15	1.47	1.36
23	b	611	CLA	C3C-C2C	5.16	1.47	1.36
23	b	608	CLA	C3C-C2C	5.16	1.47	1.36
23	C	514	CLA	C3C-C2C	5.16	1.47	1.36
23	B	612	CLA	C3C-C2C	5.18	1.47	1.36
23	A	404	CLA	C3C-C2C	5.18	1.47	1.36
23	C	510	CLA	C3C-C2C	5.20	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	C3C-C2C	5.21	1.47	1.36
23	a	408	CLA	C3C-C2C	5.22	1.47	1.36
23	C	507	CLA	O2D-CGD	5.22	1.46	1.33
23	b	601	CLA	C3C-C2C	5.22	1.47	1.36
23	c	505	CLA	C3C-C2C	5.22	1.47	1.36
23	D	405	CLA	C3C-C2C	5.23	1.48	1.36
23	C	505	CLA	C3C-C2C	5.24	1.48	1.36
23	B	606	CLA	C3C-C2C	5.25	1.48	1.36
23	C	511	CLA	C3C-C2C	5.27	1.48	1.36
23	C	503	CLA	C3C-C2C	5.28	1.48	1.36
23	b	602	CLA	C3C-C2C	5.28	1.48	1.36
23	A	405	CLA	C3C-C2C	5.28	1.48	1.36
23	b	616	CLA	C3C-C2C	5.28	1.48	1.36
23	c	509	CLA	C3C-C2C	5.29	1.48	1.36
23	d	401	CLA	C3C-C2C	5.29	1.48	1.36
23	d	404	CLA	C3C-C2C	5.29	1.48	1.36
23	B	614	CLA	C3C-C2C	5.30	1.48	1.36
23	D	404	CLA	C3C-C2C	5.30	1.48	1.36
23	b	607	CLA	C3B-C2B	5.30	1.47	1.40
23	c	501	CLA	C3C-C2C	5.30	1.48	1.36
23	B	610	CLA	OBD-CAD	5.31	1.30	1.22
23	b	612	CLA	C3C-C2C	5.32	1.48	1.36
23	a	405	CLA	C3C-C2C	5.34	1.48	1.36
23	B	607	CLA	C3C-C2C	5.34	1.48	1.36
23	b	606	CLA	C3C-C2C	5.34	1.48	1.36
23	A	406	CLA	C3B-C2B	5.36	1.47	1.40
23	b	615	CLA	C3C-C2C	5.38	1.48	1.36
23	C	504	CLA	C3C-C2C	5.39	1.48	1.36
23	A	406	CLA	C3C-C2C	5.41	1.48	1.36
23	B	603	CLA	C3C-C2C	5.42	1.48	1.36
23	C	508	CLA	C3B-C2B	5.43	1.47	1.40
23	B	615	CLA	C3B-C2B	5.43	1.47	1.40
23	b	605	CLA	C3C-C2C	5.44	1.48	1.36
23	B	608	CLA	C3C-C2C	5.45	1.48	1.36
23	B	610	CLA	C3C-C2C	5.45	1.48	1.36
23	c	508	CLA	C3C-C2C	5.45	1.48	1.36
23	b	615	CLA	C3B-C2B	5.45	1.47	1.40
23	c	507	CLA	C3B-C2B	5.45	1.47	1.40
23	B	616	CLA	C3C-C2C	5.46	1.48	1.36
23	C	513	CLA	C3C-C2C	5.46	1.48	1.36
23	b	613	CLA	C3C-C2C	5.48	1.48	1.36
23	B	602	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	601	CLA	C3C-C2C	5.53	1.48	1.36
23	A	408	CLA	C3C-C2C	5.53	1.48	1.36
24	a	407	PHO	CHC-C1C	5.57	1.49	1.38
23	C	508	CLA	C3C-C2C	5.58	1.48	1.36
23	c	512	CLA	C3B-C2B	5.59	1.47	1.40
23	C	509	CLA	C3C-C2C	5.59	1.48	1.36
23	b	603	CLA	C3B-C2B	5.59	1.47	1.40
23	C	504	CLA	C3B-C2B	5.61	1.47	1.40
23	B	606	CLA	C3B-C2B	5.62	1.47	1.40
23	D	405	CLA	C3B-C2B	5.62	1.47	1.40
23	b	603	CLA	C3C-C2C	5.63	1.48	1.36
23	c	501	CLA	C3B-C2B	5.67	1.47	1.40
23	a	408	CLA	C3B-C2B	5.68	1.47	1.40
23	b	609	CLA	C3B-C2B	5.70	1.47	1.40
23	c	512	CLA	C3C-C2C	5.71	1.49	1.36
23	b	610	CLA	C3C-C2C	5.71	1.49	1.36
23	c	505	CLA	C3B-C2B	5.71	1.47	1.40
24	a	406	PHO	C3C-C2C	5.73	1.49	1.36
24	a	407	PHO	C3C-C2C	5.77	1.49	1.36
24	A	407	PHO	C3C-C2C	5.77	1.49	1.36
23	d	403	CLA	C3B-C2B	5.82	1.48	1.40
23	b	616	CLA	C3B-C2B	5.83	1.48	1.40
23	B	614	CLA	C3B-C2B	5.84	1.48	1.40
23	B	608	CLA	C3B-C2B	5.88	1.48	1.40
23	B	604	CLA	C3B-C2B	5.92	1.48	1.40
23	C	514	CLA	C3B-C2B	5.95	1.48	1.40
23	c	510	CLA	C3B-C2B	5.96	1.48	1.40
23	c	506	CLA	C3B-C2B	5.98	1.48	1.40
23	B	610	CLA	C3B-C2B	5.98	1.48	1.40
23	c	513	CLA	C3B-C2B	6.00	1.48	1.40
23	b	606	CLA	C3B-C2B	6.01	1.48	1.40
23	A	408	CLA	C3B-C2B	6.01	1.48	1.40
23	C	511	CLA	C3B-C2B	6.03	1.48	1.40
23	b	605	CLA	C3B-C2B	6.08	1.48	1.40
23	C	507	CLA	C3B-C2B	6.13	1.48	1.40
23	c	503	CLA	C3B-C2B	6.13	1.48	1.40
23	d	404	CLA	C3B-C2B	6.14	1.48	1.40
23	C	506	CLA	C3B-C2B	6.15	1.48	1.40
23	B	602	CLA	C3B-C2B	6.18	1.48	1.40
23	B	607	CLA	C3B-C2B	6.19	1.48	1.40
23	C	513	CLA	C3B-C2B	6.19	1.48	1.40
23	b	601	CLA	C3B-C2B	6.20	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3B-C2B	6.22	1.48	1.40
24	A	407	PHO	C3B-C2B	6.23	1.48	1.37
23	B	601	CLA	C3B-C2B	6.27	1.48	1.40
23	C	503	CLA	C3B-C2B	6.27	1.48	1.40
23	A	405	CLA	C3B-C2B	6.32	1.48	1.40
23	c	509	CLA	C3B-C2B	6.34	1.48	1.40
23	C	512	CLA	C3B-C2B	6.37	1.48	1.40
23	B	616	CLA	C3B-C2B	6.41	1.48	1.40
23	d	401	CLA	C3B-C2B	6.43	1.48	1.40
23	B	603	CLA	C3B-C2B	6.44	1.48	1.40
24	a	407	PHO	C3B-C2B	6.44	1.49	1.37
23	b	604	CLA	C3B-C2B	6.49	1.48	1.40
24	a	406	PHO	C3B-C2B	6.51	1.49	1.37
23	a	404	CLA	C3B-C2B	6.52	1.49	1.40
23	b	608	CLA	C3B-C2B	6.57	1.49	1.40
24	D	401	PHO	C3B-C2B	6.59	1.49	1.37
23	B	611	CLA	C3B-C2B	6.59	1.49	1.40
23	b	602	CLA	C3B-C2B	6.60	1.49	1.40
23	c	502	CLA	C3B-C2B	6.61	1.49	1.40
23	A	404	CLA	C3B-C2B	6.62	1.49	1.40
23	c	508	CLA	C3B-C2B	6.63	1.49	1.40
23	c	511	CLA	C3B-C2B	6.63	1.49	1.40
23	b	610	CLA	C3B-C2B	6.66	1.49	1.40
23	b	611	CLA	C3B-C2B	6.70	1.49	1.40
23	B	613	CLA	C3B-C2B	6.72	1.49	1.40
23	c	504	CLA	C3B-C2B	6.72	1.49	1.40
23	b	614	CLA	C3B-C2B	6.72	1.49	1.40
23	a	405	CLA	C3B-C2B	6.73	1.49	1.40
23	b	613	CLA	C3B-C2B	6.73	1.49	1.40
23	D	404	CLA	C3B-C2B	6.76	1.49	1.40
23	b	612	CLA	C3B-C2B	6.87	1.49	1.40
23	C	502	CLA	C3B-C2B	6.89	1.49	1.40
23	C	510	CLA	C3B-C2B	7.00	1.49	1.40
23	C	509	CLA	C3B-C2B	7.07	1.49	1.40
23	C	505	CLA	C3B-C2B	7.18	1.49	1.40

All (2207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	CHD-C4C-C3C	-6.74	114.77	124.92
23	B	609	CLA	CHD-C4C-C3C	-6.47	115.16	124.92
23	C	509	CLA	C1C-NC-C4C	-6.47	103.33	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404	CLA	C1C-NC-C4C	-6.45	103.34	107.06
23	B	612	CLA	C1C-NC-C4C	-6.40	103.37	107.06
23	b	616	CLA	CHD-C4C-C3C	-6.38	115.31	124.92
23	c	505	CLA	CHD-C4C-C3C	-6.38	115.31	124.92
23	D	405	CLA	CHD-C4C-C3C	-6.37	115.32	124.92
23	B	608	CLA	CHD-C4C-C3C	-6.35	115.34	124.92
23	B	604	CLA	C1C-NC-C4C	-6.30	103.43	107.06
23	C	506	CLA	CHD-C4C-C3C	-6.27	115.47	124.92
23	B	616	CLA	CHD-C4C-C3C	-6.26	115.48	124.92
23	B	613	CLA	C1C-NC-C4C	-6.25	103.46	107.06
23	B	612	CLA	CHD-C4C-C3C	-6.18	115.60	124.92
23	b	604	CLA	CHD-C4C-C3C	-6.18	115.61	124.92
23	b	604	CLA	C1C-NC-C4C	-6.16	103.51	107.06
23	C	505	CLA	C1C-NC-C4C	-6.13	103.53	107.06
23	B	615	CLA	CHD-C4C-C3C	-6.13	115.68	124.92
23	C	506	CLA	C1C-NC-C4C	-6.13	103.53	107.06
23	B	606	CLA	CHD-C4C-C3C	-6.13	115.69	124.92
23	B	611	CLA	CHD-C4C-C3C	-6.12	115.69	124.92
23	B	604	CLA	CHD-C4C-C3C	-6.12	115.70	124.92
23	B	610	CLA	CHD-C4C-C3C	-6.11	115.70	124.92
23	b	608	CLA	CHD-C4C-C3C	-6.05	115.81	124.92
23	b	606	CLA	CHD-C4C-C3C	-6.03	115.83	124.92
23	d	401	CLA	CHD-C4C-C3C	-6.03	115.84	124.92
23	b	613	CLA	CHD-C4C-C3C	-5.98	115.90	124.92
23	c	503	CLA	CHD-C4C-C3C	-5.98	115.90	124.92
23	b	605	CLA	CHD-C4C-C3C	-5.96	115.93	124.92
23	C	512	CLA	CHD-C4C-C3C	-5.94	115.96	124.92
23	b	607	CLA	C1C-NC-C4C	-5.93	103.65	107.06
23	a	405	CLA	CHD-C4C-C3C	-5.91	116.02	124.92
25	D	406	BCR	C7-C8-C9	-5.88	117.38	126.21
23	B	605	CLA	CHD-C4C-C3C	-5.85	116.10	124.92
23	C	510	CLA	CHD-C4C-C3C	-5.85	116.10	124.92
23	c	511	CLA	CHD-C4C-C3C	-5.85	116.10	124.92
23	a	404	CLA	C1C-NC-C4C	-5.83	103.70	107.06
24	D	401	PHO	C3D-C2D-C1D	-5.82	97.19	105.82
23	c	505	CLA	C1C-NC-C4C	-5.79	103.72	107.06
23	A	406	CLA	CHD-C4C-C3C	-5.79	116.19	124.92
23	C	514	CLA	CHD-C4C-C3C	-5.77	116.22	124.92
23	C	505	CLA	CHD-C4C-C3C	-5.77	116.23	124.92
23	b	603	CLA	CHD-C4C-C3C	-5.75	116.26	124.92
23	d	404	CLA	CHD-C4C-C3C	-5.74	116.27	124.92
23	c	507	CLA	CHD-C4C-C3C	-5.73	116.29	124.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	CHD-C4C-C3C	-5.71	116.31	124.92
23	B	613	CLA	CHD-C4C-C3C	-5.71	116.31	124.92
23	c	503	CLA	C1C-NC-C4C	-5.70	103.78	107.06
23	c	512	CLA	CHD-C4C-C3C	-5.69	116.34	124.92
23	b	613	CLA	C1C-NC-C4C	-5.69	103.78	107.06
23	C	513	CLA	CHD-C4C-C3C	-5.69	116.35	124.92
23	B	614	CLA	CHD-C4C-C3C	-5.68	116.35	124.92
23	b	602	CLA	CHD-C4C-C3C	-5.67	116.37	124.92
23	b	601	CLA	CHD-C4C-C3C	-5.66	116.39	124.92
23	c	508	CLA	CHD-C4C-C3C	-5.63	116.44	124.92
23	c	506	CLA	CHD-C4C-C3C	-5.62	116.45	124.92
23	B	601	CLA	CHD-C4C-C3C	-5.62	116.45	124.92
23	b	615	CLA	CHD-C4C-C3C	-5.62	116.45	124.92
25	Y	101	BCR	C33-C5-C6	-5.61	118.22	124.51
23	b	614	CLA	CHD-C4C-C3C	-5.61	116.46	124.92
23	b	612	CLA	CHD-C4C-C3C	-5.59	116.49	124.92
23	c	513	CLA	CHD-C4C-C3C	-5.58	116.50	124.92
23	C	502	CLA	C1C-NC-C4C	-5.58	103.85	107.06
23	C	503	CLA	CHD-C4C-C3C	-5.58	116.51	124.92
23	d	403	CLA	C1C-NC-C4C	-5.57	103.85	107.06
23	c	506	CLA	C1C-NC-C4C	-5.57	103.85	107.06
23	C	502	CLA	CHD-C4C-C3C	-5.56	116.53	124.92
23	b	607	CLA	CHD-C4C-C3C	-5.55	116.55	124.92
23	c	504	CLA	CHD-C4C-C3C	-5.53	116.59	124.92
23	b	610	CLA	CHD-C4C-C3C	-5.51	116.62	124.92
23	c	502	CLA	CHD-C4C-C3C	-5.50	116.63	124.92
23	B	611	CLA	C1C-NC-C4C	-5.47	103.91	107.06
23	B	607	CLA	CHD-C4C-C3C	-5.47	116.68	124.92
23	c	502	CLA	C1C-NC-C4C	-5.44	103.93	107.06
23	C	508	CLA	CHD-C4C-C3C	-5.43	116.73	124.92
23	b	611	CLA	C1C-NC-C4C	-5.38	103.96	107.06
23	b	611	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
23	c	510	CLA	CHD-C4C-C3C	-5.38	116.81	124.92
23	C	509	CLA	CHD-C4C-C3C	-5.37	116.82	124.92
23	b	614	CLA	C1C-NC-C4C	-5.35	103.98	107.06
23	a	408	CLA	CHD-C4C-C3C	-5.30	116.93	124.92
23	B	609	CLA	C1C-NC-C4C	-5.28	104.02	107.06
26	A	410	SQD	C1-C2-C3	-5.27	100.18	109.98
23	c	508	CLA	C1C-NC-C4C	-5.26	104.03	107.06
24	a	406	PHO	C3D-C2D-C1D	-5.26	98.02	105.82
23	b	609	CLA	CHD-C4C-C3C	-5.23	117.04	124.92
23	B	615	CLA	C1C-NC-C4C	-5.22	104.05	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	501	CLA	CHD-C4C-C3C	-5.18	117.11	124.92
23	c	509	CLA	CHD-C4C-C3C	-5.15	117.15	124.92
24	A	407	PHO	C3D-C2D-C1D	-5.13	98.21	105.82
23	C	511	CLA	CHD-C4C-C3C	-5.11	117.21	124.92
23	B	610	CLA	C1C-NC-C4C	-5.10	104.12	107.06
23	a	404	CLA	CHD-C4C-C3C	-5.10	117.23	124.92
23	c	509	CLA	C1C-NC-C4C	-5.10	104.12	107.06
23	D	404	CLA	CHD-C4C-C3C	-5.03	117.34	124.92
25	t	101	BCR	C33-C5-C6	-5.03	118.88	124.51
23	c	507	CLA	C1C-NC-C4C	-4.99	104.19	107.06
23	B	602	CLA	CHD-C4C-C3C	-4.99	117.41	124.92
23	B	614	CLA	C1C-NC-C4C	-4.98	104.19	107.06
23	B	603	CLA	CHD-C4C-C3C	-4.97	117.42	124.92
23	C	512	CLA	C1C-NC-C4C	-4.96	104.20	107.06
23	c	510	CLA	C1-C2-C3	-4.95	116.84	125.96
25	c	515	BCR	C7-C8-C9	-4.94	118.79	126.21
23	B	607	CLA	C1C-NC-C4C	-4.93	104.22	107.06
23	C	504	CLA	CHD-C4C-C3C	-4.93	117.49	124.92
23	C	507	CLA	CHD-C4C-C3C	-4.92	117.51	124.92
23	b	615	CLA	C1C-NC-C4C	-4.91	104.23	107.06
23	B	606	CLA	C1C-NC-C4C	-4.89	104.24	107.06
24	a	407	PHO	C3D-C2D-C1D	-4.88	98.58	105.82
23	d	403	CLA	CHD-C4C-C3C	-4.87	117.58	124.92
23	b	610	CLA	C1C-NC-C4C	-4.84	104.27	107.06
23	A	404	CLA	C1C-NC-C4C	-4.83	104.28	107.06
23	c	513	CLA	C1C-NC-C4C	-4.80	104.29	107.06
23	A	404	CLA	CHD-C4C-C3C	-4.80	117.69	124.92
23	C	508	CLA	C1C-NC-C4C	-4.79	104.30	107.06
23	C	507	CLA	C1C-NC-C4C	-4.75	104.32	107.06
25	y	101	BCR	C33-C5-C6	-4.73	119.21	124.51
23	C	503	CLA	C1C-NC-C4C	-4.71	104.35	107.06
23	b	609	CLA	C1C-NC-C4C	-4.70	104.35	107.06
24	A	407	PHO	C1-C2-C3	-4.70	117.30	125.96
24	a	407	PHO	C1-C2-C3	-4.69	117.31	125.96
23	B	602	CLA	C1C-NC-C4C	-4.67	104.37	107.06
23	B	603	CLA	C1C-NC-C4C	-4.66	104.38	107.06
23	b	612	CLA	C1C-NC-C4C	-4.66	104.38	107.06
25	T	101	BCR	C15-C16-C17	-4.65	113.55	123.46
23	c	512	CLA	C1C-NC-C4C	-4.62	104.40	107.06
23	d	401	CLA	C1C-C2C-C3C	-4.61	101.80	106.92
23	b	605	CLA	C1C-NC-C4C	-4.60	104.41	107.06
23	C	510	CLA	C1C-NC-C4C	-4.58	104.42	107.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C1C-NC-C4C	-4.57	104.43	107.06
26	A	410	SQD	C1-O5-C5	-4.56	105.12	113.72
23	b	601	CLA	C1C-NC-C4C	-4.56	104.43	107.06
23	a	408	CLA	C1C-NC-C4C	-4.55	104.44	107.06
23	c	504	CLA	C1C-NC-C4C	-4.54	104.44	107.06
25	H	101	BCR	C11-C10-C9	-4.52	120.86	127.31
23	D	404	CLA	C1-C2-C3	-4.52	117.63	125.96
25	c	514	BCR	C11-C10-C9	-4.52	120.86	127.31
25	T	101	BCR	C33-C5-C6	-4.51	119.46	124.51
25	d	405	BCR	C15-C14-C13	-4.50	120.89	127.31
23	c	509	CLA	C1-C2-C3	-4.44	117.78	125.96
23	b	606	CLA	C1C-NC-C4C	-4.42	104.51	107.06
23	D	404	CLA	C1C-C2C-C3C	-4.41	102.03	106.92
25	B	617	BCR	C33-C5-C6	-4.40	119.59	124.51
23	c	508	CLA	O2D-CGD-O1D	-4.40	114.98	123.82
23	C	505	CLA	C1C-C2C-C3C	-4.39	102.05	106.92
23	a	404	CLA	C1C-C2C-C3C	-4.39	102.05	106.92
29	D	407	PL9	C42-C43-C44	-4.37	116.71	127.68
23	b	616	CLA	C1D-CHD-C4C	-4.36	116.52	122.48
23	b	610	CLA	C1-C2-C3	-4.31	118.01	125.96
23	c	501	CLA	C1C-NC-C4C	-4.30	104.58	107.06
23	b	609	CLA	C1-C2-C3	-4.29	118.05	125.96
25	b	619	BCR	C3-C4-C5	-4.27	106.43	113.78
23	c	502	CLA	C1C-C2C-C3C	-4.26	102.20	106.92
23	c	511	CLA	C1C-NC-C4C	-4.25	104.61	107.06
23	C	511	CLA	C1C-NC-C4C	-4.25	104.61	107.06
25	d	405	BCR	C28-C27-C26	-4.23	106.50	113.78
25	C	515	BCR	C15-C14-C13	-4.22	121.29	127.31
23	c	510	CLA	C1C-NC-C4C	-4.22	104.63	107.06
25	B	617	BCR	C7-C8-C9	-4.22	119.88	126.21
23	A	408	CLA	C1C-NC-C4C	-4.21	104.64	107.06
23	B	605	CLA	C1C-NC-C4C	-4.19	104.64	107.06
23	C	513	CLA	C1C-NC-C4C	-4.19	104.65	107.06
23	b	608	CLA	C1C-NC-C4C	-4.18	104.65	107.06
23	B	614	CLA	C1D-CHD-C4C	-4.16	116.79	122.48
23	c	501	CLA	O2D-CGD-O1D	-4.14	115.49	123.82
23	B	601	CLA	C1C-NC-C4C	-4.14	104.67	107.06
23	C	514	CLA	C1C-NC-C4C	-4.13	104.68	107.06
23	B	613	CLA	C1-C2-C3	-4.13	118.35	125.96
23	B	616	CLA	C1C-NC-C4C	-4.11	104.69	107.06
23	C	504	CLA	C1C-NC-C4C	-4.10	104.70	107.06
25	b	617	BCR	C33-C5-C6	-4.09	119.93	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C1D-CHD-C4C	-4.08	116.90	122.48
23	a	404	CLA	C1D-CHD-C4C	-4.08	116.91	122.48
25	H	101	BCR	C7-C8-C9	-4.07	120.10	126.21
23	C	502	CLA	C1C-C2C-C3C	-4.07	102.41	106.92
25	b	619	BCR	C7-C8-C9	-4.07	120.10	126.21
26	a	410	SQD	C45-O47-C7	-4.06	108.28	117.88
25	k	101	BCR	C11-C10-C9	-4.05	121.53	127.31
23	D	405	CLA	O2D-CGD-O1D	-4.05	115.67	123.82
23	C	508	CLA	C1D-CHD-C4C	-4.05	116.95	122.48
23	d	401	CLA	C1C-NC-C4C	-4.05	104.73	107.06
23	B	608	CLA	C1C-NC-C4C	-4.04	104.73	107.06
24	a	406	PHO	C4C-C3C-C2C	-4.04	102.27	106.81
23	d	403	CLA	C1C-C2C-C3C	-4.04	102.44	106.92
23	b	606	CLA	C1D-CHD-C4C	-4.01	117.00	122.48
25	c	514	BCR	C20-C21-C22	-4.00	121.61	127.31
29	a	414	PL9	C32-C33-C34	-3.99	117.67	127.68
23	B	603	CLA	C1D-CHD-C4C	-3.97	117.06	122.48
23	c	503	CLA	C1D-CHD-C4C	-3.96	117.07	122.48
23	C	502	CLA	C1D-CHD-C4C	-3.96	117.07	122.48
25	b	618	BCR	C7-C8-C9	-3.94	120.28	126.21
26	A	410	SQD	C44-O6-C1	-3.94	105.67	113.76
25	H	101	BCR	C16-C17-C18	-3.94	121.69	127.31
23	B	612	CLA	O2D-CGD-O1D	-3.93	115.91	123.82
23	c	510	CLA	C1C-C2C-C3C	-3.92	102.57	106.92
23	A	404	CLA	CAA-C2A-C3A	-3.90	102.12	112.81
23	A	405	CLA	C1C-C2C-C3C	-3.87	102.63	106.92
29	A	414	PL9	C7-C8-C9	-3.87	120.25	126.71
23	a	404	CLA	CAA-C2A-C3A	-3.85	102.24	112.81
23	B	614	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
23	C	507	CLA	C1C-C2C-C3C	-3.85	102.65	106.92
25	C	515	BCR	C16-C17-C18	-3.84	121.82	127.31
23	C	503	CLA	O2D-CGD-O1D	-3.84	116.09	123.82
23	b	613	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
23	B	605	CLA	O2D-CGD-O1D	-3.84	116.09	123.82
25	B	618	BCR	C15-C14-C13	-3.82	121.85	127.31
23	b	616	CLA	C1C-NC-C4C	-3.82	104.86	107.06
25	d	405	BCR	C7-C8-C9	-3.81	120.48	126.21
26	a	410	SQD	C1-C2-C3	-3.81	102.91	109.98
23	b	606	CLA	O2D-CGD-O1D	-3.80	116.17	123.82
23	B	613	CLA	C1C-C2C-C3C	-3.79	102.71	106.92
25	B	618	BCR	C37-C22-C21	-3.78	117.63	122.92
25	c	514	BCR	C15-C14-C13	-3.78	121.92	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C1D-CHD-C4C	-3.78	117.32	122.48
23	b	611	CLA	C1-C2-C3	-3.77	119.01	125.96
29	a	414	PL9	C27-C28-C29	-3.77	118.21	127.68
23	B	611	CLA	C1C-C2C-C3C	-3.76	102.75	106.92
23	B	608	CLA	C1C-C2C-C3C	-3.76	102.75	106.92
23	B	607	CLA	C1C-C2C-C3C	-3.76	102.75	106.92
26	a	410	SQD	C1-O5-C5	-3.75	106.66	113.72
23	a	405	CLA	C1C-NC-C4C	-3.74	104.90	107.06
25	b	619	BCR	C38-C26-C25	-3.74	120.32	124.51
23	B	612	CLA	C1-C2-C3	-3.74	119.07	125.96
29	d	406	PL9	C7-C8-C9	-3.73	120.48	126.71
23	d	401	CLA	C1D-CHD-C4C	-3.72	117.40	122.48
23	B	610	CLA	CAA-C2A-C3A	-3.72	102.61	112.81
25	c	514	BCR	C16-C17-C18	-3.71	122.01	127.31
23	B	604	CLA	C1C-C2C-C3C	-3.71	102.81	106.92
23	b	603	CLA	C1D-CHD-C4C	-3.70	117.42	122.48
23	C	511	CLA	C1C-C2C-C3C	-3.70	102.81	106.92
29	a	414	PL9	C22-C23-C24	-3.70	118.39	127.68
23	D	405	CLA	C1D-CHD-C4C	-3.69	117.44	122.48
23	D	405	CLA	C1C-NC-C4C	-3.68	104.94	107.06
23	B	616	CLA	C1D-CHD-C4C	-3.68	117.45	122.48
23	B	606	CLA	C1D-CHD-C4C	-3.68	117.46	122.48
23	a	408	CLA	C1-C2-C3	-3.67	119.19	125.96
23	c	512	CLA	C1-C2-C3	-3.67	119.20	125.96
25	Y	101	BCR	C15-C14-C13	-3.66	122.08	127.31
23	b	614	CLA	O2D-CGD-O1D	-3.66	116.45	123.82
23	C	508	CLA	O2D-CGD-O1D	-3.66	116.46	123.82
23	C	513	CLA	C1D-CHD-C4C	-3.66	117.49	122.48
29	d	406	PL9	C42-C43-C44	-3.66	118.50	127.68
38	E	103	HEM	CBD-CAD-C3D	-3.65	105.50	112.47
23	c	506	CLA	C1C-C2C-C3C	-3.65	102.87	106.92
25	C	516	BCR	C7-C8-C9	-3.65	120.73	126.21
24	D	401	PHO	C1-C2-C3	-3.64	119.26	125.96
23	D	405	CLA	C1-C2-C3	-3.63	119.26	125.96
25	k	101	BCR	C24-C23-C22	-3.63	120.75	126.21
24	A	407	PHO	C4C-C3C-C2C	-3.63	102.73	106.81
23	b	615	CLA	C1C-C2C-C3C	-3.63	102.90	106.92
23	B	603	CLA	O2A-CGA-O1A	-3.63	114.55	123.55
23	b	605	CLA	O2D-CGD-O1D	-3.62	116.53	123.82
25	h	101	BCR	C7-C8-C9	-3.62	120.77	126.21
23	C	507	CLA	C1-C2-C3	-3.62	119.28	125.96
23	C	502	CLA	C1-C2-C3	-3.61	119.31	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	C1C-NC-C4C	-3.61	104.98	107.06
23	b	604	CLA	C1C-C2C-C3C	-3.60	102.92	106.92
23	B	602	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
23	B	612	CLA	C4C-C3C-C2C	-3.59	101.41	106.91
23	B	615	CLA	C1D-CHD-C4C	-3.58	117.58	122.48
25	H	101	BCR	C24-C23-C22	-3.58	120.83	126.21
23	d	404	CLA	O2D-CGD-O1D	-3.58	116.62	123.82
25	K	102	BCR	C7-C8-C9	-3.57	120.85	126.21
23	b	603	CLA	C1C-NC-C4C	-3.57	105.00	107.06
23	d	401	CLA	CAA-C2A-C3A	-3.57	103.03	112.81
23	C	509	CLA	O2D-CGD-O1D	-3.56	116.65	123.82
23	B	614	CLA	CHC-C1C-C2C	-3.55	116.98	126.65
23	b	612	CLA	C1-C2-C3	-3.55	119.42	125.96
23	b	608	CLA	C1C-C2C-C3C	-3.55	102.99	106.92
29	a	414	PL9	C7-C3-C2	-3.54	118.19	123.23
23	b	613	CLA	C1D-CHD-C4C	-3.54	117.64	122.48
23	b	614	CLA	C1D-CHD-C4C	-3.54	117.64	122.48
23	c	508	CLA	C1C-C2C-C3C	-3.54	102.99	106.92
23	b	602	CLA	C1C-C2C-C3C	-3.54	102.99	106.92
23	a	405	CLA	C1C-C2C-C3C	-3.53	103.00	106.92
23	c	506	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
25	h	101	BCR	C16-C17-C18	-3.52	122.28	127.31
23	B	610	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
23	c	513	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
23	C	502	CLA	O2D-CGD-O1D	-3.52	116.74	123.82
23	A	404	CLA	C1C-C2C-C3C	-3.52	103.02	106.92
23	B	605	CLA	C1-C2-C3	-3.52	119.47	125.96
23	C	510	CLA	C1-C2-C3	-3.52	119.47	125.96
25	A	409	BCR	C33-C5-C6	-3.52	120.57	124.51
23	b	611	CLA	C1C-C2C-C3C	-3.52	103.02	106.92
23	C	506	CLA	C1D-CHD-C4C	-3.51	117.68	122.48
23	B	603	CLA	CAA-C2A-C3A	-3.51	103.19	112.81
23	B	608	CLA	O2A-CGA-O1A	-3.51	114.84	123.55
23	C	509	CLA	C4C-C3C-C2C	-3.51	101.53	106.91
23	a	405	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
29	a	414	PL9	C37-C38-C39	-3.50	118.88	127.68
23	b	612	CLA	C1D-CHD-C4C	-3.50	117.70	122.48
23	b	608	CLA	O2D-CGD-O1D	-3.50	116.78	123.82
23	c	511	CLA	C1-C2-C3	-3.49	119.52	125.96
25	C	516	BCR	C11-C10-C9	-3.49	122.33	127.31
23	b	605	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
25	H	101	BCR	C38-C26-C25	-3.47	120.62	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C1C-C2C-C3C	-3.47	103.07	106.92
29	A	414	PL9	C27-C28-C29	-3.46	118.98	127.68
23	b	609	CLA	O2D-CGD-O1D	-3.46	116.86	123.82
25	b	617	BCR	C7-C8-C9	-3.46	121.01	126.21
23	B	612	CLA	C1D-CHD-C4C	-3.46	117.76	122.48
23	c	511	CLA	C1D-CHD-C4C	-3.45	117.77	122.48
23	B	614	CLA	O2D-CGD-O1D	-3.45	116.88	123.82
38	V	202	HEM	CBA-CAA-C2A	-3.45	105.90	112.48
23	B	605	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
23	b	602	CLA	C1D-CHD-C4C	-3.44	117.78	122.48
25	K	102	BCR	C24-C23-C22	-3.43	121.05	126.21
23	B	610	CLA	C4C-C3C-C2C	-3.43	101.64	106.91
23	b	615	CLA	C1D-CHD-C4C	-3.43	117.79	122.48
24	a	407	PHO	C4C-C3C-C2C	-3.43	102.95	106.81
23	B	616	CLA	C4C-C3C-C2C	-3.43	101.64	106.91
23	B	603	CLA	C1C-C2C-C3C	-3.41	103.14	106.92
23	a	408	CLA	CAA-C2A-C3A	-3.41	103.46	112.81
23	C	509	CLA	C1C-C2C-C3C	-3.41	103.14	106.92
23	B	607	CLA	CAA-C2A-C3A	-3.41	103.47	112.81
23	B	614	CLA	O2A-CGA-O1A	-3.41	115.09	123.55
23	c	504	CLA	C1C-C2C-C3C	-3.41	103.14	106.92
23	B	601	CLA	C1-C2-C3	-3.41	119.68	125.96
23	c	505	CLA	C1D-CHD-C4C	-3.40	117.84	122.48
25	d	405	BCR	C33-C5-C6	-3.39	120.71	124.51
23	B	608	CLA	C1D-CHD-C4C	-3.38	117.86	122.48
23	c	512	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
25	t	101	BCR	C11-C10-C9	-3.38	122.49	127.31
23	B	601	CLA	C1C-C2C-C3C	-3.37	103.18	106.92
23	b	607	CLA	C1C-C2C-C3C	-3.37	103.18	106.92
23	b	615	CLA	C11-C10-C8	-3.37	104.67	115.73
23	C	503	CLA	C1C-C2C-C3C	-3.37	103.19	106.92
23	C	507	CLA	CBC-CAC-C3C	-3.36	102.86	112.41
23	C	502	CLA	CBC-CAC-C3C	-3.36	102.86	112.41
25	A	409	BCR	C24-C23-C22	-3.36	121.17	126.21
29	A	414	PL9	C7-C3-C2	-3.35	118.46	123.23
23	B	608	CLA	C1-C2-C3	-3.35	119.78	125.96
23	A	408	CLA	C1-C2-C3	-3.34	119.80	125.96
25	D	406	BCR	C38-C26-C25	-3.34	120.77	124.51
23	B	611	CLA	C1D-CHD-C4C	-3.34	117.92	122.48
23	d	401	CLA	CBC-CAC-C3C	-3.33	102.95	112.41
23	C	503	CLA	C1D-CHD-C4C	-3.33	117.94	122.48
25	D	406	BCR	C24-C23-C22	-3.33	121.22	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C1C-C2C-C3C	-3.32	103.24	106.92
23	b	604	CLA	C1-C2-C3	-3.32	119.84	125.96
23	B	601	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
23	A	408	CLA	C1D-CHD-C4C	-3.32	117.95	122.48
29	A	414	PL9	C22-C23-C24	-3.32	119.35	127.68
23	b	603	CLA	C1C-C2C-C3C	-3.31	103.25	106.92
25	h	101	BCR	C38-C26-C25	-3.30	120.81	124.51
24	D	401	PHO	CHC-C1C-C2C	-3.30	118.04	125.62
25	T	101	BCR	C7-C8-C9	-3.30	121.25	126.21
23	C	514	CLA	C1D-CHD-C4C	-3.30	117.97	122.48
23	a	408	CLA	C1C-C2C-C3C	-3.30	103.26	106.92
25	t	101	BCR	C21-C20-C19	-3.30	113.11	123.23
25	y	101	BCR	C38-C26-C25	-3.30	120.81	124.51
23	b	616	CLA	C4C-C3C-C2C	-3.29	101.86	106.91
23	B	604	CLA	C1-C2-C3	-3.29	119.89	125.96
31	A	416	LHG	O8-C23-O10	-3.29	115.38	123.55
23	C	513	CLA	C1C-C2C-C3C	-3.29	103.27	106.92
23	c	505	CLA	C4C-C3C-C2C	-3.29	101.87	106.91
23	b	601	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
23	C	506	CLA	C1C-C2C-C3C	-3.28	103.28	106.92
23	A	404	CLA	O2A-CGA-O1A	-3.28	115.41	123.55
23	B	609	CLA	C1C-C2C-C3C	-3.28	103.28	106.92
23	c	510	CLA	C1D-CHD-C4C	-3.28	118.01	122.48
23	c	513	CLA	C1C-C2C-C3C	-3.27	103.29	106.92
23	c	502	CLA	CHC-C1C-C2C	-3.27	117.73	126.65
23	b	609	CLA	C1D-CHD-C4C	-3.27	118.02	122.48
23	c	503	CLA	C1C-C2C-C3C	-3.27	103.30	106.92
23	c	512	CLA	C1D-CHD-C4C	-3.27	118.02	122.48
24	a	407	PHO	CHC-C1C-C2C	-3.26	118.13	125.62
23	b	615	CLA	CHC-C1C-C2C	-3.26	117.75	126.65
23	b	610	CLA	C1C-C2C-C3C	-3.26	103.30	106.92
23	A	405	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
23	C	512	CLA	C1C-C2C-C3C	-3.26	103.31	106.92
23	B	615	CLA	C1C-C2C-C3C	-3.26	103.31	106.92
25	c	515	BCR	C38-C26-C25	-3.26	120.86	124.51
25	A	409	BCR	C15-C14-C13	-3.25	122.67	127.31
23	c	502	CLA	O2D-CGD-O1D	-3.25	117.29	123.82
25	d	405	BCR	C16-C17-C18	-3.24	122.68	127.31
23	A	404	CLA	C1D-CHD-C4C	-3.24	118.06	122.48
23	b	601	CLA	C1C-C2C-C3C	-3.24	103.33	106.92
23	a	408	CLA	O2D-CGD-O1D	-3.22	117.33	123.82
25	D	406	BCR	C3-C4-C5	-3.22	108.24	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CHC-C1C-C2C	-3.22	117.86	126.65
25	C	515	BCR	C33-C5-C6	-3.22	120.90	124.51
25	b	617	BCR	C16-C17-C18	-3.22	122.71	127.31
26	f	101	SQD	C5-C6-S	-3.22	109.85	114.34
25	T	101	BCR	C12-C13-C14	-3.21	114.01	118.94
23	b	603	CLA	CAA-C2A-C3A	-3.21	104.02	112.81
23	C	502	CLA	CHC-C1C-C2C	-3.20	117.92	126.65
23	c	501	CLA	C1C-C2C-C3C	-3.20	103.37	106.92
23	d	404	CLA	C1C-NC-C4C	-3.20	105.22	107.06
23	B	606	CLA	C1C-C2C-C3C	-3.20	103.38	106.92
23	b	609	CLA	CBC-CAC-C3C	-3.19	103.34	112.41
23	c	502	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
23	a	404	CLA	O2A-CGA-O1A	-3.19	115.64	123.55
29	A	414	PL9	C32-C33-C34	-3.18	119.69	127.68
23	C	510	CLA	C1C-C2C-C3C	-3.18	103.39	106.92
23	b	613	CLA	O2A-CGA-O1A	-3.18	115.65	123.55
23	b	605	CLA	C1C-C2C-C3C	-3.18	103.39	106.92
23	C	512	CLA	C1D-CHD-C4C	-3.18	118.14	122.48
23	C	504	CLA	C1C-C2C-C3C	-3.18	103.40	106.92
25	D	406	BCR	C28-C27-C26	-3.18	108.32	113.78
23	B	602	CLA	CHC-C1C-C2C	-3.17	118.00	126.65
23	C	509	CLA	O2A-CGA-O1A	-3.17	115.68	123.55
23	c	509	CLA	C1C-C2C-C3C	-3.16	103.41	106.92
23	C	509	CLA	CHC-C1C-C2C	-3.16	118.03	126.65
23	C	514	CLA	C1C-C2C-C3C	-3.16	103.42	106.92
23	a	404	CLA	CHC-C1C-C2C	-3.16	118.03	126.65
23	B	609	CLA	C1D-CHD-C4C	-3.15	118.17	122.48
23	A	408	CLA	C4C-C3C-C2C	-3.15	102.08	106.91
23	c	506	CLA	CHC-C1C-C2C	-3.15	118.06	126.65
23	b	610	CLA	C4C-C3C-C2C	-3.15	102.08	106.91
23	c	510	CLA	CHC-C1C-C2C	-3.14	118.07	126.65
23	B	607	CLA	O2D-CGD-O1D	-3.14	117.49	123.82
23	b	611	CLA	CHC-C1C-C2C	-3.14	118.08	126.65
24	D	401	PHO	C1C-C2C-C3C	-3.14	102.87	106.51
23	D	405	CLA	CAA-C2A-C3A	-3.14	104.20	112.81
23	c	513	CLA	CAA-C2A-C3A	-3.13	104.23	112.81
23	C	514	CLA	C1-C2-C3	-3.13	120.19	125.96
23	B	607	CLA	C1D-CHD-C4C	-3.13	118.21	122.48
25	c	515	BCR	C15-C14-C13	-3.13	122.84	127.31
23	C	511	CLA	C1D-CHD-C4C	-3.13	118.21	122.48
24	a	406	PHO	CHC-C1C-C2C	-3.13	118.45	125.62
23	D	404	CLA	CHC-C1C-C2C	-3.12	118.13	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	CAA-C2A-C3A	-3.12	104.25	112.81
23	B	603	CLA	CHC-C1C-C2C	-3.12	118.14	126.65
23	C	511	CLA	C1-C2-C3	-3.12	120.21	125.96
23	c	509	CLA	C4C-C3C-C2C	-3.12	102.13	106.91
23	b	610	CLA	C1D-CHD-C4C	-3.12	118.23	122.48
23	b	602	CLA	O2D-CGD-O1D	-3.11	117.55	123.82
24	A	407	PHO	CHC-C1C-C2C	-3.11	118.48	125.62
23	c	510	CLA	CBC-CAC-C3C	-3.11	103.58	112.41
23	d	403	CLA	C1-C2-C3	-3.09	120.26	125.96
23	d	404	CLA	C1D-CHD-C4C	-3.09	118.26	122.48
25	k	101	BCR	C15-C14-C13	-3.09	122.90	127.31
23	b	612	CLA	C1C-C2C-C3C	-3.09	103.49	106.92
29	A	414	PL9	C37-C38-C39	-3.09	119.92	127.68
23	B	611	CLA	OBD-CAD-C3D	-3.09	122.34	128.03
25	T	101	BCR	C11-C10-C9	-3.09	122.91	127.31
25	A	409	BCR	C37-C22-C21	-3.08	118.60	122.92
23	d	401	CLA	CHC-C1C-C2C	-3.08	118.25	126.65
23	b	605	CLA	C4C-C3C-C2C	-3.08	102.19	106.91
26	D	413	SQD	C1-C2-C3	-3.08	104.26	109.98
23	B	605	CLA	C1C-C2C-C3C	-3.08	103.51	106.92
29	a	414	PL9	C42-C43-C44	-3.08	119.95	127.68
23	c	507	CLA	C1C-C2C-C3C	-3.08	103.51	106.92
25	C	516	BCR	C15-C14-C13	-3.07	122.92	127.31
23	c	508	CLA	C1D-CHD-C4C	-3.07	118.29	122.48
23	C	509	CLA	C1-C2-C3	-3.07	120.30	125.96
29	d	406	PL9	C36-C37-C38	-3.06	101.46	111.97
23	A	408	CLA	C1C-C2C-C3C	-3.06	103.53	106.92
23	c	502	CLA	CBC-CAC-C3C	-3.06	103.73	112.41
23	B	616	CLA	O2D-CGD-O1D	-3.05	117.67	123.82
23	b	614	CLA	C1-C2-C3	-3.05	120.33	125.96
23	b	605	CLA	O2A-CGA-O1A	-3.05	115.98	123.55
25	C	516	BCR	C33-C5-C6	-3.05	121.09	124.51
23	C	510	CLA	C1D-CHD-C4C	-3.05	118.32	122.48
26	a	410	SQD	C5-C6-S	-3.05	110.09	114.34
23	A	406	CLA	C1C-C2C-C3C	-3.05	103.54	106.92
25	B	618	BCR	C3-C4-C5	-3.04	108.55	113.78
36	c	516	DGD	C2G-O2G-C1B	-3.04	110.69	117.88
23	b	607	CLA	CHC-C1C-C2C	-3.04	118.37	126.65
23	a	405	CLA	CHC-C1C-C2C	-3.04	118.37	126.65
23	b	612	CLA	C4C-C3C-C2C	-3.03	102.25	106.91
25	b	619	BCR	C15-C14-C13	-3.03	122.98	127.31
24	A	407	PHO	C4D-ND-C1D	-3.03	101.52	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C4C-C3C-C2C	-3.03	102.27	106.91
23	D	404	CLA	O2D-CGD-O1D	-3.03	117.73	123.82
23	b	605	CLA	CHC-C1C-C2C	-3.02	118.40	126.65
25	a	409	BCR	C11-C10-C9	-3.02	122.99	127.31
25	Y	101	BCR	C16-C17-C18	-3.02	123.00	127.31
23	A	406	CLA	C4C-C3C-C2C	-3.02	102.28	106.91
26	a	410	SQD	O47-C7-O49	-3.02	116.14	123.68
23	c	504	CLA	C1D-CHD-C4C	-3.02	118.36	122.48
23	c	512	CLA	C4C-C3C-C2C	-3.02	102.28	106.91
23	a	408	CLA	O2A-CGA-O1A	-3.02	116.06	123.55
23	b	607	CLA	C4C-C3C-C2C	-3.01	102.29	106.91
23	B	601	CLA	O2D-CGD-O1D	-3.01	117.76	123.82
25	D	406	BCR	C16-C17-C18	-3.01	123.02	127.31
23	C	507	CLA	CHC-C1C-C2C	-3.01	118.45	126.65
38	v	201	HEM	CBA-CAA-C2A	-3.01	106.74	112.48
23	b	611	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
23	B	601	CLA	CHC-C1C-C2C	-3.01	118.45	126.65
38	E	103	HEM	CBA-CAA-C2A	-3.00	106.74	112.48
23	C	506	CLA	C4C-C3C-C2C	-3.00	102.30	106.91
26	B	620	SQD	C5-C6-S	-3.00	110.16	114.34
23	A	406	CLA	C1C-NC-C4C	-3.00	105.33	107.06
33	j	101	LMG	C8-O7-C10	-3.00	110.79	117.88
23	b	604	CLA	C1D-CHD-C4C	-3.00	118.39	122.48
23	A	404	CLA	CHC-C1C-C2C	-3.00	118.48	126.65
23	c	501	CLA	CHC-C1C-C2C	-2.99	118.49	126.65
23	b	614	CLA	C4C-C3C-C2C	-2.99	102.32	106.91
23	c	506	CLA	C1-C2-C3	-2.99	120.45	125.96
23	B	610	CLA	C1C-C2C-C3C	-2.99	103.61	106.92
23	C	506	CLA	O2D-CGD-O1D	-2.99	117.81	123.82
23	C	511	CLA	CBC-CAC-C3C	-2.98	103.94	112.41
23	D	405	CLA	C1C-C2C-C3C	-2.98	103.61	106.92
24	A	407	PHO	C4D-CHA-C1A	-2.98	118.44	125.06
23	b	611	CLA	C1D-CHD-C4C	-2.98	118.41	122.48
23	c	513	CLA	C1-C2-C3	-2.98	120.47	125.96
24	D	401	PHO	C4C-C3C-C2C	-2.98	103.46	106.81
23	c	512	CLA	CHC-C1C-C2C	-2.98	118.53	126.65
23	C	504	CLA	C1D-CHD-C4C	-2.98	118.41	122.48
23	c	508	CLA	C4C-C3C-C2C	-2.98	102.34	106.91
33	b	620	LMG	C1-C2-C3	-2.98	104.45	109.98
23	b	606	CLA	C4C-C3C-C2C	-2.97	102.35	106.91
23	d	403	CLA	CHC-C1C-C2C	-2.97	118.55	126.65
23	c	507	CLA	O2D-CGD-O1D	-2.97	117.84	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	CAA-C2A-C3A	-2.97	104.67	112.81
23	b	601	CLA	O1D-CGD-CBD	-2.97	119.27	124.60
23	b	606	CLA	C1C-C2C-C3C	-2.96	103.64	106.92
29	D	407	PL9	C12-C13-C14	-2.96	120.24	127.68
23	c	507	CLA	C4C-C3C-C2C	-2.96	102.37	106.91
23	C	514	CLA	C2A-C1A-CHA	-2.96	118.67	123.92
26	a	410	SQD	C44-O6-C1	-2.96	107.69	113.76
23	A	406	CLA	C1D-CHD-C4C	-2.96	118.44	122.48
23	D	404	CLA	O2A-CGA-O1A	-2.96	116.21	123.55
25	B	619	BCR	C37-C22-C21	-2.96	118.78	122.92
23	B	610	CLA	C1-C2-C3	-2.96	120.51	125.96
38	e	103	HEM	CBD-CAD-C3D	-2.95	106.84	112.47
23	b	608	CLA	C1D-CHD-C4C	-2.95	118.46	122.48
23	B	606	CLA	C4C-C3C-C2C	-2.95	102.39	106.91
23	a	408	CLA	C1D-CHD-C4C	-2.95	118.46	122.48
25	H	101	BCR	C3-C4-C5	-2.95	108.72	113.78
25	t	101	BCR	C7-C6-C5	-2.95	114.52	121.54
23	A	406	CLA	C1-C2-C3	-2.94	120.53	125.96
25	A	409	BCR	C11-C10-C9	-2.94	123.11	127.31
23	b	614	CLA	C1C-C2C-C3C	-2.94	103.66	106.92
25	c	514	BCR	C24-C23-C22	-2.94	121.80	126.21
23	C	511	CLA	CHC-C1C-C2C	-2.94	118.64	126.65
25	A	409	BCR	C38-C26-C25	-2.94	121.22	124.51
23	c	505	CLA	C1C-C2C-C3C	-2.94	103.66	106.92
23	B	602	CLA	CAA-C2A-C3A	-2.93	104.78	112.81
23	b	616	CLA	O2D-CGD-O1D	-2.93	117.93	123.82
25	B	618	BCR	C38-C26-C25	-2.93	121.23	124.51
23	B	614	CLA	CBC-CAC-C3C	-2.93	104.10	112.41
23	c	511	CLA	C1C-C2C-C3C	-2.92	103.68	106.92
23	c	507	CLA	C1D-CHD-C4C	-2.92	118.49	122.48
29	D	407	PL9	C22-C23-C24	-2.92	120.35	127.68
25	t	101	BCR	C19-C18-C17	-2.92	114.47	118.94
23	b	607	CLA	CBC-CAC-C3C	-2.91	104.14	112.41
23	c	510	CLA	O1D-CGD-CBD	-2.91	119.38	124.60
23	d	404	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
23	C	510	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
25	B	619	BCR	C24-C23-C22	-2.90	121.85	126.21
23	b	603	CLA	O2D-CGD-O1D	-2.90	117.98	123.82
23	B	611	CLA	C1-C2-C3	-2.90	120.62	125.96
25	y	101	BCR	C21-C20-C19	-2.89	114.35	123.23
23	C	512	CLA	C4C-C3C-C2C	-2.89	102.47	106.91
23	A	406	CLA	O2A-CGA-O1A	-2.89	116.37	123.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	O2A-CGA-O1A	-2.89	116.37	123.55
24	D	401	PHO	C4D-ND-C1D	-2.89	101.76	106.98
23	B	604	CLA	C4C-C3C-C2C	-2.89	102.47	106.91
31	d	409	LHG	O8-C23-O10	-2.89	116.37	123.55
23	c	512	CLA	O2D-CGD-O1D	-2.89	118.01	123.82
23	B	612	CLA	C1C-C2C-C3C	-2.89	103.72	106.92
25	c	514	BCR	C38-C26-C25	-2.89	121.28	124.51
23	B	609	CLA	C4C-C3C-C2C	-2.89	102.48	106.91
23	a	404	CLA	C1-C2-C3	-2.88	120.65	125.96
23	a	408	CLA	C4C-C3C-C2C	-2.88	102.49	106.91
23	c	511	CLA	C4C-C3C-C2C	-2.88	102.49	106.91
33	b	620	LMG	C7-O1-C1	-2.88	107.85	113.76
26	D	413	SQD	C44-O6-C1	-2.88	107.85	113.76
23	b	604	CLA	C4C-C3C-C2C	-2.88	102.49	106.91
23	c	501	CLA	C1D-CHD-C4C	-2.88	118.55	122.48
23	b	608	CLA	C1-C2-C3	-2.87	120.67	125.96
23	B	602	CLA	C1D-CHD-C4C	-2.87	118.56	122.48
25	c	514	BCR	C34-C9-C10	-2.87	118.90	122.92
23	b	613	CLA	O2D-CGD-O1D	-2.87	118.05	123.82
23	B	610	CLA	CHC-C1C-C2C	-2.87	118.83	126.65
23	C	513	CLA	O1D-CGD-CBD	-2.87	119.45	124.60
23	B	605	CLA	O2A-CGA-O1A	-2.87	116.43	123.55
23	C	512	CLA	C1-C2-C3	-2.87	120.68	125.96
23	B	605	CLA	C4C-C3C-C2C	-2.86	102.52	106.91
23	C	513	CLA	CHC-C1C-C2C	-2.86	118.84	126.65
23	b	614	CLA	O2A-CGA-O1A	-2.86	116.45	123.55
26	A	410	SQD	C5-C6-S	-2.86	110.35	114.34
23	C	508	CLA	CHC-C1C-C2C	-2.86	118.85	126.65
23	b	604	CLA	O1D-CGD-CBD	-2.86	119.47	124.60
25	t	101	BCR	C7-C8-C9	-2.85	121.93	126.21
25	c	515	BCR	C16-C17-C18	-2.85	123.24	127.31
23	b	614	CLA	CHC-C1C-C2C	-2.85	118.88	126.65
29	D	407	PL9	C7-C8-C9	-2.85	121.95	126.71
23	c	501	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
23	C	514	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
23	A	405	CLA	CAA-C2A-C3A	-2.84	105.02	112.81
23	D	405	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
25	K	102	BCR	C3-C4-C5	-2.84	108.90	113.78
25	a	409	BCR	C15-C14-C13	-2.84	123.26	127.31
23	B	606	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
23	b	609	CLA	CHC-C1C-C2C	-2.84	118.91	126.65
23	d	401	CLA	C1-C2-C3	-2.84	120.73	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C4C-C3C-C2C	-2.83	102.56	106.91
23	c	506	CLA	C4C-C3C-C2C	-2.83	102.56	106.91
24	A	407	PHO	C1C-C2C-C3C	-2.83	103.23	106.51
23	c	513	CLA	C4C-C3C-C2C	-2.83	102.57	106.91
23	b	603	CLA	O2A-CGA-O1A	-2.83	116.53	123.55
23	c	505	CLA	O2D-CGD-O1D	-2.83	118.13	123.82
25	Y	101	BCR	C38-C26-C25	-2.83	121.34	124.51
23	b	601	CLA	C4C-C3C-C2C	-2.82	102.58	106.91
23	B	604	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
23	C	513	CLA	CBC-CAC-C3C	-2.82	104.40	112.41
23	C	504	CLA	C4C-C3C-C2C	-2.82	102.58	106.91
25	y	101	BCR	C15-C14-C13	-2.82	123.29	127.31
23	b	613	CLA	C4C-C3C-C2C	-2.82	102.59	106.91
23	A	404	CLA	C2A-C1A-CHA	-2.82	118.92	123.92
23	c	509	CLA	C1D-CHD-C4C	-2.82	118.64	122.48
23	c	503	CLA	O2D-CGD-O1D	-2.82	118.15	123.82
23	B	615	CLA	O2D-CGD-O1D	-2.81	118.16	123.82
25	c	515	BCR	C21-C20-C19	-2.81	114.61	123.23
23	c	501	CLA	O2A-CGA-O1A	-2.81	116.58	123.55
23	B	601	CLA	C4C-C3C-C2C	-2.81	102.60	106.91
23	b	613	CLA	CHC-C1C-C2C	-2.81	119.00	126.65
23	C	503	CLA	CHC-C1C-C2C	-2.81	119.00	126.65
25	a	409	BCR	C20-C21-C22	-2.80	123.31	127.31
36	c	516	DGD	O3G-C3G-C2G	-2.80	104.32	110.99
23	A	404	CLA	CAA-CBA-CGA	-2.79	104.93	113.35
25	B	617	BCR	C38-C26-C25	-2.79	121.38	124.51
23	b	606	CLA	CHC-C1C-C2C	-2.79	119.05	126.65
25	b	618	BCR	C38-C26-C25	-2.79	121.39	124.51
31	E	101	LHG	C5-O7-C7	-2.79	111.30	117.88
23	C	505	CLA	CHC-C1C-C2C	-2.78	119.06	126.65
25	d	405	BCR	C40-C30-C25	-2.78	105.79	110.31
25	B	619	BCR	C15-C14-C13	-2.78	123.34	127.31
23	B	615	CLA	CHC-C1C-C2C	-2.78	119.07	126.65
26	L	101	SQD	C44-O6-C1	-2.78	108.06	113.76
23	C	509	CLA	C1D-CHD-C4C	-2.78	118.69	122.48
24	a	406	PHO	C4D-ND-C1D	-2.78	101.97	106.98
23	C	507	CLA	C2A-C1A-CHA	-2.78	119.00	123.92
23	C	514	CLA	O2D-CGD-O1D	-2.78	118.23	123.82
23	c	507	CLA	CHC-C1C-C2C	-2.77	119.08	126.65
23	B	615	CLA	C4C-C3C-C2C	-2.77	102.65	106.91
25	C	515	BCR	C23-C24-C25	-2.77	119.49	127.25
23	b	610	CLA	CAA-C2A-C3A	-2.77	105.21	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	CHC-C1C-C2C	-2.77	119.09	126.65
23	B	613	CLA	C1D-CHD-C4C	-2.77	118.70	122.48
23	b	604	CLA	O2D-CGD-O1D	-2.77	118.25	123.82
23	B	613	CLA	CHC-C1C-C2C	-2.77	119.11	126.65
23	B	605	CLA	C2A-C1A-CHA	-2.77	119.02	123.92
23	a	408	CLA	CMA-C3A-C2A	-2.76	102.55	113.77
25	B	619	BCR	C38-C26-C25	-2.76	121.42	124.51
25	b	619	BCR	C24-C23-C22	-2.76	122.06	126.21
23	a	405	CLA	C4C-C3C-C2C	-2.76	102.67	106.91
23	A	406	CLA	CAA-C2A-C3A	-2.76	105.24	112.81
23	b	601	CLA	CHC-C1C-C2C	-2.76	119.12	126.65
23	c	501	CLA	C1-C2-C3	-2.76	120.87	125.96
23	a	408	CLA	CHC-C1C-C2C	-2.76	119.13	126.65
23	d	404	CLA	C1C-C2C-C3C	-2.75	103.87	106.92
23	c	509	CLA	CHC-C1C-C2C	-2.75	119.14	126.65
23	A	405	CLA	C2A-C1A-CHA	-2.75	119.04	123.92
23	D	405	CLA	CBC-CAC-C3C	-2.75	104.60	112.41
23	C	503	CLA	C4C-C3C-C2C	-2.75	102.69	106.91
24	a	407	PHO	C4D-CHA-C1A	-2.75	118.95	125.06
23	c	504	CLA	C2A-C1A-CHA	-2.75	119.05	123.92
23	c	506	CLA	CGD-CBD-CAD	-2.75	101.51	110.71
25	B	617	BCR	C11-C10-C9	-2.74	123.39	127.31
29	d	406	PL9	C22-C23-C24	-2.74	120.79	127.68
25	b	617	BCR	C15-C14-C13	-2.74	123.40	127.31
29	A	414	PL9	C42-C43-C44	-2.74	120.79	127.68
25	Y	101	BCR	C16-C15-C14	-2.74	117.61	123.46
23	B	613	CLA	O2A-CGA-O1A	-2.74	116.75	123.55
23	B	607	CLA	CHC-C1C-C2C	-2.74	119.18	126.65
23	B	610	CLA	O1D-CGD-CBD	-2.74	119.69	124.60
23	c	504	CLA	C4C-C3C-C2C	-2.74	102.71	106.91
23	B	611	CLA	C2A-C1A-CHA	-2.73	119.07	123.92
23	a	404	CLA	CAA-C2A-C1A	-2.73	103.03	111.97
33	b	620	LMG	C8-O7-C10	-2.73	111.43	117.88
23	b	615	CLA	C4C-C3C-C2C	-2.73	102.72	106.91
25	a	409	BCR	C37-C22-C21	-2.73	119.10	122.92
24	a	406	PHO	CHD-C1D-C2D	-2.73	119.36	125.62
23	B	611	CLA	CHC-C1C-C2C	-2.73	119.21	126.65
23	c	508	CLA	CHC-C1C-C2C	-2.73	119.22	126.65
23	B	614	CLA	C4C-C3C-C2C	-2.72	102.73	106.91
25	A	409	BCR	C20-C21-C22	-2.72	123.42	127.31
23	b	603	CLA	C4C-C3C-C2C	-2.72	102.73	106.91
23	A	408	CLA	CHC-C1C-C2C	-2.72	119.22	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C2A-C1A-CHA	-2.72	119.09	123.92
24	D	401	PHO	C4D-CHA-C1A	-2.72	119.01	125.06
23	D	404	CLA	C2A-C1A-CHA	-2.72	119.09	123.92
25	D	406	BCR	C33-C5-C6	-2.72	121.46	124.51
23	a	405	CLA	CAA-C2A-C3A	-2.72	105.35	112.81
23	A	408	CLA	CMA-C3A-C2A	-2.72	102.74	113.77
23	b	610	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
23	B	616	CLA	CHC-C1C-C2C	-2.72	119.24	126.65
23	B	604	CLA	O2D-CGD-O1D	-2.72	118.36	123.82
23	b	612	CLA	CHC-C1C-C2C	-2.71	119.25	126.65
23	C	513	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
23	B	608	CLA	CHC-C1C-C2C	-2.71	119.26	126.65
24	a	407	PHO	C3A-C4A-CHB	-2.71	117.18	121.75
23	B	602	CLA	C4C-C3C-C2C	-2.71	102.76	106.91
23	b	602	CLA	CHC-C1C-C2C	-2.71	119.27	126.65
23	c	511	CLA	CAA-CBA-CGA	-2.71	105.20	113.35
26	A	410	SQD	C45-O47-C7	-2.70	111.49	117.88
23	B	603	CLA	O2D-CGD-O1D	-2.70	118.38	123.82
23	c	509	CLA	O2D-CGD-O1D	-2.70	118.38	123.82
23	b	611	CLA	CBC-CAC-C3C	-2.70	104.74	112.41
23	b	607	CLA	C1D-CHD-C4C	-2.70	118.80	122.48
23	b	611	CLA	C4C-C3C-C2C	-2.70	102.77	106.91
23	C	512	CLA	CHC-C1C-C2C	-2.70	119.30	126.65
25	A	409	BCR	C8-C7-C6	-2.70	119.70	127.25
25	k	101	BCR	C20-C21-C22	-2.69	123.47	127.31
31	D	409	LHG	O8-C23-O10	-2.69	116.87	123.55
23	b	608	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
23	b	604	CLA	O2A-CGA-O1A	-2.69	116.87	123.55
25	k	101	BCR	C3-C4-C5	-2.69	109.16	113.78
23	C	507	CLA	C1D-CHD-C4C	-2.69	118.81	122.48
23	c	512	CLA	CBA-CAA-C2A	-2.69	105.76	113.80
23	b	605	CLA	C2A-C1A-CHA	-2.69	119.16	123.92
23	A	406	CLA	C2A-C1A-CHA	-2.68	119.16	123.92
24	A	407	PHO	CHD-C1D-C2D	-2.68	119.46	125.62
25	c	515	BCR	C33-C5-C6	-2.68	121.50	124.51
23	c	504	CLA	CHC-C1C-C2C	-2.68	119.33	126.65
26	D	413	SQD	O47-C7-O49	-2.68	116.99	123.68
33	C	501	LMG	C7-O1-C1	-2.68	108.26	113.76
25	b	619	BCR	C10-C11-C12	-2.68	115.01	123.23
33	C	501	LMG	C9-C8-C7	-2.68	105.82	111.86
23	c	511	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
25	C	515	BCR	C7-C8-C9	-2.68	122.19	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C1-C2-C3	-2.68	121.03	125.96
23	B	603	CLA	C4C-C3C-C2C	-2.67	102.82	106.91
23	A	405	CLA	CBC-CAC-C3C	-2.67	104.84	112.41
24	a	407	PHO	C4D-ND-C1D	-2.67	102.17	106.98
23	b	610	CLA	CHC-C1C-C2C	-2.67	119.38	126.65
23	c	503	CLA	O2A-CGA-O1A	-2.66	116.94	123.55
23	B	613	CLA	C4C-C3C-C2C	-2.66	102.82	106.91
26	L	101	SQD	C1-C2-C3	-2.66	105.03	109.98
25	b	617	BCR	C20-C21-C22	-2.66	123.51	127.31
24	D	401	PHO	O1D-CGD-CBD	-2.66	119.82	124.60
23	B	609	CLA	CHC-C1C-C2C	-2.66	119.40	126.65
25	d	405	BCR	C39-C30-C25	-2.66	106.00	110.31
31	D	408	LHG	O8-C23-O10	-2.66	116.95	123.55
25	d	405	BCR	C21-C20-C19	-2.66	115.08	123.23
23	c	508	CLA	C2A-C1A-CHA	-2.66	119.21	123.92
25	B	619	BCR	C21-C20-C19	-2.66	115.08	123.23
25	a	409	BCR	C32-C1-C6	-2.66	106.00	110.31
23	b	616	CLA	C2A-C1A-CHA	-2.65	119.21	123.92
23	b	614	CLA	CAA-C2A-C3A	-2.65	105.54	112.81
23	C	506	CLA	O1D-CGD-CBD	-2.65	119.84	124.60
25	K	102	BCR	C15-C14-C13	-2.65	123.53	127.31
23	b	615	CLA	C11-C12-C13	-2.65	107.04	115.73
25	d	405	BCR	C16-C15-C14	-2.65	117.81	123.46
26	A	412	SQD	O48-C23-O10	-2.65	116.98	123.55
23	C	502	CLA	OBD-CAD-C3D	-2.64	123.16	128.03
23	b	608	CLA	C2A-C1A-CHA	-2.64	119.23	123.92
25	Y	101	BCR	C10-C11-C12	-2.64	115.14	123.23
23	a	405	CLA	O2D-CGD-O1D	-2.64	118.51	123.82
25	A	409	BCR	C16-C17-C18	-2.64	123.55	127.31
23	b	604	CLA	CHC-C1C-C2C	-2.63	119.47	126.65
23	b	603	CLA	C2A-C1A-CHA	-2.63	119.26	123.92
23	C	505	CLA	O2D-CGD-O1D	-2.63	118.53	123.82
23	d	404	CLA	C2A-C1A-CHA	-2.63	119.26	123.92
23	B	607	CLA	C4C-C3C-C2C	-2.62	102.88	106.91
35	D	403	LMT	O1B-C4'-C5'	-2.62	102.90	109.34
33	Z	102	LMG	C9-C8-C7	-2.62	105.95	111.86
25	D	406	BCR	C40-C30-C25	-2.62	106.06	110.31
31	d	407	LHG	O8-C23-O10	-2.62	117.05	123.55
23	A	404	CLA	C4C-C3C-C2C	-2.62	102.90	106.91
23	d	404	CLA	CAA-C2A-C3A	-2.61	105.64	112.81
24	a	406	PHO	O2D-CGD-O1D	-2.61	118.56	123.82
23	B	616	CLA	O1D-CGD-CBD	-2.61	119.92	124.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C4C-C3C-C2C	-2.61	102.91	106.91
25	h	101	BCR	C10-C11-C12	-2.61	115.24	123.23
23	B	608	CLA	C2A-C1A-CHA	-2.60	119.30	123.92
23	c	506	CLA	O2D-CGD-O1D	-2.60	118.58	123.82
23	C	513	CLA	CBA-CAA-C2A	-2.60	106.00	113.80
23	B	607	CLA	CBC-CAC-C3C	-2.60	105.02	112.41
36	C	518	DGD	C2G-O2G-C1B	-2.60	111.73	117.88
24	A	407	PHO	C6-C5-C3	-2.60	106.76	112.66
23	b	602	CLA	C11-C10-C8	-2.60	107.21	115.73
29	A	414	PL9	C12-C13-C14	-2.60	121.16	127.68
23	c	507	CLA	C6-C7-C8	-2.60	107.21	115.73
29	D	407	PL9	C27-C28-C29	-2.60	121.16	127.68
23	B	604	CLA	O2A-CGA-O1A	-2.59	117.11	123.55
36	C	519	DGD	O1G-C1A-O1A	-2.59	117.11	123.55
23	A	406	CLA	CHC-C1C-C2C	-2.59	119.58	126.65
23	B	602	CLA	C2A-C1A-CHA	-2.59	119.32	123.92
23	B	606	CLA	CHC-C1C-C2C	-2.59	119.58	126.65
24	a	406	PHO	C4D-CHA-C1A	-2.59	119.31	125.06
23	D	404	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
23	B	608	CLA	C4C-C3C-C2C	-2.59	102.94	106.91
23	c	502	CLA	C1-C2-C3	-2.59	121.19	125.96
23	d	404	CLA	CHC-C1C-C2C	-2.58	119.60	126.65
29	D	407	PL9	C36-C37-C38	-2.58	103.10	111.97
25	D	406	BCR	C15-C14-C13	-2.58	123.62	127.31
24	a	407	PHO	O2D-CGD-O1D	-2.58	118.62	123.82
25	B	617	BCR	C16-C17-C18	-2.58	123.63	127.31
23	B	603	CLA	CBC-CAC-C3C	-2.58	105.08	112.41
25	T	101	BCR	C7-C6-C5	-2.58	115.39	121.54
36	c	516	DGD	C3G-C2G-C1G	-2.57	106.06	111.86
25	b	619	BCR	C39-C30-C25	-2.57	106.14	110.31
23	B	602	CLA	O2D-CGD-O1D	-2.57	118.65	123.82
24	a	406	PHO	C1C-C2C-C3C	-2.57	103.53	106.51
23	d	401	CLA	CMA-C3A-C2A	-2.57	103.36	113.77
36	C	518	DGD	O1G-C1A-O1A	-2.56	117.18	123.55
25	b	618	BCR	C24-C23-C22	-2.56	122.36	126.21
23	B	604	CLA	O1D-CGD-CBD	-2.56	120.00	124.60
25	h	101	BCR	C37-C22-C21	-2.56	119.33	122.92
23	c	511	CLA	CBC-CAC-C3C	-2.56	105.14	112.41
25	k	101	BCR	C7-C8-C9	-2.56	122.37	126.21
23	b	602	CLA	C11-C12-C13	-2.56	107.33	115.73
23	b	608	CLA	CHC-C1C-C2C	-2.56	119.67	126.65
29	d	406	PL9	C31-C32-C33	-2.55	103.21	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	CAA-C2A-C3A	-2.55	105.82	112.81
25	c	515	BCR	C3-C4-C5	-2.55	109.40	113.78
23	C	505	CLA	CBC-CAC-C3C	-2.55	105.18	112.41
23	A	408	CLA	CBC-CAC-C3C	-2.54	105.19	112.41
23	C	505	CLA	OBD-CAD-C3D	-2.54	123.34	128.03
25	c	514	BCR	C28-C27-C26	-2.54	109.41	113.78
23	c	512	CLA	O1D-CGD-CBD	-2.54	120.04	124.60
26	A	412	SQD	C5-C6-S	-2.54	110.80	114.34
23	c	509	CLA	C2A-C1A-CHA	-2.54	119.42	123.92
23	B	612	CLA	CHC-C1C-C2C	-2.54	119.73	126.65
23	a	404	CLA	C2A-C1A-CHA	-2.54	119.42	123.92
25	B	617	BCR	C31-C1-C6	-2.54	106.20	110.31
23	C	506	CLA	CHC-C1C-C2C	-2.54	119.73	126.65
36	h	102	DGD	C3G-O3G-C1D	-2.53	108.56	113.76
23	c	507	CLA	C1-C2-C3	-2.53	121.29	125.96
29	A	414	PL9	C17-C18-C19	-2.53	121.32	127.68
23	b	612	CLA	O2D-CGD-O1D	-2.53	118.73	123.82
24	a	406	PHO	C1-C2-C3	-2.53	121.30	125.96
23	C	507	CLA	CAA-C2A-C3A	-2.53	105.88	112.81
26	D	413	SQD	C5-C6-S	-2.53	110.82	114.34
23	c	503	CLA	C1-C2-C3	-2.52	121.31	125.96
35	M	101	LMT	C1-O1'-C1'	-2.52	109.54	113.87
23	b	610	CLA	C2A-C1A-CHA	-2.52	119.45	123.92
23	c	513	CLA	C2A-C1A-CHA	-2.52	119.45	123.92
25	b	618	BCR	C28-C27-C26	-2.52	109.45	113.78
23	B	610	CLA	O2A-CGA-O1A	-2.52	117.30	123.55
23	b	611	CLA	O2A-CGA-O1A	-2.51	117.31	123.55
25	b	619	BCR	C4-C5-C6	-2.51	119.05	122.74
23	B	615	CLA	CBC-CAC-C3C	-2.51	105.27	112.41
23	a	404	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
23	b	611	CLA	C2A-C1A-CHA	-2.51	119.46	123.92
25	y	101	BCR	C10-C11-C12	-2.51	115.53	123.23
25	C	516	BCR	C38-C26-C25	-2.51	121.70	124.51
25	y	101	BCR	C24-C23-C22	-2.51	122.44	126.21
38	v	201	HEM	CBD-CAD-C3D	-2.51	107.69	112.47
23	b	603	CLA	CHC-C1C-C2C	-2.51	119.81	126.65
23	b	615	CLA	O2D-CGD-O1D	-2.50	118.79	123.82
25	t	101	BCR	C3-C4-C5	-2.50	109.48	113.78
26	A	410	SQD	O48-C23-O10	-2.50	117.34	123.55
23	b	602	CLA	C2A-C1A-CHA	-2.50	119.49	123.92
23	d	403	CLA	C4C-C3C-C2C	-2.50	103.08	106.91
23	d	403	CLA	C1D-CHD-C4C	-2.50	119.07	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	101	LMG	O8-C28-O10	-2.50	117.35	123.55
25	B	618	BCR	C28-C27-C26	-2.50	109.49	113.78
23	C	511	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
23	b	609	CLA	C4C-C3C-C2C	-2.49	103.08	106.91
23	c	506	CLA	O2A-CGA-O1A	-2.49	117.36	123.55
23	C	507	CLA	O2D-CGD-O1D	-2.49	118.80	123.82
23	C	510	CLA	CHC-C1C-C2C	-2.49	119.85	126.65
23	d	401	CLA	C11-C12-C13	-2.49	107.56	115.73
25	c	514	BCR	C33-C5-C6	-2.49	121.72	124.51
25	C	516	BCR	C15-C16-C17	-2.49	118.15	123.46
25	K	102	BCR	C33-C5-C6	-2.49	121.72	124.51
23	b	602	CLA	CAA-C2A-C3A	-2.49	106.00	112.81
23	C	514	CLA	CHC-C1C-C2C	-2.49	119.87	126.65
25	d	405	BCR	C38-C26-C25	-2.48	121.73	124.51
33	c	520	LMG	O8-C28-O10	-2.48	117.39	123.55
23	b	616	CLA	O2A-CGA-O1A	-2.48	117.39	123.55
36	c	518	DGD	O5D-C6D-C5D	-2.48	104.80	108.94
23	c	503	CLA	CHC-C1C-C2C	-2.48	119.89	126.65
23	b	613	CLA	C1-C2-C3	-2.48	121.39	125.96
23	D	405	CLA	CHC-C1C-C2C	-2.48	119.89	126.65
23	b	601	CLA	O2D-CGD-O1D	-2.48	118.84	123.82
23	B	606	CLA	C4A-NA-C1A	-2.48	103.38	106.45
23	B	611	CLA	C4C-C3C-C2C	-2.48	103.11	106.91
25	C	515	BCR	C11-C10-C9	-2.47	123.78	127.31
25	C	515	BCR	C20-C21-C22	-2.47	123.78	127.31
23	B	616	CLA	C1C-C2C-C3C	-2.47	104.18	106.92
23	c	501	CLA	C2A-C1A-CHA	-2.47	119.54	123.92
23	C	502	CLA	O2A-CGA-O1A	-2.47	117.42	123.55
23	B	607	CLA	C2A-C1A-CHA	-2.47	119.54	123.92
23	a	404	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
23	B	606	CLA	CAA-C2A-C3A	-2.46	106.07	112.81
23	B	606	CLA	C2A-C1A-CHA	-2.46	119.56	123.92
24	A	407	PHO	O2D-CGD-O1D	-2.46	118.87	123.82
23	A	405	CLA	O2D-CGD-O1D	-2.46	118.87	123.82
23	d	403	CLA	CBC-CAC-C3C	-2.45	105.44	112.41
36	c	516	DGD	C6D-O5D-C1E	-2.45	108.72	113.76
23	b	612	CLA	O2A-CGA-O1A	-2.45	117.46	123.55
23	c	504	CLA	C1-C2-C3	-2.45	121.44	125.96
26	D	413	SQD	C46-C45-C44	-2.45	106.33	111.86
23	c	502	CLA	C4C-C3C-C2C	-2.45	103.15	106.91
38	v	201	HEM	CMA-C3A-C4A	-2.45	124.70	128.46
23	A	405	CLA	CHC-C1C-C2C	-2.45	119.97	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CAA-CBA-CGA	-2.45	105.98	113.35
25	B	618	BCR	C36-C18-C17	-2.44	119.50	122.92
23	C	506	CLA	CBC-CAC-C3C	-2.44	105.49	112.41
36	H	102	DGD	C2G-O2G-C1B	-2.44	112.11	117.88
23	C	504	CLA	C1-C2-C3	-2.44	121.47	125.96
23	b	609	CLA	O2A-CGA-O1A	-2.44	117.50	123.55
36	c	518	DGD	O3G-C3G-C2G	-2.43	105.20	110.99
23	a	405	CLA	C1-C2-C3	-2.43	121.47	125.96
23	d	401	CLA	C2A-C1A-CHA	-2.43	119.61	123.92
25	b	617	BCR	C32-C1-C6	-2.43	106.36	110.31
25	B	619	BCR	C7-C8-C9	-2.43	122.56	126.21
23	C	510	CLA	O2D-CGD-O1D	-2.43	118.93	123.82
23	b	616	CLA	CHC-C1C-C2C	-2.43	120.02	126.65
25	b	618	BCR	C37-C22-C21	-2.43	119.52	122.92
25	b	617	BCR	C37-C22-C21	-2.43	119.52	122.92
33	z	101	LMG	C8-O7-C10	-2.43	112.14	117.88
35	D	403	LMT	C1-O1'-C1'	-2.43	109.70	113.87
33	C	520	LMG	O8-C28-O10	-2.42	117.54	123.55
25	t	101	BCR	C37-C22-C21	-2.42	119.53	122.92
23	B	605	CLA	CHC-C1C-C2C	-2.42	120.05	126.65
23	c	507	CLA	O1D-CGD-CBD	-2.42	120.26	124.60
33	b	620	LMG	O8-C28-O10	-2.42	117.54	123.55
23	b	606	CLA	CAA-C2A-C3A	-2.42	106.18	112.81
31	A	416	LHG	C5-O7-C7	-2.41	112.17	117.88
25	a	409	BCR	C8-C7-C6	-2.41	120.50	127.25
26	a	410	SQD	O48-C23-O10	-2.41	117.56	123.55
23	A	405	CLA	CMA-C3A-C2A	-2.41	104.01	113.77
23	D	404	CLA	OBD-CAD-C3D	-2.40	123.60	128.03
23	C	513	CLA	O2D-CGD-O1D	-2.40	118.98	123.82
23	B	616	CLA	C2A-C1A-CHA	-2.40	119.66	123.92
23	B	614	CLA	C1-C2-C3	-2.40	121.53	125.96
23	d	403	CLA	CAA-C2A-C3A	-2.40	106.23	112.81
23	C	506	CLA	C1-C2-C3	-2.40	121.54	125.96
23	C	504	CLA	C4A-NA-C1A	-2.40	103.48	106.45
25	a	409	BCR	C15-C16-C17	-2.39	118.35	123.46
23	B	601	CLA	C2A-C1A-CHA	-2.39	119.68	123.92
29	D	407	PL9	C37-C38-C39	-2.39	121.67	127.68
23	B	608	CLA	CBC-CAC-C3C	-2.39	105.62	112.41
23	b	606	CLA	C1-C2-C3	-2.39	121.55	125.96
23	C	503	CLA	C1-C2-C3	-2.39	121.55	125.96
25	C	516	BCR	C16-C17-C18	-2.39	123.90	127.31
23	c	505	CLA	CHC-C1C-C2C	-2.39	120.14	126.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	O2A-CGA-O1A	-2.39	117.63	123.55
29	d	406	PL9	C37-C38-C39	-2.38	121.69	127.68
23	a	408	CLA	OBD-CAD-C3D	-2.38	123.64	128.03
23	b	602	CLA	C1-C2-C3	-2.38	121.57	125.96
23	C	507	CLA	O2A-CGA-O1A	-2.38	117.65	123.55
23	b	608	CLA	CBC-CAC-C3C	-2.38	105.66	112.41
34	B	622	HTG	O2-C2-C3	-2.38	105.19	110.36
23	B	606	CLA	O2A-CGA-O1A	-2.37	117.66	123.55
29	d	406	PL9	C17-C18-C19	-2.37	121.72	127.68
23	C	511	CLA	O1D-CGD-CBD	-2.37	120.34	124.60
25	k	101	BCR	C10-C11-C12	-2.37	115.96	123.23
23	b	602	CLA	O1D-CGD-CBD	-2.37	120.35	124.60
23	A	408	CLA	C4A-NA-C1A	-2.37	103.51	106.45
25	h	101	BCR	C16-C15-C14	-2.37	118.41	123.46
29	d	406	PL9	C12-C13-C14	-2.36	121.75	127.68
25	C	516	BCR	C3-C4-C5	-2.36	109.72	113.78
25	B	618	BCR	C10-C11-C12	-2.36	116.00	123.23
25	C	515	BCR	C38-C26-C25	-2.36	121.87	124.51
24	D	401	PHO	O2D-CGD-O1D	-2.35	119.08	123.82
23	C	511	CLA	C4C-C3C-C2C	-2.35	103.30	106.91
23	c	510	CLA	C4-C3-C2	-2.35	117.41	123.69
29	a	414	PL9	C7-C8-C9	-2.35	122.78	126.71
25	c	515	BCR	C32-C1-C6	-2.35	106.50	110.31
23	b	602	CLA	O2A-CGA-O1A	-2.35	117.72	123.55
23	C	505	CLA	C4C-C3C-C2C	-2.35	103.31	106.91
23	d	403	CLA	C2A-C1A-CHA	-2.35	119.75	123.92
23	b	616	CLA	C4A-NA-C1A	-2.35	103.54	106.45
36	C	517	DGD	C4E-C3E-C2E	-2.35	106.70	110.84
23	a	405	CLA	CBC-CAC-C3C	-2.35	105.75	112.41
23	B	608	CLA	O2D-CGD-O1D	-2.34	119.11	123.82
23	c	513	CLA	CHC-C1C-C2C	-2.34	120.26	126.65
23	B	614	CLA	C2A-C1A-CHA	-2.34	119.77	123.92
23	a	408	CLA	CMA-C3A-C4A	-2.34	105.48	111.77
26	f	101	SQD	C4-C3-C2	-2.34	106.71	110.84
25	a	409	BCR	C33-C5-C6	-2.34	121.89	124.51
35	D	403	LMT	C1B-O5B-C5B	-2.34	109.31	113.72
29	D	407	PL9	C42-C41-C39	-2.34	105.02	112.93
23	c	504	CLA	CBC-CAC-C3C	-2.34	105.78	112.41
23	b	601	CLA	C2A-C1A-CHA	-2.34	119.78	123.92
23	C	502	CLA	C4C-C3C-C2C	-2.33	103.33	106.91
23	B	602	CLA	CBC-CAC-C3C	-2.33	105.78	112.41
23	c	504	CLA	OBD-CAD-C3D	-2.33	123.73	128.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
23	a	408	CLA	C2A-C1A-CHA	-2.33	119.79	123.92
23	B	607	CLA	C4A-NA-C1A	-2.33	103.56	106.45
25	t	101	BCR	C20-C21-C22	-2.32	123.99	127.31
23	B	610	CLA	O2D-CGD-O1D	-2.32	119.14	123.82
36	h	102	DGD	O1G-C1A-O1A	-2.32	117.78	123.55
23	b	616	CLA	CBC-CAC-C3C	-2.32	105.82	112.41
23	c	506	CLA	C2A-C1A-CHA	-2.32	119.81	123.92
23	b	606	CLA	O2A-CGA-O1A	-2.32	117.79	123.55
24	A	407	PHO	C3B-C2B-C1B	-2.32	101.62	106.30
23	D	404	CLA	C4A-NA-C1A	-2.32	103.58	106.45
23	c	510	CLA	O2A-CGA-O1A	-2.32	117.80	123.55
23	C	511	CLA	C2A-C1A-CHA	-2.31	119.82	123.92
23	c	505	CLA	C1-C2-C3	-2.31	121.70	125.96
23	C	514	CLA	CBC-CAC-C3C	-2.31	105.85	112.41
23	C	513	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
23	B	612	CLA	C11-C12-C13	-2.31	108.15	115.73
25	y	101	BCR	C40-C30-C25	-2.31	106.56	110.31
23	D	405	CLA	C2A-C1A-CHA	-2.31	119.82	123.92
23	C	508	CLA	C1-C2-C3	-2.31	121.70	125.96
23	c	501	CLA	OBD-CAD-C3D	-2.31	123.77	128.03
25	y	101	BCR	C28-C27-C26	-2.31	109.81	113.78
23	B	609	CLA	C2A-C1A-CHA	-2.31	119.83	123.92
23	B	616	CLA	CBC-CAC-C3C	-2.30	105.87	112.41
35	b	627	LMT	C3'-C4'-C5'	-2.30	105.99	110.88
36	C	517	DGD	O3G-C3G-C2G	-2.30	105.51	110.99
23	B	601	CLA	O1D-CGD-CBD	-2.30	120.47	124.60
23	B	613	CLA	CBC-CAC-C3C	-2.30	105.88	112.41
31	d	408	LHG	O8-C23-O10	-2.30	117.84	123.55
25	c	515	BCR	C11-C10-C9	-2.30	124.03	127.31
33	j	101	LMG	O8-C28-O10	-2.30	117.84	123.55
23	A	405	CLA	C4C-C3C-C2C	-2.30	103.39	106.91
23	B	611	CLA	O2D-CGD-O1D	-2.29	119.20	123.82
24	a	406	PHO	C3B-C2B-C1B	-2.29	101.67	106.30
38	V	202	HEM	CBD-CAD-C3D	-2.29	108.09	112.47
23	b	616	CLA	O1D-CGD-CBD	-2.29	120.48	124.60
23	D	404	CLA	CAA-C2A-C3A	-2.29	106.53	112.81
36	C	517	DGD	O1G-C1A-O1A	-2.29	117.86	123.55
23	C	507	CLA	CGD-CBD-CAD	-2.29	103.04	110.71
26	D	413	SQD	O5-C1-C2	-2.29	105.88	110.30
25	k	101	BCR	C39-C30-C25	-2.29	106.60	110.31
23	c	513	CLA	O2D-CGD-O1D	-2.29	119.22	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CAA-C2A-C3A	-2.28	106.55	112.81
25	Y	101	BCR	C40-C30-C25	-2.28	106.61	110.31
25	c	515	BCR	C35-C13-C14	-2.28	119.73	122.92
25	D	406	BCR	C21-C20-C19	-2.28	116.23	123.23
25	b	617	BCR	C24-C23-C22	-2.28	122.78	126.21
25	C	516	BCR	C21-C20-C19	-2.28	116.24	123.23
25	a	409	BCR	C38-C26-C25	-2.28	121.96	124.51
23	b	606	CLA	C2A-C1A-CHA	-2.28	119.88	123.92
33	B	621	LMG	C7-O1-C1	-2.27	109.10	113.76
38	E	103	HEM	C3C-C4C-NC	-2.27	106.66	110.94
23	c	508	CLA	C1-C2-C3	-2.27	121.77	125.96
23	b	616	CLA	C1-C2-C3	-2.27	121.78	125.96
23	b	607	CLA	O1D-CGD-CBD	-2.27	120.53	124.60
23	A	405	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
23	C	504	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
33	b	620	LMG	C4-C3-C2	-2.27	106.84	110.84
23	d	404	CLA	O2A-CGA-O1A	-2.26	117.93	123.55
23	d	403	CLA	O2D-CGD-O1D	-2.26	119.26	123.82
23	B	613	CLA	CAA-C2A-C3A	-2.26	106.61	112.81
23	C	514	CLA	CAA-C2A-C3A	-2.26	106.61	112.81
23	c	510	CLA	CMA-C3A-C4A	-2.26	105.70	111.77
23	D	404	CLA	C1D-CHD-C4C	-2.26	119.39	122.48
36	C	517	DGD	O1G-C1G-C2G	-2.26	102.98	108.66
23	C	511	CLA	O2A-CGA-O1A	-2.26	117.94	123.55
25	B	619	BCR	C10-C11-C12	-2.26	116.31	123.23
23	A	406	CLA	O2D-CGD-O1D	-2.25	119.28	123.82
23	b	614	CLA	CBC-CAC-C3C	-2.25	106.01	112.41
23	B	612	CLA	C2A-C1A-CHA	-2.25	119.92	123.92
23	A	404	CLA	CAA-C2A-C1A	-2.25	104.60	111.97
23	C	506	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
23	C	508	CLA	C6-C7-C8	-2.25	108.35	115.73
23	c	513	CLA	C4A-NA-C1A	-2.25	103.66	106.45
25	c	515	BCR	C20-C21-C22	-2.25	124.10	127.31
25	y	101	BCR	C11-C10-C9	-2.25	124.10	127.31
23	B	611	CLA	CBC-CAC-C3C	-2.24	106.04	112.41
26	f	101	SQD	O47-C7-O49	-2.24	118.09	123.68
33	c	520	LMG	C9-C8-C7	-2.24	106.81	111.86
23	C	503	CLA	C2A-C1A-CHA	-2.24	119.95	123.92
26	A	412	SQD	C46-C45-C44	-2.24	106.81	111.86
23	C	512	CLA	C11-C10-C8	-2.24	108.39	115.73
23	C	502	CLA	C2A-C1A-CHA	-2.23	119.96	123.92
23	b	609	CLA	CAA-C2A-C3A	-2.23	106.69	112.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C37-C22-C21	-2.23	119.80	122.92
23	b	601	CLA	CBC-CAC-C3C	-2.23	106.08	112.41
33	j	101	LMG	O7-C10-O9	-2.23	118.11	123.68
31	d	407	LHG	C5-O7-C7	-2.23	112.61	117.88
23	A	408	CLA	C2A-C1A-CHA	-2.23	119.97	123.92
23	B	606	CLA	O1D-CGD-CBD	-2.23	120.60	124.60
23	C	507	CLA	C4C-C3C-C2C	-2.23	103.49	106.91
36	C	519	DGD	O6D-C1D-O3G	-2.22	104.75	110.02
23	b	603	CLA	O1D-CGD-CBD	-2.22	120.61	124.60
25	c	515	BCR	C40-C30-C25	-2.22	106.71	110.31
23	a	405	CLA	O2A-CGA-O1A	-2.22	118.04	123.55
23	b	601	CLA	CAA-C2A-C3A	-2.22	106.73	112.81
26	B	620	SQD	O5-C1-C2	-2.22	106.02	110.30
23	b	602	CLA	CBC-CAC-C3C	-2.21	106.12	112.41
23	C	503	CLA	CBC-CAC-C3C	-2.21	106.13	112.41
23	c	513	CLA	O2A-CGA-O1A	-2.21	118.06	123.55
25	c	514	BCR	C37-C22-C21	-2.21	119.83	122.92
25	b	619	BCR	C21-C20-C19	-2.21	116.46	123.23
31	E	101	LHG	O8-C23-O10	-2.21	118.07	123.55
23	d	404	CLA	CBC-CAC-C3C	-2.21	106.15	112.41
23	c	510	CLA	C2A-C1A-CHA	-2.20	120.01	123.92
23	C	508	CLA	C2A-C1A-CHA	-2.20	120.01	123.92
25	H	101	BCR	C31-C1-C6	-2.20	106.74	110.31
25	b	618	BCR	C20-C21-C22	-2.20	124.17	127.31
23	c	503	CLA	CBC-CAC-C3C	-2.20	106.17	112.41
23	C	512	CLA	O2D-CGD-O1D	-2.19	119.41	123.82
26	B	620	SQD	C1-C2-C3	-2.19	105.90	109.98
25	A	409	BCR	C31-C1-C6	-2.19	106.75	110.31
23	B	610	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
25	H	101	BCR	C36-C18-C17	-2.19	119.86	122.92
23	c	505	CLA	C2A-C1A-CHA	-2.19	120.04	123.92
26	L	101	SQD	O47-C7-O49	-2.19	118.22	123.68
24	A	407	PHO	O2A-CGA-O1A	-2.18	118.14	123.55
23	c	512	CLA	CMA-C3A-C4A	-2.18	105.92	111.77
24	a	406	PHO	CBA-CAA-C2A	-2.18	107.28	113.80
23	B	609	CLA	O2D-CGD-O1D	-2.17	119.44	123.82
23	C	509	CLA	CAA-C2A-C3A	-2.17	106.85	112.81
24	D	401	PHO	CBA-CAA-C2A	-2.17	107.30	113.80
23	a	405	CLA	C2A-C1A-CHA	-2.17	120.07	123.92
23	B	603	CLA	C2A-C1A-CHA	-2.17	120.07	123.92
25	C	516	BCR	C34-C9-C10	-2.17	119.89	122.92
25	B	617	BCR	C28-C27-C26	-2.17	110.05	113.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	C4A-NA-C1A	-2.17	103.76	106.45
23	b	610	CLA	C4-C3-C2	-2.17	117.91	123.69
23	C	513	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
36	c	516	DGD	C1E-C2E-C3E	-2.16	105.97	109.98
23	c	504	CLA	O1D-CGD-CBD	-2.16	120.72	124.60
23	B	602	CLA	O2A-CGA-O1A	-2.16	118.19	123.55
25	t	101	BCR	C16-C15-C14	-2.16	118.86	123.46
23	b	611	CLA	O1D-CGD-CBD	-2.16	120.73	124.60
23	B	609	CLA	CBC-CAC-C3C	-2.16	106.29	112.41
24	a	407	PHO	O1D-CGD-CBD	-2.15	120.73	124.60
25	B	618	BCR	C16-C17-C18	-2.15	124.24	127.31
23	c	502	CLA	O2A-CGA-O1A	-2.15	118.22	123.55
24	D	401	PHO	C3B-C2B-C1B	-2.15	101.96	106.30
36	c	518	DGD	C3G-C2G-C1G	-2.15	107.01	111.86
23	a	404	CLA	C4C-C3C-C2C	-2.15	103.62	106.91
24	a	407	PHO	CBA-CAA-C2A	-2.15	107.38	113.80
23	c	501	CLA	CBC-CAC-C3C	-2.14	106.32	112.41
33	J	101	LMG	C8-O7-C10	-2.14	112.82	117.88
23	C	505	CLA	C1-C2-C3	-2.14	122.01	125.96
23	b	616	CLA	C11-C12-C13	-2.14	108.71	115.73
26	A	410	SQD	O47-C7-O49	-2.14	118.34	123.68
25	h	101	BCR	C20-C21-C22	-2.14	124.26	127.31
36	C	519	DGD	C3G-C2G-C1G	-2.13	107.04	111.86
25	C	515	BCR	C11-C12-C13	-2.13	120.42	126.42
24	D	401	PHO	CHD-C1D-C2D	-2.13	120.73	125.62
25	B	619	BCR	C2-C3-C4	-2.13	106.27	111.34
23	b	606	CLA	CBC-CAC-C3C	-2.13	106.36	112.41
25	c	515	BCR	C15-C16-C17	-2.13	118.91	123.46
23	B	616	CLA	C4A-NA-C1A	-2.13	103.81	106.45
24	a	406	PHO	O2A-CGA-O1A	-2.13	118.27	123.55
25	H	101	BCR	C2-C3-C4	-2.13	106.28	111.34
23	C	507	CLA	C4A-NA-C1A	-2.13	103.81	106.45
23	B	611	CLA	O2A-CGA-O1A	-2.13	118.27	123.55
31	d	407	LHG	O7-C7-O9	-2.12	118.38	123.68
24	a	406	PHO	O1D-CGD-CBD	-2.12	120.79	124.60
31	l	101	LHG	O8-C23-O10	-2.12	118.28	123.55
23	C	504	CLA	CBC-CAC-C3C	-2.12	106.39	112.41
23	B	608	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
35	a	417	LMT	C1B-O1B-C4'	-2.12	112.84	118.00
25	y	101	BCR	C16-C15-C14	-2.12	118.95	123.46
23	d	403	CLA	C4A-NA-C1A	-2.12	103.83	106.45
23	A	406	CLA	CMA-C3A-C4A	-2.11	106.09	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
33	c	519	LMG	O8-C28-O10	-2.11	118.31	123.55
23	B	612	CLA	O2A-CGA-O1A	-2.11	118.31	123.55
23	B	604	CLA	CGD-CBD-CAD	-2.11	103.64	110.71
23	d	404	CLA	C1-C2-C3	-2.11	122.07	125.96
23	A	404	CLA	OBD-CAD-C3D	-2.11	124.14	128.03
26	D	413	SQD	O48-C23-O10	-2.11	118.32	123.55
23	A	406	CLA	CBC-CAC-C3C	-2.11	106.43	112.41
23	B	613	CLA	O2D-CGD-O1D	-2.10	119.58	123.82
23	c	513	CLA	O1D-CGD-CBD	-2.10	120.82	124.60
23	C	513	CLA	C1-C2-C3	-2.10	122.08	125.96
25	K	102	BCR	C11-C10-C9	-2.10	124.31	127.31
23	b	610	CLA	O1D-CGD-CBD	-2.10	120.83	124.60
31	D	409	LHG	C6-C5-C4	-2.10	107.12	111.86
25	B	617	BCR	C36-C18-C17	-2.10	119.98	122.92
36	C	519	DGD	O6E-C1E-O5D	-2.10	105.04	110.02
36	H	102	DGD	O1G-C1A-O1A	-2.10	118.34	123.55
23	B	603	CLA	C5-C3-C2	-2.10	116.81	121.10
24	a	407	PHO	C3B-C2B-C1B	-2.09	102.07	106.30
23	b	613	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
23	a	404	CLA	O2D-CGD-O1D	-2.09	119.61	123.82
23	c	502	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
23	C	510	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
29	A	414	PL9	C47-C48-C49	-2.09	120.34	127.80
23	B	614	CLA	CAA-C2A-C3A	-2.09	107.08	112.81
23	b	606	CLA	OBD-CAD-C3D	-2.09	124.18	128.03
25	D	406	BCR	C10-C11-C12	-2.09	116.83	123.23
23	c	504	CLA	O2D-CGD-O1D	-2.09	119.62	123.82
31	D	409	LHG	O7-C7-O9	-2.09	118.47	123.68
23	C	506	CLA	C2A-C1A-CHA	-2.09	120.22	123.92
23	A	408	CLA	OBD-CAD-C3D	-2.09	124.18	128.03
25	t	101	BCR	C29-C28-C27	-2.09	106.37	111.34
29	D	407	PL9	C7-C3-C2	-2.08	120.27	123.23
23	A	404	CLA	CMA-C3A-C2A	-2.08	105.32	113.77
25	H	101	BCR	C16-C15-C14	-2.08	119.02	123.46
25	b	617	BCR	C11-C10-C9	-2.08	124.34	127.31
23	c	504	CLA	O2A-CGA-O1A	-2.08	118.38	123.55
36	H	102	DGD	C3G-O3G-C1D	-2.08	109.49	113.76
23	b	614	CLA	C2A-C1A-CHA	-2.08	120.23	123.92
25	B	618	BCR	C35-C13-C14	-2.08	120.01	122.92
29	D	407	PL9	C17-C18-C19	-2.08	122.46	127.68
23	c	510	CLA	C4C-C3C-C2C	-2.08	103.72	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C11-C12-C13	-2.07	108.93	115.73
33	z	101	LMG	C7-O1-C1	-2.07	109.51	113.76
25	c	514	BCR	C3-C4-C5	-2.07	110.22	113.78
25	h	101	BCR	C15-C14-C13	-2.07	124.35	127.31
24	D	401	PHO	C4A-NA-C1A	-2.07	106.49	108.16
25	k	101	BCR	C34-C9-C10	-2.07	120.02	122.92
33	B	621	LMG	O8-C28-O10	-2.07	118.42	123.55
23	B	607	CLA	O2A-CGA-O1A	-2.07	118.42	123.55
23	d	401	CLA	O2D-CGD-O1D	-2.06	119.67	123.82
38	e	103	HEM	C3C-C4C-NC	-2.06	107.05	110.94
35	D	403	LMT	O3'-C3'-C2'	-2.06	105.87	110.36
23	b	614	CLA	OBD-CAD-C3D	-2.06	124.23	128.03
26	B	620	SQD	O48-C23-O10	-2.06	118.43	123.55
23	C	509	CLA	OBD-CAD-C3D	-2.06	124.23	128.03
23	B	607	CLA	OBD-CAD-C3D	-2.06	124.23	128.03
25	c	514	BCR	C21-C20-C19	-2.06	116.91	123.23
23	a	408	CLA	CBC-CAC-C3C	-2.06	106.56	112.41
24	a	407	PHO	C4A-NA-C1A	-2.06	106.50	108.16
25	b	619	BCR	C20-C21-C22	-2.06	124.37	127.31
23	C	505	CLA	CAA-C2A-C3A	-2.06	107.17	112.81
23	C	513	CLA	C4A-NA-C1A	-2.06	103.90	106.45
36	c	518	DGD	O6D-C1D-O3G	-2.06	105.14	110.02
23	B	602	CLA	C11-C12-C13	-2.06	108.98	115.73
23	b	616	CLA	C1C-C2C-C3C	-2.06	104.64	106.92
23	b	613	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
36	h	102	DGD	C3B-C2B-C1B	-2.05	106.08	113.58
23	A	404	CLA	C1B-CHB-C4A	-2.05	126.05	130.12
36	C	517	DGD	C3G-C2G-C1G	-2.05	107.22	111.86
23	b	609	CLA	C7-C6-C5	-2.05	107.40	113.11
29	d	406	PL9	C27-C28-C29	-2.05	122.53	127.68
24	a	406	PHO	C3A-C4A-CHB	-2.05	118.29	121.75
25	b	617	BCR	C38-C26-C25	-2.05	122.21	124.51
23	b	603	CLA	CBC-CAC-C3C	-2.05	106.59	112.41
23	c	503	CLA	C2A-C1A-CHA	-2.05	120.28	123.92
33	C	520	LMG	C9-C8-C7	-2.05	107.23	111.86
23	B	612	CLA	OBD-CAD-C3D	-2.05	124.25	128.03
23	C	512	CLA	C2A-C1A-CHA	-2.05	120.29	123.92
23	b	610	CLA	C11-C12-C13	-2.05	109.02	115.73
23	b	602	CLA	C4A-NA-C1A	-2.05	103.91	106.45
23	D	404	CLA	C4-C3-C2	-2.05	118.23	123.69
23	c	506	CLA	CBC-CAC-C3C	-2.04	106.61	112.41
23	C	512	CLA	CBC-CAC-C3C	-2.04	106.62	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	409	BCR	C7-C8-C9	-2.04	123.15	126.21
25	a	409	BCR	C28-C27-C26	-2.04	110.28	113.78
25	T	101	BCR	C10-C11-C12	-2.04	116.99	123.23
23	B	602	CLA	C1-C2-C3	-2.03	122.21	125.96
23	B	601	CLA	CAA-C2A-C3A	-2.03	107.24	112.81
23	b	607	CLA	O2D-CGD-O1D	-2.03	119.74	123.82
31	l	101	LHG	C5-O7-C7	-2.03	113.08	117.88
36	c	517	DGD	O1G-C1A-O1A	-2.03	118.52	123.55
33	J	101	LMG	O7-C10-O9	-2.02	118.63	123.68
26	a	410	SQD	O5-C1-C2	-2.02	106.39	110.30
23	C	510	CLA	CBC-CAC-C3C	-2.02	106.67	112.41
33	B	621	LMG	C8-O7-C10	-2.02	113.10	117.88
23	b	607	CLA	O2A-CGA-O1A	-2.02	118.53	123.55
25	b	618	BCR	C15-C16-C17	-2.02	119.15	123.46
25	K	102	BCR	C38-C26-C25	-2.02	122.25	124.51
24	a	407	PHO	C1C-C2C-C3C	-2.02	104.17	106.51
26	a	412	SQD	O48-C23-O10	-2.01	118.55	123.55
23	b	615	CLA	C2A-C1A-CHA	-2.01	120.35	123.92
23	c	503	CLA	C4A-NA-C1A	-2.01	103.95	106.45
36	c	516	DGD	O6D-C1D-O3G	-2.01	105.26	110.02
23	b	601	CLA	C4A-NA-C1A	-2.01	103.96	106.45
25	d	405	BCR	C35-C13-C14	-2.00	120.12	122.92
23	b	603	CLA	C4A-NA-C1A	-2.00	103.97	106.45
23	B	601	CLA	CBC-CAC-C3C	-2.00	106.73	112.41
23	b	610	CLA	C4A-NA-C1A	-2.00	103.97	106.45
25	t	101	BCR	C28-C27-C26	-2.00	110.34	113.78
25	C	515	BCR	C21-C20-C19	-2.00	117.09	123.23
23	A	405	CLA	C11-C10-C8	-2.00	109.17	115.73
23	b	609	CLA	CHB-C4A-NA	2.00	127.28	124.51
26	B	620	SQD	O5-C5-C4	2.00	113.35	109.66
25	B	619	BCR	C29-C30-C25	2.00	113.61	110.48
35	I	101	LMT	O5'-C5'-C4'	2.00	113.85	109.75
23	C	505	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	C	507	CLA	CMB-C2B-C3B	2.02	128.63	124.89
23	C	511	CLA	C1-O2A-CGA	2.03	121.63	116.77
23	d	403	CLA	CHB-C4A-NA	2.03	127.31	124.51
23	C	508	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	d	404	CLA	CHB-C4A-NA	2.03	127.33	124.51
23	a	408	CLA	CHB-C4A-NA	2.03	127.33	124.51
23	b	608	CLA	CAC-C3C-C4C	2.04	127.70	124.83
23	C	513	CLA	CAC-C3C-C4C	2.04	127.70	124.83
25	B	619	BCR	C37-C22-C23	2.04	121.35	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	406	PHO	CMC-C2C-C1C	2.04	128.22	125.04
23	B	614	CLA	CHB-C4A-NA	2.04	127.34	124.51
23	B	611	CLA	CAC-C3C-C4C	2.04	127.71	124.83
25	B	617	BCR	C29-C30-C25	2.04	113.67	110.48
29	D	407	PL9	C30-C29-C31	2.05	118.84	115.29
23	B	606	CLA	CMB-C2B-C3B	2.05	128.69	124.89
24	D	401	PHO	C3C-C4C-NC	2.05	113.55	110.19
25	Y	101	BCR	C33-C5-C4	2.05	117.35	113.45
23	b	610	CLA	CMC-C2C-C1C	2.06	128.14	125.02
35	E	102	LMT	C2'-C3'-C4'	2.06	113.87	109.61
23	B	602	CLA	CMB-C2B-C3B	2.06	128.71	124.89
25	k	101	BCR	C34-C9-C8	2.06	121.38	118.10
23	a	405	CLA	CAC-C3C-C4C	2.06	127.73	124.83
23	C	510	CLA	C4-C3-C5	2.06	118.86	115.29
25	D	406	BCR	C30-C25-C24	2.06	121.52	115.73
36	c	517	DGD	O5D-C1E-C2E	2.06	111.60	108.23
25	T	101	BCR	C33-C5-C4	2.06	117.36	113.45
23	c	510	CLA	CHB-C4A-NA	2.06	127.37	124.51
23	B	602	CLA	CHB-C4A-NA	2.06	127.37	124.51
35	I	101	LMT	O1'-C1'-C2'	2.07	111.61	108.23
25	h	101	BCR	C37-C22-C23	2.07	121.39	118.10
23	c	511	CLA	CMB-C2B-C3B	2.07	128.74	124.89
34	V	203	HTG	C1-O5-C5	2.07	115.02	112.17
23	B	606	CLA	C1-O2A-CGA	2.07	121.75	116.77
23	A	406	CLA	C4-C3-C5	2.07	118.89	115.29
23	d	401	CLA	CMC-C2C-C1C	2.08	128.17	125.02
23	B	607	CLA	C1-O2A-CGA	2.08	121.76	116.77
24	a	407	PHO	CHC-C1C-NC	2.08	128.71	124.64
23	B	605	CLA	CAC-C3C-C4C	2.08	127.76	124.83
25	c	515	BCR	C35-C13-C12	2.08	121.42	118.10
24	a	406	PHO	C4D-C3D-CAD	2.09	109.28	105.41
24	D	401	PHO	C4D-C3D-CAD	2.09	109.28	105.41
24	A	407	PHO	CED-O2D-CGD	2.09	120.86	115.97
35	D	402	LMT	O5B-C5B-C4B	2.09	113.51	109.66
23	c	506	CLA	CMC-C2C-C1C	2.09	128.19	125.02
23	C	502	CLA	C3D-CAD-CBD	2.09	110.56	107.60
23	C	508	CLA	CMB-C2B-C1B	2.10	131.69	128.46
29	D	407	PL9	C45-C44-C46	2.10	118.93	115.29
29	d	406	PL9	C45-C44-C46	2.11	118.94	115.29
35	D	402	LMT	O1B-C1B-C2B	2.11	112.85	108.11
36	C	518	DGD	O6E-C5E-C6E	2.11	111.45	106.41
23	c	510	CLA	CMB-C2B-C3B	2.11	128.80	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CAC-C3C-C4C	2.11	127.80	124.83
23	B	611	CLA	CED-O2D-CGD	2.11	120.92	115.97
23	A	404	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	d	401	CLA	CAA-CBA-CGA	2.11	119.71	113.35
34	b	628	HTG	O5-C1-C2	2.11	113.17	110.28
23	a	404	CLA	CAC-C3C-C4C	2.12	127.81	124.83
25	Y	101	BCR	C36-C18-C19	2.12	121.47	118.10
23	c	502	CLA	CHB-C4A-NA	2.12	127.44	124.51
24	A	407	PHO	CMB-C2B-C1B	2.12	128.34	125.04
36	H	102	DGD	O6E-C5E-C6E	2.12	111.49	106.41
25	T	101	BCR	C37-C22-C23	2.12	121.48	118.10
24	a	407	PHO	O2A-CGA-CBA	2.13	118.10	111.90
25	k	101	BCR	C36-C18-C19	2.13	121.49	118.10
23	B	605	CLA	CMB-C2B-C1B	2.13	131.74	128.46
34	C	522	HTG	O5-C1-C2	2.13	113.20	110.28
23	a	405	CLA	CMC-C2C-C1C	2.13	128.25	125.02
23	B	609	CLA	CED-O2D-CGD	2.13	120.97	115.97
24	a	406	PHO	CMB-C2B-C1B	2.14	128.37	125.04
23	B	601	CLA	CHB-C4A-NA	2.14	127.47	124.51
29	a	414	PL9	C45-C44-C46	2.14	119.00	115.29
35	B	631	LMT	O1'-C1'-C2'	2.15	111.73	108.23
23	b	614	CLA	C4-C3-C5	2.15	119.01	115.29
36	c	517	DGD	C1D-O6D-C5D	2.15	117.77	113.72
23	a	405	CLA	CHB-C4A-NA	2.15	127.49	124.51
23	b	605	CLA	CAC-C3C-C4C	2.16	127.88	124.83
35	B	630	LMT	C1'-O5'-C5'	2.16	117.79	113.72
23	C	511	CLA	CMB-C2B-C3B	2.16	128.91	124.89
29	a	414	PL9	C40-C39-C41	2.16	119.04	115.29
23	C	505	CLA	O2A-CGA-CBA	2.17	118.20	111.90
29	D	407	PL9	C25-C24-C26	2.17	119.05	115.29
23	d	401	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	B	615	CLA	CMB-C2B-C1B	2.17	131.80	128.46
23	a	405	CLA	CMB-C2B-C3B	2.17	128.92	124.89
23	c	510	CLA	CAC-C3C-C4C	2.17	127.89	124.83
25	b	619	BCR	C37-C22-C23	2.17	121.56	118.10
35	D	403	LMT	C3B-C4B-C5B	2.17	114.05	110.22
24	D	401	PHO	C1-O2A-CGA	2.17	121.98	116.77
23	D	404	CLA	CMB-C2B-C3B	2.18	128.93	124.89
35	M	103	LMT	O5'-C5'-C4'	2.18	114.21	109.75
35	D	403	LMT	C1B-C2B-C3B	2.18	114.03	109.98
23	c	506	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	c	507	CLA	CHB-C4A-NA	2.18	127.53	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C16-C15-C14	2.18	128.12	123.46
23	B	607	CLA	CAA-CBA-CGA	2.18	119.92	113.35
35	I	101	LMT	O5'-C1'-C2'	2.19	114.51	110.30
23	d	403	CLA	CAC-C3C-C4C	2.19	127.92	124.83
29	D	407	PL9	C2-C1-C6	2.19	121.50	117.82
23	c	509	CLA	C4-C3-C5	2.19	119.09	115.29
29	d	406	PL9	C30-C29-C31	2.19	119.09	115.29
23	b	608	CLA	C4-C3-C5	2.20	119.10	115.29
23	B	615	CLA	C1-O2A-CGA	2.20	122.04	116.77
23	C	510	CLA	C1-O2A-CGA	2.20	122.05	116.77
23	b	601	CLA	CAC-C3C-C4C	2.20	127.93	124.83
23	b	607	CLA	CMC-C2C-C1C	2.20	128.35	125.02
23	A	404	CLA	C4-C3-C5	2.20	119.11	115.29
23	B	616	CLA	CAC-C3C-C4C	2.20	127.94	124.83
23	B	606	CLA	CMC-C2C-C1C	2.21	128.37	125.02
23	c	502	CLA	CAC-C3C-C4C	2.21	127.94	124.83
25	B	617	BCR	C33-C5-C4	2.21	117.64	113.45
23	A	408	CLA	CAC-C3C-C4C	2.21	127.95	124.83
23	a	405	CLA	C4-C3-C5	2.22	119.13	115.29
36	C	517	DGD	O1G-C1A-C2A	2.22	118.35	111.90
23	C	503	CLA	C4-C3-C5	2.22	119.13	115.29
35	m	102	LMT	C1B-O5B-C5B	2.22	117.89	113.72
23	B	605	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	C	512	CLA	CHB-C4A-NA	2.22	127.59	124.51
23	b	602	CLA	C4-C3-C5	2.22	119.15	115.29
23	c	504	CLA	CHB-C4A-NA	2.23	127.59	124.51
23	A	405	CLA	O2A-CGA-CBA	2.23	118.38	111.90
23	A	405	CLA	C4-C3-C5	2.23	119.15	115.29
25	t	101	BCR	C33-C5-C4	2.23	117.69	113.45
25	H	101	BCR	C7-C6-C5	2.23	126.86	121.54
23	d	404	CLA	C4-C3-C5	2.23	119.16	115.29
33	Z	101	LMG	C4-C3-C2	2.24	114.78	110.84
23	C	504	CLA	CMB-C2B-C3B	2.24	129.04	124.89
23	c	503	CLA	CAC-C3C-C4C	2.24	127.99	124.83
29	A	414	PL9	C51-C49-C50	2.24	119.83	114.60
23	d	404	CLA	C1-O2A-CGA	2.24	122.15	116.77
24	A	407	PHO	CBD-CHA-C1A	2.25	131.65	126.36
26	f	101	SQD	O8-S-C6	2.25	108.75	106.01
23	D	405	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	C	505	CLA	C4-C3-C5	2.26	119.21	115.29
24	A	407	PHO	C4-C3-C5	2.26	119.21	115.29
23	d	403	CLA	CMB-C2B-C3B	2.26	129.09	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	CHB-C4A-NA	2.26	127.64	124.51
25	c	514	BCR	C2-C1-C6	2.26	114.02	110.48
23	B	608	CLA	CMB-C2B-C3B	2.26	129.09	124.89
25	T	101	BCR	C2-C1-C6	2.27	114.02	110.48
23	c	501	CLA	CMC-C2C-C1C	2.27	128.46	125.02
23	b	606	CLA	C1-O2A-CGA	2.27	122.21	116.77
23	B	602	CLA	C1-O2A-CGA	2.27	122.22	116.77
23	B	615	CLA	CAC-C3C-C4C	2.27	128.04	124.83
23	B	611	CLA	CMB-C2B-C3B	2.28	129.12	124.89
23	C	508	CLA	CMC-C2C-C1C	2.28	128.47	125.02
29	a	414	PL9	C51-C49-C50	2.28	119.91	114.60
23	c	504	CLA	C4-C3-C5	2.28	119.24	115.29
23	C	513	CLA	CMC-C2C-C1C	2.28	128.48	125.02
23	b	615	CLA	CAC-C3C-C4C	2.29	128.05	124.83
23	C	513	CLA	CHB-C4A-NA	2.29	127.67	124.51
23	B	616	CLA	C4-C3-C5	2.29	119.26	115.29
23	B	601	CLA	CAC-C3C-C4C	2.30	128.07	124.83
23	A	406	CLA	CHB-C4A-NA	2.30	127.69	124.51
35	e	102	LMT	O1B-C1B-C2B	2.30	113.29	108.11
23	B	605	CLA	C4-C3-C5	2.30	119.28	115.29
23	C	513	CLA	CMB-C2B-C3B	2.30	129.17	124.89
23	B	614	CLA	CMC-C2C-C1C	2.30	128.51	125.02
25	H	101	BCR	C2-C1-C6	2.31	114.08	110.48
23	c	504	CLA	CMB-C2B-C3B	2.31	129.17	124.89
34	V	203	HTG	C1-C2-C3	2.31	112.58	109.65
23	b	606	CLA	CAC-C3C-C4C	2.31	128.09	124.83
23	B	610	CLA	C4-C3-C5	2.31	119.30	115.29
23	B	601	CLA	CMB-C2B-C3B	2.32	129.19	124.89
25	T	101	BCR	C35-C13-C12	2.32	121.80	118.10
35	e	102	LMT	C1B-C2B-C3B	2.32	114.29	109.98
23	A	404	CLA	CED-O2D-CGD	2.32	121.42	115.97
23	B	608	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	a	410	SQD	C3-C4-C5	2.33	114.32	110.22
23	B	607	CLA	O2A-CGA-CBA	2.33	118.68	111.90
23	b	616	CLA	CMC-C2C-C1C	2.33	128.56	125.02
23	C	504	CLA	CAC-C3C-C4C	2.33	128.12	124.83
23	B	615	CLA	C4-C3-C5	2.34	119.34	115.29
23	A	405	CLA	CMB-C2B-C3B	2.34	129.23	124.89
23	C	502	CLA	C4-C3-C5	2.34	119.35	115.29
23	a	404	CLA	CMC-C2C-C1C	2.35	128.58	125.02
23	C	503	CLA	O2A-CGA-CBA	2.35	118.73	111.90
23	B	605	CLA	O2A-CGA-CBA	2.35	118.73	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	408	CLA	C4-C3-C5	2.35	119.36	115.29
23	c	505	CLA	C4-C3-C5	2.35	119.37	115.29
26	B	620	SQD	O48-C46-C45	2.35	114.57	108.66
23	c	512	CLA	C1-O2A-CGA	2.36	122.43	116.77
23	C	512	CLA	CMB-C2B-C3B	2.36	129.28	124.89
23	B	601	CLA	C4-C3-C5	2.36	119.39	115.29
36	c	518	DGD	O2G-C1B-C2B	2.36	116.46	111.55
23	a	405	CLA	C1-O2A-CGA	2.37	122.45	116.77
24	A	407	PHO	C3C-C4C-NC	2.37	114.06	110.19
23	D	405	CLA	CAC-C3C-C4C	2.37	128.17	124.83
24	a	407	PHO	CAC-C3C-C4C	2.37	127.99	125.21
23	c	505	CLA	C1-O2A-CGA	2.37	122.46	116.77
25	c	515	BCR	C37-C22-C23	2.37	121.88	118.10
24	a	407	PHO	CBD-CHA-C1A	2.37	131.95	126.36
23	B	610	CLA	CHB-C4A-NA	2.38	127.80	124.51
29	D	407	PL9	C15-C14-C16	2.38	119.41	115.29
33	C	501	LMG	O8-C28-C29	2.38	118.82	111.90
23	c	505	CLA	CED-O2D-CGD	2.38	121.55	115.97
23	b	601	CLA	CMC-C2C-C1C	2.38	128.63	125.02
23	A	405	CLA	C3B-C4B-NB	2.38	112.29	109.21
35	m	102	LMT	O1B-C1B-C2B	2.38	113.48	108.11
23	c	507	CLA	CMC-C2C-C1C	2.38	128.64	125.02
25	T	101	BCR	C1-C6-C7	2.39	122.44	115.73
23	B	613	CLA	CED-O2D-CGD	2.39	121.57	115.97
23	c	508	CLA	CMC-C2C-C1C	2.39	128.64	125.02
31	D	408	LHG	O8-C23-C24	2.39	118.85	111.90
24	D	401	PHO	CBD-CHA-C1A	2.39	131.99	126.36
23	B	602	CLA	CED-O2D-CGD	2.39	121.57	115.97
23	a	405	CLA	O2A-CGA-CBA	2.39	118.86	111.90
23	A	405	CLA	CAA-CBA-CGA	2.39	120.55	113.35
26	f	101	SQD	O5-C5-C4	2.40	114.07	109.66
23	B	615	CLA	O2A-CGA-CBA	2.40	118.87	111.90
23	C	503	CLA	CAC-C3C-C4C	2.40	128.22	124.83
23	c	508	CLA	C4-C3-C5	2.40	119.45	115.29
23	d	404	CLA	CMB-C2B-C3B	2.40	129.35	124.89
23	c	502	CLA	CMC-C2C-C1C	2.40	128.66	125.02
23	c	508	CLA	CAC-C3C-C4C	2.41	128.22	124.83
23	D	405	CLA	O2A-CGA-CBA	2.42	118.94	111.90
24	a	407	PHO	C4D-C3D-CAD	2.42	109.90	105.41
23	A	408	CLA	O2A-CGA-CBA	2.42	118.95	111.90
25	H	101	BCR	C29-C30-C25	2.42	114.27	110.48
23	b	612	CLA	CMC-C2C-C1C	2.42	128.69	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	CAC-C3C-C4C	2.43	128.25	124.83
23	b	615	CLA	O2A-CGA-CBA	2.43	118.96	111.90
23	C	503	CLA	CMC-C2C-C1C	2.43	128.70	125.02
23	C	509	CLA	CHB-C4A-NA	2.43	127.87	124.51
23	b	614	CLA	CMB-C2B-C3B	2.43	129.40	124.89
29	d	406	PL9	C53-C6-C1	2.43	120.00	114.84
23	b	604	CLA	C4-C3-C5	2.43	119.51	115.29
25	A	409	BCR	C36-C18-C19	2.43	121.98	118.10
23	c	509	CLA	CMC-C2C-C1C	2.44	128.72	125.02
24	A	407	PHO	C4D-C3D-CAD	2.45	109.95	105.41
36	c	518	DGD	O1G-C1A-C2A	2.45	119.02	111.90
23	b	606	CLA	CMC-C2C-C1C	2.45	128.73	125.02
23	B	612	CLA	CMB-C2B-C3B	2.45	129.44	124.89
23	c	507	CLA	O2A-CGA-CBA	2.45	119.04	111.90
23	b	611	CLA	CMC-C2C-C1C	2.46	128.74	125.02
25	K	102	BCR	C36-C18-C19	2.46	122.01	118.10
23	B	608	CLA	CMC-C2C-C1C	2.46	128.75	125.02
25	y	101	BCR	C37-C22-C23	2.46	122.02	118.10
23	A	408	CLA	CMB-C2B-C3B	2.46	129.46	124.89
33	a	416	LMG	O8-C28-C29	2.47	119.09	111.90
25	Y	101	BCR	C37-C22-C23	2.47	122.04	118.10
23	C	508	CLA	CAC-C3C-C4C	2.48	128.32	124.83
23	C	509	CLA	C4-C3-C5	2.48	119.60	115.29
23	B	607	CLA	C4-C3-C5	2.49	119.60	115.29
29	D	407	PL9	C51-C49-C50	2.49	120.40	114.60
23	c	509	CLA	CMB-C2B-C3B	2.49	129.51	124.89
25	B	618	BCR	C36-C18-C19	2.49	122.06	118.10
34	C	521	HTG	C1-O5-C5	2.49	117.48	112.69
23	b	604	CLA	CAC-C3C-C4C	2.49	128.34	124.83
29	A	414	PL9	C45-C44-C46	2.50	119.62	115.29
25	b	618	BCR	C29-C30-C25	2.50	114.39	110.48
29	d	406	PL9	C15-C14-C16	2.50	119.63	115.29
23	b	606	CLA	CMB-C2B-C3B	2.50	129.54	124.89
23	C	506	CLA	C4-C3-C5	2.51	119.64	115.29
29	A	414	PL9	C40-C39-C41	2.51	119.64	115.29
23	C	511	CLA	CMC-C2C-C1C	2.51	128.83	125.02
33	a	416	LMG	O6-C5-C4	2.51	114.29	109.66
25	b	619	BCR	C2-C1-C6	2.52	114.42	110.48
23	C	514	CLA	O2A-CGA-CBA	2.52	119.23	111.90
23	b	603	CLA	C4-C3-C5	2.52	119.67	115.29
23	B	607	CLA	CMC-C2C-C1C	2.53	128.85	125.02
25	d	405	BCR	C38-C26-C27	2.53	118.25	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	O2A-CGA-CBA	2.53	119.27	111.90
23	b	602	CLA	CAC-C3C-C4C	2.53	128.40	124.83
24	D	401	PHO	CMC-C2C-C1C	2.54	128.99	125.04
25	D	406	BCR	C37-C22-C23	2.54	122.14	118.10
26	A	410	SQD	O8-S-C6	2.54	109.11	106.01
23	d	401	CLA	C1-O2A-CGA	2.54	122.87	116.77
23	b	613	CLA	CMC-C2C-C1C	2.54	128.88	125.02
34	c	522	HTG	O5-C1-C2	2.54	113.77	110.28
33	Z	102	LMG	C1-O6-C5	2.55	118.51	113.72
24	A	407	PHO	CAC-C3C-C4C	2.55	128.20	125.21
26	a	412	SQD	O5-C5-C4	2.55	114.35	109.66
24	a	406	PHO	CBD-CHA-C1A	2.55	132.36	126.36
23	b	605	CLA	CED-O2D-CGD	2.55	121.94	115.97
23	a	408	CLA	CMC-C2C-C1C	2.55	128.89	125.02
23	d	401	CLA	C4-C3-C5	2.55	119.72	115.29
29	A	414	PL9	C35-C34-C36	2.55	119.72	115.29
38	v	201	HEM	CAD-CBD-CGD	2.56	117.03	112.66
24	D	401	PHO	C4-C3-C5	2.56	119.73	115.29
23	B	602	CLA	CAC-C3C-C4C	2.57	128.45	124.83
29	A	414	PL9	C25-C24-C26	2.57	119.74	115.29
29	D	407	PL9	C20-C19-C21	2.57	119.74	115.29
25	D	406	BCR	C29-C30-C25	2.57	114.49	110.48
23	b	602	CLA	CMB-C2B-C3B	2.57	129.66	124.89
23	D	405	CLA	C4-C3-C5	2.57	119.75	115.29
23	C	502	CLA	CMB-C2B-C3B	2.57	129.67	124.89
25	K	102	BCR	C2-C1-C6	2.58	114.50	110.48
29	a	414	PL9	C53-C6-C1	2.58	120.31	114.84
34	B	622	HTG	O5-C1-C2	2.58	113.81	110.28
29	A	414	PL9	C53-C6-C1	2.58	120.32	114.84
23	C	511	CLA	C4-C3-C5	2.58	119.77	115.29
23	b	616	CLA	C3B-C4B-NB	2.59	112.56	109.21
29	a	414	PL9	C25-C24-C26	2.59	119.78	115.29
25	B	618	BCR	C37-C22-C23	2.59	122.22	118.10
25	a	409	BCR	C37-C22-C23	2.59	122.23	118.10
33	j	101	LMG	O8-C28-C29	2.59	119.45	111.90
23	c	504	CLA	CED-O2D-CGD	2.60	122.06	115.97
23	B	603	CLA	CAC-C3C-C4C	2.60	128.49	124.83
23	b	611	CLA	CMB-C2B-C3B	2.60	129.72	124.89
23	C	514	CLA	C4-C3-C5	2.61	119.81	115.29
23	a	404	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	b	606	CLA	O2A-CGA-CBA	2.61	119.49	111.90
23	C	511	CLA	CAC-C3C-C4C	2.61	128.51	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	C4-C3-C5	2.61	119.82	115.29
23	c	507	CLA	CAC-C3C-C4C	2.61	128.51	124.83
35	b	627	LMT	O5'-C1'-C2'	2.61	115.34	110.30
23	b	607	CLA	C4-C3-C5	2.61	119.83	115.29
23	b	613	CLA	CMB-C2B-C3B	2.62	129.75	124.89
23	b	601	CLA	CMB-C2B-C3B	2.62	129.75	124.89
23	d	403	CLA	C4-C3-C5	2.62	119.83	115.29
34	C	522	HTG	C3-C4-C5	2.62	114.84	110.22
24	a	406	PHO	C3C-C4C-NC	2.62	114.48	110.19
29	a	414	PL9	C35-C34-C36	2.63	119.84	115.29
31	d	408	LHG	O8-C23-C24	2.63	119.54	111.90
23	B	602	CLA	O2A-CGA-CBA	2.63	119.54	111.90
23	C	506	CLA	CAC-C3C-C4C	2.63	128.54	124.83
34	C	521	HTG	O5-C1-C2	2.63	113.88	110.28
23	D	404	CLA	C4-C3-C5	2.63	119.85	115.29
29	d	406	PL9	C51-C49-C50	2.63	120.74	114.60
23	B	608	CLA	C4-C3-C5	2.63	119.85	115.29
36	H	102	DGD	O1G-C1A-C2A	2.64	119.58	111.90
23	B	609	CLA	CMC-C2C-C1C	2.64	129.03	125.02
23	B	605	CLA	CMC-C2C-C1C	2.65	129.04	125.02
35	D	403	LMT	C4B-C3B-C2B	2.66	115.52	110.84
23	c	511	CLA	CMC-C2C-C1C	2.66	129.05	125.02
23	C	514	CLA	CAC-C3C-C4C	2.66	128.58	124.83
23	c	512	CLA	C4-C3-C5	2.66	119.90	115.29
23	C	513	CLA	C4-C3-C5	2.66	119.90	115.29
23	C	509	CLA	CMB-C2B-C3B	2.66	129.83	124.89
24	a	407	PHO	C2A-C1A-NA	2.66	115.14	111.91
23	B	614	CLA	C4-C3-C5	2.67	119.92	115.29
23	A	404	CLA	CMC-C2C-C1C	2.67	129.07	125.02
23	b	610	CLA	CAC-C3C-C4C	2.67	128.60	124.83
24	D	401	PHO	C2B-C1B-NB	2.68	113.78	109.82
23	B	605	CLA	C3B-C4B-NB	2.68	112.68	109.21
33	Z	102	LMG	O6-C1-C2	2.68	115.47	110.30
23	B	612	CLA	C4-C3-C5	2.68	119.95	115.29
23	C	510	CLA	O2A-CGA-CBA	2.69	119.72	111.90
23	B	604	CLA	C4-C3-C5	2.69	119.95	115.29
23	c	503	CLA	C4-C3-C5	2.69	119.95	115.29
23	b	616	CLA	CAC-C3C-C4C	2.69	128.63	124.83
25	k	101	BCR	C2-C1-C6	2.69	114.69	110.48
23	B	604	CLA	C1-O2A-CGA	2.69	123.23	116.77
23	B	612	CLA	CAC-C3C-C4C	2.70	128.63	124.83
26	a	410	SQD	O48-C23-C24	2.70	119.75	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	C2A-C1A-NA	2.70	115.18	111.91
23	b	603	CLA	CMC-C2C-C1C	2.70	129.12	125.02
23	C	502	CLA	CAC-C3C-C4C	2.70	128.64	124.83
31	d	407	LHG	O8-C23-C24	2.71	119.78	111.90
24	A	407	PHO	O2A-CGA-CBA	2.71	119.78	111.90
23	B	611	CLA	O2A-CGA-CBA	2.71	119.78	111.90
23	d	404	CLA	C3B-C4B-NB	2.71	112.72	109.21
35	D	402	LMT	O1'-C1'-C2'	2.71	112.66	108.23
23	b	610	CLA	C3B-C4B-NB	2.72	112.73	109.21
23	C	508	CLA	O2A-CGA-CBA	2.72	119.81	111.90
35	D	403	LMT	O5'-C5'-C4'	2.72	115.32	109.75
33	Z	102	LMG	O6-C5-C4	2.72	114.67	109.66
23	C	508	CLA	C4-C3-C5	2.72	120.01	115.29
23	C	502	CLA	CMC-C2C-C1C	2.72	129.15	125.02
23	d	404	CLA	CMC-C2C-C1C	2.72	129.15	125.02
23	c	501	CLA	C3B-C4B-NB	2.72	112.73	109.21
23	c	512	CLA	CHB-C4A-NA	2.72	128.28	124.51
23	C	508	CLA	C3B-C4B-NB	2.72	112.73	109.21
26	D	413	SQD	O48-C23-C24	2.73	119.83	111.90
34	b	628	HTG	O5-C5-C4	2.73	114.69	109.66
23	c	505	CLA	CAC-C3C-C4C	2.75	128.70	124.83
23	B	606	CLA	O2A-CGA-CBA	2.75	119.89	111.90
23	A	404	CLA	CMB-C2B-C3B	2.75	129.99	124.89
23	c	501	CLA	C4-C3-C5	2.75	120.06	115.29
23	c	508	CLA	CMB-C2B-C3B	2.76	130.01	124.89
36	c	517	DGD	O1G-C1A-C2A	2.76	119.93	111.90
23	d	401	CLA	CMB-C2B-C3B	2.76	130.01	124.89
29	D	407	PL9	C10-C9-C11	2.76	120.08	115.29
23	c	506	CLA	CAC-C3C-C4C	2.76	128.73	124.83
33	b	620	LMG	O6-C5-C4	2.77	114.76	109.66
23	b	612	CLA	CMB-C2B-C3B	2.78	130.05	124.89
36	C	519	DGD	O2G-C1B-C2B	2.78	117.33	111.55
23	b	613	CLA	C4-C3-C5	2.78	120.12	115.29
35	b	627	LMT	C1'-C2'-C3'	2.79	115.17	109.98
23	C	502	CLA	O2A-CGA-CBA	2.79	120.02	111.90
35	B	630	LMT	O5'-C5'-C4'	2.79	115.46	109.75
23	b	612	CLA	CAC-C3C-C4C	2.79	128.77	124.83
29	D	407	PL9	C7-C3-C4	2.79	119.15	116.88
23	B	613	CLA	O2D-CGD-CBD	2.80	116.29	111.30
23	b	608	CLA	O2A-CGA-CBA	2.80	120.04	111.90
29	D	407	PL9	C40-C39-C41	2.80	120.14	115.29
23	c	511	CLA	CAC-C3C-C4C	2.80	128.78	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	O2A-CGA-CBA	2.80	120.04	111.90
23	b	601	CLA	O2A-CGA-CBA	2.80	120.04	111.90
23	B	612	CLA	CMC-C2C-C1C	2.80	129.26	125.02
24	A	407	PHO	C2C-C1C-NC	2.80	113.97	109.82
29	d	406	PL9	C35-C34-C36	2.81	120.16	115.29
23	b	605	CLA	O2A-CGA-CBA	2.81	120.08	111.90
23	D	404	CLA	CMC-C2C-C1C	2.81	129.28	125.02
23	a	404	CLA	C4-C3-C5	2.81	120.17	115.29
34	b	625	HTG	O5-C5-C4	2.82	114.86	109.66
24	a	406	PHO	C2B-C1B-NB	2.82	114.00	109.82
25	t	101	BCR	C1-C6-C7	2.82	123.67	115.73
23	c	510	CLA	CMC-C2C-C1C	2.83	129.31	125.02
23	A	406	CLA	C3B-C4B-NB	2.83	112.87	109.21
23	b	607	CLA	CAC-C3C-C4C	2.83	128.82	124.83
23	C	509	CLA	O2A-CGA-CBA	2.83	120.14	111.90
33	Z	101	LMG	O8-C28-C29	2.83	120.14	111.90
26	f	101	SQD	O48-C23-C24	2.83	120.15	111.90
23	C	510	CLA	CMB-C2B-C3B	2.84	130.15	124.89
23	a	408	CLA	CAC-C3C-C4C	2.84	128.83	124.83
23	b	611	CLA	CAC-C3C-C4C	2.84	128.84	124.83
34	B	624	HTG	O5-C1-C2	2.84	114.17	110.28
23	c	507	CLA	C3B-C4B-NB	2.85	112.89	109.21
29	A	414	PL9	C10-C9-C11	2.85	120.23	115.29
25	c	515	BCR	C2-C1-C6	2.85	114.94	110.48
31	e	101	LHG	O8-C23-C24	2.85	120.20	111.90
29	a	414	PL9	C20-C19-C21	2.86	120.25	115.29
26	D	413	SQD	C3-C4-C5	2.86	115.26	110.22
23	b	609	CLA	CMC-C2C-C1C	2.86	129.36	125.02
23	C	514	CLA	CMC-C2C-C1C	2.87	129.37	125.02
23	b	601	CLA	C3B-C4B-NB	2.87	112.92	109.21
23	C	504	CLA	O2A-CGA-CBA	2.87	120.25	111.90
23	b	615	CLA	C4-C3-C5	2.87	120.27	115.29
23	c	508	CLA	O2A-CGA-CBA	2.87	120.25	111.90
23	c	506	CLA	C4-C3-C5	2.88	120.28	115.29
23	d	404	CLA	CAC-C3C-C4C	2.88	128.89	124.83
23	c	510	CLA	O2A-CGA-CBA	2.88	120.28	111.90
23	C	512	CLA	O2A-CGA-CBA	2.88	120.29	111.90
23	c	501	CLA	O2A-CGA-CBA	2.88	120.29	111.90
23	C	505	CLA	CMB-C2B-C3B	2.88	130.24	124.89
23	c	506	CLA	O2A-CGA-CBA	2.88	120.29	111.90
25	d	405	BCR	C37-C22-C23	2.89	122.70	118.10
23	B	604	CLA	O2A-CGA-CBA	2.89	120.31	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	b	604	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	c	503	CLA	C3B-C4B-NB	2.89	112.95	109.21
23	B	606	CLA	C3B-C4B-NB	2.90	112.95	109.21
25	t	101	BCR	C35-C13-C12	2.90	122.72	118.10
23	C	509	CLA	CAC-C3C-C4C	2.90	128.92	124.83
23	b	601	CLA	C4-C3-C5	2.90	120.33	115.29
23	c	513	CLA	C4-C3-C5	2.91	120.33	115.29
23	c	504	CLA	O2A-CGA-CBA	2.91	120.36	111.90
31	d	408	LHG	O7-C7-C8	2.91	117.59	111.55
23	B	612	CLA	O2A-CGA-CBA	2.91	120.37	111.90
23	c	509	CLA	CAC-C3C-C4C	2.91	128.94	124.83
23	d	404	CLA	O2A-CGA-CBA	2.91	120.37	111.90
23	c	513	CLA	O2A-CGA-CBA	2.91	120.38	111.90
23	c	509	CLA	C1-O2A-CGA	2.92	123.77	116.77
23	b	614	CLA	CMC-C2C-C1C	2.92	129.45	125.02
23	C	510	CLA	CAC-C3C-C4C	2.92	128.95	124.83
23	B	604	CLA	CMC-C2C-C1C	2.92	129.45	125.02
24	a	406	PHO	C2C-C1C-NC	2.93	114.15	109.82
23	C	506	CLA	O2A-CGA-CBA	2.93	120.42	111.90
23	C	505	CLA	C1-O2A-CGA	2.93	123.80	116.77
26	L	101	SQD	O8-S-C6	2.94	109.59	106.01
24	a	407	PHO	C2B-C1B-NB	2.94	114.18	109.82
23	b	616	CLA	C4-C3-C5	2.95	120.41	115.29
34	B	622	HTG	C1-O5-C5	2.95	118.37	112.69
23	C	514	CLA	C3B-C4B-NB	2.95	113.03	109.21
23	B	609	CLA	C3B-C4B-NB	2.96	113.03	109.21
23	B	615	CLA	CMC-C2C-C1C	2.96	129.50	125.02
23	C	507	CLA	O2A-CGA-CBA	2.96	120.51	111.90
23	c	512	CLA	O2A-CGA-CBA	2.96	120.51	111.90
36	C	518	DGD	O1G-C1A-C2A	2.97	120.54	111.90
23	C	506	CLA	C3B-C4B-NB	2.97	113.05	109.21
36	h	102	DGD	O2G-C1B-C2B	2.98	117.73	111.55
33	c	519	LMG	O8-C28-C29	2.98	120.56	111.90
23	B	606	CLA	C4-C3-C5	2.98	120.46	115.29
24	D	401	PHO	C2A-C1A-NA	2.99	115.54	111.91
26	B	620	SQD	O9-S-C6	2.99	109.38	106.83
31	D	409	LHG	O8-C23-C24	2.99	120.61	111.90
23	c	513	CLA	CAC-C3C-C4C	3.00	129.05	124.83
23	C	503	CLA	C3B-C4B-NB	3.00	113.08	109.21
31	D	408	LHG	O7-C7-C8	3.00	117.78	111.55
23	B	607	CLA	C3B-C4B-NB	3.00	113.09	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	509	CLA	O2A-CGA-CBA	3.01	120.64	111.90
29	d	406	PL9	C40-C39-C41	3.01	120.50	115.29
23	c	513	CLA	CMB-C2B-C3B	3.01	130.48	124.89
23	B	614	CLA	CAC-C3C-C4C	3.01	129.07	124.83
23	B	610	CLA	C3B-C4B-NB	3.01	113.11	109.21
23	D	404	CLA	CAC-C3C-C4C	3.01	129.08	124.83
23	B	616	CLA	O2A-CGA-CBA	3.02	120.69	111.90
26	B	620	SQD	C3-C4-C5	3.02	115.54	110.22
34	c	522	HTG	C1-O5-C5	3.03	118.52	112.69
23	b	602	CLA	CMC-C2C-C1C	3.03	129.61	125.02
23	b	602	CLA	O2A-CGA-CBA	3.04	120.73	111.90
23	D	405	CLA	C3B-C4B-NB	3.04	113.14	109.21
23	c	503	CLA	O2A-CGA-CBA	3.04	120.75	111.90
23	C	507	CLA	C4-C3-C5	3.04	120.57	115.29
34	b	623	HTG	O5-C1-C2	3.05	114.46	110.28
26	A	412	SQD	O47-C7-C8	3.06	117.90	111.55
24	a	407	PHO	C4-C3-C5	3.06	120.59	115.29
23	b	610	CLA	C4-C3-C5	3.06	120.59	115.29
26	a	412	SQD	C1-O5-C5	3.06	119.48	113.72
35	M	101	LMT	O1'-C1'-C2'	3.06	113.23	108.23
23	b	608	CLA	C3B-C4B-NB	3.07	113.18	109.21
29	d	406	PL9	C25-C24-C26	3.07	120.62	115.29
23	c	505	CLA	C3B-C4B-NB	3.07	113.18	109.21
26	L	101	SQD	C3-C4-C5	3.07	115.63	110.22
23	C	511	CLA	C3B-C4B-NB	3.08	113.19	109.21
24	a	406	PHO	O2A-CGA-CBA	3.09	120.88	111.90
24	a	406	PHO	CAC-C3C-C4C	3.09	128.84	125.21
23	c	513	CLA	C3B-C4B-NB	3.10	113.21	109.21
23	B	613	CLA	C4-C3-C5	3.10	120.66	115.29
26	D	413	SQD	O8-S-C6	3.10	109.79	106.01
31	A	417	LHG	O8-C23-C24	3.10	120.92	111.90
33	J	101	LMG	O8-C28-C29	3.10	120.93	111.90
23	C	507	CLA	C3B-C4B-NB	3.10	113.22	109.21
24	D	401	PHO	C2C-C1C-NC	3.11	114.42	109.82
26	A	412	SQD	O9-S-C6	3.11	109.48	106.83
23	B	616	CLA	C3B-C4B-NB	3.11	113.24	109.21
23	b	610	CLA	CMB-C2B-C3B	3.12	130.67	124.89
23	c	503	CLA	CMC-C2C-C1C	3.12	129.75	125.02
23	C	510	CLA	C3B-C4B-NB	3.12	113.24	109.21
23	C	505	CLA	CMC-C2C-C1C	3.12	129.75	125.02
36	C	519	DGD	O1G-C1A-C2A	3.13	121.00	111.90
36	h	102	DGD	O1G-C1A-C2A	3.13	121.00	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	C1-O2A-CGA	3.13	124.28	116.77
23	b	612	CLA	C4-C3-C5	3.13	120.72	115.29
23	B	611	CLA	CMC-C2C-C1C	3.13	129.77	125.02
33	z	101	LMG	O8-C28-C29	3.14	121.03	111.90
23	b	614	CLA	CAC-C3C-C4C	3.14	129.26	124.83
23	b	603	CLA	C3B-C4B-NB	3.14	113.27	109.21
34	b	622	HTG	O5-C1-C2	3.15	114.59	110.28
23	b	612	CLA	C3B-C4B-NB	3.15	113.28	109.21
23	B	601	CLA	O2A-CGA-CBA	3.15	121.06	111.90
23	C	504	CLA	C3B-C4B-NB	3.15	113.28	109.21
23	b	609	CLA	C3B-C4B-NB	3.15	113.28	109.21
25	B	618	BCR	C2-C1-C6	3.15	115.41	110.48
23	A	404	CLA	O2D-CGD-CBD	3.15	116.93	111.30
23	b	602	CLA	C3B-C4B-NB	3.15	113.29	109.21
29	A	414	PL9	C20-C19-C21	3.16	120.77	115.29
23	b	611	CLA	O2A-CGA-CBA	3.17	121.11	111.90
31	d	409	LHG	O8-C23-C24	3.17	121.12	111.90
23	c	505	CLA	CMC-C2C-C1C	3.17	129.82	125.02
26	L	101	SQD	O48-C23-C24	3.17	121.12	111.90
38	V	202	HEM	CAD-CBD-CGD	3.17	118.08	112.66
23	C	513	CLA	O2A-CGA-CBA	3.17	121.12	111.90
23	C	512	CLA	C4-C3-C5	3.17	120.79	115.29
29	a	414	PL9	C30-C29-C31	3.18	120.81	115.29
33	c	520	LMG	O8-C28-C29	3.19	121.17	111.90
23	B	615	CLA	C3B-C4B-NB	3.19	113.33	109.21
23	C	512	CLA	CAC-C3C-C4C	3.19	129.33	124.83
23	b	614	CLA	O2A-CGA-CBA	3.19	121.18	111.90
23	b	608	CLA	CMB-C2B-C3B	3.19	130.82	124.89
23	c	502	CLA	O2A-CGA-CBA	3.20	121.20	111.90
23	c	510	CLA	C4-C3-C5	3.20	120.84	115.29
26	a	412	SQD	C3-C4-C5	3.20	115.86	110.22
33	C	520	LMG	O7-C10-C11	3.20	118.20	111.55
23	c	501	CLA	CAC-C3C-C4C	3.21	129.35	124.83
23	B	614	CLA	O2A-CGA-CBA	3.21	121.23	111.90
29	A	414	PL9	C30-C29-C31	3.21	120.86	115.29
23	A	406	CLA	O2A-CGA-CBA	3.21	121.24	111.90
23	B	612	CLA	C3B-C4B-NB	3.21	113.36	109.21
31	l	101	LHG	O8-C23-C24	3.21	121.25	111.90
31	E	101	LHG	O8-C23-C24	3.21	121.25	111.90
26	a	412	SQD	O48-C23-C24	3.22	121.26	111.90
23	b	606	CLA	C3B-C4B-NB	3.22	113.37	109.21
25	T	101	BCR	C15-C14-C13	3.22	131.91	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	e	101	LHG	O7-C7-C8	3.22	118.25	111.55
29	A	414	PL9	C15-C14-C16	3.23	120.89	115.29
33	b	620	LMG	O7-C10-C11	3.23	118.25	111.55
33	B	621	LMG	O8-C28-C29	3.23	121.29	111.90
23	b	609	CLA	CAC-C3C-C4C	3.23	129.39	124.83
33	C	520	LMG	O8-C28-C29	3.24	121.32	111.90
29	d	406	PL9	C20-C19-C21	3.24	120.91	115.29
23	a	408	CLA	O2A-CGA-CBA	3.24	121.34	111.90
35	I	101	LMT	O1B-C4'-C3'	3.24	115.00	107.19
23	c	512	CLA	C3B-C4B-NB	3.25	113.41	109.21
23	B	609	CLA	O2A-CGA-CBA	3.25	121.36	111.90
24	A	407	PHO	C2B-C1B-NB	3.25	114.64	109.82
23	b	608	CLA	CMC-C2C-C1C	3.26	129.96	125.02
31	A	416	LHG	O7-C7-C8	3.26	118.32	111.55
23	B	613	CLA	O2A-CGA-CBA	3.26	121.39	111.90
23	a	404	CLA	CMB-C2B-C3B	3.26	130.95	124.89
23	C	511	CLA	O2A-CGA-CBA	3.27	121.40	111.90
23	b	604	CLA	CMC-C2C-C1C	3.27	129.98	125.02
23	B	615	CLA	CED-O2D-CGD	3.27	123.64	115.97
26	A	410	SQD	O48-C23-C24	3.27	121.42	111.90
23	B	603	CLA	C4-C3-C5	3.28	120.97	115.29
33	Z	102	LMG	C4-C3-C2	3.28	116.63	110.84
23	b	606	CLA	C4-C3-C5	3.29	120.99	115.29
29	a	414	PL9	C10-C9-C11	3.29	121.00	115.29
23	B	601	CLA	C3B-C4B-NB	3.31	113.49	109.21
33	b	620	LMG	O8-C28-C29	3.32	121.56	111.90
23	b	605	CLA	C4-C3-C5	3.33	121.06	115.29
23	b	612	CLA	O2A-CGA-CBA	3.33	121.58	111.90
23	B	608	CLA	C3B-C4B-NB	3.33	113.51	109.21
23	c	504	CLA	CAC-C3C-C4C	3.33	129.53	124.83
23	A	408	CLA	C3B-C4B-NB	3.33	113.52	109.21
23	B	613	CLA	CAC-C3C-C4C	3.33	129.53	124.83
23	a	405	CLA	C3B-C4B-NB	3.34	113.53	109.21
24	D	401	PHO	CAC-C3C-C4C	3.34	129.13	125.21
23	D	405	CLA	CMC-C2C-C1C	3.34	130.08	125.02
26	B	620	SQD	O48-C23-C24	3.35	121.65	111.90
23	b	604	CLA	O2A-CGA-CBA	3.36	121.67	111.90
23	b	616	CLA	O2A-CGA-CBA	3.36	121.68	111.90
23	B	608	CLA	O2A-CGA-CBA	3.36	121.68	111.90
25	k	101	BCR	C29-C30-C25	3.36	115.74	110.48
25	t	101	BCR	C37-C22-C23	3.37	123.47	118.10
23	b	603	CLA	O2A-CGA-CBA	3.37	121.72	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	C4-C3-C5	3.38	121.15	115.29
23	a	404	CLA	O2A-CGA-CBA	3.39	121.76	111.90
23	B	611	CLA	C3B-C4B-NB	3.40	113.60	109.21
26	a	412	SQD	O47-C7-C8	3.41	118.63	111.55
33	c	520	LMG	C3-C4-C5	3.42	116.24	110.22
23	c	504	CLA	C3B-C4B-NB	3.43	113.64	109.21
26	f	101	SQD	C1-O5-C5	3.43	120.18	113.72
23	C	506	CLA	CMC-C2C-C1C	3.45	130.25	125.02
23	c	504	CLA	CMC-C2C-C1C	3.46	130.26	125.02
23	D	404	CLA	O2A-CGA-CBA	3.46	121.97	111.90
23	B	613	CLA	CMB-C2B-C3B	3.47	131.32	124.89
23	b	610	CLA	O2A-CGA-CBA	3.48	122.01	111.90
23	c	511	CLA	C3B-C4B-NB	3.48	113.70	109.21
23	B	603	CLA	O2A-CGA-CBA	3.48	122.02	111.90
23	C	507	CLA	CMC-C2C-C1C	3.48	130.30	125.02
23	c	509	CLA	C3B-C4B-NB	3.48	113.71	109.21
23	B	613	CLA	C3B-C4B-NB	3.49	113.72	109.21
35	D	403	LMT	O1B-C4'-C3'	3.49	115.60	107.19
29	D	407	PL9	C53-C6-C1	3.51	122.30	114.84
23	b	615	CLA	C3B-C4B-NB	3.52	113.75	109.21
23	b	609	CLA	O2A-CGA-CBA	3.52	122.14	111.90
23	B	603	CLA	C3B-C4B-NB	3.52	113.76	109.21
23	C	512	CLA	CMC-C2C-C1C	3.52	130.36	125.02
23	b	613	CLA	C3B-C4B-NB	3.53	113.77	109.21
23	C	507	CLA	CAC-C3C-C4C	3.53	129.81	124.83
23	B	604	CLA	C3B-C4B-NB	3.53	113.78	109.21
23	B	602	CLA	C3B-C4B-NB	3.56	113.81	109.21
23	D	404	CLA	C3B-C4B-NB	3.56	113.81	109.21
34	B	622	HTG	C1'-S1-C1	3.58	105.58	100.28
23	b	614	CLA	C3B-C4B-NB	3.59	113.86	109.21
23	c	508	CLA	C3B-C4B-NB	3.60	113.86	109.21
23	c	513	CLA	CMC-C2C-C1C	3.61	130.49	125.02
26	A	412	SQD	O48-C23-C24	3.61	122.40	111.90
31	A	416	LHG	O8-C23-C24	3.61	122.41	111.90
25	B	618	BCR	C29-C30-C25	3.61	116.13	110.48
23	C	504	CLA	O2D-CGD-CBD	3.61	117.76	111.30
23	C	510	CLA	CMC-C2C-C1C	3.62	130.50	125.02
31	d	409	LHG	O7-C7-C8	3.62	119.07	111.55
23	b	611	CLA	C3B-C4B-NB	3.62	113.89	109.21
33	Z	101	LMG	O6-C5-C4	3.62	116.33	109.66
23	c	510	CLA	C3B-C4B-NB	3.63	113.90	109.21
23	A	404	CLA	CAC-C3C-C4C	3.65	129.97	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	l	101	LHG	O7-C7-C8	3.65	119.13	111.55
23	b	607	CLA	C3B-C4B-NB	3.65	113.93	109.21
23	d	401	CLA	O2D-CGD-CBD	3.66	117.84	111.30
34	C	522	HTG	O5-C5-C4	3.66	116.40	109.66
23	C	502	CLA	C3B-C4B-NB	3.66	113.94	109.21
31	d	407	LHG	O7-C7-C8	3.67	119.17	111.55
36	c	517	DGD	O2G-C1B-C2B	3.67	119.18	111.55
23	b	605	CLA	C3B-C4B-NB	3.68	113.97	109.21
36	C	517	DGD	O2G-C1B-C2B	3.68	119.19	111.55
33	z	101	LMG	O7-C10-C11	3.68	119.20	111.55
29	d	406	PL9	C10-C9-C11	3.69	121.68	115.29
36	C	518	DGD	O2G-C1B-C2B	3.69	119.21	111.55
23	a	408	CLA	C3B-C4B-NB	3.69	113.99	109.21
33	c	520	LMG	O6-C5-C4	3.70	116.47	109.66
23	d	403	CLA	C3B-C4B-NB	3.70	114.00	109.21
23	b	613	CLA	O2A-CGA-CBA	3.72	122.72	111.90
33	Z	102	LMG	C3-C4-C5	3.72	116.77	110.22
23	B	610	CLA	O2A-CGA-CBA	3.74	122.77	111.90
23	d	401	CLA	C3B-C4B-NB	3.75	114.06	109.21
23	c	510	CLA	C3C-C4C-NC	3.77	114.03	110.21
34	b	625	HTG	C1-O5-C5	3.78	119.97	112.69
23	C	512	CLA	C3B-C4B-NB	3.80	114.12	109.21
33	a	416	LMG	O7-C10-C11	3.82	119.49	111.55
23	a	404	CLA	O2D-CGD-CBD	3.86	118.20	111.30
33	j	101	LMG	O7-C10-C11	3.86	119.57	111.55
23	d	403	CLA	O2A-CGA-CBA	3.87	123.16	111.90
31	A	417	LHG	O7-C7-C8	3.87	119.59	111.55
25	d	405	BCR	C29-C30-C25	3.88	116.54	110.48
23	c	511	CLA	C4-C3-C5	3.89	122.04	115.29
23	A	405	CLA	CMC-C2C-C1C	3.90	130.93	125.02
33	c	519	LMG	O7-C10-C11	3.92	119.68	111.55
29	a	414	PL9	C15-C14-C16	3.93	122.10	115.29
33	B	621	LMG	O7-C10-C11	3.93	119.71	111.55
23	C	512	CLA	O2D-CGD-CBD	3.94	118.34	111.30
23	B	614	CLA	C3B-C4B-NB	3.94	114.31	109.21
23	A	404	CLA	C3B-C4B-NB	3.95	114.31	109.21
23	B	613	CLA	CMC-C2C-C1C	3.96	131.02	125.02
33	Z	102	LMG	C1-C2-C3	3.97	117.36	109.98
23	C	511	CLA	C3C-C4C-NC	3.99	114.25	110.21
23	c	502	CLA	C3B-C4B-NB	4.01	114.39	109.21
23	A	408	CLA	O2D-CGD-CBD	4.02	118.47	111.30
23	C	507	CLA	C3C-C4C-NC	4.02	114.28	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	Z	101	LMG	O7-C10-C11	4.03	119.92	111.55
36	H	102	DGD	O2G-C1B-C2B	4.04	119.94	111.55
23	c	506	CLA	C3B-C4B-NB	4.04	114.44	109.21
23	d	401	CLA	C3C-C4C-NC	4.07	114.33	110.21
34	b	628	HTG	C1-O5-C5	4.08	120.54	112.69
26	A	410	SQD	O9-S-C6	4.08	110.31	106.83
23	c	511	CLA	O2D-CGD-CBD	4.08	118.59	111.30
26	A	412	SQD	O8-S-C6	4.09	111.00	106.01
23	a	404	CLA	C3B-C4B-NB	4.09	114.49	109.21
29	A	414	PL9	C7-C3-C4	4.09	120.20	116.88
23	A	405	CLA	O2D-CGD-CBD	4.09	118.61	111.30
23	C	505	CLA	C3B-C4B-NB	4.10	114.51	109.21
35	I	101	LMT	C1'-O5'-C5'	4.11	121.45	113.72
33	J	101	LMG	O7-C10-C11	4.12	120.11	111.55
23	A	408	CLA	C4-C3-C5	4.13	122.45	115.29
31	E	101	LHG	O7-C7-C8	4.13	120.14	111.55
33	c	520	LMG	O7-C10-C11	4.15	120.18	111.55
23	c	506	CLA	O2D-CGD-CBD	4.18	118.77	111.30
23	A	404	CLA	C3C-C4C-NC	4.18	114.45	110.21
23	B	603	CLA	C3C-C4C-NC	4.19	114.46	110.21
35	D	402	LMT	O5'-C5'-C4'	4.21	118.36	109.75
23	B	611	CLA	O2D-CGD-CBD	4.23	118.85	111.30
23	C	504	CLA	C3C-C4C-NC	4.23	114.50	110.21
36	c	516	DGD	O2G-C1B-C2B	4.25	120.37	111.55
33	Z	101	LMG	C3-C4-C5	4.26	117.72	110.22
23	d	403	CLA	O2D-CGD-CBD	4.27	118.93	111.30
23	C	509	CLA	C3B-C4B-NB	4.27	114.73	109.21
23	B	609	CLA	O2D-CGD-CBD	4.28	118.95	111.30
23	C	514	CLA	O2D-CGD-CBD	4.29	118.97	111.30
23	b	613	CLA	O2D-CGD-CBD	4.29	118.97	111.30
23	C	507	CLA	O2D-CGD-CBD	4.31	119.00	111.30
26	a	412	SQD	O9-S-C6	4.32	110.52	106.83
23	b	615	CLA	O2D-CGD-CBD	4.33	119.04	111.30
23	B	602	CLA	C3C-C4C-NC	4.33	114.60	110.21
23	A	404	CLA	O2A-CGA-CBA	4.36	124.60	111.90
26	a	412	SQD	O7-S-C6	4.37	110.56	106.83
23	b	609	CLA	C3C-C4C-NC	4.39	114.65	110.21
35	D	402	LMT	C1'-O5'-C5'	4.39	121.98	113.72
26	L	101	SQD	O6-C1-C2	4.41	115.43	108.23
23	d	404	CLA	C3C-C4C-NC	4.44	114.71	110.21
23	B	608	CLA	O2D-CGD-CBD	4.45	119.24	111.30
23	B	601	CLA	C3C-C4C-NC	4.45	114.72	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405	CLA	C3C-C4C-NC	4.46	114.73	110.21
23	c	510	CLA	O2D-CGD-CBD	4.48	119.30	111.30
23	a	404	CLA	C3C-C4C-NC	4.48	114.75	110.21
26	B	620	SQD	O47-C7-C8	4.48	120.86	111.55
23	c	511	CLA	C3C-C4C-NC	4.51	114.78	110.21
23	b	616	CLA	C2C-C1C-NC	4.51	113.33	110.22
23	B	614	CLA	C3C-C4C-NC	4.53	114.80	110.21
23	A	406	CLA	O2D-CGD-CBD	4.53	119.40	111.30
23	B	605	CLA	C3C-C4C-NC	4.53	114.81	110.21
23	a	405	CLA	O2D-CGD-CBD	4.54	119.41	111.30
33	Z	102	LMG	O7-C10-C11	4.54	120.97	111.55
24	A	407	PHO	O2D-CGD-CBD	4.54	119.41	111.30
23	b	603	CLA	C3C-C4C-NC	4.56	114.83	110.21
23	c	501	CLA	C3C-C4C-NC	4.58	114.85	110.21
23	b	611	CLA	C3C-C4C-NC	4.59	114.86	110.21
23	B	602	CLA	O2D-CGD-CBD	4.59	119.50	111.30
23	b	602	CLA	C3C-C4C-NC	4.59	114.86	110.21
23	B	615	CLA	O2D-CGD-CBD	4.59	119.51	111.30
23	c	502	CLA	C3C-C4C-NC	4.61	114.88	110.21
23	d	403	CLA	C3C-C4C-NC	4.63	114.90	110.21
23	C	513	CLA	C3C-C4C-NC	4.63	114.90	110.21
23	C	502	CLA	C3C-C4C-NC	4.64	114.91	110.21
23	b	615	CLA	C3C-C4C-NC	4.64	114.91	110.21
23	A	405	CLA	C3C-C4C-NC	4.66	114.93	110.21
23	c	504	CLA	C3C-C4C-NC	4.66	114.94	110.21
23	b	601	CLA	C3C-C4C-NC	4.67	114.94	110.21
34	C	522	HTG	C1-O5-C5	4.67	121.68	112.69
23	c	504	CLA	O2D-CGD-CBD	4.67	119.65	111.30
23	B	608	CLA	C3C-C4C-NC	4.69	114.97	110.21
23	B	607	CLA	C3C-C4C-NC	4.71	114.98	110.21
23	b	607	CLA	O2D-CGD-CBD	4.71	119.72	111.30
23	C	503	CLA	C3C-C4C-NC	4.72	114.99	110.21
23	D	404	CLA	O2D-CGD-CBD	4.73	119.75	111.30
23	b	608	CLA	C3C-C4C-NC	4.73	115.01	110.21
31	D	409	LHG	O7-C7-C8	4.74	121.39	111.55
23	a	408	CLA	C3C-C4C-NC	4.75	115.02	110.21
24	a	407	PHO	C2D-C1D-ND	4.76	116.87	109.82
26	a	410	SQD	O9-S-C6	4.77	110.90	106.83
26	B	620	SQD	O6-C1-C2	4.77	116.01	108.23
23	b	605	CLA	C3C-C4C-NC	4.77	115.04	110.21
23	C	514	CLA	C3C-C4C-NC	4.77	115.05	110.21
23	A	406	CLA	C3C-C4C-NC	4.79	115.06	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	410	SQD	O8-S-C6	4.80	111.87	106.01
23	c	506	CLA	C3C-C4C-NC	4.82	115.09	110.21
26	A	410	SQD	O47-C7-C8	4.82	121.56	111.55
26	f	101	SQD	O7-S-C6	4.83	110.95	106.83
23	c	513	CLA	O2D-CGD-CBD	4.84	119.95	111.30
23	C	510	CLA	O2D-CGD-CBD	4.86	119.99	111.30
23	c	512	CLA	C3C-C4C-NC	4.88	115.15	110.21
23	b	612	CLA	O2D-CGD-CBD	4.88	120.03	111.30
26	A	410	SQD	O7-S-C6	4.89	111.01	106.83
26	a	410	SQD	O6-C1-C2	4.89	116.22	108.23
23	b	612	CLA	C3C-C4C-NC	4.90	115.17	110.21
23	D	405	CLA	C3C-C4C-NC	4.90	115.18	110.21
23	C	512	CLA	C3C-C4C-NC	4.91	115.19	110.21
23	c	505	CLA	O2D-CGD-CBD	4.92	120.08	111.30
23	A	408	CLA	C3C-C4C-NC	4.93	115.20	110.21
23	b	606	CLA	C3C-C4C-NC	4.93	115.21	110.21
23	C	510	CLA	C3C-C4C-NC	4.95	115.22	110.21
23	b	614	CLA	C3C-C4C-NC	4.97	115.25	110.21
23	B	611	CLA	C3C-C4C-NC	4.98	115.26	110.21
23	C	508	CLA	C3C-C4C-NC	4.98	115.26	110.21
23	c	509	CLA	C3C-C4C-NC	4.99	115.27	110.21
33	C	501	LMG	O7-C10-C11	5.02	121.98	111.55
23	b	616	CLA	C3C-C4C-NC	5.04	115.32	110.21
23	b	610	CLA	C3C-C4C-NC	5.04	115.32	110.21
23	c	513	CLA	C3C-C4C-NC	5.05	115.32	110.21
23	B	615	CLA	C3C-C4C-NC	5.05	115.33	110.21
23	d	404	CLA	O2D-CGD-CBD	5.06	120.35	111.30
26	D	413	SQD	O7-S-C6	5.07	111.16	106.83
23	B	603	CLA	O2D-CGD-CBD	5.08	120.38	111.30
23	a	408	CLA	O2D-CGD-CBD	5.08	120.38	111.30
23	D	405	CLA	C2C-C1C-NC	5.09	113.72	110.22
23	c	507	CLA	C3C-C4C-NC	5.09	115.37	110.21
23	D	404	CLA	C3C-C4C-NC	5.11	115.39	110.21
23	b	609	CLA	O2D-CGD-CBD	5.11	120.43	111.30
23	c	509	CLA	O2D-CGD-CBD	5.11	120.43	111.30
23	d	404	CLA	C2C-C1C-NC	5.15	113.76	110.22
23	C	505	CLA	C3C-C4C-NC	5.15	115.43	110.21
26	f	101	SQD	O47-C7-C8	5.15	122.25	111.55
26	L	101	SQD	O47-C7-C8	5.16	122.27	111.55
23	B	607	CLA	O2D-CGD-CBD	5.16	120.53	111.30
23	B	616	CLA	C3C-C4C-NC	5.18	115.46	110.21
23	A	406	CLA	C2C-C1C-NC	5.19	113.79	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C3C-C4C-NC	5.19	115.47	110.21
23	c	502	CLA	O2D-CGD-CBD	5.21	120.60	111.30
24	a	406	PHO	O2D-CGD-CBD	5.22	120.63	111.30
24	A	407	PHO	C2D-C1D-ND	5.22	117.56	109.82
24	a	407	PHO	O2D-CGD-CBD	5.23	120.64	111.30
23	b	608	CLA	O2D-CGD-CBD	5.23	120.64	111.30
23	C	505	CLA	O2D-CGD-CBD	5.24	120.66	111.30
23	B	606	CLA	C3C-C4C-NC	5.24	115.52	110.21
23	b	613	CLA	C3C-C4C-NC	5.24	115.52	110.21
23	b	606	CLA	O2D-CGD-CBD	5.25	120.69	111.30
23	c	508	CLA	C3C-C4C-NC	5.25	115.53	110.21
23	B	613	CLA	C3C-C4C-NC	5.27	115.55	110.21
26	B	620	SQD	O7-S-C6	5.28	111.34	106.83
23	C	509	CLA	O2D-CGD-CBD	5.29	120.76	111.30
23	c	503	CLA	O2D-CGD-CBD	5.31	120.79	111.30
23	B	605	CLA	O2D-CGD-CBD	5.33	120.82	111.30
23	b	610	CLA	O2D-CGD-CBD	5.33	120.82	111.30
26	D	413	SQD	O6-C1-C2	5.34	116.94	108.23
23	C	511	CLA	O2D-CGD-CBD	5.35	120.86	111.30
23	B	609	CLA	C3C-C4C-NC	5.38	115.66	110.21
23	b	605	CLA	O2D-CGD-CBD	5.39	120.94	111.30
29	a	414	PL9	C7-C3-C4	5.40	121.27	116.88
24	a	406	PHO	C2D-C1D-ND	5.47	117.92	109.82
23	b	607	CLA	C3C-C4C-NC	5.48	115.76	110.21
24	D	401	PHO	O2D-CGD-CBD	5.48	121.10	111.30
23	C	503	CLA	O2D-CGD-CBD	5.48	121.10	111.30
24	D	401	PHO	C2D-C1D-ND	5.50	117.96	109.82
23	B	610	CLA	C3C-C4C-NC	5.50	115.79	110.21
26	a	410	SQD	O47-C7-C8	5.51	122.99	111.55
23	B	610	CLA	O2D-CGD-CBD	5.52	121.17	111.30
23	B	616	CLA	C2C-C1C-NC	5.53	114.03	110.22
38	e	103	HEM	CAD-CBD-CGD	5.55	122.15	112.66
23	B	606	CLA	O2D-CGD-CBD	5.57	121.25	111.30
23	C	502	CLA	O2D-CGD-CBD	5.59	121.29	111.30
23	c	501	CLA	O2D-CGD-CBD	5.59	121.29	111.30
23	A	405	CLA	C2C-C1C-NC	5.60	114.07	110.22
23	b	603	CLA	O2D-CGD-CBD	5.62	121.34	111.30
23	B	604	CLA	C3C-C4C-NC	5.70	115.98	110.21
23	b	611	CLA	O2D-CGD-CBD	5.70	121.49	111.30
23	C	506	CLA	C3C-C4C-NC	5.72	116.00	110.21
23	B	604	CLA	O2D-CGD-CBD	5.74	121.56	111.30
23	C	513	CLA	O2D-CGD-CBD	5.74	121.57	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C2C-C1C-NC	5.75	114.18	110.22
23	b	616	CLA	O2D-CGD-CBD	5.76	121.59	111.30
23	B	612	CLA	O2D-CGD-CBD	5.77	121.61	111.30
23	B	614	CLA	O2D-CGD-CBD	5.83	121.73	111.30
23	B	601	CLA	O2D-CGD-CBD	5.86	121.77	111.30
23	C	509	CLA	C3C-C4C-NC	5.86	116.15	110.21
23	b	604	CLA	C3C-C4C-NC	5.87	116.16	110.21
23	c	505	CLA	C3C-C4C-NC	5.87	116.16	110.21
23	b	614	CLA	O2D-CGD-CBD	5.88	121.81	111.30
23	c	507	CLA	O2D-CGD-CBD	5.92	121.88	111.30
23	b	606	CLA	C2C-C1C-NC	5.92	114.30	110.22
23	b	601	CLA	O2D-CGD-CBD	5.92	121.89	111.30
23	C	514	CLA	C2C-C1C-NC	5.93	114.30	110.22
23	c	512	CLA	O2D-CGD-CBD	5.96	121.96	111.30
23	D	405	CLA	O2D-CGD-CBD	6.01	122.04	111.30
34	C	521	HTG	C1'-S1-C1	6.02	109.21	100.28
23	b	602	CLA	O2D-CGD-CBD	6.04	122.09	111.30
34	c	522	HTG	C1'-S1-C1	6.05	109.25	100.28
26	D	413	SQD	O47-C7-C8	6.07	124.15	111.55
23	b	604	CLA	O2D-CGD-CBD	6.11	122.22	111.30
23	C	513	CLA	C2C-C1C-NC	6.12	114.43	110.22
23	c	511	CLA	C2C-C1C-NC	6.14	114.44	110.22
23	C	506	CLA	O2D-CGD-CBD	6.17	122.33	111.30
34	B	627	HTG	C1'-S1-C1	6.17	109.43	100.28
23	B	606	CLA	C2C-C1C-NC	6.17	114.47	110.22
26	L	101	SQD	O7-S-C6	6.20	112.12	106.83
23	c	513	CLA	C2C-C1C-NC	6.20	114.49	110.22
23	B	616	CLA	O2D-CGD-CBD	6.22	122.41	111.30
26	A	410	SQD	O6-C1-C2	6.22	118.38	108.23
23	C	508	CLA	O2D-CGD-CBD	6.24	122.45	111.30
23	C	510	CLA	C2C-C1C-NC	6.24	114.51	110.22
23	c	508	CLA	O2D-CGD-CBD	6.26	122.48	111.30
23	B	605	CLA	C2C-C1C-NC	6.26	114.53	110.22
34	b	622	HTG	C1'-S1-C1	6.26	109.57	100.28
23	B	609	CLA	C2C-C1C-NC	6.30	114.55	110.22
23	A	408	CLA	C2C-C1C-NC	6.31	114.56	110.22
23	c	507	CLA	C2C-C1C-NC	6.31	114.56	110.22
34	C	522	HTG	C1'-S1-C1	6.32	109.65	100.28
23	b	608	CLA	C2C-C1C-NC	6.32	114.57	110.22
23	c	505	CLA	C2C-C1C-NC	6.33	114.58	110.22
23	B	612	CLA	C3C-C4C-NC	6.35	116.65	110.21
24	a	406	PHO	CMD-C2D-C1D	6.36	134.95	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	628	HTG	C1'-S1-C1	6.37	109.73	100.28
38	E	103	HEM	CAD-CBD-CGD	6.37	123.55	112.66
23	B	608	CLA	C2C-C1C-NC	6.38	114.61	110.22
23	c	501	CLA	C2C-C1C-NC	6.44	114.65	110.22
23	B	615	CLA	C2C-C1C-NC	6.46	114.66	110.22
23	b	612	CLA	C2C-C1C-NC	6.50	114.69	110.22
23	a	405	CLA	C2C-C1C-NC	6.50	114.69	110.22
23	b	601	CLA	C2C-C1C-NC	6.53	114.71	110.22
23	c	504	CLA	C2C-C1C-NC	6.60	114.76	110.22
23	C	503	CLA	C2C-C1C-NC	6.63	114.78	110.22
23	a	408	CLA	C2C-C1C-NC	6.63	114.78	110.22
23	b	614	CLA	C2C-C1C-NC	6.64	114.79	110.22
23	b	602	CLA	C2C-C1C-NC	6.66	114.80	110.22
23	C	504	CLA	C2C-C1C-NC	6.67	114.81	110.22
23	B	601	CLA	C2C-C1C-NC	6.70	114.83	110.22
23	C	512	CLA	C2C-C1C-NC	6.71	114.84	110.22
23	b	609	CLA	C2C-C1C-NC	6.71	114.84	110.22
23	B	610	CLA	C2C-C1C-NC	6.72	114.84	110.22
23	B	612	CLA	C2C-C1C-NC	6.74	114.86	110.22
23	C	506	CLA	C2C-C1C-NC	6.76	114.87	110.22
23	c	503	CLA	C2C-C1C-NC	6.77	114.88	110.22
23	b	604	CLA	C2C-C1C-NC	6.82	114.91	110.22
23	C	508	CLA	C2C-C1C-NC	6.84	114.93	110.22
23	b	605	CLA	C2C-C1C-NC	6.90	114.97	110.22
23	B	611	CLA	C2C-C1C-NC	6.91	114.97	110.22
23	c	512	CLA	C2C-C1C-NC	6.94	115.00	110.22
23	C	511	CLA	C2C-C1C-NC	6.99	115.03	110.22
23	b	610	CLA	C2C-C1C-NC	6.99	115.03	110.22
23	c	510	CLA	C2C-C1C-NC	7.00	115.04	110.22
23	c	509	CLA	C2C-C1C-NC	7.05	115.07	110.22
34	b	625	HTG	C1'-S1-C1	7.08	110.78	100.28
34	d	411	HTG	C1'-S1-C1	7.09	110.80	100.28
23	c	508	CLA	C2C-C1C-NC	7.10	115.10	110.22
23	b	607	CLA	C2C-C1C-NC	7.13	115.13	110.22
23	B	607	CLA	C2C-C1C-NC	7.18	115.16	110.22
23	d	401	CLA	C2C-C1C-NC	7.19	115.16	110.22
34	D	412	HTG	C1'-S1-C1	7.19	110.95	100.28
23	B	603	CLA	C2C-C1C-NC	7.26	115.21	110.22
24	a	407	PHO	CMD-C2D-C1D	7.27	136.36	125.04
23	b	615	CLA	C2C-C1C-NC	7.29	115.23	110.22
23	C	507	CLA	C2C-C1C-NC	7.29	115.24	110.22
34	c	521	HTG	C1'-S1-C1	7.35	111.18	100.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	PHO	CMD-C2D-C1D	7.38	136.53	125.04
23	B	604	CLA	C2C-C1C-NC	7.39	115.31	110.22
23	B	602	CLA	C2C-C1C-NC	7.42	115.33	110.22
23	A	404	CLA	C2C-C1C-NC	7.48	115.36	110.22
23	b	611	CLA	C2C-C1C-NC	7.51	115.38	110.22
23	b	613	CLA	C2C-C1C-NC	7.59	115.44	110.22
23	B	613	CLA	C2C-C1C-NC	7.61	115.45	110.22
23	C	502	CLA	C2C-C1C-NC	7.69	115.51	110.22
23	c	506	CLA	C2C-C1C-NC	7.85	115.62	110.22
23	B	614	CLA	C2C-C1C-NC	7.86	115.63	110.22
24	D	401	PHO	CMD-C2D-C1D	7.92	137.38	125.04
23	C	505	CLA	C2C-C1C-NC	7.95	115.69	110.22
23	d	403	CLA	C2C-C1C-NC	7.98	115.71	110.22
23	c	502	CLA	C2C-C1C-NC	8.18	115.84	110.22
23	C	509	CLA	C2C-C1C-NC	8.18	115.85	110.22
23	a	404	CLA	C2C-C1C-NC	8.22	115.88	110.22
34	B	623	HTG	C1'-S1-C1	8.24	112.50	100.28
34	b	623	HTG	C1'-S1-C1	8.40	112.73	100.28
34	B	624	HTG	C1'-S1-C1	8.52	112.91	100.28
23	D	404	CLA	C2C-C1C-NC	8.79	116.26	110.22

All (196) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	a	408	CLA	NC
23	a	408	CLA	ND
23	a	408	CLA	NA
23	d	404	CLA	NC
23	d	404	CLA	ND
23	d	404	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA

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Mol	Chain	Res	Type	Atom
23	c	513	CLA	NC
23	c	513	CLA	ND
23	c	513	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	A	406	CLA	NC
23	A	406	CLA	ND
23	A	406	CLA	NA
23	D	405	CLA	NC
23	D	405	CLA	ND
23	D	405	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	B	616	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	613	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	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	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	B	615	CLA	NA
23	B	615	CLA	NC
23	B	615	CLA	ND
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	503	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	C	514	CLA	NC
23	C	514	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	A	408	CLA	NC
23	A	408	CLA	ND
23	A	408	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	D	404	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	609	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	C	506	CLA	ND
23	c	501	CLA	NC
23	c	501	CLA	ND
23	c	501	CLA	NA
23	b	601	CLA	NC
23	b	601	CLA	ND
23	b	601	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
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	c	505	CLA	ND
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	b	612	CLA	NC
23	b	612	CLA	ND
23	b	612	CLA	NA
23	c	502	CLA	NC
23	c	502	CLA	ND
23	c	502	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	B	610	CLA	NC

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Mol	Chain	Res	Type	Atom
23	B	610	CLA	ND
23	B	610	CLA	NA
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	b	602	CLA	NC
23	b	602	CLA	ND
23	b	602	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	NA
23	d	403	CLA	ND
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	c	506	CLA	ND
23	c	506	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	601	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	c	504	CLA	NC

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Mol	Chain	Res	Type	Atom
23	c	504	CLA	ND
23	c	504	CLA	NA
23	b	603	CLA	NC
23	b	603	CLA	ND
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Z	102	LMG	C8-O7-C10-O9
33	Z	102	LMG	C8-O7-C10-C11
26	f	101	SQD	C45-O47-C7-O49
26	D	413	SQD	C45-O47-C7-O49
26	f	101	SQD	C45-O47-C7-C8
26	D	413	SQD	C45-O47-C7-C8

There are no ring outliers.

86 monomers are involved in 300 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	404	CLA	5	0
23	A	405	CLA	4	0
23	A	406	CLA	4	0
24	A	407	PHO	6	0
23	A	408	CLA	9	0
25	A	409	BCR	2	0
26	A	410	SQD	7	0
27	A	411	GOL	1	0
26	A	412	SQD	3	0
29	A	414	PL9	9	0
31	A	416	LHG	2	0
31	A	417	LHG	2	0
23	B	601	CLA	4	0
23	B	602	CLA	5	0
23	B	603	CLA	4	0
23	B	604	CLA	6	0
23	B	605	CLA	11	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	606	CLA	4	0
23	B	607	CLA	3	0
23	B	608	CLA	3	0
23	B	609	CLA	7	0
23	B	610	CLA	2	0
23	B	611	CLA	4	0
23	B	612	CLA	6	0
23	B	613	CLA	7	0
23	B	614	CLA	7	0
23	B	615	CLA	6	0
23	B	616	CLA	8	0
25	B	617	BCR	3	0
25	B	618	BCR	6	0
25	B	619	BCR	3	0
26	B	620	SQD	2	0
33	B	621	LMG	1	0
34	B	622	HTG	5	0
34	B	623	HTG	1	0
27	B	625	GOL	1	0
27	B	626	GOL	1	0
35	B	629	LMT	1	0
35	B	630	LMT	3	0
33	C	501	LMG	7	0
23	C	502	CLA	7	0
23	C	503	CLA	4	0
23	C	504	CLA	7	0
23	C	505	CLA	7	0
23	C	506	CLA	14	0
23	C	507	CLA	13	0
23	C	508	CLA	13	0
23	C	509	CLA	8	0
23	C	510	CLA	6	0
23	C	511	CLA	4	0
23	C	512	CLA	8	0
23	C	513	CLA	9	0
23	C	514	CLA	7	0
25	C	515	BCR	5	0
25	C	516	BCR	3	0
36	C	517	DGD	8	0
36	C	518	DGD	5	0
36	C	519	DGD	1	0
33	C	520	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	521	HTG	1	0
34	C	522	HTG	1	0
27	C	523	GOL	1	0
24	D	401	PHO	1	0
35	D	402	LMT	1	0
35	D	403	LMT	2	0
23	D	404	CLA	8	0
25	D	406	BCR	2	0
29	D	407	PL9	3	0
31	D	408	LHG	3	0
31	D	409	LHG	11	0
26	D	413	SQD	1	0
31	E	101	LHG	3	0
35	E	102	LMT	1	0
38	E	103	HEM	5	0
25	H	101	BCR	7	0
36	H	102	DGD	1	0
35	I	101	LMT	1	0
33	J	101	LMG	4	0
25	K	102	BCR	1	0
26	L	101	SQD	5	0
35	M	101	LMT	2	0
35	M	103	LMT	1	0
25	T	101	BCR	6	0
25	Y	101	BCR	2	0
33	Z	101	LMG	3	0
33	Z	102	LMG	1	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	9 (2%) 55 58	21, 31, 53, 100	0
1	a	334/344 (97%)	0.09	11 (3%) 47 50	23, 33, 62, 108	0
2	B	504/505 (99%)	0.21	50 (9%) 8 7	21, 36, 65, 109	0
2	b	504/505 (99%)	0.35	58 (11%) 5 5	23, 37, 74, 118	0
3	C	451/455 (99%)	0.51	64 (14%) 3 2	26, 45, 67, 117	0
3	c	455/455 (100%)	0.31	49 (10%) 6 6	30, 48, 69, 109	0
4	D	342/342 (100%)	-0.04	7 (2%) 65 67	21, 32, 53, 108	0
4	d	341/342 (99%)	0.22	25 (7%) 16 16	23, 36, 54, 123	0
5	E	81/84 (96%)	0.22	7 (8%) 11 11	37, 54, 82, 120	0
5	e	79/84 (94%)	1.06	19 (24%) 1 0	42, 58, 97, 120	0
6	F	34/44 (77%)	-0.22	0 100 100	38, 46, 78, 92	0
6	f	31/44 (70%)	-0.19	4 (12%) 4 3	44, 50, 86, 122	0
7	H	64/65 (98%)	0.25	5 (7%) 14 14	34, 47, 68, 101	0
7	h	65/65 (100%)	1.09	16 (24%) 1 0	37, 51, 74, 141	0
8	I	37/38 (97%)	0.42	7 (18%) 1 1	37, 46, 88, 130	0
8	i	37/38 (97%)	0.21	4 (10%) 6 6	38, 46, 93, 135	0
9	J	38/39 (97%)	0.20	5 (13%) 4 3	32, 52, 106, 147	0
9	j	39/39 (100%)	0.77	9 (23%) 1 0	40, 51, 107, 129	0
10	K	37/37 (100%)	0.00	3 (8%) 13 12	44, 53, 76, 91	0
10	k	37/37 (100%)	0.29	2 (5%) 26 27	47, 54, 78, 93	0
11	L	36/37 (97%)	0.59	7 (19%) 1 1	20, 26, 89, 129	0
11	l	36/37 (97%)	0.23	3 (8%) 12 12	22, 28, 87, 128	0
12	M	32/36 (88%)	-0.03	1 (3%) 49 52	22, 29, 49, 117	0
12	m	33/36 (91%)	-0.23	3 (9%) 10 10	24, 29, 72, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	0.25	28 (11%) 5 5	22, 45, 100, 157	0
13	o	243/244 (99%)	0.62	52 (21%) 1 1	24, 46, 99, 144	0
14	T	29/32 (90%)	0.21	0 100 100	23, 28, 60, 96	0
14	t	29/32 (90%)	-0.15	0 100 100	23, 29, 61, 97	0
15	U	96/104 (92%)	0.47	14 (14%) 3 2	31, 40, 66, 84	0
15	u	97/104 (93%)	-0.17	5 (5%) 28 29	32, 43, 68, 101	0
16	V	137/137 (100%)	0.08	3 (2%) 62 64	29, 43, 70, 100	0
16	v	137/137 (100%)	0.46	21 (15%) 2 2	34, 50, 74, 101	0
17	X	38/40 (95%)	0.20	4 (10%) 7 6	44, 56, 82, 110	0
17	x	38/40 (95%)	1.15	9 (23%) 1 0	47, 58, 83, 112	0
18	Y	29/30 (96%)	1.76	12 (41%) 0 0	56, 71, 112, 114	0
18	y	29/30 (96%)	0.95	5 (17%) 2 1	58, 70, 110, 114	0
19	Z	62/62 (100%)	1.08	14 (22%) 1 1	57, 72, 117, 152	0
19	z	62/62 (100%)	1.30	16 (25%) 1 0	60, 74, 117, 153	0
20	R	34/34 (100%)	6.09	34 (100%) 0 0	89, 108, 128, 135	0
All	All	5284/5384 (98%)	0.34	585 (11%) 6 5	20, 41, 82, 157	0

All (585) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	18	TRP	10.4
20	R	35	LEU	9.2
20	R	19	ALA	8.8
20	R	20	VAL	8.7
9	J	5	GLY	8.7
17	x	38	GLN	8.6
20	R	23	ILE	8.4
20	R	6	LEU	8.3
20	R	14	LEU	8.2
2	b	495	PHE	8.1
1	A	11	ALA	7.7
20	R	15	ALA	7.5
7	h	66	GLY	7.5
9	j	3	GLU	7.3
20	R	8	VAL	7.1
9	j	2	SER	7.0
8	I	38	GLU	6.9

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Mol	Chain	Res	Type	RSRZ
20	R	5	VAL	6.8
20	R	13	LEU	6.7
20	R	31	VAL	6.6
20	R	16	ALA	6.6
20	R	3	TRP	6.5
9	j	5	GLY	6.5
20	R	17	GLY	6.4
2	b	487	SER	6.4
13	o	27	ARG	6.3
17	x	37	VAL	6.2
2	b	218	LEU	6.2
20	R	24	LEU	6.1
2	b	494	GLY	6.0
20	R	7	VAL	5.9
20	R	22	ASN	5.9
20	R	34	LEU	5.9
20	R	4	ARG	5.9
2	b	493	TRP	5.9
18	Y	19	ILE	5.8
3	C	437	PHE	5.7
1	A	13	LEU	5.7
13	o	142	PHE	5.7
19	Z	32	ASP	5.7
2	b	491	VAL	5.6
19	z	1	MET	5.6
3	C	253	LEU	5.6
20	R	21	ARG	5.6
18	y	19	ILE	5.5
2	b	486	LEU	5.4
20	R	11	PRO	5.4
3	C	181	PHE	5.4
8	I	37	LEU	5.3
20	R	10	LEU	5.3
13	o	4	THR	5.3
2	b	504	THR	5.3
2	b	497	GLN	5.2
2	B	496	TYR	5.2
2	b	492	GLU	5.2
19	z	7	LEU	5.2
17	x	34	ILE	5.2
3	C	60	ILE	5.2
7	h	6	TRP	5.1

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Mol	Chain	Res	Type	RSRZ
20	R	33	LYS	5.1
17	x	36	LYS	5.1
8	i	37	LEU	5.1
19	z	3	ILE	5.0
4	D	238	THR	5.0
7	h	65	LEU	5.0
17	x	33	GLN	5.0
2	b	488	PRO	4.9
13	o	22	LEU	4.9
19	Z	31	GLN	4.9
20	R	26	TYR	4.9
3	C	276	LEU	4.9
19	z	4	LEU	4.9
2	B	495	PHE	4.9
3	C	433	LEU	4.8
19	Z	33	TRP	4.8
3	c	143	TYR	4.8
11	l	3	PRO	4.8
2	b	499	VAL	4.8
20	R	27	ALA	4.8
5	E	84	LYS	4.8
2	b	161	LEU	4.7
17	x	3	ILE	4.7
4	d	12	ARG	4.7
20	R	12	VAL	4.7
3	C	23	ALA	4.7
19	z	57	LEU	4.7
13	o	36	GLN	4.7
19	z	61	VAL	4.6
3	C	279	LEU	4.6
4	d	17	ILE	4.6
13	o	243	ILE	4.6
13	o	32	ILE	4.6
17	x	2	THR	4.5
3	C	143	TYR	4.5
20	R	2	ASP	4.5
18	Y	18	VAL	4.5
13	o	211	ILE	4.5
20	R	32	GLN	4.5
13	o	26	ALA	4.4
2	B	494	GLY	4.4
1	A	12	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
18	Y	46	LEU	4.4
3	c	200	THR	4.4
2	b	496	TYR	4.3
2	b	489	GLU	4.3
7	h	22	ALA	4.3
19	Z	30	PRO	4.3
3	c	60	ILE	4.3
3	c	20	SER	4.3
3	C	281	MET	4.3
13	o	38	TYR	4.3
9	j	7	ILE	4.2
11	L	2	GLU	4.2
19	Z	34	ASP	4.2
9	j	1	MET	4.2
11	L	7	ARG	4.2
13	O	27	ARG	4.2
3	C	283	GLY	4.2
19	z	5	PHE	4.1
2	b	295	GLY	4.1
2	B	461	LEU	4.1
1	A	15	GLU	4.1
2	B	489	GLU	4.1
3	C	282	MET	4.1
20	R	28	VAL	4.1
3	c	146	PHE	4.1
3	C	198	VAL	4.0
3	C	155	ASN	4.0
15	U	62	LEU	4.0
19	z	2	THR	4.0
15	U	58	VAL	4.0
2	b	502	VAL	4.0
4	d	154	VAL	4.0
3	c	426	LEU	3.9
4	D	12	ARG	3.9
3	C	280	SER	3.9
3	C	285	ILE	3.9
2	b	484	PRO	3.9
2	B	251	VAL	3.9
19	z	60	PHE	3.9
13	o	246	ALA	3.9
2	B	505	ARG	3.9
19	z	62	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	b	298	LEU	3.9
2	b	293	ALA	3.8
17	x	39	ARG	3.8
3	c	140	LEU	3.8
8	I	36	ASP	3.8
13	o	57	LYS	3.8
13	o	87	VAL	3.8
3	C	438	LEU	3.8
7	h	12	ARG	3.8
3	C	61	VAL	3.8
20	R	9	LEU	3.8
3	C	284	PHE	3.8
3	C	434	ALA	3.7
3	c	199	ILE	3.7
13	o	39	ARG	3.7
18	Y	43	ARG	3.7
13	o	85	LEU	3.7
12	m	33	GLN	3.7
16	v	21	LEU	3.7
2	b	503	THR	3.7
13	o	133	VAL	3.7
2	B	454	ALA	3.7
3	c	279	LEU	3.6
15	U	70	ARG	3.6
2	B	488	PRO	3.6
18	y	41	VAL	3.6
3	C	180	MET	3.6
13	o	60	ARG	3.6
2	B	296	ALA	3.6
5	e	20	TRP	3.6
2	b	249	ALA	3.6
16	v	17	LYS	3.6
5	e	79	PHE	3.6
3	c	433	LEU	3.6
1	a	11	ALA	3.6
3	C	432	VAL	3.6
2	B	298	LEU	3.5
2	b	246	PHE	3.5
18	Y	21	GLN	3.5
2	B	253	ALA	3.5
2	b	248	ALA	3.5
2	b	296	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	C	262	ARG	3.5
4	d	148	ALA	3.5
13	o	35	SER	3.5
13	o	134	THR	3.5
3	C	430	HIS	3.5
2	B	462	PHE	3.5
3	c	63	TRP	3.5
13	O	25	THR	3.5
3	c	430	HIS	3.5
3	C	147	PHE	3.5
11	L	9	PRO	3.5
15	U	79	LEU	3.5
13	o	25	THR	3.4
3	c	427	ALA	3.4
8	i	38	GLU	3.4
13	o	37	THR	3.4
3	C	59	LEU	3.4
2	b	498	LYS	3.4
5	E	15	THR	3.4
12	m	34	LYS	3.4
3	C	436	PHE	3.4
13	O	93	LEU	3.4
7	h	64	ALA	3.4
3	c	22	PHE	3.3
4	D	11	GLU	3.3
1	A	16	ARG	3.3
13	O	62	GLU	3.3
2	B	458	PHE	3.3
2	B	252	VAL	3.3
3	c	191	PRO	3.3
5	e	83	LEU	3.3
16	v	4	THR	3.3
2	B	161	LEU	3.3
10	k	17	ILE	3.3
18	Y	45	ASN	3.3
7	H	6	TRP	3.3
2	b	292	LEU	3.3
2	B	250	PHE	3.3
3	C	255	THR	3.3
3	c	155	ASN	3.3
2	b	245	VAL	3.3
11	L	10	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	b	123	PHE	3.2
17	X	2	THR	3.2
4	d	155	SER	3.2
15	U	73	GLN	3.2
19	Z	36	SER	3.2
2	b	244	ALA	3.2
10	k	18	PHE	3.2
3	C	57	ALA	3.2
1	a	265	PHE	3.2
6	f	15	ILE	3.2
13	O	24	ASP	3.2
3	C	146	PHE	3.2
2	b	505	ARG	3.2
3	C	429	SER	3.2
13	O	144	GLY	3.2
16	v	5	PRO	3.2
2	b	288	VAL	3.2
16	v	107	LEU	3.2
13	o	24	ASP	3.2
13	o	33	ASP	3.2
2	B	457	VAL	3.2
3	C	439	VAL	3.2
4	d	152	VAL	3.2
3	C	145[A]	SER	3.1
3	C	254	THR	3.1
3	C	286	ALA	3.1
20	R	30	GLN	3.1
9	j	4	GLY	3.1
3	c	284	PHE	3.1
9	J	6	ARG	3.1
15	U	59	GLU	3.1
5	E	17	VAL	3.1
13	O	133	VAL	3.1
3	C	275	SER	3.1
11	l	2	GLU	3.1
13	O	5	LEU	3.1
3	C	201	ASN	3.1
13	o	209	GLY	3.1
4	d	149	PRO	3.1
2	B	504	THR	3.1
5	E	83	LEU	3.1
18	Y	20	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
11	L	8	GLN	3.0
18	y	37	PHE	3.0
15	U	104	LYS	3.0
4	d	13	GLY	3.0
3	c	280	SER	3.0
18	Y	22	LEU	3.0
4	d	150	ILE	3.0
17	X	3	ILE	3.0
2	b	412	THR	3.0
3	C	63	TRP	3.0
3	C	278	ALA	3.0
19	z	6	GLN	3.0
1	a	262	TYR	3.0
2	b	294	SER	3.0
15	U	74	ILE	3.0
13	O	139	SER	3.0
3	c	283	GLY	3.0
3	C	200	THR	3.0
9	j	9	LEU	3.0
3	c	198	VAL	2.9
4	d	156	VAL	2.9
2	b	462	PHE	2.9
4	d	159	ILE	2.9
5	e	25	ILE	2.9
19	Z	35	ARG	2.9
2	b	250	PHE	2.9
2	b	490	GLN	2.9
2	B	290	ALA	2.9
7	H	2	ALA	2.9
2	B	487	SER	2.9
3	c	87	ILE	2.9
2	B	459	ALA	2.9
13	o	212	ALA	2.9
2	b	457	VAL	2.9
8	I	34	ARG	2.9
16	V	135	VAL	2.9
3	C	204	LEU	2.9
5	e	36	LEU	2.9
13	o	199	LEU	2.9
6	f	42	PHE	2.9
9	J	4	GLY	2.9
5	e	59	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	435	PHE	2.9
7	h	10	ILE	2.9
13	O	22	LEU	2.9
16	v	95	LEU	2.9
3	c	201	ASN	2.8
13	o	58	ASN	2.8
3	c	202	PRO	2.8
13	O	29	ALA	2.8
18	Y	40	ALA	2.8
2	B	490	GLN	2.8
4	D	150	ILE	2.8
4	d	157	PHE	2.8
16	v	16	GLY	2.8
2	B	491	VAL	2.8
15	U	103	TYR	2.8
2	B	451	PHE	2.8
9	J	3	GLU	2.8
19	Z	28	ALA	2.8
13	O	28	GLY	2.8
13	o	204	VAL	2.8
2	b	290	ALA	2.8
5	e	15	THR	2.8
13	o	5	LEU	2.8
16	v	110	LYS	2.8
16	v	1	ALA	2.8
4	d	147	SER	2.8
3	c	196	VAL	2.8
13	o	245	PRO	2.8
1	a	224	ILE	2.8
3	c	64	ALA	2.8
8	I	6	ILE	2.8
2	B	460	LEU	2.8
13	O	91	GLY	2.7
13	o	30	TYR	2.7
2	B	249	ALA	2.7
3	C	252	ILE	2.7
13	O	26	ALA	2.7
2	b	247	PHE	2.7
9	J	7	ILE	2.7
19	Z	29	SER	2.7
5	e	24	SER	2.7
16	v	19	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
15	U	99	ASN	2.7
2	B	502	VAL	2.7
3	c	61	VAL	2.7
3	c	203	THR	2.7
16	v	12	LEU	2.7
3	C	196	VAL	2.7
3	c	429	SER	2.7
13	o	140	THR	2.7
1	a	225	ARG	2.7
2	B	294	SER	2.6
7	h	58	VAL	2.6
5	e	14	ILE	2.6
2	b	501	ASP	2.6
13	O	204	VAL	2.6
2	b	500	GLY	2.6
5	e	42	LEU	2.6
4	d	153	PHE	2.6
13	o	136	ILE	2.6
13	O	135	SER	2.6
13	o	34	SER	2.6
2	B	297	THR	2.6
19	z	59	PHE	2.6
9	j	6	ARG	2.6
13	o	59	LYS	2.6
2	B	248	ALA	2.6
16	v	10	VAL	2.6
19	z	56	VAL	2.6
3	c	257	PHE	2.6
20	R	25	PRO	2.6
15	u	103	TYR	2.6
16	v	106	ASN	2.6
20	R	29	LYS	2.6
3	C	56	HIS	2.6
7	h	8	GLY	2.6
16	v	26	TYR	2.6
7	h	9	ASP	2.6
3	c	255	THR	2.6
13	o	98	GLU	2.6
2	B	247	PHE	2.6
17	X	34	ILE	2.6
2	b	289	GLN	2.6
3	C	440	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
3	c	144	SER	2.6
1	a	13	LEU	2.5
19	z	9	LEU	2.5
3	C	182	PHE	2.5
1	A	14	TRP	2.5
4	d	151	ALA	2.5
13	o	93	LEU	2.5
18	Y	42	ARG	2.5
4	d	123	ILE	2.5
13	o	86	LYS	2.5
3	c	141	GLU	2.5
7	h	57	GLY	2.5
13	O	207	ARG	2.5
1	a	15	GLU	2.5
3	C	431	PHE	2.5
2	b	413	ASP	2.5
2	b	414	PRO	2.5
2	B	292	LEU	2.5
19	Z	62	VAL	2.5
7	h	13	PRO	2.5
3	C	277	GLY	2.5
13	o	207	ARG	2.4
15	u	9	LEU	2.4
19	z	46	LEU	2.4
13	O	30	TYR	2.4
5	e	22	ILE	2.4
2	b	485	GLU	2.4
3	C	148	GLY	2.4
7	h	23	PRO	2.4
17	x	8	LYS	2.4
18	y	43	ARG	2.4
19	Z	39	LEU	2.4
3	C	135	ARG	2.4
4	D	122	LEU	2.4
3	C	199	ILE	2.4
4	d	119	ALA	2.4
2	B	241	SER	2.4
15	U	57	SER	2.4
18	Y	38	LEU	2.4
15	U	76	ARG	2.4
2	b	482	ILE	2.4
13	o	95	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
5	e	39	SER	2.4
2	B	245	VAL	2.4
5	e	21	VAL	2.4
12	M	33	GLN	2.4
15	u	66	GLY	2.4
13	o	40	ILE	2.4
13	o	241	ALA	2.4
13	o	198	SER	2.4
18	Y	25	ILE	2.4
5	e	57	ALA	2.4
5	E	74	GLN	2.4
16	v	25	GLN	2.4
1	A	19	ASN	2.3
6	f	43	ILE	2.3
19	Z	27	TYR	2.3
12	m	31	SER	2.3
13	O	138	THR	2.3
16	V	12	LEU	2.3
2	b	252	VAL	2.3
10	K	29	PRO	2.3
2	b	458	PHE	2.3
3	c	437	PHE	2.3
19	Z	60	PHE	2.3
4	d	68	LEU	2.3
3	c	425	TRP	2.3
2	b	126	PRO	2.3
11	l	5	PRO	2.3
13	O	131	PRO	2.3
3	C	154	LYS	2.3
13	o	203	LYS	2.3
3	C	25	ASN	2.3
2	B	242	ILE	2.3
4	D	123	ILE	2.3
2	B	295	GLY	2.3
5	e	17	VAL	2.3
5	e	7	GLU	2.3
15	u	101	GLY	2.3
13	o	141	ASP	2.3
7	H	46	LEU	2.3
3	c	192	GLY	2.3
13	O	130	GLN	2.3
3	C	287	THR	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	149	TYR	2.3
16	v	8	LEU	2.3
2	b	251	VAL	2.2
13	o	91	GLY	2.2
13	o	226	GLY	2.2
2	B	501	ASP	2.2
4	d	14	TRP	2.2
2	B	85	GLY	2.2
2	B	219	VAL	2.2
1	a	16	ARG	2.2
2	b	238	LEU	2.2
3	C	272	LEU	2.2
3	c	204	LEU	2.2
3	c	195	ASP	2.2
3	c	282	MET	2.2
16	v	135	VAL	2.2
3	c	260	ALA	2.2
10	K	14	ALA	2.2
11	L	4	ASN	2.2
2	b	459	ALA	2.2
4	d	283	ALA	2.2
13	o	138	THR	2.2
4	d	37	LEU	2.2
7	H	43	LEU	2.2
3	c	452	ALA	2.2
2	b	217	ILE	2.2
3	C	58	GLY	2.2
1	a	121[A]	LEU	2.2
3	c	59	LEU	2.2
5	e	38	VAL	2.1
13	O	63	ALA	2.1
16	v	22	THR	2.1
19	Z	3	ILE	2.1
4	D	149	PRO	2.1
6	f	16	PHE	2.1
16	v	79	PRO	2.1
19	z	38	GLN	2.1
11	L	6	ASN	2.1
1	A	152	ALA	2.1
2	B	456	ALA	2.1
3	c	24	THR	2.1
3	c	259	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
10	K	28	ILE	2.1
2	b	162	PHE	2.1
5	E	11	SER	2.1
3	c	197	ARG	2.1
7	h	56	ASP	2.1
1	a	266	ASN	2.1
8	i	2	GLU	2.1
8	I	26	GLY	2.1
13	O	134	THR	2.1
16	v	18	THR	2.1
3	C	455	PHE	2.1
7	H	42	LEU	2.1
13	O	15	LEU	2.1
5	e	77	GLU	2.1
13	O	143	LYS	2.1
4	d	126	MET	2.1
1	A	249	VAL	2.1
1	a	285	PHE	2.1
3	C	257	PHE	2.1
3	c	253	LEU	2.1
7	h	3	ARG	2.1
7	h	42	LEU	2.1
18	y	22	LEU	2.1
5	e	82	GLN	2.1
2	B	304	ALA	2.1
8	I	29	ALA	2.1
3	C	340	TYR	2.1
2	B	162	PHE	2.1
2	B	214	LEU	2.1
15	U	9	LEU	2.1
13	O	87	VAL	2.1
17	X	37	VAL	2.1
3	c	21	ILE	2.1
2	B	246	PHE	2.1
2	B	411	PHE	2.1
3	C	426	LEU	2.1
2	B	293	ALA	2.0
2	b	297	THR	2.0
9	j	12	VAL	2.0
15	u	79	LEU	2.0
5	E	73	LYS	2.0
3	C	64	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
4	d	158	LEU	2.0
4	d	279	LEU	2.0
8	i	6	ILE	2.0
15	U	101	GLY	2.0
4	d	146	PHE	2.0
13	o	23	ASP	2.0
2	b	121	GLU	2.0
13	o	84	GLU	2.0
2	B	455	HIS	2.0
13	O	4	THR	2.0
2	b	124	ARG	2.0
3	C	261	ARG	2.0
13	O	60	ARG	2.0
13	o	83	GLY	2.0
13	o	184	ARG	2.0
16	v	96	ARG	2.0
2	B	86	ILE	2.0
2	B	463	PHE	2.0
3	c	147	PHE	2.0
16	V	137	TYR	2.0
3	c	67	MET	2.0
3	c	281	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
12	FME	M	1	10/11	0.97	0.15	-	18,38,70,79	0
14	FME	T	1	10/11	0.98	0.09	-	18,32,46,47	0
8	FME	I	1	10/11	0.98	0.22	-	31,47,56,62	0
8	FME	i	1	10/11	0.97	0.09	-	37,49,57,62	0
14	FME	t	1	10/11	0.98	0.10	-	21,32,41,71	0
12	FME	m	1	10/11	0.96	0.11	-	30,42,63,78	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
27	GOL	d	402	6/6	0.80	0.60	20.72	33,50,65,68	0
34	HTG	b	622	19/19	0.76	0.89	15.38	74,95,125,130	0
30	UNL	i	101	40/-	0.70	0.42	13.74	48,88,140,147	0
30	UNL	J	102	10/-	0.71	0.39	10.13	55,64,89,90	0
35	LMT	D	402	35/35	0.65	0.37	9.47	31,97,113,115	0
34	HTG	V	203	11/19	0.82	0.56	9.01	71,92,107,108	0
35	LMT	B	630	35/35	0.55	0.46	8.54	33,105,126,134	0
35	LMT	E	102	35/35	0.72	0.55	7.55	78,120,147,150	0
35	LMT	M	103	35/35	0.68	0.34	7.10	40,120,148,154	0
30	UNL	j	102	10/-	0.74	0.29	6.91	60,75,88,89	0
34	HTG	c	522	19/19	0.74	0.85	6.47	79,124,142,146	0
35	LMT	e	102	35/35	0.67	0.79	6.36	76,134,147,156	0
29	PL9	A	414	55/55	0.71	0.40	6.31	41,88,105,119	0
34	HTG	D	412	16/19	0.54	0.43	5.45	48,115,128,130	0
34	HTG	b	623	19/19	0.62	0.66	5.23	71,109,141,169	0
27	GOL	B	625	6/6	0.95	0.29	5.22	48,76,85,89	0
34	HTG	B	623	19/19	0.76	0.41	5.21	60,84,110,115	0
30	UNL	D	411	40/-	0.83	0.24	5.19	40,77,117,122	0
34	HTG	C	522	19/19	0.68	0.91	5.19	58,139,157,179	0
27	GOL	B	626	6/6	0.86	0.31	4.97	38,51,55,62	0
34	HTG	b	628	19/19	0.85	0.25	4.41	34,65,115,119	0
35	LMT	a	417	35/35	0.84	0.55	4.29	78,114,130,131	0
30	UNL	D	410	17/-	0.93	0.28	4.13	44,56,91,100	0
30	UNL	K	101	34/-	0.71	0.35	4.09	55,96,114,125	0
27	GOL	a	411	6/6	0.91	0.20	4.08	52,60,62,66	0
27	GOL	A	411	6/6	0.97	0.12	4.01	50,58,65,79	0
30	UNL	I	102	40/-	0.73	0.31	3.93	40,85,135,142	0
29	PL9	a	414	55/55	0.66	0.41	3.40	57,93,112,120	0
35	LMT	I	101	35/35	0.58	0.65	2.93	74,108,131,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	LMG	Z	101	51/55	0.59	0.43	2.85	46,105,140,150	0
35	LMT	B	631	26/35	0.90	0.18	2.79	52,80,105,109	0
31	LHG	e	101	42/49	0.72	0.42	2.73	81,118,142,148	0
35	LMT	b	627	25/35	0.83	0.25	2.65	29,61,134,139	0
30	UNL	b	629	36/-	0.81	0.29	2.65	49,80,131,138	0
30	UNL	x	101	18/-	0.82	0.29	2.43	44,63,91,92	0
33	LMG	z	101	39/55	0.88	0.25	2.34	63,112,140,147	0
31	LHG	E	101	42/49	0.80	0.27	2.34	41,93,108,124	0
30	UNL	X	101	18/-	0.91	0.19	2.05	40,53,83,90	0
34	HTG	B	622	19/19	0.92	0.21	2.02	34,61,127,132	0
30	UNL	d	410	17/-	0.95	0.29	1.99	42,57,85,90	0
35	LMT	m	102	35/35	0.69	0.47	1.93	34,78,102,109	0
31	LHG	A	416	49/49	0.92	0.32	1.85	26,44,61,77	0
33	LMG	Z	102	37/55	0.74	0.38	1.75	47,97,129,137	0
23	CLA	c	503	65/65	0.94	0.41	1.72	40,51,63,78	0
23	CLA	B	601	65/65	0.94	0.23	1.71	39,57,88,119	0
35	LMT	B	629	25/35	0.84	0.24	1.65	34,68,124,125	0
33	LMG	c	520	51/55	0.70	0.36	1.63	51,102,132,138	0
26	SQD	L	101	54/54	0.77	0.27	1.61	47,71,116,121	0
31	LHG	D	408	49/49	0.96	0.23	1.59	22,34,51,68	0
26	SQD	f	101	43/54	0.77	0.36	1.56	85,111,157,164	0
23	CLA	b	601	65/65	0.93	0.24	1.54	43,69,99,126	0
29	PL9	D	407	55/55	0.95	0.23	1.54	20,31,45,54	0
31	LHG	d	408	49/49	0.93	0.22	1.54	24,35,53,70	0
23	CLA	c	502	65/65	0.91	0.41	1.51	37,48,68,73	0
35	LMT	M	101	35/35	0.70	0.35	1.47	39,80,103,109	0
35	LMT	D	403	35/35	0.81	0.32	1.38	48,91,116,117	0
25	BCR	t	101	40/40	0.96	0.23	1.32	19,42,59,62	0
24	PHO	a	406	64/64	0.98	0.20	1.31	22,31,40,51	0
29	PL9	d	406	55/55	0.94	0.19	1.28	23,30,41,58	0
26	SQD	a	412	54/54	0.88	0.22	1.27	44,73,125,133	0
31	LHG	A	417	49/49	0.94	0.24	1.27	23,37,55,66	0
23	CLA	B	610	65/65	0.97	0.22	1.13	27,36,52,69	0
33	LMG	c	519	51/55	0.88	0.27	1.12	43,77,114,124	0
25	BCR	T	101	40/40	0.96	0.22	1.11	20,36,45,53	0
27	GOL	C	523	6/6	0.93	0.24	1.10	44,54,59,60	0
31	LHG	d	409	49/49	0.94	0.20	1.10	33,50,98,110	0
26	SQD	A	412	54/54	0.89	0.21	1.08	39,65,102,118	0
23	CLA	B	605	65/65	0.96	0.20	1.07	22,30,44,48	0
33	LMG	C	501	51/55	0.83	0.28	1.02	35,74,98,102	0
23	CLA	c	501	65/65	0.95	0.23	1.01	38,49,64,71	0
25	BCR	B	618	40/40	0.97	0.23	1.01	21,36,54,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	DGD	C	519	62/66	0.93	0.17	0.98	28,44,71,95	0
36	DGD	c	516	62/66	0.95	0.23	0.95	33,43,73,95	0
25	BCR	d	405	40/40	0.93	0.16	0.93	40,50,74,81	0
25	BCR	C	516	40/40	0.93	0.21	0.91	36,48,66,73	0
33	LMG	J	101	51/55	0.92	0.18	0.89	30,51,88,99	0
31	LHG	l	101	49/49	0.92	0.17	0.88	25,38,55,60	0
23	CLA	b	604	65/65	0.95	0.31	0.88	23,31,85,96	0
23	CLA	b	605	65/65	0.96	0.23	0.85	24,34,52,97	0
24	PHO	a	407	64/64	0.97	0.26	0.85	28,35,50,52	0
31	LHG	d	407	49/49	0.96	0.20	0.85	25,44,72,87	0
23	CLA	B	603	65/65	0.97	0.26	0.84	26,39,52,57	0
36	DGD	c	518	62/66	0.95	0.19	0.81	36,46,77,96	0
34	HTG	d	411	16/19	0.78	0.37	0.81	81,112,121,122	0
36	DGD	h	102	62/66	0.89	0.27	0.79	31,46,62,73	0
31	LHG	D	409	49/49	0.95	0.19	0.79	29,47,107,124	0
23	CLA	C	511	65/65	0.95	0.42	0.79	33,44,57,61	0
23	CLA	a	408	65/65	0.95	0.19	0.78	28,40,107,115	0
23	CLA	C	506	65/65	0.96	0.26	0.78	31,40,71,78	0
26	SQD	D	413	43/54	0.91	0.27	0.76	64,97,112,116	0
33	LMG	j	101	51/55	0.93	0.18	0.75	37,53,102,123	0
24	PHO	D	401	64/64	0.98	0.18	0.74	21,27,35,45	0
23	CLA	D	405	65/65	0.93	0.19	0.73	31,46,99,111	0
25	BCR	H	101	40/40	0.84	0.23	0.72	33,42,63,67	0
23	CLA	c	511	65/65	0.92	0.21	0.70	43,56,74,82	0
23	CLA	c	508	65/65	0.93	0.19	0.70	35,48,107,118	0
23	CLA	c	509	65/65	0.91	0.24	0.68	43,52,66,73	0
36	DGD	c	517	62/66	0.92	0.22	0.67	38,53,112,129	0
26	SQD	a	410	54/54	0.93	0.18	0.65	41,64,98,105	0
33	LMG	a	416	51/55	0.85	0.25	0.64	41,77,102,118	0
23	CLA	C	513	65/65	0.84	0.27	0.64	43,59,94,101	0
23	CLA	b	608	65/65	0.97	0.28	0.63	32,41,60,68	0
23	CLA	B	612	65/65	0.95	0.23	0.63	24,29,42,51	0
23	CLA	C	509	65/65	0.94	0.29	0.61	30,43,102,115	0
23	CLA	A	408	65/65	0.97	0.14	0.61	26,36,101,109	0
36	DGD	C	517	62/66	0.93	0.23	0.61	27,36,81,92	0
23	CLA	C	503	65/65	0.93	0.35	0.61	31,42,55,73	0
25	BCR	B	619	40/40	0.94	0.15	0.59	28,42,63,67	0
22	CL	A	403	1/1	1.00	0.24	0.58	27,27,27,27	0
23	CLA	B	613	65/65	0.97	0.32	0.58	21,29,68,78	0
23	CLA	b	603	65/65	0.96	0.24	0.57	30,40,53,74	0
36	DGD	C	518	62/66	0.90	0.21	0.57	29,46,103,110	0
23	CLA	B	604	65/65	0.94	0.30	0.56	21,29,92,104	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	0.97	0.16	0.55	19,23,41,47	0
36	DGD	H	102	62/66	0.92	0.25	0.54	26,40,58,66	0
23	CLA	b	610	65/65	0.96	0.20	0.50	30,42,51,60	0
23	CLA	B	607	65/65	0.96	0.22	0.49	18,27,54,66	0
25	BCR	B	617	40/40	0.97	0.15	0.49	22,31,46,49	0
24	PHO	A	407	64/64	0.97	0.21	0.48	23,31,46,51	0
25	BCR	b	618	40/40	0.96	0.21	0.48	21,34,49,55	0
25	BCR	h	101	40/40	0.70	0.27	0.47	39,50,64,77	0
26	SQD	B	620	54/54	0.86	0.21	0.47	41,73,108,113	0
23	CLA	c	510	65/65	0.96	0.31	0.47	39,47,62,66	0
23	CLA	C	510	65/65	0.93	0.29	0.42	36,47,67,69	0
23	CLA	B	602	65/65	0.92	0.23	0.42	29,37,55,67	0
25	BCR	Y	101	40/40	0.94	0.15	0.41	37,49,59,62	0
33	LMG	C	520	51/55	0.83	0.28	0.41	37,69,104,121	0
23	CLA	B	611	65/65	0.94	0.24	0.39	23,30,41,45	0
25	BCR	D	406	40/40	0.94	0.17	0.39	32,42,87,90	0
23	CLA	c	504	65/65	0.95	0.27	0.39	37,50,89,111	0
33	LMG	b	620	51/55	0.90	0.19	0.39	29,50,88,106	0
23	CLA	b	607	65/65	0.96	0.17	0.37	20,31,53,63	0
23	CLA	c	505	65/65	0.94	0.20	0.36	32,45,68,86	0
23	CLA	a	405	65/65	0.97	0.22	0.35	27,36,105,111	0
34	HTG	B	627	19/19	0.91	0.17	0.35	45,63,74,75	0
23	CLA	b	612	65/65	0.94	0.23	0.34	25,35,48,59	0
23	CLA	B	608	65/65	0.97	0.23	0.32	27,37,51,55	0
23	CLA	b	602	65/65	0.92	0.23	0.31	32,44,60,68	0
25	BCR	A	409	40/40	0.97	0.15	0.29	22,34,46,49	0
25	BCR	b	619	40/40	0.94	0.15	0.28	32,45,61,69	0
33	LMG	B	621	51/55	0.88	0.21	0.28	32,49,79,105	0
39	MG	J	103	1/1	0.98	0.14	0.28	39,39,39,39	0
25	BCR	y	101	40/40	0.92	0.16	0.27	44,54,70,72	0
23	CLA	C	514	65/65	0.89	0.23	0.21	46,64,87,95	0
23	CLA	c	513	65/65	0.90	0.22	0.21	52,73,115,119	0
26	SQD	A	410	54/54	0.94	0.15	0.18	38,62,99,105	0
25	BCR	b	617	40/40	0.96	0.14	0.18	20,34,41,44	0
23	CLA	C	508	65/65	0.91	0.25	0.18	36,47,60,70	0
23	CLA	d	404	65/65	0.94	0.17	0.17	38,48,98,109	0
35	LMT	b	621	25/35	0.79	0.24	0.15	60,99,144,148	0
23	CLA	C	502	65/65	0.94	0.22	0.15	34,41,60,77	0
23	CLA	b	609	65/65	0.92	0.17	0.13	36,44,63,82	0
23	CLA	b	611	65/65	0.97	0.19	0.13	25,34,49,61	0
38	HEM	e	103	43/43	0.98	0.19	0.12	48,73,98,105	0
23	CLA	B	616	65/65	0.95	0.21	0.12	30,45,113,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	C	504	65/65	0.94	0.27	0.07	36,44,65,75	0
23	CLA	B	606	65/65	0.94	0.15	0.07	26,35,76,99	0
23	CLA	c	512	65/65	0.91	0.20	0.06	48,64,90,96	0
39	MG	j	103	1/1	0.96	0.15	0.05	51,51,51,51	0
23	CLA	A	404	65/65	0.96	0.17	0.04	20,23,41,58	0
23	CLA	d	403	65/65	0.97	0.22	0.04	25,29,49,62	0
27	GOL	b	624	6/6	0.94	0.13	0.03	58,76,78,86	0
25	BCR	c	515	40/40	0.96	0.14	0.03	37,52,65,75	0
25	BCR	K	102	40/40	0.94	0.17	0.02	39,47,62,65	0
23	CLA	D	404	65/65	0.96	0.17	-0.04	20,26,46,52	0
23	CLA	B	609	65/65	0.92	0.17	-0.05	29,39,53,63	0
23	CLA	B	614	65/65	0.92	0.18	-0.08	21,31,82,100	0
23	CLA	A	406	65/65	0.97	0.14	-0.09	22,29,80,89	0
23	CLA	b	613	65/65	0.97	0.23	-0.10	22,33,67,78	0
23	CLA	c	507	65/65	0.92	0.18	-0.12	41,53,65,68	0
23	CLA	c	506	65/65	0.96	0.14	-0.14	44,58,90,111	0
23	CLA	C	512	65/65	0.91	0.18	-0.15	36,52,73,84	0
23	CLA	d	401	65/65	0.97	0.15	-0.17	23,26,48,75	0
25	BCR	a	409	40/40	0.97	0.14	-0.17	24,35,45,49	0
23	CLA	b	606	65/65	0.95	0.14	-0.17	27,42,77,106	0
23	CLA	C	505	65/65	0.94	0.21	-0.20	30,41,79,104	0
23	CLA	b	614	65/65	0.95	0.14	-0.22	23,34,76,89	0
25	BCR	k	101	40/40	0.94	0.16	-0.28	47,55,79,81	0
38	HEM	v	201	43/43	0.98	0.13	-0.32	40,50,59,66	0
23	CLA	a	404	65/65	0.97	0.17	-0.39	25,30,50,60	0
37	CA	c	523	1/1	0.94	0.17	-0.40	68,68,68,68	0
23	CLA	b	615	65/65	0.93	0.17	-0.40	29,40,66,81	0
34	HTG	b	625	19/19	0.93	0.11	-0.42	43,56,83,93	0
23	CLA	C	507	65/65	0.93	0.15	-0.49	39,55,102,106	0
22	CL	a	403	1/1	0.98	0.19	-0.53	34,34,34,34	0
25	BCR	C	515	40/40	0.94	0.15	-0.54	46,61,72,73	0
32	BCT	a	418	4/4	0.99	0.10	-0.54	45,52,54,59	0
37	CA	C	524	1/1	0.98	0.24	-0.58	62,62,62,62	0
38	HEM	V	202	43/43	0.98	0.11	-0.59	30,33,44,53	0
23	CLA	B	615	65/65	0.95	0.14	-0.60	27,34,61,68	0
38	HEM	E	103	43/43	0.98	0.09	-0.71	40,54,66,73	0
23	CLA	b	616	65/65	0.92	0.18	-0.76	31,46,98,105	0
25	BCR	c	514	40/40	0.95	0.13	-0.84	52,65,76,79	0
32	BCT	A	418	4/4	0.99	0.08	-1.18	34,39,47,65	0
28	OEX	A	413	10/10	0.99	0.09	-1.60	22,30,43,45	0
37	CA	c	524	1/1	0.97	0.09	-1.85	66,66,66,66	0
22	CL	a	402	1/1	0.99	0.10	-1.95	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
28	OEX	a	413	10/10	1.00	0.09	-2.11	27,34,45,53	0
21	FE2	a	401	1/1	0.99	0.06	-2.13	45,45,45,45	0
37	CA	O	301	1/1	0.93	0.11	-2.28	87,87,87,87	0
22	CL	A	402	1/1	0.99	0.07	-2.64	24,24,24,24	0
37	CA	o	301	1/1	0.95	0.10	-3.41	85,85,85,85	0
21	FE2	A	401	1/1	0.99	0.04	-4.79	42,42,42,42	0
30	UNL	c	525	32/-	0.73	0.31	-	71,97,113,119	0
34	HTG	B	624	19/19	0.63	0.68	-	57,104,140,144	0
30	UNL	a	415	30/-	0.61	0.50	-	72,90,111,118	0
30	UNL	A	415	28/-	0.19	0.56	-	67,87,108,112	0
37	CA	V	201	1/1	0.93	0.14	-	93,93,93,93	0
30	UNL	m	101	10/-	0.75	0.30	-	40,50,55,56	0
30	UNL	B	628	33/-	0.68	0.28	-	29,76,136,139	0
30	UNL	b	626	33/-	0.58	0.43	-	44,78,131,135	0
34	HTG	c	521	19/19	0.78	0.36	-	68,112,134,140	0
30	UNL	M	102	10/-	0.85	0.26	-	33,52,59,69	0
34	HTG	C	521	19/19	0.78	0.41	-	66,101,116,120	0

6.5 Other polymers [i](#)

There are no such residues in this entry.