Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:40 PM GMT

PDB ID	:	4IL6
Title	:	Structure of Sr-substituted photosystem II
Authors	:	Koua, F.H.M.; Umena, Y.; Kawakami, K.; Kamiya, N.; Shen, J.R.
Deposited on	:	2012-12-29
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

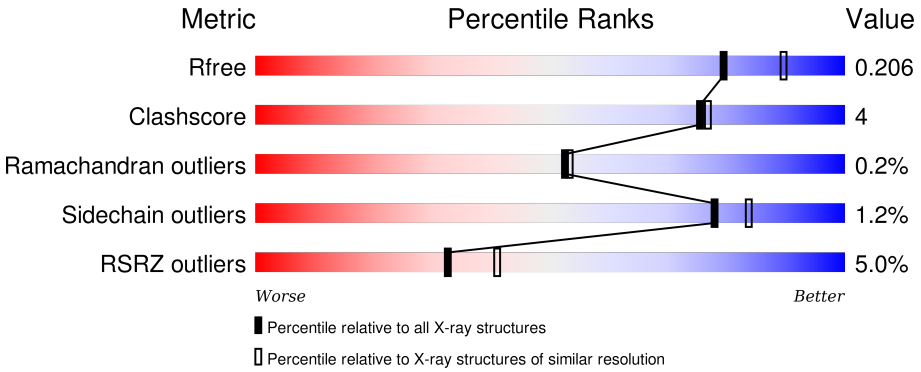
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	334	90% 10%
1	a	334	99%
2	B	505	3% 90% 10%
2	b	505	5% 98%
3	C	451	87% 13%

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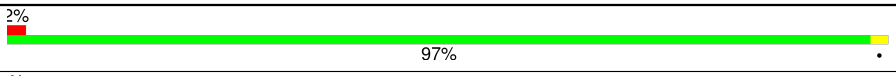
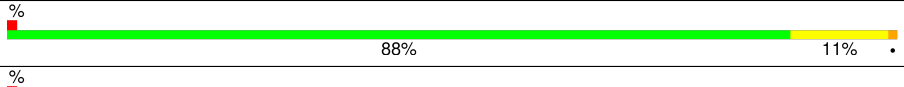
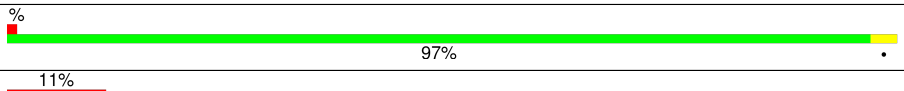
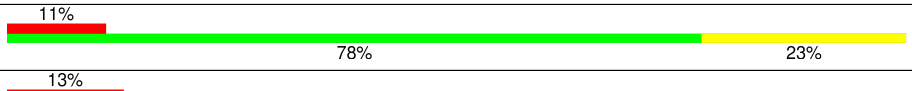
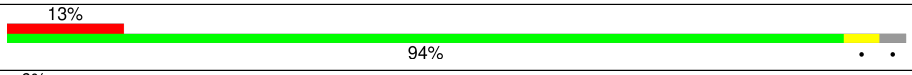
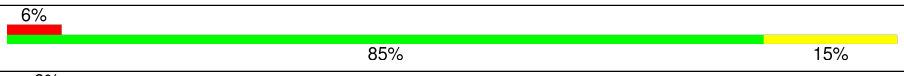
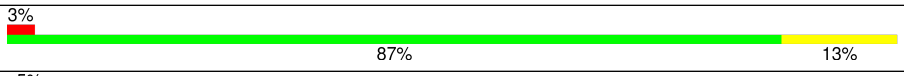
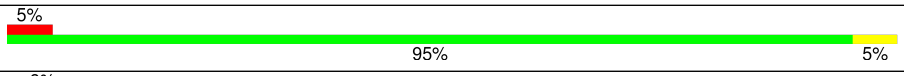
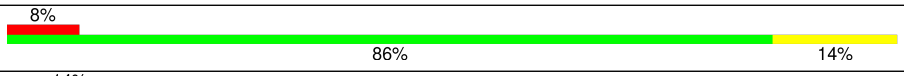
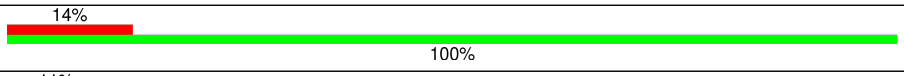
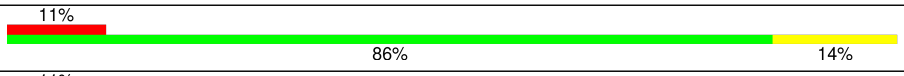
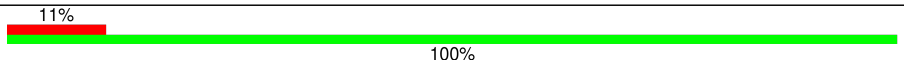
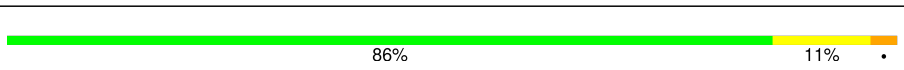
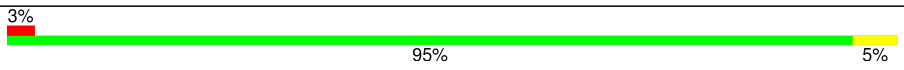
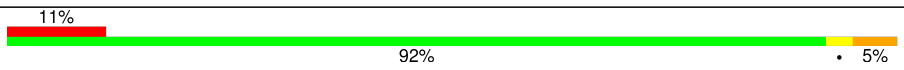
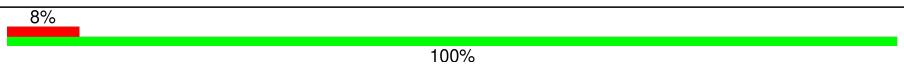
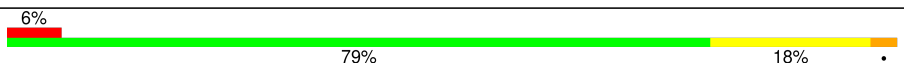
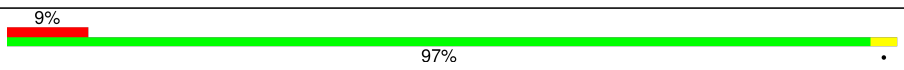
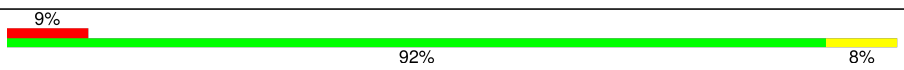
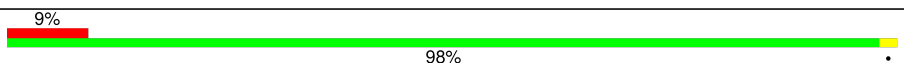
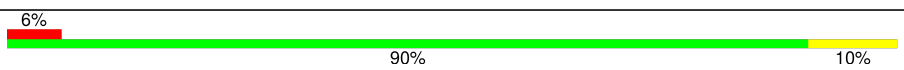
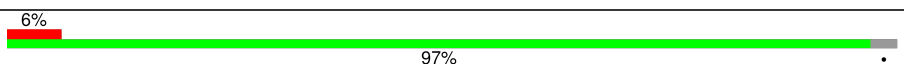
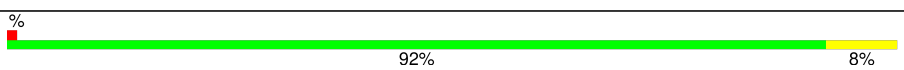
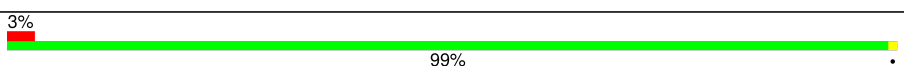
Mol	Chain	Length	Quality of chain
3	c	451	
4	D	342	
4	d	342	
5	E	80	
5	e	80	
6	F	34	
6	f	34	
7	H	63	
7	h	63	
8	I	36	
8	i	36	
9	J	37	
9	j	37	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	244	
13	o	244	
14	T	31	
14	t	31	
15	U	97	
15	u	97	

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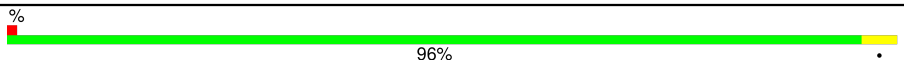
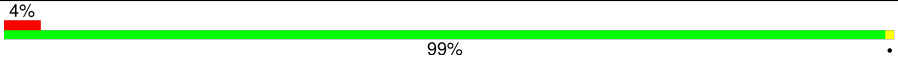
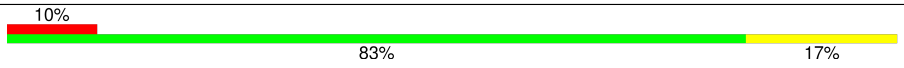
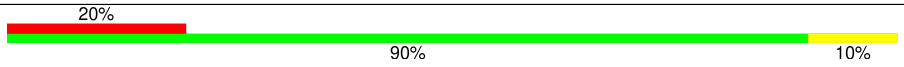
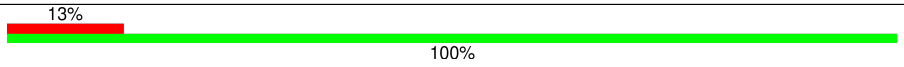
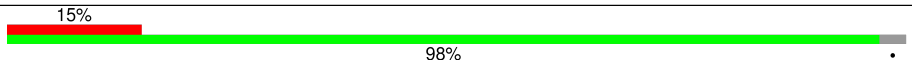
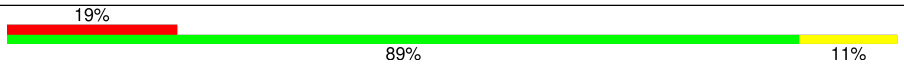
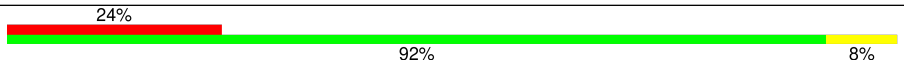
Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
24	CLA	A	1005	X	-	-	-
24	CLA	A	1006	X	-	-	-
24	CLA	A	1008	X	-	-	-
24	CLA	B	601	X	-	-	X
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	409	X	-	-	X
24	CLA	a	412	X	-	-	X
24	CLA	b	604	X	-	-	X
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	B	618	-	-	-	X
27	PL9	A	1010	-	-	-	X
27	PL9	a	414	-	-	-	X
28	SQD	B	620[A]	-	-	-	X
28	SQD	B	620[B]	-	-	-	X
28	SQD	a	401	-	-	-	X
28	SQD	b	623[A]	-	-	-	X
28	SQD	b	623[B]	-	-	-	X
29	LMG	A	1012	-	-	-	X
29	LMG	B	622	-	-	-	X
29	LMG	C	519	-	-	-	X
29	LMG	D	412	-	-	-	X
29	LMG	Z	101	-	-	-	X
29	LMG	c	519	-	-	-	X
29	LMG	c	521	-	-	-	X
29	LMG	d	409	-	-	-	X
29	LMG	m	102	-	-	-	X
30	DMS	A	1014	-	-	-	X
30	DMS	B	627	-	-	-	X
30	DMS	B	632	-	-	-	X
30	DMS	B	634	-	-	-	X
30	DMS	C	524	-	-	-	X
30	DMS	D	416	-	-	-	X
30	DMS	D	417	-	-	-	X
30	DMS	O	301	-	-	-	X
30	DMS	O	302	-	-	-	X
30	DMS	V	203	-	-	-	X
30	DMS	b	629	-	-	-	X
30	DMS	b	634	-	-	-	X
30	DMS	b	635	-	-	-	X
30	DMS	c	526	-	-	-	X
30	DMS	c	529	-	-	-	X
30	DMS	d	413	-	-	-	X
30	DMS	v	202	-	-	-	X
31	UNL	B	630	-	-	-	X
31	UNL	D	414	-	-	-	X
31	UNL	D	415	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	UNL	I	101	-	-	-	X
31	UNL	K	103	-	-	-	X
31	UNL	b	603	-	-	-	X
31	UNL	c	523	-	-	-	X
31	UNL	d	412	-	-	-	X
31	UNL	l	101	-	-	-	X
31	UNL	t	102	-	-	-	X
31	UNL	x	101	-	-	-	X
32	LMT	A	1017	-	-	-	X
32	LMT	A	1018	-	-	-	X
32	LMT	C	520	-	-	-	X
32	LMT	M	101	-	-	-	X
32	LMT	a	402	-	-	-	X
32	LMT	a	416	-	-	-	X
32	LMT	b	631	-	-	-	X
32	LMT	f	103	-	-	-	X
32	LMT	i	102	-	-	-	X
32	LMT	m	103	-	-	-	X
32	LMT	t	103	-	-	-	X
33	GOL	V	204	-	-	-	X
33	GOL	V	206	-	-	-	X
34	LHG	D	411	-	-	-	X
34	LHG	E	101	-	-	-	X
34	LHG	d	406	-	-	-	X
34	LHG	d	408	-	-	-	X
34	LHG	e	101	-	-	-	X
35	HTG	B	628	-	-	-	X
35	HTG	C	522	-	-	-	X
35	HTG	D	413	-	-	-	X
35	HTG	V	202	-	-	-	X
35	HTG	b	626	-	-	-	X
35	HTG	d	410	-	-	-	X
35	HTG	d	416	-	-	-	X
35	HTG	o	301	-	-	-	X
36	DGD	C	516	-	-	-	X
36	DGD	c	516	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 53568 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 Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	5	0
			2643	1733	431	464	15			
1	a	334	Total	C	N	O	S	0	4	0
			2637	1729	431	462	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	SEE REMARK 999	UNP P51765
a	279	PRO	ARG	SEE REMARK 999	UNP P51765

- Molecule 2 is a protein called Photosystem II core light harvesting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	10	0
			4040	2652	674	701	13			
2	b	505	Total	C	N	O	S	0	9	0
			4033	2646	676	698	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	3	0
			3500	2292	584	611	13			
3	c	450	Total	C	N	O	S	0	2	0
			3492	2287	583	609	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	342	Total	C	N	O	S	0	0	0
			2726	1805	445	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	80	Total	C	N	O	0	2	0
			660	431	105	124			
5	e	78	Total	C	N	O	0	0	0
			638	418	103	117			

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			
7	h	63	Total	C	N	O	S	0	0	0
			498	333	80	83	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			
8	i	36	Total	C	N	O	S	0	0	0
			296	200	46	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	37	Total	C	N	O	S	0	0	0
			266	179	41	45	1			
9	j	37	Total	C	N	O	S	0	0	0
			266	179	41	45	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			
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	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			
11	l	37	Total	C	N	O	S	0	0	0
			304	202	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			
12	m	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	N	O	S	0	2	0
			1883	1176	317	386	4			
13	o	243	Total	C	N	O	S	0	1	0
			1868	1167	315	382	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	31	Total	C	N	O	S	0	0	0
			267	187	38	40	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	97	Total	C	N	O	0	1	0
			780	495	129	156			
15	u	97	Total	C	N	O	0	1	0
			780	495	129	156			

- 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	3	0
			1081	687	179	211	4			
16	v	137	Total	C	N	O	S	0	2	0
			1076	683	177	212	4			

- Molecule 17 is a protein called Photosystem II reaction center protein ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			
17	y	30	Total	C	N	O	S	0	0	0
			224	147	38	36	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	0	0	0
			296	197	47	52			
18	x	39	Total	C	N	O	0	0	0
			287	191	46	50			

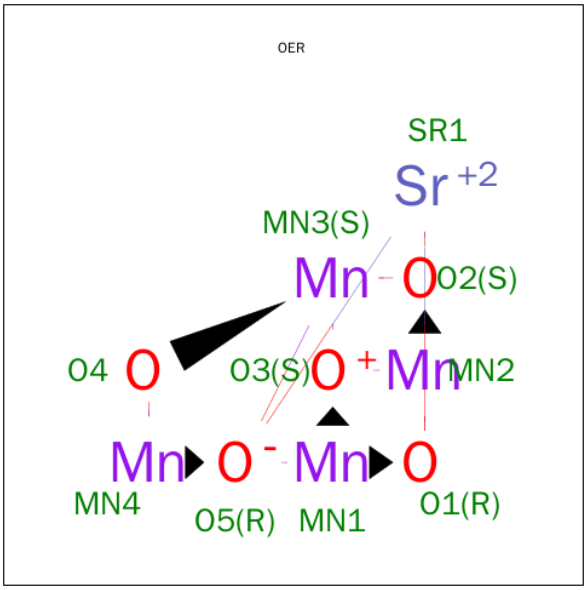
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	2			
19	z	62	Total	C	N	O	S	0	0	0
			481	329	72	78	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 SR-MN4-O5 CLUSTER (three-letter code: OER) (formula: Mn_4O_5Sr).



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

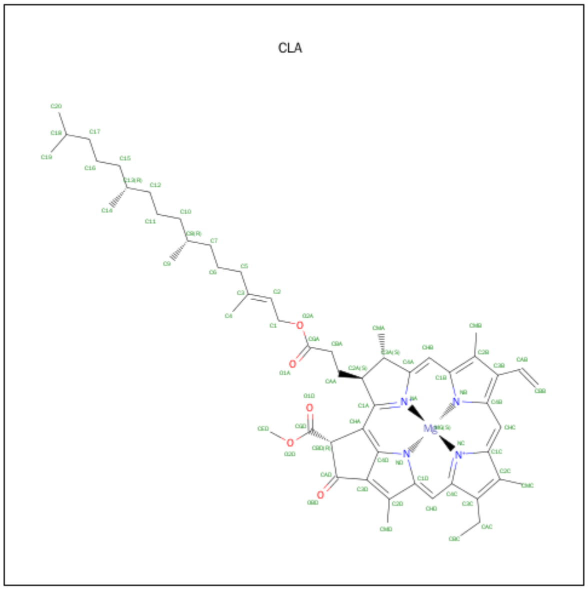
- Molecule 22 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total Fe 1 1	0	0
22	a	1	Total Fe 1 1	0	0

- Molecule 23 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 24 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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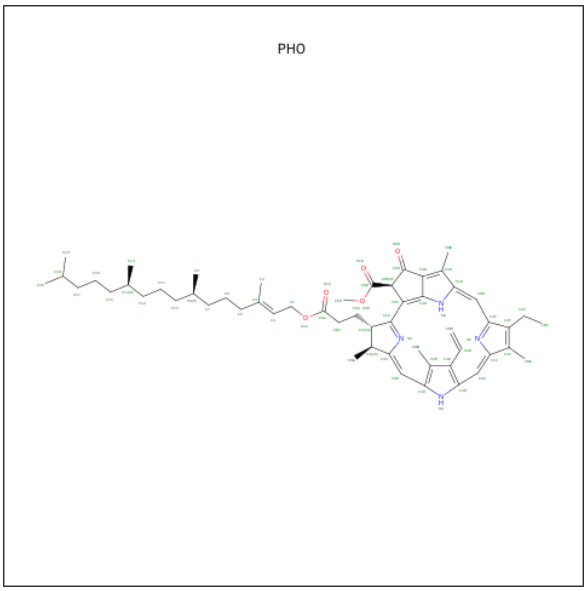
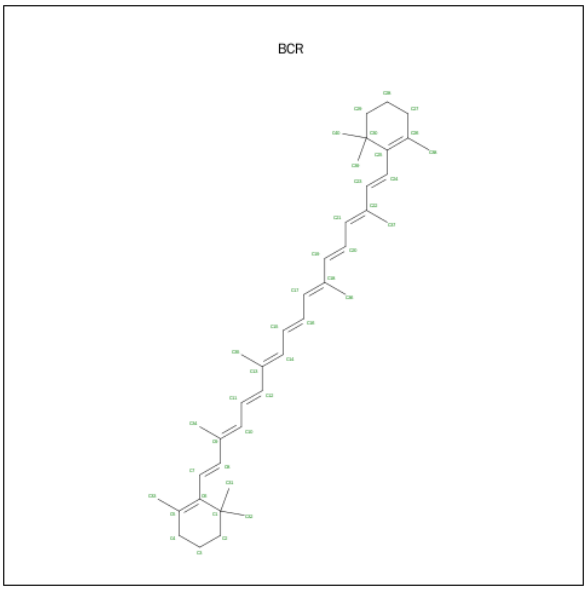
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



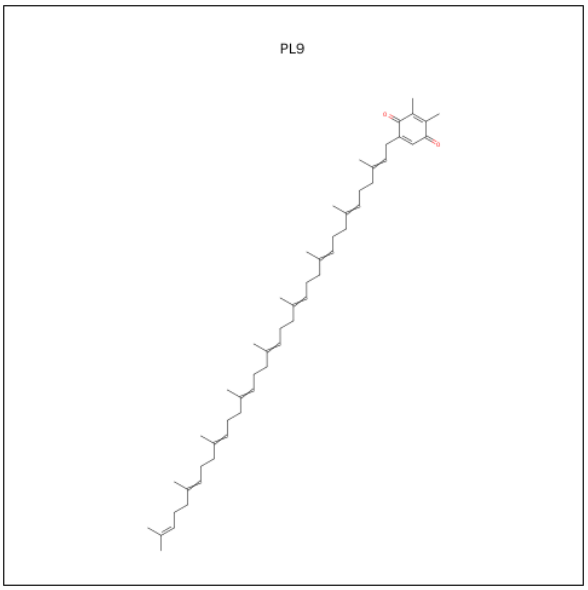
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



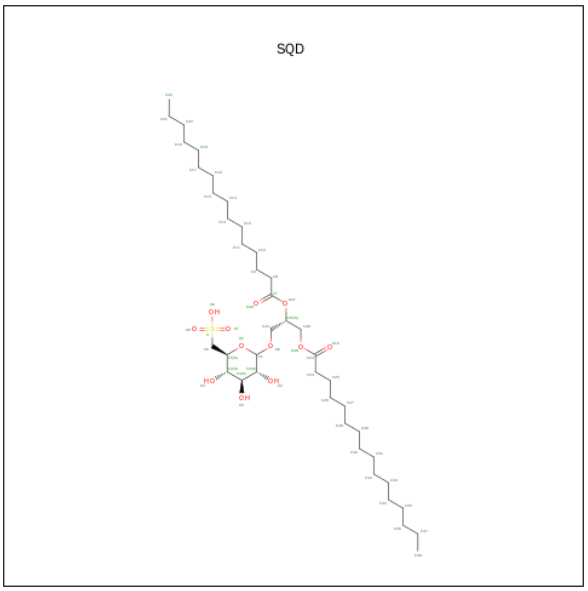
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	J	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	a	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	d	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	t	1	Total C 40 40	0	0
26	y	1	Total C 40 40	0	0

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



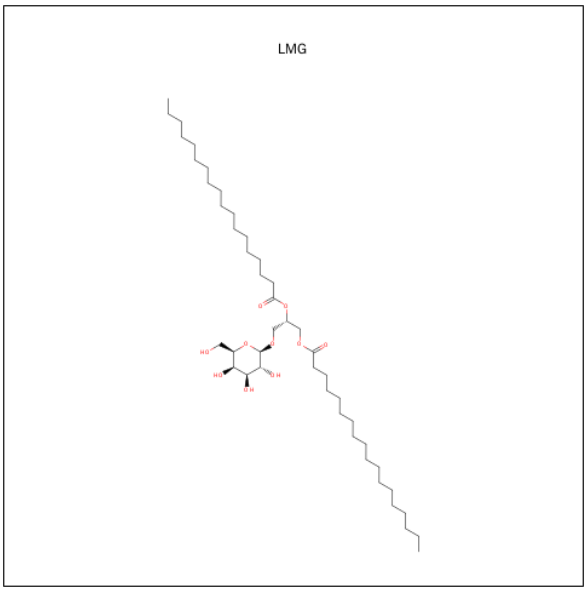
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



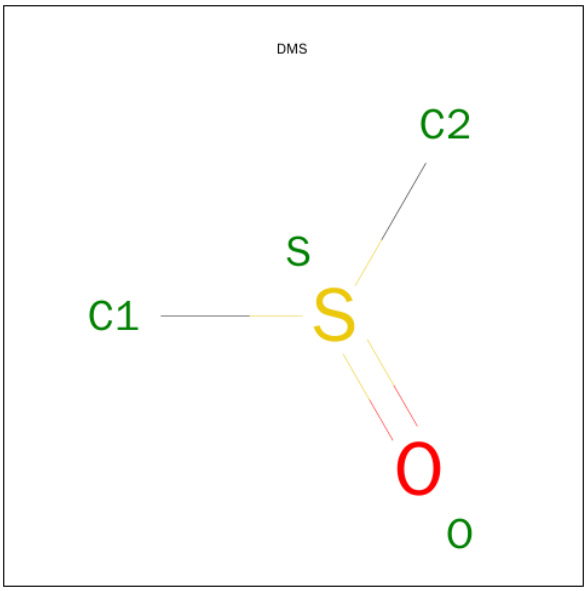
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	B	1	Total	C	O	S	0	1
			108	82	24	2		
28	D	1	Total	C	O	S	0	0
			43	30	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	1
			108	82	24	2		
28	c	1	Total	C	O	S	0	0
			54	41	12	1		
28	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	D	1	Total C O 51 41 10	0	0
29	Z	1	Total C O 51 41 10	0	0
29	a	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	d	1	Total C O 51 41 10	0	0
29	m	1	Total C O 51 41 10	0	0

- Molecule 30 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	A	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	B	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	C	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		
30	D	1	Total	C	O	S	0	0
			4	2	1	1		

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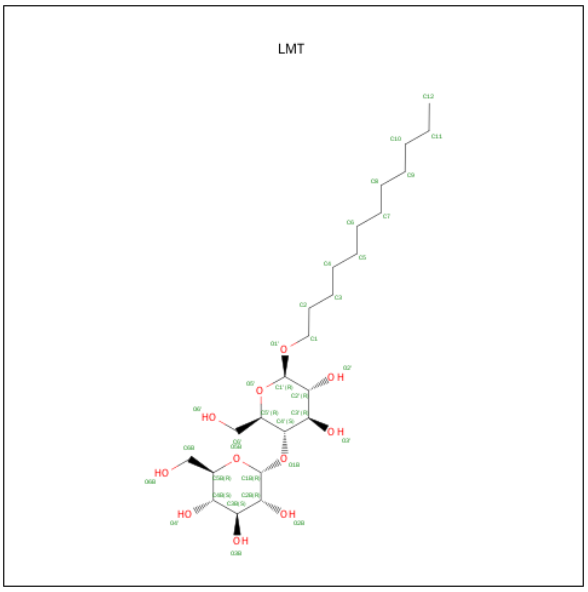
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	O	1	Total	C	O	S	0	0
			4	2	1	1		
30	O	1	Total	C	O	S	0	0
			4	2	1	1		
30	U	1	Total	C	O	S	0	0
			4	2	1	1		
30	V	1	Total	C	O	S	0	0
			4	2	1	1		
30	V	1	Total	C	O	S	0	0
			4	2	1	1		
30	a	1	Total	C	O	S	0	0
			4	2	1	1		
30	a	1	Total	C	O	S	0	0
			4	2	1	1		
30	b	1	Total	C	O	S	0	0
			4	2	1	1		
30	b	1	Total	C	O	S	0	0
			4	2	1	1		
30	b	1	Total	C	O	S	0	0
			4	2	1	1		
30	b	1	Total	C	O	S	0	0
			4	2	1	1		
30	b	1	Total	C	O	S	0	0
			4	2	1	1		
30	c	1	Total	C	O	S	0	0
			4	2	1	1		
30	c	1	Total	C	O	S	0	0
			4	2	1	1		
30	c	1	Total	C	O	S	0	0
			4	2	1	1		
30	c	1	Total	C	O	S	0	0
			4	2	1	1		
30	c	1	Total	C	O	S	0	0
			4	2	1	1		
30	d	1	Total	C	O	S	0	0
			4	2	1	1		
30	d	1	Total	C	O	S	0	0
			4	2	1	1		
30	u	1	Total	C	O	S	0	0
			4	2	1	1		
30	v	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 31 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	J	1	Total C 16 16	0	0
31	i	1	Total C 16 16	0	0
31	D	2	Total C O 56 51 5	0	0
31	K	1	Total C O 34 29 5	0	0
31	y	1	Total C 16 16	0	0
31	l	1	Total C 16 16	0	0
31	B	2	Total C 32 32	0	0
31	I	2	Total C 26 26	0	0
31	c	1	Total C O 32 27 5	0	0
31	a	1	Total C O 30 25 5	0	0
31	x	1	Total C 16 16	0	0
31	A	1	Total C O 28 23 5	0	0
31	j	1	Total C 16 16	0	0
31	X	1	Total C 16 16	0	0
31	d	2	Total C O 52 47 5	0	0
31	t	1	Total C 16 16	0	0
31	Y	1	Total C 16 16	0	0
31	L	1	Total C 16 16	0	0
31	b	2	Total C 32 32	0	0

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 35 24 11	0	0
32	A	1	Total C O 35 24 11	0	0
32	B	1	Total C O 35 24 11	0	0
32	C	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 35 24 11	0	0
32	b	1	Total C O 35 24 11	0	0
32	f	1	Total C O 35 24 11	0	0
32	i	1	Total C O 35 24 11	0	0
32	m	1	Total C O 35 24 11	0	0
32	m	1	Total C O 35 24 11	0	0

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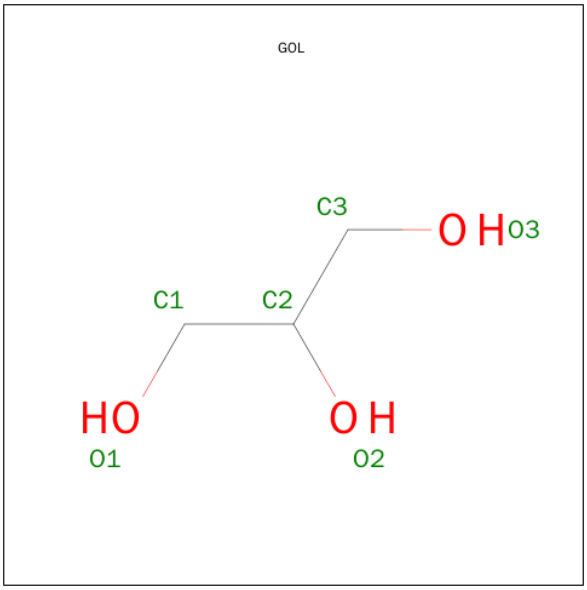
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	t	1	Total C O 35 24 11	0	0

- Molecule 33 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 6 3 3	0	0
33	B	1	Total C O 6 3 3	0	0
33	D	1	Total C O 6 3 3	0	0
33	V	1	Total C O 6 3 3	0	0
33	V	1	Total C O 6 3 3	0	0
33	V	1	Total C O 6 3 3	0	0
33	a	1	Total C O 6 3 3	0	0
33	b	1	Total C O 6 3 3	0	0
33	d	1	Total C O 6 3 3	0	0
33	d	1	Total C O 6 3 3	0	0

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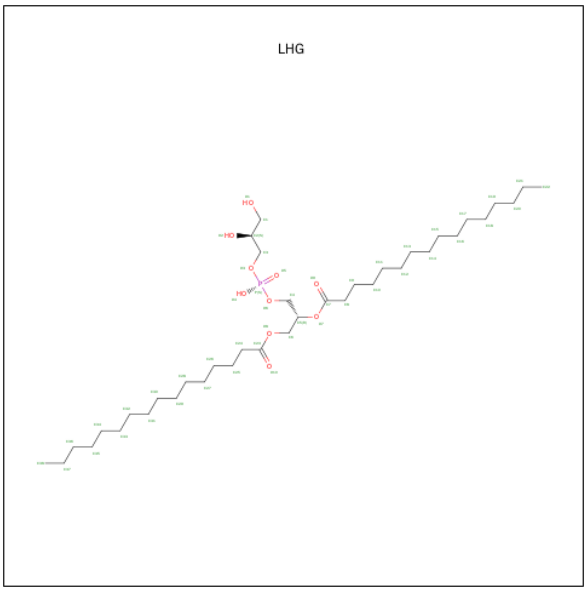
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	v	1	Total C O 6 3 3	0	0
33	v	1	Total C O 6 3 3	0	0

- Molecule 34 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O P 49 38 10 1	0	0
34	D	1	Total C O P 49 38 10 1	0	0
34	D	1	Total C O P 49 38 10 1	0	0
34	D	1	Total C O P 49 38 10 1	0	0
34	E	1	Total C O P 49 38 10 1	0	0
34	b	1	Total C O P 49 38 10 1	0	0
34	d	1	Total C O P 49 38 10 1	0	0
34	d	1	Total C O P 49 38 10 1	0	0
34	d	1	Total C O P 49 38 10 1	0	0

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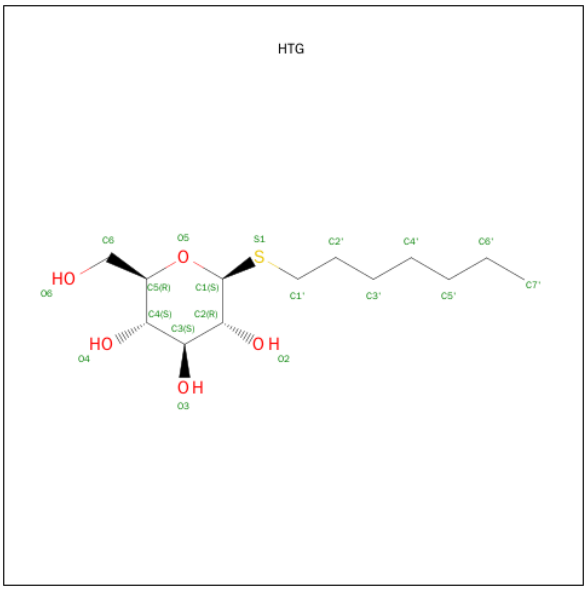
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	e	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 35 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

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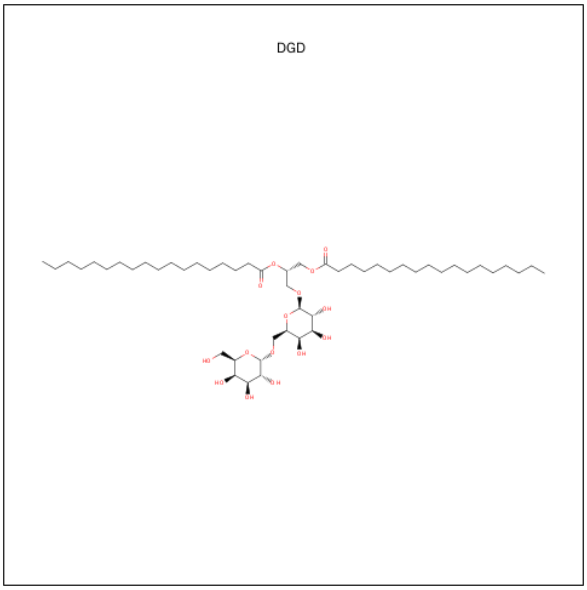
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



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		

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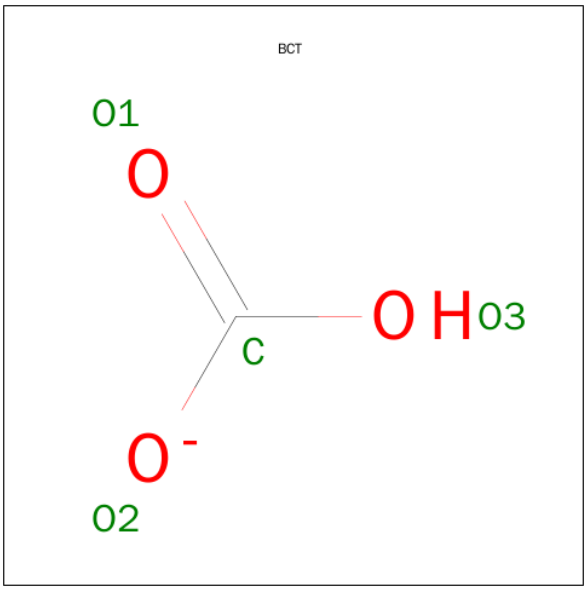
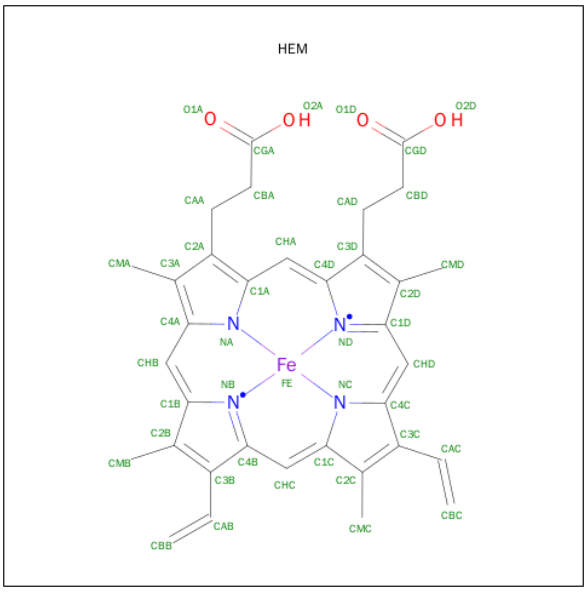
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

- Molecule 37 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O 4 1 3	0	0
37	d	1	Total C O 4 1 3	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	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
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		
39	K	1	Total	Mg	0	0
			1	1		
39	k	1	Total	Mg	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	134	Total	O	0	0
			134	134		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	B	252	Total O 253 253	0	1
40	C	168	Total O 168 168	0	0
40	D	132	Total O 132 132	0	0
40	E	22	Total O 22 22	0	0
40	F	6	Total O 6 6	0	0
40	H	31	Total O 31 31	0	0
40	I	4	Total O 4 4	0	0
40	J	7	Total O 7 7	0	0
40	K	7	Total O 7 7	0	0
40	L	11	Total O 11 11	0	0
40	M	6	Total O 6 6	0	0
40	O	119	Total O 119 119	0	0
40	T	10	Total O 10 10	0	0
40	U	63	Total O 63 63	0	0
40	V	96	Total O 96 96	0	0
40	Y	1	Total O 1 1	0	0
40	X	8	Total O 8 8	0	0
40	Z	1	Total O 1 1	0	0
40	R	1	Total O 1 1	0	0
40	a	118	Total O 118 118	0	0
40	b	209	Total O 209 209	0	0

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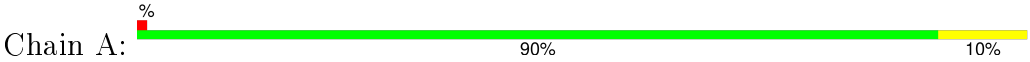
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	c	169	Total O 169 169	0	0
40	d	121	Total O 121 121	0	0
40	e	9	Total O 9 9	0	0
40	f	5	Total O 5 5	0	0
40	h	23	Total O 23 23	0	0
40	i	4	Total O 4 4	0	0
40	j	5	Total O 5 5	0	0
40	k	3	Total O 3 3	0	0
40	l	8	Total O 8 8	0	0
40	m	10	Total O 10 10	0	0
40	o	112	Total O 112 112	0	0
40	t	13	Total O 13 13	0	0
40	u	74	Total O 74 74	0	0
40	v	65	Total O 65 65	0	0
40	y	1	Total O 1 1	0	0
40	x	9	Total O 9 9	0	0

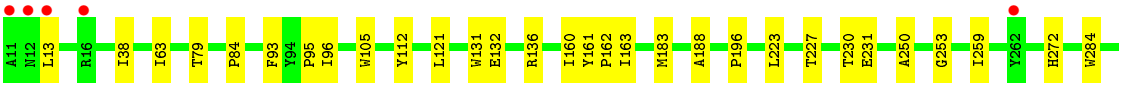
3 Residue-property plots (i)

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

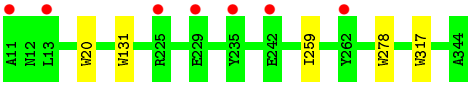
Chain A:





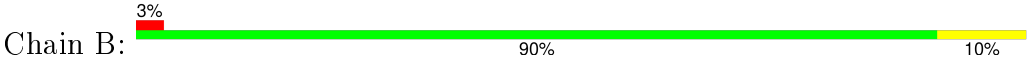
• Molecule 1: Photosystem Q(B) protein

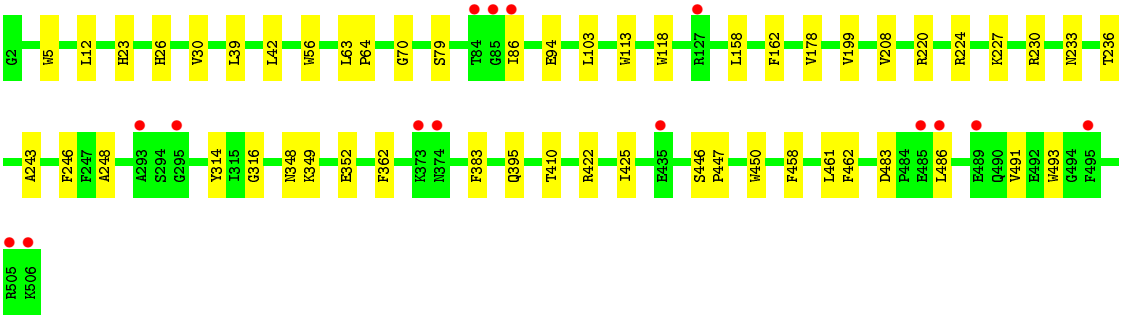
Chain a:



• Molecule 2: Photosystem II core light harvesting protein

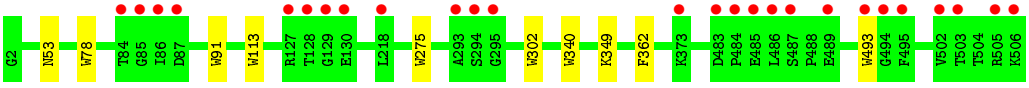
Chain B:





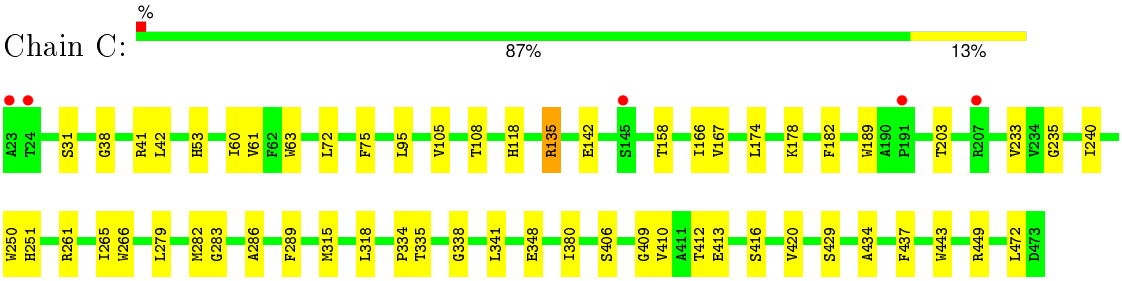
• Molecule 2: Photosystem II core light harvesting protein

Chain b:



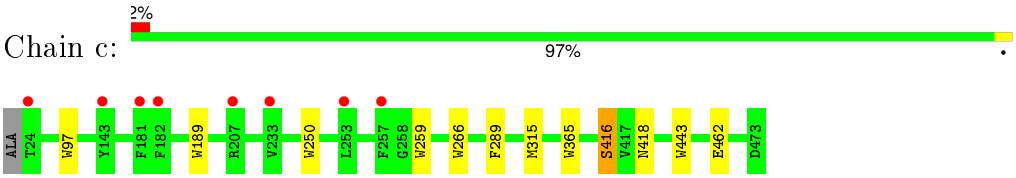
• Molecule 3: Photosystem II CP43 protein

Chain C:



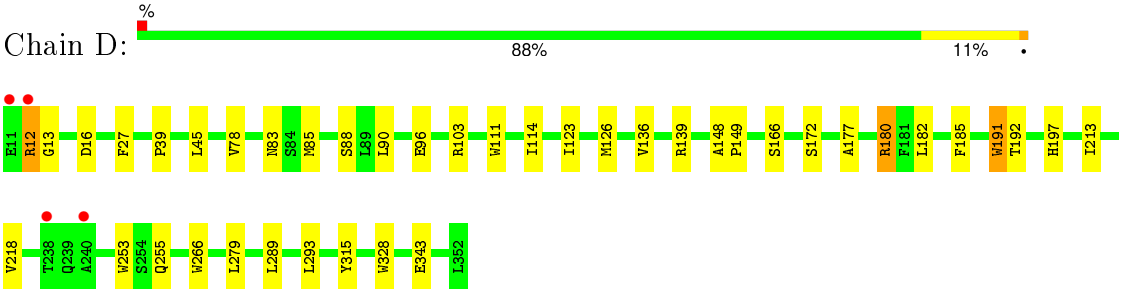
• Molecule 3: Photosystem II CP43 protein

Chain c:



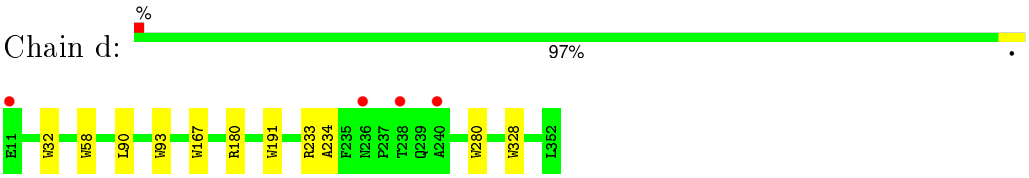
• Molecule 4: Photosystem II D2 protein

Chain D:



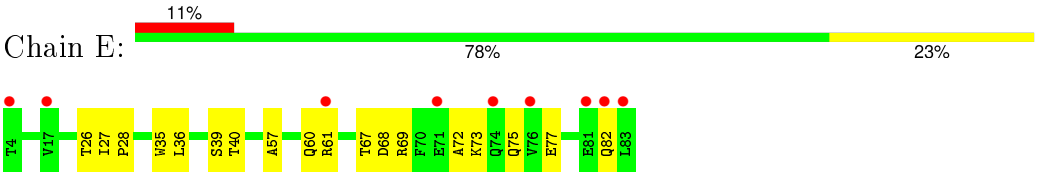
• Molecule 4: Photosystem II D2 protein

Chain d:



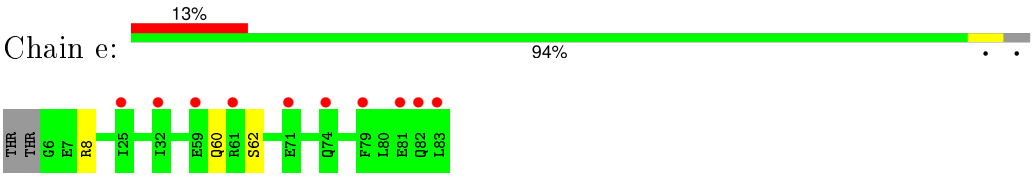
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



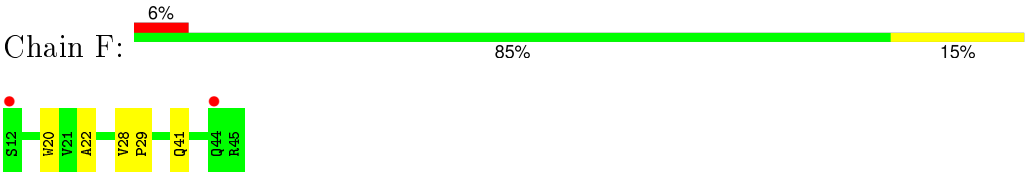
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



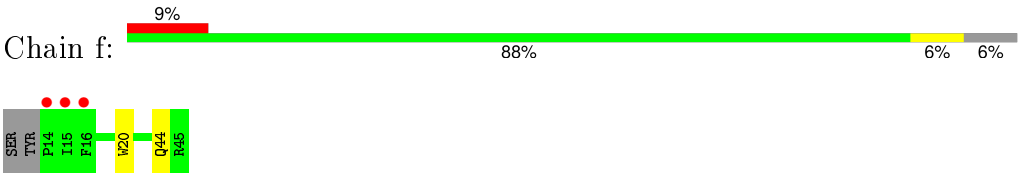
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



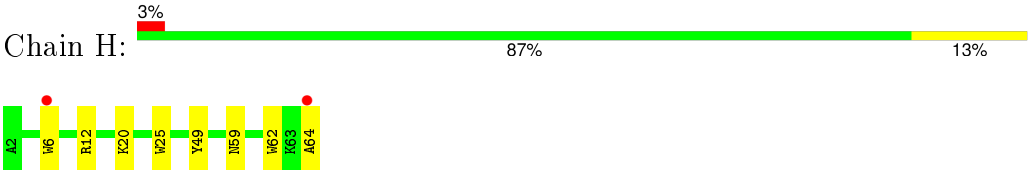
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



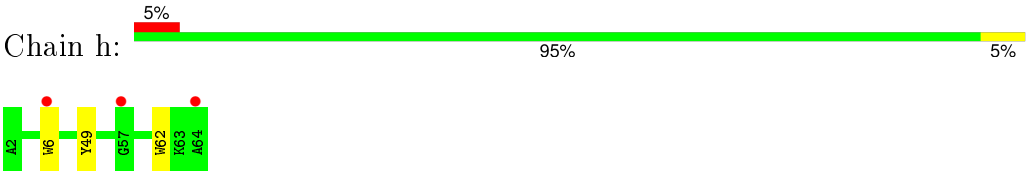
• Molecule 7: Photosystem II reaction center protein H

Chain H:



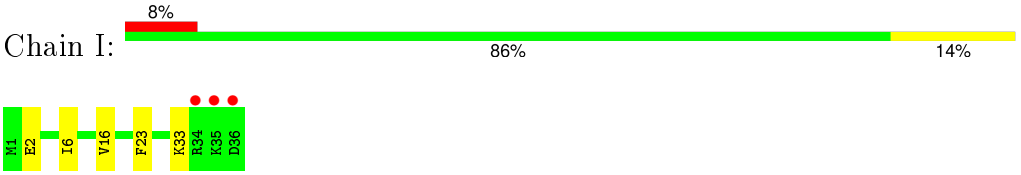
• Molecule 7: Photosystem II reaction center protein H

Chain h:



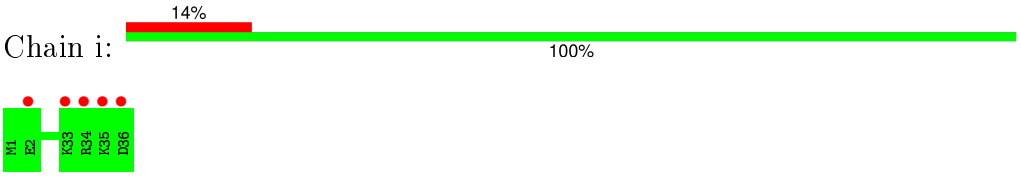
• Molecule 8: Photosystem II reaction center protein I

Chain I:



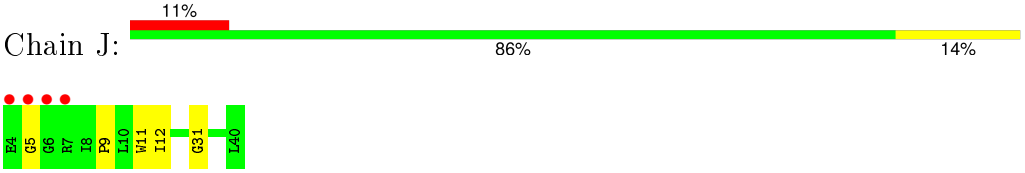
• Molecule 8: Photosystem II reaction center protein I

Chain i:



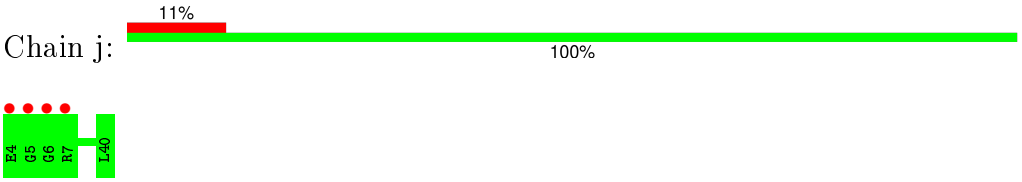
• Molecule 9: Photosystem II reaction center protein J

Chain J:



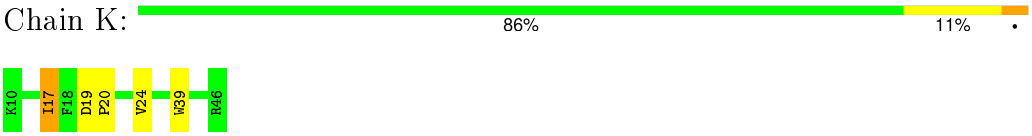
• Molecule 9: Photosystem II reaction center protein J

Chain j:



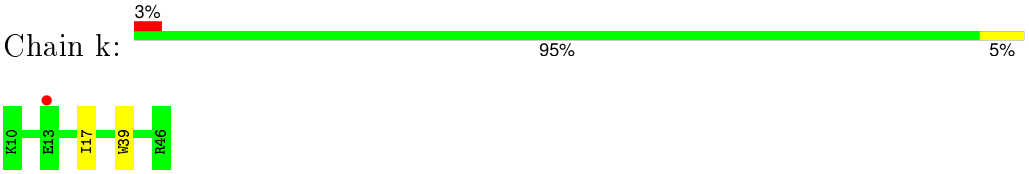
• Molecule 10: Photosystem II reaction center protein K

Chain K:



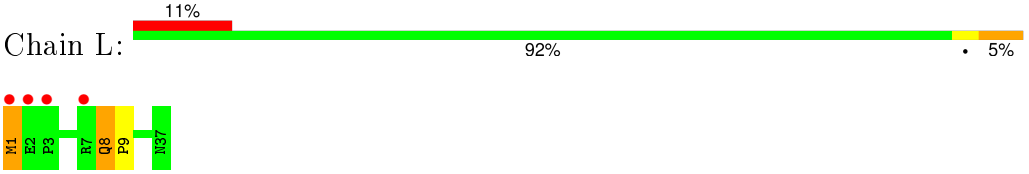
• Molecule 10: Photosystem II reaction center protein K

Chain k:



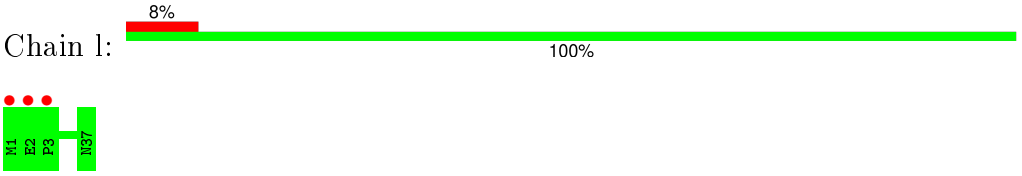
• Molecule 11: Photosystem II reaction center protein L

Chain L:



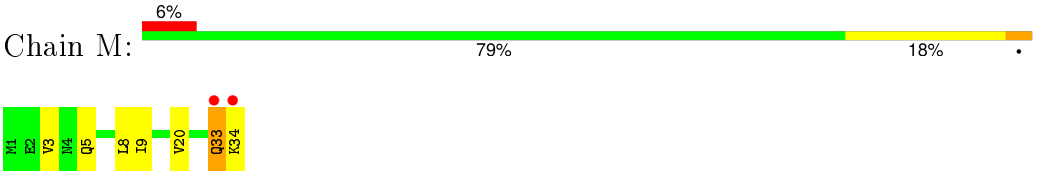
• Molecule 11: Photosystem II reaction center protein L

Chain l:



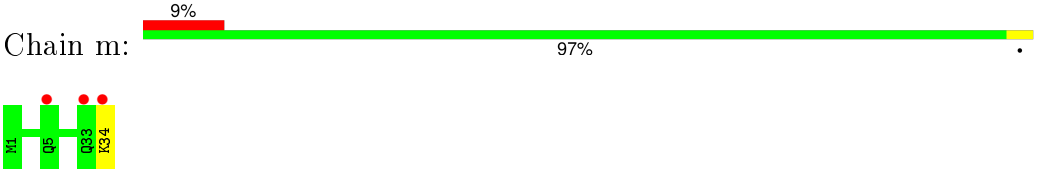
• Molecule 12: Photosystem II reaction center protein M

Chain M:



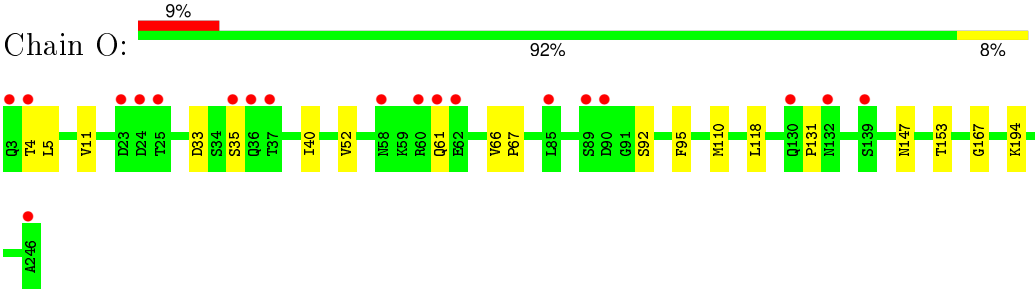
• Molecule 12: Photosystem II reaction center protein M

Chain m:



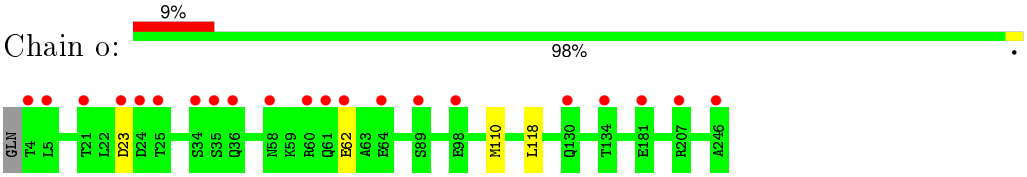
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



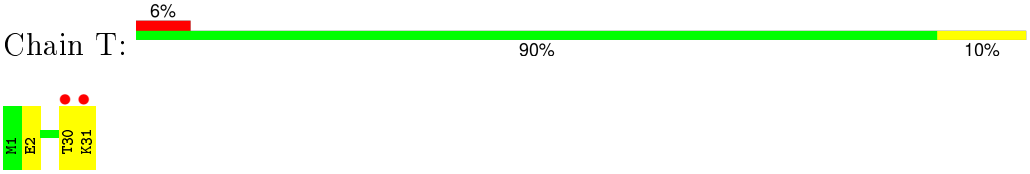
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



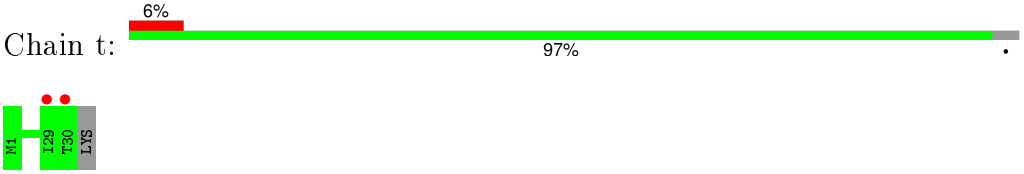
• Molecule 14: Photosystem II reaction center protein T

Chain T:



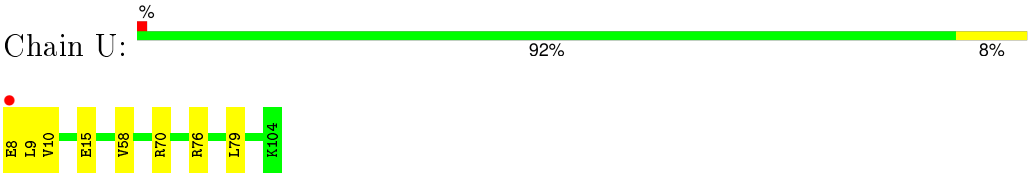
• Molecule 14: Photosystem II reaction center protein T

Chain t:



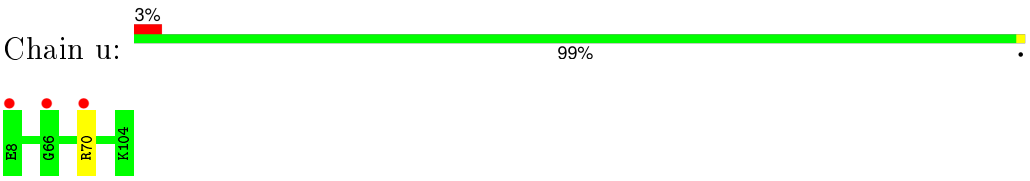
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



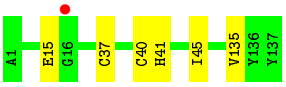
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



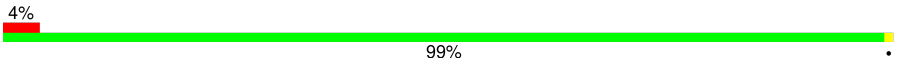
• Molecule 16: Cytochrome c-550

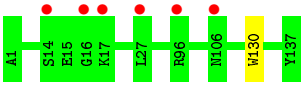
Chain V:



• Molecule 16: Cytochrome c-550

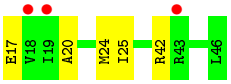
Chain v:





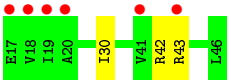
• Molecule 17: Photosystem II reaction center protein ycf12

Chain Y:



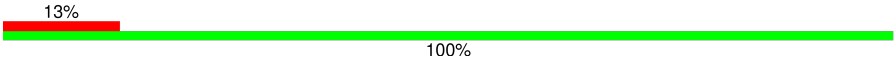
• Molecule 17: Photosystem II reaction center protein ycf12

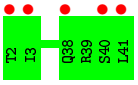
Chain y:



• Molecule 18: Photosystem II reaction center protein X

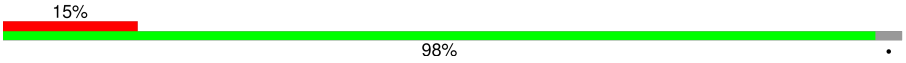
Chain X:

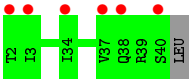




• Molecule 18: Photosystem II reaction center protein X

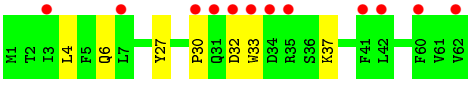
Chain x:





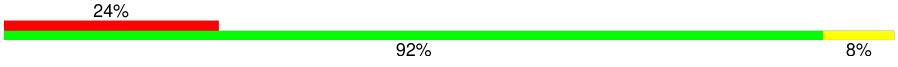
• Molecule 19: Photosystem II reaction center protein Z

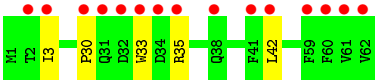
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

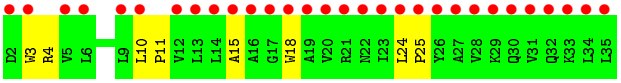
Chain z:





• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.86Å 228.79Å 285.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.96-2.10) 99.9 (19.96-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.14 (at 2.09Å)	Xtriage
Refinement program	REFMAC5.6.0117	Depositor
R, R_{free}	0.176 , 0.205 0.177 , 0.206	Depositor DCC
R_{free} test set	23034 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 460677 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	53568	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, GOL, MG, PHO, DGD, CL, OER, LMT, CLA, PL9, DMS, 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	0.57	1/2743 (0.0%)	0.52	0/3740
1	a	0.56	4/2734 (0.1%)	0.52	0/3728
2	B	0.58	6/4210 (0.1%)	0.53	0/5731
2	b	0.58	7/4200 (0.2%)	0.52	0/5719
3	C	0.58	4/3622 (0.1%)	0.52	0/4931
3	c	0.58	7/3611 (0.2%)	0.51	0/4916
4	D	0.62	3/2821 (0.1%)	0.54	0/3844
4	d	0.60	7/2821 (0.2%)	0.53	0/3844
5	E	0.51	1/685 (0.1%)	0.51	0/936
5	e	0.49	0/657	0.49	0/897
6	F	0.57	1/284 (0.4%)	0.46	0/387
6	f	0.56	1/265 (0.4%)	0.47	0/360
7	H	0.60	2/522 (0.4%)	0.52	0/712
7	h	0.60	2/511 (0.4%)	0.53	0/697
8	I	0.34	0/293	0.42	0/396
8	i	0.35	0/293	0.44	0/396
9	J	0.54	1/272 (0.4%)	0.49	0/368
9	j	0.51	0/272	0.49	0/368
10	K	0.52	1/303 (0.3%)	0.49	0/416
10	k	0.51	1/303 (0.3%)	0.52	0/416
11	L	0.38	0/311	0.46	0/422
11	l	0.36	0/311	0.47	0/422
12	M	0.30	0/270	0.48	0/368
12	m	0.33	0/270	0.47	0/368
13	O	0.34	0/1920	0.53	0/2603
13	o	0.33	0/1902	0.52	0/2579
14	T	0.40	0/266	0.45	0/360
14	t	0.38	0/257	0.45	0/349
15	U	0.36	0/794	0.51	0/1076
15	u	0.34	0/794	0.51	0/1076
16	V	0.40	0/1111	0.49	0/1507

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.40	1/1103 (0.1%)	0.48	0/1497
17	Y	0.33	0/225	0.49	0/301
17	y	0.30	0/225	0.48	0/301
18	X	0.32	0/299	0.43	0/403
18	x	0.33	0/290	0.42	0/392
19	Z	0.52	1/482 (0.2%)	0.46	0/659
19	z	0.51	1/482 (0.2%)	0.46	0/659
20	R	0.65	2/279 (0.7%)	0.52	0/383
All	All	0.53	54/43013 (0.1%)	0.51	0/58527

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	317	TRP	CD2-CE2	5.39	1.47	1.41
4	d	167	TRP	CD2-CE2	5.37	1.47	1.41
4	d	191	TRP	CD2-CE2	5.34	1.47	1.41
2	b	91	TRP	CD2-CE2	5.32	1.47	1.41
2	B	56	TRP	CD2-CE2	5.26	1.47	1.41
4	D	111	TRP	CD2-CE2	5.24	1.47	1.41
3	c	365	TRP	CD2-CE2	5.23	1.47	1.41
6	F	20	TRP	CD2-CE2	5.20	1.47	1.41
2	b	493	TRP	CD2-CE2	5.17	1.47	1.41
3	c	189	TRP	CD2-CE2	5.16	1.47	1.41
5	E	35	TRP	CD2-CE2	5.15	1.47	1.41
2	B	113	TRP	CD2-CE2	5.15	1.47	1.41
3	C	443	TRP	CD2-CE2	5.15	1.47	1.41
4	d	93	TRP	CD2-CE2	5.15	1.47	1.41
20	R	18	TRP	CD2-CE2	5.15	1.47	1.41
1	A	284	TRP	CD2-CE2	5.14	1.47	1.41
3	c	97	TRP	CD2-CE2	5.14	1.47	1.41
1	a	278	TRP	CD2-CE2	5.13	1.47	1.41
7	h	62	TRP	CD2-CE2	5.12	1.47	1.41
4	d	280	TRP	CD2-CE2	5.12	1.47	1.41
7	h	6	TRP	CD2-CE2	5.11	1.47	1.41
7	H	6	TRP	CD2-CE2	5.11	1.47	1.41
9	J	11	TRP	CD2-CE2	5.11	1.47	1.41
4	D	328	TRP	CD2-CE2	5.10	1.47	1.41
20	R	3	TRP	CD2-CE2	5.09	1.47	1.41
4	d	58	TRP	CD2-CE2	5.09	1.47	1.41
4	d	32	TRP	CD2-CE2	5.09	1.47	1.41
4	D	191	TRP	CD2-CE2	5.09	1.47	1.41
2	B	118	TRP	CD2-CE2	5.09	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	493	TRP	CD2-CE2	5.09	1.47	1.41
2	b	78	TRP	CD2-CE2	5.09	1.47	1.41
16	v	130	TRP	CD2-CE2	5.09	1.47	1.41
6	f	20	TRP	CD2-CE2	5.08	1.47	1.41
19	Z	33	TRP	CD2-CE2	5.07	1.47	1.41
19	z	33	TRP	CD2-CE2	5.07	1.47	1.41
3	c	266	TRP	CD2-CE2	5.07	1.47	1.41
3	c	259	TRP	CD2-CE2	5.06	1.47	1.41
3	c	250	TRP	CD2-CE2	5.05	1.47	1.41
7	H	62	TRP	CD2-CE2	5.05	1.47	1.41
3	c	443	TRP	CD2-CE2	5.05	1.47	1.41
3	C	250	TRP	CD2-CE2	5.04	1.47	1.41
2	b	340	TRP	CD2-CE2	5.04	1.47	1.41
10	k	39	TRP	CD2-CE2	5.04	1.47	1.41
2	b	275	TRP	CD2-CE2	5.04	1.47	1.41
2	B	450	TRP	CD2-CE2	5.04	1.47	1.41
10	K	39	TRP	CD2-CE2	5.04	1.47	1.41
3	C	63	TRP	CD2-CE2	5.03	1.47	1.41
1	a	131	TRP	CD2-CE2	5.02	1.47	1.41
2	b	113	TRP	CD2-CE2	5.02	1.47	1.41
2	B	5	TRP	CD2-CE2	5.02	1.47	1.41
1	a	20	TRP	CD2-CE2	5.01	1.47	1.41
3	C	189	TRP	CD2-CE2	5.01	1.47	1.41
2	b	302	TRP	CD2-CE2	5.00	1.47	1.41
4	d	328	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2643	0	2550	30	0
1	a	2637	0	2544	0	0
2	B	4040	0	3928	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	4033	0	3921	0	0
3	C	3500	0	3429	41	0
3	c	3492	0	3419	0	0
4	D	2726	0	2627	38	0
4	d	2726	0	2627	0	0
5	E	660	0	644	14	0
5	e	638	0	621	0	0
6	F	275	0	282	3	0
6	f	257	0	269	0	0
7	H	506	0	531	3	0
7	h	498	0	518	0	0
8	I	296	0	311	4	0
8	i	296	0	311	0	0
9	J	266	0	274	2	0
9	j	266	0	274	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	304	0	316	5	0
11	l	304	0	316	0	0
12	M	274	0	299	5	0
12	m	274	0	299	0	0
13	O	1883	0	1857	11	0
13	o	1868	0	1843	0	0
14	T	267	0	274	2	0
14	t	258	0	261	0	0
15	U	780	0	779	4	0
15	u	780	0	779	0	0
16	V	1081	0	1100	10	0
16	v	1076	0	1087	0	0
17	Y	224	0	252	6	0
17	y	224	0	252	0	0
18	X	296	0	328	0	0
18	x	287	0	317	0	0
19	Z	481	0	515	1	0
19	z	481	0	515	0	0
20	R	273	0	305	4	0
21	A	10	0	0	0	0
21	a	10	0	0	0	0
22	A	1	0	0	0	0
22	a	1	0	0	0	0
23	A	2	0	0	0	0
23	a	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	A	195	0	216	10	0
24	B	1040	0	1152	52	0
24	C	845	0	936	46	0
24	D	195	0	216	9	0
24	a	260	0	288	0	0
24	b	1040	0	1152	0	0
24	c	845	0	936	0	0
24	d	130	0	144	0	0
25	A	64	0	74	1	0
25	D	64	0	74	4	0
25	a	128	0	148	0	0
26	A	40	0	48	0	0
26	B	120	0	140	2	0
26	C	40	0	46	3	0
26	D	40	0	46	1	0
26	H	40	0	46	0	0
26	J	40	0	48	1	0
26	K	80	0	95	2	0
26	T	40	0	47	0	0
26	a	40	0	46	0	0
26	b	120	0	141	0	0
26	c	40	0	47	0	0
26	d	40	0	47	0	0
26	h	40	0	48	0	0
26	k	80	0	94	0	0
26	t	40	0	47	0	0
26	y	40	0	46	0	0
27	A	55	0	80	5	0
27	D	55	0	80	0	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	108	0	156	3	0
28	B	108	0	156	21	0
28	D	43	0	53	1	0
28	a	54	0	78	0	0
28	b	108	0	156	0	0
28	c	54	0	78	0	0
28	f	43	0	53	0	0
29	A	51	0	72	0	0
29	B	51	0	72	2	0
29	C	102	0	144	2	0
29	D	51	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Z	51	0	72	1	0
29	a	51	0	72	0	0
29	c	153	0	216	0	0
29	d	51	0	72	0	0
29	m	51	0	72	0	0
30	A	8	0	12	0	0
30	B	20	0	30	2	0
30	C	20	0	30	0	0
30	D	8	0	12	0	0
30	O	8	0	12	0	0
30	U	4	0	6	0	0
30	V	8	0	12	0	0
30	a	8	0	12	0	0
30	b	20	0	30	0	0
30	c	20	0	30	0	0
30	d	8	0	12	0	0
30	u	4	0	6	0	0
30	v	4	0	6	0	0
31	A	28	0	0	0	0
31	B	32	0	0	0	0
31	D	56	0	0	0	0
31	I	26	0	0	0	0
31	J	16	0	0	0	0
31	K	34	0	0	0	0
31	L	16	0	0	0	0
31	X	16	0	0	0	0
31	Y	16	0	0	0	0
31	a	30	0	0	0	0
31	b	32	0	0	0	0
31	c	32	0	0	0	0
31	d	52	0	0	0	0
31	i	16	0	0	0	0
31	j	16	0	0	0	0
31	l	16	0	0	0	0
31	t	16	0	0	0	0
31	x	16	0	0	0	0
31	y	16	0	0	0	0
32	A	70	0	92	3	0
32	B	35	0	46	0	0
32	C	35	0	46	0	0
32	M	70	0	92	3	0
32	a	70	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	b	70	0	92	0	0
32	f	35	0	46	0	0
32	i	35	0	46	0	0
32	m	70	0	92	0	0
32	t	35	0	46	0	0
33	A	6	0	8	0	0
33	B	6	0	8	1	0
33	D	6	0	8	0	0
33	V	18	0	24	0	0
33	a	6	0	8	0	0
33	b	6	0	8	0	0
33	d	12	0	16	0	0
33	v	12	0	16	0	0
34	B	49	0	74	1	0
34	D	147	0	222	13	0
34	E	49	0	74	3	0
34	b	49	0	74	0	0
34	d	147	0	222	0	0
34	e	49	0	74	0	0
35	B	57	0	78	1	0
35	C	38	0	52	0	0
35	D	38	0	52	1	0
35	V	19	0	26	0	0
35	b	76	0	104	0	0
35	c	38	0	52	0	0
35	d	38	0	52	0	0
35	o	19	0	26	0	0
36	C	186	0	246	5	0
36	H	62	0	82	3	0
36	c	186	0	246	0	0
36	h	62	0	82	0	0
37	D	4	0	0	0	0
37	d	4	0	0	0	0
38	F	43	0	30	3	0
38	V	43	0	30	8	0
38	f	43	0	30	0	0
38	v	43	0	30	0	0
39	J	1	0	0	0	0
39	K	1	0	0	0	0
39	j	1	0	0	0	0
39	k	1	0	0	0	0
40	A	134	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	B	253	0	0	0	0
40	C	168	0	0	2	0
40	D	132	0	0	0	0
40	E	22	0	0	1	0
40	F	6	0	0	0	0
40	H	31	0	0	1	0
40	I	4	0	0	0	0
40	J	7	0	0	0	0
40	K	7	0	0	0	0
40	L	11	0	0	0	0
40	M	6	0	0	0	0
40	O	119	0	0	1	0
40	R	1	0	0	0	0
40	T	10	0	0	0	0
40	U	63	0	0	0	0
40	V	96	0	0	0	0
40	X	8	0	0	0	0
40	Y	1	0	0	0	0
40	Z	1	0	0	0	0
40	a	118	0	0	0	0
40	b	209	0	0	0	0
40	c	169	0	0	0	0
40	d	121	0	0	0	0
40	e	9	0	0	0	0
40	f	5	0	0	0	0
40	h	23	0	0	0	0
40	i	4	0	0	0	0
40	j	5	0	0	0	0
40	k	3	0	0	0	0
40	l	8	0	0	0	0
40	m	10	0	0	0	0
40	o	112	0	0	0	0
40	t	13	0	0	0	0
40	u	74	0	0	0	0
40	v	65	0	0	0	0
40	x	9	0	0	0	0
40	y	1	0	0	0	0
All	All	53568	0	52620	319	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 4.

All (319) 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)
16:V:37:CYS:SG	38:V:201:HEM:HAB	1.58	1.53
28:B:620[B]:SQD:H141	28:B:620[B]:SQD:C38	1.48	1.42
28:B:620[B]:SQD:C14	28:B:620[B]:SQD:H382	1.52	1.39
16:V:40:CYS:SG	38:V:201:HEM:CAC	2.14	1.35
16:V:37:CYS:SG	38:V:201:HEM:CAB	2.13	1.35
16:V:40:CYS:SG	38:V:201:HEM:HAC	1.72	1.30
28:B:620[A]:SQD:H81	28:B:620[A]:SQD:C46	1.63	1.28
28:B:620[B]:SQD:H381	28:B:620[B]:SQD:C17	1.64	1.25
16:V:37:CYS:HG	38:V:201:HEM:CAB	1.54	1.21
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.43	1.12
28:B:620[A]:SQD:C8	28:B:620[A]:SQD:H462	1.63	1.11
28:B:620[B]:SQD:H381	28:B:620[B]:SQD:H172	1.06	1.04
28:B:620[B]:SQD:C38	28:B:620[B]:SQD:H172	1.96	0.93
28:B:620[A]:SQD:H81	28:B:620[A]:SQD:H462	0.93	0.92
28:B:620[A]:SQD:C8	28:B:620[A]:SQD:C46	2.26	0.91
4:D:266:TRP:CD1	34:D:410:LHG:HC32	2.09	0.86
10:K:17:ILE:H	10:K:17:ILE:HD13	1.44	0.82
17:Y:42:ARG:HG3	17:Y:42:ARG:HH11	1.45	0.81
28:B:620[A]:SQD:O10	28:B:620[A]:SQD:H442	1.82	0.79
25:D:404:PHO:HMB1	25:D:404:PHO:HBB1	1.67	0.77
2:B:230[B]:ARG:HE	30:B:634:DMS:H22	1.50	0.76
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.75	0.76
24:B:616:CLA:HBB1	24:B:616:CLA:HMB1	2.10	0.75
2:B:230[B]:ARG:HE	30:B:634:DMS:C2	2.00	0.75
24:D:403:CLA:HBB1	24:D:403:CLA:HMB1	1.80	0.72
24:A:1005:CLA:HBB1	24:A:1005:CLA:HMB1	1.71	0.72
1:A:250:ALA:HA	2:B:491:VAL:CG1	3.08	0.71
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	1.73	0.69
38:F:101:HEM:HBB2	38:F:101:HEM:HMB1	3.42	0.69
10:K:24:VAL:HG11	17:Y:25:ILE:HB	1.75	0.67
24:C:503:CLA:HAB	24:C:512:CLA:H41	3.06	0.67
24:B:607:CLA:H43	24:B:608:CLA:H2	37.08	0.66
24:C:506:CLA:HMC2	24:C:507:CLA:H101	1.77	0.66
4:D:13:GLY:HA3	35:D:413:HTG:H62	1.79	0.65
28:B:620[A]:SQD:H461	28:B:620[A]:SQD:C8	2.22	0.65
28:B:620[A]:SQD:H81	28:B:620[A]:SQD:H461	1.70	0.65
28:B:620[B]:SQD:H251	28:B:620[B]:SQD:H461	1.79	0.64
16:V:40:CYS:SG	38:V:201:HEM:C3C	2.92	0.64
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.78	0.64
5:E:40:THR:HB	20:R:4:ARG:HG2	1.80	0.64
3:C:167:VAL:HG21	24:C:512:CLA:HHB	1.95	0.63
1:A:253:GLY:HA3	2:B:491:VAL:HG12	3.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:506:CLA:HMC2	24:C:507:CLA:H102	2.95	0.63
2:B:410:THR:H	33:B:631:GOL:H2	1.61	0.63
7:H:59:ASN:HB3	7:H:64:ALA:HB3	1.81	0.63
14:T:30:THR:HG22	14:T:31:LYS:H	1.65	0.62
2:B:162:PHE:O	24:B:606:CLA:HHD	1.99	0.61
12:M:33:GLN:HG3	12:M:33:GLN:HB2	2.19	0.61
28:B:620[B]:SQD:H381	28:B:620[B]:SQD:H171	1.77	0.61
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.94	0.60
24:C:508:CLA:HBB1	24:C:508:CLA:HMB1	1.86	0.60
10:K:19:ASP:HB3	10:K:20:PRO:HD3	1.97	0.60
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.95	0.60
28:B:620[B]:SQD:C14	28:B:620[B]:SQD:C38	2.39	0.59
24:B:606:CLA:HBB1	24:B:606:CLA:HMB1	2.04	0.59
28:B:620[B]:SQD:C16	28:B:620[B]:SQD:H381	2.31	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.98	0.59
1:A:223:LEU:HD12	4:D:139:ARG:NH1	2.18	0.58
24:C:510:CLA:H41	34:D:411:LHG:H381	1.86	0.58
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.68	0.58
24:B:604:CLA:HMD2	24:B:612:CLA:H203	1.85	0.57
24:C:506:CLA:HBB1	24:C:506:CLA:HMB1	1.96	0.57
2:B:462:PHE:CE1	24:B:616:CLA:HMB3	23.13	0.57
24:C:510:CLA:HBB1	24:C:510:CLA:HMB1	2.43	0.57
24:B:614:CLA:H18	29:B:622:LMG:H421	1.86	0.57
28:B:620[B]:SQD:C17	28:B:620[B]:SQD:C38	2.59	0.57
4:D:123:ILE:HD11	36:H:102:DGD:HAH1	3.24	0.56
17:Y:42:ARG:HG3	17:Y:42:ARG:NH1	2.19	0.56
11:L:9:PRO:HA	32:M:101:LMT:H6D	41.58	0.56
3:C:60:ILE:HG22	24:C:503:CLA:HHD	1.97	0.56
24:B:613:CLA:HBB1	24:B:613:CLA:HHC	4.71	0.56
2:B:462:PHE:CE1	24:B:613:CLA:HMB3	2.40	0.56
1:A:227:THR:HB	1:A:231[A]:GLU:HG3	1.87	0.56
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.54	0.55
2:B:483:ASP:HB3	2:B:486:LEU:HB2	1.88	0.55
3:C:413[B]:GLU:HG2	40:C:628:HOH:O	2.06	0.55
28:A:1011:SQD:H272	34:D:411:LHG:H141	1.89	0.55
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.55
3:C:41:ARG:NH1	24:C:511:CLA:HMD1	2.26	0.55
24:B:607:CLA:HBA2	24:B:615:CLA:H151	37.17	0.55
24:B:615:CLA:HBB1	24:B:615:CLA:HMB1	1.89	0.54
24:B:609:CLA:HMB1	24:B:609:CLA:HBB1	4.11	0.54
25:A:1007:PHO:HBB1	25:A:1007:PHO:HMB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.89	0.53
5:E:68:ASP:H	5:E:75:GLN:HE22	3.26	0.53
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	2.25	0.53
12:M:20:VAL:HG11	12:M:20:VAL:HG22	3.04	0.53
16:V:37:CYS:SG	38:V:201:HEM:C3B	2.93	0.53
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.90	0.53
12:M:33:GLN:O	12:M:34:LYS:HB2	2.08	0.53
24:B:611:CLA:HAB	4:D:123:ILE:HG12	19.78	0.53
24:C:505:CLA:HBB1	24:C:505:CLA:HMB1	2.88	0.53
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.58	0.52
5:E:67:THR:H	5:E:75:GLN:HE22	2.62	0.52
1:A:183:MET:HA	24:A:1005:CLA:HMD2	1.92	0.52
24:A:1005:CLA:CBD	24:D:403:CLA:HAC2	2.40	0.52
2:B:248:ALA:HA	24:B:606:CLA:H42	22.91	0.51
2:B:227:LYS:O	2:B:230[B]:ARG:HD3	2.09	0.51
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.96	0.51
2:B:248:ALA:HA	24:B:603:CLA:H42	1.93	0.51
12:M:8:LEU:HG	12:M:9:ILE:HD13	5.82	0.51
10:K:17:ILE:H	10:K:17:ILE:CD1	2.20	0.51
4:D:185:PHE:CD2	24:D:402:CLA:HMD3	2.57	0.51
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.44	0.50
24:A:1006:CLA:HBB1	24:D:402:CLA:H102	1.93	0.50
38:F:101:HEM:HBB2	38:F:101:HEM:CMB	2.49	0.50
1:A:196:PRO:HB3	36:C:517:DGD:HA82	3.91	0.50
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.50
13:O:92:SER:HB3	13:O:131:PRO:HA	2.09	0.50
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.50
2:B:26:HIS:HB2	24:B:612:CLA:HMB2	1.93	0.50
4:D:85:MET:CE	4:D:96:GLU:HG2	4.87	0.50
24:C:510:CLA:H52	34:D:411:LHG:H371	1.93	0.50
24:C:502:CLA:H61	24:C:512:CLA:H42	2.15	0.50
2:B:103:LEU:HD21	24:B:605:CLA:HMC3	1.93	0.50
2:B:348:ASN:OD1	2:B:352[B]:GLU:HG3	2.10	0.50
3:C:174:LEU:HB3	24:C:502:CLA:H161	1.93	0.49
2:B:162:PHE:O	24:B:609:CLA:HHD	29.90	0.49
11:L:9:PRO:HA	32:M:102:LMT:H6D	16.56	0.49
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.01	0.49
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.95	0.49
3:C:42:LEU:HD21	24:C:511:CLA:H2A	2.04	0.49
24:B:615:CLA:H2	24:B:616:CLA:HBB2	1.94	0.49
5:E:67:THR:H	5:E:75:GLN:NE2	3.07	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:334:PRO:HA	13:O:153:THR:OG1	2.23	0.48
1:A:38:ILE:HG12	28:A:1016:SQD:H142	1.95	0.48
1:A:250:ALA:CA	2:B:491:VAL:HG11	3.19	0.48
24:B:613:CLA:H18	34:D:409:LHG:H202	1.95	0.48
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.48	0.48
24:C:510:CLA:H192	24:C:510:CLA:HBC3	2.02	0.48
24:A:1006:CLA:HMD3	4:D:182:LEU:HD11	1.96	0.48
24:B:606:CLA:HAB	24:B:608:CLA:H171	32.34	0.48
16:V:40:CYS:SG	38:V:201:HEM:CBC	2.93	0.48
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.95	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.49	0.47
24:C:513:CLA:HAB	26:K:102:BCR:H24C	3.58	0.47
2:B:103:LEU:HD21	24:B:608:CLA:HMC3	29.95	0.47
16:V:41:HIS:HA	16:V:45:ILE:O	2.21	0.47
5:E:57:ALA:HB3	5:E:60:GLN:HG2	4.64	0.47
28:B:620[A]:SQD:H442	28:B:620[A]:SQD:C23	2.45	0.47
26:C:514:BCR:HC32	8:I:23:PHE:HB3	1.95	0.47
29:C:519:LMG:H152	17:Y:25:ILE:HD13	28.08	0.47
4:D:123:ILE:HD11	36:H:102:DGD:HAE2	3.42	0.47
27:A:1010:PL9:H512	28:D:408:SQD:H321	1.97	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.20	0.47
32:A:1017:LMT:H42	2:B:39:LEU:HD22	47.58	0.47
3:C:409:GLY:HA3	3:C:413[A]:GLU:HG3	1.97	0.47
13:O:52:VAL:HB	13:O:110:MET:HE3	2.52	0.47
1:A:230:THR:HB	11:L:8:GLN:HE22	1.78	0.47
2:B:461:LEU:HD22	34:D:409:LHG:H301	1.96	0.47
3:C:142:GLU:H	3:C:142:GLU:CD	2.38	0.47
24:B:607:CLA:H42	24:B:615:CLA:H152	39.09	0.46
3:C:166:ILE:HD13	24:C:512:CLA:H191	1.97	0.46
3:C:410:VAL:HG13	40:C:742:HOH:O	2.15	0.46
3:C:472:LEU:HD11	4:D:255:GLN:HG3	2.20	0.46
1:A:79:THR:HG22	4:D:315:TYR:HB2	1.98	0.46
24:B:610:CLA:HBB1	24:B:610:CLA:HHC	1.98	0.46
2:B:233:ASN:O	2:B:236:THR:HG22	2.16	0.46
3:C:61:VAL:HG12	3:C:118:HIS:O	2.29	0.46
24:C:505:CLA:HBC2	26:C:514:BCR:H341	2.02	0.46
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.51	0.46
24:B:605:CLA:C14	24:B:610:CLA:HED2	2.46	0.46
3:C:437:PHE:CE1	24:C:510:CLA:HMB3	2.51	0.45
24:A:1008:CLA:H111	8:I:16:VAL:HG11	1.97	0.45
28:B:620[A]:SQD:H321	28:B:620[A]:SQD:H352	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:506:CLA:H122	24:C:506:CLA:H161	1.42	0.45
27:A:1010:PL9:H251	34:E:101:LHG:H211	1.98	0.45
3:C:72:LEU:HD11	3:C:108:THR:HB	2.18	0.45
5:E:36:LEU:HA	5:E:39:SER:OG	2.15	0.45
5:E:82:GLN:HB3	40:E:213:HOH:O	2.17	0.45
13:O:33:ASP:OD2	13:O:35:SER:HB3	2.17	0.45
24:C:510:CLA:H41	34:D:411:LHG:C38	2.46	0.45
10:K:24:VAL:HB	17:Y:25:ILE:HG23	6.63	0.45
1:A:121[B]:LEU:HD11	24:C:505:CLA:H152	1.98	0.45
3:C:437:PHE:CZ	24:C:510:CLA:HMB3	2.60	0.45
34:D:411:LHG:H372	34:D:411:LHG:H142	1.98	0.45
24:C:508:CLA:HBC3	24:C:510:CLA:H71	1.99	0.45
8:I:33:LYS:HA	8:I:33:LYS:HD3	4.38	0.45
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.52	0.45
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.99	0.44
4:D:185:PHE:CG	24:D:402:CLA:HMD3	2.53	0.44
24:A:1005:CLA:HBD	24:D:403:CLA:HAC2	2.00	0.44
24:A:1008:CLA:H152	24:C:505:CLA:H192	1.99	0.44
4:D:85:MET:HE3	4:D:96:GLU:HG2	5.65	0.44
32:A:1018:LMT:H3'	32:A:1018:LMT:H1B	1.54	0.44
29:B:622:LMG:HC5	32:M:101:LMT:H1'	1.99	0.44
13:O:4:THR:HG23	13:O:5:LEU:H	4.44	0.44
4:D:83:ASN:ND2	4:D:166:SER:OG	2.53	0.44
2:B:462:PHE:CZ	24:B:613:CLA:HMB3	2.52	0.44
26:B:618:BCR:H371	26:B:618:BCR:H24C	1.85	0.44
3:C:348:GLU:OE1	13:O:11:VAL:HA	2.17	0.44
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.00	0.44
3:C:75:PHE:HZ	3:C:105:VAL:HG21	2.08	0.44
36:C:515:DGD:HA82	36:C:515:DGD:HAE1	1.73	0.44
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.53	0.44
26:B:617:BCR:H371	26:B:617:BCR:H24C	1.83	0.44
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.26	0.44
17:Y:20:ALA:O	17:Y:24:MET:HG2	2.18	0.44
24:C:507:CLA:HMB1	24:C:507:CLA:HBB1	2.28	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.56	0.44
4:D:123:ILE:HD11	36:H:102:DGD:HAE1	2.00	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.43
4:D:103:ARG:HE	5:E:77:GLU:HG3	1.83	0.43
24:B:611:CLA:HBB1	24:B:611:CLA:HMB1	1.99	0.43
24:C:504:CLA:H192	24:C:510:CLA:H72	2.00	0.43
28:A:1011:SQD:H122	34:E:101:LHG:H331	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1010:PL9:H403	6:F:22:ALA:HB2	2.01	0.43
24:C:513:CLA:H171	26:K:102:BCR:H373	2.26	0.43
13:O:147:ASN:HD21	13:O:194:LYS:NZ	2.50	0.43
1:A:132:GLU:O	1:A:136:ARG:HG2	2.18	0.43
24:B:605:CLA:H143	24:B:610:CLA:HED2	2.00	0.43
2:B:70:GLY:HA2	2:B:178:VAL:HG11	2.01	0.43
5:E:68:ASP:O	5:E:72:ALA:HB2	2.18	0.43
2:B:79:SER:HB3	2:B:86:ILE:HG12	2.15	0.43
13:O:66:VAL:HB	13:O:67:PRO:HD2	2.00	0.43
20:R:24:LEU:N	20:R:25:PRO:HD2	2.33	0.43
2:B:12:LEU:HB2	24:B:615:CLA:HMC2	18.53	0.43
4:D:27:PHE:CD1	34:E:101:LHG:HC12	2.53	0.43
24:C:507:CLA:H61	24:C:507:CLA:H41	1.86	0.43
2:B:349:LYS:HG3	2:B:395:GLN:O	3.90	0.43
1:A:160:ILE:HD11	36:C:515:DGD:HBT1	2.00	0.43
9:J:9:PRO:HD2	9:J:12:ILE:HD12	2.00	0.43
13:O:228:HIS:HD2	40:O:452:HOH:O	2.32	0.43
3:C:265:ILE:HD11	3:C:449:ARG:HD3	2.01	0.43
24:D:405:CLA:HMB1	24:D:405:CLA:HBB1	2.00	0.43
24:C:504:CLA:HMC2	29:C:519:LMG:H401	24.30	0.43
24:B:601:CLA:HAB	24:B:601:CLA:H171	2.01	0.43
20:R:10:LEU:HB3	20:R:11:PRO:HD3	1.99	0.43
2:B:462:PHE:CE2	24:B:604:CLA:HMC1	2.54	0.43
25:D:404:PHO:HHD	25:D:404:PHO:HBC2	2.01	0.43
24:C:501:CLA:H42	24:C:502:CLA:HMD1	2.05	0.43
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.03	0.43
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.53	0.43
3:C:135:ARG:HG3	19:Z:27:TYR:CD1	2.53	0.43
2:B:158:LEU:HB3	2:B:199:VAL:HG22	2.18	0.43
34:B:621:LHG:HC81	34:D:409:LHG:O9	2.19	0.43
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.57	0.42
3:C:233:VAL:HA	26:C:514:BCR:H282	2.41	0.42
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.01	0.42
2:B:458:PHE:HB3	24:B:607:CLA:HBC2	15.40	0.42
4:D:279:LEU:HD22	25:D:404:PHO:HBC3	2.00	0.42
4:D:191:TRP:CZ2	4:D:197:HIS:HB2	2.54	0.42
28:B:620[B]:SQD:H211	28:B:620[B]:SQD:H182	1.86	0.42
2:B:462:PHE:CZ	24:B:616:CLA:HMB3	23.21	0.42
3:C:286:ALA:HB2	24:C:502:CLA:CMD	2.50	0.42
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.01	0.42
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.68	0.42
24:B:604:CLA:H171	24:B:604:CLA:HAB	23.24	0.42
24:B:604:CLA:C4	24:B:605:CLA:H2	2.49	0.42
15:U:8:GLU:HB2	15:U:9:LEU:H	1.71	0.42
24:B:613:CLA:CBB	24:B:613:CLA:HHC	4.03	0.42
5:E:26:THR:HA	20:R:15:ALA:HB1	2.02	0.42
3:C:318:LEU:C	3:C:318:LEU:HD23	2.40	0.42
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.42
24:C:504:CLA:H191	34:D:411:LHG:H362	2.01	0.42
1:A:230:THR:HB	11:L:8:GLN:NE2	2.34	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.01	0.42
1:A:63:ILE:HB	3:C:335:THR:HG21	2.01	0.42
29:Z:101:LMG:H171	29:Z:101:LMG:H361	2.02	0.42
1:A:322:ASN:OD1	3:C:412:THR:HA	2.32	0.42
24:B:603:CLA:HAB	24:B:605:CLA:H171	2.01	0.42
24:B:607:CLA:H91	24:B:607:CLA:H112	1.87	0.42
24:C:504:CLA:H193	24:C:508:CLA:H91	2.01	0.42
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	2.09	0.42
24:C:510:CLA:H62	24:C:510:CLA:H2	1.84	0.42
3:C:31:SER:CB	3:C:41:ARG:HG2	2.57	0.42
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.96	0.41
24:B:606:CLA:H143	35:B:629:HTG:H7'2	2.02	0.41
2:B:446:SER:HB2	2:B:447:PRO:HD2	2.02	0.41
3:C:53:HIS:CB	24:C:512:CLA:HMD1	2.51	0.41
15:U:10:VAL:HG11	15:U:15:GLU:OE2	2.20	0.41
24:B:605:CLA:NC	24:B:605:CLA:ND	2.74	0.41
24:B:604:CLA:HAB	24:B:611:CLA:H193	2.02	0.41
24:B:607:CLA:C3D	24:B:615:CLA:H161	34.53	0.41
34:D:411:LHG:H332	34:D:411:LHG:H151	2.02	0.41
24:A:1005:CLA:CAD	24:D:403:CLA:HAC2	2.50	0.41
3:C:318:LEU:HD21	3:C:380:ILE:CG2	2.59	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
4:D:12:ARG:NH1	4:D:16:ASP:HB3	2.36	0.41
3:C:95:LEU:HD21	24:C:501:CLA:OBD	2.38	0.41
3:C:38:GLY:HA3	24:C:511:CLA:HMD3	2.06	0.41
15:U:76:ARG:HA	15:U:79:LEU:HG	2.14	0.41
34:D:409:LHG:H112	34:D:409:LHG:H351	2.03	0.41
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.50	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.04	0.41
26:D:406:BCR:H383	29:D:412:LMG:H171	2.02	0.41
2:B:30:VAL:HG12	24:B:608:CLA:HHD	23.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:VAL:HG21	24:B:605:CLA:HMC1	25.62	0.41
24:B:606:CLA:H161	24:B:606:CLA:H141	4.74	0.41
24:B:612:CLA:CMB	24:B:614:CLA:HBB1	2.51	0.41
27:A:1010:PL9:H502	4:D:39:PRO:HG3	2.03	0.41
24:C:506:CLA:ND	24:C:506:CLA:NC	2.73	0.41
26:J:101:BCR:H24C	26:J:101:BCR:H371	1.93	0.41
32:A:1017:LMT:H6E	40:A:1189:HOH:O	2.21	0.41
27:A:1010:PL9:H302	4:D:45:LEU:HD22	2.03	0.41
4:D:293:LEU:HD12	4:D:293:LEU:HA	2.09	0.41
3:C:283:GLY:HA3	3:C:434:ALA:HB2	2.10	0.41
4:D:78:VAL:HG11	4:D:114:ILE:HD12	2.02	0.41
24:B:611:CLA:HMB1	4:D:126:MET:HB3	22.35	0.40
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.56	0.40
1:A:13:LEU:H	1:A:13:LEU:HD12	1.86	0.40
8:I:2:GLU:O	8:I:6:ILE:HG12	4.27	0.40
3:C:158:THR:O	3:C:251:HIS:HB3	2.22	0.40
38:F:101:HEM:HMB2	38:F:101:HEM:HBB2	2.03	0.40
3:C:282:MET:CE	24:C:507:CLA:H42	2.51	0.40
3:C:261:ARG:HA	3:C:266:TRP:CZ2	2.57	0.40
3:C:429:SER:HB3	36:C:516:DGD:HB91	2.03	0.40
28:B:620[B]:SQD:C38	28:B:620[B]:SQD:C15	2.97	0.40
2:B:23:HIS:HE1	24:B:610:CLA:H203	1.85	0.40
40:H:225:HOH:O	11:L:1:MET:HE2	2.19	0.40
24:B:612:CLA:HMB2	24:B:613:CLA:C2B	9.05	0.40
34:D:411:LHG:H381	34:D:411:LHG:H122	2.04	0.40
24:B:607:CLA:C3B	24:B:616:CLA:HMC3	27.91	0.40
25:D:404:PHO:ND	25:D:404:PHO:NC	2.70	0.40
1:A:96:ILE:HD12	24:A:1008:CLA:HMD1	2.04	0.40
1:A:163:ILE:HD11	36:C:515:DGD:HA22	2.03	0.40
3:C:338:GLY:HA3	3:C:341:LEU:O	2.24	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	337/334 (101%)	333 (99%)	3 (1%)	1 (0%)	46 45
1	a	336/334 (101%)	331 (98%)	4 (1%)	1 (0%)	46 45
2	B	513/505 (102%)	505 (98%)	8 (2%)	0	100 100
2	b	512/505 (101%)	506 (99%)	6 (1%)	0	100 100
3	C	452/451 (100%)	442 (98%)	9 (2%)	1 (0%)	52 53
3	c	450/451 (100%)	441 (98%)	8 (2%)	1 (0%)	52 53
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100 100
4	d	340/342 (99%)	333 (98%)	6 (2%)	1 (0%)	46 45
5	E	80/80 (100%)	79 (99%)	1 (1%)	0	100 100
5	e	76/80 (95%)	74 (97%)	2 (3%)	0	100 100
6	F	32/34 (94%)	32 (100%)	0	0	100 100
6	f	30/34 (88%)	30 (100%)	0	0	100 100
7	H	62/63 (98%)	59 (95%)	3 (5%)	0	100 100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100 100
8	I	34/36 (94%)	33 (97%)	1 (3%)	0	100 100
8	i	34/36 (94%)	31 (91%)	3 (9%)	0	100 100
9	J	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	6 2
9	j	35/37 (95%)	35 (100%)	0	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	33/34 (97%)	33 (100%)	0	0	100 100
12	m	33/34 (97%)	33 (100%)	0	0	100 100
13	O	244/244 (100%)	240 (98%)	4 (2%)	0	100 100
13	o	242/244 (99%)	234 (97%)	8 (3%)	0	100 100
14	T	29/31 (94%)	29 (100%)	0	0	100 100
14	t	28/31 (90%)	28 (100%)	0	0	100 100
15	U	96/97 (99%)	93 (97%)	3 (3%)	0	100 100
15	u	96/97 (99%)	94 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	V	138/137 (101%)	134 (97%)	4 (3%)	0	100 100
16	v	137/137 (100%)	134 (98%)	3 (2%)	0	100 100
17	Y	28/30 (93%)	28 (100%)	0	0	100 100
17	y	28/30 (93%)	26 (93%)	2 (7%)	0	100 100
18	X	38/40 (95%)	37 (97%)	1 (3%)	0	100 100
18	x	37/40 (92%)	37 (100%)	0	0	100 100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11 5
19	z	60/62 (97%)	57 (95%)	2 (3%)	1 (2%)	11 5
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
All	All	5258/5296 (99%)	5151 (98%)	99 (2%)	8 (0%)	52 53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
3	c	416	SER
9	J	5	GLY
4	d	234	ALA
19	z	30	PRO
19	Z	30	PRO
1	A	259	ILE
1	a	259	ILE

5.3.2 Protein sidechains (i)

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	274/269 (102%)	274 (100%)	0	100 100
1	a	273/269 (102%)	273 (100%)	0	100 100
2	B	413/403 (102%)	412 (100%)	1 (0%)	95 97
2	b	412/403 (102%)	409 (99%)	3 (1%)	88 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	355/352 (101%)	352 (99%)	3 (1%)	86 91
3	c	354/352 (101%)	349 (99%)	5 (1%)	74 80
4	D	277/277 (100%)	274 (99%)	3 (1%)	80 85
4	d	277/277 (100%)	274 (99%)	3 (1%)	80 85
5	E	73/71 (103%)	72 (99%)	1 (1%)	74 80
5	e	69/71 (97%)	66 (96%)	3 (4%)	35 34
6	F	28/28 (100%)	28 (100%)	0	100 100
6	f	26/28 (93%)	25 (96%)	1 (4%)	40 40
7	H	54/53 (102%)	51 (94%)	3 (6%)	26 22
7	h	53/53 (100%)	52 (98%)	1 (2%)	65 70
8	I	32/32 (100%)	32 (100%)	0	100 100
8	i	32/32 (100%)	32 (100%)	0	100 100
9	J	25/25 (100%)	25 (100%)	0	100 100
9	j	25/25 (100%)	25 (100%)	0	100 100
10	K	30/30 (100%)	29 (97%)	1 (3%)	45 47
10	k	30/30 (100%)	29 (97%)	1 (3%)	45 47
11	L	35/35 (100%)	33 (94%)	2 (6%)	25 22
11	l	35/35 (100%)	35 (100%)	0	100 100
12	M	31/30 (103%)	29 (94%)	2 (6%)	21 17
12	m	31/30 (103%)	30 (97%)	1 (3%)	46 48
13	O	209/207 (101%)	207 (99%)	2 (1%)	82 87
13	o	207/207 (100%)	203 (98%)	4 (2%)	65 70
14	T	27/27 (100%)	27 (100%)	0	100 100
14	t	26/27 (96%)	26 (100%)	0	100 100
15	U	85/84 (101%)	84 (99%)	1 (1%)	78 84
15	u	85/84 (101%)	84 (99%)	1 (1%)	78 84
16	V	120/117 (103%)	119 (99%)	1 (1%)	86 91
16	v	119/117 (102%)	119 (100%)	0	100 100
17	Y	23/23 (100%)	22 (96%)	1 (4%)	35 34
17	y	23/23 (100%)	20 (87%)	3 (13%)	5 2
18	X	33/33 (100%)	33 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	x	32/33 (97%)	32 (100%)	0	100 100
19	Z	51/51 (100%)	47 (92%)	4 (8%)	16 11
19	z	51/51 (100%)	48 (94%)	3 (6%)	24 20
20	R	29/29 (100%)	29 (100%)	0	100 100
All	All	4364/4323 (101%)	4310 (99%)	54 (1%)	78 84

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	PHE
3	C	135	ARG
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	90	LEU
4	D	180	ARG
5	E	61	ARG
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	17	ILE
11	L	1	MET
11	L	8	GLN
12	M	5	GLN
12	M	33	GLN
13	O	61	GLN
13	O	118	LEU
15	U	70	ARG
16	V	15	GLU
17	Y	17	GLU
19	Z	4	LEU
19	Z	6	GLN
19	Z	32	ASP
19	Z	37	LYS
2	b	53	ASN
2	b	349	LYS
2	b	362	PHE
3	c	289	PHE
3	c	315	MET
3	c	416	SER
3	c	418	ASN

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Mol	Chain	Res	Type
3	c	462	GLU
4	d	90	LEU
4	d	180	ARG
4	d	233	ARG
5	e	8	ARG
5	e	60	GLN
5	e	62	SER
6	f	44	GLN
7	h	49	TYR
10	k	17	ILE
12	m	34	LYS
13	o	23	ASP
13	o	62	GLU
13	o	110	MET
13	o	118	LEU
15	u	70	ARG
17	y	30	ILE
17	y	42	ARG
17	y	43	ARG
19	z	3	ILE
19	z	35	ARG
19	z	42	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
2	B	14	ASN
2	B	53	ASN
2	B	331	ASN
3	C	25	ASN
4	D	83	ASN
11	L	8	GLN
12	M	33	GLN
13	O	61	GLN
13	O	82	GLN
13	O	124	ASN
13	O	147	ASN
16	V	34	GLN
16	V	118	HIS
19	Z	58	ASN

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Mol	Chain	Res	Type
1	a	315	ASN
2	b	53	ASN
2	b	331	ASN
4	d	83	ASN
4	d	332	GLN
5	e	75	GLN
13	o	124	ASN
13	o	147	ASN
16	v	34	GLN
19	z	31	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

8 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	8,9,10	0.52	0	6,9,11	1.60	3 (50%)
12	FME	M	1	12	8,9,10	0.47	0	6,9,11	2.01	3 (50%)
14	FME	T	1	14	8,9,10	0.52	0	6,9,11	1.76	2 (33%)
19	FME	Z	1	19	8,9,10	0.59	0	6,9,11	2.15	3 (50%)
8	FME	i	1	8	8,9,10	0.48	0	6,9,11	1.57	3 (50%)
12	FME	m	1	12	8,9,10	0.47	0	6,9,11	2.07	2 (33%)
14	FME	t	1	14	8,9,10	0.46	0	6,9,11	1.84	3 (50%)
19	FME	z	1	19	8,9,10	0.46	0	6,9,11	2.09	3 (50%)

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
19	FME	Z	1	19	-	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
19	FME	z	1	19	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	M	1	FME	O1-CN-N	-3.44	119.80	124.76
12	m	1	FME	O1-CN-N	-3.44	119.81	124.76
19	Z	1	FME	O1-CN-N	-3.35	119.93	124.76
19	z	1	FME	O1-CN-N	-3.00	120.43	124.76
14	t	1	FME	O1-CN-N	-2.44	121.25	124.76
14	T	1	FME	O-C-CA	-2.37	119.17	125.44
8	I	1	FME	O1-CN-N	-2.33	121.40	124.76
14	t	1	FME	O-C-CA	-2.33	119.28	125.44
19	Z	1	FME	O-C-CA	-2.26	119.47	125.44
8	i	1	FME	O1-CN-N	-2.17	121.63	124.76
19	z	1	FME	O-C-CA	-2.16	119.72	125.44
8	i	1	FME	O-C-CA	-2.14	119.78	125.44
12	M	1	FME	O-C-CA	-2.03	120.09	125.44
8	I	1	FME	O-C-CA	-2.01	120.12	125.44
8	i	1	FME	CE-SD-CG	2.09	107.52	100.37
8	I	1	FME	CE-SD-CG	2.21	107.93	100.37
12	m	1	FME	CE-SD-CG	2.49	108.86	100.37
12	M	1	FME	CE-SD-CG	2.61	109.27	100.37
14	t	1	FME	CE-SD-CG	2.73	109.68	100.37
19	z	1	FME	CE-SD-CG	2.76	109.81	100.37
14	T	1	FME	CE-SD-CG	2.88	110.19	100.37
19	Z	1	FME	CE-SD-CG	3.08	110.90	100.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 261 ligands modelled in this entry, 24 are unknown and 10 are monoatomic - leaving 227 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	$\#\|Z\| > 2$
21	OER	A	1001	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
24	CLA	A	1005	-	55,73,73	1.87	11 (20%)	61,113,113	1.80	13 (21%)
24	CLA	A	1006	40	55,73,73	1.84	11 (20%)	61,113,113	1.87	14 (22%)
25	PHO	A	1007	-	67,69,69	1.99	15 (22%)	84,99,99	1.94	17 (20%)
24	CLA	A	1008	-	55,73,73	1.87	11 (20%)	61,113,113	1.82	14 (22%)
26	BCR	A	1009	-	41,41,41	3.77	14 (34%)	56,56,56	8.02	40 (71%)
27	PL9	A	1010	-	55,55,55	0.68	2 (3%)	68,69,69	1.71	17 (25%)
28	SQD	A	1011	-	53,54,54	1.36	3 (5%)	61,65,65	1.45	7 (11%)
29	LMG	A	1012	-	51,51,55	0.91	2 (3%)	59,59,63	0.93	2 (3%)
30	DMS	A	1013	-	3,3,3	2.49	1 (33%)	3,3,3	0.52	0
30	DMS	A	1014	-	3,3,3	2.63	1 (33%)	3,3,3	0.49	0
28	SQD	A	1016	-	53,54,54	1.38	3 (5%)	61,65,65	1.27	5 (8%)
32	LMT	A	1017	-	36,36,36	0.52	1 (2%)	47,47,47	0.88	1 (2%)
32	LMT	A	1018	-	36,36,36	0.52	0	47,47,47	1.03	5 (10%)
33	GOL	A	1019	-	5,5,5	0.22	0	5,5,5	0.26	0
24	CLA	B	601	40	55,73,73	1.90	12 (21%)	61,113,113	1.91	16 (26%)
24	CLA	B	602	-	55,73,73	1.88	12 (21%)	61,113,113	1.78	13 (21%)
24	CLA	B	603	-	55,73,73	1.82	11 (20%)	61,113,113	2.07	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	604	-	55,73,73	1.84	10 (18%)	61,113,113	1.89	15 (24%)
24	CLA	B	605	-	55,73,73	1.83	11 (20%)	61,113,113	1.79	14 (22%)
24	CLA	B	606	-	55,73,73	1.89	12 (21%)	61,113,113	1.88	14 (22%)
24	CLA	B	607	40	55,73,73	1.78	11 (20%)	61,113,113	1.90	14 (22%)
24	CLA	B	608	-	55,73,73	1.85	12 (21%)	61,113,113	1.86	15 (24%)
24	CLA	B	609	-	55,73,73	1.86	11 (20%)	61,113,113	1.76	11 (18%)
24	CLA	B	610	40	55,73,73	1.84	11 (20%)	61,113,113	1.80	13 (21%)
24	CLA	B	611	-	55,73,73	1.90	11 (20%)	61,113,113	1.73	13 (21%)
24	CLA	B	612	-	55,73,73	1.90	11 (20%)	61,113,113	1.75	14 (22%)
24	CLA	B	613	-	55,73,73	1.85	11 (20%)	61,113,113	1.71	13 (21%)
24	CLA	B	614	-	55,73,73	1.89	11 (20%)	61,113,113	1.93	14 (22%)
24	CLA	B	615	-	55,73,73	1.92	12 (21%)	61,113,113	1.78	14 (22%)
24	CLA	B	616	-	55,73,73	1.84	11 (20%)	61,113,113	1.87	16 (26%)
26	BCR	B	617	-	41,41,41	3.76	15 (36%)	56,56,56	7.95	39 (69%)
26	BCR	B	618	-	41,41,41	3.76	14 (34%)	56,56,56	8.23	42 (75%)
26	BCR	B	619	-	41,41,41	3.81	15 (36%)	56,56,56	7.78	36 (64%)
28	SQD	B	620[A]	-	53,54,54	1.36	3 (5%)	61,65,65	1.17	5 (8%)
28	SQD	B	620[B]	-	53,54,54	1.35	3 (5%)	61,65,65	1.22	6 (9%)
34	LHG	B	621	-	48,48,48	0.90	2 (4%)	49,54,54	0.95	2 (4%)
29	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	0.92	2 (3%)
32	LMT	B	623	-	36,36,36	0.47	0	47,47,47	1.04	2 (4%)
35	HTG	B	624	-	19,19,19	0.96	2 (10%)	22,24,24	1.94	1 (4%)
30	DMS	B	626	-	3,3,3	2.50	1 (33%)	3,3,3	0.31	0
30	DMS	B	627	-	3,3,3	2.53	1 (33%)	3,3,3	0.41	0
35	HTG	B	628	-	19,19,19	0.98	2 (10%)	22,24,24	1.60	1 (4%)
35	HTG	B	629	-	19,19,19	0.95	2 (10%)	22,24,24	1.68	1 (4%)
33	GOL	B	631	-	5,5,5	0.21	0	5,5,5	0.24	0
30	DMS	B	632	-	3,3,3	2.61	1 (33%)	3,3,3	0.44	0
30	DMS	B	633	-	3,3,3	2.64	1 (33%)	3,3,3	0.51	0
30	DMS	B	634	-	3,3,3	2.63	1 (33%)	3,3,3	0.44	0
24	CLA	C	501	-	55,73,73	1.87	12 (21%)	61,113,113	1.82	14 (22%)
24	CLA	C	502	-	55,73,73	1.84	11 (20%)	61,113,113	1.81	14 (22%)
24	CLA	C	503	-	55,73,73	1.92	11 (20%)	61,113,113	1.68	13 (21%)
24	CLA	C	504	40	55,73,73	1.89	12 (21%)	61,113,113	1.84	13 (21%)
24	CLA	C	505	-	55,73,73	1.87	12 (21%)	61,113,113	1.79	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	506	-	55,73,73	1.91	12 (21%)	61,113,113	1.78	14 (22%)
24	CLA	C	507	40	55,73,73	1.93	11 (20%)	61,113,113	1.89	13 (21%)
24	CLA	C	508	-	55,73,73	1.91	11 (20%)	61,113,113	1.64	11 (18%)
24	CLA	C	509	-	55,73,73	1.87	11 (20%)	61,113,113	1.90	13 (21%)
24	CLA	C	510	-	55,73,73	1.85	11 (20%)	61,113,113	1.90	12 (19%)
24	CLA	C	511	3	55,73,73	1.93	11 (20%)	61,113,113	1.71	11 (18%)
24	CLA	C	512	-	55,73,73	1.92	12 (21%)	61,113,113	1.76	15 (24%)
24	CLA	C	513	-	55,73,73	1.96	12 (21%)	61,113,113	1.68	14 (22%)
26	BCR	C	514	-	41,41,41	3.87	15 (36%)	56,56,56	8.06	39 (69%)
36	DGD	C	515	-	63,63,67	0.84	2 (3%)	77,77,81	0.88	2 (2%)
36	DGD	C	516	-	63,63,67	0.88	3 (4%)	77,77,81	0.96	5 (6%)
36	DGD	C	517	-	63,63,67	0.82	2 (3%)	77,77,81	0.88	3 (3%)
29	LMG	C	518	-	51,51,55	0.94	2 (3%)	59,59,63	0.88	2 (3%)
29	LMG	C	519	-	51,51,55	0.96	2 (3%)	59,59,63	1.06	4 (6%)
32	LMT	C	520	-	36,36,36	0.50	0	47,47,47	1.05	2 (4%)
35	HTG	C	521	-	19,19,19	0.98	2 (10%)	22,24,24	1.59	1 (4%)
35	HTG	C	522	-	19,19,19	0.94	1 (5%)	22,24,24	2.14	5 (22%)
30	DMS	C	523	-	3,3,3	2.50	1 (33%)	3,3,3	0.34	0
30	DMS	C	524	-	3,3,3	2.54	1 (33%)	3,3,3	0.42	0
30	DMS	C	525	-	3,3,3	2.62	1 (33%)	3,3,3	0.49	0
30	DMS	C	526	-	3,3,3	2.61	1 (33%)	3,3,3	0.45	0
30	DMS	C	527	-	3,3,3	2.61	1 (33%)	3,3,3	0.50	0
37	BCT	D	401	22	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	D	402	-	55,73,73	1.84	11 (20%)	61,113,113	1.88	15 (24%)
24	CLA	D	403	40	55,73,73	1.81	10 (18%)	61,113,113	2.00	16 (26%)
25	PHO	D	404	-	67,69,69	2.06	16 (23%)	84,99,99	1.95	22 (26%)
24	CLA	D	405	-	55,73,73	1.90	12 (21%)	61,113,113	1.68	14 (22%)
26	BCR	D	406	-	41,41,41	3.81	14 (34%)	56,56,56	7.95	45 (80%)
27	PL9	D	407	-	55,55,55	0.75	2 (3%)	68,69,69	1.53	15 (22%)
28	SQD	D	408	-	42,43,54	1.48	3 (7%)	50,54,65	1.87	9 (18%)
34	LHG	D	409	-	48,48,48	0.88	2 (4%)	49,54,54	0.98	4 (8%)
34	LHG	D	410	-	48,48,48	0.85	2 (4%)	49,54,54	0.98	3 (6%)
34	LHG	D	411	-	48,48,48	0.91	2 (4%)	49,54,54	0.95	2 (4%)
29	LMG	D	412	39	51,51,55	0.87	2 (3%)	59,59,63	0.81	1 (1%)
35	HTG	D	413	-	19,19,19	0.97	2 (10%)	22,24,24	1.63	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	DMS	D	416	-	3,3,3	2.66	1 (33%)	3,3,3	0.68	0
30	DMS	D	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.39	0
33	GOL	D	418	-	5,5,5	0.24	0	5,5,5	0.29	0
35	HTG	D	419	-	19,19,19	0.94	1 (5%)	22,24,24	2.04	1 (4%)
34	LHG	E	101	-	48,48,48	0.93	2 (4%)	49,54,54	0.98	2 (4%)
38	HEM	F	101	5,6	30,50,50	2.18	7 (23%)	24,82,82	2.39	10 (41%)
26	BCR	H	101	-	41,41,41	3.78	15 (36%)	56,56,56	8.18	41 (73%)
36	DGD	H	102	-	63,63,67	0.84	3 (4%)	77,77,81	0.83	3 (3%)
26	BCR	J	101	-	41,41,41	3.83	14 (34%)	56,56,56	8.55	40 (71%)
26	BCR	K	101	-	41,41,41	3.80	15 (36%)	56,56,56	7.81	41 (73%)
26	BCR	K	102	-	41,41,41	3.88	15 (36%)	56,56,56	8.27	41 (73%)
32	LMT	M	101	-	36,36,36	0.47	0	47,47,47	0.91	0
32	LMT	M	102	-	36,36,36	0.48	0	47,47,47	0.77	1 (2%)
30	DMS	O	301	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
30	DMS	O	302	-	3,3,3	2.62	1 (33%)	3,3,3	0.55	0
26	BCR	T	101	-	41,41,41	3.85	15 (36%)	56,56,56	7.82	39 (69%)
30	DMS	U	201	-	3,3,3	2.59	1 (33%)	3,3,3	0.44	0
38	HEM	V	201	16	30,50,50	2.30	10 (33%)	24,82,82	2.50	13 (54%)
35	HTG	V	202	-	19,19,19	0.92	2 (10%)	22,24,24	1.81	3 (13%)
30	DMS	V	203	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
33	GOL	V	204	-	5,5,5	0.24	0	5,5,5	0.20	0
30	DMS	V	205	-	3,3,3	2.62	1 (33%)	3,3,3	0.47	0
33	GOL	V	206	-	5,5,5	0.23	0	5,5,5	0.22	0
33	GOL	V	207	-	5,5,5	0.20	0	5,5,5	0.31	0
29	LMG	Z	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.02	3 (5%)
28	SQD	a	401	-	53,54,54	1.39	3 (5%)	61,65,65	1.28	5 (8%)
32	LMT	a	402	-	36,36,36	0.57	1 (2%)	47,47,47	0.88	3 (6%)
21	OER	a	403	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
24	CLA	a	407	-	55,73,73	1.88	10 (18%)	61,113,113	1.67	10 (16%)
24	CLA	a	408	40	55,73,73	1.87	10 (18%)	61,113,113	1.84	13 (21%)
24	CLA	a	409	40	55,73,73	1.79	10 (18%)	61,113,113	1.79	14 (22%)
25	PHO	a	410	-	67,69,69	2.04	15 (22%)	84,99,99	1.91	19 (22%)
25	PHO	a	411	-	67,69,69	2.06	16 (23%)	84,99,99	2.01	21 (25%)
24	CLA	a	412	-	55,73,73	1.84	11 (20%)	61,113,113	1.88	16 (26%)
26	BCR	a	413	-	41,41,41	3.69	14 (34%)	56,56,56	8.30	41 (73%)
27	PL9	a	414	-	55,55,55	0.70	2 (3%)	68,69,69	1.56	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	a	415	-	51,51,55	0.92	2 (3%)	59,59,63	0.99	3 (5%)
32	LMT	a	416	-	36,36,36	0.49	0	47,47,47	0.78	1 (2%)
30	DMS	a	417	-	3,3,3	2.51	1 (33%)	3,3,3	0.35	0
30	DMS	a	418	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
33	GOL	a	420	-	5,5,5	0.24	0	5,5,5	0.24	0
35	HTG	b	601	-	19,19,19	0.94	1 (5%)	22,24,24	1.68	1 (4%)
35	HTG	b	602	-	19,19,19	0.95	2 (10%)	22,24,24	1.79	1 (4%)
24	CLA	b	604	40	55,73,73	1.97	12 (21%)	61,113,113	1.79	14 (22%)
24	CLA	b	605	-	55,73,73	1.92	12 (21%)	61,113,113	1.69	13 (21%)
24	CLA	b	606	-	55,73,73	1.88	11 (20%)	61,113,113	1.85	14 (22%)
24	CLA	b	607	-	55,73,73	1.87	11 (20%)	61,113,113	1.88	13 (21%)
24	CLA	b	608	-	55,73,73	1.82	11 (20%)	61,113,113	1.85	13 (21%)
24	CLA	b	609	-	55,73,73	1.94	12 (21%)	61,113,113	1.84	12 (19%)
24	CLA	b	610	40	55,73,73	1.84	12 (21%)	61,113,113	1.91	16 (26%)
24	CLA	b	611	-	55,73,73	1.86	11 (20%)	61,113,113	1.88	15 (24%)
24	CLA	b	612	-	55,73,73	1.87	12 (21%)	61,113,113	1.78	12 (19%)
24	CLA	b	613	40	55,73,73	1.88	11 (20%)	61,113,113	1.69	11 (18%)
24	CLA	b	614	-	55,73,73	1.82	11 (20%)	61,113,113	1.70	14 (22%)
24	CLA	b	615	-	55,73,73	1.89	11 (20%)	61,113,113	1.84	13 (21%)
24	CLA	b	616	-	55,73,73	1.84	11 (20%)	61,113,113	1.80	13 (21%)
24	CLA	b	617	-	55,73,73	1.84	11 (20%)	61,113,113	1.92	16 (26%)
24	CLA	b	618	-	55,73,73	1.89	11 (20%)	61,113,113	1.71	14 (22%)
24	CLA	b	619	-	55,73,73	1.88	11 (20%)	61,113,113	1.80	12 (19%)
26	BCR	b	620	-	41,41,41	3.76	14 (34%)	56,56,56	7.90	41 (73%)
26	BCR	b	621	-	41,41,41	3.79	14 (34%)	56,56,56	8.23	43 (76%)
26	BCR	b	622	-	41,41,41	3.85	15 (36%)	56,56,56	7.94	36 (64%)
28	SQD	b	623[A]	-	53,54,54	1.36	3 (5%)	61,65,65	1.21	5 (8%)
28	SQD	b	623[B]	-	53,54,54	1.35	3 (5%)	61,65,65	1.14	5 (8%)
34	LHG	b	624	-	48,48,48	0.88	2 (4%)	49,54,54	0.98	2 (4%)
32	LMT	b	625	-	36,36,36	0.50	0	47,47,47	1.26	5 (10%)
35	HTG	b	626	-	19,19,19	0.92	1 (5%)	22,24,24	1.45	2 (9%)
30	DMS	b	628	-	3,3,3	2.47	1 (33%)	3,3,3	0.45	0
30	DMS	b	629	-	3,3,3	2.61	1 (33%)	3,3,3	0.40	0
35	HTG	b	630	-	19,19,19	1.00	2 (10%)	22,24,24	2.09	2 (9%)
32	LMT	b	631	-	36,36,36	0.49	0	47,47,47	0.85	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	GOL	b	632	-	5,5,5	0.18	0	5,5,5	0.23	0
30	DMS	b	633	-	3,3,3	2.62	1 (33%)	3,3,3	0.59	0
30	DMS	b	634	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
30	DMS	b	635	-	3,3,3	2.62	1 (33%)	3,3,3	0.40	0
24	CLA	c	501	-	55,73,73	1.89	12 (21%)	61,113,113	1.86	13 (21%)
24	CLA	c	502	-	55,73,73	1.89	11 (20%)	61,113,113	1.77	14 (22%)
24	CLA	c	503	-	55,73,73	1.93	12 (21%)	61,113,113	1.65	12 (19%)
24	CLA	c	504	40	55,73,73	1.89	12 (21%)	61,113,113	1.84	14 (22%)
24	CLA	c	505	-	55,73,73	1.91	12 (21%)	61,113,113	1.84	14 (22%)
24	CLA	c	506	-	55,73,73	1.92	12 (21%)	61,113,113	1.77	13 (21%)
24	CLA	c	507	40	55,73,73	1.93	11 (20%)	61,113,113	1.91	13 (21%)
24	CLA	c	508	-	55,73,73	1.93	12 (21%)	61,113,113	1.71	13 (21%)
24	CLA	c	509	-	55,73,73	1.92	12 (21%)	61,113,113	1.81	15 (24%)
24	CLA	c	510	-	55,73,73	1.89	12 (21%)	61,113,113	1.80	14 (22%)
24	CLA	c	511	3	55,73,73	1.93	11 (20%)	61,113,113	1.67	13 (21%)
24	CLA	c	512	-	55,73,73	1.94	12 (21%)	61,113,113	1.83	13 (21%)
24	CLA	c	513	-	55,73,73	1.94	12 (21%)	61,113,113	1.76	16 (26%)
26	BCR	c	514	-	41,41,41	3.85	15 (36%)	56,56,56	8.52	41 (73%)
36	DGD	c	515	-	63,63,67	0.86	3 (4%)	77,77,81	0.91	2 (2%)
36	DGD	c	516	-	63,63,67	0.89	2 (3%)	77,77,81	0.94	4 (5%)
36	DGD	c	517	-	63,63,67	0.86	2 (3%)	77,77,81	0.82	3 (3%)
28	SQD	c	518	-	53,54,54	1.36	3 (5%)	61,65,65	1.48	8 (13%)
29	LMG	c	519	-	51,51,55	0.94	2 (3%)	59,59,63	0.89	2 (3%)
29	LMG	c	520	-	51,51,55	0.96	3 (5%)	59,59,63	1.07	4 (6%)
29	LMG	c	521	-	51,51,55	0.97	2 (3%)	59,59,63	1.07	2 (3%)
35	HTG	c	522	-	19,19,19	0.93	2 (10%)	22,24,24	1.54	1 (4%)
30	DMS	c	524	-	3,3,3	2.54	1 (33%)	3,3,3	0.30	0
35	HTG	c	525	-	19,19,19	0.98	2 (10%)	22,24,24	1.51	1 (4%)
30	DMS	c	526	-	3,3,3	2.61	1 (33%)	3,3,3	0.41	0
30	DMS	c	527	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
30	DMS	c	528	-	3,3,3	2.62	1 (33%)	3,3,3	0.49	0
30	DMS	c	529	-	3,3,3	2.56	1 (33%)	3,3,3	0.44	0
37	BCT	d	401	22	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	d	402	-	55,73,73	1.83	11 (20%)	61,113,113	1.81	14 (22%)
24	CLA	d	403	-	55,73,73	1.93	12 (21%)	61,113,113	1.62	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	d	404	-	41,41,41	3.86	15 (36%)	56,56,56	8.03	42 (75%)
27	PL9	d	405	-	55,55,55	0.74	2 (3%)	68,69,69	1.46	12 (17%)
34	LHG	d	406	-	48,48,48	0.91	2 (4%)	49,54,54	0.94	3 (6%)
34	LHG	d	407	-	48,48,48	0.85	2 (4%)	49,54,54	0.93	3 (6%)
34	LHG	d	408	-	48,48,48	0.92	2 (4%)	49,54,54	0.95	2 (4%)
29	LMG	d	409	39	51,51,55	0.91	2 (3%)	59,59,63	0.87	2 (3%)
35	HTG	d	410	-	19,19,19	0.98	1 (5%)	22,24,24	1.68	1 (4%)
30	DMS	d	413	-	3,3,3	2.64	1 (33%)	3,3,3	0.54	0
30	DMS	d	414	-	3,3,3	2.61	1 (33%)	3,3,3	0.38	0
33	GOL	d	415	-	5,5,5	0.23	0	5,5,5	0.30	0
35	HTG	d	416	-	19,19,19	0.94	1 (5%)	22,24,24	2.07	1 (4%)
33	GOL	d	417	-	5,5,5	0.27	0	5,5,5	0.15	0
34	LHG	e	101	-	48,48,48	0.94	2 (4%)	49,54,54	1.01	2 (4%)
38	HEM	f	101	5,6	30,50,50	2.13	10 (33%)	24,82,82	2.43	9 (37%)
28	SQD	f	102	-	42,43,54	1.55	4 (9%)	50,54,65	1.46	7 (14%)
32	LMT	f	103	-	36,36,36	0.51	0	47,47,47	0.68	0
26	BCR	h	101	-	41,41,41	3.81	14 (34%)	56,56,56	8.27	42 (75%)
36	DGD	h	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.85	2 (2%)
32	LMT	i	102	-	36,36,36	0.50	0	47,47,47	1.04	2 (4%)
26	BCR	k	101	-	41,41,41	3.81	15 (36%)	56,56,56	8.42	41 (73%)
26	BCR	k	102	-	41,41,41	3.75	15 (36%)	56,56,56	8.19	38 (67%)
32	LMT	m	101	-	36,36,36	0.46	0	47,47,47	0.71	0
29	LMG	m	102	-	51,51,55	0.95	2 (3%)	59,59,63	1.12	4 (6%)
32	LMT	m	103	-	36,36,36	0.51	1 (2%)	47,47,47	0.84	1 (2%)
35	HTG	o	301	-	19,19,19	0.96	1 (5%)	22,24,24	1.62	1 (4%)
26	BCR	t	101	-	41,41,41	3.83	15 (36%)	56,56,56	7.88	40 (71%)
32	LMT	t	103	-	36,36,36	0.44	0	47,47,47	1.06	2 (4%)
30	DMS	u	201	-	3,3,3	2.59	1 (33%)	3,3,3	0.46	0
38	HEM	v	201	16	30,50,50	2.30	9 (30%)	24,82,82	2.37	8 (33%)
30	DMS	v	202	-	3,3,3	2.58	1 (33%)	3,3,3	0.46	0
33	GOL	v	203	-	5,5,5	0.28	0	5,5,5	0.31	0
33	GOL	v	204	-	5,5,5	0.21	0	5,5,5	0.26	0
26	BCR	y	101	-	41,41,41	3.85	15 (36%)	56,56,56	8.63	44 (78%)

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
21	OER	A	1001	1,3,40	-	0/0/68/68	0/0/6/6
24	CLA	A	1005	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	1006	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	A	1007	-	-	0/53/103/103	0/1/6/6
24	CLA	A	1008	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	A	1009	-	-	1/29/63/63	0/2/2/2
27	PL9	A	1010	-	-	0/53/73/73	0/1/1/1
28	SQD	A	1011	-	-	0/49/69/69	0/1/1/1
29	LMG	A	1012	-	-	0/46/66/70	0/1/1/1
30	DMS	A	1013	-	-	0/0/0/0	0/0/0/0
30	DMS	A	1014	-	-	0/0/0/0	0/0/0/0
28	SQD	A	1016	-	-	0/49/69/69	0/1/1/1
32	LMT	A	1017	-	-	0/21/61/61	0/2/2/2
32	LMT	A	1018	-	-	0/21/61/61	0/2/2/2
33	GOL	A	1019	-	-	0/4/4/4	0/0/0/0
24	CLA	B	601	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	617	-	-	0/29/63/63	0/2/2/2
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
28	SQD	B	620[A]	-	-	2/49/69/69	0/1/1/1
28	SQD	B	620[B]	-	-	0/49/69/69	0/1/1/1
34	LHG	B	621	-	-	0/53/53/53	0/0/0/0
29	LMG	B	622	-	-	0/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LMT	B	623	-	-	0/21/61/61	0/2/2/2
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
30	DMS	B	626	-	-	0/0/0/0	0/0/0/0
30	DMS	B	627	-	-	0/0/0/0	0/0/0/0
35	HTG	B	628	-	-	0/10/30/30	0/1/1/1
35	HTG	B	629	-	-	0/10/30/30	0/1/1/1
33	GOL	B	631	-	-	0/4/4/4	0/0/0/0
30	DMS	B	632	-	-	0/0/0/0	0/0/0/0
30	DMS	B	633	-	-	0/0/0/0	0/0/0/0
30	DMS	B	634	-	-	0/0/0/0	0/0/0/0
24	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	507	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
36	DGD	C	515	-	-	0/51/91/95	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
29	LMG	C	518	-	-	0/46/66/70	0/1/1/1
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
32	LMT	C	520	-	-	0/21/61/61	0/2/2/2
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
30	DMS	C	523	-	-	0/0/0/0	0/0/0/0
30	DMS	C	524	-	-	0/0/0/0	0/0/0/0
30	DMS	C	525	-	-	0/0/0/0	0/0/0/0
30	DMS	C	526	-	-	0/0/0/0	0/0/0/0
30	DMS	C	527	-	-	0/0/0/0	0/0/0/0
37	BCT	D	401	22	-	0/0/0/0	0/0/0/0
24	CLA	D	402	-	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	CLA	D	403	40	1/1/20/25	0/37/135/135	0/0/9/9
25	PHO	D	404	-	-	0/53/103/103	0/1/6/6
24	CLA	D	405	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
27	PL9	D	407	-	-	0/53/73/73	0/1/1/1
28	SQD	D	408	-	-	0/38/58/69	0/1/1/1
34	LHG	D	409	-	-	0/53/53/53	0/0/0/0
34	LHG	D	410	-	-	0/53/53/53	0/0/0/0
34	LHG	D	411	-	-	0/53/53/53	0/0/0/0
29	LMG	D	412	39	-	0/46/66/70	0/1/1/1
35	HTG	D	413	-	-	0/10/30/30	0/1/1/1
30	DMS	D	416	-	-	0/0/0/0	0/0/0/0
30	DMS	D	417	-	-	0/0/0/0	0/0/0/0
33	GOL	D	418	-	-	0/4/4/4	0/0/0/0
35	HTG	D	419	-	-	0/10/30/30	0/1/1/1
34	LHG	E	101	-	-	0/53/53/53	0/0/0/0
38	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
26	BCR	H	101	-	-	2/29/63/63	0/2/2/2
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	J	101	-	-	0/29/63/63	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
26	BCR	K	102	-	-	1/29/63/63	0/2/2/2
32	LMT	M	101	-	-	0/21/61/61	0/2/2/2
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
30	DMS	O	301	-	-	0/0/0/0	0/0/0/0
30	DMS	O	302	-	-	0/0/0/0	0/0/0/0
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
30	DMS	U	201	-	-	0/0/0/0	0/0/0/0
38	HEM	V	201	16	-	0/10/54/54	0/0/8/8
35	HTG	V	202	-	-	0/10/30/30	0/1/1/1
30	DMS	V	203	-	-	0/0/0/0	0/0/0/0
33	GOL	V	204	-	-	0/4/4/4	0/0/0/0
30	DMS	V	205	-	-	0/0/0/0	0/0/0/0
33	GOL	V	206	-	-	0/4/4/4	0/0/0/0
33	GOL	V	207	-	-	0/4/4/4	0/0/0/0
29	LMG	Z	101	-	-	0/46/66/70	0/1/1/1
28	SQD	a	401	-	-	0/49/69/69	0/1/1/1
32	LMT	a	402	-	-	0/21/61/61	0/2/2/2
21	OER	a	403	1,3,40	-	0/0/68/68	0/0/6/6
24	CLA	a	407	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	408	40	1/1/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	a	409	40	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	a	410	-	-	0/53/103/103	0/1/6/6
25	PHO	a	411	-	-	0/53/103/103	0/1/6/6
24	CLA	a	412	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
27	PL9	a	414	-	-	0/53/73/73	0/1/1/1
29	LMG	a	415	-	-	0/46/66/70	0/1/1/1
32	LMT	a	416	-	-	0/21/61/61	0/2/2/2
30	DMS	a	417	-	-	0/0/0/0	0/0/0/0
30	DMS	a	418	-	-	0/0/0/0	0/0/0/0
33	GOL	a	420	-	-	0/4/4/4	0/0/0/0
35	HTG	b	601	-	-	0/10/30/30	0/1/1/1
35	HTG	b	602	-	-	0/10/30/30	0/1/1/1
24	CLA	b	604	40	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	-	0/37/135/135	0/0/9/9
24	CLA	b	613	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	620	-	-	0/29/63/63	0/2/2/2
26	BCR	b	621	-	-	0/29/63/63	0/2/2/2
26	BCR	b	622	-	-	1/29/63/63	0/2/2/2
28	SQD	b	623[A]	-	-	0/49/69/69	0/1/1/1
28	SQD	b	623[B]	-	-	1/49/69/69	0/1/1/1
34	LHG	b	624	-	-	0/53/53/53	0/0/0/0
32	LMT	b	625	-	-	0/21/61/61	0/2/2/2
35	HTG	b	626	-	-	0/10/30/30	0/1/1/1
30	DMS	b	628	-	-	0/0/0/0	0/0/0/0
30	DMS	b	629	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	b	630	-	-	0/10/30/30	0/1/1/1
32	LMT	b	631	-	-	0/21/61/61	0/2/2/2
33	GOL	b	632	-	-	0/4/4/4	0/0/0/0
30	DMS	b	633	-	-	0/0/0/0	0/0/0/0
30	DMS	b	634	-	-	0/0/0/0	0/0/0/0
30	DMS	b	635	-	-	0/0/0/0	0/0/0/0
24	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	503	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	40	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	505	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	40	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	511	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	c	514	-	-	1/29/63/63	0/2/2/2
36	DGD	c	515	-	-	0/51/91/95	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
28	SQD	c	518	-	-	0/49/69/69	0/1/1/1
29	LMG	c	519	-	-	0/46/66/70	0/1/1/1
29	LMG	c	520	-	-	0/46/66/70	0/1/1/1
29	LMG	c	521	-	-	0/46/66/70	0/1/1/1
35	HTG	c	522	-	-	0/10/30/30	0/1/1/1
30	DMS	c	524	-	-	0/0/0/0	0/0/0/0
35	HTG	c	525	-	-	0/10/30/30	0/1/1/1
30	DMS	c	526	-	-	0/0/0/0	0/0/0/0
30	DMS	c	527	-	-	0/0/0/0	0/0/0/0
30	DMS	c	528	-	-	0/0/0/0	0/0/0/0
30	DMS	c	529	-	-	0/0/0/0	0/0/0/0
37	BCT	d	401	22	-	0/0/0/0	0/0/0/0
24	CLA	d	402	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	d	404	-	-	0/29/63/63	0/2/2/2
27	PL9	d	405	-	-	0/53/73/73	0/1/1/1
34	LHG	d	406	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LHG	d	407	-	-	0/53/53/53	0/0/0/0
34	LHG	d	408	-	-	0/53/53/53	0/0/0/0
29	LMG	d	409	39	-	0/46/66/70	0/1/1/1
35	HTG	d	410	-	-	0/10/30/30	0/1/1/1
30	DMS	d	413	-	-	0/0/0/0	0/0/0/0
30	DMS	d	414	-	-	0/0/0/0	0/0/0/0
33	GOL	d	415	-	-	0/4/4/4	0/0/0/0
35	HTG	d	416	-	-	0/10/30/30	0/1/1/1
33	GOL	d	417	-	-	0/4/4/4	0/0/0/0
34	LHG	e	101	-	-	0/53/53/53	0/0/0/0
38	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
28	SQD	f	102	-	-	0/38/58/69	0/1/1/1
32	LMT	f	103	-	-	0/21/61/61	0/2/2/2
26	BCR	h	101	-	-	0/29/63/63	0/2/2/2
36	DGD	h	102	-	-	0/51/91/95	0/2/2/2
32	LMT	i	102	-	-	0/21/61/61	0/2/2/2
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
32	LMT	m	101	-	-	0/21/61/61	0/2/2/2
29	LMG	m	102	-	-	0/46/66/70	0/1/1/1
32	LMT	m	103	-	-	0/21/61/61	0/2/2/2
35	HTG	o	301	-	-	0/10/30/30	0/1/1/1
26	BCR	t	101	-	-	0/29/63/63	0/2/2/2
32	LMT	t	103	-	-	0/21/61/61	0/2/2/2
30	DMS	u	201	-	-	0/0/0/0	0/0/0/0
38	HEM	v	201	16	-	0/10/54/54	0/0/8/8
30	DMS	v	202	-	-	0/0/0/0	0/0/0/0
33	GOL	v	203	-	-	0/4/4/4	0/0/0/0
33	GOL	v	204	-	-	0/4/4/4	0/0/0/0
26	BCR	y	101	-	-	1/29/63/63	0/2/2/2

All (1382) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	514	BCR	C8-C9	-8.68	1.26	1.45
26	t	101	BCR	C8-C9	-8.61	1.26	1.45
26	k	102	BCR	C12-C13	-8.59	1.26	1.45
26	K	101	BCR	C8-C9	-8.59	1.26	1.45
26	D	406	BCR	C19-C18	-8.58	1.26	1.45
26	b	622	BCR	C8-C9	-8.57	1.26	1.45
26	d	404	BCR	C19-C18	-8.56	1.26	1.45
26	B	618	BCR	C8-C9	-8.55	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	k	101	BCR	C8-C9	-8.54	1.27	1.45
26	B	619	BCR	C8-C9	-8.54	1.27	1.45
26	C	514	BCR	C8-C9	-8.54	1.27	1.45
26	k	102	BCR	C8-C9	-8.53	1.27	1.45
26	b	622	BCR	C12-C13	-8.51	1.27	1.45
26	K	102	BCR	C12-C13	-8.50	1.27	1.45
26	C	514	BCR	C19-C18	-8.49	1.27	1.45
26	c	514	BCR	C12-C13	-8.48	1.27	1.45
26	K	102	BCR	C19-C18	-8.48	1.27	1.45
26	t	101	BCR	C19-C18	-8.47	1.27	1.45
26	H	101	BCR	C8-C9	-8.47	1.27	1.45
26	B	617	BCR	C8-C9	-8.47	1.27	1.45
26	y	101	BCR	C12-C13	-8.46	1.27	1.45
26	y	101	BCR	C19-C18	-8.46	1.27	1.45
26	d	404	BCR	C8-C9	-8.45	1.27	1.45
26	T	101	BCR	C8-C9	-8.45	1.27	1.45
26	T	101	BCR	C19-C18	-8.44	1.27	1.45
26	K	102	BCR	C8-C9	-8.44	1.27	1.45
26	C	514	BCR	C12-C13	-8.41	1.27	1.45
26	b	622	BCR	C19-C18	-8.41	1.27	1.45
26	B	619	BCR	C12-C13	-8.40	1.27	1.45
26	y	101	BCR	C8-C9	-8.40	1.27	1.45
26	h	101	BCR	C19-C18	-8.39	1.27	1.45
26	t	101	BCR	C12-C13	-8.39	1.27	1.45
26	K	101	BCR	C19-C18	-8.38	1.27	1.45
26	k	102	BCR	C19-C18	-8.38	1.27	1.45
26	b	620	BCR	C8-C9	-8.37	1.27	1.45
26	J	101	BCR	C12-C13	-8.37	1.27	1.45
26	k	101	BCR	C19-C18	-8.37	1.27	1.45
26	A	1009	BCR	C8-C9	-8.36	1.27	1.45
26	B	617	BCR	C12-C13	-8.36	1.27	1.45
26	d	404	BCR	C12-C13	-8.36	1.27	1.45
26	h	101	BCR	C8-C9	-8.35	1.27	1.45
26	B	618	BCR	C12-C13	-8.35	1.27	1.45
26	k	101	BCR	C12-C13	-8.35	1.27	1.45
26	T	101	BCR	C12-C13	-8.34	1.27	1.45
26	b	620	BCR	C12-C13	-8.34	1.27	1.45
26	D	406	BCR	C8-C9	-8.33	1.27	1.45
26	h	101	BCR	C12-C13	-8.33	1.27	1.45
26	J	101	BCR	C19-C18	-8.32	1.27	1.45
26	H	101	BCR	C12-C13	-8.32	1.27	1.45
26	J	101	BCR	C8-C9	-8.32	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	406	BCR	C12-C13	-8.31	1.27	1.45
26	H	101	BCR	C19-C18	-8.30	1.27	1.45
26	b	621	BCR	C8-C9	-8.30	1.27	1.45
26	b	620	BCR	C19-C18	-8.29	1.27	1.45
26	A	1009	BCR	C19-C18	-8.29	1.27	1.45
26	c	514	BCR	C19-C18	-8.28	1.27	1.45
26	A	1009	BCR	C12-C13	-8.27	1.27	1.45
26	b	621	BCR	C19-C18	-8.27	1.27	1.45
26	B	618	BCR	C19-C18	-8.26	1.27	1.45
26	b	621	BCR	C12-C13	-8.24	1.27	1.45
26	B	619	BCR	C19-C18	-8.23	1.27	1.45
26	K	101	BCR	C12-C13	-8.22	1.27	1.45
26	a	413	BCR	C8-C9	-8.19	1.27	1.45
26	a	413	BCR	C12-C13	-8.15	1.27	1.45
26	B	617	BCR	C19-C18	-8.15	1.27	1.45
26	a	413	BCR	C19-C18	-8.04	1.28	1.45
38	v	201	HEM	C3B-C4B	-8.04	1.44	1.51
26	C	514	BCR	C20-C21	-7.84	1.19	1.43
26	K	102	BCR	C20-C21	-7.83	1.19	1.43
26	y	101	BCR	C20-C21	-7.79	1.19	1.43
26	K	102	BCR	C16-C17	-7.77	1.19	1.43
26	J	101	BCR	C16-C17	-7.77	1.19	1.43
26	d	404	BCR	C20-C21	-7.76	1.19	1.43
26	D	406	BCR	C20-C21	-7.76	1.19	1.43
26	b	622	BCR	C20-C21	-7.73	1.19	1.43
26	c	514	BCR	C16-C17	-7.71	1.19	1.43
26	B	619	BCR	C20-C21	-7.69	1.19	1.43
26	h	101	BCR	C20-C21	-7.69	1.19	1.43
26	H	101	BCR	C20-C21	-7.68	1.19	1.43
26	B	618	BCR	C20-C21	-7.68	1.19	1.43
26	T	101	BCR	C16-C17	-7.68	1.19	1.43
26	A	1009	BCR	C20-C21	-7.68	1.19	1.43
26	k	101	BCR	C20-C21	-7.67	1.19	1.43
26	C	514	BCR	C16-C17	-7.67	1.19	1.43
26	c	514	BCR	C20-C21	-7.67	1.19	1.43
26	K	101	BCR	C20-C21	-7.67	1.19	1.43
26	b	620	BCR	C20-C21	-7.66	1.19	1.43
26	J	101	BCR	C20-C21	-7.66	1.20	1.43
26	b	621	BCR	C20-C21	-7.66	1.20	1.43
26	y	101	BCR	C16-C17	-7.65	1.20	1.43
26	T	101	BCR	C20-C21	-7.63	1.20	1.43
26	K	101	BCR	C16-C17	-7.63	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	617	BCR	C16-C17	-7.62	1.20	1.43
26	t	101	BCR	C20-C21	-7.61	1.20	1.43
26	h	101	BCR	C16-C17	-7.60	1.20	1.43
26	k	101	BCR	C16-C17	-7.59	1.20	1.43
26	d	404	BCR	C16-C17	-7.58	1.20	1.43
26	D	406	BCR	C16-C17	-7.57	1.20	1.43
26	H	101	BCR	C16-C17	-7.57	1.20	1.43
26	b	622	BCR	C16-C17	-7.56	1.20	1.43
26	B	619	BCR	C16-C17	-7.56	1.20	1.43
26	t	101	BCR	C16-C17	-7.55	1.20	1.43
26	b	621	BCR	C16-C17	-7.55	1.20	1.43
26	k	102	BCR	C20-C21	-7.52	1.20	1.43
26	B	617	BCR	C20-C21	-7.50	1.20	1.43
28	a	401	SQD	C6-S	-7.46	1.66	1.77
26	b	620	BCR	C16-C17	-7.45	1.20	1.43
38	V	201	HEM	C3B-C4B	-7.43	1.45	1.51
28	A	1016	SQD	C6-S	-7.42	1.66	1.77
26	a	413	BCR	C16-C17	-7.42	1.20	1.43
26	B	618	BCR	C16-C17	-7.41	1.20	1.43
26	A	1009	BCR	C16-C17	-7.41	1.20	1.43
26	a	413	BCR	C20-C21	-7.40	1.20	1.43
28	A	1011	SQD	C6-S	-7.39	1.67	1.77
28	b	623[A]	SQD	C6-S	-7.33	1.67	1.77
28	f	102	SQD	C6-S	-7.26	1.67	1.77
28	B	620[B]	SQD	C6-S	-7.25	1.67	1.77
28	B	620[A]	SQD	C6-S	-7.21	1.67	1.77
28	c	518	SQD	C6-S	-7.21	1.67	1.77
28	b	623[B]	SQD	C6-S	-7.18	1.67	1.77
28	D	408	SQD	C6-S	-6.76	1.67	1.77
26	D	406	BCR	C21-C22	-6.72	1.26	1.35
38	F	101	HEM	C3B-C4B	-6.67	1.45	1.51
26	K	102	BCR	C21-C22	-6.66	1.27	1.35
26	d	404	BCR	C21-C22	-6.64	1.27	1.35
26	b	622	BCR	C21-C22	-6.61	1.27	1.35
26	k	102	BCR	C21-C22	-6.55	1.27	1.35
26	t	101	BCR	C17-C18	-6.51	1.27	1.35
26	c	514	BCR	C17-C18	-6.50	1.27	1.35
26	d	404	BCR	C17-C18	-6.50	1.27	1.35
26	T	101	BCR	C17-C18	-6.47	1.27	1.35
26	K	102	BCR	C17-C18	-6.46	1.27	1.35
26	b	621	BCR	C21-C22	-6.46	1.27	1.35
26	A	1009	BCR	C21-C22	-6.46	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	514	BCR	C21-C22	-6.46	1.27	1.35
26	y	101	BCR	C21-C22	-6.42	1.27	1.35
26	y	101	BCR	C17-C18	-6.39	1.27	1.35
26	B	617	BCR	C21-C22	-6.38	1.27	1.35
26	T	101	BCR	C21-C22	-6.36	1.27	1.35
26	J	101	BCR	C17-C18	-6.36	1.27	1.35
26	h	101	BCR	C21-C22	-6.36	1.27	1.35
26	b	622	BCR	C17-C18	-6.36	1.27	1.35
26	H	101	BCR	C21-C22	-6.36	1.27	1.35
26	C	514	BCR	C17-C18	-6.35	1.27	1.35
26	J	101	BCR	C21-C22	-6.32	1.27	1.35
26	K	101	BCR	C21-C22	-6.29	1.27	1.35
26	k	102	BCR	C17-C18	-6.28	1.27	1.35
26	k	102	BCR	C16-C17	-6.27	1.24	1.43
26	h	101	BCR	C17-C18	-6.26	1.27	1.35
26	b	621	BCR	C17-C18	-6.26	1.27	1.35
26	k	101	BCR	C17-C18	-6.25	1.27	1.35
26	B	619	BCR	C21-C22	-6.23	1.27	1.35
26	k	101	BCR	C21-C22	-6.21	1.27	1.35
38	f	101	HEM	C3B-C4B	-6.20	1.46	1.51
26	t	101	BCR	C21-C22	-6.19	1.27	1.35
26	B	618	BCR	C21-C22	-6.18	1.27	1.35
26	T	101	BCR	C16-C15	-6.17	1.19	1.35
26	B	619	BCR	C17-C18	-6.17	1.27	1.35
26	A	1009	BCR	C17-C18	-6.17	1.27	1.35
26	b	620	BCR	C21-C22	-6.17	1.27	1.35
26	a	413	BCR	C17-C18	-6.15	1.27	1.35
26	B	617	BCR	C17-C18	-6.15	1.27	1.35
26	c	514	BCR	C21-C22	-6.14	1.27	1.35
26	J	101	BCR	C16-C15	-6.11	1.19	1.35
26	H	101	BCR	C17-C18	-6.11	1.27	1.35
26	b	620	BCR	C17-C18	-6.10	1.27	1.35
26	c	514	BCR	C16-C15	-6.08	1.19	1.35
26	y	101	BCR	C16-C15	-6.07	1.19	1.35
26	C	514	BCR	C16-C15	-6.06	1.19	1.35
26	K	102	BCR	C16-C15	-6.06	1.19	1.35
26	B	618	BCR	C17-C18	-6.04	1.27	1.35
26	d	404	BCR	C16-C15	-6.03	1.19	1.35
26	D	406	BCR	C17-C18	-5.97	1.27	1.35
26	K	101	BCR	C17-C18	-5.97	1.27	1.35
26	t	101	BCR	C16-C15	-5.94	1.19	1.35
26	A	1009	BCR	C16-C15	-5.93	1.20	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	h	101	BCR	C16-C15	-5.91	1.20	1.35
26	a	413	BCR	C21-C22	-5.90	1.28	1.35
26	B	619	BCR	C16-C15	-5.90	1.20	1.35
26	H	101	BCR	C16-C15	-5.89	1.20	1.35
26	k	101	BCR	C16-C15	-5.89	1.20	1.35
26	K	101	BCR	C16-C15	-5.89	1.20	1.35
26	b	620	BCR	C16-C15	-5.88	1.20	1.35
26	b	621	BCR	C16-C15	-5.87	1.20	1.35
26	b	622	BCR	C16-C15	-5.84	1.20	1.35
26	B	617	BCR	C16-C15	-5.83	1.20	1.35
26	D	406	BCR	C16-C15	-5.78	1.20	1.35
26	C	514	BCR	C20-C19	-5.76	1.19	1.34
26	a	413	BCR	C16-C15	-5.76	1.20	1.35
26	k	102	BCR	C11-C12	-5.73	1.19	1.34
26	J	101	BCR	C11-C12	-5.72	1.19	1.34
26	B	619	BCR	C11-C12	-5.70	1.19	1.34
38	V	201	HEM	C3D-C4D	-5.68	1.44	1.51
26	C	514	BCR	C11-C12	-5.67	1.19	1.34
26	K	102	BCR	C20-C19	-5.66	1.19	1.34
26	t	101	BCR	C11-C12	-5.66	1.19	1.34
26	b	622	BCR	C11-C12	-5.65	1.19	1.34
26	B	618	BCR	C16-C15	-5.64	1.20	1.35
26	K	102	BCR	C11-C12	-5.63	1.19	1.34
26	h	101	BCR	C20-C19	-5.62	1.19	1.34
26	c	514	BCR	C11-C12	-5.61	1.19	1.34
26	k	101	BCR	C11-C12	-5.60	1.19	1.34
26	y	101	BCR	C11-C12	-5.60	1.19	1.34
26	y	101	BCR	C20-C19	-5.60	1.19	1.34
26	d	404	BCR	C20-C19	-5.59	1.19	1.34
26	c	514	BCR	C20-C19	-5.57	1.19	1.34
26	T	101	BCR	C20-C19	-5.57	1.19	1.34
26	T	101	BCR	C11-C12	-5.57	1.19	1.34
26	b	621	BCR	C11-C12	-5.56	1.19	1.34
26	K	101	BCR	C20-C19	-5.55	1.19	1.34
26	h	101	BCR	C11-C12	-5.55	1.19	1.34
26	B	618	BCR	C11-C12	-5.54	1.19	1.34
26	b	621	BCR	C20-C19	-5.54	1.20	1.34
26	d	404	BCR	C11-C12	-5.53	1.20	1.34
26	K	101	BCR	C11-C12	-5.53	1.20	1.34
26	D	406	BCR	C20-C19	-5.52	1.20	1.34
26	b	620	BCR	C11-C12	-5.51	1.20	1.34
26	J	101	BCR	C20-C19	-5.51	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	622	BCR	C20-C19	-5.51	1.20	1.34
26	B	619	BCR	C20-C19	-5.48	1.20	1.34
26	T	101	BCR	C11-C10	-5.47	1.26	1.43
26	k	101	BCR	C20-C19	-5.47	1.20	1.34
26	D	406	BCR	C11-C12	-5.46	1.20	1.34
26	H	101	BCR	C20-C19	-5.45	1.20	1.34
26	A	1009	BCR	C11-C12	-5.45	1.20	1.34
26	k	102	BCR	C11-C10	-5.44	1.26	1.43
26	H	101	BCR	C11-C12	-5.44	1.20	1.34
26	A	1009	BCR	C20-C19	-5.43	1.20	1.34
26	k	102	BCR	C15-C14	-5.42	1.26	1.43
26	t	101	BCR	C20-C19	-5.41	1.20	1.34
26	B	619	BCR	C11-C10	-5.39	1.27	1.43
26	h	101	BCR	C11-C10	-5.39	1.27	1.43
26	b	622	BCR	C11-C10	-5.38	1.27	1.43
26	c	514	BCR	C11-C10	-5.37	1.27	1.43
26	K	102	BCR	C11-C10	-5.37	1.27	1.43
26	B	617	BCR	C11-C12	-5.37	1.20	1.34
26	b	620	BCR	C20-C19	-5.37	1.20	1.34
26	B	618	BCR	C20-C19	-5.37	1.20	1.34
26	C	514	BCR	C11-C10	-5.37	1.27	1.43
26	k	101	BCR	C11-C10	-5.37	1.27	1.43
38	v	201	HEM	C3D-C4D	-5.35	1.44	1.51
26	c	514	BCR	C15-C14	-5.34	1.27	1.43
26	d	404	BCR	C11-C10	-5.34	1.27	1.43
26	t	101	BCR	C11-C10	-5.33	1.27	1.43
26	y	101	BCR	C11-C10	-5.33	1.27	1.43
26	J	101	BCR	C11-C10	-5.33	1.27	1.43
26	a	413	BCR	C11-C12	-5.32	1.20	1.34
26	C	514	BCR	C15-C14	-5.32	1.27	1.43
26	K	102	BCR	C15-C14	-5.32	1.27	1.43
26	T	101	BCR	C15-C14	-5.32	1.27	1.43
26	J	101	BCR	C15-C14	-5.31	1.27	1.43
26	B	618	BCR	C11-C10	-5.30	1.27	1.43
26	A	1009	BCR	C11-C10	-5.28	1.27	1.43
26	h	101	BCR	C15-C14	-5.27	1.27	1.43
26	y	101	BCR	C15-C14	-5.27	1.27	1.43
26	B	619	BCR	C15-C14	-5.26	1.27	1.43
26	k	101	BCR	C15-C14	-5.25	1.27	1.43
26	H	101	BCR	C11-C10	-5.25	1.27	1.43
26	a	413	BCR	C20-C19	-5.25	1.20	1.34
26	B	617	BCR	C11-C10	-5.24	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	101	BCR	C11-C10	-5.24	1.27	1.43
26	b	620	BCR	C11-C10	-5.24	1.27	1.43
26	t	101	BCR	C15-C14	-5.23	1.27	1.43
26	D	406	BCR	C11-C10	-5.21	1.27	1.43
26	d	404	BCR	C15-C14	-5.21	1.27	1.43
26	B	617	BCR	C15-C14	-5.20	1.27	1.43
26	B	617	BCR	C20-C19	-5.20	1.20	1.34
26	K	101	BCR	C15-C14	-5.20	1.27	1.43
26	k	102	BCR	C20-C19	-5.18	1.20	1.34
26	b	622	BCR	C15-C14	-5.18	1.27	1.43
26	b	621	BCR	C15-C14	-5.16	1.27	1.43
26	b	621	BCR	C11-C10	-5.15	1.27	1.43
26	a	413	BCR	C15-C14	-5.14	1.27	1.43
26	D	406	BCR	C15-C14	-5.14	1.27	1.43
26	H	101	BCR	C15-C14	-5.09	1.27	1.43
26	A	1009	BCR	C15-C14	-5.07	1.28	1.43
26	a	413	BCR	C11-C10	-5.07	1.28	1.43
26	B	618	BCR	C15-C14	-5.06	1.28	1.43
26	b	620	BCR	C15-C14	-5.03	1.28	1.43
26	k	102	BCR	C16-C15	-5.01	1.22	1.35
38	f	101	HEM	C3D-C4D	-4.94	1.45	1.51
38	F	101	HEM	C3D-C4D	-4.90	1.45	1.51
26	d	404	BCR	C23-C22	-4.84	1.35	1.45
26	D	406	BCR	C23-C22	-4.80	1.35	1.45
26	a	413	BCR	C23-C22	-4.80	1.35	1.45
26	k	101	BCR	C23-C22	-4.73	1.35	1.45
26	k	102	BCR	C23-C22	-4.73	1.35	1.45
26	b	621	BCR	C23-C22	-4.72	1.35	1.45
26	y	101	BCR	C23-C22	-4.72	1.35	1.45
26	T	101	BCR	C23-C22	-4.70	1.35	1.45
26	K	102	BCR	C23-C22	-4.69	1.35	1.45
26	t	101	BCR	C23-C22	-4.65	1.35	1.45
26	B	619	BCR	C23-C22	-4.64	1.35	1.45
26	b	620	BCR	C23-C22	-4.64	1.35	1.45
26	J	101	BCR	C23-C22	-4.64	1.35	1.45
26	H	101	BCR	C23-C22	-4.62	1.35	1.45
26	B	617	BCR	C23-C22	-4.59	1.35	1.45
26	K	101	BCR	C23-C22	-4.59	1.35	1.45
26	C	514	BCR	C23-C22	-4.58	1.35	1.45
26	h	101	BCR	C23-C22	-4.58	1.35	1.45
26	c	514	BCR	C23-C22	-4.54	1.35	1.45
26	b	622	BCR	C23-C22	-4.54	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	411	PHO	C1A-NA	-4.46	1.27	1.37
26	B	618	BCR	C23-C22	-4.45	1.36	1.45
26	A	1009	BCR	C23-C22	-4.44	1.36	1.45
25	A	1007	PHO	C1A-NA	-4.38	1.27	1.37
25	D	404	PHO	C1A-NA	-4.38	1.27	1.37
25	a	410	PHO	C1A-NA	-4.25	1.27	1.37
38	f	101	HEM	C2C-C1C	-3.87	1.45	1.52
38	F	101	HEM	C2C-C1C	-3.81	1.45	1.52
38	V	201	HEM	C2C-C1C	-3.74	1.45	1.52
38	v	201	HEM	C2C-C1C	-3.70	1.45	1.52
35	o	301	HTG	C1'-S1	-3.52	1.76	1.81
35	b	630	HTG	C1'-S1	-3.51	1.76	1.81
35	d	410	HTG	C1'-S1	-3.44	1.76	1.81
35	b	626	HTG	C1'-S1	-3.42	1.76	1.81
35	D	413	HTG	C1'-S1	-3.41	1.76	1.81
35	B	628	HTG	C1'-S1	-3.38	1.76	1.81
35	c	525	HTG	C1'-S1	-3.36	1.76	1.81
35	C	521	HTG	C1'-S1	-3.34	1.76	1.81
35	b	601	HTG	C1'-S1	-3.33	1.76	1.81
35	B	629	HTG	C1'-S1	-3.31	1.76	1.81
35	B	624	HTG	C1'-S1	-3.28	1.76	1.81
35	D	419	HTG	C1'-S1	-3.26	1.76	1.81
35	d	416	HTG	C1'-S1	-3.24	1.77	1.81
35	b	602	HTG	C1'-S1	-3.22	1.77	1.81
35	c	522	HTG	C1'-S1	-3.17	1.77	1.81
35	V	202	HTG	C1'-S1	-3.16	1.77	1.81
35	C	522	HTG	C1'-S1	-3.10	1.77	1.81
25	a	410	PHO	CHB-C4A	-3.00	1.34	1.40
25	a	411	PHO	C3D-C4D	-2.97	1.34	1.43
25	D	404	PHO	C3D-C4D	-2.91	1.34	1.43
25	a	411	PHO	CHB-C4A	-2.86	1.35	1.40
25	D	404	PHO	CHB-C4A	-2.82	1.35	1.40
25	A	1007	PHO	C3D-C4D	-2.76	1.34	1.43
26	K	101	BCR	C24-C25	-2.72	1.35	1.45
26	k	102	BCR	C24-C25	-2.71	1.35	1.45
26	y	101	BCR	C24-C25	-2.69	1.35	1.45
25	a	410	PHO	C3D-C4D	-2.68	1.35	1.43
25	A	1007	PHO	CHB-C4A	-2.67	1.35	1.40
26	K	102	BCR	C24-C25	-2.66	1.35	1.45
26	J	101	BCR	C24-C25	-2.64	1.35	1.45
26	b	621	BCR	C24-C25	-2.63	1.35	1.45
26	c	514	BCR	C24-C25	-2.63	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	404	BCR	C24-C25	-2.63	1.35	1.45
26	b	622	BCR	C24-C25	-2.60	1.36	1.45
26	b	620	BCR	C24-C25	-2.59	1.36	1.45
26	t	101	BCR	C24-C25	-2.59	1.36	1.45
26	k	101	BCR	C24-C25	-2.59	1.36	1.45
26	D	406	BCR	C24-C25	-2.57	1.36	1.45
26	C	514	BCR	C24-C25	-2.56	1.36	1.45
26	h	101	BCR	C24-C25	-2.55	1.36	1.45
26	B	619	BCR	C24-C25	-2.53	1.36	1.45
26	A	1009	BCR	C24-C25	-2.53	1.36	1.45
26	B	618	BCR	C24-C25	-2.51	1.36	1.45
26	B	617	BCR	C24-C25	-2.51	1.36	1.45
26	a	413	BCR	C24-C25	-2.48	1.36	1.45
26	H	101	BCR	C24-C25	-2.48	1.36	1.45
26	T	101	BCR	C24-C25	-2.44	1.36	1.45
35	C	521	HTG	C1-S1	-2.29	1.77	1.80
35	B	628	HTG	C1-S1	-2.22	1.77	1.80
35	b	630	HTG	C1-S1	-2.20	1.77	1.80
35	c	525	HTG	C1-S1	-2.20	1.77	1.80
35	c	522	HTG	C1-S1	-2.20	1.77	1.80
38	V	201	HEM	C2B-C1B	-2.15	1.44	1.51
26	b	622	BCR	C8-C7	-2.14	1.26	1.33
35	D	413	HTG	C1-S1	-2.13	1.77	1.80
35	b	602	HTG	C1-S1	-2.12	1.77	1.80
35	V	202	HTG	C1-S1	-2.11	1.77	1.80
26	K	101	BCR	C8-C7	-2.10	1.26	1.33
26	d	404	BCR	C8-C7	-2.10	1.26	1.33
26	K	102	BCR	C8-C7	-2.09	1.26	1.33
26	c	514	BCR	C8-C7	-2.09	1.26	1.33
26	t	101	BCR	C8-C7	-2.09	1.26	1.33
35	B	624	HTG	C1-S1	-2.07	1.77	1.80
26	k	101	BCR	C8-C7	-2.07	1.26	1.33
26	C	514	BCR	C8-C7	-2.06	1.26	1.33
26	B	617	BCR	C8-C7	-2.05	1.26	1.33
26	k	102	BCR	C8-C7	-2.05	1.26	1.33
26	y	101	BCR	C8-C7	-2.04	1.26	1.33
38	v	201	HEM	C2B-C1B	-2.04	1.45	1.51
26	T	101	BCR	C8-C7	-2.04	1.26	1.33
26	B	619	BCR	C8-C7	-2.04	1.27	1.33
35	B	629	HTG	C1-S1	-2.04	1.77	1.80
38	v	201	HEM	C2D-C1D	-2.02	1.45	1.51
26	H	101	BCR	C8-C7	-2.01	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	V	201	HEM	C2D-C1D	-2.01	1.45	1.51
32	A	1017	LMT	O1'-C1'	2.00	1.43	1.40
24	A	1005	CLA	C1C-C2C	2.00	1.48	1.44
29	c	520	LMG	O1-C1	2.01	1.43	1.40
24	c	512	CLA	C4C-C3C	2.01	1.48	1.45
24	B	601	CLA	C4C-C3C	2.02	1.48	1.45
24	A	1006	CLA	C1C-C2C	2.02	1.48	1.44
36	C	516	DGD	O5D-C1E	2.02	1.43	1.40
24	d	403	CLA	C4C-C3C	2.02	1.48	1.45
24	C	512	CLA	C4C-C3C	2.03	1.48	1.45
24	B	616	CLA	C1C-C2C	2.03	1.48	1.44
25	D	404	PHO	C1B-C2B	2.03	1.50	1.45
24	C	513	CLA	C4C-C3C	2.03	1.48	1.45
24	b	616	CLA	C1C-C2C	2.03	1.48	1.44
24	B	603	CLA	C1C-C2C	2.03	1.48	1.44
24	b	619	CLA	C1C-C2C	2.04	1.48	1.44
36	c	515	DGD	O5D-C1E	2.04	1.43	1.40
24	C	504	CLA	C4C-C3C	2.04	1.48	1.45
24	c	510	CLA	C4C-C3C	2.05	1.48	1.45
24	C	509	CLA	C1C-C2C	2.06	1.48	1.44
24	C	502	CLA	C1C-C2C	2.06	1.48	1.44
24	b	612	CLA	C4C-C3C	2.07	1.48	1.45
38	v	201	HEM	C4C-NC	2.07	1.38	1.36
38	f	101	HEM	C3C-CAC	2.07	1.55	1.51
24	c	502	CLA	C4C-C3C	2.08	1.48	1.45
25	a	411	PHO	C4C-C3C	2.08	1.49	1.45
24	B	608	CLA	C1C-C2C	2.08	1.48	1.44
24	c	505	CLA	C4C-C3C	2.08	1.48	1.45
32	a	402	LMT	O1'-C1'	2.09	1.43	1.40
24	b	608	CLA	C1C-C2C	2.09	1.48	1.44
32	m	103	LMT	O1'-C1'	2.09	1.43	1.40
24	B	602	CLA	C4C-C3C	2.10	1.48	1.45
38	f	101	HEM	C4C-NC	2.10	1.38	1.36
24	B	615	CLA	C4C-C3C	2.10	1.48	1.45
24	b	610	CLA	C1C-C2C	2.11	1.48	1.44
25	a	410	PHO	C3B-C4B	2.11	1.48	1.43
36	h	102	DGD	O5D-C1E	2.11	1.43	1.40
27	d	405	PL9	C2-C3	2.11	1.40	1.34
28	f	102	SQD	O6-C1	2.12	1.44	1.40
24	b	607	CLA	C1C-C2C	2.12	1.48	1.44
38	F	101	HEM	C3C-CAC	2.12	1.55	1.51
24	B	609	CLA	C1C-C2C	2.12	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	C4C-C3C	2.13	1.48	1.45
38	V	201	HEM	FE-NB	2.13	2.08	1.97
24	b	615	CLA	C1C-C2C	2.13	1.48	1.44
25	A	1007	PHO	C3B-C4B	2.14	1.48	1.43
24	b	612	CLA	C1C-C2C	2.15	1.48	1.44
24	C	504	CLA	C1C-C2C	2.15	1.48	1.44
38	f	101	HEM	FE-NB	2.15	2.08	1.97
24	c	509	CLA	C1C-C2C	2.16	1.48	1.44
24	b	614	CLA	C1C-C2C	2.17	1.48	1.44
24	c	501	CLA	C1C-C2C	2.17	1.48	1.44
24	c	506	CLA	C1C-C2C	2.17	1.48	1.44
24	d	402	CLA	C1C-C2C	2.17	1.48	1.44
24	b	611	CLA	C1C-C2C	2.18	1.48	1.44
24	B	607	CLA	C1C-C2C	2.18	1.49	1.44
24	C	506	CLA	C1C-C2C	2.18	1.49	1.44
24	b	610	CLA	C4C-C3C	2.18	1.49	1.45
27	a	414	PL9	C2-C3	2.18	1.40	1.34
24	B	613	CLA	C1C-C2C	2.19	1.49	1.44
24	C	506	CLA	C4C-C3C	2.19	1.49	1.45
24	C	501	CLA	C4C-C3C	2.19	1.49	1.45
24	D	405	CLA	C4C-C3C	2.20	1.49	1.45
24	c	513	CLA	C4C-C3C	2.20	1.49	1.45
24	c	503	CLA	C4C-C3C	2.21	1.49	1.45
24	b	613	CLA	C1C-C2C	2.21	1.49	1.44
24	B	606	CLA	C4C-C3C	2.21	1.49	1.45
24	c	501	CLA	C4C-C3C	2.21	1.49	1.45
24	B	611	CLA	C1C-C2C	2.22	1.49	1.44
25	D	404	PHO	C3B-C4B	2.22	1.48	1.43
38	V	201	HEM	C3C-CAC	2.22	1.55	1.51
24	B	608	CLA	C4C-C3C	2.22	1.49	1.45
24	B	615	CLA	C1C-C2C	2.22	1.49	1.44
24	C	510	CLA	C1C-C2C	2.23	1.49	1.44
24	a	412	CLA	C1C-C2C	2.23	1.49	1.44
24	c	504	CLA	C4C-C3C	2.24	1.49	1.45
24	C	505	CLA	C1C-C2C	2.24	1.49	1.44
24	c	504	CLA	C1C-C2C	2.24	1.49	1.44
36	H	102	DGD	O5D-C1E	2.26	1.44	1.40
38	V	201	HEM	C4C-NC	2.26	1.38	1.36
24	b	604	CLA	C4C-C3C	2.26	1.49	1.45
24	B	610	CLA	C1C-C2C	2.26	1.49	1.44
24	c	506	CLA	C4C-C3C	2.27	1.49	1.45
24	C	501	CLA	C1C-C2C	2.27	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	C4C-C3C	2.28	1.49	1.45
27	A	1010	PL9	C2-C3	2.29	1.40	1.34
27	D	407	PL9	C2-C3	2.29	1.40	1.34
38	V	201	HEM	C3B-CAB	2.29	1.55	1.51
24	B	612	CLA	C1C-C2C	2.29	1.49	1.44
24	b	605	CLA	C4C-C3C	2.29	1.49	1.45
38	v	201	HEM	FE-ND	2.30	2.09	1.97
24	A	1008	CLA	C1C-C2C	2.30	1.49	1.44
24	c	510	CLA	C1C-C2C	2.31	1.49	1.44
24	B	601	CLA	C1C-C2C	2.31	1.49	1.44
24	c	508	CLA	C4C-C3C	2.31	1.49	1.45
24	C	508	CLA	C1C-C2C	2.32	1.49	1.44
38	f	101	HEM	FE-ND	2.33	2.09	1.97
24	C	505	CLA	C4C-C3C	2.33	1.49	1.45
38	V	201	HEM	C1C-NC	2.35	1.38	1.36
38	F	101	HEM	C3B-CAB	2.35	1.55	1.51
38	f	101	HEM	C3B-CAB	2.35	1.55	1.51
24	B	602	CLA	C1C-C2C	2.35	1.49	1.44
25	a	411	PHO	C3B-C4B	2.35	1.48	1.43
38	F	101	HEM	FE-ND	2.36	2.10	1.97
24	b	618	CLA	C1C-C2C	2.36	1.49	1.44
24	b	605	CLA	C1C-C2C	2.38	1.49	1.44
27	d	405	PL9	C6-C5	2.38	1.49	1.35
24	c	511	CLA	C1C-C2C	2.38	1.49	1.44
24	c	508	CLA	C1C-C2C	2.38	1.49	1.44
24	b	609	CLA	C1C-C2C	2.39	1.49	1.44
24	C	503	CLA	C1C-C2C	2.40	1.49	1.44
24	b	604	CLA	C1C-C2C	2.41	1.49	1.44
27	A	1010	PL9	C6-C5	2.42	1.49	1.35
24	b	606	CLA	C1C-C2C	2.42	1.49	1.44
24	c	513	CLA	C1C-C2C	2.42	1.49	1.44
27	a	414	PL9	C6-C5	2.43	1.49	1.35
27	D	407	PL9	C6-C5	2.43	1.49	1.35
24	c	505	CLA	C1C-C2C	2.44	1.49	1.44
24	D	405	CLA	C1C-C2C	2.45	1.49	1.44
24	b	617	CLA	C3D-C2D	2.45	1.46	1.40
24	D	402	CLA	C1C-C2C	2.45	1.49	1.44
38	f	101	HEM	C1C-NC	2.45	1.39	1.36
24	d	403	CLA	C1C-C2C	2.46	1.49	1.44
24	C	507	CLA	C1C-C2C	2.46	1.49	1.44
24	B	605	CLA	C1C-C2C	2.47	1.49	1.44
24	d	402	CLA	C3D-C2D	2.48	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	v	201	HEM	C3C-CAC	2.48	1.56	1.51
24	B	614	CLA	C3D-C2D	2.48	1.46	1.40
24	c	503	CLA	C1C-C2C	2.51	1.49	1.44
24	c	510	CLA	C3D-C2D	2.51	1.46	1.40
24	D	402	CLA	C3D-C2D	2.51	1.46	1.40
24	C	511	CLA	C1C-C2C	2.51	1.49	1.44
38	v	201	HEM	FE-NC	2.52	2.05	1.95
24	B	606	CLA	C1C-C2C	2.52	1.49	1.44
24	c	507	CLA	C1C-C2C	2.53	1.49	1.44
24	c	505	CLA	C3D-C2D	2.53	1.46	1.40
24	B	610	CLA	C3D-C2D	2.55	1.46	1.40
24	B	603	CLA	C3D-C2D	2.55	1.46	1.40
24	C	502	CLA	CHD-C4C	2.56	1.47	1.41
24	b	613	CLA	C3D-C2D	2.56	1.46	1.40
24	C	507	CLA	C3D-C2D	2.57	1.46	1.40
24	B	616	CLA	C3D-C2D	2.57	1.46	1.40
24	b	617	CLA	C1C-C2C	2.58	1.49	1.44
24	b	615	CLA	C3D-C2D	2.59	1.46	1.40
24	B	613	CLA	CHD-C4C	2.59	1.47	1.41
38	f	101	HEM	FE-NC	2.60	2.06	1.95
24	B	614	CLA	C1C-C2C	2.60	1.49	1.44
24	c	512	CLA	C3D-C2D	2.61	1.46	1.40
24	D	403	CLA	C4B-CHC	2.61	1.47	1.39
24	C	512	CLA	C1C-C2C	2.62	1.49	1.44
24	B	614	CLA	CHD-C4C	2.63	1.47	1.41
24	c	501	CLA	C3D-C2D	2.64	1.46	1.40
24	D	402	CLA	CHD-C4C	2.64	1.47	1.41
24	B	613	CLA	C3D-C2D	2.64	1.46	1.40
24	c	507	CLA	C3D-C2D	2.64	1.46	1.40
24	b	617	CLA	CHD-C4C	2.66	1.47	1.41
24	C	502	CLA	C3D-C2D	2.66	1.46	1.40
24	B	604	CLA	C3D-C2D	2.66	1.46	1.40
24	C	508	CLA	C3D-C2D	2.67	1.46	1.40
24	b	619	CLA	C3D-C2D	2.67	1.46	1.40
24	b	611	CLA	C3D-C2D	2.67	1.46	1.40
24	c	511	CLA	C3D-C2D	2.68	1.46	1.40
24	A	1008	CLA	C3D-C2D	2.68	1.46	1.40
24	B	611	CLA	CHD-C4C	2.69	1.47	1.41
24	B	601	CLA	C3D-C2D	2.70	1.46	1.40
24	b	614	CLA	CHD-C4C	2.70	1.47	1.41
24	C	510	CLA	C3D-C2D	2.70	1.46	1.40
24	b	619	CLA	CHD-C4C	2.70	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	512	CLA	C1C-C2C	2.70	1.50	1.44
24	b	616	CLA	C3D-C2D	2.71	1.46	1.40
24	C	505	CLA	C3D-C2D	2.71	1.46	1.40
24	B	605	CLA	C3D-C2D	2.71	1.46	1.40
24	b	618	CLA	C3D-C2D	2.71	1.46	1.40
24	b	606	CLA	C3D-C2D	2.72	1.46	1.40
24	a	407	CLA	CHD-C4C	2.72	1.47	1.41
24	c	509	CLA	C3D-C2D	2.72	1.46	1.40
24	b	607	CLA	C3D-C2D	2.72	1.46	1.40
24	c	503	CLA	C3D-C2D	2.72	1.46	1.40
24	c	506	CLA	C3D-C2D	2.73	1.46	1.40
24	c	507	CLA	CHD-C4C	2.74	1.47	1.41
24	c	508	CLA	C3D-C2D	2.74	1.46	1.40
24	D	405	CLA	C3D-C2D	2.74	1.46	1.40
24	C	513	CLA	C3D-C2D	2.74	1.46	1.40
24	b	604	CLA	C3D-C2D	2.74	1.46	1.40
24	B	609	CLA	C3D-C2D	2.74	1.46	1.40
24	b	605	CLA	C3D-C2D	2.75	1.46	1.40
24	c	502	CLA	C3D-C2D	2.75	1.46	1.40
24	C	506	CLA	C3D-C2D	2.75	1.46	1.40
24	B	612	CLA	CHD-C4C	2.75	1.47	1.41
24	a	412	CLA	CHD-C4C	2.75	1.47	1.41
24	B	611	CLA	C3D-C2D	2.76	1.46	1.40
24	C	513	CLA	C1C-C2C	2.76	1.50	1.44
24	B	606	CLA	C3D-C2D	2.76	1.46	1.40
24	B	607	CLA	C3D-C2D	2.76	1.46	1.40
24	a	407	CLA	C3D-C2D	2.76	1.46	1.40
25	A	1007	PHO	C3D-C2D	2.77	1.46	1.38
24	B	616	CLA	CHD-C4C	2.77	1.47	1.41
24	c	513	CLA	C3D-C2D	2.77	1.46	1.40
24	A	1008	CLA	CHD-C4C	2.77	1.47	1.41
24	d	403	CLA	C3D-C2D	2.78	1.46	1.40
24	C	508	CLA	CHD-C4C	2.78	1.47	1.41
24	a	412	CLA	C4B-CHC	2.78	1.47	1.39
24	B	612	CLA	C3D-C2D	2.78	1.46	1.40
24	B	610	CLA	CHD-C4C	2.79	1.47	1.41
24	C	509	CLA	C3D-C2D	2.79	1.46	1.40
24	A	1005	CLA	C4B-CHC	2.80	1.47	1.39
24	b	608	CLA	C3D-C2D	2.80	1.46	1.40
24	B	615	CLA	C4B-CHC	2.80	1.47	1.39
24	B	605	CLA	CHD-C4C	2.80	1.47	1.41
24	A	1005	CLA	C3D-C2D	2.80	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C3D-C2D	2.80	1.46	1.40
24	C	512	CLA	C3D-C2D	2.81	1.46	1.40
24	C	512	CLA	CHD-C4C	2.81	1.47	1.41
24	a	408	CLA	C4B-CHC	2.81	1.47	1.39
24	C	501	CLA	C3D-C2D	2.81	1.46	1.40
24	B	606	CLA	CHD-C4C	2.81	1.47	1.41
24	b	609	CLA	C3D-C2D	2.82	1.46	1.40
24	C	510	CLA	CHD-C4C	2.82	1.47	1.41
24	b	612	CLA	C3D-C2D	2.82	1.46	1.40
24	a	412	CLA	C3D-C2D	2.82	1.46	1.40
24	A	1006	CLA	CHD-C4C	2.83	1.47	1.41
24	C	503	CLA	C3D-C2D	2.84	1.46	1.40
24	b	610	CLA	CHD-C4C	2.84	1.47	1.41
24	d	402	CLA	CHD-C4C	2.85	1.47	1.41
24	a	408	CLA	CHD-C4C	2.86	1.47	1.41
24	B	608	CLA	C3D-C2D	2.87	1.47	1.40
24	b	606	CLA	CHD-C4C	2.87	1.47	1.41
24	B	615	CLA	CHD-C4C	2.88	1.47	1.41
24	a	408	CLA	C3D-C2D	2.88	1.47	1.40
24	b	615	CLA	CHD-C4C	2.89	1.48	1.41
24	B	615	CLA	C3D-C2D	2.89	1.47	1.40
24	B	603	CLA	CHD-C4C	2.90	1.48	1.41
25	a	411	PHO	C3D-C2D	2.90	1.46	1.38
24	C	511	CLA	CHD-C4C	2.91	1.48	1.41
24	b	607	CLA	CHD-C4C	2.91	1.48	1.41
24	C	509	CLA	C4B-CHC	2.92	1.47	1.39
24	C	507	CLA	CHD-C4C	2.92	1.48	1.41
24	b	608	CLA	CHD-C4C	2.92	1.48	1.41
24	b	608	CLA	C4B-CHC	2.92	1.47	1.39
25	a	410	PHO	C3D-C2D	2.92	1.46	1.38
24	B	607	CLA	CHD-C4C	2.92	1.48	1.41
24	C	504	CLA	C3D-C2D	2.93	1.47	1.40
24	c	504	CLA	C3D-C2D	2.93	1.47	1.40
24	b	611	CLA	CHD-C4C	2.93	1.48	1.41
24	b	613	CLA	CHD-C4C	2.93	1.48	1.41
24	C	509	CLA	CHD-C4C	2.93	1.48	1.41
24	A	1006	CLA	C3D-C2D	2.93	1.47	1.40
25	D	404	PHO	C3D-C2D	2.93	1.46	1.38
24	c	510	CLA	CHD-C4C	2.93	1.48	1.41
24	C	510	CLA	C4B-CHC	2.94	1.47	1.39
24	B	604	CLA	CHD-C4C	2.94	1.48	1.41
24	a	407	CLA	C4B-CHC	2.94	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1007	PHO	CHC-C4B	2.94	1.47	1.40
24	B	609	CLA	CHD-C4C	2.94	1.48	1.41
24	c	511	CLA	CHD-C4C	2.94	1.48	1.41
24	d	402	CLA	C4B-CHC	2.95	1.48	1.39
24	B	604	CLA	C4B-CHC	2.95	1.48	1.39
24	b	610	CLA	C4B-CHC	2.95	1.48	1.39
24	c	512	CLA	CHD-C4C	2.96	1.48	1.41
24	C	506	CLA	CHD-C4C	2.97	1.48	1.41
24	a	409	CLA	C3D-C2D	2.97	1.47	1.40
24	B	603	CLA	C4B-CHC	2.97	1.48	1.39
24	C	513	CLA	CHD-C4C	2.97	1.48	1.41
24	A	1005	CLA	CHD-C4C	2.97	1.48	1.41
24	B	608	CLA	CHD-C4C	2.97	1.48	1.41
24	C	502	CLA	C4B-CHC	2.97	1.48	1.39
24	b	616	CLA	CHD-C4C	2.97	1.48	1.41
25	A	1007	PHO	CHD-C4C	2.98	1.47	1.40
24	A	1006	CLA	C4B-CHC	2.98	1.48	1.39
24	d	403	CLA	CHD-C4C	2.98	1.48	1.41
24	C	504	CLA	C4B-CHC	2.98	1.48	1.39
24	D	403	CLA	CHD-C4C	2.99	1.48	1.41
24	D	402	CLA	C4B-CHC	2.99	1.48	1.39
24	c	508	CLA	CHD-C4C	2.99	1.48	1.41
24	B	608	CLA	C4B-CHC	3.00	1.48	1.39
24	B	613	CLA	C4B-CHC	3.00	1.48	1.39
24	B	602	CLA	C3D-C2D	3.00	1.47	1.40
24	c	509	CLA	C4B-CHC	3.01	1.48	1.39
24	b	618	CLA	CHD-C4C	3.01	1.48	1.41
24	C	511	CLA	C3D-C2D	3.01	1.47	1.40
24	D	403	CLA	C3D-C2D	3.02	1.47	1.40
24	c	502	CLA	CHD-C4C	3.02	1.48	1.41
24	B	612	CLA	C4B-CHC	3.03	1.48	1.39
24	C	505	CLA	C4B-CHC	3.03	1.48	1.39
24	b	609	CLA	CHD-C4C	3.03	1.48	1.41
24	c	501	CLA	CHD-C4C	3.03	1.48	1.41
24	a	409	CLA	CHD-C4C	3.03	1.48	1.41
24	B	607	CLA	C4B-CHC	3.04	1.48	1.39
24	C	509	CLA	C1B-CHB	3.05	1.48	1.39
24	c	505	CLA	CHD-C4C	3.06	1.48	1.41
24	b	615	CLA	C4B-CHC	3.06	1.48	1.39
24	b	610	CLA	C3D-C2D	3.06	1.47	1.40
24	b	616	CLA	C4B-CHC	3.06	1.48	1.39
24	b	619	CLA	C4B-CHC	3.07	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C4B-CHC	3.07	1.48	1.39
24	a	409	CLA	C4B-CHC	3.07	1.48	1.39
24	D	405	CLA	CHD-C4C	3.08	1.48	1.41
24	C	504	CLA	CHD-C4C	3.08	1.48	1.41
24	c	506	CLA	C4B-CHC	3.09	1.48	1.39
24	A	1008	CLA	C4B-CHC	3.09	1.48	1.39
25	a	411	PHO	CHC-C4B	3.09	1.48	1.40
24	c	502	CLA	C4B-CHC	3.11	1.48	1.39
24	B	616	CLA	C4B-CHC	3.11	1.48	1.39
24	c	504	CLA	CHD-C4C	3.11	1.48	1.41
24	b	614	CLA	C4B-CHC	3.11	1.48	1.39
24	B	601	CLA	CHD-C4C	3.11	1.48	1.41
24	C	506	CLA	C4B-CHC	3.12	1.48	1.39
25	a	411	PHO	CHD-C4C	3.12	1.48	1.40
24	b	612	CLA	C4B-CHC	3.12	1.48	1.39
24	C	508	CLA	C4B-CHC	3.12	1.48	1.39
24	c	506	CLA	CHD-C4C	3.12	1.48	1.41
25	a	410	PHO	CHD-C4C	3.12	1.48	1.40
25	D	404	PHO	CHD-C4C	3.12	1.48	1.40
24	b	607	CLA	C4B-CHC	3.12	1.48	1.39
25	a	410	PHO	CHC-C4B	3.13	1.48	1.40
24	C	503	CLA	CHD-C4C	3.13	1.48	1.41
24	b	605	CLA	C4B-CHC	3.14	1.48	1.39
24	b	609	CLA	C4B-CHC	3.14	1.48	1.39
24	B	609	CLA	C4B-CHC	3.14	1.48	1.39
24	B	606	CLA	C4B-CHC	3.14	1.48	1.39
24	b	612	CLA	CHD-C4C	3.14	1.48	1.41
24	B	611	CLA	C4B-CHC	3.14	1.48	1.39
24	c	509	CLA	CHD-C4C	3.15	1.48	1.41
24	B	602	CLA	C4B-CHC	3.15	1.48	1.39
24	b	604	CLA	CHD-C4C	3.16	1.48	1.41
24	d	402	CLA	C1B-CHB	3.16	1.48	1.39
24	c	505	CLA	C4B-CHC	3.17	1.48	1.39
24	B	601	CLA	C4B-CHC	3.17	1.48	1.39
24	B	607	CLA	C1B-CHB	3.17	1.48	1.39
24	c	504	CLA	C4B-CHC	3.17	1.48	1.39
24	b	606	CLA	C4B-CHC	3.18	1.48	1.39
24	C	501	CLA	C4B-CHC	3.18	1.48	1.39
24	D	405	CLA	C4B-CHC	3.18	1.48	1.39
24	d	403	CLA	C4B-CHC	3.18	1.48	1.39
24	b	608	CLA	C1B-CHB	3.19	1.48	1.39
24	C	501	CLA	CHD-C4C	3.19	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	CLA	C1B-CHB	3.19	1.48	1.39
24	C	505	CLA	CHD-C4C	3.20	1.48	1.41
25	D	404	PHO	CHC-C4B	3.20	1.48	1.40
24	a	412	CLA	C1B-CHB	3.20	1.48	1.39
24	A	1005	CLA	C1B-CHB	3.21	1.48	1.39
24	c	510	CLA	C4B-CHC	3.21	1.48	1.39
24	D	403	CLA	C1B-CHB	3.21	1.48	1.39
24	c	503	CLA	CHD-C4C	3.22	1.48	1.41
24	B	610	CLA	C4B-CHC	3.22	1.48	1.39
24	c	513	CLA	C4B-CHC	3.23	1.48	1.39
24	b	617	CLA	C4B-CHC	3.24	1.48	1.39
24	B	605	CLA	C4B-CHC	3.24	1.48	1.39
24	c	508	CLA	C4B-CHC	3.24	1.48	1.39
24	C	511	CLA	C4B-CHC	3.24	1.48	1.39
24	c	501	CLA	C4B-CHC	3.24	1.48	1.39
24	B	602	CLA	C1B-CHB	3.25	1.48	1.39
24	B	616	CLA	C1B-CHB	3.25	1.48	1.39
24	b	605	CLA	CHD-C4C	3.25	1.48	1.41
24	c	502	CLA	C1B-CHB	3.26	1.48	1.39
24	b	614	CLA	C1B-CHB	3.26	1.48	1.39
24	b	611	CLA	C4B-CHC	3.26	1.48	1.39
24	c	513	CLA	CHD-C4C	3.27	1.48	1.41
24	a	409	CLA	C1B-CHB	3.27	1.48	1.39
24	B	608	CLA	C1B-CHB	3.27	1.48	1.39
24	B	614	CLA	C4B-CHC	3.28	1.48	1.39
24	b	613	CLA	C4B-CHC	3.29	1.48	1.39
24	D	402	CLA	C1B-CHB	3.29	1.48	1.39
24	B	602	CLA	CHD-C4C	3.29	1.48	1.41
24	b	617	CLA	C1B-CHB	3.30	1.48	1.39
24	B	605	CLA	C1B-CHB	3.30	1.48	1.39
24	b	611	CLA	C1B-CHB	3.31	1.49	1.39
24	B	601	CLA	C1B-CHB	3.32	1.49	1.39
24	C	508	CLA	C1B-CHB	3.32	1.49	1.39
24	C	503	CLA	C4B-CHC	3.33	1.49	1.39
24	A	1006	CLA	C1B-CHB	3.33	1.49	1.39
24	B	603	CLA	C1B-CHB	3.33	1.49	1.39
24	b	604	CLA	C4B-CHC	3.33	1.49	1.39
24	c	507	CLA	C4B-CHC	3.33	1.49	1.39
24	C	512	CLA	C4B-CHC	3.33	1.49	1.39
24	a	409	CLA	OBD-CAD	3.33	1.27	1.22
24	C	506	CLA	C1B-CHB	3.34	1.49	1.39
24	d	403	CLA	C1B-CHB	3.34	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	504	CLA	C1B-CHB	3.35	1.49	1.39
24	c	503	CLA	C4B-CHC	3.35	1.49	1.39
24	C	501	CLA	C1B-CHB	3.35	1.49	1.39
24	c	512	CLA	C4B-CHC	3.35	1.49	1.39
24	c	511	CLA	C4B-CHC	3.35	1.49	1.39
24	c	508	CLA	C1B-CHB	3.36	1.49	1.39
24	B	606	CLA	C1B-CHB	3.36	1.49	1.39
24	c	511	CLA	C1B-CHB	3.36	1.49	1.39
24	c	503	CLA	C1B-CHB	3.37	1.49	1.39
24	c	512	CLA	C1B-CHB	3.37	1.49	1.39
24	c	504	CLA	C1B-CHB	3.37	1.49	1.39
24	B	611	CLA	C1B-CHB	3.37	1.49	1.39
24	B	604	CLA	C1B-CHB	3.37	1.49	1.39
24	B	610	CLA	C1B-CHB	3.38	1.49	1.39
24	b	612	CLA	C1B-CHB	3.38	1.49	1.39
24	b	613	CLA	C1B-CHB	3.38	1.49	1.39
24	b	605	CLA	C1B-CHB	3.39	1.49	1.39
24	C	513	CLA	C4B-CHC	3.39	1.49	1.39
24	b	606	CLA	C1B-CHB	3.39	1.49	1.39
24	C	502	CLA	C1B-CHB	3.39	1.49	1.39
24	b	619	CLA	C1B-CHB	3.40	1.49	1.39
24	b	609	CLA	C1B-CHB	3.40	1.49	1.39
24	D	405	CLA	C1B-CHB	3.40	1.49	1.39
24	b	616	CLA	C1B-CHB	3.41	1.49	1.39
24	C	507	CLA	C4B-CHC	3.41	1.49	1.39
24	C	503	CLA	C1B-CHB	3.41	1.49	1.39
24	b	604	CLA	C1B-CHB	3.41	1.49	1.39
24	b	607	CLA	C1B-CHB	3.41	1.49	1.39
24	B	609	CLA	C1B-CHB	3.41	1.49	1.39
24	c	509	CLA	C1B-CHB	3.42	1.49	1.39
24	A	1008	CLA	C1B-CHB	3.42	1.49	1.39
24	C	507	CLA	C1B-CHB	3.44	1.49	1.39
25	A	1007	PHO	OBD-CAD	3.44	1.28	1.22
24	c	501	CLA	C1B-CHB	3.45	1.49	1.39
24	c	505	CLA	C1B-CHB	3.45	1.49	1.39
34	D	409	LHG	O7-C7	3.45	1.44	1.34
24	c	506	CLA	C1B-CHB	3.45	1.49	1.39
24	c	513	CLA	C1B-CHB	3.45	1.49	1.39
24	C	510	CLA	C1B-CHB	3.46	1.49	1.39
24	b	610	CLA	OBD-CAD	3.47	1.27	1.22
24	C	512	CLA	C1B-CHB	3.47	1.49	1.39
24	C	505	CLA	C1B-CHB	3.47	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C1B-CHB	3.47	1.49	1.39
24	c	507	CLA	C1B-CHB	3.48	1.49	1.39
24	B	614	CLA	C1B-CHB	3.48	1.49	1.39
24	b	618	CLA	C1B-CHB	3.49	1.49	1.39
24	C	511	CLA	C1B-CHB	3.49	1.49	1.39
24	a	408	CLA	C1B-CHB	3.49	1.49	1.39
34	D	410	LHG	O7-C7	3.49	1.44	1.34
25	D	404	PHO	OBD-CAD	3.51	1.28	1.22
25	a	411	PHO	OBD-CAD	3.51	1.28	1.22
24	B	615	CLA	C1B-CHB	3.51	1.49	1.39
24	c	510	CLA	C1B-CHB	3.52	1.49	1.39
24	C	513	CLA	C1B-CHB	3.53	1.49	1.39
34	d	407	LHG	O7-C7	3.55	1.44	1.34
24	B	613	CLA	C1B-CHB	3.55	1.49	1.39
24	b	610	CLA	C1B-CHB	3.56	1.49	1.39
24	b	615	CLA	C1B-CHB	3.57	1.49	1.39
34	d	406	LHG	O7-C7	3.59	1.45	1.34
34	b	624	LHG	O7-C7	3.60	1.45	1.34
36	H	102	DGD	O2G-C1B	3.62	1.45	1.34
25	a	410	PHO	OBD-CAD	3.64	1.29	1.22
24	B	607	CLA	OBD-CAD	3.66	1.27	1.22
24	B	603	CLA	O2A-CGA	3.66	1.44	1.33
24	D	403	CLA	CHC-C1C	3.69	1.46	1.35
38	F	101	HEM	FE-NC	3.72	2.10	1.95
24	B	605	CLA	OBD-CAD	3.72	1.28	1.22
24	b	614	CLA	OBD-CAD	3.73	1.28	1.22
36	c	515	DGD	O2G-C1B	3.74	1.45	1.34
24	a	407	CLA	O2A-CGA	3.74	1.44	1.33
24	B	605	CLA	O2A-CGA	3.75	1.44	1.33
34	D	410	LHG	O8-C23	3.76	1.44	1.33
36	C	516	DGD	O2G-C1B	3.77	1.45	1.34
29	D	412	LMG	O7-C10	3.78	1.45	1.34
36	C	515	DGD	O2G-C1B	3.78	1.45	1.34
24	B	608	CLA	CHC-C1C	3.79	1.47	1.35
24	b	606	CLA	O2A-CGA	3.80	1.44	1.33
24	d	402	CLA	OBD-CAD	3.81	1.28	1.22
34	B	621	LHG	O7-C7	3.81	1.45	1.34
24	B	610	CLA	O2A-CGA	3.82	1.44	1.33
36	c	517	DGD	O2G-C1B	3.82	1.45	1.34
34	D	411	LHG	O7-C7	3.83	1.45	1.34
24	B	612	CLA	O2A-CGA	3.83	1.44	1.33
34	d	407	LHG	O8-C23	3.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	O2A-CGA	3.83	1.44	1.33
24	B	607	CLA	O2A-CGA	3.84	1.44	1.33
24	b	616	CLA	O2A-CGA	3.84	1.44	1.33
24	a	408	CLA	CHC-C1C	3.86	1.47	1.35
36	c	516	DGD	O2G-C1B	3.86	1.45	1.34
24	B	606	CLA	O2A-CGA	3.86	1.44	1.33
24	b	608	CLA	OBD-CAD	3.86	1.28	1.22
24	B	608	CLA	OBD-CAD	3.87	1.28	1.22
24	B	616	CLA	OBD-CAD	3.87	1.28	1.22
25	A	1007	PHO	O2A-CGA	3.87	1.45	1.33
36	C	515	DGD	O1G-C1A	3.87	1.45	1.33
28	A	1011	SQD	O47-C7	3.87	1.45	1.34
36	H	102	DGD	O1G-C1A	3.88	1.45	1.33
29	D	412	LMG	O8-C28	3.88	1.45	1.33
24	D	402	CLA	CHC-C1C	3.89	1.47	1.35
36	C	517	DGD	O2G-C1B	3.89	1.45	1.34
24	B	606	CLA	OBD-CAD	3.89	1.28	1.22
24	C	512	CLA	OBD-CAD	3.90	1.28	1.22
36	C	516	DGD	O1G-C1A	3.91	1.45	1.33
24	A	1006	CLA	OBD-CAD	3.91	1.28	1.22
28	b	623[B]	SQD	O47-C7	3.91	1.46	1.34
24	b	617	CLA	OBD-CAD	3.92	1.28	1.22
24	b	608	CLA	O2A-CGA	3.92	1.45	1.33
36	C	517	DGD	O1G-C1A	3.92	1.45	1.33
28	B	620[B]	SQD	O47-C7	3.93	1.46	1.34
24	C	509	CLA	CHC-C1C	3.93	1.47	1.35
36	h	102	DGD	O2G-C1B	3.93	1.46	1.34
24	B	607	CLA	CHC-C1C	3.93	1.47	1.35
24	C	510	CLA	CHC-C1C	3.93	1.47	1.35
29	Z	101	LMG	O7-C10	3.93	1.46	1.34
24	B	602	CLA	O2A-CGA	3.94	1.45	1.33
24	B	615	CLA	CHC-C1C	3.94	1.47	1.35
24	c	502	CLA	O2A-CGA	3.94	1.45	1.33
24	b	610	CLA	O2A-CGA	3.94	1.45	1.33
24	C	503	CLA	O2A-CGA	3.95	1.45	1.33
24	B	610	CLA	OBD-CAD	3.95	1.28	1.22
24	B	603	CLA	CHC-C1C	3.95	1.47	1.35
24	C	504	CLA	OBD-CAD	3.95	1.28	1.22
24	b	610	CLA	CHC-C1C	3.95	1.47	1.35
24	B	603	CLA	OBD-CAD	3.95	1.28	1.22
34	d	408	LHG	O7-C7	3.96	1.46	1.34
24	A	1006	CLA	O2A-CGA	3.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	m	102	LMG	O7-C10	3.96	1.46	1.34
28	b	623[A]	SQD	O47-C7	3.96	1.46	1.34
28	B	620[A]	SQD	O47-C7	3.96	1.46	1.34
25	a	410	PHO	O2A-CGA	3.96	1.45	1.33
24	b	613	CLA	O2A-CGA	3.97	1.45	1.33
24	B	615	CLA	O2A-CGA	3.97	1.45	1.33
24	b	615	CLA	O2A-CGA	3.97	1.45	1.33
24	C	504	CLA	O2A-CGA	3.97	1.45	1.33
24	c	501	CLA	OBD-CAD	3.97	1.28	1.22
24	C	502	CLA	O2A-CGA	3.98	1.45	1.33
34	E	101	LHG	O7-C7	3.98	1.46	1.34
24	c	504	CLA	O2A-CGA	3.98	1.45	1.33
24	b	611	CLA	O2A-CGA	3.99	1.45	1.33
24	b	607	CLA	O2A-CGA	3.99	1.45	1.33
29	d	409	LMG	O7-C10	4.00	1.46	1.34
29	c	520	LMG	O7-C10	4.00	1.46	1.34
24	b	611	CLA	OBD-CAD	4.00	1.28	1.22
29	A	1012	LMG	O7-C10	4.01	1.46	1.34
24	c	501	CLA	CHC-C1C	4.01	1.47	1.35
24	C	511	CLA	O2A-CGA	4.02	1.45	1.33
24	C	510	CLA	O2A-CGA	4.02	1.45	1.33
28	f	102	SQD	O47-C7	4.02	1.46	1.34
24	b	606	CLA	OBD-CAD	4.02	1.28	1.22
24	b	617	CLA	O2A-CGA	4.03	1.45	1.33
24	B	611	CLA	O2A-CGA	4.03	1.45	1.33
24	c	508	CLA	O2A-CGA	4.03	1.45	1.33
24	b	614	CLA	O2A-CGA	4.03	1.45	1.33
24	a	409	CLA	O2A-CGA	4.03	1.45	1.33
24	B	614	CLA	CHC-C1C	4.03	1.48	1.35
24	C	501	CLA	O2A-CGA	4.04	1.45	1.33
24	c	503	CLA	O2A-CGA	4.04	1.45	1.33
34	b	624	LHG	O8-C23	4.04	1.45	1.33
24	b	619	CLA	OBD-CAD	4.04	1.28	1.22
24	c	503	CLA	OBD-CAD	4.05	1.28	1.22
34	B	621	LHG	O8-C23	4.05	1.45	1.33
28	A	1016	SQD	O47-C7	4.05	1.46	1.34
24	B	613	CLA	O2A-CGA	4.05	1.45	1.33
24	C	504	CLA	CHC-C1C	4.05	1.48	1.35
24	a	407	CLA	CHC-C1C	4.05	1.48	1.35
24	c	510	CLA	O2A-CGA	4.05	1.45	1.33
24	C	501	CLA	OBD-CAD	4.06	1.28	1.22
34	d	408	LHG	O8-C23	4.06	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	CHC-C1C	4.06	1.48	1.35
29	C	518	LMG	O7-C10	4.06	1.46	1.34
24	b	612	CLA	O2A-CGA	4.06	1.45	1.33
34	D	411	LHG	O8-C23	4.06	1.45	1.33
24	b	614	CLA	CHC-C1C	4.06	1.48	1.35
24	c	506	CLA	CHC-C1C	4.06	1.48	1.35
28	a	401	SQD	O47-C7	4.07	1.46	1.34
29	a	415	LMG	O7-C10	4.07	1.46	1.34
24	A	1006	CLA	CHC-C1C	4.07	1.48	1.35
24	C	505	CLA	O2A-CGA	4.07	1.45	1.33
36	h	102	DGD	O1G-C1A	4.07	1.45	1.33
24	c	510	CLA	CHC-C1C	4.08	1.48	1.35
34	e	101	LHG	O7-C7	4.08	1.46	1.34
24	B	604	CLA	CHC-C1C	4.08	1.48	1.35
36	c	515	DGD	O1G-C1A	4.08	1.45	1.33
29	C	519	LMG	O7-C10	4.09	1.46	1.34
24	b	609	CLA	O2A-CGA	4.09	1.45	1.33
24	b	617	CLA	CHC-C1C	4.09	1.48	1.35
24	B	602	CLA	CHC-C1C	4.09	1.48	1.35
24	b	619	CLA	CHC-C1C	4.09	1.48	1.35
28	c	518	SQD	O47-C7	4.10	1.46	1.34
29	d	409	LMG	O8-C28	4.10	1.45	1.33
24	D	405	CLA	OBD-CAD	4.10	1.28	1.22
24	C	505	CLA	OBD-CAD	4.10	1.28	1.22
24	C	512	CLA	O2A-CGA	4.10	1.45	1.33
24	D	402	CLA	O2A-CGA	4.11	1.45	1.33
24	C	507	CLA	O2A-CGA	4.11	1.45	1.33
24	c	505	CLA	O2A-CGA	4.11	1.45	1.33
24	c	511	CLA	O2A-CGA	4.11	1.45	1.33
34	D	409	LHG	O8-C23	4.11	1.45	1.33
24	b	618	CLA	O2A-CGA	4.11	1.45	1.33
29	B	622	LMG	O7-C10	4.12	1.46	1.34
24	b	618	CLA	CHC-C1C	4.12	1.48	1.35
24	B	616	CLA	O2A-CGA	4.12	1.45	1.33
24	A	1005	CLA	O2A-CGA	4.12	1.45	1.33
24	C	508	CLA	O2A-CGA	4.12	1.45	1.33
30	b	628	DMS	O-S	4.12	1.78	1.50
24	D	403	CLA	O2A-CGA	4.13	1.45	1.33
25	a	411	PHO	O2A-CGA	4.13	1.45	1.33
25	D	404	PHO	O2A-CGA	4.13	1.45	1.33
24	B	616	CLA	CHC-C1C	4.13	1.48	1.35
24	c	504	CLA	OBD-CAD	4.13	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	516	DGD	O1G-C1A	4.13	1.45	1.33
24	B	613	CLA	OBD-CAD	4.13	1.28	1.22
24	A	1008	CLA	CHC-C1C	4.13	1.48	1.35
24	D	405	CLA	O2A-CGA	4.13	1.45	1.33
24	c	513	CLA	O2A-CGA	4.14	1.45	1.33
24	A	1005	CLA	CHC-C1C	4.14	1.48	1.35
24	b	616	CLA	CHC-C1C	4.14	1.48	1.35
24	c	509	CLA	CHC-C1C	4.14	1.48	1.35
24	a	412	CLA	OBD-CAD	4.14	1.28	1.22
24	c	508	CLA	CHC-C1C	4.14	1.48	1.35
29	c	519	LMG	O7-C10	4.14	1.46	1.34
24	b	615	CLA	CHC-C1C	4.15	1.48	1.35
29	a	415	LMG	O8-C28	4.15	1.45	1.33
24	b	613	CLA	OBD-CAD	4.15	1.28	1.22
24	c	506	CLA	O2A-CGA	4.15	1.45	1.33
24	d	402	CLA	CHC-C1C	4.15	1.48	1.35
24	b	608	CLA	CHC-C1C	4.16	1.48	1.35
28	b	623[A]	SQD	O48-C23	4.16	1.45	1.33
36	c	517	DGD	O1G-C1A	4.16	1.45	1.33
24	A	1008	CLA	O2A-CGA	4.16	1.45	1.33
30	A	1013	DMS	O-S	4.16	1.78	1.50
24	B	610	CLA	CHC-C1C	4.16	1.48	1.35
24	C	505	CLA	CHC-C1C	4.17	1.48	1.35
24	C	506	CLA	OBD-CAD	4.17	1.28	1.22
28	c	518	SQD	O48-C23	4.17	1.45	1.33
24	C	502	CLA	CHC-C1C	4.17	1.48	1.35
28	B	620[B]	SQD	O48-C23	4.17	1.45	1.33
24	B	609	CLA	OBD-CAD	4.17	1.28	1.22
24	b	605	CLA	O2A-CGA	4.18	1.45	1.33
24	A	1008	CLA	OBD-CAD	4.18	1.28	1.22
24	a	412	CLA	CHC-C1C	4.18	1.48	1.35
24	b	618	CLA	OBD-CAD	4.18	1.28	1.22
24	B	612	CLA	CHC-C1C	4.18	1.48	1.35
28	D	408	SQD	O47-C7	4.18	1.46	1.34
28	B	620[A]	SQD	O48-C23	4.18	1.45	1.33
28	A	1011	SQD	O48-C23	4.19	1.45	1.33
24	c	512	CLA	OBD-CAD	4.19	1.28	1.22
30	C	523	DMS	O-S	4.19	1.79	1.50
24	C	508	CLA	OBD-CAD	4.19	1.28	1.22
24	a	409	CLA	CHC-C1C	4.19	1.48	1.35
24	C	506	CLA	O2A-CGA	4.19	1.45	1.33
30	a	417	DMS	O-S	4.19	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	1016	SQD	O48-C23	4.19	1.45	1.33
29	A	1012	LMG	O8-C28	4.20	1.46	1.33
24	B	606	CLA	CHC-C1C	4.20	1.48	1.35
30	B	626	DMS	O-S	4.20	1.79	1.50
24	C	501	CLA	CHC-C1C	4.20	1.48	1.35
24	B	611	CLA	CHC-C1C	4.20	1.48	1.35
28	b	623[B]	SQD	O48-C23	4.21	1.46	1.33
24	B	601	CLA	O2A-CGA	4.21	1.46	1.33
24	B	614	CLA	O2A-CGA	4.21	1.46	1.33
28	D	408	SQD	O48-C23	4.21	1.46	1.33
24	C	513	CLA	O2A-CGA	4.21	1.46	1.33
24	C	513	CLA	OBD-CAD	4.21	1.28	1.22
24	C	511	CLA	OBD-CAD	4.21	1.28	1.22
24	b	609	CLA	CHC-C1C	4.22	1.48	1.35
24	c	504	CLA	CHC-C1C	4.22	1.48	1.35
24	d	403	CLA	OBD-CAD	4.22	1.28	1.22
24	c	509	CLA	O2A-CGA	4.22	1.46	1.33
24	b	612	CLA	CHC-C1C	4.22	1.48	1.35
24	B	609	CLA	O2A-CGA	4.23	1.46	1.33
24	b	607	CLA	OBD-CAD	4.23	1.28	1.22
24	c	512	CLA	O2A-CGA	4.23	1.46	1.33
34	E	101	LHG	O8-C23	4.23	1.46	1.33
24	c	506	CLA	OBD-CAD	4.23	1.28	1.22
24	a	412	CLA	O2A-CGA	4.23	1.46	1.33
24	C	503	CLA	OBD-CAD	4.23	1.28	1.22
29	c	519	LMG	O8-C28	4.23	1.46	1.33
24	D	403	CLA	OBD-CAD	4.24	1.28	1.22
24	c	502	CLA	CHC-C1C	4.24	1.48	1.35
28	a	401	SQD	O48-C23	4.24	1.46	1.33
24	C	512	CLA	CHC-C1C	4.24	1.48	1.35
24	B	613	CLA	CHC-C1C	4.24	1.48	1.35
34	e	101	LHG	O8-C23	4.24	1.46	1.33
24	C	509	CLA	OBD-CAD	4.24	1.28	1.22
24	b	613	CLA	CHC-C1C	4.24	1.48	1.35
30	C	524	DMS	O-S	4.25	1.79	1.50
30	B	627	DMS	O-S	4.26	1.79	1.50
24	c	507	CLA	O2A-CGA	4.26	1.46	1.33
24	a	408	CLA	OBD-CAD	4.26	1.28	1.22
24	B	601	CLA	CHC-C1C	4.26	1.48	1.35
24	c	513	CLA	OBD-CAD	4.26	1.28	1.22
24	B	601	CLA	OBD-CAD	4.26	1.28	1.22
24	a	408	CLA	O2A-CGA	4.26	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	CHC-C1C	4.27	1.48	1.35
24	c	501	CLA	O2A-CGA	4.27	1.46	1.33
24	d	403	CLA	O2A-CGA	4.27	1.46	1.33
24	c	507	CLA	OBD-CAD	4.27	1.28	1.22
24	c	505	CLA	CHC-C1C	4.27	1.48	1.35
29	c	521	LMG	O7-C10	4.27	1.47	1.34
30	c	524	DMS	O-S	4.27	1.79	1.50
24	C	506	CLA	CHC-C1C	4.28	1.48	1.35
24	b	611	CLA	CHC-C1C	4.28	1.48	1.35
30	c	529	DMS	O-S	4.28	1.79	1.50
24	B	615	CLA	OBD-CAD	4.28	1.28	1.22
24	b	612	CLA	OBD-CAD	4.28	1.28	1.22
24	B	609	CLA	CHC-C1C	4.29	1.48	1.35
24	c	513	CLA	CHC-C1C	4.29	1.48	1.35
29	C	519	LMG	O8-C28	4.29	1.46	1.33
28	f	102	SQD	O48-C23	4.29	1.46	1.33
24	B	602	CLA	OBD-CAD	4.29	1.28	1.22
24	b	605	CLA	OBD-CAD	4.29	1.28	1.22
24	c	505	CLA	OBD-CAD	4.29	1.28	1.22
24	c	511	CLA	OBD-CAD	4.29	1.28	1.22
24	b	605	CLA	CHC-C1C	4.30	1.48	1.35
24	B	612	CLA	OBD-CAD	4.30	1.28	1.22
24	D	405	CLA	CHC-C1C	4.30	1.48	1.35
24	c	508	CLA	OBD-CAD	4.30	1.28	1.22
24	C	513	CLA	CHC-C1C	4.31	1.48	1.35
24	d	403	CLA	CHC-C1C	4.31	1.48	1.35
24	b	604	CLA	OBD-CAD	4.31	1.28	1.22
24	b	616	CLA	OBD-CAD	4.31	1.28	1.22
34	d	406	LHG	O8-C23	4.31	1.46	1.33
29	c	521	LMG	O8-C28	4.31	1.46	1.33
24	C	509	CLA	O2A-CGA	4.32	1.46	1.33
29	C	518	LMG	O8-C28	4.32	1.46	1.33
24	B	604	CLA	OBD-CAD	4.32	1.29	1.22
24	c	507	CLA	CHC-C1C	4.32	1.48	1.35
24	B	605	CLA	CHC-C1C	4.33	1.48	1.35
24	b	609	CLA	OBD-CAD	4.33	1.29	1.22
24	c	510	CLA	OBD-CAD	4.33	1.29	1.22
30	v	202	DMS	O-S	4.33	1.80	1.50
24	B	608	CLA	O2A-CGA	4.34	1.46	1.33
30	u	201	DMS	O-S	4.34	1.80	1.50
24	b	619	CLA	O2A-CGA	4.35	1.46	1.33
24	B	614	CLA	OBD-CAD	4.35	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	U	201	DMS	O-S	4.36	1.80	1.50
24	c	512	CLA	CHC-C1C	4.36	1.49	1.35
24	C	510	CLA	OBD-CAD	4.37	1.29	1.22
24	C	507	CLA	CHC-C1C	4.37	1.49	1.35
29	B	622	LMG	O8-C28	4.37	1.46	1.33
24	b	604	CLA	CHC-C1C	4.37	1.49	1.35
24	C	502	CLA	OBD-CAD	4.37	1.29	1.22
24	d	402	CLA	O2A-CGA	4.37	1.46	1.33
30	c	526	DMS	O-S	4.37	1.80	1.50
24	C	508	CLA	CHC-C1C	4.38	1.49	1.35
24	C	507	CLA	OBD-CAD	4.38	1.29	1.22
29	c	520	LMG	O8-C28	4.38	1.46	1.33
30	d	414	DMS	O-S	4.38	1.80	1.50
30	C	527	DMS	O-S	4.38	1.80	1.50
30	B	632	DMS	O-S	4.38	1.80	1.50
30	C	526	DMS	O-S	4.38	1.80	1.50
29	Z	101	LMG	O8-C28	4.39	1.46	1.33
30	c	528	DMS	O-S	4.39	1.80	1.50
25	A	1007	PHO	O2D-CGD	4.39	1.44	1.33
30	b	633	DMS	O-S	4.40	1.80	1.50
24	b	606	CLA	CHC-C1C	4.40	1.49	1.35
30	C	525	DMS	O-S	4.40	1.80	1.50
24	C	503	CLA	CHC-C1C	4.40	1.49	1.35
25	a	411	PHO	CHD-C1D	4.40	1.47	1.38
30	b	635	DMS	O-S	4.41	1.80	1.50
30	b	629	DMS	O-S	4.41	1.80	1.50
30	V	205	DMS	O-S	4.41	1.80	1.50
30	O	302	DMS	O-S	4.41	1.80	1.50
29	m	102	LMG	O8-C28	4.42	1.46	1.33
30	c	527	DMS	O-S	4.42	1.80	1.50
30	O	301	DMS	O-S	4.42	1.80	1.50
24	c	503	CLA	CHC-C1C	4.43	1.49	1.35
30	V	203	DMS	O-S	4.43	1.80	1.50
30	A	1014	DMS	O-S	4.43	1.80	1.50
30	a	418	DMS	O-S	4.44	1.80	1.50
30	B	633	DMS	O-S	4.44	1.80	1.50
30	B	634	DMS	O-S	4.44	1.80	1.50
24	B	607	CLA	O2D-CGD	4.44	1.44	1.33
30	d	413	DMS	O-S	4.44	1.80	1.50
30	D	417	DMS	O-S	4.45	1.80	1.50
24	c	511	CLA	CHC-C1C	4.45	1.49	1.35
25	A	1007	PHO	CHD-C1D	4.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D	416	DMS	O-S	4.46	1.80	1.50
30	b	634	DMS	O-S	4.47	1.81	1.50
24	D	403	CLA	O2D-CGD	4.47	1.44	1.33
24	B	611	CLA	OBD-CAD	4.50	1.29	1.22
24	B	602	CLA	O2D-CGD	4.51	1.44	1.33
24	a	407	CLA	OBD-CAD	4.51	1.29	1.22
24	a	409	CLA	O2D-CGD	4.51	1.44	1.33
24	a	408	CLA	O2D-CGD	4.52	1.44	1.33
24	A	1005	CLA	OBD-CAD	4.52	1.29	1.22
24	c	502	CLA	OBD-CAD	4.53	1.29	1.22
25	D	404	PHO	CHD-C1D	4.53	1.47	1.38
24	b	604	CLA	O2A-CGA	4.53	1.47	1.33
24	c	509	CLA	OBD-CAD	4.53	1.29	1.22
24	D	402	CLA	OBD-CAD	4.55	1.29	1.22
24	D	402	CLA	O2D-CGD	4.55	1.44	1.33
24	B	613	CLA	O2D-CGD	4.58	1.44	1.33
24	d	403	CLA	O2D-CGD	4.58	1.44	1.33
24	B	610	CLA	O2D-CGD	4.60	1.44	1.33
24	B	608	CLA	O2D-CGD	4.62	1.45	1.33
24	b	616	CLA	O2D-CGD	4.63	1.45	1.33
24	c	505	CLA	O2D-CGD	4.63	1.45	1.33
24	D	405	CLA	O2D-CGD	4.64	1.45	1.33
24	C	507	CLA	O2D-CGD	4.65	1.45	1.33
24	b	605	CLA	O2D-CGD	4.66	1.45	1.33
25	a	410	PHO	O2D-CGD	4.67	1.45	1.33
24	b	611	CLA	O2D-CGD	4.69	1.45	1.33
24	a	412	CLA	O2D-CGD	4.69	1.45	1.33
24	C	505	CLA	O2D-CGD	4.70	1.45	1.33
24	b	615	CLA	OBD-CAD	4.71	1.29	1.22
24	A	1008	CLA	O2D-CGD	4.72	1.45	1.33
24	A	1006	CLA	O2D-CGD	4.73	1.45	1.33
24	C	502	CLA	O2D-CGD	4.74	1.45	1.33
24	c	502	CLA	O2D-CGD	4.74	1.45	1.33
24	a	407	CLA	O2D-CGD	4.75	1.45	1.33
24	B	614	CLA	O2D-CGD	4.75	1.45	1.33
24	C	503	CLA	O2D-CGD	4.75	1.45	1.33
24	c	503	CLA	O2D-CGD	4.76	1.45	1.33
24	b	617	CLA	O2D-CGD	4.76	1.45	1.33
24	C	509	CLA	O2D-CGD	4.76	1.45	1.33
24	B	616	CLA	O2D-CGD	4.76	1.45	1.33
24	b	619	CLA	O2D-CGD	4.77	1.45	1.33
24	d	402	CLA	O2D-CGD	4.78	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	O2D-CGD	4.78	1.45	1.33
24	b	609	CLA	O2D-CGD	4.80	1.45	1.33
24	C	501	CLA	O2D-CGD	4.80	1.45	1.33
24	B	604	CLA	O2D-CGD	4.80	1.45	1.33
24	c	501	CLA	O2D-CGD	4.80	1.45	1.33
25	A	1007	PHO	CHC-C1C	4.80	1.48	1.38
24	b	614	CLA	O2D-CGD	4.81	1.45	1.33
24	D	402	CLA	C3C-C2C	4.82	1.47	1.36
24	D	403	CLA	C3C-C2C	4.82	1.47	1.36
24	B	612	CLA	O2D-CGD	4.82	1.45	1.33
24	c	507	CLA	O2D-CGD	4.83	1.45	1.33
24	b	610	CLA	O2D-CGD	4.83	1.45	1.33
24	A	1005	CLA	O2D-CGD	4.84	1.45	1.33
25	a	411	PHO	O2D-CGD	4.84	1.45	1.33
24	b	612	CLA	O2D-CGD	4.84	1.45	1.33
25	a	410	PHO	CHC-C1C	4.85	1.48	1.38
24	b	619	CLA	C3C-C2C	4.85	1.47	1.36
24	c	502	CLA	C3C-C2C	4.86	1.47	1.36
25	a	410	PHO	CHD-C1D	4.86	1.48	1.38
24	c	512	CLA	O2D-CGD	4.86	1.45	1.33
24	C	510	CLA	C3C-C2C	4.88	1.47	1.36
24	b	614	CLA	C3C-C2C	4.89	1.47	1.36
24	B	613	CLA	C3C-C2C	4.89	1.47	1.36
24	b	608	CLA	O2D-CGD	4.89	1.45	1.33
24	c	510	CLA	O2D-CGD	4.90	1.45	1.33
24	b	615	CLA	O2D-CGD	4.90	1.45	1.33
24	B	605	CLA	O2D-CGD	4.90	1.45	1.33
24	C	512	CLA	O2D-CGD	4.90	1.45	1.33
24	b	613	CLA	O2D-CGD	4.91	1.45	1.33
25	D	404	PHO	O2D-CGD	4.92	1.45	1.33
24	b	607	CLA	O2D-CGD	4.92	1.45	1.33
24	c	506	CLA	O2D-CGD	4.92	1.45	1.33
24	C	510	CLA	O2D-CGD	4.92	1.45	1.33
24	b	607	CLA	C3C-C2C	4.93	1.47	1.36
24	C	502	CLA	C3C-C2C	4.93	1.47	1.36
24	B	606	CLA	O2D-CGD	4.93	1.45	1.33
24	C	504	CLA	O2D-CGD	4.95	1.45	1.33
24	A	1005	CLA	C3C-C2C	4.95	1.47	1.36
24	B	616	CLA	C3C-C2C	4.95	1.47	1.36
24	A	1006	CLA	C3C-C2C	4.95	1.47	1.36
24	B	609	CLA	O2D-CGD	4.96	1.45	1.33
24	B	603	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	509	CLA	O2D-CGD	4.97	1.45	1.33
24	B	607	CLA	C3B-C2B	4.97	1.46	1.40
24	b	616	CLA	C3C-C2C	4.99	1.47	1.36
24	c	513	CLA	O2D-CGD	5.00	1.46	1.33
24	B	609	CLA	C3C-C2C	5.01	1.47	1.36
24	C	511	CLA	O2D-CGD	5.01	1.46	1.33
24	B	609	CLA	C3B-C2B	5.01	1.46	1.40
24	b	606	CLA	O2D-CGD	5.02	1.46	1.33
24	c	509	CLA	C3C-C2C	5.02	1.47	1.36
24	B	615	CLA	C3C-C2C	5.02	1.47	1.36
24	B	601	CLA	O2D-CGD	5.03	1.46	1.33
24	C	513	CLA	O2D-CGD	5.03	1.46	1.33
24	C	506	CLA	O2D-CGD	5.03	1.46	1.33
24	B	605	CLA	C3C-C2C	5.03	1.47	1.36
24	a	408	CLA	C3C-C2C	5.04	1.47	1.36
24	B	611	CLA	O2D-CGD	5.04	1.46	1.33
24	a	409	CLA	C3C-C2C	5.05	1.47	1.36
24	c	511	CLA	O2D-CGD	5.05	1.46	1.33
24	B	612	CLA	C3C-C2C	5.05	1.47	1.36
24	B	607	CLA	C3C-C2C	5.07	1.47	1.36
24	b	612	CLA	C3B-C2B	5.07	1.47	1.40
24	a	409	CLA	C3B-C2B	5.07	1.47	1.40
24	C	508	CLA	O2D-CGD	5.07	1.46	1.33
25	D	404	PHO	CHC-C1C	5.07	1.48	1.38
24	B	615	CLA	O2D-CGD	5.08	1.46	1.33
24	B	604	CLA	C3B-C2B	5.08	1.47	1.40
24	b	617	CLA	C3C-C2C	5.10	1.47	1.36
24	a	412	CLA	C3C-C2C	5.10	1.47	1.36
24	c	507	CLA	C3C-C2C	5.12	1.47	1.36
24	b	612	CLA	C3C-C2C	5.12	1.47	1.36
24	C	501	CLA	C3C-C2C	5.13	1.47	1.36
24	b	610	CLA	C3C-C2C	5.13	1.47	1.36
24	b	618	CLA	C3C-C2C	5.15	1.47	1.36
24	d	403	CLA	C3C-C2C	5.15	1.47	1.36
24	C	505	CLA	C3C-C2C	5.16	1.47	1.36
24	c	508	CLA	O2D-CGD	5.16	1.46	1.33
24	d	402	CLA	C3C-C2C	5.16	1.47	1.36
24	c	504	CLA	O2D-CGD	5.17	1.46	1.33
25	a	411	PHO	C3C-C2C	5.17	1.47	1.36
24	b	615	CLA	C3C-C2C	5.17	1.47	1.36
24	c	510	CLA	C3C-C2C	5.18	1.47	1.36
25	a	411	PHO	CHC-C1C	5.18	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C3C-C2C	5.18	1.47	1.36
24	b	606	CLA	C3C-C2C	5.18	1.47	1.36
24	c	505	CLA	C3C-C2C	5.18	1.47	1.36
24	d	402	CLA	C3B-C2B	5.19	1.47	1.40
24	B	614	CLA	C3C-C2C	5.19	1.47	1.36
24	B	604	CLA	C3C-C2C	5.19	1.47	1.36
24	b	604	CLA	O2D-CGD	5.20	1.46	1.33
24	B	611	CLA	C3C-C2C	5.20	1.48	1.36
24	b	608	CLA	C3C-C2C	5.21	1.48	1.36
24	C	507	CLA	C3C-C2C	5.21	1.48	1.36
25	D	404	PHO	C3C-C2C	5.22	1.48	1.36
24	A	1008	CLA	C3C-C2C	5.22	1.48	1.36
25	a	410	PHO	C3B-C2B	5.22	1.47	1.36
24	c	506	CLA	C3C-C2C	5.23	1.48	1.36
24	C	509	CLA	C3C-C2C	5.23	1.48	1.36
24	C	503	CLA	C3C-C2C	5.25	1.48	1.36
24	b	609	CLA	C3C-C2C	5.25	1.48	1.36
24	b	613	CLA	C3C-C2C	5.25	1.48	1.36
24	a	407	CLA	C3C-C2C	5.26	1.48	1.36
24	b	604	CLA	C3C-C2C	5.26	1.48	1.36
24	B	601	CLA	C3C-C2C	5.26	1.48	1.36
24	B	603	CLA	C3C-C2C	5.27	1.48	1.36
24	B	605	CLA	C3B-C2B	5.27	1.47	1.40
24	b	605	CLA	C3C-C2C	5.28	1.48	1.36
24	b	610	CLA	C3B-C2B	5.28	1.47	1.40
24	a	412	CLA	C3B-C2B	5.28	1.47	1.40
24	c	511	CLA	C3C-C2C	5.28	1.48	1.36
24	B	606	CLA	C3C-C2C	5.29	1.48	1.36
24	C	508	CLA	C3C-C2C	5.29	1.48	1.36
24	D	405	CLA	C3C-C2C	5.30	1.48	1.36
24	C	504	CLA	C3C-C2C	5.30	1.48	1.36
24	B	610	CLA	C3C-C2C	5.30	1.48	1.36
24	B	608	CLA	C3C-C2C	5.30	1.48	1.36
25	A	1007	PHO	CHB-C1B	5.31	1.49	1.38
24	C	506	CLA	C3C-C2C	5.31	1.48	1.36
24	B	602	CLA	C3C-C2C	5.31	1.48	1.36
24	C	505	CLA	C3B-C2B	5.31	1.47	1.40
24	c	513	CLA	C3C-C2C	5.31	1.48	1.36
24	b	611	CLA	C3C-C2C	5.31	1.48	1.36
24	B	603	CLA	C3B-C2B	5.31	1.47	1.40
24	c	512	CLA	C3C-C2C	5.32	1.48	1.36
24	C	501	CLA	C3B-C2B	5.32	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C3C-C2C	5.32	1.48	1.36
24	C	511	CLA	C3C-C2C	5.33	1.48	1.36
25	a	411	PHO	CHB-C1B	5.34	1.49	1.38
24	C	510	CLA	C3B-C2B	5.34	1.47	1.40
24	b	613	CLA	C3B-C2B	5.34	1.47	1.40
24	b	617	CLA	C3B-C2B	5.35	1.47	1.40
25	A	1007	PHO	C3B-C2B	5.35	1.48	1.36
24	B	601	CLA	C3B-C2B	5.35	1.47	1.40
24	c	504	CLA	C3B-C2B	5.36	1.47	1.40
24	c	501	CLA	C3C-C2C	5.37	1.48	1.36
24	C	513	CLA	C3C-C2C	5.37	1.48	1.36
24	b	608	CLA	C3B-C2B	5.38	1.47	1.40
24	C	512	CLA	C3C-C2C	5.38	1.48	1.36
25	a	410	PHO	C3C-C2C	5.39	1.48	1.36
24	B	608	CLA	C3B-C2B	5.39	1.47	1.40
25	a	410	PHO	CHB-C1B	5.39	1.49	1.38
24	A	1008	CLA	C3B-C2B	5.39	1.47	1.40
24	D	402	CLA	C3B-C2B	5.40	1.47	1.40
24	b	606	CLA	C3B-C2B	5.40	1.47	1.40
25	a	411	PHO	C3B-C2B	5.41	1.48	1.36
24	c	508	CLA	C3C-C2C	5.42	1.48	1.36
25	A	1007	PHO	C3C-C2C	5.44	1.48	1.36
24	c	501	CLA	C3B-C2B	5.44	1.47	1.40
24	b	611	CLA	C3B-C2B	5.44	1.47	1.40
25	D	404	PHO	C3B-C2B	5.45	1.48	1.36
24	c	510	CLA	C3B-C2B	5.45	1.47	1.40
24	B	614	CLA	C3B-C2B	5.46	1.47	1.40
25	D	404	PHO	CHB-C1B	5.49	1.49	1.38
24	C	506	CLA	C3B-C2B	5.50	1.47	1.40
24	b	616	CLA	C3B-C2B	5.50	1.47	1.40
24	B	610	CLA	C3B-C2B	5.51	1.47	1.40
24	B	602	CLA	C3B-C2B	5.51	1.47	1.40
24	C	502	CLA	C3B-C2B	5.54	1.47	1.40
24	b	614	CLA	C3B-C2B	5.55	1.47	1.40
24	B	611	CLA	C3B-C2B	5.55	1.47	1.40
24	D	403	CLA	C3B-C2B	5.56	1.47	1.40
24	C	508	CLA	C3B-C2B	5.57	1.47	1.40
24	c	508	CLA	C3B-C2B	5.58	1.47	1.40
24	C	504	CLA	C3B-C2B	5.59	1.47	1.40
24	C	509	CLA	C3B-C2B	5.59	1.47	1.40
24	D	405	CLA	C3B-C2B	5.60	1.47	1.40
24	b	615	CLA	C3B-C2B	5.61	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1005	CLA	C3B-C2B	5.65	1.47	1.40
24	b	604	CLA	C3B-C2B	5.66	1.47	1.40
24	B	613	CLA	C3B-C2B	5.69	1.47	1.40
24	B	616	CLA	C3B-C2B	5.70	1.47	1.40
24	c	506	CLA	C3B-C2B	5.71	1.47	1.40
24	b	605	CLA	C3B-C2B	5.72	1.47	1.40
24	b	607	CLA	C3B-C2B	5.73	1.47	1.40
24	c	502	CLA	C3B-C2B	5.75	1.47	1.40
24	c	511	CLA	C3B-C2B	5.75	1.47	1.40
24	c	509	CLA	C3B-C2B	5.76	1.47	1.40
24	c	513	CLA	C3B-C2B	5.78	1.47	1.40
24	B	606	CLA	C3B-C2B	5.78	1.47	1.40
24	C	512	CLA	C3B-C2B	5.78	1.47	1.40
24	a	407	CLA	C3B-C2B	5.79	1.48	1.40
24	c	512	CLA	C3B-C2B	5.80	1.48	1.40
24	C	503	CLA	C3B-C2B	5.80	1.48	1.40
24	c	505	CLA	C3B-C2B	5.80	1.48	1.40
24	C	511	CLA	C3B-C2B	5.80	1.48	1.40
24	b	618	CLA	C3B-C2B	5.81	1.48	1.40
24	c	503	CLA	C3B-C2B	5.85	1.48	1.40
24	C	513	CLA	C3B-C2B	5.95	1.48	1.40
24	A	1006	CLA	C3B-C2B	5.96	1.48	1.40
24	b	619	CLA	C3B-C2B	6.01	1.48	1.40
24	c	507	CLA	C3B-C2B	6.03	1.48	1.40
24	b	609	CLA	C3B-C2B	6.06	1.48	1.40
24	d	403	CLA	C3B-C2B	6.06	1.48	1.40
24	a	408	CLA	C3B-C2B	6.14	1.48	1.40
24	B	615	CLA	C3B-C2B	6.17	1.48	1.40
24	B	612	CLA	C3B-C2B	6.18	1.48	1.40
24	C	507	CLA	C3B-C2B	6.20	1.48	1.40

All (2212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	617	BCR	C36-C18-C17	-9.42	108.99	122.90
26	J	101	BCR	C36-C18-C17	-9.27	109.20	122.90
26	a	413	BCR	C36-C18-C17	-8.55	110.27	122.90
26	B	619	BCR	C36-C18-C17	-8.34	110.58	122.90
26	J	101	BCR	C33-C5-C4	-8.34	97.62	113.43
26	c	514	BCR	C36-C18-C17	-8.14	110.88	122.90
26	t	101	BCR	C36-C18-C17	-7.91	111.22	122.90
26	C	514	BCR	C37-C22-C21	-7.89	111.25	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	BCR	C36-C18-C19	-7.76	105.18	118.10
26	k	102	BCR	C37-C22-C21	-7.71	111.51	122.90
26	b	620	BCR	C38-C26-C27	-7.34	99.52	113.43
26	y	101	BCR	C33-C5-C4	-7.28	99.62	113.43
26	k	101	BCR	C36-C18-C17	-7.22	112.23	122.90
26	h	101	BCR	C37-C22-C21	-7.00	112.56	122.90
26	d	404	BCR	C30-C25-C26	-6.90	112.53	122.66
26	c	514	BCR	C38-C26-C27	-6.89	100.36	113.43
26	A	1009	BCR	C36-C18-C17	-6.73	112.96	122.90
26	A	1009	BCR	C36-C18-C19	-6.62	107.08	118.10
26	B	618	BCR	C36-C18-C19	-6.59	107.13	118.10
26	b	622	BCR	C37-C22-C21	-6.41	113.43	122.90
26	H	101	BCR	C37-C22-C21	-6.38	113.47	122.90
26	k	101	BCR	C38-C26-C27	-6.30	101.48	113.43
26	K	102	BCR	C38-C26-C27	-6.29	101.50	113.43
26	k	102	BCR	C33-C5-C4	-6.24	101.60	113.43
26	T	101	BCR	C36-C18-C17	-6.20	113.74	122.90
26	K	101	BCR	C37-C22-C21	-6.19	113.77	122.90
26	h	101	BCR	C38-C26-C27	-6.08	101.90	113.43
26	k	101	BCR	C33-C5-C4	-6.04	101.98	113.43
26	b	621	BCR	C36-C18-C19	-6.02	108.08	118.10
26	B	618	BCR	C38-C26-C27	-6.01	102.03	113.43
26	k	102	BCR	C36-C18-C17	-5.94	114.13	122.90
26	B	618	BCR	C35-C13-C12	-5.90	108.28	118.10
26	H	101	BCR	C36-C18-C19	-5.89	108.30	118.10
26	B	618	BCR	C36-C18-C17	-5.82	114.31	122.90
26	c	514	BCR	C37-C22-C21	-5.81	114.31	122.90
26	y	101	BCR	C38-C26-C27	-5.81	102.41	113.43
26	K	101	BCR	C36-C18-C17	-5.79	114.35	122.90
26	A	1009	BCR	C38-C26-C27	-5.78	102.47	113.43
26	H	101	BCR	C36-C18-C17	-5.75	114.41	122.90
26	B	619	BCR	C30-C25-C26	-5.65	114.36	122.66
26	b	622	BCR	C35-C13-C12	-5.61	108.77	118.10
26	b	621	BCR	C36-C18-C17	-5.60	114.64	122.90
26	b	620	BCR	C35-C13-C12	-5.60	108.78	118.10
26	C	514	BCR	C38-C26-C27	-5.57	102.86	113.43
26	y	101	BCR	C37-C22-C21	-5.57	114.68	122.90
26	b	622	BCR	C36-C18-C17	-5.56	114.68	122.90
26	K	102	BCR	C37-C22-C21	-5.53	114.73	122.90
26	y	101	BCR	C36-C18-C17	-5.47	114.82	122.90
26	A	1009	BCR	C37-C22-C21	-5.44	114.87	122.90
26	h	101	BCR	C36-C18-C17	-5.43	114.88	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	413	BCR	C38-C26-C27	-5.41	103.17	113.43
26	a	413	BCR	C33-C5-C4	-5.40	103.19	113.43
26	d	404	BCR	C37-C22-C21	-5.38	114.96	122.90
26	H	101	BCR	C38-C26-C27	-5.37	103.24	113.43
26	b	620	BCR	C36-C18-C19	-5.37	109.16	118.10
26	b	622	BCR	C38-C26-C27	-5.36	103.27	113.43
26	k	102	BCR	C38-C26-C27	-5.34	103.31	113.43
26	b	621	BCR	C37-C22-C21	-5.33	115.03	122.90
26	T	101	BCR	C38-C26-C27	-5.32	103.35	113.43
26	D	406	BCR	C38-C26-C27	-5.25	103.48	113.43
26	J	101	BCR	C1-C6-C5	-5.23	114.97	122.66
26	B	618	BCR	C30-C25-C26	-5.23	114.97	122.66
26	b	621	BCR	C38-C26-C27	-5.23	103.52	113.43
26	d	404	BCR	C36-C18-C19	-5.18	109.48	118.10
26	a	413	BCR	C37-C22-C23	-5.14	109.54	118.10
26	b	620	BCR	C36-C18-C17	-5.11	115.35	122.90
26	t	101	BCR	C35-C13-C12	-5.11	109.59	118.10
26	h	101	BCR	C36-C18-C19	-5.10	109.61	118.10
26	D	406	BCR	C33-C5-C4	-5.09	103.77	113.43
26	B	619	BCR	C35-C13-C12	-5.06	109.67	118.10
26	t	101	BCR	C38-C26-C27	-5.04	103.88	113.43
26	B	618	BCR	C34-C9-C8	-5.01	109.76	118.10
26	B	617	BCR	C38-C26-C27	-5.00	103.94	113.43
26	B	617	BCR	C37-C22-C21	-5.00	115.52	122.90
26	d	404	BCR	C32-C1-C2	-4.98	90.97	108.79
26	K	102	BCR	C33-C5-C4	-4.97	104.01	113.43
26	c	514	BCR	C33-C5-C4	-4.95	104.05	113.43
26	a	413	BCR	C36-C18-C19	-4.94	109.88	118.10
26	H	101	BCR	C30-C25-C26	-4.92	115.44	122.66
26	c	514	BCR	C1-C6-C5	-4.90	115.46	122.66
26	C	514	BCR	C36-C18-C19	-4.89	109.95	118.10
26	D	406	BCR	C30-C25-C26	-4.89	115.48	122.66
26	B	617	BCR	C37-C22-C23	-4.84	110.05	118.10
26	t	101	BCR	C33-C5-C4	-4.83	104.27	113.43
26	k	101	BCR	C37-C22-C23	-4.81	110.09	118.10
26	B	618	BCR	C37-C22-C21	-4.81	115.80	122.90
26	b	622	BCR	C36-C18-C19	-4.79	110.12	118.10
26	b	621	BCR	C35-C13-C14	-4.79	115.83	122.90
26	b	622	BCR	C30-C25-C26	-4.78	115.64	122.66
26	b	621	BCR	C30-C25-C26	-4.77	115.65	122.66
26	K	102	BCR	C36-C18-C17	-4.75	115.89	122.90
26	H	101	BCR	C35-C13-C12	-4.73	110.22	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	404	BCR	C33-C5-C4	-4.68	104.55	113.43
26	c	514	BCR	C30-C25-C26	-4.68	115.78	122.66
26	h	101	BCR	C30-C25-C26	-4.67	115.80	122.66
26	A	1009	BCR	C30-C25-C26	-4.64	115.84	122.66
26	J	101	BCR	C37-C22-C21	-4.61	116.09	122.90
26	T	101	BCR	C33-C5-C4	-4.61	104.68	113.43
24	D	403	CLA	C1C-C2C-C3C	-4.58	101.43	106.91
26	H	101	BCR	C33-C5-C4	-4.54	104.82	113.43
26	h	101	BCR	C35-C13-C12	-4.52	110.58	118.10
26	K	101	BCR	C36-C18-C19	-4.51	110.60	118.10
26	k	101	BCR	C35-C13-C12	-4.51	110.60	118.10
26	D	406	BCR	C37-C22-C21	-4.49	116.26	122.90
26	b	620	BCR	C33-C5-C4	-4.47	104.96	113.43
26	y	101	BCR	C36-C18-C19	-4.47	110.66	118.10
26	J	101	BCR	C38-C26-C27	-4.46	104.97	113.43
26	T	101	BCR	C37-C22-C21	-4.45	116.32	122.90
26	A	1009	BCR	C37-C22-C23	-4.45	110.69	118.10
26	T	101	BCR	C30-C25-C26	-4.43	116.16	122.66
26	A	1009	BCR	C35-C13-C14	-4.41	116.38	122.90
26	y	101	BCR	C30-C25-C26	-4.41	116.18	122.66
26	d	404	BCR	C40-C30-C29	-4.37	93.14	108.79
26	K	102	BCR	C36-C18-C19	-4.35	110.85	118.10
26	J	101	BCR	C30-C25-C26	-4.33	116.30	122.66
26	J	101	BCR	C35-C13-C12	-4.33	110.89	118.10
26	C	514	BCR	C31-C1-C2	-4.27	93.48	108.79
26	B	619	BCR	C38-C26-C27	-4.27	105.33	113.43
26	K	101	BCR	C35-C13-C14	-4.27	116.59	122.90
26	b	620	BCR	C37-C22-C21	-4.25	116.62	122.90
26	K	101	BCR	C38-C26-C27	-4.23	105.41	113.43
25	D	404	PHO	C3D-C2D-C1D	-4.22	98.99	105.77
26	D	406	BCR	C35-C13-C12	-4.21	111.08	118.10
26	A	1009	BCR	C33-C5-C4	-4.20	105.47	113.43
24	a	408	CLA	C1C-C2C-C3C	-4.19	101.89	106.91
25	a	411	PHO	C3D-C2D-C1D	-4.18	99.05	105.77
26	D	406	BCR	C1-C6-C5	-4.18	116.53	122.66
26	h	101	BCR	C33-C5-C4	-4.15	105.57	113.43
26	B	619	BCR	C39-C30-C29	-4.15	93.94	108.79
24	B	614	CLA	O1D-CGD-CBD	-4.13	118.70	124.62
26	H	101	BCR	C35-C13-C14	-4.12	116.82	122.90
26	t	101	BCR	C37-C22-C23	-4.11	111.26	118.10
38	V	201	HEM	CBD-CAD-C3D	-4.11	101.60	113.55
26	D	406	BCR	C36-C18-C17	-4.10	116.84	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	O1D-CGD-CBD	-4.09	118.75	124.62
24	B	607	CLA	C1C-C2C-C3C	-4.09	102.01	106.91
26	C	514	BCR	C30-C25-C26	-4.08	116.66	122.66
38	f	101	HEM	CBD-CAD-C3D	-4.03	101.82	113.55
26	d	404	BCR	C35-C13-C12	-4.03	111.39	118.10
25	a	410	PHO	C3D-C2D-C1D	-4.02	99.31	105.77
26	K	101	BCR	C34-C9-C8	-4.02	111.41	118.10
24	A	1006	CLA	C1C-C2C-C3C	-4.01	102.11	106.91
24	C	510	CLA	C1C-C2C-C3C	-4.01	102.11	106.91
25	A	1007	PHO	C3D-C2D-C1D	-4.00	99.35	105.77
26	b	621	BCR	C35-C13-C12	-3.99	111.46	118.10
26	K	101	BCR	C30-C25-C26	-3.99	116.81	122.66
25	D	404	PHO	C4C-C3C-C2C	-3.97	102.38	106.81
26	H	101	BCR	C34-C9-C10	-3.97	117.04	122.90
24	A	1005	CLA	C1C-C2C-C3C	-3.96	102.17	106.91
26	k	101	BCR	C30-C25-C26	-3.94	116.87	122.66
27	A	1010	PL9	C7-C3-C2	-3.92	120.17	123.42
26	h	101	BCR	C39-C30-C29	-3.85	95.00	108.79
25	A	1007	PHO	C4C-C3C-C2C	-3.84	102.52	106.81
24	c	507	CLA	O1D-CGD-CBD	-3.84	119.12	124.62
24	c	501	CLA	C1C-C2C-C3C	-3.84	102.32	106.91
26	D	406	BCR	C40-C30-C29	-3.83	95.05	108.79
26	B	619	BCR	C36-C18-C19	-3.83	111.72	118.10
26	K	102	BCR	C40-C30-C29	-3.83	95.07	108.79
24	A	1008	CLA	C1C-C2C-C3C	-3.82	102.34	106.91
25	a	411	PHO	C4C-C3C-C2C	-3.81	102.56	106.81
24	b	610	CLA	C1C-C2C-C3C	-3.80	102.36	106.91
24	B	603	CLA	C1C-C2C-C3C	-3.80	102.36	106.91
26	b	620	BCR	C30-C25-C26	-3.80	117.08	122.66
24	D	402	CLA	C1C-C2C-C3C	-3.79	102.37	106.91
26	B	617	BCR	C35-C13-C12	-3.79	111.78	118.10
26	B	617	BCR	C30-C25-C26	-3.79	117.09	122.66
26	B	617	BCR	C36-C18-C19	-3.77	111.82	118.10
26	a	413	BCR	C37-C22-C21	-3.76	117.35	122.90
26	C	514	BCR	C1-C6-C5	-3.75	117.15	122.66
26	c	514	BCR	C31-C1-C2	-3.74	95.38	108.79
24	a	407	CLA	C1C-C2C-C3C	-3.73	102.44	106.91
26	a	413	BCR	C30-C25-C26	-3.73	117.18	122.66
26	y	101	BCR	C1-C6-C5	-3.69	117.23	122.66
26	b	620	BCR	C1-C6-C5	-3.69	117.24	122.66
25	a	410	PHO	C4C-C3C-C2C	-3.66	102.72	106.81
24	b	609	CLA	C1C-C2C-C3C	-3.66	102.53	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	507	CLA	C1C-C2C-C3C	-3.66	102.53	106.91
38	F	101	HEM	CBA-CAA-C2A	-3.65	105.99	112.53
26	a	413	BCR	C35-C13-C14	-3.64	117.52	122.90
24	b	608	CLA	C1C-C2C-C3C	-3.64	102.56	106.91
24	c	512	CLA	O1D-CGD-CBD	-3.63	119.42	124.62
24	a	409	CLA	C1C-C2C-C3C	-3.62	102.57	106.91
38	F	101	HEM	CBD-CAD-C3D	-3.62	103.03	113.55
27	A	1010	PL9	C37-C38-C39	-3.61	119.90	127.76
24	b	612	CLA	C1C-C2C-C3C	-3.61	102.59	106.91
26	A	1009	BCR	C35-C13-C12	-3.61	112.08	118.10
24	b	606	CLA	C1C-C2C-C3C	-3.59	102.61	106.91
24	a	412	CLA	C1C-C2C-C3C	-3.59	102.62	106.91
24	C	509	CLA	C1C-C2C-C3C	-3.58	102.62	106.91
24	C	507	CLA	O1D-CGD-CBD	-3.57	119.50	124.62
24	b	616	CLA	C1C-C2C-C3C	-3.56	102.65	106.91
26	t	101	BCR	C1-C6-C5	-3.56	117.43	122.66
26	K	102	BCR	C30-C25-C26	-3.56	117.43	122.66
26	K	101	BCR	C31-C1-C2	-3.55	96.06	108.79
24	c	510	CLA	C1C-C2C-C3C	-3.55	102.66	106.91
25	a	411	PHO	O2D-CGD-O1D	-3.55	116.47	123.79
26	D	406	BCR	C35-C13-C14	-3.54	117.68	122.90
26	y	101	BCR	C35-C13-C12	-3.53	112.22	118.10
26	C	514	BCR	C33-C5-C4	-3.53	106.74	113.43
24	B	606	CLA	C1C-C2C-C3C	-3.53	102.69	106.91
24	B	608	CLA	C1C-C2C-C3C	-3.53	102.69	106.91
24	d	403	CLA	C1C-C2C-C3C	-3.52	102.69	106.91
24	C	501	CLA	C1C-C2C-C3C	-3.52	102.70	106.91
24	C	504	CLA	C1C-C2C-C3C	-3.52	102.70	106.91
26	H	101	BCR	C39-C30-C29	-3.51	96.21	108.79
24	B	604	CLA	C1C-C2C-C3C	-3.50	102.72	106.91
24	d	402	CLA	C1C-C2C-C3C	-3.50	102.72	106.91
26	k	102	BCR	C30-C25-C26	-3.50	117.52	122.66
26	K	101	BCR	C33-C5-C4	-3.50	106.79	113.43
24	c	507	CLA	C1C-C2C-C3C	-3.50	102.72	106.91
26	C	514	BCR	C35-C13-C12	-3.50	112.28	118.10
24	C	505	CLA	C1C-C2C-C3C	-3.49	102.73	106.91
24	c	504	CLA	O1D-CGD-CBD	-3.49	119.62	124.62
24	B	613	CLA	C1C-C2C-C3C	-3.49	102.74	106.91
26	K	102	BCR	C35-C13-C12	-3.48	112.30	118.10
24	B	602	CLA	C1C-C2C-C3C	-3.48	102.75	106.91
26	B	618	BCR	C33-C5-C4	-3.48	106.84	113.43
24	B	603	CLA	O1D-CGD-CBD	-3.48	119.64	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	C1C-C2C-C3C	-3.47	102.75	106.91
24	B	614	CLA	C1C-C2C-C3C	-3.47	102.76	106.91
26	t	101	BCR	C36-C18-C19	-3.44	112.36	118.10
24	b	607	CLA	C1C-C2C-C3C	-3.44	102.79	106.91
26	D	406	BCR	C39-C30-C25	-3.44	104.91	110.30
24	B	614	CLA	O2D-CGD-O1D	-3.44	116.69	123.79
26	y	101	BCR	C39-C30-C29	-3.43	96.51	108.79
24	c	503	CLA	O1D-CGD-CBD	-3.43	119.71	124.62
26	k	101	BCR	C39-C30-C29	-3.42	96.52	108.79
26	a	413	BCR	C34-C9-C8	-3.42	112.40	118.10
26	J	101	BCR	C34-C9-C10	-3.41	117.86	122.90
24	b	611	CLA	C1C-C2C-C3C	-3.41	102.83	106.91
24	c	505	CLA	C1C-C2C-C3C	-3.39	102.85	106.91
24	c	510	CLA	O1D-CGD-CBD	-3.39	119.76	124.62
26	c	514	BCR	C39-C30-C29	-3.39	96.65	108.79
27	a	414	PL9	C7-C3-C2	-3.38	120.62	123.42
26	a	413	BCR	C35-C13-C12	-3.38	112.48	118.10
26	B	618	BCR	C39-C30-C29	-3.37	96.70	108.79
35	V	202	HTG	O5-C1-C2	-3.37	105.61	110.19
24	D	405	CLA	C1C-C2C-C3C	-3.36	102.89	106.91
26	K	101	BCR	C35-C13-C12	-3.36	112.50	118.10
24	c	506	CLA	C1C-C2C-C3C	-3.35	102.90	106.91
26	K	102	BCR	C39-C30-C29	-3.35	96.79	108.79
24	b	613	CLA	O1D-CGD-CBD	-3.35	119.82	124.62
24	b	618	CLA	C1C-C2C-C3C	-3.35	102.91	106.91
24	b	617	CLA	O1D-CGD-CBD	-3.34	119.84	124.62
24	c	509	CLA	C1C-C2C-C3C	-3.33	102.92	106.91
24	b	606	CLA	O1D-CGD-CBD	-3.32	119.86	124.62
26	B	618	BCR	C31-C1-C2	-3.31	96.92	108.79
38	v	201	HEM	C3B-CAB-CBB	-3.31	119.38	124.46
24	C	509	CLA	O1D-CGD-CBD	-3.31	119.88	124.62
26	D	406	BCR	C34-C9-C10	-3.31	118.02	122.90
24	B	601	CLA	O1D-CGD-CBD	-3.31	119.88	124.62
24	c	512	CLA	C1C-C2C-C3C	-3.30	102.96	106.91
26	d	404	BCR	C35-C13-C14	-3.30	118.02	122.90
24	b	619	CLA	O1D-CGD-CBD	-3.30	119.89	124.62
24	B	609	CLA	C3B-CAB-CBB	-3.30	119.57	126.32
24	B	601	CLA	C1C-C2C-C3C	-3.29	102.97	106.91
26	b	622	BCR	C39-C30-C29	-3.28	97.05	108.79
26	k	102	BCR	C39-C30-C29	-3.28	97.06	108.79
26	A	1009	BCR	C1-C6-C5	-3.27	117.85	122.66
24	B	615	CLA	C1C-C2C-C3C	-3.27	103.00	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	601	CLA	C3B-CAB-CBB	-3.26	119.64	126.32
24	c	513	CLA	C1C-C2C-C3C	-3.26	103.01	106.91
27	A	1010	PL9	C32-C33-C34	-3.25	120.69	127.76
26	D	406	BCR	C34-C9-C8	-3.25	112.69	118.10
24	B	609	CLA	C1C-C2C-C3C	-3.25	103.03	106.91
24	c	509	CLA	O1D-CGD-CBD	-3.24	119.98	124.62
24	b	604	CLA	O1D-CGD-CBD	-3.23	119.99	124.62
24	C	512	CLA	C1C-C2C-C3C	-3.23	103.04	106.91
24	c	512	CLA	C3B-CAB-CBB	-3.23	119.71	126.32
38	v	201	HEM	CBD-CAD-C3D	-3.23	104.16	113.55
26	b	621	BCR	C33-C5-C4	-3.22	107.32	113.43
24	a	412	CLA	O2D-CGD-O1D	-3.22	117.14	123.79
24	B	611	CLA	C1C-C2C-C3C	-3.22	103.06	106.91
24	c	504	CLA	C1C-C2C-C3C	-3.21	103.06	106.91
24	c	503	CLA	C1C-C2C-C3C	-3.21	103.08	106.91
26	k	101	BCR	C36-C18-C19	-3.20	112.76	118.10
26	B	618	BCR	C35-C13-C14	-3.20	118.18	122.90
26	B	619	BCR	C37-C22-C21	-3.20	118.18	122.90
24	C	502	CLA	C1C-C2C-C3C	-3.19	103.09	106.91
24	A	1006	CLA	O1D-CGD-CBD	-3.19	120.05	124.62
24	C	503	CLA	C1C-C2C-C3C	-3.19	103.10	106.91
24	C	506	CLA	C1C-C2C-C3C	-3.18	103.10	106.91
24	B	607	CLA	O2D-CGD-O1D	-3.18	117.22	123.79
26	y	101	BCR	C35-C13-C14	-3.17	118.22	122.90
24	b	613	CLA	C1C-C2C-C3C	-3.16	103.12	106.91
25	A	1007	PHO	C4D-ND-C1D	-3.16	101.26	107.05
28	D	408	SQD	C1-O5-C5	-3.16	107.62	113.75
24	c	505	CLA	O1D-CGD-CBD	-3.15	120.11	124.62
26	k	101	BCR	C37-C22-C21	-3.15	118.25	122.90
26	d	404	BCR	C39-C30-C29	-3.14	97.52	108.79
26	b	622	BCR	C1-C6-C5	-3.14	118.05	122.66
25	A	1007	PHO	O1D-CGD-CBD	-3.14	120.12	124.62
24	b	615	CLA	C1C-C2C-C3C	-3.13	103.16	106.91
26	d	404	BCR	C36-C18-C17	-3.13	118.28	122.90
27	d	405	PL9	C7-C8-C9	-3.13	121.40	126.70
26	b	620	BCR	C31-C1-C2	-3.13	97.59	108.79
26	B	617	BCR	C33-C5-C4	-3.12	107.50	113.43
24	C	513	CLA	C1C-C2C-C3C	-3.12	103.18	106.91
24	B	610	CLA	C1C-C2C-C3C	-3.12	103.18	106.91
26	c	514	BCR	C35-C13-C12	-3.11	112.92	118.10
24	b	604	CLA	C1C-C2C-C3C	-3.10	103.20	106.91
26	b	620	BCR	C35-C13-C14	-3.09	118.34	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C1C-C2C-C3C	-3.09	103.21	106.91
24	c	511	CLA	C1C-C2C-C3C	-3.08	103.23	106.91
24	b	610	CLA	C3B-CAB-CBB	-3.07	120.03	126.32
25	a	410	PHO	C1C-C2C-C3C	-3.06	102.84	106.50
24	c	502	CLA	C1C-C2C-C3C	-3.06	103.25	106.91
24	B	616	CLA	C1C-C2C-C3C	-3.05	103.26	106.91
24	b	605	CLA	C1C-C2C-C3C	-3.05	103.26	106.91
24	c	508	CLA	C1C-C2C-C3C	-3.05	103.26	106.91
25	a	410	PHO	O1D-CGD-CBD	-3.03	120.28	124.62
26	D	406	BCR	C32-C1-C2	-3.03	97.94	108.79
24	c	508	CLA	C4C-C3C-C2C	-3.03	102.03	106.94
26	k	101	BCR	C31-C1-C2	-3.02	97.96	108.79
24	B	612	CLA	C4C-C3C-C2C	-3.02	102.05	106.94
26	T	101	BCR	C1-C6-C5	-3.01	118.24	122.66
24	C	501	CLA	O2D-CGD-O1D	-3.01	117.58	123.79
24	c	501	CLA	O2D-CGD-O1D	-3.00	117.59	123.79
24	B	616	CLA	O1D-CGD-CBD	-3.00	120.32	124.62
26	B	619	BCR	C31-C1-C2	-3.00	98.05	108.79
24	B	609	CLA	O1D-CGD-CBD	-3.00	120.33	124.62
24	C	511	CLA	C1C-C2C-C3C	-2.99	103.33	106.91
24	B	605	CLA	C4C-C3C-C2C	-2.99	102.09	106.94
24	b	614	CLA	C1C-C2C-C3C	-2.99	103.33	106.91
24	C	508	CLA	C4C-C3C-C2C	-2.99	102.09	106.94
24	b	618	CLA	C3B-CAB-CBB	-2.98	120.22	126.32
25	A	1007	PHO	C1C-C2C-C3C	-2.98	102.94	106.50
24	B	612	CLA	C1C-C2C-C3C	-2.98	103.35	106.91
24	C	502	CLA	O1D-CGD-CBD	-2.98	120.36	124.62
26	D	406	BCR	C39-C30-C29	-2.98	98.13	108.79
26	h	101	BCR	C1-C6-C5	-2.97	118.29	122.66
27	a	414	PL9	C37-C38-C39	-2.97	121.30	127.76
26	J	101	BCR	C40-C30-C29	-2.97	98.17	108.79
24	D	403	CLA	C1C-NC-C4C	-2.96	102.67	106.27
24	b	611	CLA	O1D-CGD-CBD	-2.96	120.38	124.62
24	b	619	CLA	C1C-C2C-C3C	-2.96	103.37	106.91
26	b	622	BCR	C32-C1-C2	-2.96	98.20	108.79
24	B	610	CLA	C4C-C3C-C2C	-2.95	102.15	106.94
24	D	405	CLA	O1D-CGD-CBD	-2.95	120.39	124.62
24	C	511	CLA	C4C-C3C-C2C	-2.95	102.16	106.94
24	b	612	CLA	C3B-CAB-CBB	-2.93	120.32	126.32
24	d	403	CLA	O2D-CGD-O1D	-2.93	117.75	123.79
24	B	615	CLA	C4C-C3C-C2C	-2.92	102.20	106.94
24	b	605	CLA	O2D-CGD-O1D	-2.92	117.77	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	603	CLA	O2D-CGD-O1D	-2.92	117.77	123.79
24	C	513	CLA	C4C-C3C-C2C	-2.92	102.21	106.94
24	C	510	CLA	O1D-CGD-CBD	-2.91	120.44	124.62
24	B	616	CLA	C4C-C3C-C2C	-2.91	102.21	106.94
24	C	506	CLA	C4C-C3C-C2C	-2.91	102.22	106.94
24	A	1005	CLA	O2D-CGD-O1D	-2.91	117.78	123.79
24	b	619	CLA	C4C-C3C-C2C	-2.91	102.23	106.94
26	b	621	BCR	C34-C9-C8	-2.90	113.27	118.10
24	B	602	CLA	C3B-CAB-CBB	-2.89	120.40	126.32
24	B	605	CLA	O1D-CGD-CBD	-2.89	120.48	124.62
24	C	509	CLA	O2D-CGD-O1D	-2.88	117.84	123.79
24	B	604	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
24	b	608	CLA	O1D-CGD-CBD	-2.88	120.50	124.62
24	b	612	CLA	O1D-CGD-CBD	-2.88	120.50	124.62
26	b	620	BCR	C34-C9-C10	-2.87	118.66	122.90
26	h	101	BCR	C34-C9-C10	-2.87	118.66	122.90
24	b	614	CLA	C4C-C3C-C2C	-2.87	102.29	106.94
24	b	613	CLA	C4C-C3C-C2C	-2.87	102.29	106.94
24	C	506	CLA	O1D-CGD-CBD	-2.87	120.52	124.62
24	a	409	CLA	O1D-CGD-CBD	-2.86	120.52	124.62
24	b	609	CLA	O2D-CGD-O1D	-2.86	117.89	123.79
25	D	404	PHO	O2D-CGD-O1D	-2.86	117.89	123.79
24	B	614	CLA	C4C-C3C-C2C	-2.86	102.31	106.94
24	b	615	CLA	C4C-C3C-C2C	-2.86	102.31	106.94
24	C	502	CLA	C4C-C3C-C2C	-2.86	102.31	106.94
24	c	504	CLA	C3B-CAB-CBB	-2.85	120.48	126.32
24	c	506	CLA	O1D-CGD-CBD	-2.85	120.54	124.62
24	B	606	CLA	O2D-CGD-O1D	-2.85	117.91	123.79
24	B	610	CLA	O1D-CGD-CBD	-2.85	120.54	124.62
26	K	101	BCR	C39-C30-C29	-2.84	98.61	108.79
26	b	620	BCR	C39-C30-C29	-2.84	98.62	108.79
24	a	409	CLA	C3B-CAB-CBB	-2.84	120.51	126.32
25	a	410	PHO	C4D-ND-C1D	-2.84	101.84	107.05
24	B	605	CLA	C1C-C2C-C3C	-2.84	103.52	106.91
24	C	512	CLA	C4C-C3C-C2C	-2.83	102.35	106.94
26	B	617	BCR	C39-C30-C29	-2.83	98.66	108.79
24	D	402	CLA	C1C-NC-C4C	-2.82	102.83	106.27
25	a	411	PHO	C4D-ND-C1D	-2.82	101.87	107.05
35	V	202	HTG	C1-C2-C3	-2.82	104.44	110.69
24	b	604	CLA	C4C-C3C-C2C	-2.82	102.37	106.94
26	K	102	BCR	C32-C1-C2	-2.82	98.70	108.79
24	B	611	CLA	C4C-C3C-C2C	-2.82	102.37	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	404	BCR	C34-C9-C10	-2.81	118.75	122.90
24	B	607	CLA	C3B-CAB-CBB	-2.80	120.59	126.32
26	A	1009	BCR	C40-C30-C29	-2.80	98.76	108.79
25	a	411	PHO	O1D-CGD-CBD	-2.80	120.61	124.62
25	D	404	PHO	C4D-ND-C1D	-2.80	101.92	107.05
24	A	1005	CLA	C3B-CAB-CBB	-2.79	120.60	126.32
26	k	101	BCR	C34-C9-C8	-2.79	113.45	118.10
24	B	608	CLA	O2D-CGD-O1D	-2.78	118.04	123.79
24	c	506	CLA	C4C-C3C-C2C	-2.78	102.43	106.94
26	C	514	BCR	C36-C18-C17	-2.78	118.79	122.90
25	a	411	PHO	CHD-C1D-ND	-2.78	119.47	124.66
24	c	512	CLA	C4C-C3C-C2C	-2.78	102.44	106.94
24	d	403	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
27	D	407	PL9	C37-C38-C39	-2.78	121.72	127.76
24	c	511	CLA	C4C-C3C-C2C	-2.78	102.44	106.94
24	c	509	CLA	O2D-CGD-O1D	-2.78	118.06	123.79
24	c	510	CLA	O2D-CGD-O1D	-2.76	118.08	123.79
27	d	405	PL9	C22-C23-C24	-2.76	121.77	127.76
24	C	512	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
26	t	101	BCR	C31-C1-C2	-2.76	98.92	108.79
26	B	617	BCR	C34-C9-C10	-2.75	118.83	122.90
25	D	404	PHO	CHD-C1D-ND	-2.75	119.53	124.66
27	d	405	PL9	C7-C3-C2	-2.75	121.14	123.42
24	b	617	CLA	C4C-C3C-C2C	-2.74	102.49	106.94
24	C	504	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
24	b	611	CLA	C3B-CAB-CBB	-2.74	120.72	126.32
24	B	611	CLA	O1D-CGD-CBD	-2.73	120.71	124.62
24	c	502	CLA	C4C-C3C-C2C	-2.73	102.51	106.94
24	c	511	CLA	O1D-CGD-CBD	-2.73	120.71	124.62
24	C	505	CLA	O1D-CGD-CBD	-2.73	120.71	124.62
24	c	513	CLA	O1D-CGD-CBD	-2.73	120.72	124.62
26	d	404	BCR	C34-C9-C8	-2.72	113.57	118.10
24	B	608	CLA	C4C-C3C-C2C	-2.71	102.54	106.94
24	D	402	CLA	C4C-C3C-C2C	-2.71	102.54	106.94
26	b	621	BCR	C31-C1-C2	-2.71	99.07	108.79
27	a	414	PL9	C32-C33-C34	-2.71	121.87	127.76
24	D	405	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
24	B	606	CLA	C4C-C3C-C2C	-2.71	102.55	106.94
24	C	501	CLA	O1D-CGD-CBD	-2.71	120.74	124.62
27	D	407	PL9	C22-C23-C24	-2.70	121.89	127.76
26	t	101	BCR	C37-C22-C21	-2.70	118.92	122.90
24	d	402	CLA	C4C-C3C-C2C	-2.70	102.57	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	601	CLA	C4C-C3C-C2C	-2.69	102.58	106.94
24	b	618	CLA	C4C-C3C-C2C	-2.69	102.58	106.94
24	c	507	CLA	C4C-C3C-C2C	-2.69	102.58	106.94
26	b	620	BCR	C37-C22-C23	-2.68	113.64	118.10
27	A	1010	PL9	C42-C43-C44	-2.67	121.95	127.76
24	b	611	CLA	C4C-C3C-C2C	-2.67	102.61	106.94
24	c	509	CLA	C4C-C3C-C2C	-2.67	102.61	106.94
28	D	408	SQD	C44-O6-C1	-2.67	108.21	113.82
24	b	607	CLA	C4C-C3C-C2C	-2.67	102.62	106.94
25	a	411	PHO	C1C-C2C-C3C	-2.67	103.31	106.50
24	b	606	CLA	O2D-CGD-O1D	-2.66	118.29	123.79
26	H	101	BCR	C1-C6-C5	-2.66	118.75	122.66
24	C	503	CLA	C4C-C3C-C2C	-2.66	102.62	106.94
24	D	403	CLA	CHD-C4C-C3C	-2.66	120.83	124.94
26	h	101	BCR	C35-C13-C14	-2.66	118.97	122.90
24	b	615	CLA	O1D-CGD-CBD	-2.66	120.81	124.62
24	B	604	CLA	C4C-C3C-C2C	-2.66	102.63	106.94
24	C	509	CLA	C4C-C3C-C2C	-2.66	102.63	106.94
26	T	101	BCR	C36-C18-C19	-2.65	113.68	118.10
24	b	613	CLA	C3B-CAB-CBB	-2.65	120.90	126.32
24	a	407	CLA	C4C-C3C-C2C	-2.65	102.65	106.94
26	b	621	BCR	C1-C6-C5	-2.64	118.78	122.66
24	b	605	CLA	C4C-C3C-C2C	-2.64	102.65	106.94
24	B	602	CLA	O2D-CGD-O1D	-2.64	118.34	123.79
24	C	504	CLA	C4C-C3C-C2C	-2.64	102.66	106.94
24	D	403	CLA	O1D-CGD-CBD	-2.64	120.84	124.62
26	H	101	BCR	C32-C1-C2	-2.64	99.35	108.79
24	D	405	CLA	C4C-C3C-C2C	-2.63	102.67	106.94
24	c	510	CLA	C4C-C3C-C2C	-2.63	102.67	106.94
24	c	512	CLA	O2D-CGD-O1D	-2.63	118.36	123.79
24	b	607	CLA	O1D-CGD-CBD	-2.63	120.85	124.62
24	b	610	CLA	C4C-C3C-C2C	-2.63	102.68	106.94
24	B	609	CLA	C4C-C3C-C2C	-2.62	102.69	106.94
24	c	503	CLA	C4C-C3C-C2C	-2.62	102.69	106.94
24	c	504	CLA	C4C-C3C-C2C	-2.62	102.70	106.94
24	b	617	CLA	O2D-CGD-O1D	-2.61	118.39	123.79
24	C	513	CLA	O2D-CGD-O1D	-2.61	118.39	123.79
24	B	601	CLA	C4-C3-C2	-2.61	118.38	123.50
24	a	412	CLA	C4C-C3C-C2C	-2.61	102.71	106.94
26	d	404	BCR	C38-C26-C27	-2.60	108.49	113.43
26	b	620	BCR	C34-C9-C8	-2.60	113.76	118.10
26	t	101	BCR	C40-C30-C29	-2.60	99.47	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	C4C-C3C-C2C	-2.60	102.72	106.94
26	T	101	BCR	C35-C13-C12	-2.60	113.77	118.10
24	B	616	CLA	O2D-CGD-O1D	-2.60	118.42	123.79
24	b	604	CLA	C3B-CAB-CBB	-2.60	121.00	126.32
38	f	101	HEM	C3C-CAC-CBC	-2.59	120.48	124.46
24	c	505	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
24	C	505	CLA	C4C-C3C-C2C	-2.58	102.76	106.94
24	C	510	CLA	CBC-CAC-C3C	-2.58	104.52	112.39
24	B	607	CLA	CBC-CAC-C3C	-2.58	104.52	112.39
24	B	602	CLA	C4C-C3C-C2C	-2.58	102.76	106.94
24	C	502	CLA	C3B-CAB-CBB	-2.58	121.05	126.32
24	c	513	CLA	C4C-C3C-C2C	-2.57	102.77	106.94
24	c	501	CLA	C3B-CAB-CBB	-2.57	121.07	126.32
24	b	609	CLA	C4C-C3C-C2C	-2.56	102.78	106.94
24	b	616	CLA	C4C-C3C-C2C	-2.56	102.78	106.94
24	B	607	CLA	O1D-CGD-CBD	-2.56	120.96	124.62
26	y	101	BCR	C34-C9-C8	-2.56	113.84	118.10
24	B	601	CLA	O2D-CGD-O1D	-2.55	118.53	123.79
27	D	407	PL9	C7-C3-C2	-2.54	121.31	123.42
24	D	403	CLA	CBC-CAC-C3C	-2.54	104.64	112.39
24	c	502	CLA	O1D-CGD-CBD	-2.53	120.99	124.62
24	A	1008	CLA	C4C-C3C-C2C	-2.53	102.84	106.94
24	B	603	CLA	C4C-C3C-C2C	-2.53	102.84	106.94
24	B	603	CLA	C5-C3-C2	-2.53	116.26	121.05
26	k	102	BCR	C1-C6-C5	-2.52	118.96	122.66
26	k	102	BCR	C31-C1-C2	-2.52	99.78	108.79
24	B	606	CLA	O1D-CGD-CBD	-2.50	121.03	124.62
26	A	1009	BCR	C32-C1-C2	-2.50	99.82	108.79
24	B	603	CLA	C3B-CAB-CBB	-2.50	121.20	126.32
24	b	606	CLA	C4C-C3C-C2C	-2.50	102.89	106.94
26	a	413	BCR	C1-C6-C5	-2.49	119.00	122.66
24	B	612	CLA	O1D-CGD-CBD	-2.49	121.05	124.62
25	a	411	PHO	C3B-C2B-C1B	-2.49	100.94	106.33
24	d	403	CLA	C4C-C3C-C2C	-2.49	102.91	106.94
24	A	1008	CLA	O1D-CGD-CBD	-2.48	121.06	124.62
24	c	507	CLA	O2D-CGD-O1D	-2.48	118.67	123.79
24	b	619	CLA	CBC-CAC-C3C	-2.47	104.84	112.39
24	B	614	CLA	C3B-CAB-CBB	-2.47	121.26	126.32
24	B	604	CLA	C3B-CAB-CBB	-2.47	121.27	126.32
26	b	621	BCR	C37-C22-C23	-2.45	114.01	118.10
26	B	619	BCR	C1-C6-C5	-2.45	119.06	122.66
24	C	503	CLA	C3B-CAB-CBB	-2.44	121.32	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	102	BCR	C1-C6-C5	-2.44	119.07	122.66
24	b	612	CLA	C4C-C3C-C2C	-2.44	102.98	106.94
24	b	611	CLA	C6-C5-C3	-2.44	107.13	112.48
24	B	608	CLA	C3B-CAB-CBB	-2.44	121.33	126.32
24	C	507	CLA	C4C-C3C-C2C	-2.43	102.99	106.94
24	C	501	CLA	C4C-C3C-C2C	-2.43	103.00	106.94
24	B	613	CLA	C4C-C3C-C2C	-2.43	103.00	106.94
24	a	408	CLA	CHD-C4C-C3C	-2.42	121.20	124.94
24	d	402	CLA	C3B-CAB-CBB	-2.42	121.36	126.32
24	B	603	CLA	O2A-CGA-O1A	-2.42	117.25	123.49
28	c	518	SQD	O5-C1-C2	-2.42	105.32	110.28
26	c	514	BCR	C40-C30-C29	-2.41	100.14	108.79
27	A	1010	PL9	C27-C28-C29	-2.41	122.52	127.76
26	a	413	BCR	C31-C1-C2	-2.41	100.15	108.79
26	D	406	BCR	C37-C22-C23	-2.41	114.09	118.10
26	c	514	BCR	C34-C9-C8	-2.40	114.09	118.10
26	D	406	BCR	C31-C1-C2	-2.40	100.18	108.79
24	a	408	CLA	O1D-CGD-CBD	-2.40	121.19	124.62
24	A	1005	CLA	C4C-C3C-C2C	-2.39	103.06	106.94
24	C	510	CLA	C3B-CAB-CBB	-2.39	121.42	126.32
27	D	407	PL9	C42-C43-C44	-2.39	122.56	127.76
25	D	404	PHO	C1C-C2C-C3C	-2.39	103.64	106.50
24	b	608	CLA	C4C-C3C-C2C	-2.39	103.07	106.94
24	c	501	CLA	C4C-C3C-C2C	-2.39	103.07	106.94
34	D	410	LHG	C5-O7-C7	-2.38	112.19	117.89
26	t	101	BCR	C34-C9-C8	-2.37	114.15	118.10
24	c	504	CLA	O2D-CGD-O1D	-2.37	118.90	123.79
24	C	505	CLA	C3B-CAB-CBB	-2.37	121.47	126.32
24	C	501	CLA	C3B-CAB-CBB	-2.37	121.48	126.32
24	c	506	CLA	O2D-CGD-O1D	-2.36	118.91	123.79
24	c	513	CLA	C3B-CAB-CBB	-2.36	121.49	126.32
26	y	101	BCR	C40-C30-C29	-2.36	100.34	108.79
36	H	102	DGD	O1G-C1A-O1A	-2.36	117.40	123.49
28	B	620[B]	SQD	C45-O47-C7	-2.35	112.25	117.89
26	J	101	BCR	C39-C30-C29	-2.35	100.36	108.79
24	D	402	CLA	CHD-C4C-C3C	-2.35	121.31	124.94
26	B	619	BCR	C34-C9-C8	-2.35	114.19	118.10
24	A	1006	CLA	CBC-CAC-C3C	-2.35	105.22	112.39
24	c	502	CLA	C3B-CAB-CBB	-2.35	121.52	126.32
26	k	102	BCR	C35-C13-C12	-2.34	114.19	118.10
28	A	1011	SQD	C45-O47-C7	-2.34	112.27	117.89
26	B	619	BCR	C37-C22-C23	-2.34	114.20	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	O2D-CGD-O1D	-2.34	118.95	123.79
26	b	621	BCR	C40-C30-C29	-2.34	100.40	108.79
24	b	608	CLA	C3B-CAB-CBB	-2.34	121.53	126.32
24	b	611	CLA	O2D-CGD-O1D	-2.33	118.97	123.79
27	D	407	PL9	C12-C13-C14	-2.33	122.69	127.76
32	A	1017	LMT	C3'-C4'-C5'	-2.33	105.58	110.84
24	c	505	CLA	C3B-CAB-CBB	-2.33	121.56	126.32
25	D	404	PHO	C3B-C2B-C1B	-2.32	101.30	106.33
24	B	612	CLA	O2D-CGD-O1D	-2.32	119.00	123.79
24	b	614	CLA	O2D-CGD-O1D	-2.32	119.00	123.79
24	a	409	CLA	C4C-C3C-C2C	-2.32	103.18	106.94
24	c	502	CLA	O2D-CGD-O1D	-2.32	119.01	123.79
27	D	407	PL9	C40-C39-C38	-2.31	118.96	123.50
24	b	618	CLA	O1D-CGD-CBD	-2.31	121.31	124.62
38	V	201	HEM	C3B-CAB-CBB	-2.30	120.92	124.46
26	B	617	BCR	C35-C13-C14	-2.30	119.50	122.90
26	T	101	BCR	C31-C1-C2	-2.30	100.53	108.79
26	B	618	BCR	C37-C22-C23	-2.30	114.27	118.10
27	D	407	PL9	C31-C32-C33	-2.29	105.68	111.69
24	C	503	CLA	O1D-CGD-CBD	-2.29	121.34	124.62
25	a	410	PHO	C3B-C2B-C1B	-2.29	101.37	106.33
24	b	607	CLA	O2D-CGD-O1D	-2.29	119.07	123.79
26	J	101	BCR	C36-C18-C19	-2.28	114.30	118.10
24	b	616	CLA	O2D-CGD-O1D	-2.28	119.08	123.79
24	B	608	CLA	O1D-CGD-CBD	-2.28	121.36	124.62
24	b	610	CLA	O2D-CGD-O1D	-2.28	119.09	123.79
24	B	607	CLA	C4C-C3C-C2C	-2.27	103.27	106.94
24	C	513	CLA	O1D-CGD-CBD	-2.27	121.37	124.62
24	c	513	CLA	O2D-CGD-O1D	-2.27	119.11	123.79
24	C	506	CLA	O2D-CGD-O1D	-2.26	119.11	123.79
24	C	508	CLA	O2D-CGD-O1D	-2.26	119.11	123.79
24	b	617	CLA	O2A-CGA-O1A	-2.26	117.65	123.49
24	B	616	CLA	C4-C3-C2	-2.26	119.06	123.50
25	a	410	PHO	CHD-C1D-ND	-2.26	120.44	124.66
24	C	507	CLA	O2D-CGD-O1D	-2.26	119.13	123.79
27	A	1010	PL9	C17-C18-C19	-2.26	122.86	127.76
26	k	101	BCR	C1-C6-C5	-2.26	119.35	122.66
29	C	519	LMG	O7-C10-O9	-2.25	117.62	123.67
27	a	414	PL9	C27-C28-C29	-2.25	122.87	127.76
28	A	1011	SQD	O5-C1-C2	-2.25	105.66	110.28
24	a	409	CLA	O2D-CGD-O1D	-2.25	119.15	123.79
24	a	407	CLA	C3B-CAB-CBB	-2.24	121.73	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	CBC-CAC-C3C	-2.24	105.55	112.39
24	B	605	CLA	C3B-CAB-CBB	-2.24	121.73	126.32
24	b	608	CLA	O2D-CGD-O1D	-2.24	119.17	123.79
28	D	408	SQD	O5-C1-C2	-2.24	105.68	110.28
25	A	1007	PHO	CHD-C1D-ND	-2.24	120.48	124.66
24	C	510	CLA	C4C-C3C-C2C	-2.23	103.32	106.94
24	b	605	CLA	C3B-CAB-CBB	-2.23	121.76	126.32
24	B	613	CLA	O2D-CGD-O1D	-2.23	119.19	123.79
24	c	511	CLA	C3B-CAB-CBB	-2.23	121.76	126.32
28	b	623[A]	SQD	C45-O47-C7	-2.23	112.55	117.89
26	b	622	BCR	C31-C1-C2	-2.22	100.82	108.79
24	b	604	CLA	O2D-CGD-O1D	-2.22	119.20	123.79
27	a	414	PL9	C42-C43-C44	-2.22	122.93	127.76
25	A	1007	PHO	C3B-C2B-C1B	-2.22	101.52	106.33
24	b	610	CLA	O1D-CGD-CBD	-2.22	121.44	124.62
26	h	101	BCR	C32-C1-C31	-2.22	101.26	108.37
24	C	512	CLA	O2D-CGD-O1D	-2.22	119.21	123.79
24	B	610	CLA	O2D-CGD-O1D	-2.22	119.22	123.79
25	D	404	PHO	CMD-C2D-C3D	-2.21	122.88	128.04
26	H	101	BCR	C37-C22-C23	-2.21	114.41	118.10
26	T	101	BCR	C37-C22-C23	-2.21	114.42	118.10
24	D	403	CLA	CHC-C1C-C2C	-2.21	120.55	126.35
36	C	516	DGD	O1G-C1A-O1A	-2.21	117.80	123.49
24	A	1006	CLA	C1C-NC-C4C	-2.20	103.59	106.27
26	B	618	BCR	C40-C30-C29	-2.20	100.90	108.79
24	C	506	CLA	C3B-CAB-CBB	-2.20	121.82	126.32
24	D	402	CLA	O2D-CGD-O1D	-2.20	119.25	123.79
25	a	411	PHO	CMD-C2D-C3D	-2.20	122.93	128.04
27	D	407	PL9	C27-C28-C29	-2.19	123.00	127.76
25	a	410	PHO	O2D-CGD-O1D	-2.19	119.27	123.79
34	d	407	LHG	O8-C23-O10	-2.19	117.85	123.49
32	a	402	LMT	C3'-C4'-C5'	-2.18	105.91	110.84
24	B	615	CLA	O1D-CGD-CBD	-2.18	121.50	124.62
24	a	412	CLA	C1C-NC-C4C	-2.18	103.62	106.27
38	V	201	HEM	C3C-CAC-CBC	-2.17	121.12	124.46
28	b	623[B]	SQD	C45-O47-C7	-2.17	112.67	117.89
26	B	619	BCR	C32-C1-C2	-2.17	101.02	108.79
24	A	1008	CLA	C3B-CAB-CBB	-2.17	121.88	126.32
24	d	402	CLA	O2D-CGD-O1D	-2.17	119.31	123.79
24	b	617	CLA	CBC-CAC-C3C	-2.17	105.77	112.39
27	d	405	PL9	C42-C43-C44	-2.17	123.05	127.76
24	c	510	CLA	C3B-CAB-CBB	-2.17	121.88	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1008	CLA	O2D-CGD-O1D	-2.17	119.32	123.79
24	A	1005	CLA	C1C-NC-C4C	-2.16	103.64	106.27
24	A	1006	CLA	C3B-CAB-CBB	-2.16	121.89	126.32
24	C	511	CLA	O2D-CGD-O1D	-2.16	119.33	123.79
28	A	1011	SQD	C1-O5-C5	-2.16	109.56	113.75
36	c	517	DGD	O1G-C1A-O1A	-2.16	117.93	123.49
38	V	201	HEM	CMA-C3A-C4A	-2.15	124.80	128.36
24	B	616	CLA	O2A-CGA-O1A	-2.15	117.95	123.49
26	t	101	BCR	C30-C25-C26	-2.14	119.51	122.66
24	D	403	CLA	O2D-CGD-O1D	-2.14	119.37	123.79
25	D	404	PHO	O1D-CGD-CBD	-2.14	121.56	124.62
24	B	615	CLA	O2D-CGD-O1D	-2.14	119.38	123.79
28	D	408	SQD	C1-C2-C3	-2.13	105.77	109.97
34	d	406	LHG	O8-C23-O10	-2.13	117.98	123.49
24	a	412	CLA	O1D-CGD-CBD	-2.13	121.56	124.62
24	B	606	CLA	C3B-CAB-CBB	-2.12	121.98	126.32
26	A	1009	BCR	C34-C9-C8	-2.12	114.58	118.10
27	A	1010	PL9	C22-C23-C24	-2.12	123.16	127.76
38	F	101	HEM	CAA-C2A-C1A	-2.11	124.72	127.01
24	a	408	CLA	C1C-NC-C4C	-2.11	103.70	106.27
24	B	610	CLA	O2A-CGA-O1A	-2.11	118.05	123.49
24	a	412	CLA	C3B-CAB-CBB	-2.11	122.00	126.32
24	A	1006	CLA	CHD-C4C-C3C	-2.11	121.69	124.94
38	V	201	HEM	CBA-CAA-C2A	-2.11	108.75	112.53
24	c	508	CLA	O1D-CGD-CBD	-2.10	121.61	124.62
26	C	514	BCR	C34-C9-C8	-2.10	114.60	118.10
28	B	620[A]	SQD	C45-O47-C7	-2.10	112.86	117.89
26	C	514	BCR	C40-C30-C29	-2.10	101.28	108.79
26	C	514	BCR	C35-C13-C14	-2.09	119.81	122.90
24	b	610	CLA	CBC-CAC-C3C	-2.09	106.00	112.39
26	K	102	BCR	C31-C1-C2	-2.09	101.30	108.79
26	B	617	BCR	C40-C30-C29	-2.09	101.30	108.79
24	b	614	CLA	CBC-CAC-C3C	-2.09	106.02	112.39
25	D	404	PHO	C4-C3-C2	-2.08	119.41	123.50
36	C	517	DGD	C3G-C2G-C1G	-2.08	107.20	112.07
34	D	409	LHG	O8-C23-O10	-2.08	118.12	123.49
28	c	518	SQD	C1-C2-C3	-2.08	105.87	109.97
24	B	613	CLA	CHD-C4C-C3C	-2.08	121.73	124.94
24	c	509	CLA	C3B-CAB-CBB	-2.08	122.07	126.32
26	T	101	BCR	C39-C30-C29	-2.07	101.36	108.79
24	C	512	CLA	C3B-CAB-CBB	-2.07	122.08	126.32
24	b	610	CLA	C1C-NC-C4C	-2.07	103.75	106.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	O2D-CGD-O1D	-2.07	119.51	123.79
27	d	405	PL9	C37-C38-C39	-2.07	123.26	127.76
24	D	405	CLA	C3B-CAB-CBB	-2.07	122.08	126.32
24	B	605	CLA	O2A-CGA-O1A	-2.07	118.15	123.49
24	B	611	CLA	C3B-CAB-CBB	-2.07	122.09	126.32
38	V	201	HEM	C3B-C4B-NB	-2.06	107.68	111.63
26	a	413	BCR	C40-C30-C29	-2.06	101.40	108.79
38	F	101	HEM	C3C-CAC-CBC	-2.06	121.30	124.46
24	D	403	CLA	C4C-C3C-C2C	-2.05	103.61	106.94
24	B	605	CLA	CHD-C4C-C3C	-2.05	121.77	124.94
24	c	510	CLA	C4-C3-C2	-2.05	119.47	123.50
26	J	101	BCR	C31-C1-C2	-2.05	101.44	108.79
34	D	409	LHG	C5-O7-C7	-2.05	112.97	117.89
24	c	513	CLA	O2A-CGA-O1A	-2.05	118.21	123.49
24	b	614	CLA	C1C-NC-C4C	-2.05	103.78	106.27
24	d	402	CLA	C1C-NC-C4C	-2.05	103.78	106.27
24	b	606	CLA	C3B-CAB-CBB	-2.04	122.13	126.32
26	b	620	BCR	C32-C1-C2	-2.04	101.47	108.79
26	B	617	BCR	C32-C1-C2	-2.04	101.47	108.79
36	c	516	DGD	O1G-C1A-O1A	-2.04	118.22	123.49
26	T	101	BCR	C35-C13-C14	-2.04	119.89	122.90
36	C	516	DGD	O2G-C1B-O1B	-2.04	118.19	123.67
24	c	507	CLA	CBC-CAC-C3C	-2.04	106.16	112.39
29	m	102	LMG	O8-C28-O10	-2.04	118.23	123.49
24	b	606	CLA	O2A-CGA-O1A	-2.04	118.23	123.49
26	b	621	BCR	C32-C1-C31	-2.04	101.84	108.37
25	a	410	PHO	CMD-C2D-C3D	-2.04	123.30	128.04
24	B	608	CLA	C1C-NC-C4C	-2.04	103.79	106.27
24	B	603	CLA	C1C-NC-C4C	-2.03	103.79	106.27
24	D	402	CLA	C3B-CAB-CBB	-2.03	122.16	126.32
24	B	610	CLA	C1C-NC-C4C	-2.03	103.80	106.27
24	c	508	CLA	O2D-CGD-O1D	-2.03	119.59	123.79
32	C	520	LMT	C2'-C3'-C4'	-2.03	105.14	109.60
27	A	1010	PL9	C7-C8-C9	-2.03	123.26	126.70
24	b	614	CLA	O1D-CGD-CBD	-2.02	121.72	124.62
24	B	611	CLA	CBC-CAC-C3C	-2.02	106.23	112.39
24	A	1006	CLA	C4C-C3C-C2C	-2.02	103.67	106.94
24	b	607	CLA	C1C-NC-C4C	-2.01	103.82	106.27
26	k	102	BCR	C40-C30-C29	-2.01	101.59	108.79
24	C	505	CLA	O2D-CGD-O1D	-2.01	119.64	123.79
24	C	511	CLA	O1D-CGD-CBD	-2.01	121.75	124.62
28	c	518	SQD	C46-O48-C23	2.00	122.44	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	601	CLA	CAC-C3C-C4C	2.00	127.74	124.83
24	B	609	CLA	CED-O2D-CGD	2.01	120.70	115.99
32	b	625	LMT	O5B-C5B-C6B	2.01	111.43	106.36
35	b	626	HTG	O5-C5-C6	2.01	111.43	106.36
24	a	409	CLA	CMB-C2B-C3B	2.01	129.03	125.09
24	a	409	CLA	O2A-CGA-CBA	2.02	118.04	111.90
28	A	1016	SQD	O7-S-C6	2.02	108.64	106.94
26	k	101	BCR	C32-C1-C6	2.02	113.46	110.30
24	a	412	CLA	CED-O2D-CGD	2.02	120.73	115.99
24	b	610	CLA	O2A-CGA-CBA	2.02	118.06	111.90
24	c	503	CLA	O2A-CGA-CBA	2.02	118.07	111.90
32	a	402	LMT	O5'-C5'-C6'	2.03	111.48	106.36
29	c	520	LMG	C9-O8-C28	2.03	122.52	116.85
26	h	101	BCR	C28-C29-C30	2.03	122.35	114.83
24	B	611	CLA	CMB-C2B-C3B	2.03	129.06	125.09
26	d	404	BCR	C31-C1-C6	2.04	113.49	110.30
24	B	604	CLA	CMB-C2B-C3B	2.04	129.07	125.09
24	C	512	CLA	CED-O2D-CGD	2.04	120.77	115.99
27	a	414	PL9	C51-C49-C50	2.04	119.65	114.64
25	A	1007	PHO	CED-O2D-CGD	2.04	120.77	115.99
24	c	505	CLA	O2A-CGA-CBA	2.04	118.12	111.90
24	C	511	CLA	CMC-C2C-C1C	2.04	128.18	125.02
24	a	408	CLA	CED-O2D-CGD	2.05	120.79	115.99
24	c	501	CLA	CMB-C2B-C3B	2.05	129.09	125.09
24	b	604	CLA	CMB-C2B-C3B	2.06	129.11	125.09
32	M	102	LMT	C2'-C3'-C4'	2.06	114.12	109.60
35	C	522	HTG	O5-C5-C6	2.06	111.56	106.36
24	C	503	CLA	CAC-C3C-C4C	2.06	127.82	124.83
32	A	1018	LMT	O5B-C5B-C4B	2.06	113.55	109.68
24	D	403	CLA	O2A-CGA-CBA	2.06	118.19	111.90
24	c	508	CLA	CED-O2D-CGD	2.07	120.85	115.99
29	C	519	LMG	O6-C5-C6	2.07	111.59	106.36
24	B	614	CLA	CED-O2D-CGD	2.07	120.85	115.99
24	b	618	CLA	CED-O2D-CGD	2.08	120.86	115.99
24	c	505	CLA	CED-O2D-CGD	2.08	120.86	115.99
26	k	102	BCR	C2-C3-C4	2.08	116.77	111.53
24	b	605	CLA	CED-O2D-CGD	2.08	120.87	115.99
24	b	609	CLA	O2A-CGA-CBA	2.08	118.24	111.90
24	b	612	CLA	CED-O2D-CGD	2.08	120.87	115.99
24	b	618	CLA	O2A-CGA-CBA	2.08	118.25	111.90
24	B	601	CLA	CMB-C2B-C3B	2.09	129.17	125.09
24	c	504	CLA	CMC-C2C-C1C	2.09	128.25	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	CED-O2D-CGD	2.09	120.90	115.99
24	b	619	CLA	CED-O2D-CGD	2.10	120.90	115.99
26	a	413	BCR	C1-C6-C7	2.10	121.69	115.82
27	D	407	PL9	C45-C44-C46	2.10	118.61	115.41
25	a	411	PHO	CED-O2D-CGD	2.10	120.92	115.99
24	C	513	CLA	CAC-C3C-C4C	2.11	127.89	124.83
24	B	606	CLA	O2A-CGA-CBA	2.11	118.32	111.90
24	c	511	CLA	CAC-C3C-C4C	2.11	127.89	124.83
24	B	612	CLA	CED-O2D-CGD	2.11	120.94	115.99
26	K	102	BCR	C39-C30-C25	2.11	113.61	110.30
32	a	416	LMT	C1B-O5B-C5B	2.11	117.85	113.75
24	C	504	CLA	CMC-C2C-C1C	2.11	128.29	125.02
27	d	405	PL9	C15-C14-C16	2.11	118.64	115.41
24	B	601	CLA	CED-O2D-CGD	2.11	120.95	115.99
26	T	101	BCR	C1-C6-C7	2.12	121.74	115.82
27	D	407	PL9	C53-C6-C1	2.12	120.00	114.94
24	B	613	CLA	CED-O2D-CGD	2.12	120.97	115.99
24	b	612	CLA	O2A-CGA-CBA	2.12	118.37	111.90
26	K	102	BCR	C29-C28-C27	2.12	116.89	111.53
26	C	514	BCR	C30-C25-C24	2.13	121.77	115.82
24	D	402	CLA	CED-O2D-CGD	2.13	120.98	115.99
24	D	402	CLA	CMB-C2B-C3B	2.13	129.25	125.09
32	b	631	LMT	O5B-C5B-C6B	2.13	111.74	106.36
24	B	615	CLA	O2A-CGA-CBA	2.13	118.41	111.90
24	B	611	CLA	CMC-C2C-C1C	2.14	128.33	125.02
24	b	607	CLA	CMB-C2B-C3B	2.14	129.27	125.09
26	A	1009	BCR	C1-C6-C7	2.14	121.82	115.82
32	B	623	LMT	C1B-O5B-C5B	2.14	117.91	113.75
26	K	101	BCR	C1-C6-C7	2.14	121.82	115.82
24	B	602	CLA	CAC-C3C-C4C	2.15	127.94	124.83
24	C	502	CLA	CMB-C2B-C3B	2.15	129.28	125.09
26	b	622	BCR	C30-C25-C24	2.15	121.83	115.82
24	B	616	CLA	CMC-C2C-C1C	2.15	128.34	125.02
29	Z	101	LMG	O1-C1-C2	2.15	110.75	108.04
24	c	502	CLA	O2A-CGA-CBA	2.15	118.45	111.90
24	B	608	CLA	O2A-CGA-CBA	2.15	118.45	111.90
24	b	605	CLA	CAC-C3C-C4C	2.15	127.95	124.83
29	m	102	LMG	O1-C1-C2	2.15	110.76	108.04
26	D	406	BCR	C40-C30-C39	2.15	115.27	108.37
24	b	618	CLA	CMB-C2B-C3B	2.16	129.31	125.09
24	C	508	CLA	O2A-CGA-CBA	2.16	118.48	111.90
24	b	610	CLA	CMC-C2C-C1C	2.16	128.37	125.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	CAC-C3C-C4C	2.16	127.97	124.83
26	K	101	BCR	C4-C5-C6	2.16	125.54	122.78
24	A	1008	CLA	CMB-C2B-C3B	2.16	129.32	125.09
24	C	502	CLA	O2A-CGA-CBA	2.17	118.50	111.90
26	K	101	BCR	C40-C30-C25	2.17	113.70	110.30
24	B	606	CLA	CAC-C3C-C4C	2.17	127.98	124.83
26	J	101	BCR	C1-C6-C7	2.17	121.91	115.82
24	a	412	CLA	O2A-CGA-CBA	2.18	118.53	111.90
24	d	403	CLA	C4-C3-C5	2.18	118.73	115.41
26	d	404	BCR	C3-C2-C1	2.18	122.90	114.83
26	h	101	BCR	C30-C25-C24	2.18	121.92	115.82
24	B	611	CLA	CED-O2D-CGD	2.18	121.11	115.99
24	C	509	CLA	CED-O2D-CGD	2.18	121.11	115.99
24	D	403	CLA	C4-C3-C5	2.18	118.74	115.41
24	b	608	CLA	CMB-C2B-C3B	2.19	129.36	125.09
24	C	501	CLA	CMB-C2B-C3B	2.19	129.37	125.09
26	d	404	BCR	C3-C4-C5	2.19	117.34	113.87
26	k	101	BCR	C28-C27-C26	2.19	117.34	113.87
24	C	512	CLA	CAC-C3C-C4C	2.19	128.01	124.83
34	B	621	LHG	O8-C23-C24	2.19	118.57	111.90
24	b	616	CLA	CMB-C2B-C3B	2.19	129.38	125.09
26	y	101	BCR	C39-C30-C25	2.19	113.74	110.30
24	b	617	CLA	CAC-C3C-C4C	2.19	128.01	124.83
27	a	414	PL9	C15-C14-C16	2.20	118.76	115.41
24	D	405	CLA	CAC-C3C-C4C	2.20	128.02	124.83
24	b	618	CLA	CAC-C3C-C4C	2.20	128.02	124.83
24	C	501	CLA	CMC-C2C-C1C	2.20	128.42	125.02
29	d	409	LMG	O8-C28-C29	2.20	118.59	111.90
24	B	601	CLA	CMC-C2C-C1C	2.20	128.42	125.02
24	b	614	CLA	CED-O2D-CGD	2.20	121.16	115.99
26	K	102	BCR	C3-C4-C5	2.20	117.36	113.87
24	B	610	CLA	CMB-C2B-C3B	2.20	129.40	125.09
24	a	409	CLA	CAC-C3C-C4C	2.21	128.03	124.83
26	b	621	BCR	C3-C4-C5	2.21	117.37	113.87
26	b	621	BCR	C30-C25-C24	2.21	122.01	115.82
26	y	101	BCR	C1-C6-C7	2.21	122.01	115.82
24	B	607	CLA	CMB-C2B-C3B	2.21	129.41	125.09
24	b	616	CLA	CAC-C3C-C4C	2.21	128.04	124.83
24	b	608	CLA	CED-O2D-CGD	2.21	121.18	115.99
26	t	101	BCR	C31-C1-C6	2.21	113.77	110.30
24	B	606	CLA	CMC-C2C-C1C	2.21	128.45	125.02
24	c	508	CLA	O2A-CGA-CBA	2.22	118.66	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	J	101	BCR	C32-C1-C6	2.22	113.79	110.30
24	a	407	CLA	C4-C3-C5	2.23	118.81	115.41
24	c	501	CLA	O2A-CGA-CBA	2.23	118.69	111.90
24	c	503	CLA	CAC-C3C-C4C	2.23	128.06	124.83
28	c	518	SQD	O48-C23-C24	2.23	118.69	111.90
24	B	604	CLA	CMC-C2C-C1C	2.23	128.47	125.02
24	C	501	CLA	CED-O2D-CGD	2.23	121.22	115.99
24	c	513	CLA	CED-O2D-CGD	2.23	121.22	115.99
24	D	405	CLA	O2A-CGA-CBA	2.23	118.70	111.90
24	A	1005	CLA	C4-C3-C5	2.23	118.82	115.41
24	c	511	CLA	O2A-CGA-CBA	2.24	118.71	111.90
24	b	616	CLA	CED-O2D-CGD	2.24	121.24	115.99
26	y	101	BCR	C30-C25-C24	2.24	122.10	115.82
24	B	614	CLA	O2A-CGA-CBA	2.25	118.74	111.90
24	d	402	CLA	CED-O2D-CGD	2.25	121.26	115.99
26	c	514	BCR	C28-C29-C30	2.25	123.15	114.83
26	B	618	BCR	C28-C27-C26	2.25	117.44	113.87
24	C	513	CLA	CED-O2D-CGD	2.25	121.28	115.99
28	A	1011	SQD	O48-C23-C24	2.25	118.77	111.90
24	C	506	CLA	O2A-CGA-CBA	2.26	118.78	111.90
24	b	612	CLA	CMC-C2C-C1C	2.26	128.51	125.02
24	C	508	CLA	CED-O2D-CGD	2.26	121.29	115.99
24	c	511	CLA	CMB-C2B-C3B	2.26	129.51	125.09
24	B	615	CLA	CMC-C2C-C1C	2.26	128.52	125.02
26	K	102	BCR	C23-C24-C25	2.26	134.12	127.32
26	H	101	BCR	C30-C25-C24	2.27	122.16	115.82
24	a	407	CLA	CAC-C3C-C4C	2.27	128.12	124.83
24	B	612	CLA	O2A-CGA-CBA	2.27	118.81	111.90
24	D	405	CLA	CMC-C2C-C1C	2.27	128.53	125.02
24	b	610	CLA	CAC-C3C-C4C	2.27	128.13	124.83
27	d	405	PL9	C53-C6-C1	2.28	120.38	114.94
24	c	506	CLA	CED-O2D-CGD	2.28	121.34	115.99
25	a	410	PHO	CED-O2D-CGD	2.28	121.34	115.99
24	C	502	CLA	CMC-C2C-C1C	2.28	128.55	125.02
26	h	101	BCR	C40-C30-C25	2.28	113.88	110.30
24	c	512	CLA	CMB-C2B-C3B	2.29	129.56	125.09
28	f	102	SQD	C4-C3-C2	2.29	115.06	110.79
24	c	503	CLA	CMC-C2C-C1C	2.29	128.56	125.02
24	a	408	CLA	CMB-C2B-C3B	2.29	129.57	125.09
24	B	616	CLA	CMB-C2B-C3B	2.29	129.57	125.09
24	c	506	CLA	CMB-C2B-C3B	2.29	129.57	125.09
24	C	513	CLA	C4-C3-C5	2.29	118.91	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	O2A-CGA-CBA	2.29	118.89	111.90
26	a	413	BCR	C4-C5-C6	2.30	125.71	122.78
24	b	609	CLA	CAC-C3C-C4C	2.30	128.16	124.83
24	b	615	CLA	CMB-C2B-C3B	2.30	129.58	125.09
26	C	514	BCR	C33-C5-C6	2.30	126.86	124.61
24	B	607	CLA	CED-O2D-CGD	2.31	121.40	115.99
34	b	624	LHG	O8-C23-C24	2.31	118.93	111.90
25	a	411	PHO	CMB-C2B-C1B	2.31	128.81	125.06
26	A	1009	BCR	C23-C24-C25	2.31	134.25	127.32
24	b	609	CLA	CMB-C2B-C3B	2.31	129.61	125.09
32	A	1018	LMT	O1B-C4'-C3'	2.31	113.13	107.17
24	c	501	CLA	CMC-C2C-C1C	2.31	128.60	125.02
32	a	402	LMT	C1B-O5B-C5B	2.31	118.24	113.75
26	K	101	BCR	C38-C26-C25	2.31	126.88	124.61
24	C	509	CLA	O2A-CGA-CBA	2.32	118.96	111.90
24	b	614	CLA	CMC-C2C-C1C	2.32	128.61	125.02
26	B	619	BCR	C30-C25-C24	2.32	122.31	115.82
24	c	509	CLA	CMC-C2C-C1C	2.32	128.61	125.02
26	c	514	BCR	C39-C30-C25	2.32	113.95	110.30
24	B	611	CLA	CAC-C3C-C4C	2.33	128.21	124.83
24	b	604	CLA	CAC-C3C-C4C	2.33	128.22	124.83
24	b	611	CLA	CAC-C3C-C4C	2.33	128.22	124.83
24	c	504	CLA	CED-O2D-CGD	2.33	121.46	115.99
24	b	611	CLA	CMC-C2C-C1C	2.34	128.64	125.02
24	a	408	CLA	O2A-CGA-CBA	2.34	119.03	111.90
24	c	509	CLA	O2A-CGA-CBA	2.34	119.04	111.90
24	b	619	CLA	O2A-CGA-CBA	2.34	119.04	111.90
26	y	101	BCR	C31-C1-C6	2.35	113.98	110.30
24	C	507	CLA	CED-O2D-CGD	2.35	121.50	115.99
24	A	1008	CLA	O2A-CGA-CBA	2.35	119.07	111.90
24	c	512	CLA	C3B-C4B-NB	2.35	112.25	109.21
28	a	401	SQD	O7-S-C6	2.35	108.92	106.94
24	b	613	CLA	CMB-C2B-C3B	2.35	129.69	125.09
24	c	511	CLA	CMC-C2C-C1C	2.36	128.66	125.02
28	c	518	SQD	O7-S-C6	2.36	108.93	106.94
26	B	618	BCR	C2-C1-C6	2.36	114.09	110.36
32	b	625	LMT	C4B-C3B-C2B	2.36	115.19	110.79
36	C	516	DGD	O1G-C1A-C2A	2.36	119.08	111.90
26	B	618	BCR	C32-C1-C6	2.36	114.00	110.30
26	k	102	BCR	C30-C25-C24	2.36	122.42	115.82
24	B	608	CLA	CMC-C2C-C1C	2.36	128.67	125.02
26	J	101	BCR	C27-C26-C25	2.37	125.80	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	504	CLA	CMB-C2B-C3B	2.37	129.72	125.09
24	B	609	CLA	CMC-C2C-C1C	2.37	128.69	125.02
24	c	509	CLA	CED-O2D-CGD	2.37	121.55	115.99
24	B	614	CLA	CMC-C2C-C1C	2.37	128.69	125.02
24	c	502	CLA	CMC-C2C-C1C	2.37	128.69	125.02
24	C	504	CLA	CED-O2D-CGD	2.37	121.55	115.99
24	C	503	CLA	CMC-C2C-C1C	2.37	128.69	125.02
24	b	606	CLA	CMB-C2B-C3B	2.37	129.73	125.09
38	F	101	HEM	C2D-C3D-C4D	2.38	105.54	101.50
24	c	510	CLA	CMC-C2C-C1C	2.39	128.71	125.02
24	c	505	CLA	CMB-C2B-C3B	2.39	129.76	125.09
36	C	516	DGD	O3G-C1D-C2D	2.39	111.06	108.04
26	J	101	BCR	C28-C27-C26	2.39	117.66	113.87
24	B	605	CLA	CAC-C3C-C4C	2.39	128.30	124.83
24	B	614	CLA	CMB-C2B-C3B	2.39	129.77	125.09
24	B	613	CLA	C4-C3-C5	2.39	119.06	115.41
26	K	101	BCR	C30-C25-C24	2.40	122.53	115.82
24	b	613	CLA	O2A-CGA-CBA	2.40	119.20	111.90
24	c	513	CLA	CAC-C3C-C4C	2.40	128.31	124.83
25	a	410	PHO	CMB-C2B-C1B	2.40	128.97	125.06
24	C	503	CLA	CMB-C2B-C3B	2.40	129.78	125.09
24	D	405	CLA	CMB-C2B-C3B	2.40	129.79	125.09
26	T	101	BCR	C30-C25-C24	2.40	122.55	115.82
26	b	621	BCR	C28-C29-C30	2.40	123.73	114.83
24	d	403	CLA	CMC-C2C-C1C	2.40	128.74	125.02
24	D	402	CLA	O2A-CGA-CBA	2.40	119.22	111.90
24	a	412	CLA	CMB-C2B-C3B	2.41	129.79	125.09
24	B	605	CLA	CED-O2D-CGD	2.41	121.64	115.99
24	c	504	CLA	CMB-C2B-C3B	2.41	129.80	125.09
24	C	509	CLA	CAC-C3C-C4C	2.42	128.34	124.83
24	C	508	CLA	C4-C3-C5	2.42	119.10	115.41
24	b	617	CLA	CMB-C2B-C3B	2.42	129.81	125.09
26	B	619	BCR	C31-C1-C6	2.42	114.09	110.30
25	D	404	PHO	CMB-C2B-C1B	2.42	128.99	125.06
24	B	605	CLA	C3B-C4B-NB	2.42	112.34	109.21
24	A	1005	CLA	CMC-C2C-C1C	2.42	128.76	125.02
24	c	508	CLA	CAC-C3C-C4C	2.42	128.34	124.83
27	D	407	PL9	C35-C34-C36	2.42	119.11	115.41
27	a	414	PL9	C45-C44-C46	2.43	119.11	115.41
24	a	407	CLA	C4A-NA-C1A	2.43	109.50	106.36
24	c	501	CLA	CAC-C3C-C4C	2.43	128.36	124.83
24	b	617	CLA	O2A-CGA-CBA	2.43	119.31	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	414	PL9	C53-C6-C1	2.43	120.75	114.94
24	b	609	CLA	CMC-C2C-C1C	2.43	128.78	125.02
26	b	621	BCR	C24-C23-C22	2.44	129.93	126.22
24	b	614	CLA	CMB-C2B-C3B	2.44	129.86	125.09
24	c	513	CLA	CMC-C2C-C1C	2.44	128.79	125.02
27	A	1010	PL9	C53-C6-C1	2.44	120.77	114.94
28	f	102	SQD	O9-S-C6	2.44	109.00	106.94
24	C	507	CLA	CMC-C2C-C1C	2.44	128.80	125.02
24	b	611	CLA	O2A-CGA-CBA	2.44	119.35	111.90
24	A	1005	CLA	O2A-CGA-CBA	2.44	119.35	111.90
24	b	616	CLA	C4-C3-C5	2.44	119.14	115.41
24	C	506	CLA	CAC-C3C-C4C	2.44	128.38	124.83
25	D	404	PHO	CED-O2D-CGD	2.45	121.72	115.99
26	k	101	BCR	C40-C30-C25	2.45	114.14	110.30
24	C	512	CLA	CMB-C2B-C3B	2.45	129.88	125.09
36	c	516	DGD	O1G-C1A-C2A	2.45	119.36	111.90
24	B	615	CLA	CAC-C3C-C4C	2.46	128.40	124.83
24	B	612	CLA	CAC-C3C-C4C	2.46	128.40	124.83
38	f	101	HEM	C2D-C3D-C4D	2.46	105.67	101.50
24	c	510	CLA	CMB-C2B-C3B	2.46	129.90	125.09
24	b	604	CLA	C4-C3-C5	2.46	119.17	115.41
24	B	613	CLA	CMB-C2B-C3B	2.46	129.90	125.09
36	H	102	DGD	O1G-C1A-C2A	2.46	119.40	111.90
24	c	503	CLA	CMB-C2B-C3B	2.46	129.91	125.09
24	C	508	CLA	CMB-C2B-C3B	2.47	129.91	125.09
24	C	513	CLA	O2A-CGA-CBA	2.47	119.42	111.90
27	a	414	PL9	C20-C19-C21	2.47	119.18	115.41
24	c	506	CLA	CAC-C3C-C4C	2.47	128.42	124.83
28	D	408	SQD	O48-C23-C24	2.47	119.43	111.90
24	c	502	CLA	CMB-C2B-C3B	2.47	129.92	125.09
24	A	1006	CLA	C4A-NA-C1A	2.47	109.56	106.36
24	d	402	CLA	CMB-C2B-C3B	2.48	129.93	125.09
24	b	604	CLA	CED-O2D-CGD	2.48	121.81	115.99
24	B	612	CLA	CMC-C2C-C1C	2.48	128.86	125.02
24	B	616	CLA	CAC-C3C-C4C	2.48	128.43	124.83
24	C	505	CLA	CMC-C2C-C1C	2.48	128.86	125.02
24	C	506	CLA	CMB-C2B-C3B	2.49	129.95	125.09
24	c	506	CLA	O2A-CGA-CBA	2.49	119.48	111.90
24	A	1008	CLA	CED-O2D-CGD	2.49	121.82	115.99
24	b	607	CLA	CMC-C2C-C1C	2.49	128.87	125.02
24	b	617	CLA	CED-O2D-CGD	2.49	121.83	115.99
24	C	503	CLA	C3B-C4B-NB	2.49	112.43	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	CMC-C2C-C1C	2.49	128.88	125.02
26	c	514	BCR	C8-C9-C10	2.49	123.00	118.98
26	d	404	BCR	C4-C5-C6	2.49	125.96	122.78
24	B	615	CLA	CMB-C2B-C3B	2.49	129.97	125.09
24	B	602	CLA	CMB-C2B-C3B	2.50	129.97	125.09
26	c	514	BCR	C7-C6-C5	2.51	127.11	121.37
36	C	515	DGD	O1G-C1A-C2A	2.51	119.54	111.90
24	B	615	CLA	C4-C3-C5	2.51	119.24	115.41
24	B	613	CLA	O2A-CGA-CBA	2.51	119.55	111.90
24	a	412	CLA	CAC-C3C-C4C	2.51	128.47	124.83
24	B	602	CLA	CMC-C2C-C1C	2.51	128.91	125.02
24	B	606	CLA	CMB-C2B-C3B	2.51	130.00	125.09
24	C	513	CLA	CMC-C2C-C1C	2.51	128.91	125.02
24	c	509	CLA	CMB-C2B-C3B	2.51	130.01	125.09
24	c	507	CLA	CMB-C2B-C3B	2.52	130.01	125.09
24	c	508	CLA	CMB-C2B-C3B	2.52	130.01	125.09
24	b	606	CLA	O2A-CGA-CBA	2.52	119.57	111.90
24	B	603	CLA	O2A-CGA-CBA	2.52	119.58	111.90
24	A	1008	CLA	CMC-C2C-C1C	2.52	128.92	125.02
26	B	619	BCR	C23-C24-C25	2.52	134.90	127.32
36	c	516	DGD	O3G-C1D-C2D	2.53	111.23	108.04
27	A	1010	PL9	C15-C14-C16	2.53	119.27	115.41
29	a	415	LMG	O1-C1-C2	2.53	111.23	108.04
24	b	608	CLA	CMC-C2C-C1C	2.53	128.93	125.02
24	c	502	CLA	C4-C3-C5	2.54	119.28	115.41
24	B	602	CLA	C4-C3-C5	2.54	119.28	115.41
24	C	504	CLA	CAC-C3C-C4C	2.54	128.51	124.83
26	a	413	BCR	C40-C30-C25	2.54	114.28	110.30
26	J	101	BCR	C2-C1-C6	2.54	114.38	110.36
24	c	503	CLA	C3B-C4B-NB	2.54	112.50	109.21
24	c	513	CLA	C3B-C4B-NB	2.54	112.50	109.21
27	d	405	PL9	C10-C9-C11	2.54	119.29	115.41
26	b	622	BCR	C28-C27-C26	2.55	117.91	113.87
24	C	512	CLA	C3B-C4B-NB	2.55	112.50	109.21
34	d	408	LHG	O8-C23-C24	2.55	119.68	111.90
25	a	411	PHO	CAC-C3C-C4C	2.55	128.14	125.16
24	C	507	CLA	CMB-C2B-C3B	2.56	130.09	125.09
24	c	507	CLA	O2A-CGA-CBA	2.56	119.69	111.90
24	b	613	CLA	C4-C3-C5	2.56	119.32	115.41
26	k	102	BCR	C8-C9-C10	2.56	123.11	118.98
34	D	410	LHG	O8-C23-C24	2.56	119.70	111.90
24	b	611	CLA	C4-C3-C5	2.56	119.32	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1007	PHO	CMB-C2B-C1B	2.56	129.23	125.06
24	b	609	CLA	C4-C3-C5	2.57	119.33	115.41
24	b	605	CLA	C4-C3-C5	2.57	119.33	115.41
32	t	103	LMT	C1'-C2'-C3'	2.57	115.04	109.97
24	c	505	CLA	CAC-C3C-C4C	2.57	128.56	124.83
24	A	1005	CLA	C4A-NA-C1A	2.58	109.69	106.36
24	B	612	CLA	CMB-C2B-C3B	2.58	130.13	125.09
24	b	619	CLA	CMB-C2B-C3B	2.58	130.14	125.09
24	b	618	CLA	CMC-C2C-C1C	2.59	129.02	125.02
24	C	501	CLA	CAC-C3C-C4C	2.59	128.59	124.83
24	b	605	CLA	CMB-C2B-C3B	2.59	130.15	125.09
26	D	406	BCR	C3-C4-C5	2.59	117.98	113.87
26	B	619	BCR	C28-C27-C26	2.60	117.99	113.87
24	c	513	CLA	C4-C3-C5	2.60	119.38	115.41
24	c	507	CLA	C4-C3-C5	2.60	119.38	115.41
26	h	101	BCR	C2-C1-C6	2.60	114.49	110.36
34	d	407	LHG	O7-C7-C8	2.61	117.19	111.53
24	c	509	CLA	CAC-C3C-C4C	2.61	128.62	124.83
24	b	616	CLA	O2A-CGA-CBA	2.62	119.89	111.90
24	c	505	CLA	CMC-C2C-C1C	2.62	129.08	125.02
24	c	512	CLA	CMC-C2C-C1C	2.62	129.08	125.02
38	f	101	HEM	C3B-C4B-CHC	2.62	126.86	123.16
27	D	407	PL9	C10-C9-C11	2.63	119.42	115.41
24	B	608	CLA	C4-C3-C5	2.63	119.42	115.41
24	b	604	CLA	C3B-C4B-NB	2.63	112.61	109.21
29	c	519	LMG	O8-C28-C29	2.63	119.91	111.90
34	d	407	LHG	O8-C23-C24	2.63	119.92	111.90
24	C	502	CLA	CAC-C3C-C4C	2.63	128.65	124.83
25	D	404	PHO	CAC-C3C-C4C	2.63	128.24	125.16
32	A	1018	LMT	C1'-C2'-C3'	2.64	115.17	109.97
24	d	403	CLA	CMB-C2B-C3B	2.64	130.25	125.09
27	A	1010	PL9	C20-C19-C21	2.64	119.44	115.41
36	h	102	DGD	O1G-C1A-C2A	2.64	119.95	111.90
24	d	402	CLA	CMC-C2C-C1C	2.64	129.11	125.02
27	A	1010	PL9	C45-C44-C46	2.64	119.44	115.41
24	b	605	CLA	O2A-CGA-CBA	2.64	119.95	111.90
24	C	509	CLA	C4-C3-C5	2.65	119.45	115.41
24	c	512	CLA	O2A-CGA-CBA	2.65	119.96	111.90
24	b	618	CLA	C4-C3-C5	2.65	119.45	115.41
27	d	405	PL9	C20-C19-C21	2.65	119.45	115.41
24	c	513	CLA	CMB-C2B-C3B	2.65	130.27	125.09
24	b	612	CLA	CAC-C3C-C4C	2.65	128.68	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	413	BCR	C23-C24-C25	2.65	135.29	127.32
24	C	507	CLA	O2A-CGA-CBA	2.66	119.99	111.90
24	C	510	CLA	CMC-C2C-C1C	2.66	129.13	125.02
24	c	510	CLA	C4-C3-C5	2.66	119.47	115.41
28	B	620[B]	SQD	O9-S-C6	2.66	109.18	106.94
24	b	608	CLA	C4A-NA-C1A	2.66	109.80	106.36
24	B	602	CLA	O2A-CGA-CBA	2.66	120.00	111.90
24	b	615	CLA	CED-O2D-CGD	2.66	122.24	115.99
24	b	611	CLA	CMB-C2B-C3B	2.67	130.30	125.09
24	C	513	CLA	CMB-C2B-C3B	2.67	130.31	125.09
36	C	517	DGD	O1G-C1A-C2A	2.67	120.04	111.90
29	D	412	LMG	O7-C10-C11	2.67	117.33	111.53
24	a	409	CLA	CMC-C2C-C1C	2.67	129.15	125.02
34	e	101	LHG	O8-C23-C24	2.67	120.05	111.90
28	b	623[B]	SQD	O7-S-C6	2.68	109.20	106.94
24	a	408	CLA	CMC-C2C-C1C	2.68	129.16	125.02
24	c	509	CLA	C4-C3-C5	2.68	119.50	115.41
29	c	520	LMG	O8-C28-C29	2.68	120.06	111.90
24	C	509	CLA	CMB-C2B-C3B	2.68	130.33	125.09
24	b	616	CLA	CMC-C2C-C1C	2.69	129.18	125.02
24	d	402	CLA	C4A-NA-C1A	2.69	109.84	106.36
29	C	519	LMG	O8-C28-C29	2.69	120.10	111.90
24	B	605	CLA	CMC-C2C-C1C	2.69	129.19	125.02
24	C	510	CLA	O2A-CGA-CBA	2.70	120.11	111.90
24	c	510	CLA	O2A-CGA-CBA	2.70	120.13	111.90
28	B	620[A]	SQD	O48-C23-C24	2.70	120.13	111.90
24	C	512	CLA	O2A-CGA-CBA	2.70	120.13	111.90
27	a	414	PL9	C30-C29-C31	2.70	119.53	115.41
27	A	1010	PL9	C40-C39-C41	2.70	119.53	115.41
24	C	512	CLA	CMC-C2C-C1C	2.70	129.20	125.02
24	b	615	CLA	CAC-C3C-C4C	2.71	128.76	124.83
24	b	615	CLA	O2A-CGA-CBA	2.71	120.15	111.90
24	c	511	CLA	C3B-C4B-NB	2.71	112.71	109.21
28	B	620[B]	SQD	O48-C23-C24	2.71	120.16	111.90
29	Z	101	LMG	O8-C28-C29	2.71	120.17	111.90
32	A	1018	LMT	C2'-C3'-C4'	2.71	115.56	109.60
24	b	611	CLA	C3B-C4B-NB	2.72	112.72	109.21
27	D	407	PL9	C20-C19-C21	2.72	119.56	115.41
26	b	622	BCR	C8-C9-C10	2.72	123.37	118.98
24	a	412	CLA	CMC-C2C-C1C	2.72	129.23	125.02
24	C	502	CLA	C4-C3-C5	2.72	119.57	115.41
28	f	102	SQD	O48-C23-C24	2.72	120.20	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	f	101	HEM	CMD-C2D-C3D	2.73	126.41	114.35
24	b	617	CLA	CMC-C2C-C1C	2.73	129.24	125.02
24	B	604	CLA	O2A-CGA-CBA	2.73	120.22	111.90
38	V	201	HEM	C2D-C3D-C4D	2.73	106.13	101.50
24	c	513	CLA	O2A-CGA-CBA	2.73	120.22	111.90
25	D	404	PHO	C4D-C3D-CAD	2.73	110.42	105.51
28	a	401	SQD	O48-C23-C24	2.73	120.23	111.90
26	A	1009	BCR	C3-C4-C5	2.74	118.21	113.87
26	H	101	BCR	C2-C1-C6	2.74	114.70	110.36
24	b	615	CLA	CMC-C2C-C1C	2.74	129.27	125.02
24	B	601	CLA	C4-C3-C5	2.75	119.60	115.41
29	a	415	LMG	O8-C28-C29	2.75	120.28	111.90
24	B	604	CLA	CAC-C3C-C4C	2.75	128.82	124.83
24	C	513	CLA	C3B-C4B-NB	2.75	112.77	109.21
26	d	404	BCR	C30-C25-C24	2.75	123.53	115.82
24	b	610	CLA	CED-O2D-CGD	2.76	122.46	115.99
26	B	618	BCR	C3-C4-C5	2.76	118.24	113.87
26	t	101	BCR	C4-C5-C6	2.76	126.30	122.78
26	K	102	BCR	C8-C9-C10	2.76	123.43	118.98
32	m	103	LMT	O1'-C1'-C2'	2.76	111.53	108.04
24	b	614	CLA	CAC-C3C-C4C	2.76	128.84	124.83
38	v	201	HEM	C2D-C3D-C4D	2.76	106.19	101.50
24	B	603	CLA	CMB-C2B-C3B	2.77	130.50	125.09
38	F	101	HEM	CMD-C2D-C3D	2.77	126.60	114.35
24	B	609	CLA	CAC-C3C-C4C	2.77	128.85	124.83
38	v	201	HEM	CMD-C2D-C3D	2.77	126.61	114.35
24	b	613	CLA	C3B-C4B-NB	2.78	112.80	109.21
24	B	610	CLA	O2A-CGA-CBA	2.78	120.36	111.90
27	d	405	PL9	C35-C34-C36	2.78	119.65	115.41
24	B	602	CLA	C3B-C4B-NB	2.78	112.80	109.21
34	D	411	LHG	O8-C23-C24	2.78	120.38	111.90
25	D	404	PHO	C4-C3-C5	2.78	119.66	115.41
29	A	1012	LMG	O8-C28-C29	2.79	120.39	111.90
28	A	1016	SQD	O48-C23-C24	2.79	120.39	111.90
26	T	101	BCR	C4-C5-C6	2.79	126.33	122.78
24	B	615	CLA	CED-O2D-CGD	2.79	122.53	115.99
24	c	506	CLA	C4-C3-C5	2.79	119.67	115.41
26	d	404	BCR	C23-C24-C25	2.79	135.69	127.32
24	a	408	CLA	C4-C3-C5	2.79	119.67	115.41
24	C	507	CLA	C3B-C4B-NB	2.79	112.82	109.21
25	a	411	PHO	C4D-C3D-CAD	2.80	110.54	105.51
27	d	405	PL9	C25-C24-C26	2.80	119.68	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	518	LMG	O8-C28-C29	2.80	120.43	111.90
26	A	1009	BCR	C32-C1-C6	2.80	114.69	110.30
26	K	102	BCR	C27-C26-C25	2.80	126.35	122.78
24	b	606	CLA	CMC-C2C-C1C	2.81	129.38	125.02
24	B	614	CLA	C3B-C4B-NB	2.82	112.85	109.21
32	A	1018	LMT	C1B-O5B-C5B	2.82	119.22	113.75
26	t	101	BCR	C1-C6-C7	2.82	123.71	115.82
24	B	616	CLA	C4-C3-C5	2.82	119.72	115.41
24	C	506	CLA	C4-C3-C5	2.82	119.72	115.41
26	T	101	BCR	C8-C9-C10	2.82	123.53	118.98
24	C	505	CLA	CAC-C3C-C4C	2.83	128.93	124.83
27	a	414	PL9	C35-C34-C36	2.83	119.73	115.41
24	b	610	CLA	C4-C3-C5	2.83	119.73	115.41
24	b	605	CLA	C3B-C4B-NB	2.83	112.87	109.21
24	B	601	CLA	C3B-C4B-NB	2.84	112.88	109.21
24	c	503	CLA	C4-C3-C5	2.84	119.74	115.41
27	A	1010	PL9	C30-C29-C31	2.84	119.74	115.41
25	D	404	PHO	C4A-NA-C1A	2.84	110.75	108.21
26	C	514	BCR	C4-C5-C6	2.84	126.40	122.78
24	B	608	CLA	CMB-C2B-C3B	2.84	130.65	125.09
27	a	414	PL9	C10-C9-C11	2.84	119.75	115.41
24	D	403	CLA	CMC-C2C-C1C	2.84	129.42	125.02
24	b	607	CLA	CAC-C3C-C4C	2.84	128.96	124.83
29	c	521	LMG	O8-C28-C29	2.84	120.56	111.90
24	a	409	CLA	C4-C3-C5	2.85	119.75	115.41
24	b	612	CLA	C3B-C4B-NB	2.85	112.89	109.21
24	C	511	CLA	C4-C3-C5	2.85	119.76	115.41
24	B	613	CLA	CMC-C2C-C1C	2.86	129.44	125.02
32	b	625	LMT	C3B-C4B-C5B	2.86	115.17	110.20
26	D	406	BCR	C28-C27-C26	2.86	118.40	113.87
34	d	406	LHG	O7-C7-C8	2.86	117.74	111.53
26	t	101	BCR	C8-C9-C10	2.87	123.60	118.98
24	d	402	CLA	O2A-CGA-CBA	2.87	120.64	111.90
36	H	102	DGD	O2G-C1B-C2B	2.87	117.77	111.53
24	B	612	CLA	C4A-NA-C1A	2.87	110.07	106.36
28	b	623[A]	SQD	O9-S-C6	2.87	109.36	106.94
26	y	101	BCR	C3-C4-C5	2.87	118.43	113.87
24	d	403	CLA	O2D-CGD-CBD	2.88	115.24	111.30
24	a	412	CLA	C4A-NA-C1A	2.88	110.08	106.36
24	c	505	CLA	C3B-C4B-NB	2.88	112.93	109.21
24	B	608	CLA	C4A-NA-C1A	2.88	110.08	106.36
27	a	414	PL9	C40-C39-C41	2.88	119.81	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	504	CLA	CAC-C3C-C4C	2.88	129.01	124.83
34	D	410	LHG	O7-C7-C8	2.88	117.80	111.53
24	b	607	CLA	O2A-CGA-CBA	2.89	120.69	111.90
24	B	604	CLA	C4-C3-C5	2.89	119.83	115.41
24	D	405	CLA	C3B-C4B-NB	2.90	112.95	109.21
24	B	607	CLA	CMC-C2C-C1C	2.90	129.50	125.02
24	C	507	CLA	C4-C3-C5	2.90	119.83	115.41
38	V	201	HEM	CMD-C2D-C3D	2.90	127.17	114.35
24	D	405	CLA	C4-C3-C5	2.90	119.84	115.41
26	D	406	BCR	C27-C26-C25	2.90	126.48	122.78
24	a	408	CLA	C4A-NA-C1A	2.90	110.11	106.36
24	B	604	CLA	CED-O2D-CGD	2.90	122.80	115.99
28	b	623[B]	SQD	O48-C23-C24	2.90	120.74	111.90
24	a	412	CLA	C4-C3-C5	2.90	119.84	115.41
24	B	608	CLA	CAC-C3C-C4C	2.91	129.05	124.83
24	b	619	CLA	CAC-C3C-C4C	2.91	129.05	124.83
26	t	101	BCR	C3-C4-C5	2.91	118.48	113.87
24	c	507	CLA	C3B-C4B-NB	2.91	112.97	109.21
26	K	101	BCR	C39-C30-C25	2.91	114.86	110.30
24	B	611	CLA	C3B-C4B-NB	2.91	112.98	109.21
34	E	101	LHG	O8-C23-C24	2.91	120.78	111.90
24	C	511	CLA	C3B-C4B-NB	2.91	112.98	109.21
36	c	517	DGD	O1G-C1A-C2A	2.92	120.78	111.90
25	a	411	PHO	C4A-NA-C1A	2.92	110.82	108.21
25	a	410	PHO	C4D-C3D-CAD	2.92	110.76	105.51
26	b	620	BCR	C4-C5-C6	2.92	126.50	122.78
26	k	101	BCR	C4-C5-C6	2.92	126.50	122.78
24	C	501	CLA	C4-C3-C5	2.92	119.87	115.41
24	b	604	CLA	O2A-CGA-CBA	2.92	120.81	111.90
24	A	1006	CLA	CMB-C2B-C3B	2.92	130.81	125.09
24	B	616	CLA	O2A-CGA-CBA	2.93	120.82	111.90
24	B	603	CLA	C4A-NA-C1A	2.93	110.15	106.36
26	h	101	BCR	C28-C27-C26	2.94	118.52	113.87
32	B	623	LMT	C2'-C3'-C4'	2.94	116.05	109.60
24	c	504	CLA	C4-C3-C5	2.94	119.89	115.41
24	B	610	CLA	C4A-NA-C1A	2.94	110.16	106.36
24	b	606	CLA	C3B-C4B-NB	2.94	113.02	109.21
35	C	522	HTG	O5-C5-C4	2.95	115.21	109.68
24	C	503	CLA	C4-C3-C5	2.95	119.92	115.41
26	B	619	BCR	C27-C26-C25	2.95	126.55	122.78
24	C	506	CLA	C3B-C4B-NB	2.96	113.03	109.21
24	b	618	CLA	C3B-C4B-NB	2.96	113.03	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	510	CLA	C4-C3-C5	2.96	119.93	115.41
24	a	407	CLA	CMB-C2B-C3B	2.96	130.88	125.09
24	B	610	CLA	C3B-C4B-NB	2.97	113.04	109.21
26	y	101	BCR	C2-C1-C6	2.97	115.06	110.36
24	c	501	CLA	C4-C3-C5	2.97	119.94	115.41
24	D	403	CLA	CMB-C2B-C3B	2.97	130.90	125.09
28	b	623[A]	SQD	O48-C23-C24	2.97	120.95	111.90
36	c	515	DGD	O1G-C1A-C2A	2.97	120.96	111.90
24	c	502	CLA	C3B-C4B-NB	2.97	113.06	109.21
26	T	101	BCR	C3-C4-C5	2.98	118.59	113.87
25	D	404	PHO	C3C-C4C-NC	2.98	115.05	110.24
34	D	409	LHG	O7-C7-C8	2.99	118.02	111.53
24	b	609	CLA	C3B-C4B-NB	2.99	113.07	109.21
26	K	102	BCR	C4-C5-C6	2.99	126.59	122.78
24	b	611	CLA	C4A-NA-C1A	2.99	110.23	106.36
25	A	1007	PHO	C4D-C3D-CAD	3.00	110.90	105.51
24	B	616	CLA	C4A-NA-C1A	3.00	110.24	106.36
24	d	403	CLA	C4A-NA-C1A	3.01	110.25	106.36
26	h	101	BCR	C8-C9-C10	3.01	123.84	118.98
24	b	614	CLA	C4A-NA-C1A	3.01	110.25	106.36
24	B	612	CLA	C4-C3-C5	3.02	120.02	115.41
26	t	101	BCR	C39-C30-C25	3.03	115.05	110.30
24	B	609	CLA	C3B-C4B-NB	3.03	113.12	109.21
34	B	621	LHG	O7-C7-C8	3.03	118.11	111.53
24	B	614	CLA	C4-C3-C5	3.03	120.04	115.41
24	c	511	CLA	C4-C3-C5	3.03	120.04	115.41
24	B	606	CLA	C4-C3-C5	3.04	120.05	115.41
24	B	610	CLA	C4-C3-C5	3.04	120.05	115.41
24	c	501	CLA	C3B-C4B-NB	3.05	113.15	109.21
32	i	102	LMT	O5'-C5'-C4'	3.05	116.19	109.75
24	a	409	CLA	C4A-NA-C1A	3.06	110.31	106.36
29	B	622	LMG	O8-C28-C29	3.06	121.22	111.90
26	h	101	BCR	C4-C5-C6	3.06	126.68	122.78
24	c	510	CLA	C4A-NA-C1A	3.06	110.31	106.36
26	a	413	BCR	C3-C4-C5	3.06	118.73	113.87
26	B	618	BCR	C39-C30-C25	3.06	115.11	110.30
24	A	1008	CLA	C4A-NA-C1A	3.07	110.32	106.36
24	b	617	CLA	C3B-C4B-NB	3.07	113.18	109.21
24	B	606	CLA	C3B-C4B-NB	3.07	113.18	109.21
32	b	625	LMT	O1'-C1'-C2'	3.07	111.92	108.04
24	A	1006	CLA	C4-C3-C5	3.07	120.10	115.41
34	b	624	LHG	O7-C7-C8	3.07	118.21	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	403	CLA	C4A-NA-C1A	3.07	110.33	106.36
34	D	409	LHG	O8-C23-C24	3.07	121.27	111.90
28	a	401	SQD	O6-C1-C2	3.08	111.92	108.04
38	V	201	HEM	C3B-C4B-CHC	3.08	127.50	123.16
26	B	617	BCR	C39-C30-C25	3.08	115.13	110.30
36	C	517	DGD	O2G-C1B-C2B	3.08	118.22	111.53
24	b	607	CLA	C3B-C4B-NB	3.08	113.20	109.21
24	b	617	CLA	C4A-NA-C1A	3.08	110.34	106.36
24	A	1006	CLA	CMC-C2C-C1C	3.09	129.80	125.02
24	b	608	CLA	C3B-C4B-NB	3.09	113.20	109.21
24	a	409	CLA	C3B-C4B-NB	3.09	113.21	109.21
26	D	406	BCR	C33-C5-C6	3.10	127.64	124.61
27	A	1010	PL9	C35-C34-C36	3.10	120.14	115.41
24	B	602	CLA	C4A-NA-C1A	3.11	110.37	106.36
32	b	631	LMT	C1B-O5B-C5B	3.11	119.78	113.75
26	A	1009	BCR	C33-C5-C6	3.11	127.66	124.61
26	K	101	BCR	C33-C5-C6	3.12	127.67	124.61
24	C	504	CLA	C4-C3-C5	3.12	120.17	115.41
27	D	407	PL9	C25-C24-C26	3.12	120.17	115.41
24	c	502	CLA	CAC-C3C-C4C	3.12	129.36	124.83
28	B	620[B]	SQD	O6-C1-C2	3.13	111.99	108.04
24	B	612	CLA	C3B-C4B-NB	3.13	113.25	109.21
24	c	510	CLA	C3B-C4B-NB	3.13	113.26	109.21
26	T	101	BCR	C23-C24-C25	3.13	136.72	127.32
24	B	601	CLA	O2A-CGA-CBA	3.14	121.46	111.90
26	b	621	BCR	C33-C5-C6	3.14	127.69	124.61
24	A	1008	CLA	C4-C3-C5	3.14	120.20	115.41
26	B	617	BCR	C2-C1-C6	3.14	115.34	110.36
26	b	621	BCR	C31-C1-C6	3.15	115.23	110.30
27	d	405	PL9	C40-C39-C41	3.15	120.21	115.41
25	a	411	PHO	C3C-C4C-NC	3.15	115.32	110.24
27	a	414	PL9	C25-C24-C26	3.15	120.22	115.41
25	a	410	PHO	C3C-C4C-NC	3.15	115.33	110.24
34	d	406	LHG	O8-C23-C24	3.15	121.51	111.90
24	c	512	CLA	C4-C3-C5	3.16	120.23	115.41
26	K	101	BCR	C28-C27-C26	3.16	118.88	113.87
24	B	607	CLA	C4A-NA-C1A	3.16	110.45	106.36
26	b	622	BCR	C32-C1-C6	3.16	115.26	110.30
26	H	101	BCR	C23-C24-C25	3.16	136.82	127.32
24	c	508	CLA	C3B-C4B-NB	3.17	113.30	109.21
24	C	505	CLA	C3B-C4B-NB	3.17	113.31	109.21
35	C	522	HTG	O5-C1-C2	3.17	114.49	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t	101	BCR	C23-C24-C25	3.17	136.84	127.32
24	B	605	CLA	C4A-NA-C1A	3.18	110.47	106.36
26	t	101	BCR	C27-C26-C25	3.18	126.83	122.78
24	c	508	CLA	C4-C3-C5	3.18	120.26	115.41
26	y	101	BCR	C28-C27-C26	3.18	118.91	113.87
24	d	402	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	c	504	CLA	C3B-C4B-NB	3.18	113.33	109.21
25	D	404	PHO	C2C-C1C-NC	3.19	114.50	109.73
26	d	404	BCR	C2-C1-C6	3.19	115.41	110.36
24	C	512	CLA	C4-C3-C5	3.19	120.28	115.41
24	A	1005	CLA	CMB-C2B-C3B	3.19	131.33	125.09
26	c	514	BCR	C31-C1-C6	3.19	115.31	110.30
26	C	514	BCR	C23-C24-C25	3.19	136.91	127.32
25	A	1007	PHO	C3C-C4C-NC	3.19	115.40	110.24
24	B	616	CLA	C3B-C4B-NB	3.20	113.35	109.21
26	h	101	BCR	C33-C5-C6	3.20	127.75	124.61
24	D	405	CLA	C4A-NA-C1A	3.21	110.50	106.36
24	C	501	CLA	C3B-C4B-NB	3.21	113.35	109.21
26	A	1009	BCR	C4-C5-C6	3.21	126.87	122.78
24	c	513	CLA	C4A-NA-C1A	3.21	110.51	106.36
27	A	1010	PL9	C10-C9-C11	3.22	120.32	115.41
25	a	410	PHO	C2B-C1B-NB	3.23	114.57	109.73
24	C	502	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	A	1008	CLA	C3B-C4B-NB	3.24	113.39	109.21
24	b	619	CLA	C4A-NA-C1A	3.24	110.54	106.36
25	D	404	PHO	C2B-C1B-NB	3.24	114.59	109.73
24	c	509	CLA	C3B-C4B-NB	3.24	113.40	109.21
24	d	403	CLA	C3B-C4B-NB	3.25	113.41	109.21
24	D	402	CLA	C4A-NA-C1A	3.25	110.56	106.36
28	f	102	SQD	C3-C4-C5	3.25	115.86	110.20
24	c	506	CLA	C3B-C4B-NB	3.25	113.42	109.21
28	B	620[A]	SQD	O7-S-C6	3.26	109.69	106.94
24	d	402	CLA	C4-C3-C5	3.26	120.39	115.41
26	b	621	BCR	C38-C26-C25	3.27	127.82	124.61
26	B	618	BCR	C40-C30-C25	3.27	115.44	110.30
25	a	411	PHO	C4-C3-C5	3.28	120.42	115.41
26	b	622	BCR	C23-C24-C25	3.28	137.17	127.32
29	B	622	LMG	O7-C10-C11	3.28	118.66	111.53
26	y	101	BCR	C27-C26-C25	3.28	126.96	122.78
26	b	620	BCR	C23-C24-C25	3.29	137.18	127.32
24	C	510	CLA	C4A-NA-C1A	3.29	110.61	106.36
24	b	606	CLA	C4A-NA-C1A	3.29	110.61	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	B	620[B]	SQD	O7-S-C6	3.29	109.72	106.94
35	b	630	HTG	C1-O5-C5	3.30	119.03	112.74
24	B	604	CLA	C3B-C4B-NB	3.30	113.48	109.21
24	b	614	CLA	C3B-C4B-NB	3.31	113.48	109.21
26	b	620	BCR	C40-C30-C25	3.31	115.49	110.30
24	C	508	CLA	C4A-NA-C1A	3.31	110.64	106.36
24	C	508	CLA	C3B-C4B-NB	3.31	113.49	109.21
24	B	615	CLA	C3B-C4B-NB	3.32	113.50	109.21
24	b	605	CLA	C4A-NA-C1A	3.32	110.66	106.36
34	D	411	LHG	O7-C7-C8	3.33	118.77	111.53
24	b	615	CLA	C3B-C4B-NB	3.33	113.52	109.21
24	a	407	CLA	C3B-C4B-NB	3.33	113.52	109.21
26	A	1009	BCR	C29-C30-C25	3.34	115.65	110.36
25	a	411	PHO	C2C-C1C-NC	3.34	114.74	109.73
24	D	402	CLA	CMC-C2C-C1C	3.34	130.19	125.02
26	T	101	BCR	C38-C26-C25	3.35	127.89	124.61
25	A	1007	PHO	C2B-C1B-NB	3.35	114.74	109.73
29	C	518	LMG	O7-C10-C11	3.35	118.81	111.53
26	K	101	BCR	C8-C7-C6	3.35	137.39	127.32
24	D	402	CLA	C4-C3-C5	3.36	120.54	115.41
24	b	615	CLA	C4-C3-C5	3.37	120.55	115.41
24	c	505	CLA	C4A-NA-C1A	3.37	110.72	106.36
24	C	509	CLA	C4A-NA-C1A	3.38	110.73	106.36
24	C	502	CLA	C4A-NA-C1A	3.38	110.73	106.36
26	H	101	BCR	C33-C5-C6	3.38	127.93	124.61
25	a	411	PHO	C2D-C1D-ND	3.39	114.80	109.73
24	A	1005	CLA	C3B-C4B-NB	3.39	113.59	109.21
28	b	623[B]	SQD	O9-S-C6	3.39	109.80	106.94
24	b	615	CLA	C4A-NA-C1A	3.39	110.74	106.36
25	a	410	PHO	C2D-C1D-ND	3.40	114.82	109.73
24	b	613	CLA	C4A-NA-C1A	3.40	110.75	106.36
26	C	514	BCR	C8-C9-C10	3.40	124.46	118.98
29	c	520	LMG	O7-C10-C11	3.40	118.92	111.53
32	t	103	LMT	C2'-C3'-C4'	3.41	117.10	109.60
24	C	513	CLA	C4A-NA-C1A	3.42	110.78	106.36
24	B	613	CLA	C3B-C4B-NB	3.42	113.63	109.21
29	m	102	LMG	O8-C28-C29	3.43	122.35	111.90
26	d	404	BCR	C40-C30-C39	3.43	119.36	108.37
24	c	504	CLA	C4A-NA-C1A	3.43	110.80	106.36
29	A	1012	LMG	O7-C10-C11	3.43	118.99	111.53
24	a	412	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	c	502	CLA	C4A-NA-C1A	3.45	110.82	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	415	LMG	O7-C10-C11	3.46	119.04	111.53
24	A	1006	CLA	C3B-C4B-NB	3.46	113.68	109.21
25	D	404	PHO	C2D-C1D-ND	3.46	114.92	109.73
29	c	520	LMG	O1-C1-C2	3.46	112.41	108.04
36	c	517	DGD	O2G-C1B-C2B	3.46	119.05	111.53
25	a	410	PHO	C4A-NA-C1A	3.46	111.30	108.21
29	d	409	LMG	O7-C10-C11	3.46	119.06	111.53
26	k	102	BCR	C4-C5-C6	3.47	127.20	122.78
26	B	617	BCR	C33-C5-C6	3.47	128.01	124.61
24	B	607	CLA	C3B-C4B-NB	3.47	113.70	109.21
26	k	101	BCR	C2-C1-C6	3.47	115.86	110.36
24	C	504	CLA	C3B-C4B-NB	3.48	113.70	109.21
24	C	510	CLA	C3B-C4B-NB	3.48	113.71	109.21
26	a	413	BCR	C31-C1-C6	3.49	115.77	110.30
26	k	101	BCR	C39-C30-C25	3.49	115.77	110.30
24	B	608	CLA	C3B-C4B-NB	3.49	113.73	109.21
24	b	610	CLA	C3B-C4B-NB	3.49	113.73	109.21
24	C	501	CLA	C4A-NA-C1A	3.50	110.88	106.36
26	H	101	BCR	C4-C5-C6	3.51	127.25	122.78
27	A	1010	PL9	C25-C24-C26	3.52	120.78	115.41
24	B	609	CLA	C4A-NA-C1A	3.52	110.91	106.36
26	A	1009	BCR	C38-C26-C25	3.52	128.06	124.61
24	b	616	CLA	C4A-NA-C1A	3.52	110.91	106.36
24	c	508	CLA	C4A-NA-C1A	3.52	110.91	106.36
24	b	616	CLA	C3B-C4B-NB	3.53	113.77	109.21
28	B	620[A]	SQD	O9-S-C6	3.53	109.92	106.94
26	y	101	BCR	C8-C9-C10	3.53	124.67	118.98
26	H	101	BCR	C28-C27-C26	3.53	119.47	113.87
24	B	603	CLA	C3B-C4B-NB	3.53	113.78	109.21
24	C	504	CLA	C4A-NA-C1A	3.53	110.93	106.36
24	B	614	CLA	C4A-NA-C1A	3.54	110.93	106.36
26	k	102	BCR	C39-C30-C25	3.54	115.86	110.30
36	c	515	DGD	O2G-C1B-C2B	3.55	119.25	111.53
28	A	1016	SQD	O6-C1-C2	3.56	112.53	108.04
29	c	519	LMG	O7-C10-C11	3.56	119.26	111.53
24	C	512	CLA	C4A-NA-C1A	3.56	110.97	106.36
26	y	101	BCR	C32-C1-C6	3.56	115.89	110.30
24	C	506	CLA	C4A-NA-C1A	3.57	110.97	106.36
25	a	411	PHO	C2B-C1B-NB	3.58	115.09	109.73
24	b	619	CLA	C3B-C4B-NB	3.58	113.83	109.21
24	B	611	CLA	C4A-NA-C1A	3.58	110.98	106.36
26	K	101	BCR	C24-C23-C22	3.58	131.67	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	619	BCR	C38-C26-C25	3.58	128.12	124.61
26	A	1009	BCR	C2-C1-C6	3.59	116.05	110.36
24	b	608	CLA	C4-C3-C5	3.60	120.90	115.41
24	B	607	CLA	C4-C3-C5	3.63	120.95	115.41
32	i	102	LMT	C1'-O5'-C5'	3.63	120.79	113.75
24	b	610	CLA	C4A-NA-C1A	3.63	111.05	106.36
24	c	509	CLA	C4A-NA-C1A	3.63	111.06	106.36
24	D	402	CLA	C3B-C4B-NB	3.64	113.91	109.21
24	B	601	CLA	C4A-NA-C1A	3.64	111.06	106.36
24	c	506	CLA	C4A-NA-C1A	3.65	111.08	106.36
28	a	401	SQD	O47-C7-C8	3.66	119.47	111.53
24	C	509	CLA	C3B-C4B-NB	3.66	113.94	109.21
25	A	1007	PHO	C2C-C1C-NC	3.66	115.22	109.73
24	c	501	CLA	C4A-NA-C1A	3.66	111.09	106.36
36	h	102	DGD	O2G-C1B-C2B	3.66	119.49	111.53
34	d	408	LHG	O7-C7-C8	3.67	119.50	111.53
28	f	102	SQD	O6-C1-C2	3.67	112.67	108.04
26	h	101	BCR	C39-C30-C25	3.67	116.06	110.30
24	b	604	CLA	C4A-NA-C1A	3.68	111.11	106.36
26	b	620	BCR	C39-C30-C25	3.68	116.08	110.30
25	A	1007	PHO	C2D-C1D-ND	3.69	115.26	109.73
26	b	620	BCR	C29-C30-C25	3.71	116.23	110.36
26	k	102	BCR	C23-C24-C25	3.71	138.46	127.32
24	a	407	CLA	O2D-CGD-CBD	3.71	116.39	111.30
25	a	410	PHO	C2C-C1C-NC	3.72	115.30	109.73
26	c	514	BCR	C33-C5-C6	3.72	128.26	124.61
25	A	1007	PHO	C4A-NA-C1A	3.72	111.53	108.21
24	c	512	CLA	C4A-NA-C1A	3.73	111.18	106.36
24	B	613	CLA	C4A-NA-C1A	3.73	111.18	106.36
26	y	101	BCR	C4-C5-C6	3.74	127.55	122.78
24	b	606	CLA	C4-C3-C5	3.74	121.12	115.41
26	K	101	BCR	C29-C30-C25	3.75	116.29	110.36
26	B	617	BCR	C29-C30-C25	3.75	116.30	110.36
26	H	101	BCR	C38-C26-C25	3.75	128.29	124.61
28	A	1016	SQD	O47-C7-C8	3.77	119.73	111.53
26	c	514	BCR	C28-C27-C26	3.77	119.86	113.87
26	K	101	BCR	C23-C24-C25	3.78	138.67	127.32
34	E	101	LHG	O7-C7-C8	3.78	119.75	111.53
36	C	515	DGD	O2G-C1B-C2B	3.79	119.76	111.53
24	B	606	CLA	C4A-NA-C1A	3.79	111.26	106.36
24	a	408	CLA	C3B-C4B-NB	3.79	114.11	109.21
26	B	617	BCR	C38-C26-C25	3.80	128.33	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	413	BCR	C29-C30-C25	3.80	116.38	110.36
38	F	101	HEM	CMC-C2C-C3C	3.82	126.06	116.53
26	b	622	BCR	C38-C26-C25	3.82	128.35	124.61
26	B	617	BCR	C32-C1-C6	3.83	116.31	110.30
26	c	514	BCR	C23-C24-C25	3.84	138.85	127.32
26	C	514	BCR	C2-C1-C6	3.85	116.47	110.36
26	c	514	BCR	C4-C5-C6	3.86	127.69	122.78
24	B	604	CLA	C4A-NA-C1A	3.86	111.35	106.36
26	h	101	BCR	C23-C24-C25	3.86	138.92	127.32
26	K	101	BCR	C27-C26-C25	3.87	127.71	122.78
24	B	605	CLA	C4-C3-C5	3.87	121.32	115.41
26	B	617	BCR	C27-C26-C25	3.88	127.73	122.78
26	k	102	BCR	C12-C13-C14	3.88	125.24	118.98
24	C	505	CLA	C4A-NA-C1A	3.88	111.38	106.36
26	b	622	BCR	C39-C30-C25	3.89	116.40	110.30
26	k	102	BCR	C40-C30-C25	3.92	116.45	110.30
26	b	621	BCR	C2-C1-C6	3.92	116.58	110.36
26	C	514	BCR	C29-C30-C25	3.93	116.58	110.36
36	c	516	DGD	O2G-C1B-C2B	3.93	120.07	111.53
28	f	102	SQD	O7-S-C6	3.93	110.25	106.94
32	b	625	LMT	O1B-C1B-C2B	3.93	117.67	108.10
26	k	101	BCR	C27-C26-C25	3.94	127.80	122.78
24	c	511	CLA	C4A-NA-C1A	3.94	111.46	106.36
26	A	1009	BCR	C8-C9-C10	3.95	125.35	118.98
24	b	612	CLA	C4A-NA-C1A	3.96	111.48	106.36
38	f	101	HEM	CMC-C2C-C3C	3.97	126.43	116.53
38	V	201	HEM	CMC-C2C-C3C	3.97	126.44	116.53
28	D	408	SQD	O47-C7-C8	3.99	120.19	111.53
24	c	503	CLA	C4A-NA-C1A	3.99	111.52	106.36
26	c	514	BCR	C40-C30-C25	4.00	116.57	110.30
38	V	201	HEM	CAD-C3D-C4D	4.00	126.58	112.47
26	b	620	BCR	C33-C5-C6	4.01	128.54	124.61
26	B	617	BCR	C23-C24-C25	4.01	139.35	127.32
34	e	101	LHG	O7-C7-C8	4.01	120.24	111.53
24	D	403	CLA	C3B-C4B-NB	4.01	114.40	109.21
26	D	406	BCR	C23-C24-C25	4.01	139.38	127.32
26	y	101	BCR	C24-C23-C22	4.03	132.35	126.22
28	B	620[B]	SQD	O47-C7-C8	4.03	120.29	111.53
28	f	102	SQD	O47-C7-C8	4.04	120.31	111.53
24	b	617	CLA	C4-C3-C5	4.04	121.58	115.41
38	F	101	HEM	CMB-C2B-C3B	4.04	126.63	116.53
29	Z	101	LMG	O7-C10-C11	4.05	120.33	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	609	CLA	C4A-NA-C1A	4.06	111.61	106.36
26	b	621	BCR	C8-C9-C10	4.06	125.52	118.98
26	a	413	BCR	C38-C26-C25	4.07	128.60	124.61
28	b	623[A]	SQD	O47-C7-C8	4.07	120.38	111.53
26	y	101	BCR	C23-C24-C25	4.08	139.58	127.32
26	a	413	BCR	C2-C1-C6	4.10	116.86	110.36
26	B	618	BCR	C27-C26-C25	4.10	128.01	122.78
27	D	407	PL9	C40-C39-C41	4.10	121.67	115.41
26	b	622	BCR	C29-C30-C25	4.10	116.86	110.36
26	B	617	BCR	C8-C9-C10	4.11	125.61	118.98
24	B	615	CLA	C4A-NA-C1A	4.12	111.69	106.36
26	b	621	BCR	C29-C30-C25	4.12	116.88	110.36
26	J	101	BCR	C8-C9-C10	4.12	125.62	118.98
28	b	623[A]	SQD	O7-S-C6	4.13	110.42	106.94
28	b	623[B]	SQD	O47-C7-C8	4.13	120.51	111.53
24	C	503	CLA	C4A-NA-C1A	4.14	111.71	106.36
24	b	618	CLA	C4A-NA-C1A	4.15	111.72	106.36
38	v	201	HEM	CAD-C3D-C4D	4.15	127.10	112.47
38	f	101	HEM	CAD-C3D-C4D	4.15	127.11	112.47
24	A	1005	CLA	O2D-CGD-CBD	4.16	117.01	111.30
26	K	101	BCR	C2-C1-C6	4.17	116.97	110.36
28	c	518	SQD	O47-C7-C8	4.19	120.63	111.53
26	B	618	BCR	C8-C7-C6	4.22	139.99	127.32
36	C	516	DGD	O2G-C1B-C2B	4.22	120.70	111.53
26	J	101	BCR	C23-C24-C25	4.24	140.06	127.32
29	m	102	LMG	O7-C10-C11	4.25	120.76	111.53
24	B	603	CLA	C4-C3-C5	4.25	121.89	115.41
26	B	618	BCR	C8-C9-C10	4.25	125.83	118.98
24	D	405	CLA	O2D-CGD-CBD	4.25	117.13	111.30
26	C	514	BCR	C27-C26-C25	4.27	128.22	122.78
26	k	101	BCR	C23-C24-C25	4.27	140.14	127.32
26	a	413	BCR	C27-C26-C25	4.28	128.23	122.78
38	v	201	HEM	CMB-C2B-C3B	4.28	127.23	116.53
26	D	406	BCR	C32-C1-C6	4.29	117.02	110.30
24	C	507	CLA	C4A-NA-C1A	4.29	111.91	106.36
26	K	102	BCR	C12-C13-C14	4.29	125.89	118.98
24	D	402	CLA	O2D-CGD-CBD	4.29	117.19	111.30
26	C	514	BCR	C24-C23-C22	4.29	132.76	126.22
38	v	201	HEM	CMC-C2C-C3C	4.30	127.26	116.53
32	C	520	LMT	O1B-C4'-C3'	4.35	118.40	107.17
26	k	102	BCR	C32-C1-C6	4.35	117.12	110.30
26	h	101	BCR	C38-C26-C25	4.36	128.89	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	F	101	HEM	CAD-C3D-C4D	4.37	127.88	112.47
28	B	620[A]	SQD	O47-C7-C8	4.38	121.04	111.53
26	c	514	BCR	C27-C26-C25	4.38	128.36	122.78
26	b	622	BCR	C27-C26-C25	4.39	128.38	122.78
26	C	514	BCR	C38-C26-C25	4.39	128.92	124.61
24	b	618	CLA	O2D-CGD-CBD	4.39	117.33	111.30
24	c	507	CLA	C4A-NA-C1A	4.41	112.07	106.36
28	A	1011	SQD	O47-C7-C8	4.42	121.13	111.53
26	k	101	BCR	C29-C30-C25	4.43	117.37	110.36
24	C	511	CLA	C4A-NA-C1A	4.44	112.09	106.36
26	k	102	BCR	C8-C7-C6	4.45	140.68	127.32
26	T	101	BCR	C33-C5-C6	4.46	128.99	124.61
26	H	101	BCR	C27-C26-C25	4.47	128.47	122.78
26	H	101	BCR	C29-C30-C25	4.48	117.46	110.36
26	k	102	BCR	C29-C30-C25	4.48	117.46	110.36
24	B	613	CLA	O2D-CGD-CBD	4.49	117.46	111.30
38	f	101	HEM	CMB-C2B-C3B	4.50	127.75	116.53
26	B	619	BCR	C8-C7-C6	4.50	140.83	127.32
26	K	101	BCR	C8-C9-C10	4.51	126.24	118.98
38	V	201	HEM	CMB-C2B-C3B	4.51	127.78	116.53
26	k	101	BCR	C31-C1-C6	4.52	117.38	110.30
28	c	518	SQD	O6-C1-C2	4.53	113.76	108.04
24	b	607	CLA	C4A-NA-C1A	4.54	112.24	106.36
26	D	406	BCR	C4-C5-C6	4.55	128.58	122.78
26	T	101	BCR	C12-C13-C14	4.57	126.35	118.98
28	D	408	SQD	O9-S-C6	4.57	110.80	106.94
26	C	514	BCR	C31-C1-C6	4.59	117.50	110.30
28	A	1011	SQD	O6-C1-C2	4.59	113.84	108.04
26	H	101	BCR	C39-C30-C25	4.60	117.52	110.30
26	b	621	BCR	C27-C26-C25	4.61	128.66	122.78
26	d	404	BCR	C24-C23-C22	4.61	133.25	126.22
26	K	102	BCR	C23-C22-C21	4.62	126.43	118.98
26	T	101	BCR	C29-C30-C25	4.63	117.69	110.36
26	b	621	BCR	C23-C24-C25	4.63	141.23	127.32
38	F	101	HEM	CAD-C3D-C2D	4.63	126.54	113.22
24	c	503	CLA	O2D-CGD-CBD	4.64	117.66	111.30
29	C	519	LMG	O7-C10-C11	4.66	121.66	111.53
26	t	101	BCR	C2-C1-C6	4.66	117.74	110.36
26	J	101	BCR	C29-C30-C25	4.66	117.75	110.36
24	C	508	CLA	O2D-CGD-CBD	4.67	117.71	111.30
26	y	101	BCR	C40-C30-C25	4.68	117.64	110.30
26	B	617	BCR	C40-C30-C25	4.68	117.64	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k	101	BCR	C8-C9-C10	4.68	126.53	118.98
26	K	102	BCR	C2-C1-C6	4.68	117.78	110.36
26	D	406	BCR	C8-C7-C6	4.68	141.38	127.32
38	v	201	HEM	CAD-C3D-C2D	4.69	126.69	113.22
26	d	404	BCR	C38-C26-C25	4.69	129.21	124.61
26	T	101	BCR	C27-C26-C25	4.69	128.76	122.78
28	A	1016	SQD	O9-S-C6	4.70	110.91	106.94
26	K	102	BCR	C40-C30-C25	4.71	117.69	110.30
24	B	607	CLA	O2D-CGD-CBD	4.71	117.76	111.30
26	J	101	BCR	C38-C26-C25	4.72	129.24	124.61
26	b	621	BCR	C32-C1-C6	4.73	117.71	110.30
26	J	101	BCR	C8-C7-C6	4.73	141.54	127.32
26	t	101	BCR	C40-C30-C25	4.74	117.73	110.30
26	t	101	BCR	C38-C26-C25	4.77	129.29	124.61
26	c	514	BCR	C2-C1-C6	4.78	117.93	110.36
26	a	413	BCR	C8-C7-C6	4.78	141.67	127.32
26	b	620	BCR	C27-C26-C25	4.78	128.87	122.78
28	a	401	SQD	O9-S-C6	4.79	110.98	106.94
29	c	521	LMG	O7-C10-C11	4.80	121.96	111.53
26	d	404	BCR	C8-C7-C6	4.81	141.77	127.32
26	y	101	BCR	C23-C22-C21	4.83	126.77	118.98
24	b	613	CLA	O2D-CGD-CBD	4.85	117.95	111.30
24	B	604	CLA	O2D-CGD-CBD	4.85	117.96	111.30
38	f	101	HEM	CAD-C3D-C2D	4.85	127.17	113.22
24	B	615	CLA	O2D-CGD-CBD	4.85	117.96	111.30
26	K	102	BCR	C8-C7-C6	4.85	141.90	127.32
26	c	514	BCR	C12-C13-C14	4.86	126.81	118.98
26	a	413	BCR	C8-C9-C10	4.86	126.82	118.98
26	b	621	BCR	C8-C7-C6	4.87	141.93	127.32
26	k	102	BCR	C2-C1-C6	4.87	118.07	110.36
38	V	201	HEM	CAD-C3D-C2D	4.87	127.23	113.22
26	H	101	BCR	C8-C9-C10	4.88	126.84	118.98
26	K	102	BCR	C33-C5-C6	4.88	129.40	124.61
26	k	101	BCR	C8-C7-C6	4.88	141.99	127.32
28	D	408	SQD	O6-C1-C2	4.91	114.24	108.04
35	C	522	HTG	C1-O5-C5	4.92	122.11	112.74
26	t	101	BCR	C33-C5-C6	4.92	129.44	124.61
26	K	101	BCR	C31-C1-C6	4.94	118.05	110.30
24	C	503	CLA	O2D-CGD-CBD	4.97	118.11	111.30
26	d	404	BCR	C33-C5-C6	4.98	129.49	124.61
26	B	619	BCR	C2-C1-C6	4.98	118.25	110.36
26	H	101	BCR	C32-C1-C6	5.01	118.16	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	h	101	BCR	C27-C26-C25	5.04	129.21	122.78
24	c	506	CLA	O2D-CGD-CBD	5.06	118.24	111.30
24	b	614	CLA	O2D-CGD-CBD	5.07	118.25	111.30
26	A	1009	BCR	C8-C7-C6	5.07	142.54	127.32
24	d	402	CLA	O2D-CGD-CBD	5.09	118.28	111.30
24	b	616	CLA	O2D-CGD-CBD	5.12	118.32	111.30
24	B	608	CLA	O2D-CGD-CBD	5.12	118.33	111.30
26	T	101	BCR	C2-C1-C6	5.13	118.49	110.36
26	k	102	BCR	C23-C22-C21	5.13	127.25	118.98
26	c	514	BCR	C8-C7-C6	5.15	142.78	127.32
28	A	1011	SQD	O9-S-C6	5.19	111.31	106.94
26	K	102	BCR	C24-C23-C22	5.20	134.14	126.22
24	c	509	CLA	O2D-CGD-CBD	5.22	118.46	111.30
26	B	618	BCR	C31-C1-C6	5.22	118.48	110.30
26	t	101	BCR	C8-C7-C6	5.23	143.02	127.32
24	c	511	CLA	O2D-CGD-CBD	5.23	118.47	111.30
26	b	620	BCR	C8-C7-C6	5.23	143.03	127.32
26	J	101	BCR	C12-C13-C14	5.23	127.42	118.98
26	y	101	BCR	C8-C7-C6	5.23	143.04	127.32
26	b	622	BCR	C8-C7-C6	5.24	143.06	127.32
26	A	1009	BCR	C27-C26-C25	5.25	129.47	122.78
26	h	101	BCR	C8-C7-C6	5.25	143.09	127.32
24	c	511	CLA	C2C-C1C-NC	5.28	114.18	110.24
24	c	510	CLA	O2D-CGD-CBD	5.29	118.56	111.30
26	C	514	BCR	C40-C30-C25	5.31	118.62	110.30
26	h	101	BCR	C29-C30-C25	5.32	118.78	110.36
24	C	513	CLA	C2C-C1C-NC	5.34	114.22	110.24
26	b	620	BCR	C8-C9-C10	5.34	127.58	118.98
26	B	617	BCR	C8-C7-C6	5.34	143.37	127.32
26	h	101	BCR	C32-C1-C6	5.35	118.68	110.30
26	B	619	BCR	C23-C22-C21	5.36	127.62	118.98
24	C	512	CLA	C2C-C1C-NC	5.37	114.24	110.24
24	D	403	CLA	O2D-CGD-CBD	5.38	118.68	111.30
26	d	404	BCR	C8-C9-C10	5.39	127.67	118.98
24	c	503	CLA	C2C-C1C-NC	5.40	114.26	110.24
26	D	406	BCR	C40-C30-C25	5.41	118.78	110.30
26	d	404	BCR	C23-C22-C21	5.44	127.75	118.98
26	B	618	BCR	C38-C26-C25	5.45	129.96	124.61
24	c	508	CLA	O2D-CGD-CBD	5.45	118.78	111.30
26	J	101	BCR	C23-C22-C21	5.48	127.81	118.98
24	b	605	CLA	O2D-CGD-CBD	5.49	118.84	111.30
24	B	609	CLA	O2D-CGD-CBD	5.50	118.84	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	408	CLA	O2D-CGD-CBD	5.51	118.85	111.30
26	y	101	BCR	C29-C30-C25	5.51	119.08	110.36
24	C	503	CLA	C2C-C1C-NC	5.51	114.35	110.24
26	J	101	BCR	C40-C30-C25	5.52	118.96	110.30
24	B	605	CLA	C2C-C1C-NC	5.53	114.36	110.24
24	C	511	CLA	O2D-CGD-CBD	5.54	118.89	111.30
26	D	406	BCR	C38-C26-C25	5.54	130.04	124.61
24	c	512	CLA	C2C-C1C-NC	5.54	114.37	110.24
26	C	514	BCR	C12-C13-C14	5.54	127.91	118.98
24	C	511	CLA	C2C-C1C-NC	5.54	114.37	110.24
24	b	605	CLA	C2C-C1C-NC	5.56	114.38	110.24
24	C	513	CLA	O2D-CGD-CBD	5.56	118.93	111.30
24	B	610	CLA	O2D-CGD-CBD	5.57	118.94	111.30
24	b	610	CLA	O2D-CGD-CBD	5.59	118.97	111.30
24	c	513	CLA	C2C-C1C-NC	5.59	114.40	110.24
24	A	1006	CLA	O2D-CGD-CBD	5.60	118.98	111.30
24	b	612	CLA	O2D-CGD-CBD	5.60	118.99	111.30
24	b	604	CLA	C2C-C1C-NC	5.62	114.43	110.24
26	B	618	BCR	C33-C5-C6	5.63	130.13	124.61
26	k	102	BCR	C24-C23-C22	5.63	134.79	126.22
24	a	409	CLA	O2D-CGD-CBD	5.64	119.04	111.30
26	b	620	BCR	C24-C23-C22	5.65	134.82	126.22
24	b	615	CLA	O2D-CGD-CBD	5.66	119.06	111.30
26	b	621	BCR	C40-C30-C25	5.69	119.22	110.30
26	b	622	BCR	C24-C23-C22	5.70	134.91	126.22
24	C	508	CLA	C2C-C1C-NC	5.72	114.50	110.24
26	C	514	BCR	C8-C7-C6	5.72	144.50	127.32
24	B	611	CLA	O2D-CGD-CBD	5.77	119.22	111.30
24	B	612	CLA	C2C-C1C-NC	5.79	114.55	110.24
24	c	508	CLA	C2C-C1C-NC	5.80	114.56	110.24
24	A	1008	CLA	O2D-CGD-CBD	5.81	119.27	111.30
24	C	510	CLA	O2D-CGD-CBD	5.82	119.28	111.30
26	D	406	BCR	C23-C22-C21	5.82	128.36	118.98
24	C	512	CLA	O2D-CGD-CBD	5.83	119.30	111.30
26	K	102	BCR	C32-C1-C6	5.85	119.48	110.30
26	B	618	BCR	C23-C24-C25	5.85	144.90	127.32
24	D	405	CLA	C2C-C1C-NC	5.85	114.60	110.24
24	b	613	CLA	C2C-C1C-NC	5.87	114.61	110.24
26	H	101	BCR	C24-C23-C22	5.87	135.16	126.22
26	B	619	BCR	C12-C13-C14	5.88	128.45	118.98
24	c	502	CLA	C2C-C1C-NC	5.88	114.62	110.24
24	B	612	CLA	O2D-CGD-CBD	5.89	119.39	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	602	CLA	O2D-CGD-CBD	5.90	119.39	111.30
24	C	506	CLA	O2D-CGD-CBD	5.90	119.40	111.30
24	B	601	CLA	C2C-C1C-NC	5.91	114.64	110.24
24	c	505	CLA	C2C-C1C-NC	5.93	114.66	110.24
24	c	504	CLA	C2C-C1C-NC	5.95	114.67	110.24
26	c	514	BCR	C29-C30-C25	5.95	119.78	110.36
24	b	607	CLA	O2D-CGD-CBD	5.95	119.46	111.30
24	C	501	CLA	O2D-CGD-CBD	5.96	119.48	111.30
26	B	618	BCR	C29-C30-C25	5.97	119.81	110.36
24	B	616	CLA	C2C-C1C-NC	5.97	114.69	110.24
26	c	514	BCR	C23-C22-C21	5.97	128.60	118.98
35	b	626	HTG	C1'-S1-C1	5.98	108.54	100.30
26	H	101	BCR	C8-C7-C6	5.98	145.28	127.32
26	b	622	BCR	C2-C1-C6	5.99	119.85	110.36
24	C	505	CLA	O2D-CGD-CBD	6.00	119.53	111.30
24	d	403	CLA	C2C-C1C-NC	6.00	114.71	110.24
24	b	617	CLA	C2C-C1C-NC	6.02	114.72	110.24
24	b	618	CLA	C2C-C1C-NC	6.02	114.72	110.24
24	C	507	CLA	C2C-C1C-NC	6.02	114.73	110.24
26	B	617	BCR	C12-C13-C14	6.04	128.72	118.98
24	c	512	CLA	O2D-CGD-CBD	6.05	119.60	111.30
26	K	102	BCR	C29-C30-C25	6.06	119.95	110.36
24	B	611	CLA	C2C-C1C-NC	6.07	114.76	110.24
24	c	513	CLA	O2D-CGD-CBD	6.08	119.64	111.30
26	J	101	BCR	C33-C5-C6	6.08	130.57	124.61
24	b	619	CLA	C2C-C1C-NC	6.09	114.78	110.24
24	B	614	CLA	C2C-C1C-NC	6.10	114.78	110.24
24	c	507	CLA	C2C-C1C-NC	6.10	114.79	110.24
24	b	606	CLA	O2D-CGD-CBD	6.11	119.68	111.30
24	b	606	CLA	C2C-C1C-NC	6.12	114.80	110.24
26	y	101	BCR	C38-C26-C25	6.13	130.63	124.61
26	k	101	BCR	C24-C23-C22	6.14	135.57	126.22
24	C	504	CLA	O2D-CGD-CBD	6.15	119.73	111.30
26	t	101	BCR	C12-C13-C14	6.15	128.89	118.98
24	B	605	CLA	O2D-CGD-CBD	6.15	119.74	111.30
26	D	406	BCR	C2-C1-C6	6.15	120.10	110.36
26	b	620	BCR	C2-C1-C6	6.17	120.12	110.36
25	a	410	PHO	O2D-CGD-CBD	6.17	119.77	111.30
24	B	613	CLA	C2C-C1C-NC	6.18	114.85	110.24
24	C	502	CLA	O2D-CGD-CBD	6.19	119.80	111.30
26	k	102	BCR	C15-C14-C13	6.22	136.19	127.20
26	k	101	BCR	C38-C26-C25	6.23	130.72	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	O2D-CGD-CBD	6.23	119.85	111.30
26	b	622	BCR	C12-C13-C14	6.25	129.05	118.98
24	b	614	CLA	C2C-C1C-NC	6.25	114.90	110.24
24	b	617	CLA	O2D-CGD-CBD	6.25	119.88	111.30
26	B	617	BCR	C7-C8-C9	6.26	135.76	126.22
26	B	618	BCR	C24-C23-C22	6.27	135.77	126.22
26	T	101	BCR	C23-C22-C21	6.27	129.08	118.98
24	B	606	CLA	C2C-C1C-NC	6.27	114.91	110.24
24	b	608	CLA	O2D-CGD-CBD	6.28	119.92	111.30
24	c	502	CLA	O2D-CGD-CBD	6.28	119.92	111.30
24	B	602	CLA	C2C-C1C-NC	6.29	114.93	110.24
26	J	101	BCR	C24-C23-C22	6.29	135.81	126.22
24	C	501	CLA	C2C-C1C-NC	6.30	114.93	110.24
24	a	412	CLA	O2D-CGD-CBD	6.31	119.95	111.30
24	C	506	CLA	C2C-C1C-NC	6.31	114.94	110.24
24	b	611	CLA	C2C-C1C-NC	6.32	114.95	110.24
24	C	502	CLA	C2C-C1C-NC	6.32	114.95	110.24
24	b	609	CLA	O2D-CGD-CBD	6.33	119.98	111.30
26	A	1009	BCR	C24-C23-C22	6.33	135.86	126.22
24	B	609	CLA	C2C-C1C-NC	6.33	114.96	110.24
26	k	101	BCR	C12-C13-C14	6.34	129.20	118.98
35	V	202	HTG	C1'-S1-C1	6.35	109.05	100.30
26	t	101	BCR	C24-C23-C22	6.35	135.89	126.22
24	b	619	CLA	O2D-CGD-CBD	6.35	120.01	111.30
28	c	518	SQD	O9-S-C6	6.36	112.30	106.94
24	b	615	CLA	C2C-C1C-NC	6.36	114.98	110.24
24	a	409	CLA	C2C-C1C-NC	6.36	114.98	110.24
26	K	101	BCR	C23-C22-C21	6.37	129.24	118.98
24	B	610	CLA	C2C-C1C-NC	6.37	114.99	110.24
24	b	609	CLA	C2C-C1C-NC	6.38	114.99	110.24
26	D	406	BCR	C8-C9-C10	6.40	129.29	118.98
24	C	507	CLA	O2D-CGD-CBD	6.40	120.08	111.30
26	T	101	BCR	C8-C7-C6	6.41	146.56	127.32
24	c	509	CLA	C2C-C1C-NC	6.41	115.01	110.24
24	c	510	CLA	C2C-C1C-NC	6.42	115.02	110.24
25	A	1007	PHO	O2D-CGD-CBD	6.43	120.12	111.30
25	a	411	PHO	O2D-CGD-CBD	6.46	120.17	111.30
24	B	606	CLA	O2D-CGD-CBD	6.47	120.18	111.30
24	C	504	CLA	C2C-C1C-NC	6.50	115.08	110.24
24	c	501	CLA	C2C-C1C-NC	6.51	115.09	110.24
26	t	101	BCR	C23-C22-C21	6.52	129.49	118.98
35	c	525	HTG	C1'-S1-C1	6.53	109.30	100.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	612	CLA	C2C-C1C-NC	6.54	115.11	110.24
24	b	608	CLA	C2C-C1C-NC	6.55	115.12	110.24
26	b	620	BCR	C23-C22-C21	6.56	129.54	118.98
24	b	604	CLA	O2D-CGD-CBD	6.56	120.30	111.30
26	y	101	BCR	C12-C13-C14	6.57	129.56	118.98
24	d	402	CLA	C2C-C1C-NC	6.57	115.13	110.24
26	b	621	BCR	C23-C22-C21	6.57	129.57	118.98
24	b	616	CLA	C2C-C1C-NC	6.59	115.15	110.24
24	B	604	CLA	C2C-C1C-NC	6.61	115.16	110.24
24	c	501	CLA	O2D-CGD-CBD	6.62	120.38	111.30
26	a	413	BCR	C33-C5-C6	6.62	131.10	124.61
24	c	506	CLA	C2C-C1C-NC	6.65	115.19	110.24
24	b	611	CLA	O2D-CGD-CBD	6.65	120.43	111.30
24	B	615	CLA	C2C-C1C-NC	6.66	115.20	110.24
26	d	404	BCR	C29-C30-C25	6.66	120.91	110.36
25	D	404	PHO	O2D-CGD-CBD	6.68	120.46	111.30
24	b	607	CLA	C2C-C1C-NC	6.68	115.22	110.24
24	C	505	CLA	C2C-C1C-NC	6.70	115.23	110.24
26	k	102	BCR	C33-C5-C6	6.72	131.20	124.61
24	c	504	CLA	O2D-CGD-CBD	6.75	120.56	111.30
28	D	408	SQD	O7-S-C6	6.76	112.64	106.94
24	c	507	CLA	O2D-CGD-CBD	6.78	120.60	111.30
24	B	614	CLA	O2D-CGD-CBD	6.78	120.61	111.30
35	c	522	HTG	C1'-S1-C1	6.79	109.65	100.30
26	c	514	BCR	C24-C23-C22	6.79	136.56	126.22
26	B	618	BCR	C23-C22-C21	6.80	129.93	118.98
26	c	514	BCR	C38-C26-C25	6.80	131.28	124.61
24	A	1008	CLA	C2C-C1C-NC	6.81	115.31	110.24
24	a	412	CLA	C2C-C1C-NC	6.83	115.33	110.24
35	o	301	HTG	C1'-S1-C1	6.83	109.71	100.30
26	a	413	BCR	C12-C13-C14	6.84	130.00	118.98
24	C	509	CLA	C2C-C1C-NC	6.86	115.35	110.24
26	B	619	BCR	C24-C23-C22	6.88	136.70	126.22
35	B	628	HTG	C1'-S1-C1	6.89	109.79	100.30
24	a	407	CLA	C2C-C1C-NC	6.92	115.39	110.24
24	B	601	CLA	O2D-CGD-CBD	6.95	120.83	111.30
35	b	601	HTG	C1'-S1-C1	7.00	109.95	100.30
24	A	1006	CLA	C2C-C1C-NC	7.00	115.46	110.24
24	B	616	CLA	O2D-CGD-CBD	7.01	120.92	111.30
35	C	522	HTG	C1'-S1-C1	7.03	109.99	100.30
26	B	619	BCR	C29-C30-C25	7.04	121.51	110.36
26	k	101	BCR	C33-C5-C6	7.04	131.52	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	514	BCR	C23-C22-C21	7.05	130.33	118.98
35	C	521	HTG	C1'-S1-C1	7.06	110.03	100.30
35	D	413	HTG	C1'-S1-C1	7.07	110.05	100.30
26	J	101	BCR	C4-C5-C6	7.08	131.81	122.78
26	b	622	BCR	C23-C22-C21	7.09	130.40	118.98
24	B	603	CLA	C2C-C1C-NC	7.09	115.52	110.24
26	h	101	BCR	C12-C13-C14	7.12	130.45	118.98
24	C	510	CLA	C2C-C1C-NC	7.13	115.55	110.24
26	h	101	BCR	C23-C22-C21	7.13	130.46	118.98
26	b	620	BCR	C38-C26-C25	7.13	131.61	124.61
35	B	629	HTG	C1'-S1-C1	7.14	110.14	100.30
24	c	505	CLA	O2D-CGD-CBD	7.16	121.12	111.30
24	B	607	CLA	C2C-C1C-NC	7.20	115.60	110.24
26	d	404	BCR	C12-C13-C14	7.20	130.59	118.98
26	k	102	BCR	C38-C26-C25	7.20	131.68	124.61
24	B	608	CLA	C2C-C1C-NC	7.25	115.64	110.24
24	D	402	CLA	C2C-C1C-NC	7.30	115.68	110.24
26	k	102	BCR	C19-C18-C17	7.34	130.80	118.98
24	A	1005	CLA	C2C-C1C-NC	7.36	115.72	110.24
26	k	102	BCR	C11-C10-C9	7.36	137.83	127.20
24	a	408	CLA	C2C-C1C-NC	7.38	115.74	110.24
25	A	1007	PHO	CMD-C2D-C1D	7.39	137.09	125.06
26	t	101	BCR	C11-C10-C9	7.39	137.88	127.20
26	K	101	BCR	C12-C13-C14	7.40	130.91	118.98
24	b	610	CLA	C2C-C1C-NC	7.42	115.76	110.24
26	d	404	BCR	C11-C10-C9	7.57	138.13	127.20
35	d	410	HTG	C1'-S1-C1	7.57	110.73	100.30
25	a	410	PHO	CMD-C2D-C1D	7.57	137.39	125.06
26	A	1009	BCR	C23-C22-C21	7.59	131.21	118.98
26	a	413	BCR	C23-C22-C21	7.60	131.23	118.98
26	D	406	BCR	C12-C13-C14	7.61	131.24	118.98
26	C	514	BCR	C19-C18-C17	7.62	131.26	118.98
26	B	617	BCR	C24-C23-C22	7.67	137.90	126.22
26	K	102	BCR	C38-C26-C25	7.69	132.15	124.61
26	h	101	BCR	C7-C8-C9	7.77	138.06	126.22
26	A	1009	BCR	C12-C13-C14	7.79	131.53	118.98
24	B	603	CLA	O2D-CGD-CBD	7.81	122.02	111.30
26	k	101	BCR	C23-C22-C21	7.84	131.62	118.98
26	H	101	BCR	C23-C22-C21	7.91	131.72	118.98
25	a	411	PHO	CMD-C2D-C1D	7.96	138.02	125.06
35	b	602	HTG	C1'-S1-C1	8.00	111.32	100.30
25	D	404	PHO	CMD-C2D-C1D	8.03	138.13	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	413	BCR	C24-C23-C22	8.03	138.46	126.22
26	H	101	BCR	C10-C11-C12	8.10	147.83	123.13
26	d	404	BCR	C19-C18-C17	8.23	132.25	118.98
26	D	406	BCR	C29-C30-C25	8.25	123.42	110.36
26	J	101	BCR	C15-C14-C13	8.31	139.20	127.20
26	y	101	BCR	C15-C14-C13	8.34	139.25	127.20
26	y	101	BCR	C33-C5-C6	8.38	132.83	124.61
26	d	404	BCR	C32-C1-C6	8.38	123.45	110.30
26	T	101	BCR	C19-C18-C17	8.44	132.58	118.98
35	B	624	HTG	C1'-S1-C1	8.46	111.96	100.30
24	D	403	CLA	C2C-C1C-NC	8.48	116.55	110.24
26	B	617	BCR	C11-C12-C13	8.49	151.30	126.32
26	T	101	BCR	C7-C8-C9	8.49	139.16	126.22
26	b	621	BCR	C12-C13-C14	8.52	132.71	118.98
26	H	101	BCR	C7-C8-C9	8.61	139.34	126.22
26	b	620	BCR	C12-C13-C14	8.63	132.88	118.98
26	h	101	BCR	C24-C23-C22	8.63	139.37	126.22
26	c	514	BCR	C11-C10-C9	8.65	139.69	127.20
35	b	630	HTG	C1'-S1-C1	8.66	112.24	100.30
26	H	101	BCR	C12-C13-C14	8.67	132.96	118.98
26	h	101	BCR	C10-C11-C12	8.67	149.57	123.13
26	J	101	BCR	C11-C10-C9	8.73	139.80	127.20
26	B	617	BCR	C23-C22-C21	8.74	133.06	118.98
26	y	101	BCR	C11-C10-C9	8.82	139.94	127.20
26	T	101	BCR	C24-C23-C22	8.83	139.68	126.22
26	K	102	BCR	C19-C18-C17	8.86	133.26	118.98
26	C	514	BCR	C7-C8-C9	8.91	139.79	126.22
26	K	102	BCR	C11-C10-C9	9.00	140.19	127.20
26	d	404	BCR	C10-C11-C12	9.02	150.61	123.13
26	c	514	BCR	C19-C18-C17	9.02	133.52	118.98
26	B	618	BCR	C12-C13-C14	9.04	133.54	118.98
26	B	618	BCR	C11-C12-C13	9.12	153.16	126.32
26	b	621	BCR	C7-C8-C9	9.13	140.13	126.22
26	h	101	BCR	C15-C14-C13	9.14	140.39	127.20
35	d	416	HTG	C1'-S1-C1	9.23	113.02	100.30
35	D	419	HTG	C1'-S1-C1	9.26	113.06	100.30
26	B	618	BCR	C11-C10-C9	9.28	140.60	127.20
26	t	101	BCR	C15-C14-C13	9.29	140.61	127.20
26	b	620	BCR	C7-C8-C9	9.36	140.48	126.22
26	C	514	BCR	C15-C14-C13	9.40	140.78	127.20
26	c	514	BCR	C15-C14-C13	9.41	140.79	127.20
26	B	619	BCR	C11-C10-C9	9.42	140.80	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	622	BCR	C11-C10-C9	9.47	140.87	127.20
26	K	102	BCR	C15-C14-C13	9.56	141.01	127.20
26	y	101	BCR	C19-C18-C17	9.64	134.52	118.98
26	b	621	BCR	C11-C12-C13	9.67	154.79	126.32
26	T	101	BCR	C15-C14-C13	9.77	141.31	127.20
26	B	619	BCR	C7-C8-C9	9.78	141.12	126.22
26	k	101	BCR	C11-C10-C9	9.89	141.48	127.20
26	k	101	BCR	C19-C18-C17	9.94	135.00	118.98
26	H	101	BCR	C15-C14-C13	9.95	141.57	127.20
26	D	406	BCR	C10-C11-C12	9.96	153.49	123.13
26	K	101	BCR	C19-C18-C17	9.98	135.06	118.98
26	b	622	BCR	C7-C8-C9	9.98	141.43	126.22
26	b	621	BCR	C15-C14-C13	10.03	141.68	127.20
26	B	619	BCR	C15-C14-C13	10.05	141.72	127.20
26	b	620	BCR	C11-C12-C13	10.05	155.91	126.32
26	b	622	BCR	C19-C18-C17	10.07	135.20	118.98
26	J	101	BCR	C7-C8-C9	10.07	141.56	126.22
26	c	514	BCR	C7-C8-C9	10.07	141.56	126.22
26	D	406	BCR	C11-C10-C9	10.08	141.76	127.20
26	A	1009	BCR	C15-C14-C13	10.10	141.78	127.20
26	K	102	BCR	C7-C8-C9	10.11	141.62	126.22
26	H	101	BCR	C11-C12-C13	10.11	156.08	126.32
26	b	620	BCR	C11-C10-C9	10.12	141.81	127.20
26	K	101	BCR	C7-C8-C9	10.14	141.67	126.22
26	b	622	BCR	C15-C14-C13	10.16	141.87	127.20
26	d	404	BCR	C15-C14-C13	10.19	141.91	127.20
26	b	620	BCR	C19-C18-C17	10.24	135.49	118.98
26	h	101	BCR	C19-C18-C17	10.26	135.51	118.98
26	T	101	BCR	C11-C10-C9	10.26	142.02	127.20
26	T	101	BCR	C11-C12-C13	10.28	156.58	126.32
26	b	620	BCR	C20-C19-C18	10.29	156.60	126.32
26	c	514	BCR	C11-C12-C13	10.32	156.70	126.32
26	t	101	BCR	C7-C8-C9	10.34	141.98	126.22
26	B	618	BCR	C15-C14-C13	10.38	142.19	127.20
26	B	619	BCR	C20-C19-C18	10.41	156.95	126.32
26	h	101	BCR	C11-C12-C13	10.41	156.97	126.32
26	h	101	BCR	C11-C10-C9	10.43	142.26	127.20
26	b	620	BCR	C15-C14-C13	10.47	142.32	127.20
26	D	406	BCR	C11-C12-C13	10.48	157.16	126.32
26	A	1009	BCR	C11-C12-C13	10.49	157.19	126.32
26	K	101	BCR	C11-C10-C9	10.50	142.36	127.20
26	B	618	BCR	C10-C11-C12	10.51	155.16	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	BCR	C20-C19-C18	10.55	157.38	126.32
26	d	404	BCR	C7-C8-C9	10.56	142.31	126.22
26	A	1009	BCR	C11-C10-C9	10.58	142.48	127.20
26	B	617	BCR	C10-C11-C12	10.71	155.77	123.13
26	b	621	BCR	C20-C19-C18	10.72	157.88	126.32
26	C	514	BCR	C11-C12-C13	10.72	157.88	126.32
26	k	101	BCR	C15-C14-C13	10.80	142.80	127.20
26	t	101	BCR	C19-C18-C17	10.82	136.42	118.98
26	a	413	BCR	C7-C8-C9	10.84	142.74	126.22
26	J	101	BCR	C19-C18-C17	10.87	136.50	118.98
26	a	413	BCR	C11-C12-C13	10.89	158.38	126.32
26	A	1009	BCR	C7-C8-C9	10.89	142.82	126.22
26	k	101	BCR	C20-C19-C18	10.93	158.50	126.32
26	T	101	BCR	C10-C11-C12	10.98	156.60	123.13
26	b	620	BCR	C10-C11-C12	11.00	156.66	123.13
26	y	101	BCR	C10-C11-C12	11.08	156.89	123.13
26	B	618	BCR	C20-C19-C18	11.09	158.96	126.32
26	B	617	BCR	C20-C19-C18	11.12	159.04	126.32
26	B	618	BCR	C7-C8-C9	11.12	143.17	126.22
26	J	101	BCR	C20-C19-C18	11.17	159.21	126.32
26	d	404	BCR	C20-C19-C18	11.24	159.40	126.32
26	k	101	BCR	C7-C8-C9	11.27	143.40	126.22
26	D	406	BCR	C7-C8-C9	11.29	143.42	126.22
26	C	514	BCR	C11-C10-C9	11.35	143.59	127.20
26	b	621	BCR	C19-C18-C17	11.36	137.28	118.98
26	H	101	BCR	C19-C18-C17	11.37	137.30	118.98
26	K	102	BCR	C11-C12-C13	11.47	160.07	126.32
26	k	101	BCR	C11-C12-C13	11.47	160.09	126.32
26	y	101	BCR	C11-C12-C13	11.48	160.11	126.32
26	A	1009	BCR	C10-C11-C12	11.51	158.21	123.13
26	b	622	BCR	C10-C11-C12	11.53	158.28	123.13
26	k	102	BCR	C20-C19-C18	11.54	160.27	126.32
26	d	404	BCR	C11-C12-C13	11.55	160.31	126.32
26	B	619	BCR	C19-C18-C17	11.61	137.69	118.98
26	C	514	BCR	C20-C19-C18	11.64	160.58	126.32
26	D	406	BCR	C15-C14-C13	11.66	144.04	127.20
26	b	622	BCR	C11-C12-C13	11.67	160.68	126.32
26	t	101	BCR	C20-C19-C18	11.70	160.77	126.32
26	B	617	BCR	C11-C10-C9	11.74	144.15	127.20
26	b	622	BCR	C20-C19-C18	11.75	160.91	126.32
26	D	406	BCR	C19-C18-C17	11.79	137.98	118.98
26	T	101	BCR	C20-C19-C18	11.85	161.21	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	101	BCR	C20-C19-C18	11.90	161.35	126.32
26	a	413	BCR	C20-C19-C18	12.00	161.64	126.32
26	B	617	BCR	C15-C14-C13	12.03	144.57	127.20
26	B	618	BCR	C19-C18-C17	12.14	138.55	118.98
26	H	101	BCR	C11-C10-C9	12.21	144.83	127.20
26	J	101	BCR	C10-C11-C12	12.23	160.42	123.13
26	b	621	BCR	C10-C11-C12	12.35	160.78	123.13
26	H	101	BCR	C20-C19-C18	12.43	162.91	126.32
26	B	619	BCR	C11-C12-C13	12.44	162.94	126.32
26	B	617	BCR	C19-C18-C17	12.54	139.19	118.98
26	k	102	BCR	C11-C12-C13	12.58	163.35	126.32
26	a	413	BCR	C15-C14-C13	12.70	145.54	127.20
26	K	101	BCR	C10-C11-C12	12.75	162.00	123.13
26	c	514	BCR	C10-C11-C12	12.81	162.17	123.13
26	h	101	BCR	C20-C19-C18	12.85	164.13	126.32
26	K	101	BCR	C15-C14-C13	12.86	145.77	127.20
26	K	101	BCR	C11-C12-C13	12.88	164.22	126.32
26	K	102	BCR	C20-C19-C18	12.94	164.41	126.32
26	A	1009	BCR	C20-C19-C18	12.94	164.41	126.32
26	a	413	BCR	C11-C10-C9	12.95	145.91	127.20
26	a	413	BCR	C19-C18-C17	12.95	139.85	118.98
26	A	1009	BCR	C19-C18-C17	13.02	139.97	118.98
26	c	514	BCR	C20-C19-C18	13.03	164.66	126.32
26	y	101	BCR	C20-C19-C18	13.04	164.70	126.32
26	b	621	BCR	C11-C10-C9	13.12	146.15	127.20
26	t	101	BCR	C10-C11-C12	13.18	163.31	123.13
26	J	101	BCR	C11-C12-C13	13.32	165.52	126.32
26	k	101	BCR	C10-C11-C12	13.34	163.80	123.13
26	t	101	BCR	C11-C12-C13	13.37	165.68	126.32
26	B	619	BCR	C10-C11-C12	13.46	164.16	123.13
26	C	514	BCR	C10-C11-C12	13.53	164.38	123.13
26	y	101	BCR	C7-C8-C9	13.73	147.14	126.22
26	a	413	BCR	C10-C11-C12	13.84	165.31	123.13
26	K	102	BCR	C10-C11-C12	14.05	165.95	123.13
26	b	620	BCR	C21-C20-C19	14.19	166.39	123.13
26	t	101	BCR	C21-C20-C19	14.43	167.12	123.13
26	k	102	BCR	C7-C8-C9	14.60	148.46	126.22
26	D	406	BCR	C16-C15-C14	14.75	156.00	123.39
26	b	622	BCR	C21-C20-C19	14.90	168.54	123.13
26	D	406	BCR	C21-C20-C19	14.91	168.57	123.13
26	k	102	BCR	C10-C11-C12	14.96	168.72	123.13
26	A	1009	BCR	C21-C20-C19	15.36	169.96	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	617	BCR	C21-C20-C19	15.38	170.02	123.13
26	C	514	BCR	C21-C20-C19	15.81	171.32	123.13
26	k	102	BCR	C21-C20-C19	16.02	171.96	123.13
26	B	619	BCR	C21-C20-C19	16.06	172.09	123.13
26	d	404	BCR	C21-C20-C19	16.13	172.31	123.13
26	a	413	BCR	C21-C20-C19	16.18	172.44	123.13
26	b	621	BCR	C21-C20-C19	16.19	172.49	123.13
26	b	621	BCR	C16-C15-C14	16.37	159.58	123.39
26	c	514	BCR	C21-C20-C19	16.41	173.15	123.13
26	J	101	BCR	C21-C20-C19	16.53	173.53	123.13
26	T	101	BCR	C21-C20-C19	16.73	174.13	123.13
26	K	101	BCR	C21-C20-C19	17.00	174.96	123.13
26	h	101	BCR	C21-C20-C19	17.13	175.34	123.13
26	b	620	BCR	C16-C15-C14	17.26	161.56	123.39
26	H	101	BCR	C21-C20-C19	17.27	175.76	123.13
26	A	1009	BCR	C16-C15-C14	17.38	161.83	123.39
26	B	618	BCR	C21-C20-C19	17.41	176.20	123.13
26	H	101	BCR	C16-C15-C14	17.46	161.99	123.39
26	k	101	BCR	C21-C20-C19	17.75	177.23	123.13
26	B	619	BCR	C16-C15-C14	17.99	163.17	123.39
26	K	102	BCR	C21-C20-C19	18.00	178.01	123.13
26	K	101	BCR	C16-C15-C14	18.11	163.44	123.39
26	B	618	BCR	C16-C15-C14	18.13	163.48	123.39
26	k	102	BCR	C16-C15-C14	18.17	163.56	123.39
26	y	101	BCR	C21-C20-C19	18.24	178.74	123.13
26	A	1009	BCR	C15-C16-C17	18.38	164.03	123.39
26	h	101	BCR	C16-C15-C14	18.47	164.24	123.39
26	B	617	BCR	C16-C15-C14	18.52	164.35	123.39
26	a	413	BCR	C16-C15-C14	18.76	164.87	123.39
26	k	101	BCR	C16-C15-C14	18.98	165.36	123.39
26	J	101	BCR	C16-C15-C14	19.00	165.41	123.39
26	y	101	BCR	C16-C15-C14	19.01	165.43	123.39
26	c	514	BCR	C16-C15-C14	19.21	165.86	123.39
26	t	101	BCR	C16-C15-C14	19.56	166.63	123.39
26	d	404	BCR	C16-C15-C14	19.69	166.94	123.39
26	T	101	BCR	C16-C17-C18	19.90	155.94	127.20
26	b	622	BCR	C16-C17-C18	20.14	156.28	127.20
26	K	101	BCR	C15-C16-C17	20.15	167.94	123.39
26	B	619	BCR	C16-C17-C18	20.34	156.57	127.20
26	K	102	BCR	C16-C15-C14	20.35	168.38	123.39
26	B	617	BCR	C15-C16-C17	20.38	168.46	123.39
26	d	404	BCR	C16-C17-C18	20.41	156.68	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	514	BCR	C16-C17-C18	20.64	157.00	127.20
26	B	619	BCR	C15-C16-C17	20.67	169.09	123.39
26	C	514	BCR	C16-C15-C14	20.72	169.22	123.39
26	D	406	BCR	C15-C16-C17	20.75	169.28	123.39
26	A	1009	BCR	C16-C17-C18	20.79	157.22	127.20
26	K	101	BCR	C16-C17-C18	20.90	157.38	127.20
26	t	101	BCR	C16-C17-C18	20.99	157.52	127.20
26	T	101	BCR	C16-C15-C14	21.13	170.11	123.39
26	b	622	BCR	C16-C15-C14	21.15	170.15	123.39
26	B	618	BCR	C15-C16-C17	21.16	170.19	123.39
26	b	620	BCR	C15-C16-C17	21.25	170.39	123.39
26	t	101	BCR	C15-C16-C17	21.47	170.87	123.39
26	a	413	BCR	C15-C16-C17	21.51	170.97	123.39
26	b	620	BCR	C16-C17-C18	21.54	158.31	127.20
26	K	102	BCR	C16-C17-C18	21.65	158.46	127.20
26	a	413	BCR	C20-C21-C22	21.69	158.52	127.20
26	B	617	BCR	C16-C17-C18	22.25	159.34	127.20
26	T	101	BCR	C15-C16-C17	22.40	172.93	123.39
26	b	621	BCR	C15-C16-C17	22.41	172.95	123.39
26	K	101	BCR	C20-C21-C22	22.48	159.66	127.20
26	H	101	BCR	C15-C16-C17	22.56	173.27	123.39
26	h	101	BCR	C15-C16-C17	22.66	173.49	123.39
26	B	618	BCR	C16-C17-C18	23.14	160.62	127.20
26	k	102	BCR	C15-C16-C17	23.15	174.58	123.39
26	D	406	BCR	C16-C17-C18	23.35	160.92	127.20
26	J	101	BCR	C15-C16-C17	23.41	175.15	123.39
26	k	101	BCR	C20-C21-C22	23.46	161.08	127.20
26	b	622	BCR	C15-C16-C17	23.61	175.61	123.39
26	H	101	BCR	C16-C17-C18	23.65	161.35	127.20
26	y	101	BCR	C15-C16-C17	23.68	175.76	123.39
26	D	406	BCR	C20-C21-C22	23.81	161.59	127.20
26	T	101	BCR	C20-C21-C22	23.94	161.78	127.20
26	k	102	BCR	C16-C17-C18	23.96	161.80	127.20
26	b	622	BCR	C20-C21-C22	24.01	161.88	127.20
26	d	404	BCR	C15-C16-C17	24.07	176.62	123.39
26	k	101	BCR	C16-C17-C18	24.14	162.07	127.20
26	a	413	BCR	C16-C17-C18	24.27	162.26	127.20
26	K	102	BCR	C15-C16-C17	24.29	177.10	123.39
26	C	514	BCR	C15-C16-C17	24.35	177.23	123.39
26	t	101	BCR	C20-C21-C22	24.46	162.52	127.20
26	c	514	BCR	C15-C16-C17	24.48	177.52	123.39
26	B	619	BCR	C20-C21-C22	24.61	162.75	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	621	BCR	C16-C17-C18	24.68	162.84	127.20
26	k	102	BCR	C20-C21-C22	24.88	163.13	127.20
26	H	101	BCR	C20-C21-C22	24.93	163.20	127.20
26	h	101	BCR	C16-C17-C18	25.01	163.32	127.20
26	K	102	BCR	C20-C21-C22	25.01	163.32	127.20
26	k	101	BCR	C15-C16-C17	25.07	178.83	123.39
26	C	514	BCR	C20-C21-C22	25.14	163.51	127.20
26	B	617	BCR	C20-C21-C22	25.42	163.91	127.20
26	J	101	BCR	C20-C21-C22	25.75	164.40	127.20
26	d	404	BCR	C20-C21-C22	25.77	164.42	127.20
26	b	620	BCR	C20-C21-C22	25.94	164.67	127.20
26	c	514	BCR	C20-C21-C22	26.13	164.94	127.20
26	B	618	BCR	C20-C21-C22	26.16	164.98	127.20
26	y	101	BCR	C16-C17-C18	26.38	165.30	127.20
26	h	101	BCR	C20-C21-C22	26.43	165.37	127.20
26	b	621	BCR	C20-C21-C22	26.72	165.78	127.20
26	c	514	BCR	C16-C17-C18	26.75	165.84	127.20
26	y	101	BCR	C20-C21-C22	26.95	166.12	127.20
26	J	101	BCR	C16-C17-C18	27.78	167.31	127.20
26	A	1009	BCR	C20-C21-C22	27.83	167.39	127.20

All (166) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	503	CLA	NC
24	C	503	CLA	NA
24	B	612	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND
24	c	502	CLA	NA
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	A	1005	CLA	NC
24	A	1005	CLA	ND
24	A	1005	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	ND
24	C	504	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	b	607	CLA	NA

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Mol	Chain	Res	Type	Atom
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	a	408	CLA	NA
24	B	601	CLA	NC
24	B	601	CLA	ND
24	B	601	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	b	608	CLA	NC
24	b	608	CLA	ND
24	b	608	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA
24	c	501	CLA	NC
24	c	501	CLA	ND
24	c	501	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	NA
24	c	512	CLA	ND
24	b	614	CLA	NC
24	B	608	CLA	NC
24	c	513	CLA	NC
24	d	403	CLA	NC
24	d	403	CLA	NA
24	A	1006	CLA	NC
24	A	1006	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	613	CLA	NA
24	c	503	CLA	NC
24	a	409	CLA	NC
24	a	409	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	B	602	CLA	NA
24	c	507	CLA	NC
24	c	507	CLA	ND
24	c	507	CLA	NA
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	A	1008	CLA	NC
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	NA
24	C	512	CLA	ND
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	c	505	CLA	ND
24	c	505	CLA	NA
24	b	615	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	c	511	CLA	NC
24	c	511	CLA	NA
24	C	502	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA
24	a	407	CLA	NC
24	a	407	CLA	ND

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Mol	Chain	Res	Type	Atom
24	a	407	CLA	NA
24	C	501	CLA	NC
24	C	501	CLA	ND
24	C	501	CLA	NA
24	D	402	CLA	ND
24	D	402	CLA	NA
24	C	505	CLA	ND
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	604	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	B	610	CLA	NA
24	c	504	CLA	NC
24	c	504	CLA	NA
24	c	510	CLA	NC
24	c	510	CLA	ND
24	c	510	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	NA
24	B	609	CLA	NC
24	B	609	CLA	ND
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	603	CLA	NA
24	b	611	CLA	NC
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	606	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	b	609	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	D	405	CLA	NC

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Mol	Chain	Res	Type	Atom
24	D	405	CLA	NA
24	d	402	CLA	ND
24	b	618	CLA	NC
24	b	618	CLA	ND
24	b	618	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND
24	B	616	CLA	NA
24	C	507	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	511	CLA	NC
24	C	511	CLA	NA
24	b	619	CLA	NC
24	b	619	CLA	ND
24	b	619	CLA	NA
24	D	403	CLA	NA
24	b	604	CLA	NA
24	a	412	CLA	NC
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	y	101	BCR	C21-C20-C19-C18
26	H	101	BCR	C21-C20-C19-C18
26	b	622	BCR	C17-C16-C15-C14
26	H	101	BCR	C17-C16-C15-C14
26	k	102	BCR	C21-C20-C19-C18
26	c	514	BCR	C21-C20-C19-C18
26	A	1009	BCR	C21-C20-C19-C18
26	K	102	BCR	C21-C20-C19-C18
28	b	623[B]	SQD	C45-O47-C7-C8
28	B	620[A]	SQD	C45-O47-C7-O49
28	B	620[A]	SQD	C45-O47-C7-C8

There are no ring outliers.

71 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1005	CLA	5	0
24	A	1006	CLA	2	0
25	A	1007	PHO	1	0
24	A	1008	CLA	3	0
27	A	1010	PL9	5	0
28	A	1011	SQD	2	0
28	A	1016	SQD	1	0
32	A	1017	LMT	2	0
32	A	1018	LMT	1	0
24	B	601	CLA	1	0
24	B	603	CLA	2	0
24	B	604	CLA	5	0
24	B	605	CLA	7	0
24	B	606	CLA	6	0
24	B	607	CLA	7	0
24	B	608	CLA	4	0
24	B	609	CLA	2	0
24	B	610	CLA	4	0
24	B	611	CLA	4	0
24	B	612	CLA	4	0
24	B	613	CLA	7	0
24	B	614	CLA	3	0
24	B	615	CLA	6	0
24	B	616	CLA	5	0
26	B	617	BCR	1	0
26	B	618	BCR	1	0
28	B	620[A]	SQD	9	0
28	B	620[B]	SQD	12	0
34	B	621	LHG	1	0
29	B	622	LMG	2	0
35	B	629	HTG	1	0
33	B	631	GOL	1	0
30	B	634	DMS	2	0
24	C	501	CLA	3	0
24	C	502	CLA	4	0
24	C	503	CLA	3	0
24	C	504	CLA	4	0
24	C	505	CLA	6	0
24	C	506	CLA	5	0
24	C	507	CLA	5	0
24	C	508	CLA	3	0
24	C	509	CLA	2	0
24	C	510	CLA	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	511	CLA	3	0
24	C	512	CLA	5	0
24	C	513	CLA	2	0
26	C	514	BCR	3	0
36	C	515	DGD	3	0
36	C	516	DGD	1	0
36	C	517	DGD	1	0
29	C	519	LMG	2	0
24	D	402	CLA	4	0
24	D	403	CLA	4	0
25	D	404	PHO	4	0
24	D	405	CLA	1	0
26	D	406	BCR	1	0
28	D	408	SQD	1	0
34	D	409	LHG	4	0
34	D	410	LHG	1	0
34	D	411	LHG	8	0
29	D	412	LMG	1	0
35	D	413	HTG	1	0
34	E	101	LHG	3	0
38	F	101	HEM	3	0
36	H	102	DGD	3	0
26	J	101	BCR	1	0
26	K	102	BCR	2	0
32	M	101	LMT	2	0
32	M	102	LMT	1	0
38	V	201	HEM	8	0
29	Z	101	LMG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	334/334 (100%)	-0.69	5 (1%) 76 81	19, 25, 44, 64	0
1	a	334/334 (100%)	-0.55	7 (2%) 67 72	21, 28, 51, 72	0
2	B	505/505 (100%)	-0.49	15 (2%) 54 62	20, 29, 50, 69	0
2	b	505/505 (100%)	-0.30	26 (5%) 32 40	21, 31, 59, 88	0
3	C	451/451 (100%)	-0.50	5 (1%) 82 86	22, 33, 47, 72	0
3	c	450/451 (99%)	-0.34	8 (1%) 71 76	26, 38, 51, 68	0
4	D	342/342 (100%)	-0.67	4 (1%) 81 85	18, 26, 39, 88	0
4	d	342/342 (100%)	-0.63	4 (1%) 81 85	21, 29, 46, 80	0
5	E	80/80 (100%)	0.29	9 (11%) 7 9	29, 43, 65, 74	0
5	e	78/80 (97%)	0.58	10 (12%) 5 6	35, 47, 68, 75	0
6	F	34/34 (100%)	-0.32	2 (5%) 26 34	29, 34, 55, 67	0
6	f	32/34 (94%)	0.02	3 (9%) 11 14	33, 40, 69, 78	0
7	H	63/63 (100%)	-0.15	2 (3%) 51 60	27, 36, 45, 54	0
7	h	63/63 (100%)	-0.08	3 (4%) 34 43	30, 39, 49, 56	0
8	I	35/36 (97%)	0.02	3 (8%) 13 18	32, 37, 71, 87	0
8	i	35/36 (97%)	0.06	5 (14%) 4 5	32, 37, 71, 92	0
9	J	37/37 (100%)	-0.08	4 (10%) 8 10	28, 37, 84, 92	0
9	j	37/37 (100%)	0.20	4 (10%) 8 10	33, 44, 68, 75	0
10	K	37/37 (100%)	-0.50	0 100 100	33, 38, 50, 52	0
10	k	37/37 (100%)	0.00	1 (2%) 58 65	38, 44, 61, 71	0
11	L	37/37 (100%)	-0.31	4 (10%) 8 10	21, 24, 57, 73	0
11	l	37/37 (100%)	-0.21	3 (8%) 15 20	22, 25, 63, 88	0
12	M	33/34 (97%)	-0.25	2 (6%) 25 33	24, 27, 51, 76	0
12	m	33/34 (97%)	-0.31	3 (9%) 11 16	25, 29, 52, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	244/244 (100%)	0.13	21 (8%) 13 18	20, 37, 68, 88	0
13	o	243/244 (99%)	0.07	21 (8%) 13 18	24, 38, 68, 78	0
14	T	30/31 (96%)	-0.22	2 (6%) 21 28	22, 27, 56, 84	0
14	t	29/31 (93%)	-0.29	2 (6%) 20 27	23, 27, 53, 66	0
15	U	97/97 (100%)	-0.28	1 (1%) 84 87	25, 31, 48, 66	0
15	u	97/97 (100%)	-0.33	3 (3%) 52 61	28, 32, 42, 71	0
16	V	137/137 (100%)	-0.53	1 (0%) 89 91	24, 30, 43, 62	0
16	v	137/137 (100%)	-0.07	6 (4%) 38 47	30, 40, 57, 66	0
17	Y	30/30 (100%)	0.52	3 (10%) 9 13	40, 47, 58, 63	0
17	y	30/30 (100%)	0.71	6 (20%) 1 2	45, 56, 69, 75	0
18	X	40/40 (100%)	0.26	5 (12%) 5 7	33, 40, 65, 80	0
18	x	39/40 (97%)	0.43	6 (15%) 3 4	38, 47, 76, 83	0
19	Z	61/62 (98%)	0.59	12 (19%) 1 2	37, 45, 77, 86	0
19	z	61/62 (98%)	1.11	15 (24%) 1 1	49, 59, 90, 96	0
20	R	34/34 (100%)	4.14	30 (88%) 0 0	71, 86, 100, 101	0
All	All	5280/5296 (99%)	-0.27	266 (5%) 32 41	18, 33, 61, 101	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	9.0
19	z	62	VAL	8.5
18	x	2	THR	7.8
20	R	18	TRP	7.6
3	C	23	ALA	7.5
20	R	6	LEU	7.1
18	X	41	LEU	7.0
11	l	1	MET	7.0
20	R	28	VAL	6.7
14	T	30	THR	6.7
2	b	85	GLY	6.6
7	H	64	ALA	6.5
1	a	11	ALA	6.4
2	b	503	THR	6.3
8	I	36	ASP	6.3
19	Z	31	GLN	6.2
2	b	486	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
20	R	16	ALA	6.2
19	z	31	GLN	6.2
13	O	60	ARG	6.1
12	M	33	GLN	6.1
20	R	13	LEU	6.1
18	X	2	THR	6.1
20	R	20	VAL	6.1
13	o	4	THR	5.9
12	M	34	LYS	5.9
7	h	64	ALA	5.8
20	R	35	LEU	5.8
18	x	40	SER	5.8
20	R	25	PRO	5.7
4	D	11	GLU	5.7
6	f	14	PRO	5.7
9	J	4	GLU	5.7
19	z	3	ILE	5.7
2	b	495	PHE	5.5
1	A	11	ALA	5.5
5	e	61	ARG	5.5
20	R	32	GLN	5.4
13	o	35	SER	5.3
14	T	31	LYS	5.3
8	i	36	ASP	5.3
13	O	61	GLN	5.3
9	J	5	GLY	5.3
2	b	84	THR	5.3
2	b	506	LYS	5.2
17	y	18	VAL	5.1
13	O	3	GLN	5.1
20	R	3	TRP	5.1
13	o	246	ALA	5.1
15	u	8	GLU	5.1
19	z	32	ASP	5.0
19	z	61	VAL	5.0
20	R	26	TYR	5.0
2	b	127	ARG	4.9
11	L	1	MET	4.9
16	v	16	GLY	4.8
17	y	19	ILE	4.8
20	R	10	LEU	4.8
12	m	33	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
2	b	86	ILE	4.8
20	R	14	LEU	4.7
2	B	86	ILE	4.7
13	O	4	THR	4.7
19	z	60	PHE	4.7
20	R	24	LEU	4.7
20	R	31	VAL	4.7
17	Y	19	ILE	4.6
19	Z	32	ASP	4.6
18	x	38	GLN	4.6
13	o	62	GLU	4.5
2	b	484	PRO	4.5
11	l	2	GLU	4.5
9	j	6	GLY	4.5
14	t	29	ILE	4.5
6	F	12	SER	4.5
2	B	85	GLY	4.4
13	o	36	GLN	4.4
8	I	34	ARG	4.3
14	t	30	THR	4.3
9	j	4	GLU	4.3
20	R	29	LYS	4.2
5	E	61	ARG	4.2
19	Z	62	VAL	4.2
19	Z	30	PRO	4.2
13	O	246	ALA	4.2
5	E	83	LEU	4.1
8	i	35	LYS	4.1
17	y	41	VAL	4.1
3	C	24	THR	4.1
2	b	502	VAL	4.1
13	O	35	SER	4.1
11	l	3	PRO	4.1
4	d	11	GLU	4.1
2	B	485	GLU	4.0
20	R	17	GLY	4.0
1	A	13	LEU	4.0
2	b	485	GLU	4.0
3	c	207	ARG	4.0
13	O	62	GLU	4.0
9	j	5	GLY	3.9
20	R	33	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
2	b	87	ASP	3.9
19	z	35	ARG	3.9
20	R	21	ARG	3.9
20	R	23	ILE	3.8
2	b	295	GLY	3.8
19	Z	7	LEU	3.8
12	m	34	LYS	3.8
11	L	2	GLU	3.8
19	Z	34	ASP	3.8
13	o	207	ARG	3.7
20	R	27	ALA	3.7
19	Z	33	TRP	3.7
20	R	15	ALA	3.7
20	R	12	VAL	3.7
5	e	59	GLU	3.7
15	U	8	GLU	3.6
5	e	25	ILE	3.6
20	R	34	LEU	3.6
13	o	58	ASN	3.6
6	f	15	ILE	3.5
5	E	82	GLN	3.5
13	O	36	GLN	3.5
5	E	81	GLU	3.5
4	D	240	ALA	3.5
9	J	6	GLY	3.5
9	J	7	ARG	3.4
13	o	23	ASP	3.4
13	o	5	LEU	3.4
19	z	34	ASP	3.4
3	C	145	SER	3.4
20	R	2	ASP	3.4
13	O	89	SER	3.3
13	o	61	GLN	3.3
18	X	40	SER	3.3
4	D	12	ARG	3.3
1	A	262	TYR	3.3
9	j	7	ARG	3.3
19	Z	60	PHE	3.3
2	b	129	GLY	3.3
20	R	9	LEU	3.3
3	C	207	ARG	3.3
13	O	132	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
5	e	71	GLU	3.2
1	a	235	TYR	3.2
13	o	25	THR	3.2
19	Z	3	ILE	3.2
6	f	16	PHE	3.2
2	B	506	LYS	3.2
3	c	143	TYR	3.2
13	O	130	GLN	3.1
2	b	128	THR	3.1
13	o	130	GLN	3.1
1	a	262	TYR	3.1
2	B	127[A]	ARG	3.1
13	O	85	LEU	3.1
13	o	60	ARG	3.1
4	d	240	ALA	3.0
3	c	24	THR	3.0
13	O	58	ASN	3.0
17	y	43	ARG	3.0
2	B	486	LEU	3.0
19	z	38	GLN	3.0
8	I	35	LYS	2.9
19	Z	41	PHE	2.9
2	B	295	GLY	2.9
2	b	218	LEU	2.9
3	c	257	PHE	2.9
19	z	2	THR	2.9
5	e	81	GLU	2.9
13	O	207	ARG	2.9
16	v	106	ASN	2.9
17	Y	18	VAL	2.9
4	d	236	ASN	2.9
1	A	16	ARG	2.8
17	Y	43	ARG	2.8
19	Z	35	ARG	2.8
2	b	493	TRP	2.8
8	i	34	ARG	2.8
5	E	4	THR	2.8
2	B	293	ALA	2.8
4	D	238	THR	2.8
18	x	34	ILE	2.8
13	o	34	SER	2.7
17	y	20	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
5	e	82	GLN	2.7
19	z	30	PRO	2.7
20	R	5	VAL	2.7
20	R	30	GLN	2.7
2	b	487	SER	2.7
5	E	74	GLN	2.7
19	z	33	TRP	2.7
13	o	24	ASP	2.7
3	C	191	PRO	2.7
19	Z	42	LEU	2.6
5	e	83	LEU	2.6
2	B	373	LYS	2.6
13	O	25	THR	2.6
7	h	57	GLY	2.6
16	v	17	LYS	2.6
2	b	489	GLU	2.6
11	L	7	ARG	2.6
18	X	38	GLN	2.6
3	c	182	PHE	2.5
3	c	253	LEU	2.5
10	k	13	GLU	2.5
18	X	3	ILE	2.5
2	B	505	ARG	2.5
16	v	96	ARG	2.5
11	L	3	PRO	2.5
13	O	90	ASP	2.5
1	a	229	GLU	2.5
1	a	242	GLU	2.4
5	E	71	GLU	2.4
7	H	6	TRP	2.5
2	B	495	PHE	2.4
12	m	5	GLN	2.4
3	c	233	VAL	2.4
13	O	139	SER	2.4
4	d	238	THR	2.4
16	v	14	SER	2.4
13	O	24	ASP	2.4
18	x	37	VAL	2.3
15	u	66	GLY	2.3
13	o	21	THR	2.3
1	A	12	ASN	2.3
19	z	41	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	a	225	ARG	2.3
1	a	13	LEU	2.3
2	B	489[A]	GLU	2.3
20	R	19	ALA	2.3
5	E	76	VAL	2.3
19	z	59	PHE	2.3
13	o	64	GLU	2.3
16	v	27	LEU	2.3
13	O	206	GLY	2.2
2	b	130[A]	GLU	2.2
13	O	37	THR	2.2
2	b	294	SER	2.2
2	b	505[A]	ARG	2.2
20	R	22	ASN	2.2
5	E	17	VAL	2.2
17	y	17	GLU	2.1
18	x	3	ILE	2.1
13	O	23	ASP	2.1
2	B	84	THR	2.1
13	o	134	THR	2.1
19	z	42	LEU	2.1
6	F	44	GLN	2.1
2	B	435[A]	GLU	2.1
2	b	483	ASP	2.1
5	e	32	ILE	2.1
8	i	2	GLU	2.1
3	c	181	PHE	2.1
13	o	98	GLU	2.1
16	V	16	GLY	2.1
7	h	6	TRP	2.1
2	B	374	ASN	2.1
2	b	373	LYS	2.0
15	u	70	ARG	2.0
5	e	74	GLN	2.0
5	e	79	PHE	2.0
2	b	293	ALA	2.0
13	o	181	GLU	2.0
13	o	89	SER	2.0
8	i	33	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
19	FME	Z	1	10/11	0.75	0.23	-	69,71,74,78	0
8	FME	I	1	10/11	0.97	0.07	-	34,39,40,40	0
12	FME	m	1	10/11	0.92	0.12	-	35,38,49,54	0
14	FME	T	1	10/11	0.95	0.09	-	27,29,44,46	0
8	FME	i	1	10/11	0.95	0.08	-	36,38,40,40	0
19	FME	z	1	10/11	0.71	0.34	-	87,91,94,95	0
12	FME	M	1	10/11	0.91	0.12	-	33,36,43,49	0
14	FME	t	1	10/11	0.89	0.14	-	28,30,46,49	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
32	LMT	a	402	35/35	0.50	0.31	15.44	52,65,69,70	0
32	LMT	A	1017	35/35	0.62	0.31	13.83	54,72,75,80	0
35	HTG	D	413	19/19	0.53	0.31	12.19	69,80,85,86	0
33	GOL	V	206	6/6	0.84	0.29	9.13	53,56,57,58	0
32	LMT	b	631	35/35	0.59	0.28	8.96	40,74,94,96	0
30	DMS	O	302	4/4	0.94	0.27	8.95	58,59,62,62	0
32	LMT	t	103	35/35	0.53	0.30	8.91	46,75,96,99	0
35	HTG	o	301	19/19	0.80	0.18	8.17	47,49,53,53	0
32	LMT	f	103	35/35	0.59	0.35	7.27	71,92,104,104	0
32	LMT	A	1018	35/35	0.24	0.44	7.08	51,93,113,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	DMS	D	416	4/4	0.91	0.26	6.94	55,55,56,59	0
31	UNL	t	102	16/-	0.74	0.18	6.66	68,72,74,74	0
28	SQD	a	401	54/54	0.84	0.16	6.43	42,60,74,76	0
27	PL9	a	414	55/55	0.80	0.21	5.54	53,63,77,78	0
28	SQD	b	623[A]	54/54	0.75	0.25	5.33	41,53,70,71	54
31	UNL	D	414	40/-	0.64	0.24	5.17	48,58,72,73	0
31	UNL	b	603	16/-	0.46	0.36	5.08	64,67,71,71	0
30	DMS	O	301	4/4	0.73	0.30	5.05	72,73,75,76	0
30	DMS	A	1014	4/4	0.92	0.20	4.84	54,54,55,61	0
30	DMS	c	529	4/4	0.96	0.20	4.80	51,51,53,54	0
28	SQD	b	623[B]	54/54	0.75	0.25	4.80	49,57,77,80	54
27	PL9	A	1010	55/55	0.82	0.20	4.66	43,55,72,72	0
33	GOL	V	204	6/6	0.70	0.34	4.65	57,58,59,60	0
31	UNL	d	412	16/-	0.89	0.18	4.48	48,53,62,63	0
29	LMG	c	521	51/55	0.57	0.30	4.48	53,81,93,97	0
35	HTG	d	416	19/19	0.69	0.33	4.10	70,92,94,96	0
30	DMS	d	413	4/4	0.88	0.21	4.09	57,62,62,63	0
35	HTG	V	202	19/19	0.81	0.29	4.00	56,63,77,77	0
30	DMS	D	417	4/4	0.91	0.20	3.99	57,58,62,64	0
35	HTG	d	410	19/19	0.58	0.33	3.81	74,84,91,91	0
24	CLA	B	601	65/65	0.84	0.16	3.62	34,42,66,69	0
29	LMG	Z	101	51/55	0.47	0.35	3.58	47,77,104,110	0
32	LMT	i	102	35/35	0.22	0.41	3.54	52,88,111,111	0
30	DMS	c	526	4/4	0.95	0.19	3.54	73,74,74,75	0
35	HTG	b	626	19/19	0.81	0.17	3.49	43,48,51,51	0
29	LMG	B	622	51/55	0.86	0.14	3.48	38,47,58,64	0
30	DMS	b	635	4/4	0.61	0.29	3.47	66,70,72,74	0
31	UNL	D	415	16/-	0.89	0.13	3.39	39,42,48,49	0
34	LHG	e	101	49/49	0.61	0.31	3.38	66,97,101,102	0
30	DMS	B	634	4/4	0.92	0.27	3.34	54,57,59,59	0
35	HTG	C	522	19/19	0.81	0.26	3.33	65,75,80,80	0
34	LHG	D	411	49/49	0.95	0.14	3.29	29,38,73,76	0
29	LMG	D	412	51/55	0.90	0.15	3.28	27,38,77,78	0
31	UNL	l	101	16/-	0.80	0.21	3.14	49,58,68,69	0
34	LHG	d	408	49/49	0.93	0.15	3.13	32,41,72,74	0
36	DGD	C	516	62/66	0.92	0.10	3.06	28,36,70,72	0
30	DMS	b	634	4/4	0.70	0.25	3.04	61,63,65,68	0
29	LMG	d	409	51/55	0.86	0.16	3.01	33,42,72,76	0
32	LMT	a	416	35/35	0.79	0.32	3.01	73,75,79,79	0
28	SQD	B	620[A]	54/54	0.78	0.24	2.92	42,56,75,76	54
31	UNL	K	103	34/-	0.57	0.24	2.90	57,76,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	LMG	A	1012	51/55	0.83	0.17	2.90	49,56,67,71	0
30	DMS	C	524	4/4	0.97	0.17	2.83	40,41,41,42	0
31	UNL	x	101	16/-	0.78	0.17	2.78	41,45,59,60	0
30	DMS	B	632	4/4	0.97	0.18	2.72	57,58,60,61	0
29	LMG	C	519	51/55	0.73	0.28	2.71	38,74,84,85	0
31	UNL	B	630	16/-	0.81	0.24	2.68	53,56,60,60	0
24	CLA	a	409	65/65	0.94	0.12	2.60	24,26,85,90	0
31	UNL	c	523	32/-	0.64	0.30	2.59	63,75,84,87	0
31	UNL	I	101	13/-	0.81	0.27	2.59	54,56,56,57	0
29	LMG	m	102	51/55	0.87	0.13	2.58	35,49,57,59	0
28	SQD	B	620[B]	54/54	0.78	0.24	2.54	40,54,66,66	54
29	LMG	c	519	51/55	0.80	0.18	2.46	45,62,77,80	0
34	LHG	E	101	49/49	0.66	0.26	2.45	51,77,83,85	0
30	DMS	b	629	4/4	0.96	0.12	2.44	48,49,52,53	0
32	LMT	M	101	35/35	0.55	0.29	2.41	52,85,95,97	0
30	DMS	V	203	4/4	0.96	0.14	2.40	50,51,51,52	0
24	CLA	b	604	65/65	0.83	0.17	2.36	40,48,69,70	0
32	LMT	m	103	35/35	0.52	0.29	2.34	55,90,100,101	0
36	DGD	c	516	62/66	0.90	0.12	2.32	36,42,75,79	0
24	CLA	a	412	65/65	0.93	0.15	2.32	26,28,90,92	0
30	DMS	v	202	4/4	0.95	0.14	2.21	55,56,58,58	0
26	BCR	B	618	40/40	0.93	0.09	2.21	27,32,41,41	0
35	HTG	B	628	19/19	0.77	0.20	2.20	45,68,72,74	0
32	LMT	C	520	35/35	0.78	0.27	2.07	68,75,79,79	0
30	DMS	B	627	4/4	0.97	0.09	2.05	41,41,42,44	0
34	LHG	d	406	49/49	0.94	0.13	2.01	38,41,46,46	0
24	CLA	d	403	65/65	0.89	0.14	1.99	31,34,76,77	0
37	BCT	D	401	4/4	0.97	0.16	1.98	37,38,38,41	0
36	DGD	C	515	62/66	0.94	0.11	1.97	27,36,63,64	0
31	UNL	d	411	36/-	0.65	0.21	1.96	46,56,78,79	0
24	CLA	A	1008	65/65	0.93	0.13	1.96	25,27,79,81	0
36	DGD	H	102	62/66	0.93	0.11	1.95	27,34,38,39	0
30	DMS	b	633	4/4	0.87	0.15	1.92	55,55,56,62	0
28	SQD	f	102	43/54	0.78	0.28	1.87	61,80,89,91	0
35	HTG	D	419	19/19	0.62	0.27	1.85	59,79,83,84	0
31	UNL	j	101	16/-	0.68	0.16	1.81	58,60,62,63	0
30	DMS	C	526	4/4	0.91	0.18	1.81	71,71,72,72	0
24	CLA	C	504	65/65	0.94	0.10	1.80	27,30,55,57	0
36	DGD	c	515	62/66	0.93	0.12	1.78	28,38,69,71	0
36	DGD	C	517	62/66	0.94	0.10	1.76	24,33,62,69	0
35	HTG	b	630	19/19	0.59	0.35	1.76	66,83,88,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	UNL	X	101	16/-	0.85	0.14	1.74	39,43,51,51	0
36	DGD	h	102	62/66	0.91	0.11	1.73	32,38,46,48	0
34	LHG	d	407	49/49	0.95	0.11	1.73	26,31,40,45	0
24	CLA	b	612	65/65	0.93	0.13	1.67	30,34,37,38	0
28	SQD	A	1016	54/54	0.82	0.17	1.63	46,60,72,73	0
26	BCR	K	101	40/40	0.91	0.13	1.60	32,35,37,38	0
34	LHG	D	410	49/49	0.96	0.11	1.57	26,30,38,41	0
29	LMG	a	415	51/55	0.81	0.17	1.56	50,60,70,71	0
24	CLA	A	1006	65/65	0.95	0.10	1.56	22,23,66,69	0
36	DGD	c	517	62/66	0.92	0.12	1.54	29,38,64,73	0
25	PHO	a	411	64/64	0.95	0.11	1.51	24,30,35,36	0
28	SQD	A	1011	54/54	0.91	0.15	1.48	43,57,69,69	0
31	UNL	Y	101	16/-	0.58	0.27	1.47	66,68,70,70	0
32	LMT	b	625	35/35	0.53	0.29	1.44	52,82,103,104	0
29	LMG	C	518	51/55	0.83	0.18	1.40	36,62,70,70	0
24	CLA	B	604	65/65	0.96	0.10	1.40	22,24,53,55	0
38	HEM	V	201	43/43	0.98	0.12	1.40	25,26,28,29	0
24	CLA	D	405	65/65	0.92	0.12	1.39	28,30,70,71	0
24	CLA	B	607	65/65	0.96	0.09	1.36	20,22,36,37	0
24	CLA	B	606	65/65	0.92	0.12	1.36	27,30,51,53	0
32	LMT	B	623	35/35	0.70	0.24	1.32	48,65,71,72	0
26	BCR	t	101	40/40	0.93	0.09	1.29	26,39,46,47	0
24	CLA	a	407	65/65	0.97	0.10	1.28	21,23,30,35	0
34	LHG	D	409	49/49	0.94	0.11	1.24	35,38,43,45	0
26	BCR	A	1009	40/40	0.93	0.10	1.21	25,29,32,32	0
24	CLA	A	1005	65/65	0.97	0.10	1.20	17,20,29,33	0
26	BCR	D	406	40/40	0.90	0.11	1.19	28,32,50,51	0
24	CLA	B	616	65/65	0.89	0.16	1.16	27,31,79,80	0
24	CLA	C	512	65/65	0.88	0.13	1.15	39,42,71,72	0
24	CLA	C	513	65/65	0.85	0.15	1.14	41,48,66,68	0
24	CLA	c	509	65/65	0.96	0.11	1.14	33,35,50,51	0
24	CLA	C	509	65/65	0.96	0.10	1.13	28,31,52,53	0
24	CLA	C	508	65/65	0.94	0.10	1.09	28,31,65,70	0
30	DMS	u	201	4/4	0.93	0.24	1.07	56,57,57,59	0
24	CLA	b	619	65/65	0.88	0.15	1.06	31,35,80,81	0
28	SQD	c	518	54/54	0.90	0.14	1.04	41,59,74,76	0
27	PL9	D	407	55/55	0.95	0.09	1.03	21,25,32,33	0
29	LMG	c	520	51/55	0.69	0.26	1.03	42,74,84,89	0
33	GOL	v	203	6/6	0.81	0.20	1.02	48,52,53,53	0
31	UNL	L	101	16/-	0.83	0.21	0.96	53,56,63,63	0
24	CLA	B	613	65/65	0.97	0.08	0.95	23,25,49,53	0
24	CLA	d	402	65/65	0.97	0.10	0.95	21,23,39,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	BCR	K	102	40/40	0.85	0.12	0.88	39,49,52,52	0
24	CLA	c	504	65/65	0.94	0.10	0.85	32,35,57,59	0
26	BCR	d	404	40/40	0.89	0.11	0.84	31,36,59,59	0
24	CLA	C	507	65/65	0.94	0.11	0.82	34,37,51,53	0
24	CLA	C	505	65/65	0.94	0.10	0.81	32,35,44,48	0
24	CLA	b	609	65/65	0.91	0.12	0.80	29,32,65,68	0
24	CLA	c	513	65/65	0.86	0.16	0.79	45,54,69,70	0
24	CLA	c	508	65/65	0.93	0.10	0.77	32,35,65,72	0
30	DMS	V	205	4/4	0.89	0.17	0.73	61,62,64,65	0
28	SQD	D	408	43/54	0.91	0.18	0.71	41,67,74,76	0
24	CLA	b	607	65/65	0.96	0.09	0.71	24,26,50,51	0
24	CLA	B	614	65/65	0.95	0.10	0.70	24,27,67,68	0
24	CLA	c	512	65/65	0.91	0.12	0.67	42,46,65,67	0
27	PL9	d	405	55/55	0.95	0.09	0.67	21,27,32,33	0
24	CLA	b	608	65/65	0.96	0.10	0.66	24,26,35,35	0
26	BCR	b	622	40/40	0.94	0.09	0.66	33,36,40,41	0
26	BCR	k	101	40/40	0.93	0.12	0.65	36,45,47,48	0
24	CLA	b	605	65/65	0.95	0.10	0.56	29,32,37,37	0
24	CLA	c	506	65/65	0.88	0.15	0.54	38,40,78,81	0
26	BCR	k	102	40/40	0.87	0.14	0.53	48,54,64,66	0
24	CLA	b	616	65/65	0.97	0.09	0.53	25,25,50,52	0
24	CLA	C	510	65/65	0.97	0.09	0.53	27,31,38,39	0
24	CLA	B	605	65/65	0.96	0.10	0.52	23,26,31,32	0
38	HEM	f	101	43/43	0.95	0.12	0.50	42,44,57,63	0
32	LMT	m	101	35/35	0.73	0.20	0.50	38,51,56,57	0
26	BCR	a	413	40/40	0.93	0.09	0.50	24,30,34,34	0
24	CLA	c	505	65/65	0.95	0.10	0.49	34,36,48,48	0
24	CLA	b	610	65/65	0.96	0.08	0.47	23,25,34,35	0
26	BCR	B	619	40/40	0.94	0.08	0.46	31,34,42,43	0
26	BCR	J	101	40/40	0.92	0.09	0.46	35,37,41,41	0
24	CLA	D	402	65/65	0.97	0.09	0.44	17,20,35,37	0
24	CLA	B	610	65/65	0.96	0.09	0.44	24,26,34,36	0
24	CLA	c	507	65/65	0.94	0.12	0.43	33,34,50,51	0
24	CLA	B	609	65/65	0.95	0.11	0.43	28,31,33,35	0
24	CLA	b	613	65/65	0.95	0.10	0.40	28,31,38,40	0
24	CLA	a	408	65/65	0.97	0.08	0.38	20,23,31,34	0
24	CLA	b	617	65/65	0.96	0.10	0.38	24,28,67,68	0
24	CLA	B	615	65/65	0.95	0.10	0.37	27,28,44,46	0
24	CLA	C	506	65/65	0.92	0.11	0.36	36,43,73,76	0
24	CLA	D	403	65/65	0.97	0.07	0.35	18,20,29,33	0
34	LHG	b	624	49/49	0.96	0.09	0.32	27,32,48,53	0
26	BCR	b	621	40/40	0.94	0.08	0.32	28,31,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	LHG	B	621	49/49	0.97	0.09	0.32	26,32,45,49	0
25	PHO	D	404	64/64	0.96	0.09	0.31	22,25,29,30	0
26	BCR	T	101	40/40	0.95	0.08	0.30	27,37,42,43	0
33	GOL	V	207	6/6	0.75	0.18	0.28	60,63,64,64	0
24	CLA	b	614	65/65	0.96	0.09	0.26	24,26,40,41	0
32	LMT	M	102	35/35	0.73	0.20	0.26	39,58,64,66	0
35	HTG	b	601	19/19	0.89	0.14	0.23	44,60,67,67	0
30	DMS	d	414	4/4	0.96	0.11	0.23	58,59,59,60	0
24	CLA	B	602	65/65	0.96	0.09	0.21	25,27,34,35	0
26	BCR	C	514	40/40	0.94	0.11	0.18	31,38,41,41	0
31	UNL	y	102	16/-	0.72	0.21	0.18	63,65,67,67	0
24	CLA	C	502	65/65	0.96	0.09	0.15	26,28,42,44	0
26	BCR	c	514	40/40	0.92	0.11	0.10	34,41,43,44	0
24	CLA	B	612	65/65	0.97	0.08	0.08	24,26,30,31	0
24	CLA	c	510	65/65	0.96	0.08	0.08	33,35,41,43	0
30	DMS	U	201	4/4	0.91	0.19	0.07	56,56,58,58	0
24	CLA	c	501	65/65	0.95	0.11	0.06	35,36,43,44	0
30	DMS	B	626	4/4	0.98	0.07	0.05	25,26,26,27	0
25	PHO	A	1007	64/64	0.97	0.08	0.05	21,24,26,28	0
26	BCR	b	620	40/40	0.96	0.09	0.05	28,34,35,35	0
38	HEM	v	201	43/43	0.97	0.10	0.00	31,32,36,37	0
24	CLA	B	611	65/65	0.97	0.09	-0.01	22,24,36,37	0
25	PHO	a	410	64/64	0.97	0.08	-0.03	22,24,29,31	0
24	CLA	b	611	65/65	0.96	0.08	-0.03	26,28,38,39	0
24	CLA	c	503	65/65	0.95	0.09	-0.04	33,39,42,44	0
26	BCR	B	617	40/40	0.95	0.08	-0.05	28,30,33,33	0
24	CLA	b	606	65/65	0.97	0.09	-0.06	26,29,35,39	0
24	CLA	c	502	65/65	0.96	0.09	-0.08	28,31,50,51	0
26	BCR	h	101	40/40	0.90	0.12	-0.10	32,39,47,48	0
24	CLA	B	603	65/65	0.97	0.08	-0.12	25,26,32,34	0
26	BCR	y	101	40/40	0.92	0.09	-0.14	40,44,46,47	0
24	CLA	b	615	65/65	0.95	0.08	-0.15	25,28,32,35	0
30	DMS	b	628	4/4	0.98	0.07	-0.19	30,31,31,32	0
24	CLA	C	511	65/65	0.95	0.10	-0.19	29,35,40,42	0
37	BCT	d	401	4/4	0.96	0.09	-0.22	40,40,41,42	0
26	BCR	H	101	40/40	0.93	0.09	-0.27	27,36,42,42	0
38	HEM	F	101	43/43	0.96	0.11	-0.33	39,41,44,46	0
24	CLA	C	501	65/65	0.96	0.08	-0.43	31,35,41,42	0
24	CLA	c	511	65/65	0.95	0.10	-0.53	36,39,43,46	0
24	CLA	B	608	65/65	0.97	0.08	-0.56	25,27,31,31	0
24	CLA	C	503	65/65	0.96	0.08	-0.58	28,33,36,38	0
24	CLA	b	618	65/65	0.96	0.08	-0.75	30,32,44,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
21	OER	A	1001	10/10	1.00	0.06	-1.06	24,25,28,28	1
22	FE2	a	404	1/1	1.00	0.05	-1.12	29,29,29,29	0
21	OER	a	403	10/10	1.00	0.05	-1.76	27,28,29,31	1
39	MG	j	102	1/1	0.94	0.06	-1.87	37,37,37,37	0
22	FE2	A	1002	1/1	1.00	0.03	-2.03	29,29,29,29	0
23	CL	a	406	1/1	1.00	0.05	-2.03	27,27,27,27	0
39	MG	J	103	1/1	0.98	0.04	-2.30	32,32,32,32	0
23	CL	A	1003	1/1	0.99	0.03	-2.53	25,25,25,25	0
23	CL	a	405	1/1	0.99	0.03	-3.06	26,26,26,26	0
23	CL	A	1004	1/1	1.00	0.02	-3.95	22,22,22,22	0
31	UNL	i	101	16/-	0.69	0.23	-	55,57,62,62	0
30	DMS	B	633	4/4	0.80	0.23	-	67,69,70,75	0
30	DMS	C	527	4/4	0.88	0.26	-	75,75,77,80	0
31	UNL	A	1015	28/-	0.61	0.27	-	62,73,78,78	0
31	UNL	I	102	13/-	0.85	0.14	-	55,57,60,60	0
35	HTG	C	521	19/19	0.85	0.23	-	69,71,74,75	0
33	GOL	B	631	6/6	0.89	0.24	-	56,57,60,62	0
33	GOL	A	1019	6/6	0.86	0.21	-	60,61,62,62	0
35	HTG	c	522	19/19	0.81	0.28	-	82,85,89,90	0
33	GOL	a	420	6/6	0.90	0.15	-	53,56,57,59	0
31	UNL	a	419	30/-	0.62	0.29	-	62,74,87,89	0
30	DMS	a	417	4/4	0.97	0.09	-	31,32,33,33	0
35	HTG	c	525	19/19	0.55	0.36	-	76,90,95,96	0
30	DMS	c	528	4/4	0.84	0.21	-	83,85,86,88	0
31	UNL	B	625	16/-	0.85	0.13	-	44,46,52,54	0
31	UNL	J	102	16/-	0.78	0.16	-	50,52,58,59	0
33	GOL	d	417	6/6	0.59	0.26	-	58,61,62,62	0
35	HTG	b	602	19/19	0.59	0.26	-	60,89,94,94	0
30	DMS	a	418	4/4	0.83	0.20	-	62,63,66,69	0
39	MG	K	104	1/1	0.93	0.08	-	48,48,48,48	0
35	HTG	B	624	19/19	0.53	0.42	-	58,86,92,92	0
30	DMS	c	524	4/4	0.98	0.18	-	43,43,43,43	0
33	GOL	v	204	6/6	0.75	0.24	-	74,75,76,76	0
33	GOL	D	418	6/6	0.46	0.31	-	70,72,73,74	0
30	DMS	C	525	4/4	0.87	0.24	-	71,73,73,74	0
33	GOL	d	415	6/6	0.70	0.20	-	63,66,66,67	0
31	UNL	b	627	16/-	0.79	0.13	-	47,48,50,50	0
39	MG	k	103	1/1	0.97	0.05	-	45,45,45,45	0
30	DMS	c	527	4/4	0.88	0.25	-	65,65,66,66	0
35	HTG	B	629	19/19	0.53	0.28	-	52,86,90,90	0
30	DMS	A	1013	4/4	0.98	0.09	-	29,29,30,31	0
30	DMS	C	523	4/4	0.99	0.10	-	36,37,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
33	GOL	b	632	6/6	0.71	0.26	-	51,56,61,63	0

6.5 Other polymers (i)

There are no such residues in this entry.