Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 09:04 PM GMT

PDB ID	:	4RVY
Title	:	Serial Time resolved crystallography of Photosystem II using a femtosecond X-ray laser. The S state after two flashes (S3)
Authors	:	Kupitz, C.; Basu, S.; Grotjohann, I.; Fromme, R.; Zatsepin, N.; Rendek, K.N.; Hunter, M.; Shoeman, R.L.; White, T.A.; Wang, D.; James, D.; Yang, J.-H.; Cobb, D.E.; Reeder, B.; Sierra, R.G.; Liu, H.; Barty, A.; Aquila, A.; Deponte, D.; Kirian, R.; Bari, S.; Bergkamp, J.J.; Beyerlein, K.; Bogan, M.J.; Caleman, C.; Chao, T.-C.; Conrad, C.E.; Davis, K.M.; Fleckenstein, H.; Galli, L.; Hau-Riege, S.P.; Kassemeyer, S.; Laksmono, H.; Liang, M.; Lomb, L.; Marchesini, S.; Martin, A.V.; Messerschmidt, M.; Milathianaki, D.; Nass, K.; Ros, A.; Roy-Chowdhury, S.; Schmidt, K.; Seibert, M.; Steinbrener, J.; Stellato, F.; Yan, L.; Yoon, C.; Moore, T.A.; Moore, A.L.; Pushkar, Y.; Williams, G.J.; Boutet, S.; Doak, R.B.; Weierstall, U.; Frank, M.; Chapman, H.N.; Spence, J.C.H.; Fromme, P.
Deposited on	:	2014-11-29
Resolution	:	5.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

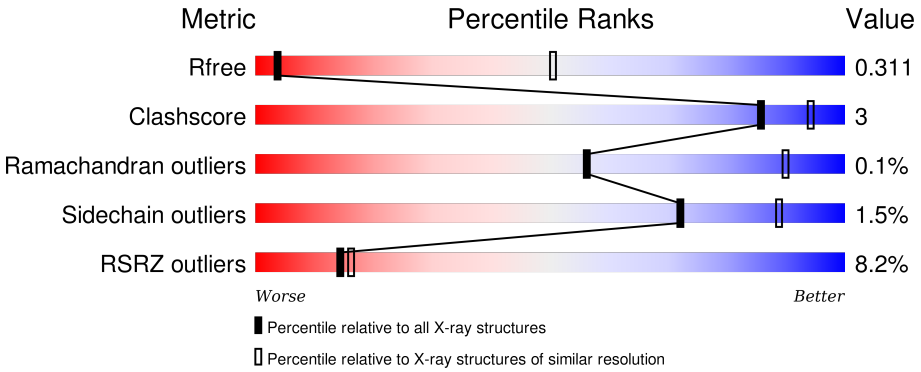
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135

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 5.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (7.38-3.62)
Clashscore	102246	1020 (7.10-3.70)
Ramachandran outliers	100387	1014 (7.36-3.64)
Sidechain outliers	100360	1013 (7.38-3.62)
RSRZ outliers	91569	1014 (7.38-3.62)

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	6% 94% 6%
1	a	334	8% 100%

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CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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Mol	Chain	Length	Quality of chain
2	B	504	6% 91% 9%
2	b	504	14% 99%
3	C	461	9% 92% 6%
3	c	461	8% 97%
4	D	342	10% 93% 6%
4	d	342	7% 99%
5	E	81	12% 94% 6%
5	e	81	11% 99%
6	F	34	3% 85% 15%
6	f	34	97%
7	H	65	14% 91% 8%
7	h	65	28% 95% 5%
8	I	38	13% 87% 11%
8	i	38	8% 97%
9	J	40	8% 93% 5%
9	j	40	95% 5%
10	K	37	5% 89% 8%
10	k	37	11% 95% 5%
11	L	37	5% 86% 11%
11	l	37	8% 95% 5%
12	M	34	18% 74% 26%
12	m	34	9% 97%
13	O	243	3% 91% 8%
13	o	243	6% 98%
14	T	30	10% 73% 23%

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Mol	Chain	Length	Quality of chain
14	t	30	3% 97%
15	U	97	2% 99%
15	u	97	6% 97%
16	V	137	% 95% 5%
16	v	137	4% 99%
17	X	39	18% 92% 8%
17	x	39	18% 100%
18	Y	29	10% 86% 14%
18	y	29	97%
19	Z	62	3% 97%
19	z	62	11% 97%

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
20	OEX	a	601	-	-	-	X
22	CLA	A	603	X	-	-	X
22	CLA	A	604	X	-	-	X
22	CLA	A	607	X	-	-	X
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	X
22	CLA	B	604	X	-	-	X
22	CLA	B	605	X	-	-	X
22	CLA	B	606	X	-	-	X
22	CLA	B	607	X	-	-	X
22	CLA	B	608	X	-	-	X
22	CLA	B	609	X	-	-	X
22	CLA	B	610	X	-	-	X
22	CLA	B	611	X	-	-	X
22	CLA	B	612	X	-	-	X
22	CLA	B	613	X	-	-	X
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	616	X	-	-	X
22	CLA	B	617	X	-	-	X
22	CLA	C	501	X	-	-	X
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	X
22	CLA	C	504	X	-	-	X
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	X
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	X
22	CLA	C	510	X	-	-	X
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	513	X	-	-	X
22	CLA	D	401	X	-	-	X
22	CLA	D	402	X	-	-	X
22	CLA	D	403	X	-	-	X
22	CLA	a	603	X	-	-	X
22	CLA	a	604	X	-	-	X
22	CLA	a	607	X	-	-	X
22	CLA	b	602	X	-	-	X
22	CLA	b	603	X	-	-	X
22	CLA	b	604	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	X
22	CLA	b	611	X	-	-	X
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	X
22	CLA	b	615	X	-	-	X
22	CLA	b	616	X	-	-	X
22	CLA	b	617	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	X
22	CLA	c	505	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	506	X	-	-	X
22	CLA	c	507	X	-	-	X
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	X
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	X
22	CLA	c	512	X	-	-	X
22	CLA	c	513	X	-	-	X
22	CLA	d	401	X	-	-	X
22	CLA	d	402	X	-	-	X
22	CLA	d	403	X	-	-	X
23	PHO	A	605	-	-	-	X
23	PHO	A	606	-	-	-	X
23	PHO	a	605	-	-	-	X
23	PHO	a	606	-	-	-	X
24	BCR	A	608	-	-	-	X
24	BCR	B	622	-	-	-	X
24	BCR	C	514	-	-	-	X
24	BCR	C	515	-	-	-	X
24	BCR	D	404	-	-	-	X
24	BCR	H	101	-	-	-	X
24	BCR	K	101	-	-	-	X
24	BCR	K	102	-	-	-	X
24	BCR	T	102	-	-	-	X
24	BCR	a	608	-	-	-	X
24	BCR	b	618	-	-	-	X
24	BCR	b	622	-	-	-	X
24	BCR	c	514	-	-	-	X
24	BCR	c	515	-	-	-	X
24	BCR	d	404	-	-	-	X
24	BCR	h	101	-	-	-	X
24	BCR	k	101	-	-	-	X
24	BCR	k	102	-	-	-	X
24	BCR	t	101	-	-	-	X
25	SQD	A	609	-	-	-	X
25	SQD	D	411	-	-	-	X
25	SQD	L	101	-	-	-	X
25	SQD	a	609	-	-	-	X
25	SQD	b	601	-	-	-	X
25	SQD	b	621	-	-	-	X
25	SQD	d	411	-	-	-	X
26	CL	A	610	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CL	a	610	-	-	-	X
27	BCT	A	612	-	-	-	X
27	BCT	a	612	-	-	-	X
28	PL9	A	613	-	-	-	X
28	PL9	D	408	-	-	-	X
28	PL9	a	613	-	-	-	X
29	LMG	A	614	-	-	-	X
29	LMG	C	519	-	-	-	X
29	LMG	C	520	-	-	-	X
29	LMG	D	406	-	-	-	X
29	LMG	Z	101	-	-	-	X
29	LMG	a	614	-	-	-	X
29	LMG	c	519	-	-	-	X
29	LMG	c	520	-	-	-	X
29	LMG	d	406	-	-	-	X
29	LMG	z	101	-	-	-	X
31	DGD	C	516	-	-	-	X
31	DGD	C	517	-	-	-	X
31	DGD	C	518	-	-	-	X
31	DGD	D	410	-	-	-	X
31	DGD	H	102	-	-	-	X
31	DGD	c	516	-	-	-	X
31	DGD	c	518	-	-	-	X
31	DGD	d	410	-	-	-	X
31	DGD	h	102	-	-	-	X
32	LHG	D	407	-	-	-	X
32	LHG	D	409	-	-	-	X
32	LHG	E	101	-	-	-	X
32	LHG	d	405	-	-	-	X
32	LHG	d	409	-	-	-	X
32	LHG	e	101	-	-	-	X
33	HEM	F	101	-	-	-	X
33	HEM	V	201	-	-	-	X
33	HEM	f	101	-	-	-	X
33	HEM	v	201	-	-	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 49594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	286	ALA	THR	CONFLICT	UNP P0A444
a	286	ALA	THR	CONFLICT	UNP P0A444

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	13			
3	c	451	Total	C	N	O	S	0	0	0
			3486	2281	584	608	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	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	81	Total	C	N	O	0	0	0
			662	432	107	123			

- 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	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			
8	i	38	Total	C	N	O	S	0	0	0
			312	210	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	38	Total	C	N	O	S	0	0	0
			272	182	42	47	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	0	0
			267	178	40	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			267	178	40	48	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	39	Total 287	C 191	N 46	O 50	0	0	0
17	x	39	Total 287	C 191	N 46	O 50	0	0	0

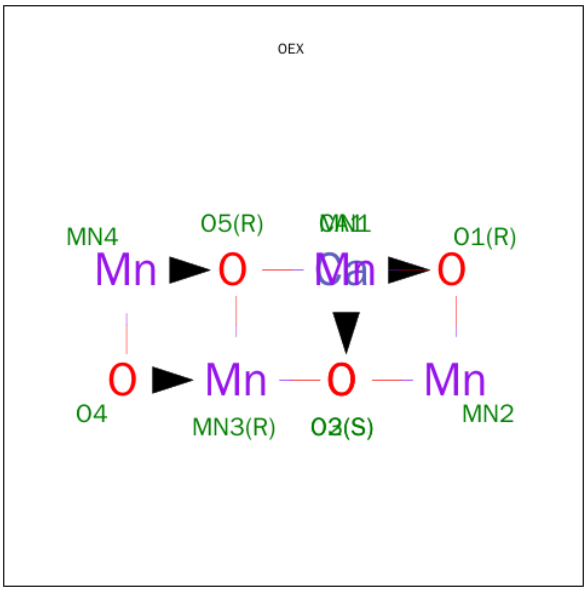
- Molecule 18 is a protein called Photosystem II reaction center protein Ycf12.

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

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

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

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).

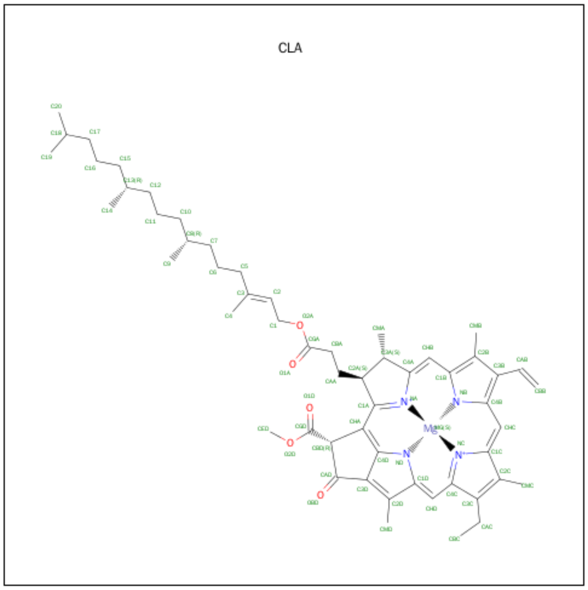


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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

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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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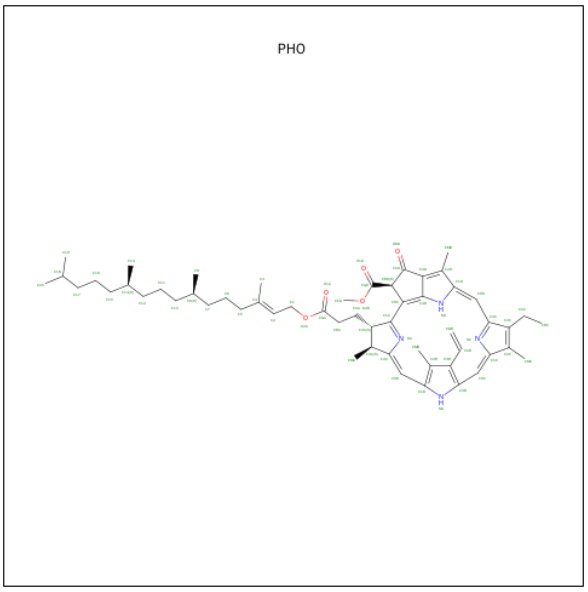
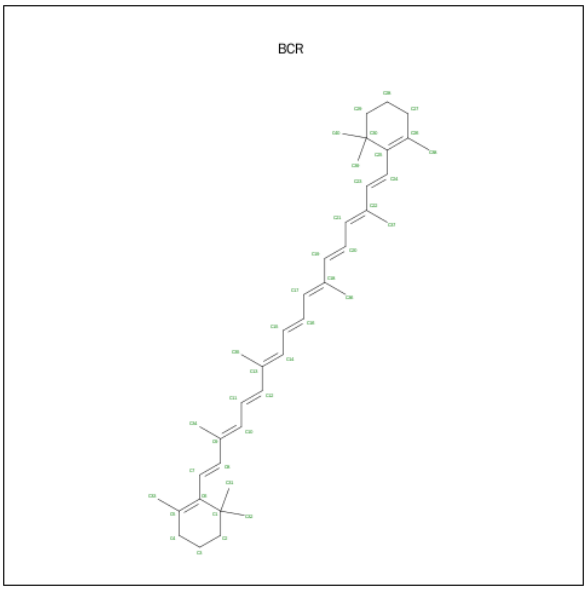
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4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

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



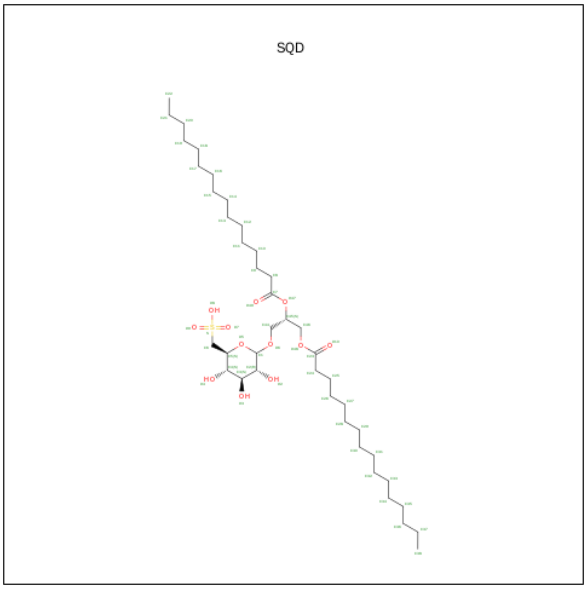
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).

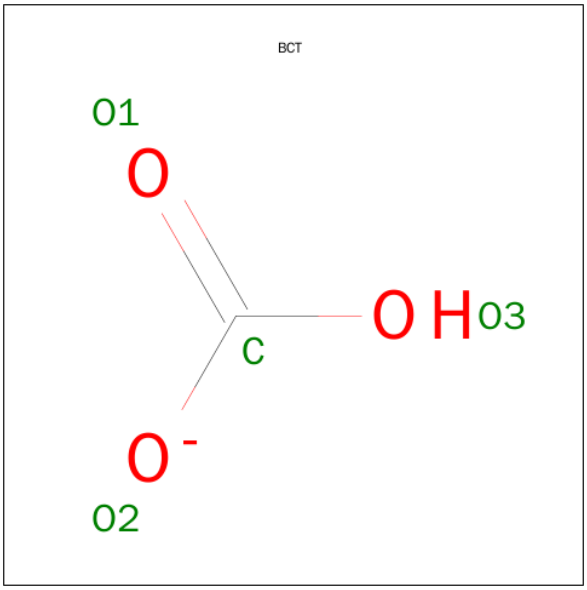


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	O	S	0	0
			54	41	12	1		
25	a	1	Total	C	O	S	0	0
			54	41	12	1		
25	B	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	b	1	Total	C	O	S	0	0
			54	41	12	1		
25	D	1	Total	C	O	S	0	0
			43	30	12	1		
25	d	1	Total	C	O	S	0	0
			43	30	12	1		
25	L	1	Total	C	O	S	0	0
			54	41	12	1		
25	l	1	Total	C	O	S	0	0
			54	41	12	1		
25	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 26 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

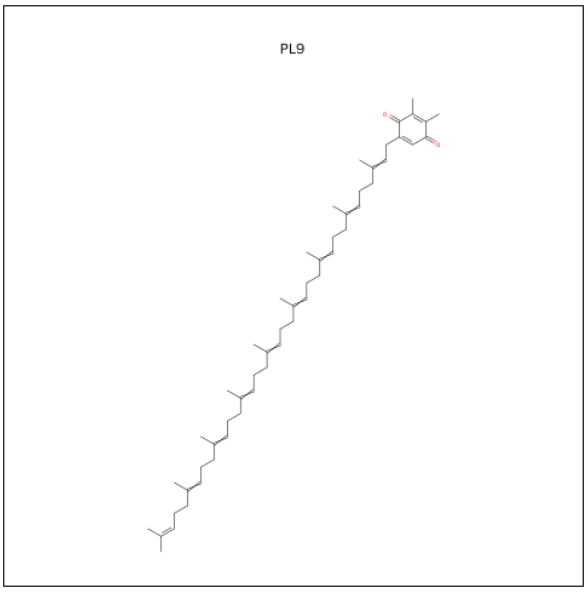
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	2	Total Cl 2 2	0	0
26	u	1	Total Cl 1 1	0	0
26	a	2	Total Cl 2 2	0	0
26	U	1	Total Cl 1 1	0	0

- Molecule 27 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



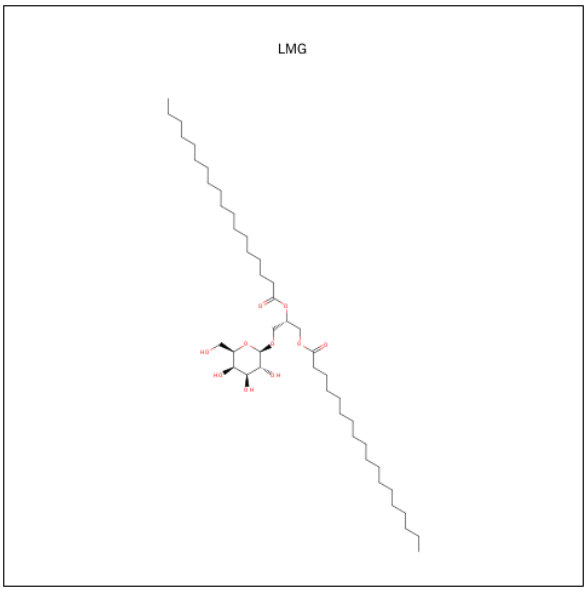
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 4 1 3	0	0
27	a	1	Total C O 4 1 3	0	0

- Molecule 28 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
28	A	1	Total C O 55 53 2	0	0
28	a	1	Total C O 55 53 2	0	0
28	D	1	Total C O 55 53 2	0	0
28	d	1	Total C O 55 53 2	0	0

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

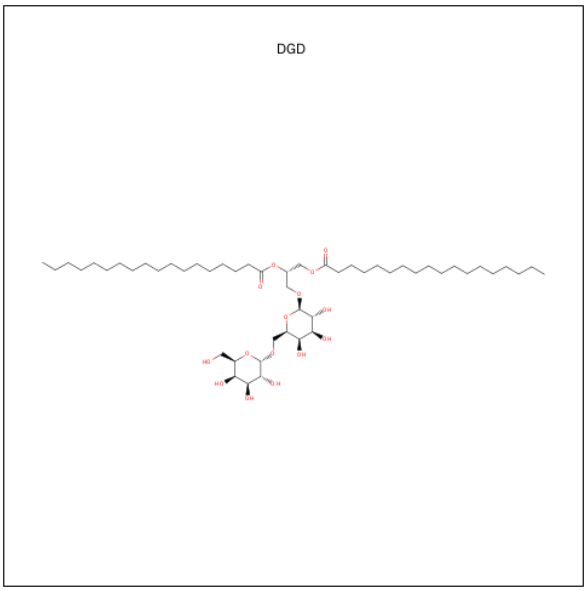


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	a	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	D	1	Total C O 51 41 10	0	0
29	d	1	Total C O 51 41 10	0	0
29	Z	1	Total C O 37 27 10	0	0
29	z	1	Total C O 37 27 10	0	0

- Molecule 30 is CALCIUM ION (three-letter code: CA) (formula: Ca).

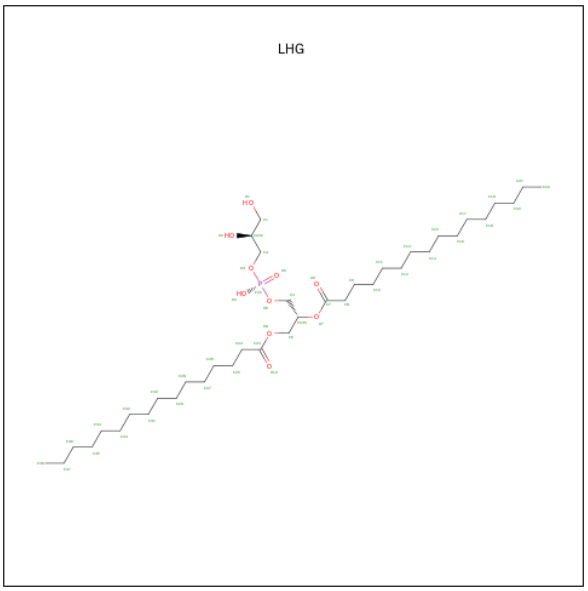
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	B	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



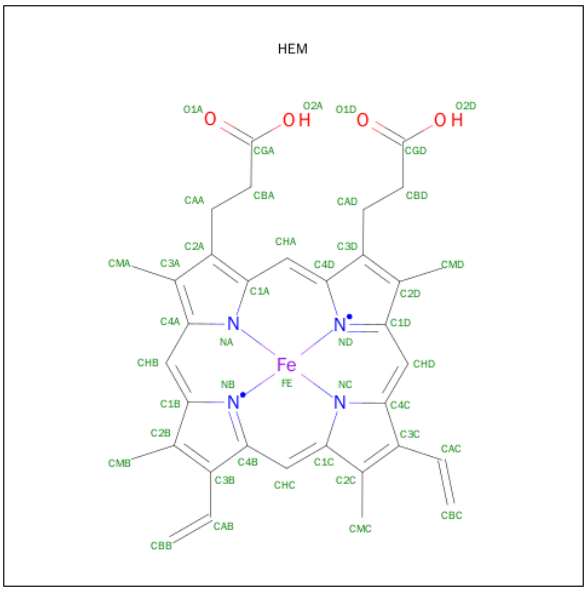
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	C	1	Total C O 62 47 15	0	0
31	C	1	Total C O 62 47 15	0	0
31	C	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	D	1	Total C O 62 47 15	0	0
31	d	1	Total C O 62 47 15	0	0
31	H	1	Total C O 62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

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
33	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
33	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
33	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

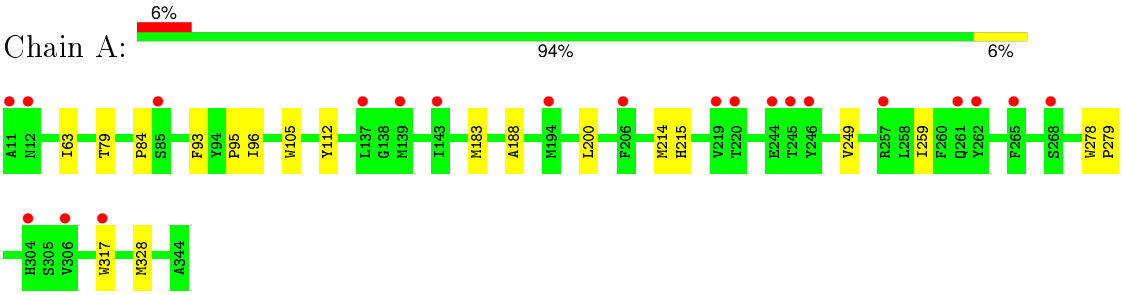
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	1	Total	Mg	0	0
			1	1		
34	j	1	Total	Mg	0	0
			1	1		

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.

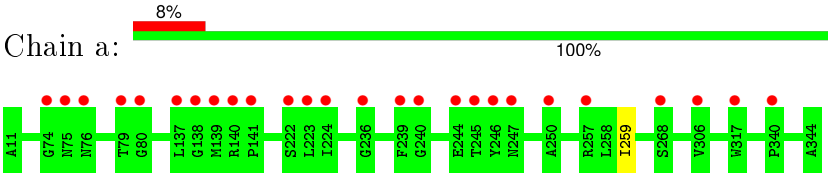
- Molecule 1: Photosystem II protein D1 1

Chain A:



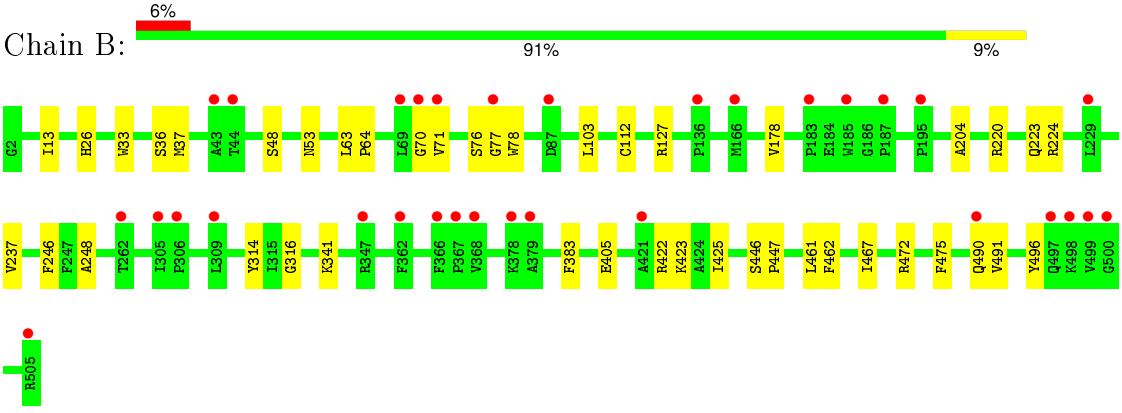
- Molecule 1: Photosystem II protein D1 1

Chain a:



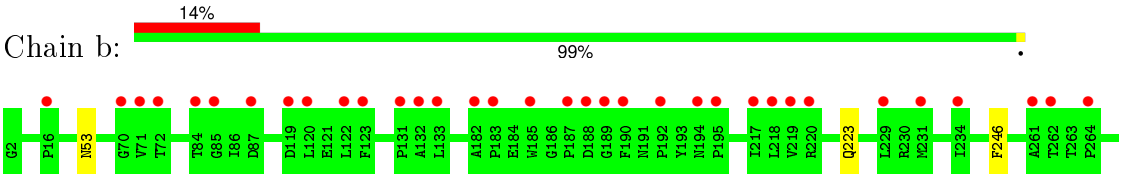
- Molecule 2: Photosystem II CP47 reaction center protein

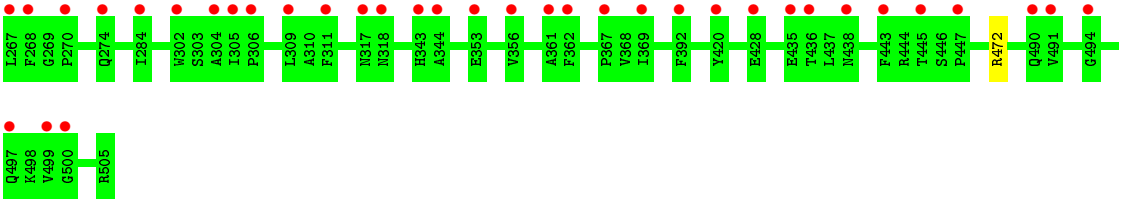
Chain B:



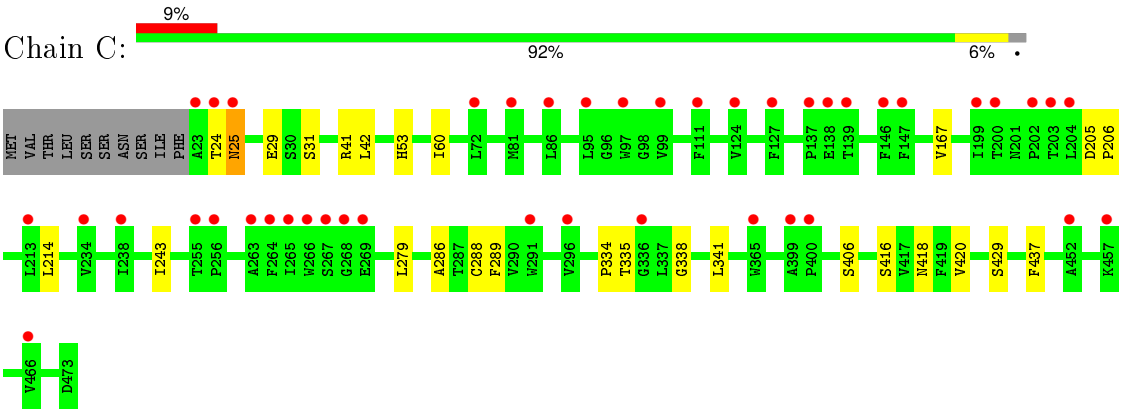
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

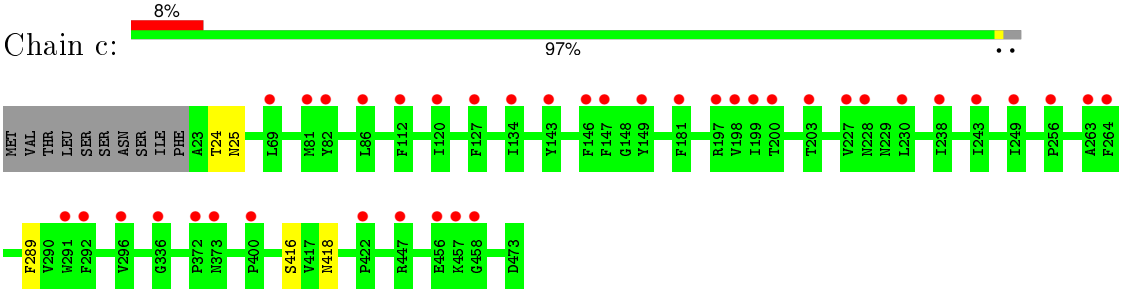




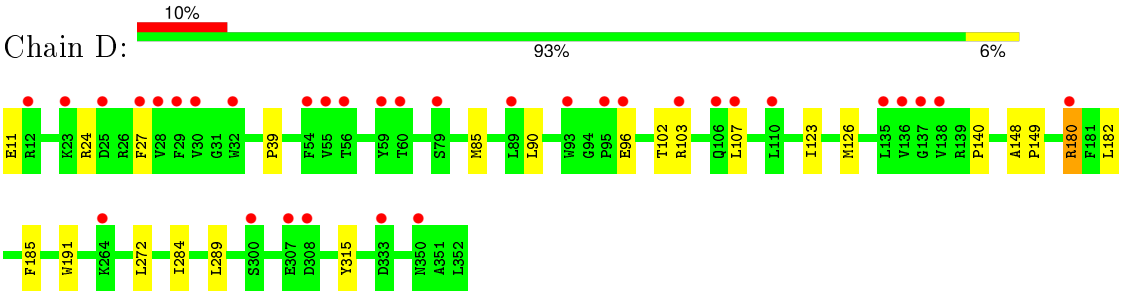
• Molecule 3: Photosystem II CP43 reaction center protein



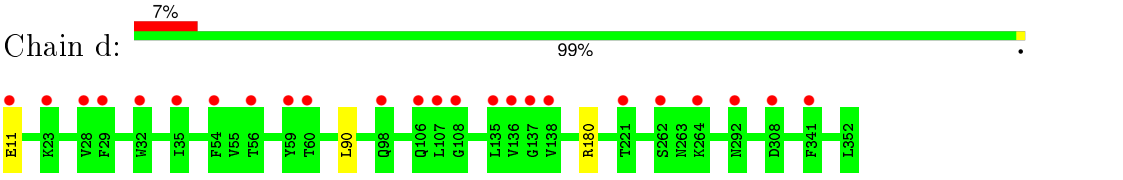
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein

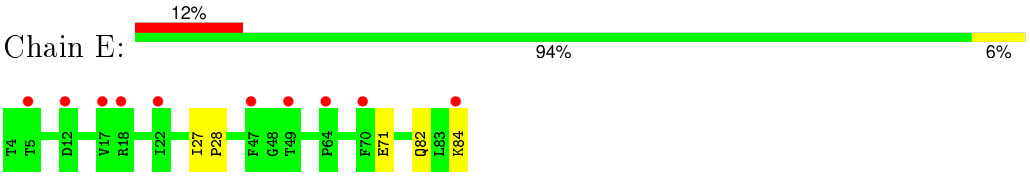


• Molecule 4: Photosystem II D2 protein



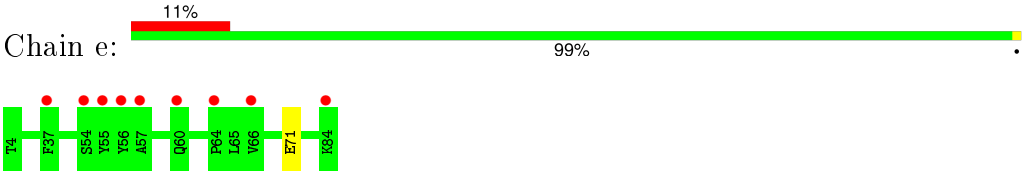
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



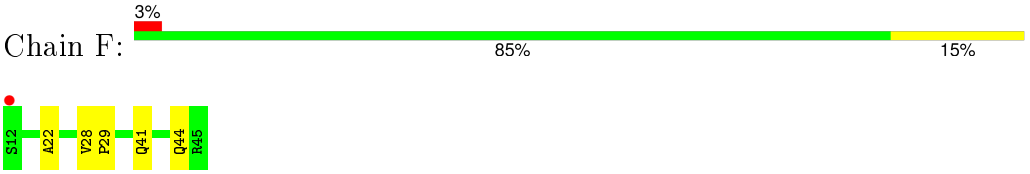
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



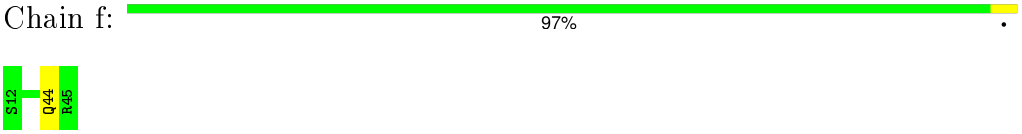
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



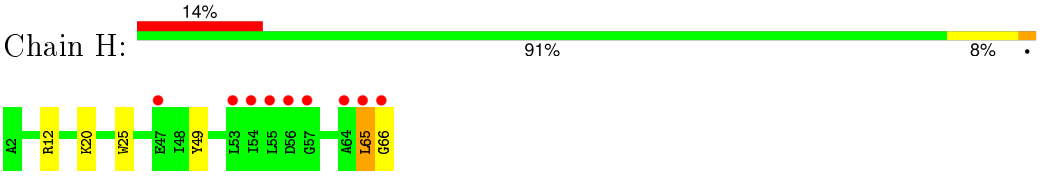
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



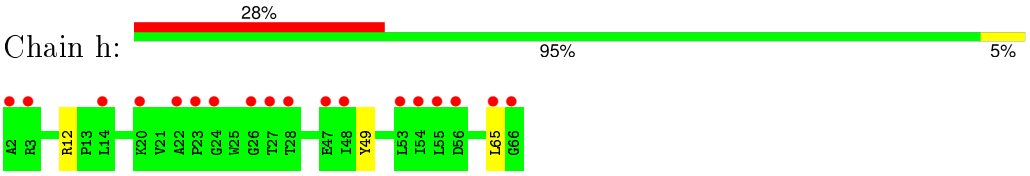
• Molecule 7: Photosystem II reaction center protein H

Chain H:



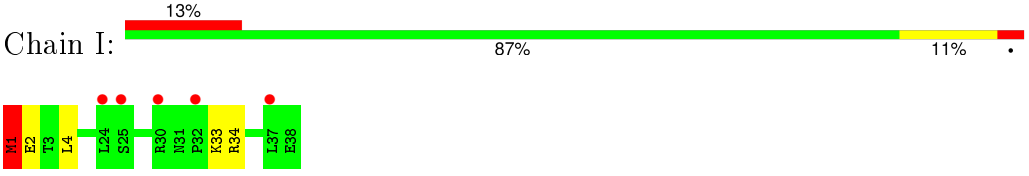
• Molecule 7: Photosystem II reaction center protein H

Chain h:



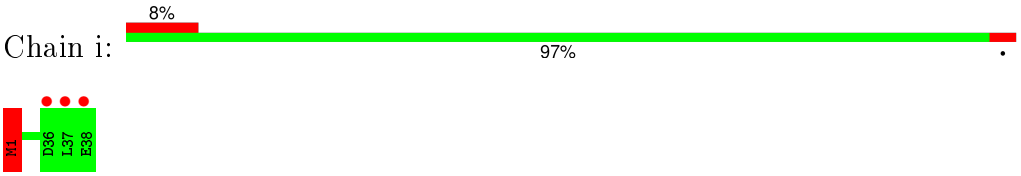
• Molecule 8: Photosystem II reaction center protein I

Chain I:



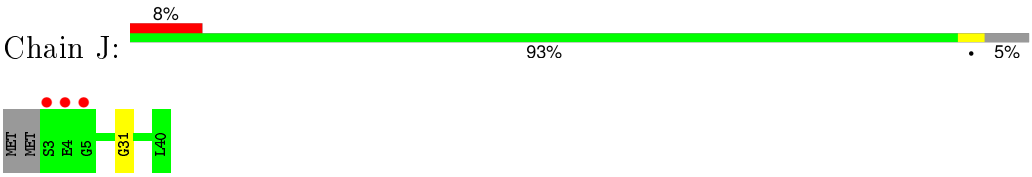
• Molecule 8: Photosystem II reaction center protein I

Chain i:



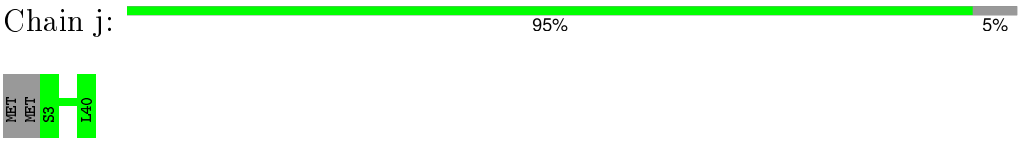
• Molecule 9: Photosystem II reaction center protein J

Chain J:



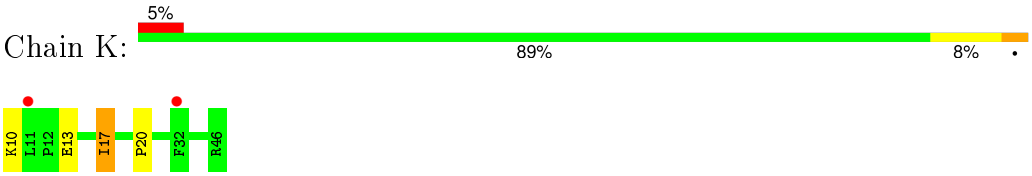
• Molecule 9: Photosystem II reaction center protein J

Chain j:



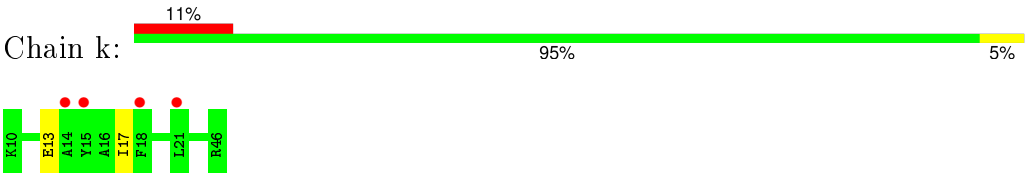
• Molecule 10: Photosystem II reaction center protein K

Chain K:



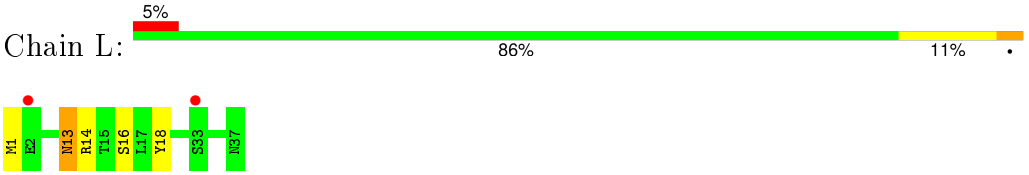
• Molecule 10: Photosystem II reaction center protein K

Chain k:



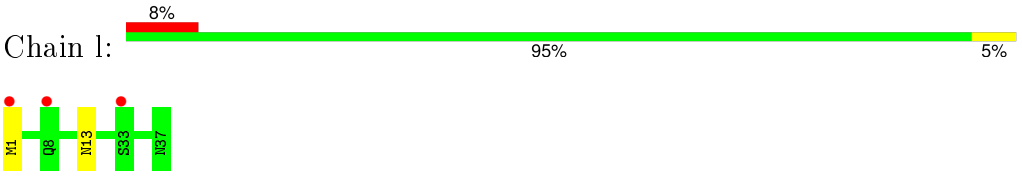
• Molecule 11: Photosystem II reaction center protein L

Chain L:



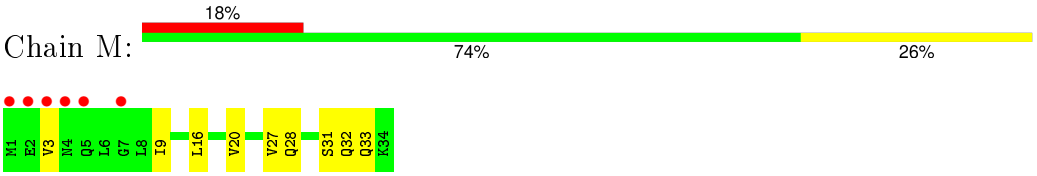
• Molecule 11: Photosystem II reaction center protein L

Chain l:



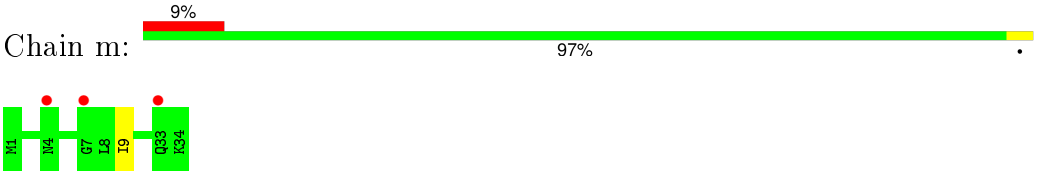
• Molecule 12: Photosystem II reaction center protein M

Chain M:



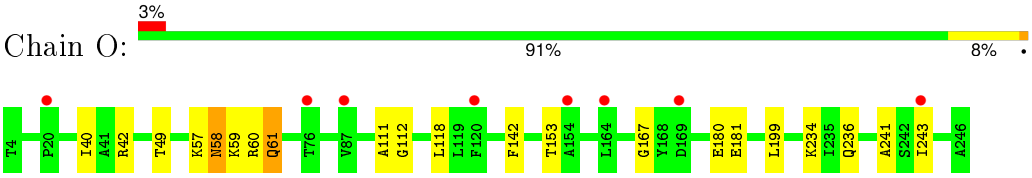
• Molecule 12: Photosystem II reaction center protein M

Chain m:



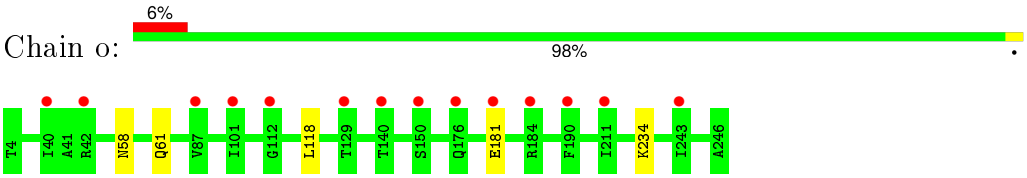
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



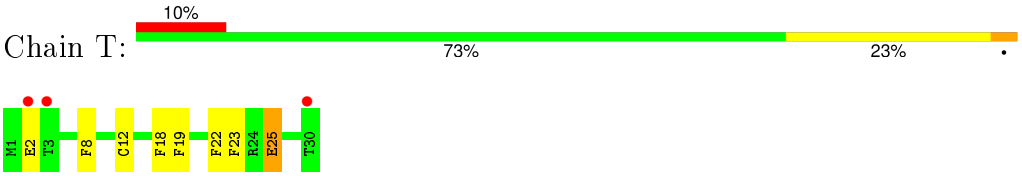
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



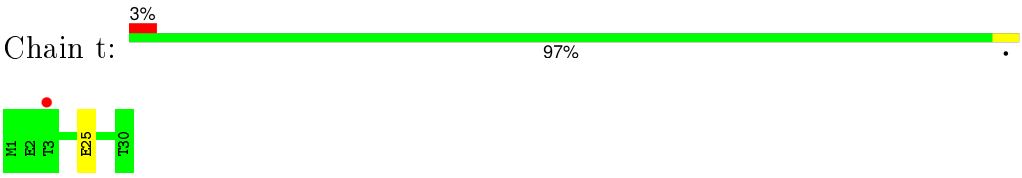
• Molecule 14: Photosystem II reaction center protein T

Chain T:



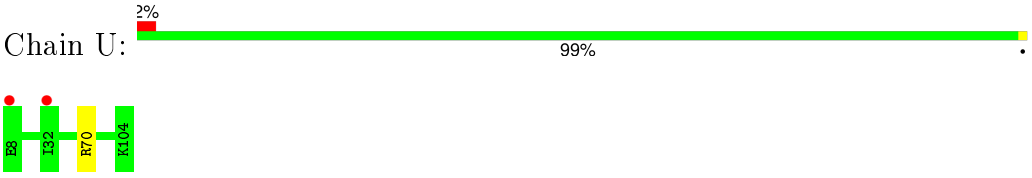
• Molecule 14: Photosystem II reaction center protein T

Chain t:



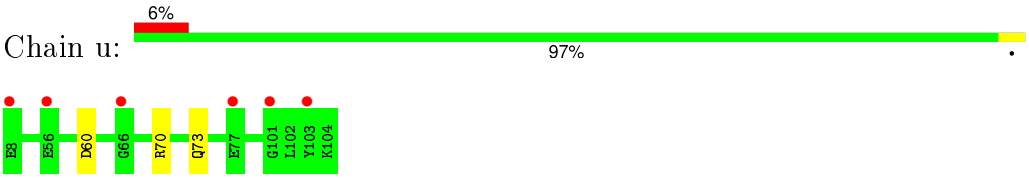
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



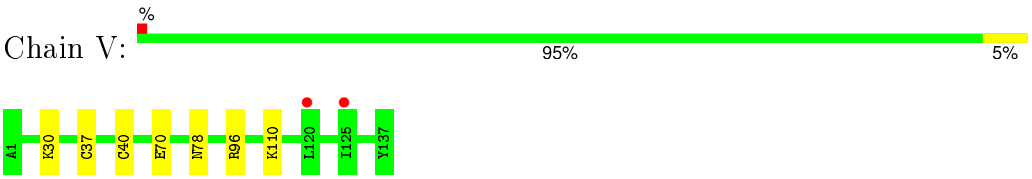
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



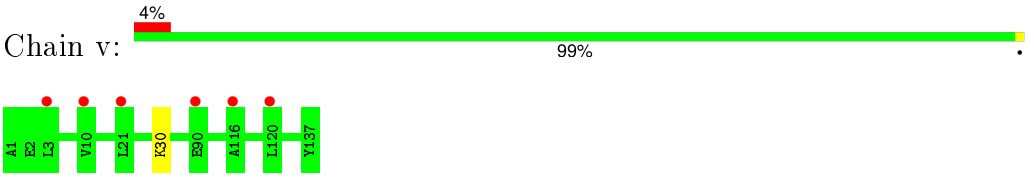
• Molecule 16: Cytochrome c-550

Chain V:



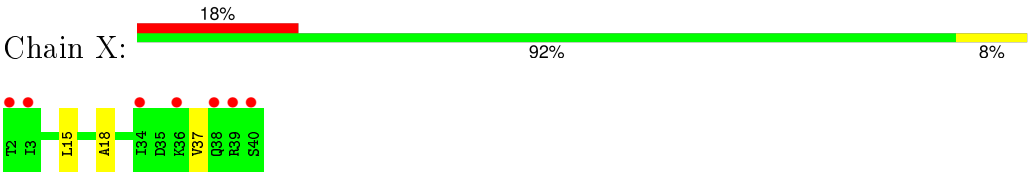
• Molecule 16: Cytochrome c-550

Chain v:



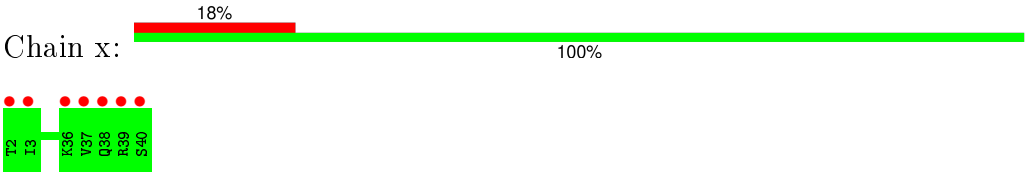
• Molecule 17: Photosystem II reaction center X protein

Chain X:



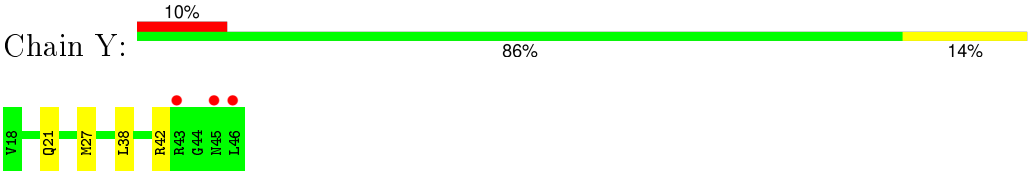
• Molecule 17: Photosystem II reaction center X protein

Chain x:



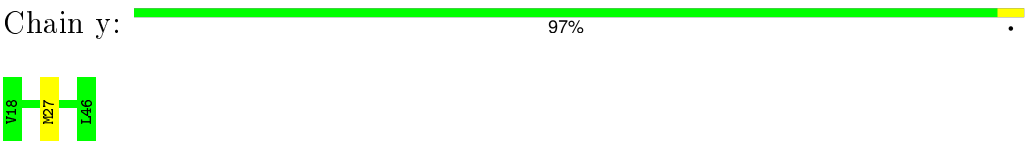
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



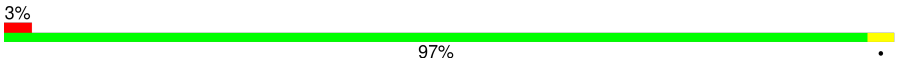
• Molecule 18: Photosystem II reaction center protein Ycf12

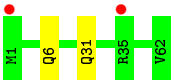
Chain y:



• Molecule 19: Photosystem II reaction center protein Z

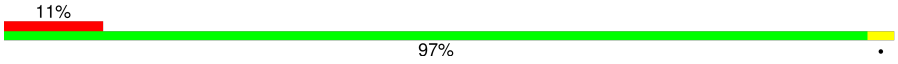
Chain Z:

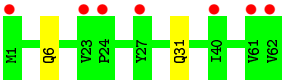




• Molecule 19: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	136.61Å 228.09Å 308.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.30 – 5.50 102.29 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (102.30-5.50) 100.0 (102.29-5.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 5.42Å)	Xtriage
Refinement program	Phenix (phenix.refine: 1.8.2_1336)	Depositor
R, R_{free}	0.281 , 0.291 0.303 , 0.311	Depositor DCC
R_{free} test set	1626 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	357.8	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 32105 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	49594	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, MG, OEX, PHO, DGD, CL, CA, CLA, PL9, FE2, BCT, HEM, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.53	0/2705	0.55	0/3689
1	a	0.53	0/2705	0.55	0/3689
2	B	0.50	0/4109	0.54	0/5600
2	b	0.50	0/4109	0.54	0/5600
3	C	0.46	0/3599	0.51	0/4900
3	c	0.46	0/3599	0.51	0/4900
4	D	0.53	0/2821	0.55	0/3844
4	d	0.53	0/2821	0.55	0/3844
5	E	0.43	0/681	0.51	0/928
5	e	0.43	0/681	0.51	0/928
6	F	0.49	0/284	0.45	0/387
6	f	0.49	0/284	0.45	0/387
7	H	0.47	0/524	0.50	0/713
7	h	0.47	0/524	0.50	0/713
8	I	2.22	2/319 (0.6%)	1.25	4/429 (0.9%)
8	i	2.22	2/319 (0.6%)	1.25	4/429 (0.9%)
9	J	0.46	0/278	0.43	0/376
9	j	0.46	0/278	0.43	0/376
10	K	0.42	0/303	0.50	0/416
10	k	0.43	0/303	0.50	0/416
11	L	0.55	0/311	0.51	0/422
11	l	0.55	0/311	0.51	0/422
12	M	0.47	0/270	0.59	0/367
12	m	0.47	0/270	0.59	0/367
13	O	0.45	0/1896	0.58	0/2571
13	o	0.45	0/1896	0.58	0/2571
14	T	0.53	0/265	0.54	0/359
14	t	0.53	0/265	0.54	0/359
15	U	0.46	0/785	0.55	0/1064
15	u	0.46	0/785	0.55	0/1064
16	V	0.47	0/1085	0.53	0/1473
16	v	0.47	0/1085	0.53	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	X	0.43	0/290	0.47	0/392
17	x	0.43	0/290	0.47	0/392
18	Y	0.41	0/216	0.45	0/289
18	y	0.41	0/216	0.45	0/289
19	Z	0.41	0/490	0.45	0/669
19	z	0.41	0/490	0.45	0/669
All	All	0.55	4/42462 (0.0%)	0.55	8/57776 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	1	1
8	i	1	1
All	All	2	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	MET	N-CA	36.97	2.20	1.46
8	I	1	MET	N-CA	36.95	2.20	1.46
8	I	1	MET	CA-C	12.27	1.84	1.52
8	i	1	MET	CA-C	12.26	1.84	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	i	1	MET	N-CA-CB	-17.88	78.41	110.60
8	I	1	MET	N-CA-CB	-17.86	78.45	110.60
8	I	1	MET	N-CA-C	-12.99	75.92	111.00
8	i	1	MET	N-CA-C	-12.98	75.94	111.00
8	I	1	MET	CA-C-N	-6.32	103.29	117.20
8	i	1	MET	CA-C-N	-6.30	103.33	117.20
8	I	1	MET	CB-CA-C	-6.21	97.97	110.40
8	i	1	MET	CB-CA-C	-6.21	97.97	110.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	I	1	MET	CA

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Mol	Chain	Res	Type	Atom
8	i	1	MET	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	I	1	MET	Mainchain
8	i	1	MET	Mainchain

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	2620	0	2517	16	0
1	a	2620	0	2517	0	0
2	B	3969	0	3828	47	0
2	b	3969	0	3828	0	0
3	C	3486	0	3407	20	0
3	c	3486	0	3407	0	0
4	D	2726	0	2627	21	0
4	d	2726	0	2627	0	0
5	E	662	0	648	3	0
5	e	662	0	648	0	0
6	F	275	0	282	3	0
6	f	275	0	282	0	0
7	H	511	0	532	4	0
7	h	511	0	532	0	0
8	I	312	0	329	16	0
8	i	312	0	329	0	0
9	J	272	0	279	1	0
9	j	272	0	279	0	0
10	K	293	0	305	5	0
10	k	293	0	305	0	0
11	L	304	0	316	6	0
11	l	304	0	316	0	0
12	M	267	0	288	21	0
12	m	267	0	287	0	0
13	O	1865	0	1838	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	o	1865	0	1838	0	0
14	T	256	0	262	12	0
14	t	256	0	262	0	0
15	U	774	0	773	0	0
15	u	774	0	773	0	7
16	V	1064	0	1073	10	7
16	v	1064	0	1073	0	0
17	X	287	0	317	3	0
17	x	287	0	317	0	0
18	Y	215	0	246	2	0
18	y	215	0	246	0	0
19	Z	479	0	516	0	0
19	z	479	0	516	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	195	0	216	10	0
22	B	1040	0	1152	32	0
22	C	845	0	936	29	0
22	D	195	0	216	8	0
22	a	195	0	216	0	0
22	b	1040	0	1152	0	0
22	c	845	0	936	0	0
22	d	195	0	216	0	0
23	A	128	0	148	6	0
23	a	128	0	148	0	0
24	A	40	0	48	1	0
24	B	120	0	140	8	0
24	C	80	0	93	0	0
24	D	40	0	48	3	0
24	H	40	0	46	1	0
24	K	80	0	93	1	0
24	T	80	0	95	9	0
24	a	40	0	48	0	0
24	b	80	0	92	0	0
24	c	80	0	93	0	0
24	d	40	0	48	0	0
24	h	40	0	46	0	0
24	k	80	0	93	0	0
24	t	40	0	47	0	0
25	A	54	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	54	0	78	4	0
25	D	43	0	53	0	0
25	L	54	0	34	5	0
25	a	54	0	78	0	0
25	b	108	0	112	0	0
25	d	43	0	53	0	0
25	l	108	0	59	0	0
26	A	2	0	0	0	0
26	U	1	0	0	0	0
26	a	2	0	0	0	0
26	u	1	0	0	0	0
27	A	4	0	0	0	0
27	a	4	0	0	0	0
28	A	55	0	80	8	0
28	D	55	0	80	0	0
28	a	55	0	80	0	0
28	d	55	0	80	0	0
29	A	51	0	72	3	0
29	B	51	0	72	3	0
29	C	102	0	144	1	0
29	D	51	0	72	2	0
29	Z	37	0	44	1	0
29	a	51	0	72	0	0
29	b	51	0	72	0	0
29	c	102	0	144	0	0
29	d	51	0	72	0	0
29	z	37	0	44	0	0
30	B	1	0	0	0	0
30	F	1	0	0	0	0
30	O	1	0	0	0	0
30	b	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	5	0
31	D	62	0	82	3	0
31	H	62	0	82	1	0
31	c	186	0	246	0	0
31	d	62	0	82	0	0
31	h	62	0	82	0	0
32	D	147	0	222	13	0
32	E	42	0	57	2	0
32	L	49	0	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	d	147	0	222	0	0
32	e	42	0	57	0	0
32	l	49	0	74	0	0
33	F	43	0	30	1	0
33	V	43	0	30	9	0
33	f	43	0	30	0	0
33	v	43	0	30	0	0
34	J	1	0	0	0	0
34	j	1	0	0	0	0
All	All	49594	0	50450	263	7

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 3.

All (263) 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	33:V:201:HEM:HAB	1.52	1.48
16:V:37:CYS:SG	33:V:201:HEM:CAB	2.02	1.47
16:V:40:CYS:SG	33:V:201:HEM:CAC	2.04	1.46
16:V:40:CYS:SG	33:V:201:HEM:HAC	1.57	1.44
8:I:1:MET:CA	8:I:1:MET:C	1.84	1.44
8:I:1:MET:HG2	8:I:1:MET:N	1.37	1.35
8:I:1:MET:CG	8:I:1:MET:N	1.89	1.35
1:A:214:MET:HG2	28:A:613:PL9:H102	1.20	1.17
12:M:16:LEU:HD22	12:M:16:LEU:HD11	2.95	1.11
12:M:16:LEU:HD13	12:M:16:LEU:HD13	0.00	1.07
8:I:1:MET:CA	8:I:1:MET:N	2.20	1.04
12:M:16:LEU:CD1	12:M:16:LEU:HD22	2.70	0.98
10:K:17:ILE:H	10:K:17:ILE:HD13	1.29	0.97
8:I:1:MET:HG2	8:I:1:MET:H1	0.87	0.97
12:M:20:VAL:CG2	12:M:20:VAL:HG11	2.72	0.95
32:D:409:LHG:H372	32:D:409:LHG:H132	1.48	0.93
2:B:76:SER:OG	13:O:112:GLY:CA	56.52	0.92
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.35	0.91
1:A:214:MET:HG2	28:A:613:PL9:C10	2.02	0.88
25:L:101:SQD:H342	14:T:12:CYS:HB3	1.90	0.87
11:L:14:ARG:HD3	25:L:101:SQD:H241	1.57	0.86
12:M:20:VAL:HG11	12:M:20:VAL:HG22	3.05	0.86
32:D:409:LHG:H352	32:D:409:LHG:H151	1.59	0.83
8:I:1:MET:CB	8:I:1:MET:N	2.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:509:CLA:HBB1	22:C:509:CLA:HMB1	1.63	0.81
8:I:1:MET:CG	8:I:1:MET:H2	1.73	0.80
8:I:1:MET:SD	8:I:1:MET:N	2.43	0.78
2:B:76:SER:OG	13:O:112:GLY:HA2	56.41	0.77
12:M:33:GLN:HB2	12:M:33:GLN:HB2	0.00	0.77
8:I:1:MET:CA	8:I:2:GLU:N	2.50	0.75
8:I:1:MET:CB	8:I:1:MET:C	2.56	0.74
12:M:20:VAL:HG11	12:M:20:VAL:HG21	2.52	0.73
13:O:57:LYS:O	13:O:58:ASN:HB2	1.87	0.73
12:M:16:LEU:CD1	12:M:16:LEU:HD13	0.97	0.73
32:D:409:LHG:H112	32:D:409:LHG:H382	1.72	0.72
22:D:402:CLA:HBB1	22:D:402:CLA:HMB1	1.71	0.72
12:M:16:LEU:CD1	12:M:16:LEU:CD2	2.49	0.71
22:A:603:CLA:HBB1	22:A:603:CLA:HMB1	1.73	0.70
22:B:614:CLA:HBB1	22:B:614:CLA:HMB1	1.73	0.70
25:B:601:SQD:H252	24:T:101:BCR:H373	44.10	0.70
16:V:37:CYS:SG	33:V:201:HEM:C3B	2.85	0.70
22:C:508:CLA:HBB1	22:C:508:CLA:HMB1	1.75	0.69
1:A:214:MET:CG	28:A:613:PL9:H102	2.12	0.69
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.75	0.69
22:B:615:CLA:H18	29:B:620:LMG:H421	1.76	0.67
12:M:28:GLN:O	12:M:31:SER:OG	3.31	0.67
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.77	0.67
23:A:606:PHO:HBB1	23:A:606:PHO:HMB1	1.76	0.67
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.76	0.67
10:K:17:ILE:HD13	10:K:17:ILE:N	2.08	0.67
22:C:506:CLA:HMC2	22:C:507:CLA:H102	1.77	0.66
16:V:40:CYS:SG	33:V:201:HEM:CBC	2.81	0.65
2:B:77:GLY:C	13:O:111:ALA:HB1	64.18	0.65
8:I:1:MET:C	8:I:1:MET:N	2.50	0.65
22:B:617:CLA:HMB1	22:B:617:CLA:HBB1	1.79	0.65
16:V:40:CYS:SG	33:V:201:HEM:C3C	2.90	0.64
2:B:33:TRP:CD1	24:B:622:BCR:H381	2.32	0.64
1:A:183:MET:HA	22:A:603:CLA:HMD2	1.81	0.63
29:Z:101:LMG:O2	29:Z:101:LMG:HC71	1.99	0.63
32:D:409:LHG:H112	32:D:409:LHG:C38	2.30	0.61
25:L:101:SQD:H45	14:T:23:PHE:CD1	2.35	0.61
24:D:404:BCR:H383	29:D:406:LMG:H172	1.83	0.60
3:C:167:VAL:HG21	22:C:512:CLA:HHB	1.83	0.60
2:B:33:TRP:HD1	24:B:622:BCR:H381	1.66	0.60
32:D:409:LHG:H372	32:D:409:LHG:C13	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:510:CLA:H43	32:D:409:LHG:H383	1.84	0.60
2:B:76:SER:OG	13:O:112:GLY:C	55.95	0.60
23:A:605:PHO:HMB1	23:A:605:PHO:HBB1	1.84	0.60
22:B:606:CLA:C14	22:B:611:CLA:HED2	2.33	0.59
11:L:13:ASN:ND2	11:L:16:SER:H	2.01	0.59
12:M:20:VAL:HG13	12:M:20:VAL:HG13	0.00	0.59
22:B:611:CLA:HBB1	22:B:611:CLA:HHC	1.85	0.59
28:A:613:PL9:H502	4:D:39:PRO:HG3	1.85	0.58
2:B:76:SER:O	13:O:111:ALA:HA	62.72	0.58
2:B:462:PHE:CE1	22:B:614:CLA:HMB3	2.38	0.58
2:B:103:LEU:HD21	22:B:606:CLA:HMC3	1.86	0.57
22:B:616:CLA:H2	22:B:617:CLA:HBB2	1.87	0.57
12:M:28:GLN:CB	12:M:28:GLN:HA	2.06	0.57
12:M:31:SER:O	12:M:32:GLN:HG2	4.82	0.56
2:B:76:SER:OG	13:O:112:GLY:N	57.94	0.56
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.40	0.56
2:B:127:ARG:NH1	2:B:127:ARG:HG3	2.12	0.56
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.42	0.55
3:C:279:LEU:HD22	22:C:509:CLA:HED2	1.89	0.55
8:I:1:MET:CE	8:I:4:LEU:HB2	2.37	0.55
10:K:17:ILE:H	10:K:17:ILE:CD1	2.00	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.89	0.55
24:D:404:BCR:H313	31:D:410:DGD:HA91	1.89	0.55
2:B:26:HIS:HB2	22:B:613:CLA:HMB2	1.89	0.55
16:V:37:CYS:SG	33:V:201:HEM:CBB	2.88	0.54
3:C:41:ARG:NH1	22:C:511:CLA:HMD1	2.22	0.54
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.54
22:B:614:CLA:H122	29:B:620:LMG:H232	1.88	0.54
22:C:501:CLA:C4D	22:C:503:CLA:H2	2.38	0.54
7:H:65:LEU:HD12	7:H:66:GLY:H	1.73	0.54
12:M:20:VAL:CG1	12:M:20:VAL:HG22	2.78	0.53
22:C:506:CLA:HBB1	22:C:506:CLA:HMB1	1.90	0.53
25:B:601:SQD:C25	24:T:101:BCR:H373	44.11	0.53
2:B:446:SER:HB2	2:B:447:PRO:CD	2.38	0.53
22:C:513:CLA:HMB1	22:C:513:CLA:HBB1	1.91	0.52
4:D:123:ILE:HD11	31:H:102:DGD:HAE1	1.92	0.52
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.92	0.52
22:C:510:CLA:C4	32:D:409:LHG:H383	2.40	0.52
2:B:76:SER:O	13:O:112:GLY:N	60.38	0.52
22:A:603:CLA:CBD	22:D:402:CLA:HAC2	2.40	0.52
22:C:503:CLA:HBB1	22:C:503:CLA:HMB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:L:101:SQD:O6	14:T:23:PHE:CD1	2.92	0.52
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.52
12:M:20:VAL:CG1	12:M:20:VAL:CG2	2.55	0.52
22:C:508:CLA:H92	32:D:409:LHG:H371	1.93	0.51
25:B:601:SQD:H252	24:T:101:BCR:C37	44.21	0.51
2:B:37:MET:CE	24:B:622:BCR:H282	2.71	0.51
2:B:248:ALA:HA	22:B:604:CLA:H42	1.92	0.51
22:D:403:CLA:H192	17:X:15:LEU:HD11	1.93	0.51
28:A:613:PL9:H403	6:F:22:ALA:HB2	1.93	0.51
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.93	0.51
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.93	0.51
11:L:13:ASN:C	11:L:13:ASN:HD22	2.15	0.50
8:I:1:MET:C	8:I:1:MET:SD	2.90	0.50
2:B:112:CYS:HG	14:T:18:PHE:HZ	45.04	0.50
11:L:13:ASN:HD22	11:L:16:SER:H	1.60	0.50
3:C:437:PHE:CZ	22:C:510:CLA:HMB3	2.47	0.50
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.47	0.50
2:B:36:SER:OG	24:B:618:BCR:H362	13.46	0.49
29:B:620:LMG:H242	4:D:284:ILE:HD13	1.94	0.49
2:B:341:LYS:HA	2:B:405:GLU:HG2	1.94	0.49
22:C:501:CLA:H42	22:C:502:CLA:HMD1	1.94	0.49
2:B:48:SER:O	13:O:57:LYS:HE3	52.61	0.49
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
32:D:409:LHG:H132	32:D:409:LHG:C37	2.33	0.49
22:B:604:CLA:HAB	22:B:606:CLA:H171	1.95	0.49
3:C:60:ILE:HG22	22:C:503:CLA:HHD	1.95	0.49
2:B:36:SER:OG	24:B:619:BCR:H362	2.12	0.49
22:A:604:CLA:HMD3	4:D:182:LEU:HD11	1.95	0.49
31:C:517:DGD:HB22	29:C:519:LMG:H302	1.95	0.49
18:Y:38:LEU:O	18:Y:42:ARG:HD3	2.13	0.48
32:D:409:LHG:C11	32:D:409:LHG:H382	2.42	0.48
22:B:615:CLA:H171	14:T:8:PHE:CE1	20.74	0.48
2:B:462:PHE:CZ	22:B:614:CLA:HMB3	2.49	0.48
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.96	0.48
13:O:49:THR:OG1	13:O:236:GLN:HB2	2.14	0.48
3:C:437:PHE:CE1	22:C:510:CLA:HMB3	2.50	0.47
22:B:615:CLA:H151	14:T:8:PHE:HE1	22.71	0.47
29:A:614:LMG:H291	3:C:214:LEU:O	2.14	0.47
3:C:25:ASN:HD21	3:C:31:SER:HA	1.79	0.47
24:K:102:BCR:H371	24:K:102:BCR:H24C	1.70	0.47
2:B:490:GLN:HA	2:B:496:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:606:PHO:HHD	23:A:606:PHO:HBC2	1.97	0.47
3:C:288:CYS:SG	31:C:516:DGD:HB32	2.55	0.47
11:L:18:TYR:OH	25:L:101:SQD:C24	2.78	0.47
14:T:18:PHE:HE1	24:T:101:BCR:H381	7.62	0.47
13:O:42:ARG:O	13:O:241:ALA:HA	2.15	0.47
22:B:609:CLA:HMB1	22:B:609:CLA:HBB1	1.97	0.47
1:A:200:LEU:HG	31:C:518:DGD:HAT2	1.97	0.47
2:B:127:ARG:CG	2:B:127:ARG:HH11	2.18	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
24:B:618:BCR:H371	24:B:618:BCR:H24C	1.83	0.46
11:L:14:ARG:HB3	14:T:25:GLU:HG2	1.97	0.46
3:C:429:SER:HB3	31:C:517:DGD:HBT2	1.98	0.46
1:A:63:ILE:HB	3:C:335:THR:HG21	1.97	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.98	0.46
4:D:27:PHE:CD1	32:E:101:LHG:HC12	2.51	0.46
2:B:237:VAL:HG12	22:B:613:CLA:HMD1	1.98	0.46
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.16	0.46
8:I:1:MET:HE1	8:I:4:LEU:HB2	1.98	0.46
22:B:617:CLA:HED2	22:B:617:CLA:H43	1.98	0.45
2:B:467:ILE:HG13	4:D:126:MET:HE2	2.04	0.45
24:T:101:BCR:H371	24:T:101:BCR:H24C	1.83	0.45
22:B:611:CLA:OBD	22:B:611:CLA:H152	2.16	0.45
22:A:607:CLA:H162	22:A:607:CLA:H122	1.76	0.45
24:T:102:BCR:H371	24:T:102:BCR:H24C	1.78	0.45
8:I:1:MET:HE3	8:I:4:LEU:HB2	1.98	0.45
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.51	0.45
22:C:510:CLA:H192	22:C:510:CLA:HBC3	1.99	0.45
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.81	0.45
1:A:215:HIS:HA	28:A:613:PL9:O1	2.17	0.44
22:B:606:CLA:H41	22:B:606:CLA:H62	1.77	0.44
22:A:607:CLA:H192	22:C:505:CLA:H142	2.00	0.44
2:B:78:TRP:N	13:O:111:ALA:HB1	63.04	0.44
12:M:27:VAL:HG12	12:M:28:GLN:HG2	6.64	0.44
22:D:403:CLA:H121	17:X:18:ALA:HB2	1.99	0.44
29:A:614:LMG:H231	29:A:614:LMG:H201	1.86	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.17	0.44
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.44
22:D:403:CLA:HBB1	22:D:403:CLA:HMB1	2.00	0.44
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.44
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.44
5:E:82:GLN:C	5:E:84:LYS:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:618:BCR:C38	14:T:19:PHE:HZ	34.43	0.44
24:A:608:BCR:H24C	24:A:608:BCR:H371	1.84	0.44
24:D:404:BCR:HC22	31:D:410:DGD:HA72	2.00	0.43
3:C:205:ASP:HA	3:C:206:PRO:HD3	1.90	0.43
22:C:506:CLA:H122	22:C:506:CLA:H162	1.72	0.43
22:B:616:CLA:H2	22:B:617:CLA:CBB	2.48	0.43
22:C:505:CLA:HAA1	22:C:505:CLA:HBD	1.99	0.43
22:A:604:CLA:HBB1	22:A:604:CLA:HMB1	2.00	0.43
2:B:13:ILE:HG12	22:B:613:CLA:HAC2	2.00	0.43
24:B:622:BCR:H371	24:B:622:BCR:H24C	1.89	0.43
2:B:467:ILE:HG13	4:D:126:MET:CE	2.48	0.43
14:T:22:PHE:HB3	24:T:102:BCR:H271	2.00	0.43
4:D:85:MET:CE	4:D:96:GLU:HG2	2.49	0.43
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.33	0.43
29:A:614:LMG:H151	31:C:516:DGD:HA62	2.01	0.43
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.52	0.43
5:E:27:ILE:HG12	33:F:101:HEM:HMC3	2.01	0.43
16:V:37:CYS:CB	33:V:201:HEM:HAB	2.43	0.43
1:A:215:HIS:ND1	28:A:613:PL9:O1	2.47	0.43
2:B:71:VAL:HG23	22:B:607:CLA:HMA2	2.01	0.43
8:I:33:LYS:HB3	8:I:34:ARG:H	1.50	0.43
4:D:102:THR:OG1	31:D:410:DGD:HG31	2.19	0.43
3:C:53:HIS:CB	22:C:512:CLA:HMD1	2.49	0.43
10:K:10:LYS:N	10:K:10:LYS:HD2	2.34	0.43
22:C:510:CLA:HBB1	22:C:510:CLA:HMB1	2.01	0.42
22:A:603:CLA:CAD	22:D:402:CLA:HAC2	2.50	0.42
12:M:20:VAL:CG1	12:M:20:VAL:HG13	0.97	0.42
22:B:605:CLA:H43	22:B:606:CLA:H2	2.01	0.42
22:A:604:CLA:H142	29:D:406:LMG:H232	2.01	0.42
22:C:504:CLA:H201	32:D:409:LHG:H342	2.01	0.42
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.42
25:A:609:SQD:O10	32:D:409:LHG:H122	2.20	0.42
22:B:614:CLA:H162	22:B:614:CLA:H121	1.88	0.42
23:A:605:PHO:ND	23:A:605:PHO:NC	2.68	0.42
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	2.01	0.42
32:D:409:LHG:H302	32:D:409:LHG:H332	1.88	0.42
4:D:27:PHE:HD1	32:E:101:LHG:HC12	1.85	0.42
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.01	0.42
4:D:272:LEU:C	4:D:272:LEU:HD23	2.40	0.42
22:B:612:CLA:H142	32:L:102:LHG:H361	2.02	0.42
13:O:59:LYS:HD2	13:O:61:GLN:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:H:101:BCR:H24C	24:H:101:BCR:H371	1.81	0.42
3:C:29:GLU:CD	3:C:29:GLU:H	2.22	0.42
4:D:185:PHE:CG	22:D:401:CLA:HMD3	2.55	0.42
2:B:204:ALA:CB	22:B:603:CLA:HAB	2.50	0.42
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.55	0.42
25:B:601:SQD:H252	24:T:101:BCR:C22	45.35	0.41
22:A:603:CLA:HBD	22:D:402:CLA:HAC2	2.02	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
22:C:502:CLA:H61	22:C:512:CLA:H42	2.03	0.41
22:B:605:CLA:H161	22:B:605:CLA:H141	1.93	0.41
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.94	0.41
12:M:16:LEU:CD1	12:M:16:LEU:CD1	0.00	0.41
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.51	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.02	0.41
23:A:606:PHO:HMA2	28:A:613:PL9:C22	2.51	0.41
22:B:611:CLA:CBB	22:B:611:CLA:HHC	2.50	0.41
12:M:28:GLN:CA	12:M:28:GLN:HA	0.97	0.41
22:B:607:CLA:HBB1	22:B:607:CLA:HMB1	2.03	0.41
3:C:243:ILE:HG22	22:C:506:CLA:HMC1	2.03	0.41
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.56	0.41
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.41
22:B:609:CLA:HMB1	4:D:126:MET:HB3	2.04	0.40
3:C:338:GLY:HA3	3:C:341:LEU:O	2.22	0.40
14:T:18:PHE:CE1	24:T:101:BCR:H381	6.90	0.40
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.56	0.40
2:B:78:TRP:HD1	13:O:112:GLY:HA2	55.87	0.40
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.04	0.40
2:B:127:ARG:NH1	2:B:127:ARG:CG	2.81	0.40
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.52	0.40
13:O:180:GLU:CD	13:O:180:GLU:H	2.24	0.40
23:A:606:PHO:ND	23:A:606:PHO:NC	2.70	0.40
25:A:609:SQD:H291	22:C:508:CLA:H71	2.03	0.40
3:C:286:ALA:HB2	22:C:502:CLA:CMD	2.51	0.40
4:D:103:ARG:O	4:D:107:LEU:HG	2.21	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:73:GLN:OE1	16:V:70:GLU:CD[3_544]	0.80	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:73:GLN:OE1	16:V:70:GLU:OE1[3_544]	1.22	0.98
15:u:73:GLN:OE1	16:V:70:GLU:OE2[3_544]	1.45	0.75
15:u:73:GLN:CD	16:V:70:GLU:OE1[3_544]	1.79	0.41
15:u:73:GLN:CD	16:V:70:GLU:CD[3_544]	1.89	0.31
15:u:73:GLN:OE1	16:V:70:GLU:CG[3_544]	1.98	0.22
15:u:60:ASP:OD2	16:V:110:LYS:CD[3_544]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	46 83
1	a	332/334 (99%)	328 (99%)	3 (1%)	1 (0%)	46 83
2	B	502/504 (100%)	497 (99%)	5 (1%)	0	100 100
2	b	502/504 (100%)	496 (99%)	6 (1%)	0	100 100
3	C	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	52 86
3	c	449/461 (97%)	440 (98%)	8 (2%)	1 (0%)	52 86
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100 100
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100 100
5	E	79/81 (98%)	78 (99%)	1 (1%)	0	100 100
5	e	79/81 (98%)	78 (99%)	1 (1%)	0	100 100
6	F	32/34 (94%)	32 (100%)	0	0	100 100
6	f	32/34 (94%)	32 (100%)	0	0	100 100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100 100
7	h	63/65 (97%)	58 (92%)	5 (8%)	0	100 100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100 100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	36/40 (90%)	36 (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	32/34 (94%)	32 (100%)	0	0	100	100
12	m	32/34 (94%)	32 (100%)	0	0	100	100
13	O	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	39	80
13	o	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	39	80
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
15	U	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
15	u	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
16	V	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
16	v	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
17	X	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
17	x	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
18	Y	27/29 (93%)	27 (100%)	0	0	100	100
18	y	27/29 (93%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5188/5288 (98%)	5085 (98%)	97 (2%)	6 (0%)	56	90

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	o	58	ASN
3	C	416	SER
3	c	416	SER
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	269/269 (100%)	269 (100%)	0	100	100
1	a	269/269 (100%)	269 (100%)	0	100	100
2	B	402/402 (100%)	398 (99%)	4 (1%)	82	92
2	b	402/402 (100%)	398 (99%)	4 (1%)	82	92
3	C	352/362 (97%)	348 (99%)	4 (1%)	80	91
3	c	352/362 (97%)	348 (99%)	4 (1%)	80	91
4	D	277/277 (100%)	274 (99%)	3 (1%)	80	91
4	d	277/277 (100%)	274 (99%)	3 (1%)	80	91
5	E	72/72 (100%)	71 (99%)	1 (1%)	74	89
5	e	72/72 (100%)	71 (99%)	1 (1%)	74	89
6	F	28/28 (100%)	27 (96%)	1 (4%)	42	74
6	f	28/28 (100%)	27 (96%)	1 (4%)	42	74
7	H	54/54 (100%)	51 (94%)	3 (6%)	26	63
7	h	54/54 (100%)	51 (94%)	3 (6%)	26	63
8	I	35/35 (100%)	34 (97%)	1 (3%)	50	78
8	i	35/35 (100%)	34 (97%)	1 (3%)	50	78
9	J	26/28 (93%)	26 (100%)	0	100	100
9	j	26/28 (93%)	26 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	57
10	k	30/30 (100%)	28 (93%)	2 (7%)	20	57
11	L	35/35 (100%)	33 (94%)	2 (6%)	25	62
11	l	35/35 (100%)	33 (94%)	2 (6%)	25	62
12	M	31/31 (100%)	30 (97%)	1 (3%)	46	77
12	m	31/31 (100%)	30 (97%)	1 (3%)	46	77
13	O	206/206 (100%)	202 (98%)	4 (2%)	65	86
13	o	206/206 (100%)	202 (98%)	4 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	27/27 (100%)	26 (96%)	1 (4%)	41	74
14	t	27/27 (100%)	26 (96%)	1 (4%)	41	74
15	U	84/84 (100%)	83 (99%)	1 (1%)	78	90
15	u	84/84 (100%)	83 (99%)	1 (1%)	78	90
16	V	117/117 (100%)	116 (99%)	1 (1%)	84	93
16	v	117/117 (100%)	116 (99%)	1 (1%)	84	93
17	X	32/32 (100%)	32 (100%)	0	100	100
17	x	32/32 (100%)	32 (100%)	0	100	100
18	Y	22/22 (100%)	21 (96%)	1 (4%)	34	69
18	y	22/22 (100%)	21 (96%)	1 (4%)	34	69
19	Z	52/52 (100%)	50 (96%)	2 (4%)	40	73
19	z	52/52 (100%)	50 (96%)	2 (4%)	40	73
All	All	4302/4326 (99%)	4238 (98%)	64 (2%)	72	89

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	223	GLN
2	B	246	PHE
2	B	472	ARG
2	b	53	ASN
2	b	223	GLN
2	b	246	PHE
2	b	472	ARG
3	C	24	THR
3	C	25	ASN
3	C	289	PHE
3	C	418	ASN
3	c	24	THR
3	c	25	ASN
3	c	289	PHE
3	c	418	ASN
4	D	11	GLU
4	D	90	LEU
4	D	180	ARG
4	d	11	GLU
4	d	90	LEU

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Mol	Chain	Res	Type
4	d	180	ARG
5	E	71	GLU
5	e	71	GLU
6	F	44	GLN
6	f	44	GLN
7	H	12	ARG
7	H	49	TYR
7	H	65	LEU
7	h	12	ARG
7	h	49	TYR
7	h	65	LEU
8	I	1	MET
8	i	1	MET
10	K	13	GLU
10	K	17	ILE
10	k	13	GLU
10	k	17	ILE
11	L	1	MET
11	L	13	ASN
11	l	1	MET
11	l	13	ASN
12	M	9	ILE
12	m	9	ILE
13	O	61	GLN
13	O	118	LEU
13	O	181	GLU
13	O	234	LYS
13	o	61	GLN
13	o	118	LEU
13	o	181	GLU
13	o	234	LYS
14	T	25	GLU
14	t	25	GLU
15	U	70	ARG
15	u	70	ARG
16	V	30	LYS
16	v	30	LYS
18	Y	27	MET
18	y	27	MET
19	Z	6	GLN
19	Z	31	GLN
19	z	6	GLN

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Mol	Chain	Res	Type
19	z	31	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
1	a	261	GLN
1	a	315	ASN
2	B	53	ASN
2	B	223	GLN
2	B	281	GLN
2	B	331	ASN
2	b	53	ASN
2	b	223	GLN
2	b	281	GLN
2	b	331	ASN
3	C	25	ASN
3	C	373	ASN
3	c	25	ASN
3	c	373	ASN
4	D	83	ASN
4	D	332	GLN
4	d	83	ASN
4	d	332	GLN
6	F	44	GLN
6	f	44	GLN
10	K	40	GLN
10	k	40	GLN
11	L	13	ASN
11	l	13	ASN
13	O	82	GLN
13	O	124	ASN
13	O	147	ASN
13	o	82	GLN
13	o	124	ASN
13	o	147	ASN
16	V	34	GLN
16	v	34	GLN
19	Z	58	ASN
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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 166 ligands modelled in this entry, 16 are monoatomic - leaving 150 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	$\#\|Z\| > 2$
20	OEX	A	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
22	CLA	A	603	-	57,73,73	1.81	10 (17%)	61,113,113	1.90	14 (22%)
22	CLA	A	604	-	57,73,73	1.73	10 (17%)	61,113,113	2.19	15 (24%)
23	PHO	A	605	-	67,69,69	1.88	13 (19%)	86,99,99	1.94	21 (24%)
23	PHO	A	606	-	67,69,69	1.99	15 (22%)	86,99,99	1.95	22 (25%)
22	CLA	A	607	-	57,73,73	1.84	10 (17%)	61,113,113	2.01	15 (24%)
24	BCR	A	608	-	41,41,41	3.76	14 (34%)	56,56,56	7.62	39 (69%)
25	SQD	A	609	-	53,54,54	1.49	3 (5%)	62,65,65	1.78	12 (19%)
27	BCT	A	612	21	0,3,3	0.00	-	0,3,3	0.00	-
28	PL9	A	613	-	54,55,55	0.66	2 (3%)	68,69,69	1.62	12 (17%)
29	LMG	A	614	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)
25	SQD	B	601	-	53,54,54	1.50	3 (5%)	62,65,65	1.42	6 (9%)
22	CLA	B	602	-	57,73,73	1.91	11 (19%)	61,113,113	2.02	15 (24%)
22	CLA	B	603	-	57,73,73	1.89	11 (19%)	61,113,113	1.82	13 (21%)
22	CLA	B	604	-	57,73,73	1.83	12 (21%)	61,113,113	2.15	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	605	-	57,73,73	1.72	12 (21%)	61,113,113	2.13	14 (22%)
22	CLA	B	606	-	57,73,73	1.77	10 (17%)	61,113,113	1.97	14 (22%)
22	CLA	B	607	-	57,73,73	1.85	11 (19%)	61,113,113	2.02	14 (22%)
22	CLA	B	608	-	57,73,73	1.80	10 (17%)	61,113,113	1.92	13 (21%)
22	CLA	B	609	-	57,73,73	1.76	10 (17%)	61,113,113	2.20	19 (31%)
22	CLA	B	610	-	57,73,73	1.79	10 (17%)	61,113,113	1.97	13 (21%)
22	CLA	B	611	-	57,73,73	1.82	11 (19%)	61,113,113	1.90	12 (19%)
22	CLA	B	612	-	57,73,73	1.66	10 (17%)	61,113,113	2.02	13 (21%)
22	CLA	B	613	-	57,73,73	1.80	11 (19%)	61,113,113	2.00	15 (24%)
22	CLA	B	614	-	57,73,73	1.80	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	B	615	-	57,73,73	1.77	12 (21%)	61,113,113	2.04	16 (26%)
22	CLA	B	616	-	57,73,73	1.83	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	B	617	-	57,73,73	1.85	10 (17%)	61,113,113	1.96	17 (27%)
24	BCR	B	618	-	41,41,41	3.70	14 (34%)	56,56,56	7.34	38 (67%)
24	BCR	B	619	-	41,41,41	3.70	14 (34%)	56,56,56	7.60	42 (75%)
29	LMG	B	620	-	51,51,55	0.91	2 (3%)	59,59,63	1.01	3 (5%)
24	BCR	B	622	-	41,41,41	3.85	14 (34%)	56,56,56	6.92	38 (67%)
22	CLA	C	501	-	57,73,73	1.85	11 (19%)	61,113,113	2.08	16 (26%)
22	CLA	C	502	-	57,73,73	1.79	11 (19%)	61,113,113	1.92	13 (21%)
22	CLA	C	503	-	57,73,73	1.87	11 (19%)	61,113,113	1.87	13 (21%)
22	CLA	C	504	-	57,73,73	1.85	10 (17%)	61,113,113	2.02	13 (21%)
22	CLA	C	505	-	57,73,73	1.85	12 (21%)	61,113,113	1.91	13 (21%)
22	CLA	C	506	-	57,73,73	1.88	11 (19%)	61,113,113	2.04	15 (24%)
22	CLA	C	507	-	57,73,73	1.94	11 (19%)	61,113,113	1.99	15 (24%)
22	CLA	C	508	-	57,73,73	1.91	12 (21%)	61,113,113	1.91	10 (16%)
22	CLA	C	509	-	57,73,73	1.85	12 (21%)	61,113,113	2.04	15 (24%)
22	CLA	C	510	-	57,73,73	1.82	11 (19%)	61,113,113	1.95	15 (24%)
22	CLA	C	511	3	57,73,73	1.88	11 (19%)	61,113,113	1.93	13 (21%)
22	CLA	C	512	-	57,73,73	1.90	12 (21%)	61,113,113	1.96	17 (27%)
22	CLA	C	513	-	57,73,73	1.97	12 (21%)	61,113,113	1.85	14 (22%)
24	BCR	C	514	-	41,41,41	3.91	14 (34%)	56,56,56	8.26	35 (62%)
24	BCR	C	515	-	41,41,41	3.87	14 (34%)	56,56,56	8.04	39 (69%)
31	DGD	C	516	-	63,63,67	0.85	2 (3%)	77,77,81	0.99	3 (3%)
31	DGD	C	517	-	63,63,67	0.85	2 (3%)	77,77,81	0.86	3 (3%)
31	DGD	C	518	-	63,63,67	0.77	2 (3%)	77,77,81	0.90	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	C	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.03	4 (6%)
29	LMG	C	520	-	51,51,55	0.98	3 (5%)	59,59,63	1.00	2 (3%)
22	CLA	D	401	-	57,73,73	1.82	13 (22%)	61,113,113	2.04	18 (29%)
22	CLA	D	402	-	57,73,73	1.76	11 (19%)	61,113,113	2.20	16 (26%)
22	CLA	D	403	-	57,73,73	1.87	12 (21%)	61,113,113	1.85	13 (21%)
24	BCR	D	404	-	41,41,41	3.86	14 (34%)	56,56,56	7.66	40 (71%)
32	LHG	D	405	-	48,48,48	0.84	2 (4%)	49,54,54	1.01	3 (6%)
29	LMG	D	406	34	51,51,55	0.85	2 (3%)	59,59,63	0.80	3 (5%)
32	LHG	D	407	-	48,48,48	0.87	2 (4%)	49,54,54	0.85	2 (4%)
28	PL9	D	408	-	54,55,55	0.76	1 (1%)	68,69,69	1.37	8 (11%)
32	LHG	D	409	-	48,48,48	0.92	2 (4%)	49,54,54	0.91	3 (6%)
31	DGD	D	410	-	63,63,67	0.96	3 (4%)	77,77,81	1.08	5 (6%)
25	SQD	D	411	-	42,43,54	1.70	3 (7%)	51,54,65	1.78	8 (15%)
32	LHG	E	101	-	41,41,48	1.03	2 (4%)	42,47,54	1.10	3 (7%)
33	HEM	F	101	5,6	24,50,50	2.26	6 (25%)	16,82,82	2.14	2 (12%)
24	BCR	H	101	-	41,41,41	3.84	14 (34%)	56,56,56	8.08	41 (73%)
31	DGD	H	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.94	5 (6%)
24	BCR	K	101	-	41,41,41	3.88	14 (34%)	56,56,56	7.89	36 (64%)
24	BCR	K	102	-	41,41,41	3.81	14 (34%)	56,56,56	7.59	40 (71%)
25	SQD	L	101	-	53,54,54	1.43	3 (5%)	62,65,65	1.63	7 (11%)
32	LHG	L	102	-	48,48,48	0.87	2 (4%)	49,54,54	0.99	2 (4%)
24	BCR	T	101	-	41,41,41	3.70	14 (34%)	56,56,56	7.34	38 (67%)
24	BCR	T	102	-	41,41,41	3.77	14 (34%)	56,56,56	8.25	42 (75%)
33	HEM	V	201	16	24,50,50	2.27	5 (20%)	16,82,82	1.88	3 (18%)
29	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.39	3 (6%)
20	OEX	a	601	1,3	0,15,15	0.00	-	0,32,32	0.00	-
22	CLA	a	603	-	57,73,73	1.81	10 (17%)	61,113,113	1.89	14 (22%)
22	CLA	a	604	-	57,73,73	1.72	10 (17%)	61,113,113	2.18	15 (24%)
23	PHO	a	605	-	67,69,69	1.88	13 (19%)	86,99,99	1.95	21 (24%)
23	PHO	a	606	-	67,69,69	1.99	15 (22%)	86,99,99	1.95	22 (25%)
22	CLA	a	607	-	57,73,73	1.83	10 (17%)	61,113,113	2.00	15 (24%)
24	BCR	a	608	-	41,41,41	3.76	14 (34%)	56,56,56	7.62	39 (69%)
25	SQD	a	609	-	53,54,54	1.49	3 (5%)	62,65,65	1.78	12 (19%)
27	BCT	a	612	21	0,3,3	0.00	-	0,3,3	0.00	-
28	PL9	a	613	-	54,55,55	0.66	2 (3%)	68,69,69	1.62	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	a	614	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)
25	SQD	b	601	-	53,54,54	1.51	3 (5%)	62,65,65	1.42	6 (9%)
22	CLA	b	602	-	57,73,73	1.91	11 (19%)	61,113,113	2.02	15 (24%)
22	CLA	b	603	-	57,73,73	1.89	11 (19%)	61,113,113	1.83	13 (21%)
22	CLA	b	604	-	57,73,73	1.84	12 (21%)	61,113,113	2.16	15 (24%)
22	CLA	b	605	-	57,73,73	1.73	12 (21%)	61,113,113	2.12	14 (22%)
22	CLA	b	606	-	57,73,73	1.77	11 (19%)	61,113,113	1.96	14 (22%)
22	CLA	b	607	-	57,73,73	1.85	11 (19%)	61,113,113	2.02	14 (22%)
22	CLA	b	608	-	57,73,73	1.80	10 (17%)	61,113,113	1.91	13 (21%)
22	CLA	b	609	-	57,73,73	1.77	10 (17%)	61,113,113	2.20	19 (31%)
22	CLA	b	610	-	57,73,73	1.79	10 (17%)	61,113,113	1.96	13 (21%)
22	CLA	b	611	-	57,73,73	1.81	11 (19%)	61,113,113	1.90	12 (19%)
22	CLA	b	612	-	57,73,73	1.66	10 (17%)	61,113,113	2.02	13 (21%)
22	CLA	b	613	-	57,73,73	1.80	11 (19%)	61,113,113	2.00	15 (24%)
22	CLA	b	614	-	57,73,73	1.80	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	b	615	-	57,73,73	1.76	12 (21%)	61,113,113	2.04	16 (26%)
22	CLA	b	616	-	57,73,73	1.83	11 (19%)	61,113,113	1.88	14 (22%)
22	CLA	b	617	-	57,73,73	1.85	10 (17%)	61,113,113	1.96	16 (26%)
24	BCR	b	618	-	41,41,41	3.70	14 (34%)	56,56,56	7.61	42 (75%)
29	LMG	b	619	-	51,51,55	0.92	2 (3%)	59,59,63	1.01	3 (5%)
25	SQD	b	621	-	53,54,54	1.48	3 (5%)	62,65,65	1.73	9 (14%)
24	BCR	b	622	-	41,41,41	3.85	14 (34%)	56,56,56	6.92	38 (67%)
22	CLA	c	501	-	57,73,73	1.85	11 (19%)	61,113,113	2.08	16 (26%)
22	CLA	c	502	-	57,73,73	1.79	11 (19%)	61,113,113	1.92	13 (21%)
22	CLA	c	503	-	57,73,73	1.87	11 (19%)	61,113,113	1.86	13 (21%)
22	CLA	c	504	-	57,73,73	1.85	10 (17%)	61,113,113	2.01	13 (21%)
22	CLA	c	505	-	57,73,73	1.86	12 (21%)	61,113,113	1.91	13 (21%)
22	CLA	c	506	-	57,73,73	1.88	11 (19%)	61,113,113	2.03	15 (24%)
22	CLA	c	507	-	57,73,73	1.94	11 (19%)	61,113,113	1.99	15 (24%)
22	CLA	c	508	-	57,73,73	1.92	12 (21%)	61,113,113	1.91	11 (18%)
22	CLA	c	509	-	57,73,73	1.86	12 (21%)	61,113,113	2.04	15 (24%)
22	CLA	c	510	-	57,73,73	1.82	11 (19%)	61,113,113	1.95	15 (24%)
22	CLA	c	511	3	57,73,73	1.87	11 (19%)	61,113,113	1.93	13 (21%)
22	CLA	c	512	-	57,73,73	1.90	12 (21%)	61,113,113	1.96	17 (27%)
22	CLA	c	513	-	57,73,73	1.97	12 (21%)	61,113,113	1.85	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	c	514	-	41,41,41	3.91	15 (36%)	56,56,56	8.26	35 (62%)
24	BCR	c	515	-	41,41,41	3.87	14 (34%)	56,56,56	8.03	39 (69%)
31	DGD	c	516	-	63,63,67	0.85	2 (3%)	77,77,81	0.99	3 (3%)
31	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	0.86	3 (3%)
31	DGD	c	518	-	63,63,67	0.77	2 (3%)	77,77,81	0.90	2 (2%)
29	LMG	c	519	-	51,51,55	0.92	2 (3%)	59,59,63	1.03	4 (6%)
29	LMG	c	520	-	51,51,55	0.98	3 (5%)	59,59,63	1.00	2 (3%)
22	CLA	d	401	-	57,73,73	1.81	12 (21%)	61,113,113	2.04	18 (29%)
22	CLA	d	402	-	57,73,73	1.76	11 (19%)	61,113,113	2.20	15 (24%)
22	CLA	d	403	-	57,73,73	1.87	13 (22%)	61,113,113	1.86	13 (21%)
24	BCR	d	404	-	41,41,41	3.86	14 (34%)	56,56,56	7.65	40 (71%)
32	LHG	d	405	-	48,48,48	0.84	2 (4%)	49,54,54	1.00	3 (6%)
29	LMG	d	406	34	51,51,55	0.85	2 (3%)	59,59,63	0.80	3 (5%)
32	LHG	d	407	-	48,48,48	0.88	2 (4%)	49,54,54	0.85	2 (4%)
28	PL9	d	408	-	54,55,55	0.76	1 (1%)	68,69,69	1.37	8 (11%)
32	LHG	d	409	-	48,48,48	0.92	2 (4%)	49,54,54	0.90	2 (4%)
31	DGD	d	410	-	63,63,67	0.96	4 (6%)	77,77,81	1.08	5 (6%)
25	SQD	d	411	-	42,43,54	1.70	3 (7%)	51,54,65	1.78	8 (15%)
32	LHG	e	101	-	41,41,48	1.03	2 (4%)	42,47,54	1.10	3 (7%)
33	HEM	f	101	5,6	24,50,50	2.26	6 (25%)	16,82,82	2.13	2 (12%)
24	BCR	h	101	-	41,41,41	3.84	14 (34%)	56,56,56	8.08	41 (73%)
31	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.94	5 (6%)
24	BCR	k	101	-	41,41,41	3.88	14 (34%)	56,56,56	7.89	36 (64%)
24	BCR	k	102	-	41,41,41	3.81	14 (34%)	56,56,56	7.59	40 (71%)
25	SQD	l	101	-	53,54,54	1.43	4 (7%)	62,65,65	1.62	7 (11%)
25	SQD	l	102	-	53,54,54	1.48	4 (7%)	62,65,65	1.73	9 (14%)
32	LHG	l	103	-	48,48,48	0.87	2 (4%)	49,54,54	0.99	2 (4%)
24	BCR	t	101	-	41,41,41	3.77	14 (34%)	56,56,56	8.25	42 (75%)
33	HEM	v	201	16	24,50,50	2.27	6 (25%)	16,82,82	1.88	3 (18%)
29	LMG	z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.40	3 (6%)

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
20	OEX	A	601	1,3	-	0/0/68/68	0/0/6/6
22	CLA	A	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	604	-	2/2/20/25	0/37/135/135	0/0/9/9
23	PHO	A	605	-	-	0/53/103/103	0/1/6/6
23	PHO	A	606	-	-	0/53/103/103	0/1/6/6
22	CLA	A	607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	BCR	A	608	-	-	0/29/63/63	0/2/2/2
25	SQD	A	609	-	-	0/49/69/69	0/1/1/1
27	BCT	A	612	21	-	0/0/0/0	0/0/0/0
28	PL9	A	613	-	-	0/53/73/73	0/1/1/1
29	LMG	A	614	-	-	0/46/66/70	0/1/1/1
25	SQD	B	601	-	-	0/49/69/69	0/1/1/1
22	CLA	B	602	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
29	LMG	B	620	-	-	0/46/66/70	0/1/1/1
24	BCR	B	622	-	-	0/29/63/63	0/2/2/2
22	CLA	C	501	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	513	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	C	514	-	-	0/29/63/63	0/2/2/2
24	BCR	C	515	-	-	0/29/63/63	0/2/2/2
31	DGD	C	516	-	-	0/51/91/95	0/2/2/2
31	DGD	C	517	-	-	0/51/91/95	0/2/2/2
31	DGD	C	518	-	-	0/51/91/95	0/2/2/2
29	LMG	C	519	-	-	0/46/66/70	0/1/1/1
29	LMG	C	520	-	-	0/46/66/70	0/1/1/1
22	CLA	D	401	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	D	402	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	D	404	-	-	0/29/63/63	0/2/2/2
32	LHG	D	405	-	-	0/53/53/53	0/0/0/0
29	LMG	D	406	34	-	0/46/66/70	0/1/1/1
32	LHG	D	407	-	-	0/53/53/53	0/0/0/0
28	PL9	D	408	-	-	0/53/73/73	0/1/1/1
32	LHG	D	409	-	-	0/53/53/53	0/0/0/0
31	DGD	D	410	-	-	0/51/91/95	0/2/2/2
25	SQD	D	411	-	-	0/38/58/69	0/1/1/1
32	LHG	E	101	-	-	0/46/46/53	0/0/0/0
33	HEM	F	101	5,6	-	0/6/54/54	0/0/8/8
24	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	DGD	H	102	-	-	0/51/91/95	0/2/2/2
24	BCR	K	101	-	-	0/29/63/63	0/2/2/2
24	BCR	K	102	-	-	0/29/63/63	0/2/2/2
25	SQD	L	101	-	-	0/49/69/69	0/1/1/1
32	LHG	L	102	-	-	0/53/53/53	0/0/0/0
24	BCR	T	101	-	-	0/29/63/63	0/2/2/2
24	BCR	T	102	-	-	0/29/63/63	0/2/2/2
33	HEM	V	201	16	-	0/6/54/54	0/0/8/8
29	LMG	Z	101	-	-	1/31/51/70	0/1/1/1
20	OEX	a	601	1,3	-	0/0/68/68	0/0/6/6
22	CLA	a	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	604	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	a	605	-	-	0/53/103/103	0/1/6/6
23	PHO	a	606	-	-	0/53/103/103	0/1/6/6
22	CLA	a	607	-	1/1/20/25	0/37/135/135	0/0/9/9
24	BCR	a	608	-	-	0/29/63/63	0/2/2/2
25	SQD	a	609	-	-	0/49/69/69	0/1/1/1
27	BCT	a	612	21	-	0/0/0/0	0/0/0/0
28	PL9	a	613	-	-	0/53/73/73	0/1/1/1
29	LMG	a	614	-	-	0/46/66/70	0/1/1/1
25	SQD	b	601	-	-	0/49/69/69	0/1/1/1
22	CLA	b	602	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
24	BCR	b	618	-	-	0/29/63/63	0/2/2/2
29	LMG	b	619	-	-	0/46/66/70	0/1/1/1
25	SQD	b	621	-	-	0/49/69/69	0/1/1/1
24	BCR	b	622	-	-	0/29/63/63	0/2/2/2
22	CLA	c	501	-	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	502	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	505	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	508	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	511	3	2/2/20/25	0/37/135/135	0/0/9/9
22	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	513	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	c	514	-	-	0/29/63/63	0/2/2/2
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
31	DGD	c	516	-	-	0/51/91/95	0/2/2/2
31	DGD	c	517	-	-	0/51/91/95	0/2/2/2
31	DGD	c	518	-	-	0/51/91/95	0/2/2/2
29	LMG	c	519	-	-	0/46/66/70	0/1/1/1
29	LMG	c	520	-	-	0/46/66/70	0/1/1/1
22	CLA	d	401	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	d	402	-	1/1/20/25	0/37/135/135	0/0/9/9
22	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	BCR	d	404	-	-	0/29/63/63	0/2/2/2
32	LHG	d	405	-	-	0/53/53/53	0/0/0/0
29	LMG	d	406	34	-	0/46/66/70	0/1/1/1
32	LHG	d	407	-	-	0/53/53/53	0/0/0/0
28	PL9	d	408	-	-	0/53/73/73	0/1/1/1
32	LHG	d	409	-	-	0/53/53/53	0/0/0/0
31	DGD	d	410	-	-	0/51/91/95	0/2/2/2
25	SQD	d	411	-	-	0/38/58/69	0/1/1/1
32	LHG	e	101	-	-	0/46/46/53	0/0/0/0
33	HEM	f	101	5,6	-	0/6/54/54	0/0/8/8
24	BCR	h	101	-	-	0/29/63/63	0/2/2/2
31	DGD	h	102	-	-	0/51/91/95	0/2/2/2
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
24	BCR	k	102	-	-	0/29/63/63	0/2/2/2
25	SQD	l	101	-	-	0/49/69/69	0/1/1/1
25	SQD	l	102	-	-	0/49/69/69	0/1/1/1
32	LHG	l	103	-	-	0/53/53/53	0/0/0/0
24	BCR	t	101	-	-	0/29/63/63	0/2/2/2
33	HEM	v	201	16	-	0/6/54/54	0/0/8/8
29	LMG	z	101	-	-	1/31/51/70	0/1/1/1

All (1272) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	609	SQD	C6-S	-8.73	1.67	1.77
25	a	609	SQD	C6-S	-8.71	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	BCR	C8-C9	-8.55	1.27	1.45
24	c	514	BCR	C8-C9	-8.51	1.27	1.45
25	b	601	SQD	C6-S	-8.50	1.67	1.77
24	d	404	BCR	C8-C9	-8.48	1.27	1.45
24	C	514	BCR	C12-C13	-8.47	1.27	1.45
24	K	102	BCR	C8-C9	-8.46	1.27	1.45
24	k	102	BCR	C8-C9	-8.45	1.27	1.45
24	D	404	BCR	C8-C9	-8.45	1.27	1.45
24	c	514	BCR	C12-C13	-8.44	1.27	1.45
25	B	601	SQD	C6-S	-8.43	1.67	1.77
24	h	101	BCR	C19-C18	-8.42	1.27	1.45
24	H	101	BCR	C19-C18	-8.40	1.27	1.45
24	k	101	BCR	C19-C18	-8.39	1.27	1.45
24	B	622	BCR	C8-C9	-8.39	1.27	1.45
24	b	622	BCR	C8-C9	-8.38	1.27	1.45
24	c	515	BCR	C8-C9	-8.37	1.27	1.45
24	C	515	BCR	C8-C9	-8.35	1.27	1.45
25	d	411	SQD	C6-S	-8.34	1.67	1.77
24	K	101	BCR	C19-C18	-8.34	1.27	1.45
24	K	101	BCR	C8-C9	-8.33	1.27	1.45
25	D	411	SQD	C6-S	-8.32	1.67	1.77
24	T	102	BCR	C8-C9	-8.31	1.27	1.45
24	k	101	BCR	C8-C9	-8.30	1.27	1.45
24	t	101	BCR	C8-C9	-8.29	1.27	1.45
24	b	622	BCR	C12-C13	-8.27	1.27	1.45
24	c	515	BCR	C19-C18	-8.25	1.27	1.45
24	B	622	BCR	C12-C13	-8.24	1.27	1.45
24	D	404	BCR	C19-C18	-8.24	1.27	1.45
24	C	514	BCR	C19-C18	-8.23	1.27	1.45
24	d	404	BCR	C19-C18	-8.23	1.27	1.45
24	K	101	BCR	C12-C13	-8.22	1.27	1.45
24	t	101	BCR	C12-C13	-8.22	1.27	1.45
24	c	514	BCR	C19-C18	-8.21	1.27	1.45
24	B	618	BCR	C8-C9	-8.21	1.27	1.45
24	k	101	BCR	C12-C13	-8.20	1.27	1.45
24	T	101	BCR	C8-C9	-8.20	1.27	1.45
24	C	515	BCR	C12-C13	-8.20	1.27	1.45
24	C	515	BCR	C19-C18	-8.20	1.27	1.45
24	H	101	BCR	C12-C13	-8.18	1.27	1.45
24	T	102	BCR	C12-C13	-8.18	1.27	1.45
24	H	101	BCR	C8-C9	-8.18	1.27	1.45
24	h	101	BCR	C8-C9	-8.17	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	BCR	C12-C13	-8.16	1.27	1.45
24	h	101	BCR	C12-C13	-8.15	1.27	1.45
24	B	619	BCR	C8-C9	-8.14	1.27	1.45
24	b	618	BCR	C8-C9	-8.13	1.27	1.45
24	k	102	BCR	C19-C18	-8.13	1.27	1.45
24	K	102	BCR	C19-C18	-8.13	1.27	1.45
24	a	608	BCR	C8-C9	-8.12	1.28	1.45
24	A	608	BCR	C8-C9	-8.10	1.28	1.45
24	b	622	BCR	C19-C18	-8.09	1.28	1.45
24	d	404	BCR	C20-C21	-8.09	1.19	1.43
24	B	622	BCR	C19-C18	-8.08	1.28	1.45
24	d	404	BCR	C12-C13	-8.07	1.28	1.45
24	k	101	BCR	C20-C21	-8.07	1.20	1.43
24	D	404	BCR	C20-C21	-8.06	1.20	1.43
24	B	619	BCR	C19-C18	-8.06	1.28	1.45
24	K	101	BCR	C20-C21	-8.05	1.20	1.43
24	D	404	BCR	C12-C13	-8.05	1.28	1.45
24	C	514	BCR	C20-C21	-8.05	1.20	1.43
24	h	101	BCR	C20-C21	-8.04	1.20	1.43
24	b	618	BCR	C19-C18	-8.04	1.28	1.45
24	c	514	BCR	C20-C21	-8.03	1.20	1.43
24	k	102	BCR	C12-C13	-8.03	1.28	1.45
24	H	101	BCR	C20-C21	-8.03	1.20	1.43
24	B	618	BCR	C12-C13	-8.03	1.28	1.45
24	T	101	BCR	C12-C13	-8.02	1.28	1.45
24	c	514	BCR	C16-C17	-8.01	1.20	1.43
24	K	102	BCR	C12-C13	-8.01	1.28	1.45
25	l	102	SQD	C6-S	-8.00	1.68	1.77
24	c	515	BCR	C16-C17	-8.00	1.20	1.43
24	C	514	BCR	C16-C17	-7.99	1.20	1.43
24	K	101	BCR	C16-C17	-7.99	1.20	1.43
24	A	608	BCR	C12-C13	-7.98	1.28	1.45
24	C	515	BCR	C16-C17	-7.98	1.20	1.43
24	C	515	BCR	C20-C21	-7.97	1.20	1.43
25	b	621	SQD	C6-S	-7.96	1.68	1.77
24	a	608	BCR	C12-C13	-7.96	1.28	1.45
24	c	515	BCR	C20-C21	-7.95	1.20	1.43
24	A	608	BCR	C19-C18	-7.95	1.28	1.45
24	k	101	BCR	C16-C17	-7.94	1.20	1.43
24	t	101	BCR	C19-C18	-7.92	1.28	1.45
24	b	618	BCR	C12-C13	-7.92	1.28	1.45
24	k	102	BCR	C20-C21	-7.91	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	102	BCR	C20-C21	-7.91	1.20	1.43
24	a	608	BCR	C19-C18	-7.90	1.28	1.45
24	B	619	BCR	C12-C13	-7.90	1.28	1.45
24	T	102	BCR	C19-C18	-7.88	1.28	1.45
24	d	404	BCR	C16-C17	-7.87	1.20	1.43
24	D	404	BCR	C16-C17	-7.87	1.20	1.43
24	H	101	BCR	C16-C17	-7.87	1.20	1.43
24	B	622	BCR	C16-C17	-7.86	1.20	1.43
24	b	622	BCR	C16-C17	-7.86	1.20	1.43
24	h	101	BCR	C16-C17	-7.86	1.20	1.43
24	b	622	BCR	C20-C21	-7.86	1.20	1.43
24	A	608	BCR	C20-C21	-7.86	1.20	1.43
24	a	608	BCR	C20-C21	-7.83	1.20	1.43
24	B	622	BCR	C20-C21	-7.83	1.20	1.43
24	B	618	BCR	C19-C18	-7.82	1.28	1.45
24	t	101	BCR	C16-C17	-7.81	1.20	1.43
24	b	618	BCR	C20-C21	-7.81	1.20	1.43
24	T	102	BCR	C16-C17	-7.81	1.20	1.43
24	B	619	BCR	C20-C21	-7.78	1.20	1.43
24	A	608	BCR	C16-C17	-7.78	1.20	1.43
24	K	102	BCR	C16-C17	-7.77	1.20	1.43
24	T	101	BCR	C19-C18	-7.77	1.28	1.45
24	k	102	BCR	C16-C17	-7.77	1.20	1.43
24	a	608	BCR	C16-C17	-7.77	1.20	1.43
24	t	101	BCR	C20-C21	-7.75	1.20	1.43
25	L	101	SQD	C6-S	-7.75	1.68	1.77
24	T	102	BCR	C20-C21	-7.74	1.21	1.43
24	B	618	BCR	C20-C21	-7.71	1.21	1.43
25	l	101	SQD	C6-S	-7.71	1.68	1.77
24	T	101	BCR	C20-C21	-7.69	1.21	1.43
24	T	101	BCR	C16-C17	-7.62	1.21	1.43
24	B	618	BCR	C16-C17	-7.61	1.21	1.43
24	B	619	BCR	C16-C17	-7.61	1.21	1.43
24	b	618	BCR	C16-C17	-7.60	1.21	1.43
24	c	514	BCR	C11-C12	-6.28	1.19	1.34
24	c	515	BCR	C21-C22	-6.28	1.27	1.35
24	k	101	BCR	C11-C12	-6.27	1.19	1.34
24	k	101	BCR	C21-C22	-6.26	1.27	1.35
24	C	514	BCR	C11-C12	-6.25	1.19	1.34
24	K	101	BCR	C11-C12	-6.24	1.19	1.34
24	a	608	BCR	C20-C19	-6.24	1.19	1.34
24	C	515	BCR	C20-C19	-6.23	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	101	BCR	C21-C22	-6.22	1.27	1.35
24	C	515	BCR	C21-C22	-6.21	1.27	1.35
24	D	404	BCR	C20-C19	-6.19	1.20	1.34
24	c	515	BCR	C20-C19	-6.19	1.20	1.34
24	A	608	BCR	C20-C19	-6.19	1.20	1.34
24	K	101	BCR	C20-C19	-6.19	1.20	1.34
24	T	102	BCR	C11-C12	-6.17	1.20	1.34
24	D	404	BCR	C21-C22	-6.16	1.27	1.35
24	h	101	BCR	C21-C22	-6.16	1.27	1.35
24	d	404	BCR	C21-C22	-6.16	1.27	1.35
24	H	101	BCR	C21-C22	-6.15	1.27	1.35
24	h	101	BCR	C20-C19	-6.15	1.20	1.34
24	H	101	BCR	C20-C19	-6.15	1.20	1.34
24	B	622	BCR	C21-C22	-6.14	1.27	1.35
24	b	622	BCR	C11-C12	-6.14	1.20	1.34
24	t	101	BCR	C11-C12	-6.14	1.20	1.34
24	k	102	BCR	C21-C22	-6.13	1.27	1.35
24	k	101	BCR	C20-C19	-6.13	1.20	1.34
24	d	404	BCR	C20-C19	-6.13	1.20	1.34
24	B	622	BCR	C11-C12	-6.13	1.20	1.34
24	c	514	BCR	C20-C19	-6.13	1.20	1.34
24	K	102	BCR	C21-C22	-6.13	1.27	1.35
24	C	514	BCR	C17-C18	-6.12	1.27	1.35
24	C	514	BCR	C20-C19	-6.12	1.20	1.34
24	c	514	BCR	C17-C18	-6.11	1.27	1.35
24	D	404	BCR	C11-C12	-6.11	1.20	1.34
24	d	404	BCR	C11-C12	-6.10	1.20	1.34
24	b	622	BCR	C21-C22	-6.09	1.27	1.35
24	K	101	BCR	C17-C18	-6.08	1.27	1.35
24	k	101	BCR	C17-C18	-6.07	1.27	1.35
24	B	622	BCR	C20-C19	-6.05	1.20	1.34
24	B	622	BCR	C16-C15	-6.05	1.19	1.35
24	c	515	BCR	C11-C12	-6.04	1.20	1.34
24	c	514	BCR	C21-C22	-6.04	1.27	1.35
24	b	622	BCR	C16-C15	-6.04	1.19	1.35
24	C	514	BCR	C21-C22	-6.03	1.27	1.35
24	c	514	BCR	C16-C15	-6.03	1.19	1.35
24	b	622	BCR	C20-C19	-6.02	1.20	1.34
24	B	619	BCR	C21-C22	-6.02	1.27	1.35
24	h	101	BCR	C11-C12	-6.02	1.20	1.34
24	C	514	BCR	C16-C15	-6.01	1.20	1.35
24	K	102	BCR	C20-C19	-6.00	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	102	BCR	C11-C12	-6.00	1.20	1.34
24	C	515	BCR	C11-C12	-5.99	1.20	1.34
24	H	101	BCR	C11-C12	-5.99	1.20	1.34
24	b	618	BCR	C21-C22	-5.99	1.27	1.35
24	k	102	BCR	C20-C19	-5.99	1.20	1.34
24	A	608	BCR	C17-C18	-5.99	1.27	1.35
24	k	102	BCR	C11-C12	-5.98	1.20	1.34
24	a	608	BCR	C17-C18	-5.97	1.27	1.35
24	T	102	BCR	C20-C19	-5.96	1.20	1.34
24	t	101	BCR	C20-C19	-5.93	1.20	1.34
24	C	515	BCR	C16-C15	-5.93	1.20	1.35
24	k	101	BCR	C16-C15	-5.92	1.20	1.35
24	c	515	BCR	C16-C15	-5.91	1.20	1.35
24	K	101	BCR	C16-C15	-5.91	1.20	1.35
24	C	515	BCR	C17-C18	-5.90	1.27	1.35
24	T	102	BCR	C21-C22	-5.89	1.27	1.35
24	d	404	BCR	C17-C18	-5.89	1.27	1.35
24	t	101	BCR	C21-C22	-5.89	1.27	1.35
24	D	404	BCR	C17-C18	-5.88	1.27	1.35
24	b	622	BCR	C17-C18	-5.87	1.27	1.35
24	B	622	BCR	C17-C18	-5.87	1.27	1.35
24	b	618	BCR	C20-C19	-5.86	1.20	1.34
24	B	619	BCR	C20-C19	-5.85	1.20	1.34
24	b	618	BCR	C11-C12	-5.84	1.20	1.34
24	c	515	BCR	C17-C18	-5.84	1.27	1.35
24	B	619	BCR	C11-C12	-5.83	1.20	1.34
24	a	608	BCR	C16-C15	-5.83	1.20	1.35
24	h	101	BCR	C16-C15	-5.82	1.20	1.35
24	T	101	BCR	C21-C22	-5.81	1.28	1.35
24	H	101	BCR	C17-C18	-5.81	1.28	1.35
24	B	618	BCR	C16-C15	-5.81	1.20	1.35
24	B	618	BCR	C11-C12	-5.80	1.20	1.34
24	H	101	BCR	C16-C15	-5.80	1.20	1.35
24	A	608	BCR	C16-C15	-5.80	1.20	1.35
24	K	102	BCR	C17-C18	-5.79	1.28	1.35
24	k	102	BCR	C17-C18	-5.79	1.28	1.35
24	T	101	BCR	C16-C15	-5.79	1.20	1.35
24	a	608	BCR	C11-C12	-5.79	1.21	1.34
24	D	404	BCR	C16-C15	-5.79	1.20	1.35
24	h	101	BCR	C17-C18	-5.78	1.28	1.35
24	d	404	BCR	C16-C15	-5.78	1.20	1.35
24	k	102	BCR	C16-C15	-5.78	1.20	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	608	BCR	C21-C22	-5.77	1.28	1.35
24	K	102	BCR	C16-C15	-5.77	1.20	1.35
24	T	102	BCR	C16-C15	-5.77	1.20	1.35
24	T	101	BCR	C11-C12	-5.76	1.21	1.34
24	A	608	BCR	C11-C12	-5.76	1.21	1.34
24	t	101	BCR	C16-C15	-5.75	1.20	1.35
24	a	608	BCR	C21-C22	-5.74	1.28	1.35
24	B	618	BCR	C21-C22	-5.72	1.28	1.35
24	C	514	BCR	C11-C10	-5.68	1.27	1.43
24	c	514	BCR	C11-C10	-5.65	1.27	1.43
24	T	102	BCR	C17-C18	-5.60	1.28	1.35
24	H	101	BCR	C11-C10	-5.59	1.27	1.43
24	t	101	BCR	C17-C18	-5.59	1.28	1.35
24	h	101	BCR	C11-C10	-5.58	1.27	1.43
24	d	404	BCR	C11-C10	-5.57	1.27	1.43
24	D	404	BCR	C11-C10	-5.57	1.27	1.43
24	T	101	BCR	C20-C19	-5.57	1.21	1.34
24	C	515	BCR	C11-C10	-5.56	1.27	1.43
24	c	515	BCR	C11-C10	-5.53	1.27	1.43
24	B	618	BCR	C20-C19	-5.53	1.21	1.34
24	b	622	BCR	C11-C10	-5.50	1.27	1.43
24	B	622	BCR	C11-C10	-5.49	1.27	1.43
24	K	101	BCR	C11-C10	-5.49	1.27	1.43
24	C	514	BCR	C15-C14	-5.49	1.27	1.43
24	k	101	BCR	C11-C10	-5.48	1.27	1.43
24	c	514	BCR	C15-C14	-5.46	1.27	1.43
24	T	101	BCR	C17-C18	-5.46	1.28	1.35
24	B	618	BCR	C17-C18	-5.44	1.28	1.35
24	B	622	BCR	C15-C14	-5.44	1.27	1.43
24	A	608	BCR	C11-C10	-5.44	1.27	1.43
24	C	515	BCR	C15-C14	-5.43	1.27	1.43
24	b	622	BCR	C15-C14	-5.43	1.27	1.43
24	a	608	BCR	C11-C10	-5.42	1.27	1.43
24	H	101	BCR	C15-C14	-5.42	1.27	1.43
24	c	515	BCR	C15-C14	-5.42	1.27	1.43
24	h	101	BCR	C15-C14	-5.41	1.27	1.43
24	k	102	BCR	C11-C10	-5.40	1.27	1.43
24	K	102	BCR	C11-C10	-5.40	1.27	1.43
24	B	619	BCR	C16-C15	-5.39	1.21	1.35
24	T	102	BCR	C11-C10	-5.37	1.27	1.43
24	b	618	BCR	C16-C15	-5.37	1.21	1.35
24	T	101	BCR	C11-C10	-5.37	1.27	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	101	BCR	C15-C14	-5.37	1.27	1.43
24	K	101	BCR	C15-C14	-5.36	1.27	1.43
24	d	404	BCR	C15-C14	-5.36	1.27	1.43
24	t	101	BCR	C11-C10	-5.36	1.27	1.43
24	B	618	BCR	C11-C10	-5.36	1.27	1.43
24	D	404	BCR	C15-C14	-5.35	1.27	1.43
24	t	101	BCR	C15-C14	-5.35	1.27	1.43
24	T	102	BCR	C15-C14	-5.35	1.27	1.43
24	k	102	BCR	C15-C14	-5.32	1.28	1.43
24	K	102	BCR	C15-C14	-5.30	1.28	1.43
24	A	608	BCR	C15-C14	-5.27	1.28	1.43
24	B	619	BCR	C11-C10	-5.26	1.28	1.43
24	b	618	BCR	C11-C10	-5.25	1.28	1.43
24	a	608	BCR	C15-C14	-5.24	1.28	1.43
24	b	618	BCR	C17-C18	-5.24	1.28	1.35
24	B	619	BCR	C17-C18	-5.23	1.28	1.35
24	B	619	BCR	C15-C14	-5.09	1.28	1.43
24	b	618	BCR	C15-C14	-5.08	1.28	1.43
24	B	618	BCR	C15-C14	-5.06	1.28	1.43
24	T	101	BCR	C15-C14	-5.06	1.28	1.43
24	B	622	BCR	C23-C22	-4.77	1.35	1.45
24	C	515	BCR	C23-C22	-4.77	1.35	1.45
24	b	622	BCR	C23-C22	-4.76	1.35	1.45
24	c	515	BCR	C23-C22	-4.73	1.35	1.45
33	v	201	HEM	C3C-C2C	-4.67	1.34	1.40
33	V	201	HEM	C3C-C2C	-4.66	1.34	1.40
24	D	404	BCR	C23-C22	-4.66	1.35	1.45
24	d	404	BCR	C23-C22	-4.66	1.35	1.45
24	K	101	BCR	C23-C22	-4.63	1.35	1.45
24	T	101	BCR	C23-C22	-4.62	1.35	1.45
24	B	618	BCR	C23-C22	-4.62	1.35	1.45
24	K	102	BCR	C23-C22	-4.61	1.35	1.45
24	k	101	BCR	C23-C22	-4.60	1.35	1.45
24	C	514	BCR	C23-C22	-4.59	1.35	1.45
24	H	101	BCR	C23-C22	-4.59	1.35	1.45
24	k	102	BCR	C23-C22	-4.59	1.35	1.45
24	c	514	BCR	C23-C22	-4.58	1.35	1.45
24	h	101	BCR	C23-C22	-4.54	1.35	1.45
33	f	101	HEM	C3C-C2C	-4.45	1.34	1.40
33	F	101	HEM	C3C-C2C	-4.43	1.34	1.40
24	b	618	BCR	C23-C22	-4.42	1.36	1.45
24	B	619	BCR	C23-C22	-4.41	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	T	102	BCR	C23-C22	-4.35	1.36	1.45
24	t	101	BCR	C23-C22	-4.35	1.36	1.45
33	f	101	HEM	C3B-C2B	-4.32	1.34	1.40
23	a	606	PHO	C1A-NA	-4.31	1.28	1.37
24	a	608	BCR	C23-C22	-4.30	1.36	1.45
23	A	606	PHO	C1A-NA	-4.29	1.28	1.37
33	F	101	HEM	C3B-C2B	-4.28	1.34	1.40
33	v	201	HEM	C3B-C2B	-4.26	1.34	1.40
24	A	608	BCR	C23-C22	-4.26	1.36	1.45
33	V	201	HEM	C3B-C2B	-4.20	1.35	1.40
23	a	605	PHO	C1A-NA	-4.11	1.28	1.37
23	A	605	PHO	C1A-NA	-4.11	1.28	1.37
23	A	606	PHO	C3D-C4D	-2.69	1.34	1.43
24	k	102	BCR	C24-C25	-2.69	1.35	1.45
24	c	515	BCR	C24-C25	-2.69	1.35	1.45
24	K	102	BCR	C24-C25	-2.69	1.35	1.45
23	a	606	PHO	C3D-C4D	-2.66	1.34	1.43
24	C	515	BCR	C24-C25	-2.66	1.36	1.45
24	c	514	BCR	C24-C25	-2.66	1.36	1.45
24	h	101	BCR	C24-C25	-2.65	1.36	1.45
24	H	101	BCR	C24-C25	-2.65	1.36	1.45
24	C	514	BCR	C24-C25	-2.65	1.36	1.45
24	k	101	BCR	C24-C25	-2.63	1.36	1.45
24	K	101	BCR	C24-C25	-2.62	1.36	1.45
23	a	605	PHO	C3D-C4D	-2.61	1.34	1.43
24	t	101	BCR	C24-C25	-2.60	1.36	1.45
24	B	618	BCR	C24-C25	-2.59	1.36	1.45
24	T	101	BCR	C24-C25	-2.59	1.36	1.45
23	A	605	PHO	C3D-C4D	-2.59	1.35	1.43
22	B	615	CLA	C1C-NC	-2.58	1.33	1.37
24	T	102	BCR	C24-C25	-2.57	1.36	1.45
24	D	404	BCR	C24-C25	-2.56	1.36	1.45
24	d	404	BCR	C24-C25	-2.55	1.36	1.45
22	b	615	CLA	C1C-NC	-2.55	1.33	1.37
24	a	608	BCR	C24-C25	-2.53	1.36	1.45
24	A	608	BCR	C24-C25	-2.53	1.36	1.45
24	b	622	BCR	C24-C25	-2.51	1.36	1.45
24	B	622	BCR	C24-C25	-2.48	1.36	1.45
24	b	618	BCR	C24-C25	-2.41	1.36	1.45
24	B	619	BCR	C24-C25	-2.39	1.37	1.45
22	c	509	CLA	C4C-NC	-2.35	1.34	1.37
22	C	509	CLA	C4C-NC	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	C1C-NC	-2.11	1.34	1.37
22	b	604	CLA	C1C-NC	-2.11	1.34	1.37
22	b	611	CLA	C1C-NC	-2.08	1.34	1.37
22	B	604	CLA	C1C-NC	-2.06	1.34	1.37
23	a	606	PHO	CHB-C4A	-2.06	1.34	1.40
23	A	606	PHO	CHB-C4A	-2.06	1.34	1.40
22	C	513	CLA	C4C-NC	-2.04	1.34	1.37
24	c	514	BCR	C8-C7	-2.02	1.26	1.32
22	d	403	CLA	C1C-NC	-2.00	1.34	1.37
22	c	513	CLA	C4C-NC	-2.00	1.34	1.37
22	b	605	CLA	C1C-C2C	2.00	1.48	1.44
22	C	505	CLA	C4C-C3C	2.01	1.48	1.45
25	l	102	SQD	O6-C1	2.01	1.43	1.40
22	c	502	CLA	C1C-C2C	2.02	1.48	1.44
22	C	502	CLA	C1C-C2C	2.02	1.48	1.44
29	C	520	LMG	O1-C1	2.02	1.43	1.40
22	B	605	CLA	C1C-C2C	2.02	1.48	1.44
22	D	401	CLA	C1C-C2C	2.02	1.48	1.44
31	d	410	DGD	O3G-C1D	2.03	1.43	1.40
22	D	401	CLA	C4C-C3C	2.03	1.48	1.45
33	v	201	HEM	CMA-C3A	2.03	1.55	1.51
22	b	606	CLA	C1C-C2C	2.03	1.48	1.44
22	b	615	CLA	C1C-C2C	2.03	1.48	1.44
25	l	101	SQD	O6-C1	2.03	1.43	1.40
22	d	401	CLA	C1C-C2C	2.04	1.48	1.44
22	b	613	CLA	C1C-C2C	2.04	1.48	1.44
31	D	410	DGD	O5D-C1E	2.05	1.43	1.40
22	D	403	CLA	C4C-C3C	2.05	1.48	1.45
29	c	520	LMG	O1-C1	2.05	1.43	1.40
22	C	509	CLA	C4C-C3C	2.06	1.48	1.45
22	B	613	CLA	C1C-C2C	2.06	1.48	1.44
22	d	403	CLA	C4C-C3C	2.07	1.48	1.45
22	c	509	CLA	C4C-C3C	2.07	1.48	1.45
22	c	505	CLA	C4C-C3C	2.07	1.48	1.45
22	B	615	CLA	C1C-C2C	2.07	1.48	1.44
22	d	402	CLA	CHB-C4A	2.08	1.36	1.33
22	c	512	CLA	C4C-C3C	2.09	1.48	1.45
22	C	512	CLA	C4C-C3C	2.09	1.48	1.45
22	D	402	CLA	CHB-C4A	2.10	1.36	1.33
31	d	410	DGD	O5D-C1E	2.11	1.44	1.40
29	z	101	LMG	O1-C1	2.11	1.44	1.40
22	b	604	CLA	C1C-C2C	2.11	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	508	CLA	C1C-C2C	2.11	1.48	1.44
33	f	101	HEM	C4D-ND	2.12	1.39	1.36
22	c	508	CLA	C1C-C2C	2.12	1.48	1.44
22	B	605	CLA	CHB-C4A	2.12	1.36	1.33
29	Z	101	LMG	O1-C1	2.12	1.44	1.40
33	F	101	HEM	C4D-ND	2.13	1.39	1.36
22	b	605	CLA	CHB-C4A	2.14	1.36	1.33
22	B	604	CLA	C1C-C2C	2.15	1.48	1.44
22	c	511	CLA	C1C-C2C	2.18	1.48	1.44
22	c	508	CLA	C4C-C3C	2.19	1.49	1.45
22	b	616	CLA	C1C-C2C	2.19	1.48	1.44
22	B	616	CLA	C1C-C2C	2.20	1.48	1.44
22	C	511	CLA	C1C-C2C	2.20	1.48	1.44
22	C	508	CLA	C4C-C3C	2.21	1.49	1.45
28	A	613	PL9	C2-C3	2.22	1.40	1.34
22	c	510	CLA	C1C-C2C	2.24	1.48	1.44
22	b	603	CLA	C1C-C2C	2.24	1.48	1.44
22	C	510	CLA	C1C-C2C	2.25	1.48	1.44
28	a	613	PL9	C2-C3	2.25	1.40	1.34
22	b	614	CLA	C1C-C2C	2.28	1.49	1.44
22	B	614	CLA	C1C-C2C	2.28	1.49	1.44
22	b	607	CLA	C1C-C2C	2.28	1.49	1.44
22	B	607	CLA	C1C-C2C	2.29	1.49	1.44
22	B	603	CLA	C1C-C2C	2.29	1.49	1.44
22	c	505	CLA	C1C-C2C	2.30	1.49	1.44
22	D	403	CLA	C1C-C2C	2.31	1.49	1.44
22	c	506	CLA	C1C-C2C	2.31	1.49	1.44
22	d	403	CLA	C1C-C2C	2.32	1.49	1.44
22	C	505	CLA	C1C-C2C	2.32	1.49	1.44
22	C	506	CLA	C1C-C2C	2.32	1.49	1.44
22	C	501	CLA	C1C-C2C	2.35	1.49	1.44
22	c	501	CLA	C1C-C2C	2.37	1.49	1.44
22	b	606	CLA	CHD-C4C	2.37	1.46	1.41
22	B	606	CLA	CHD-C4C	2.42	1.46	1.41
28	D	408	PL9	C6-C5	2.43	1.49	1.35
28	d	408	PL9	C6-C5	2.43	1.49	1.35
23	a	606	PHO	C3B-C4B	2.45	1.48	1.43
22	D	401	CLA	CHB-C4A	2.45	1.36	1.33
22	D	402	CLA	CHD-C4C	2.46	1.47	1.41
22	d	402	CLA	CHD-C4C	2.46	1.47	1.41
22	d	401	CLA	CHB-C4A	2.47	1.36	1.33
23	A	606	PHO	C3B-C4B	2.47	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	604	CLA	C4B-CHC	2.47	1.46	1.40
28	a	613	PL9	C6-C5	2.48	1.49	1.35
28	A	613	PL9	C6-C5	2.48	1.49	1.35
22	A	604	CLA	C4B-CHC	2.48	1.46	1.40
22	B	609	CLA	C4B-CHC	2.49	1.46	1.40
31	h	102	DGD	O5D-C1E	2.49	1.44	1.40
22	b	610	CLA	CHD-C4C	2.50	1.47	1.41
22	b	612	CLA	CHD-C4C	2.50	1.47	1.41
22	b	609	CLA	C4B-CHC	2.50	1.46	1.40
22	C	513	CLA	C1C-C2C	2.51	1.49	1.44
22	c	512	CLA	C1C-C2C	2.51	1.49	1.44
31	H	102	DGD	O5D-C1E	2.52	1.44	1.40
22	D	401	CLA	CHD-C4C	2.52	1.47	1.41
22	B	612	CLA	CHD-C4C	2.54	1.47	1.41
22	C	502	CLA	CHD-C4C	2.54	1.47	1.41
22	C	512	CLA	C1C-C2C	2.54	1.49	1.44
22	c	502	CLA	CHD-C4C	2.54	1.47	1.41
22	c	513	CLA	C1C-C2C	2.54	1.49	1.44
22	B	610	CLA	CHD-C4C	2.54	1.47	1.41
22	d	401	CLA	CHD-C4C	2.55	1.47	1.41
29	Z	101	LMG	O8-C28	2.55	1.46	1.33
29	z	101	LMG	O8-C28	2.56	1.46	1.33
22	b	617	CLA	CHD-C4C	2.57	1.47	1.41
22	B	617	CLA	CHD-C4C	2.58	1.47	1.41
22	B	605	CLA	C4B-CHC	2.58	1.47	1.40
22	b	605	CLA	C4B-CHC	2.59	1.47	1.40
22	B	604	CLA	CHD-C4C	2.59	1.47	1.41
22	C	507	CLA	C1C-C2C	2.61	1.49	1.44
22	b	604	CLA	CHD-C4C	2.63	1.47	1.41
22	C	504	CLA	C4B-CHC	2.64	1.47	1.40
22	b	615	CLA	C4B-CHC	2.64	1.47	1.40
22	c	507	CLA	C1C-C2C	2.65	1.49	1.44
22	B	615	CLA	C4B-CHC	2.65	1.47	1.40
23	A	605	PHO	C3D-C2D	2.66	1.46	1.38
23	A	605	PHO	CHC-C4B	2.67	1.47	1.40
22	c	504	CLA	C4B-CHC	2.67	1.47	1.40
23	A	606	PHO	CHD-C4C	2.67	1.47	1.40
22	B	615	CLA	CHD-C4C	2.68	1.47	1.41
22	B	602	CLA	C1C-C2C	2.68	1.49	1.44
23	a	605	PHO	CHC-C4B	2.68	1.47	1.40
22	b	602	CLA	C1C-C2C	2.68	1.49	1.44
22	A	607	CLA	CHD-C4C	2.69	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C4B-CHC	2.69	1.47	1.40
23	a	606	PHO	CHD-C4C	2.69	1.47	1.40
23	a	605	PHO	C3D-C2D	2.69	1.46	1.38
22	b	615	CLA	CHD-C4C	2.69	1.47	1.41
22	B	608	CLA	C4B-CHC	2.69	1.47	1.40
22	a	607	CLA	CHD-C4C	2.70	1.47	1.41
22	B	605	CLA	C3D-C2D	2.70	1.46	1.40
22	b	605	CLA	C3D-C2D	2.71	1.46	1.40
22	B	611	CLA	CHD-C4C	2.72	1.47	1.41
22	C	510	CLA	C4B-CHC	2.73	1.47	1.40
22	b	611	CLA	CHD-C4C	2.73	1.47	1.41
22	D	401	CLA	C3D-C2D	2.73	1.46	1.40
22	d	401	CLA	C3D-C2D	2.73	1.46	1.40
22	b	605	CLA	CHD-C4C	2.75	1.47	1.41
22	c	510	CLA	C4B-CHC	2.75	1.47	1.40
22	b	609	CLA	CHD-C4C	2.75	1.47	1.41
22	B	604	CLA	C4B-CHC	2.75	1.47	1.40
22	a	604	CLA	CHD-C4C	2.76	1.47	1.41
22	c	503	CLA	C1C-C2C	2.76	1.49	1.44
22	b	604	CLA	C4B-CHC	2.76	1.47	1.40
22	C	509	CLA	C4B-CHC	2.78	1.47	1.40
22	B	605	CLA	CHD-C4C	2.78	1.47	1.41
22	A	604	CLA	CHD-C4C	2.78	1.47	1.41
22	B	609	CLA	CHD-C4C	2.78	1.47	1.41
22	C	503	CLA	C1C-C2C	2.79	1.50	1.44
22	c	509	CLA	C4B-CHC	2.80	1.47	1.40
22	C	509	CLA	CHD-C4C	2.80	1.47	1.41
22	b	602	CLA	C3D-C2D	2.80	1.46	1.40
22	B	614	CLA	CHD-C4C	2.80	1.47	1.41
22	A	604	CLA	C1B-CHB	2.81	1.47	1.40
22	D	402	CLA	C1B-CHB	2.81	1.47	1.40
22	B	602	CLA	C3D-C2D	2.81	1.46	1.40
22	c	508	CLA	CHD-C4C	2.81	1.47	1.41
22	b	616	CLA	C4B-CHC	2.82	1.47	1.40
22	d	402	CLA	C1B-CHB	2.82	1.47	1.40
22	C	508	CLA	CHD-C4C	2.82	1.47	1.41
22	B	616	CLA	C4B-CHC	2.82	1.47	1.40
22	B	612	CLA	C4B-CHC	2.82	1.47	1.40
23	A	605	PHO	CHD-C4C	2.82	1.47	1.40
22	b	614	CLA	CHD-C4C	2.84	1.47	1.41
22	a	604	CLA	C1B-CHB	2.84	1.47	1.40
22	a	603	CLA	CHD-C4C	2.84	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	CHD-C4C	2.85	1.47	1.41
23	a	605	PHO	CHD-C4C	2.86	1.47	1.40
22	D	402	CLA	C4B-CHC	2.86	1.47	1.40
22	b	612	CLA	C4B-CHC	2.86	1.47	1.40
22	b	606	CLA	C4B-CHC	2.86	1.47	1.40
22	c	503	CLA	C3D-C2D	2.86	1.46	1.40
22	d	402	CLA	C4B-CHC	2.87	1.47	1.40
22	B	606	CLA	C4B-CHC	2.87	1.47	1.40
22	b	617	CLA	C4B-CHC	2.88	1.47	1.40
22	B	612	CLA	C3D-C2D	2.88	1.46	1.40
22	c	510	CLA	CHD-C4C	2.88	1.48	1.41
22	A	603	CLA	CHD-C4C	2.88	1.48	1.41
22	D	401	CLA	C1B-CHB	2.89	1.47	1.40
22	c	502	CLA	C4B-CHC	2.89	1.47	1.40
22	b	612	CLA	C3D-C2D	2.89	1.46	1.40
22	b	607	CLA	C3D-C2D	2.89	1.46	1.40
22	C	503	CLA	C3D-C2D	2.90	1.46	1.40
22	c	511	CLA	C4B-CHC	2.90	1.47	1.40
22	C	513	CLA	CHD-C4C	2.90	1.48	1.41
22	C	510	CLA	CHD-C4C	2.90	1.48	1.41
22	c	513	CLA	CHD-C4C	2.90	1.48	1.41
22	d	401	CLA	C1B-CHB	2.90	1.47	1.40
22	C	502	CLA	C4B-CHC	2.91	1.48	1.40
22	C	511	CLA	CHD-C4C	2.92	1.48	1.41
22	b	610	CLA	C4B-CHC	2.92	1.48	1.40
22	B	614	CLA	C4B-CHC	2.92	1.48	1.40
22	b	614	CLA	C4B-CHC	2.92	1.48	1.40
22	C	511	CLA	C4B-CHC	2.93	1.48	1.40
22	B	617	CLA	C4B-CHC	2.93	1.48	1.40
22	B	607	CLA	C3D-C2D	2.93	1.46	1.40
22	b	616	CLA	CHD-C4C	2.93	1.48	1.41
22	D	403	CLA	CHD-C4C	2.93	1.48	1.41
22	B	610	CLA	C4B-CHC	2.93	1.48	1.40
22	d	401	CLA	C4B-CHC	2.93	1.48	1.40
22	D	401	CLA	C4B-CHC	2.93	1.48	1.40
22	c	511	CLA	CHD-C4C	2.93	1.48	1.41
22	B	607	CLA	CHD-C4C	2.94	1.48	1.41
22	C	507	CLA	CHD-C4C	2.94	1.48	1.41
23	a	606	PHO	C3D-C2D	2.94	1.46	1.38
22	B	609	CLA	C1B-CHB	2.95	1.48	1.40
22	B	613	CLA	C3D-C2D	2.96	1.46	1.40
22	C	503	CLA	CHD-C4C	2.96	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	616	CLA	CHD-C4C	2.96	1.48	1.41
22	b	602	CLA	CHD-C4C	2.96	1.48	1.41
22	b	603	CLA	CHD-C4C	2.96	1.48	1.41
22	a	607	CLA	C3D-C2D	2.96	1.46	1.40
23	A	606	PHO	C3D-C2D	2.96	1.46	1.38
22	b	607	CLA	CHD-C4C	2.96	1.48	1.41
22	c	505	CLA	CHD-C4C	2.97	1.48	1.41
22	d	403	CLA	CHD-C4C	2.97	1.48	1.41
22	b	609	CLA	C1B-CHB	2.97	1.48	1.40
22	c	506	CLA	CHD-C4C	2.97	1.48	1.41
22	c	507	CLA	CHD-C4C	2.97	1.48	1.41
22	B	602	CLA	CHD-C4C	2.97	1.48	1.41
22	c	503	CLA	CHD-C4C	2.97	1.48	1.41
22	B	603	CLA	CHD-C4C	2.97	1.48	1.41
22	C	505	CLA	CHD-C4C	2.98	1.48	1.41
22	C	509	CLA	C3D-C2D	2.98	1.46	1.40
22	C	506	CLA	C3D-C2D	2.98	1.46	1.40
22	c	506	CLA	C3D-C2D	2.99	1.46	1.40
22	b	613	CLA	C3D-C2D	2.99	1.46	1.40
22	c	509	CLA	C3D-C2D	2.99	1.46	1.40
22	A	607	CLA	C3D-C2D	2.99	1.46	1.40
22	A	603	CLA	C3D-C2D	2.99	1.46	1.40
22	c	508	CLA	C4B-CHC	3.00	1.48	1.40
22	C	508	CLA	C4B-CHC	3.00	1.48	1.40
22	B	613	CLA	C4B-CHC	3.00	1.48	1.40
22	A	603	CLA	C4B-CHC	3.00	1.48	1.40
22	D	403	CLA	C4B-CHC	3.01	1.48	1.40
22	C	502	CLA	C3D-C2D	3.01	1.46	1.40
22	c	512	CLA	C4B-CHC	3.01	1.48	1.40
22	B	608	CLA	CHD-C4C	3.01	1.48	1.41
22	C	506	CLA	CHD-C4C	3.01	1.48	1.41
22	b	613	CLA	C4B-CHC	3.01	1.48	1.40
22	B	607	CLA	C4B-CHC	3.02	1.48	1.40
22	b	608	CLA	C3D-C2D	3.02	1.46	1.40
22	b	615	CLA	C3D-C2D	3.02	1.46	1.40
22	d	403	CLA	C4B-CHC	3.02	1.48	1.40
22	a	603	CLA	C4B-CHC	3.02	1.48	1.40
22	c	507	CLA	C3D-C2D	3.02	1.46	1.40
22	C	505	CLA	C3D-C2D	3.02	1.46	1.40
32	d	405	LHG	O7-C7	3.02	1.43	1.34
22	c	502	CLA	C3D-C2D	3.02	1.46	1.40
22	C	507	CLA	C3D-C2D	3.02	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	C3D-C2D	3.02	1.46	1.40
22	b	613	CLA	CHD-C4C	3.02	1.48	1.41
22	B	611	CLA	C4B-CHC	3.03	1.48	1.40
22	a	603	CLA	C3D-C2D	3.03	1.46	1.40
22	B	608	CLA	C3D-C2D	3.03	1.46	1.40
22	C	506	CLA	C4B-CHC	3.03	1.48	1.40
22	b	607	CLA	C4B-CHC	3.03	1.48	1.40
22	b	612	CLA	C1B-CHB	3.03	1.48	1.40
22	C	512	CLA	C4B-CHC	3.03	1.48	1.40
22	c	505	CLA	C3D-C2D	3.03	1.46	1.40
22	b	608	CLA	CHD-C4C	3.04	1.48	1.41
22	c	506	CLA	C4B-CHC	3.04	1.48	1.40
22	B	612	CLA	C1B-CHB	3.04	1.48	1.40
22	B	613	CLA	CHD-C4C	3.04	1.48	1.41
22	C	510	CLA	C3D-C2D	3.05	1.46	1.40
32	D	405	LHG	O7-C7	3.05	1.43	1.34
22	c	510	CLA	C3D-C2D	3.05	1.46	1.40
22	b	611	CLA	C4B-CHC	3.06	1.48	1.40
23	A	605	PHO	OBD-CAD	3.07	1.27	1.22
23	a	605	PHO	OBD-CAD	3.08	1.27	1.22
22	A	607	CLA	C4B-CHC	3.08	1.48	1.40
22	B	606	CLA	C3D-C2D	3.08	1.46	1.40
22	b	602	CLA	C1B-CHB	3.09	1.48	1.40
22	a	607	CLA	C4B-CHC	3.10	1.48	1.40
22	d	403	CLA	C3D-C2D	3.11	1.46	1.40
22	b	616	CLA	C3D-C2D	3.11	1.46	1.40
22	B	602	CLA	C1B-CHB	3.11	1.48	1.40
22	b	606	CLA	C3D-C2D	3.11	1.46	1.40
22	B	616	CLA	C3D-C2D	3.11	1.46	1.40
22	b	610	CLA	C3D-C2D	3.12	1.46	1.40
22	C	507	CLA	C4B-CHC	3.12	1.48	1.40
22	c	507	CLA	C4B-CHC	3.12	1.48	1.40
22	C	501	CLA	CHD-C4C	3.12	1.48	1.41
22	D	403	CLA	C3D-C2D	3.12	1.46	1.40
23	A	606	PHO	CHC-C4B	3.13	1.48	1.40
22	C	509	CLA	C1B-CHB	3.13	1.48	1.40
22	c	509	CLA	C1B-CHB	3.13	1.48	1.40
22	c	501	CLA	C4B-CHC	3.13	1.48	1.40
22	b	609	CLA	C3D-C2D	3.14	1.46	1.40
22	c	512	CLA	CHD-C4C	3.14	1.48	1.41
22	B	609	CLA	C3D-C2D	3.14	1.46	1.40
22	B	610	CLA	C3D-C2D	3.15	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	CHD-C4C	3.15	1.48	1.41
22	c	501	CLA	CHD-C4C	3.15	1.48	1.41
22	c	503	CLA	C1B-CHB	3.15	1.48	1.40
23	a	606	PHO	CHC-C4B	3.16	1.48	1.40
22	b	611	CLA	C1B-CHB	3.17	1.48	1.40
22	B	611	CLA	C1B-CHB	3.17	1.48	1.40
22	B	603	CLA	C4B-CHC	3.17	1.48	1.40
22	c	502	CLA	C1B-CHB	3.17	1.48	1.40
22	b	617	CLA	C1B-CHB	3.17	1.48	1.40
22	b	603	CLA	C4B-CHC	3.17	1.48	1.40
22	C	501	CLA	C4B-CHC	3.17	1.48	1.40
22	B	617	CLA	C1B-CHB	3.18	1.48	1.40
22	C	503	CLA	C1B-CHB	3.18	1.48	1.40
22	A	603	CLA	C1B-CHB	3.18	1.48	1.40
22	C	502	CLA	C1B-CHB	3.18	1.48	1.40
22	C	505	CLA	C4B-CHC	3.18	1.48	1.40
22	a	603	CLA	C1B-CHB	3.18	1.48	1.40
22	A	604	CLA	C3D-C2D	3.18	1.47	1.40
22	c	505	CLA	C4B-CHC	3.19	1.48	1.40
22	d	402	CLA	C3D-C2D	3.20	1.47	1.40
22	b	614	CLA	C3D-C2D	3.20	1.47	1.40
22	B	614	CLA	C3D-C2D	3.21	1.47	1.40
22	B	616	CLA	C1B-CHB	3.21	1.48	1.40
22	D	402	CLA	C3D-C2D	3.21	1.47	1.40
22	b	616	CLA	C1B-CHB	3.21	1.48	1.40
22	c	501	CLA	C3D-C2D	3.22	1.47	1.40
22	C	501	CLA	C1B-CHB	3.22	1.48	1.40
22	a	604	CLA	C3D-C2D	3.22	1.47	1.40
22	c	503	CLA	C4B-CHC	3.22	1.48	1.40
22	C	501	CLA	C3D-C2D	3.23	1.47	1.40
31	C	518	DGD	O2G-C1B	3.24	1.43	1.34
22	c	512	CLA	C3D-C2D	3.24	1.47	1.40
22	C	503	CLA	C4B-CHC	3.24	1.48	1.40
22	c	501	CLA	C1B-CHB	3.24	1.48	1.40
22	b	611	CLA	C3D-C2D	3.24	1.47	1.40
22	B	611	CLA	C3D-C2D	3.24	1.47	1.40
22	B	608	CLA	O2A-CGA	3.24	1.43	1.33
22	b	608	CLA	O2A-CGA	3.25	1.43	1.33
31	c	518	DGD	O2G-C1B	3.25	1.43	1.34
22	C	512	CLA	C3D-C2D	3.27	1.47	1.40
22	C	504	CLA	C3D-C2D	3.27	1.47	1.40
22	B	613	CLA	C1B-CHB	3.28	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	C4B-CHC	3.28	1.49	1.40
22	b	610	CLA	C1B-CHB	3.29	1.49	1.40
22	C	504	CLA	CHD-C4C	3.29	1.48	1.41
22	C	513	CLA	C4B-CHC	3.29	1.49	1.40
22	c	511	CLA	C3D-C2D	3.29	1.47	1.40
22	b	613	CLA	C1B-CHB	3.29	1.49	1.40
22	B	610	CLA	C1B-CHB	3.30	1.49	1.40
22	c	504	CLA	C3D-C2D	3.30	1.47	1.40
22	b	604	CLA	C3D-C2D	3.30	1.47	1.40
22	C	511	CLA	C3D-C2D	3.31	1.47	1.40
22	B	604	CLA	C3D-C2D	3.31	1.47	1.40
22	C	513	CLA	C3D-C2D	3.32	1.47	1.40
22	b	617	CLA	C3D-C2D	3.32	1.47	1.40
22	B	604	CLA	C1B-CHB	3.33	1.49	1.40
22	b	605	CLA	C1B-CHB	3.33	1.49	1.40
22	c	513	CLA	C3D-C2D	3.33	1.47	1.40
22	B	617	CLA	C3D-C2D	3.34	1.47	1.40
22	c	504	CLA	CHD-C4C	3.34	1.49	1.41
22	b	604	CLA	C1B-CHB	3.34	1.49	1.40
22	B	605	CLA	C1B-CHB	3.36	1.49	1.40
22	b	603	CLA	C3D-C2D	3.37	1.47	1.40
22	c	505	CLA	C1B-CHB	3.40	1.49	1.40
22	b	603	CLA	O2A-CGA	3.40	1.43	1.33
22	b	612	CLA	O2A-CGA	3.40	1.43	1.33
22	B	603	CLA	C3D-C2D	3.40	1.47	1.40
22	B	603	CLA	O2A-CGA	3.40	1.43	1.33
22	B	607	CLA	C1B-CHB	3.41	1.49	1.40
22	B	612	CLA	O2A-CGA	3.41	1.43	1.33
22	b	602	CLA	C4B-CHC	3.42	1.49	1.40
22	C	508	CLA	C3D-C2D	3.42	1.47	1.40
22	C	507	CLA	C1B-CHB	3.42	1.49	1.40
22	a	607	CLA	C1B-CHB	3.43	1.49	1.40
22	c	507	CLA	C1B-CHB	3.43	1.49	1.40
22	C	508	CLA	C1B-CHB	3.43	1.49	1.40
22	B	605	CLA	OBD-CAD	3.43	1.27	1.22
22	c	508	CLA	C1B-CHB	3.44	1.49	1.40
22	C	504	CLA	C1B-CHB	3.44	1.49	1.40
22	b	607	CLA	C1B-CHB	3.44	1.49	1.40
22	b	615	CLA	C1B-CHB	3.44	1.49	1.40
22	A	607	CLA	C1B-CHB	3.44	1.49	1.40
22	B	602	CLA	C4B-CHC	3.44	1.49	1.40
22	C	512	CLA	C1B-CHB	3.44	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	C1B-CHB	3.45	1.49	1.40
22	c	504	CLA	C1B-CHB	3.45	1.49	1.40
22	B	615	CLA	C1B-CHB	3.46	1.49	1.40
22	a	603	CLA	O2A-CGA	3.46	1.43	1.33
22	C	513	CLA	C1B-CHB	3.46	1.49	1.40
22	c	512	CLA	C1B-CHB	3.46	1.49	1.40
22	c	513	CLA	C1B-CHB	3.47	1.49	1.40
22	c	508	CLA	C3D-C2D	3.48	1.47	1.40
22	b	605	CLA	OBD-CAD	3.48	1.27	1.22
22	c	511	CLA	C1B-CHB	3.48	1.49	1.40
22	A	603	CLA	O2A-CGA	3.49	1.43	1.33
22	b	603	CLA	C1B-CHB	3.49	1.49	1.40
22	C	511	CLA	C1B-CHB	3.50	1.49	1.40
22	B	614	CLA	C1B-CHB	3.50	1.49	1.40
22	B	603	CLA	C1B-CHB	3.50	1.49	1.40
22	b	606	CLA	C1B-CHB	3.51	1.49	1.40
22	C	506	CLA	C1B-CHB	3.51	1.49	1.40
22	C	510	CLA	C1B-CHB	3.51	1.49	1.40
22	c	510	CLA	C1B-CHB	3.52	1.49	1.40
22	B	606	CLA	C1B-CHB	3.52	1.49	1.40
22	b	614	CLA	C1B-CHB	3.52	1.49	1.40
22	C	503	CLA	OBD-CAD	3.52	1.27	1.22
22	c	506	CLA	C1B-CHB	3.53	1.49	1.40
22	c	503	CLA	OBD-CAD	3.53	1.27	1.22
22	b	608	CLA	C1B-CHB	3.55	1.49	1.40
22	B	608	CLA	C1B-CHB	3.55	1.49	1.40
22	d	403	CLA	C1B-CHB	3.56	1.49	1.40
33	f	101	HEM	C3C-CAC	3.56	1.55	1.47
31	C	517	DGD	O2G-C1B	3.58	1.44	1.34
22	D	403	CLA	C1B-CHB	3.58	1.49	1.40
33	F	101	HEM	C3C-CAC	3.59	1.55	1.47
31	c	517	DGD	O2G-C1B	3.60	1.44	1.34
23	A	605	PHO	CHD-C1D	3.62	1.45	1.38
23	a	605	PHO	CHD-C1D	3.62	1.45	1.38
32	D	407	LHG	O7-C7	3.63	1.45	1.34
22	b	613	CLA	O2A-CGA	3.64	1.44	1.33
32	d	407	LHG	O7-C7	3.64	1.45	1.34
29	D	406	LMG	O8-C28	3.65	1.44	1.33
22	b	614	CLA	O2A-CGA	3.65	1.44	1.33
29	d	406	LMG	O8-C28	3.65	1.44	1.33
22	B	613	CLA	O2A-CGA	3.65	1.44	1.33
32	L	102	LHG	O7-C7	3.66	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	O2A-CGA	3.66	1.44	1.33
22	B	606	CLA	O2A-CGA	3.66	1.44	1.33
32	l	103	LHG	O7-C7	3.67	1.45	1.34
23	a	606	PHO	O2A-CGA	3.67	1.44	1.33
23	A	606	PHO	O2A-CGA	3.68	1.44	1.33
22	b	606	CLA	O2A-CGA	3.68	1.44	1.33
33	F	101	HEM	C3B-CAB	3.69	1.55	1.47
31	h	102	DGD	O2G-C1B	3.71	1.45	1.34
31	H	102	DGD	O2G-C1B	3.71	1.45	1.34
33	f	101	HEM	C3B-CAB	3.71	1.55	1.47
22	A	604	CLA	O2A-CGA	3.72	1.44	1.33
22	b	605	CLA	O2A-CGA	3.73	1.44	1.33
22	B	605	CLA	O2A-CGA	3.74	1.44	1.33
32	d	409	LHG	O7-C7	3.76	1.45	1.34
32	D	409	LHG	O7-C7	3.76	1.45	1.34
29	d	406	LMG	O7-C10	3.77	1.45	1.34
22	B	612	CLA	OBD-CAD	3.77	1.28	1.22
22	a	604	CLA	O2A-CGA	3.77	1.44	1.33
29	B	620	LMG	O7-C10	3.78	1.45	1.34
22	b	612	CLA	OBD-CAD	3.78	1.28	1.22
29	D	406	LMG	O7-C10	3.78	1.45	1.34
22	b	611	CLA	O2A-CGA	3.79	1.44	1.33
22	C	505	CLA	O2A-CGA	3.79	1.44	1.33
31	C	516	DGD	O2G-C1B	3.79	1.45	1.34
23	a	606	PHO	OBD-CAD	3.79	1.28	1.22
29	b	619	LMG	O7-C10	3.81	1.45	1.34
22	B	611	CLA	O2A-CGA	3.81	1.44	1.33
31	c	516	DGD	O2G-C1B	3.82	1.45	1.34
22	c	505	CLA	O2A-CGA	3.82	1.44	1.33
31	C	516	DGD	O1G-C1A	3.82	1.44	1.33
22	b	614	CLA	OBD-CAD	3.82	1.28	1.22
23	A	606	PHO	OBD-CAD	3.82	1.28	1.22
22	B	614	CLA	OBD-CAD	3.83	1.28	1.22
31	c	516	DGD	O1G-C1A	3.85	1.44	1.33
22	B	609	CLA	O2A-CGA	3.85	1.44	1.33
33	v	201	HEM	C3C-CAC	3.85	1.55	1.47
33	V	201	HEM	C3C-CAC	3.85	1.55	1.47
23	A	605	PHO	O2A-CGA	3.86	1.44	1.33
22	b	609	CLA	O2A-CGA	3.86	1.44	1.33
31	c	518	DGD	O1G-C1A	3.86	1.44	1.33
31	C	518	DGD	O1G-C1A	3.87	1.44	1.33
23	a	605	PHO	O2A-CGA	3.88	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	402	CLA	CHC-C1C	3.88	1.46	1.35
32	D	407	LHG	O8-C23	3.88	1.44	1.33
22	d	402	CLA	O2A-CGA	3.88	1.44	1.33
22	D	402	CLA	CHC-C1C	3.89	1.46	1.35
22	D	402	CLA	O2A-CGA	3.89	1.44	1.33
22	C	510	CLA	O2A-CGA	3.89	1.44	1.33
22	B	609	CLA	CHC-C1C	3.89	1.46	1.35
32	d	407	LHG	O8-C23	3.89	1.44	1.33
22	d	401	CLA	CHC-C1C	3.90	1.46	1.35
22	c	512	CLA	OBD-CAD	3.90	1.28	1.22
22	D	401	CLA	CHC-C1C	3.91	1.46	1.35
31	H	102	DGD	O1G-C1A	3.91	1.45	1.33
32	D	405	LHG	O8-C23	3.91	1.45	1.33
22	c	510	CLA	O2A-CGA	3.91	1.45	1.33
22	b	609	CLA	CHC-C1C	3.91	1.46	1.35
22	B	604	CLA	O2A-CGA	3.91	1.45	1.33
32	d	405	LHG	O8-C23	3.92	1.45	1.33
33	V	201	HEM	C3B-CAB	3.92	1.56	1.47
22	c	504	CLA	O2A-CGA	3.93	1.45	1.33
22	B	615	CLA	OBD-CAD	3.93	1.28	1.22
31	h	102	DGD	O1G-C1A	3.93	1.45	1.33
25	a	609	SQD	O48-C23	3.93	1.45	1.33
22	B	609	CLA	OBD-CAD	3.93	1.28	1.22
22	C	512	CLA	OBD-CAD	3.93	1.28	1.22
22	c	508	CLA	O2A-CGA	3.94	1.45	1.33
22	b	608	CLA	OBD-CAD	3.94	1.28	1.22
22	B	608	CLA	OBD-CAD	3.95	1.28	1.22
22	C	504	CLA	O2A-CGA	3.95	1.45	1.33
25	A	609	SQD	O48-C23	3.95	1.45	1.33
22	C	508	CLA	O2A-CGA	3.95	1.45	1.33
33	v	201	HEM	C3B-CAB	3.95	1.56	1.47
22	b	604	CLA	O2A-CGA	3.95	1.45	1.33
32	l	103	LHG	O8-C23	3.96	1.45	1.33
25	a	609	SQD	O47-C7	3.96	1.45	1.34
22	b	609	CLA	OBD-CAD	3.96	1.28	1.22
25	A	609	SQD	O47-C7	3.96	1.46	1.34
32	L	102	LHG	O8-C23	3.97	1.45	1.33
22	b	615	CLA	OBD-CAD	3.97	1.28	1.22
22	B	615	CLA	O2A-CGA	3.97	1.45	1.33
22	B	605	CLA	CHC-C1C	3.98	1.47	1.35
22	B	606	CLA	OBD-CAD	3.98	1.28	1.22
22	c	501	CLA	O2A-CGA	3.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	CHC-C1C	3.99	1.47	1.35
22	d	402	CLA	O2D-CGD	3.99	1.43	1.33
22	B	612	CLA	CHC-C1C	3.99	1.47	1.35
22	B	607	CLA	O2A-CGA	3.99	1.45	1.33
22	c	502	CLA	O2A-CGA	3.99	1.45	1.33
22	a	604	CLA	CHC-C1C	3.99	1.47	1.35
22	b	605	CLA	CHC-C1C	4.00	1.47	1.35
22	b	615	CLA	O2A-CGA	4.00	1.45	1.33
22	b	607	CLA	O2A-CGA	4.00	1.45	1.33
22	C	501	CLA	O2A-CGA	4.00	1.45	1.33
22	A	604	CLA	CHC-C1C	4.00	1.47	1.35
22	c	510	CLA	CHC-C1C	4.01	1.47	1.35
22	B	610	CLA	O2A-CGA	4.01	1.45	1.33
22	b	606	CLA	OBD-CAD	4.01	1.28	1.22
22	D	402	CLA	O2D-CGD	4.02	1.43	1.33
22	C	510	CLA	CHC-C1C	4.02	1.47	1.35
22	C	502	CLA	O2A-CGA	4.02	1.45	1.33
31	c	517	DGD	O1G-C1A	4.02	1.45	1.33
31	C	517	DGD	O1G-C1A	4.02	1.45	1.33
25	l	101	SQD	O48-C23	4.04	1.45	1.33
22	b	610	CLA	O2A-CGA	4.04	1.45	1.33
29	C	519	LMG	O7-C10	4.04	1.46	1.34
25	L	101	SQD	O48-C23	4.05	1.45	1.33
22	B	613	CLA	OBD-CAD	4.05	1.28	1.22
32	e	101	LHG	O7-C7	4.06	1.46	1.34
32	D	409	LHG	O8-C23	4.06	1.45	1.33
32	d	409	LHG	O8-C23	4.06	1.45	1.33
22	C	511	CLA	O2A-CGA	4.06	1.45	1.33
22	B	616	CLA	O2A-CGA	4.06	1.45	1.33
22	D	403	CLA	O2A-CGA	4.06	1.45	1.33
29	a	614	LMG	O7-C10	4.06	1.46	1.34
22	D	403	CLA	OBD-CAD	4.06	1.28	1.22
29	A	614	LMG	O7-C10	4.07	1.46	1.34
32	E	101	LHG	O7-C7	4.07	1.46	1.34
29	c	519	LMG	O7-C10	4.08	1.46	1.34
22	c	511	CLA	O2A-CGA	4.08	1.45	1.33
22	b	616	CLA	O2A-CGA	4.08	1.45	1.33
22	d	403	CLA	O2A-CGA	4.09	1.45	1.33
22	B	611	CLA	OBD-CAD	4.09	1.28	1.22
22	B	616	CLA	OBD-CAD	4.09	1.28	1.22
22	C	513	CLA	O2A-CGA	4.09	1.45	1.33
29	Z	101	LMG	O7-C10	4.09	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	613	CLA	OBD-CAD	4.09	1.28	1.22
22	A	607	CLA	O2A-CGA	4.09	1.45	1.33
22	d	403	CLA	OBD-CAD	4.09	1.28	1.22
22	c	508	CLA	OBD-CAD	4.10	1.28	1.22
25	B	601	SQD	O47-C7	4.10	1.46	1.34
25	b	601	SQD	O47-C7	4.10	1.46	1.34
22	c	503	CLA	O2A-CGA	4.10	1.45	1.33
22	c	513	CLA	O2A-CGA	4.10	1.45	1.33
22	c	506	CLA	OBD-CAD	4.10	1.28	1.22
22	b	611	CLA	OBD-CAD	4.10	1.28	1.22
22	C	505	CLA	OBD-CAD	4.11	1.28	1.22
29	z	101	LMG	O7-C10	4.11	1.46	1.34
22	A	607	CLA	O2D-CGD	4.11	1.43	1.33
22	a	607	CLA	O2D-CGD	4.12	1.43	1.33
22	C	503	CLA	O2A-CGA	4.12	1.45	1.33
22	a	607	CLA	O2A-CGA	4.12	1.45	1.33
22	C	508	CLA	OBD-CAD	4.13	1.28	1.22
22	C	507	CLA	OBD-CAD	4.13	1.28	1.22
22	b	616	CLA	OBD-CAD	4.14	1.28	1.22
22	B	604	CLA	CHC-C1C	4.14	1.47	1.35
22	B	610	CLA	OBD-CAD	4.14	1.28	1.22
22	C	506	CLA	OBD-CAD	4.14	1.28	1.22
22	C	512	CLA	O2A-CGA	4.14	1.45	1.33
22	d	401	CLA	O2A-CGA	4.15	1.45	1.33
29	a	614	LMG	O8-C28	4.16	1.45	1.33
22	c	507	CLA	OBD-CAD	4.16	1.28	1.22
22	c	507	CLA	O2A-CGA	4.16	1.45	1.33
22	C	502	CLA	OBD-CAD	4.16	1.28	1.22
29	A	614	LMG	O8-C28	4.16	1.45	1.33
22	C	507	CLA	O2A-CGA	4.16	1.45	1.33
22	C	501	CLA	OBD-CAD	4.16	1.28	1.22
22	c	505	CLA	OBD-CAD	4.16	1.28	1.22
22	c	504	CLA	CHC-C1C	4.16	1.47	1.35
22	C	504	CLA	CHC-C1C	4.17	1.47	1.35
22	B	617	CLA	O2A-CGA	4.18	1.45	1.33
22	c	509	CLA	O2A-CGA	4.18	1.45	1.33
25	L	101	SQD	O47-C7	4.18	1.46	1.34
22	c	512	CLA	O2A-CGA	4.18	1.45	1.33
29	C	519	LMG	O8-C28	4.18	1.45	1.33
22	b	604	CLA	CHC-C1C	4.18	1.47	1.35
22	c	504	CLA	OBD-CAD	4.19	1.28	1.22
22	c	501	CLA	OBD-CAD	4.19	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	617	CLA	O2A-CGA	4.19	1.45	1.33
22	C	509	CLA	O2A-CGA	4.19	1.45	1.33
22	b	608	CLA	CHC-C1C	4.19	1.47	1.35
25	l	101	SQD	O47-C7	4.20	1.46	1.34
22	b	610	CLA	OBD-CAD	4.20	1.28	1.22
22	b	602	CLA	OBD-CAD	4.20	1.28	1.22
22	b	603	CLA	O2D-CGD	4.20	1.44	1.33
29	c	519	LMG	O8-C28	4.20	1.45	1.33
22	D	401	CLA	O2A-CGA	4.20	1.45	1.33
22	B	602	CLA	OBD-CAD	4.21	1.28	1.22
25	b	621	SQD	O47-C7	4.21	1.46	1.34
22	B	605	CLA	O2D-CGD	4.22	1.44	1.33
22	b	605	CLA	O2D-CGD	4.22	1.44	1.33
22	A	604	CLA	OBD-CAD	4.22	1.28	1.22
22	B	603	CLA	O2D-CGD	4.22	1.44	1.33
22	c	502	CLA	OBD-CAD	4.23	1.28	1.22
23	A	605	PHO	CHC-C1C	4.23	1.47	1.38
25	l	102	SQD	O47-C7	4.23	1.46	1.34
22	B	608	CLA	CHC-C1C	4.24	1.47	1.35
22	C	504	CLA	OBD-CAD	4.24	1.28	1.22
22	c	509	CLA	CHC-C1C	4.24	1.47	1.35
22	C	506	CLA	O2A-CGA	4.25	1.46	1.33
22	C	509	CLA	CHC-C1C	4.25	1.47	1.35
22	C	511	CLA	CHC-C1C	4.25	1.47	1.35
29	c	520	LMG	O8-C28	4.26	1.46	1.33
22	a	603	CLA	CHC-C1C	4.26	1.47	1.35
22	A	603	CLA	CHC-C1C	4.27	1.47	1.35
22	B	610	CLA	CHC-C1C	4.27	1.47	1.35
22	B	610	CLA	O2D-CGD	4.27	1.44	1.33
22	c	511	CLA	CHC-C1C	4.28	1.47	1.35
22	b	616	CLA	CHC-C1C	4.28	1.47	1.35
22	c	506	CLA	O2A-CGA	4.28	1.46	1.33
31	d	410	DGD	O2G-C1B	4.28	1.46	1.34
22	b	612	CLA	O2D-CGD	4.28	1.44	1.33
22	B	612	CLA	O2D-CGD	4.28	1.44	1.33
22	b	610	CLA	O2D-CGD	4.28	1.44	1.33
22	a	604	CLA	OBD-CAD	4.29	1.28	1.22
23	a	605	PHO	CHC-C1C	4.29	1.47	1.38
22	B	616	CLA	CHC-C1C	4.29	1.48	1.35
22	B	617	CLA	CHC-C1C	4.29	1.48	1.35
22	b	610	CLA	CHC-C1C	4.29	1.48	1.35
25	d	411	SQD	O47-C7	4.29	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	607	CLA	OBD-CAD	4.30	1.28	1.22
31	D	410	DGD	O2G-C1B	4.30	1.46	1.34
29	C	520	LMG	O8-C28	4.30	1.46	1.33
25	D	411	SQD	O47-C7	4.30	1.47	1.34
22	b	617	CLA	CHC-C1C	4.31	1.48	1.35
22	B	614	CLA	O2D-CGD	4.31	1.44	1.33
23	A	606	PHO	CHD-C1D	4.31	1.47	1.38
22	B	615	CLA	CHC-C1C	4.32	1.48	1.35
23	a	606	PHO	CHD-C1D	4.32	1.47	1.38
22	C	513	CLA	OBD-CAD	4.32	1.28	1.22
22	b	614	CLA	O2D-CGD	4.32	1.44	1.33
22	b	615	CLA	CHC-C1C	4.32	1.48	1.35
29	c	520	LMG	O7-C10	4.33	1.47	1.34
29	C	520	LMG	O7-C10	4.33	1.47	1.34
22	b	607	CLA	OBD-CAD	4.33	1.28	1.22
22	D	403	CLA	CHC-C1C	4.34	1.48	1.35
25	b	621	SQD	O48-C23	4.34	1.46	1.33
22	b	611	CLA	O2D-CGD	4.35	1.44	1.33
23	A	605	PHO	O2D-CGD	4.35	1.44	1.33
22	B	611	CLA	O2D-CGD	4.35	1.44	1.33
22	C	508	CLA	CHC-C1C	4.35	1.48	1.35
22	b	614	CLA	CHC-C1C	4.35	1.48	1.35
22	c	513	CLA	OBD-CAD	4.35	1.28	1.22
22	c	508	CLA	CHC-C1C	4.35	1.48	1.35
22	a	607	CLA	CHC-C1C	4.36	1.48	1.35
22	C	511	CLA	OBD-CAD	4.36	1.28	1.22
22	c	511	CLA	OBD-CAD	4.36	1.28	1.22
23	a	605	PHO	O2D-CGD	4.37	1.44	1.33
25	l	102	SQD	O48-C23	4.37	1.46	1.33
22	b	603	CLA	OBD-CAD	4.37	1.28	1.22
22	B	603	CLA	OBD-CAD	4.37	1.28	1.22
22	b	611	CLA	CHC-C1C	4.37	1.48	1.35
22	B	604	CLA	OBD-CAD	4.38	1.28	1.22
22	c	505	CLA	CHC-C1C	4.38	1.48	1.35
22	d	403	CLA	CHC-C1C	4.38	1.48	1.35
22	C	501	CLA	O2D-CGD	4.38	1.44	1.33
22	B	611	CLA	CHC-C1C	4.38	1.48	1.35
22	B	614	CLA	CHC-C1C	4.38	1.48	1.35
22	c	501	CLA	O2D-CGD	4.38	1.44	1.33
22	A	607	CLA	CHC-C1C	4.39	1.48	1.35
32	E	101	LHG	O8-C23	4.39	1.46	1.33
22	B	607	CLA	CHC-C1C	4.39	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	CHC-C1C	4.40	1.48	1.35
25	B	601	SQD	O48-C23	4.40	1.46	1.33
22	d	401	CLA	OBD-CAD	4.41	1.29	1.22
22	d	401	CLA	O2D-CGD	4.41	1.44	1.33
22	b	607	CLA	CHC-C1C	4.42	1.48	1.35
32	e	101	LHG	O8-C23	4.42	1.46	1.33
25	b	601	SQD	O48-C23	4.42	1.46	1.33
22	A	603	CLA	OBD-CAD	4.42	1.29	1.22
31	d	410	DGD	O1G-C1A	4.42	1.46	1.33
22	C	506	CLA	CHC-C1C	4.42	1.48	1.35
22	D	401	CLA	OBD-CAD	4.42	1.29	1.22
22	b	604	CLA	OBD-CAD	4.42	1.29	1.22
22	a	604	CLA	O2D-CGD	4.42	1.44	1.33
22	c	506	CLA	CHC-C1C	4.43	1.48	1.35
25	d	411	SQD	O48-C23	4.43	1.46	1.33
22	b	606	CLA	CHC-C1C	4.44	1.48	1.35
22	b	617	CLA	OBD-CAD	4.44	1.29	1.22
22	d	403	CLA	O2D-CGD	4.44	1.44	1.33
31	D	410	DGD	O1G-C1A	4.44	1.46	1.33
22	B	606	CLA	CHC-C1C	4.45	1.48	1.35
22	B	617	CLA	OBD-CAD	4.45	1.29	1.22
22	c	507	CLA	CHC-C1C	4.45	1.48	1.35
22	c	501	CLA	CHC-C1C	4.45	1.48	1.35
22	D	403	CLA	O2D-CGD	4.45	1.44	1.33
22	C	501	CLA	CHC-C1C	4.46	1.48	1.35
22	C	507	CLA	CHC-C1C	4.46	1.48	1.35
22	D	402	CLA	OBD-CAD	4.46	1.29	1.22
22	D	401	CLA	O2D-CGD	4.46	1.44	1.33
22	C	504	CLA	O2D-CGD	4.46	1.44	1.33
22	A	604	CLA	O2D-CGD	4.46	1.44	1.33
22	c	504	CLA	O2D-CGD	4.47	1.44	1.33
22	B	602	CLA	CHC-C1C	4.47	1.48	1.35
29	B	620	LMG	O8-C28	4.48	1.46	1.33
25	D	411	SQD	O48-C23	4.48	1.46	1.33
22	a	603	CLA	OBD-CAD	4.48	1.29	1.22
29	b	619	LMG	O8-C28	4.50	1.46	1.33
22	d	402	CLA	OBD-CAD	4.50	1.29	1.22
22	b	615	CLA	O2D-CGD	4.50	1.44	1.33
22	b	602	CLA	CHC-C1C	4.50	1.48	1.35
22	C	503	CLA	CHC-C1C	4.51	1.48	1.35
22	c	503	CLA	CHC-C1C	4.51	1.48	1.35
22	B	615	CLA	O2D-CGD	4.51	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	513	CLA	CHC-C1C	4.51	1.48	1.35
22	b	608	CLA	O2D-CGD	4.52	1.44	1.33
22	c	513	CLA	CHC-C1C	4.52	1.48	1.35
22	C	512	CLA	CHC-C1C	4.52	1.48	1.35
22	B	608	CLA	O2D-CGD	4.52	1.44	1.33
22	c	503	CLA	O2D-CGD	4.52	1.44	1.33
22	C	503	CLA	O2D-CGD	4.52	1.44	1.33
22	b	613	CLA	O2D-CGD	4.54	1.44	1.33
22	c	512	CLA	CHC-C1C	4.54	1.48	1.35
22	C	510	CLA	OBD-CAD	4.55	1.29	1.22
22	B	613	CLA	O2D-CGD	4.55	1.44	1.33
23	a	606	PHO	CHC-C1C	4.55	1.47	1.38
23	A	606	PHO	CHC-C1C	4.56	1.47	1.38
22	c	502	CLA	CHC-C1C	4.56	1.48	1.35
22	C	502	CLA	CHC-C1C	4.57	1.48	1.35
22	b	613	CLA	CHC-C1C	4.57	1.48	1.35
22	B	613	CLA	CHC-C1C	4.58	1.48	1.35
22	b	604	CLA	O2D-CGD	4.58	1.45	1.33
22	b	616	CLA	O2D-CGD	4.59	1.45	1.33
22	c	510	CLA	OBD-CAD	4.59	1.29	1.22
22	b	617	CLA	O2D-CGD	4.59	1.45	1.33
22	a	603	CLA	O2D-CGD	4.59	1.45	1.33
22	A	603	CLA	O2D-CGD	4.60	1.45	1.33
22	a	607	CLA	OBD-CAD	4.60	1.29	1.22
22	B	617	CLA	O2D-CGD	4.60	1.45	1.33
22	B	604	CLA	O2D-CGD	4.60	1.45	1.33
22	b	612	CLA	C3C-C2C	4.61	1.46	1.36
22	b	606	CLA	O2D-CGD	4.61	1.45	1.33
22	B	616	CLA	O2D-CGD	4.61	1.45	1.33
22	B	606	CLA	O2D-CGD	4.61	1.45	1.33
22	B	612	CLA	C3C-C2C	4.62	1.46	1.36
22	C	510	CLA	O2D-CGD	4.63	1.45	1.33
22	B	603	CLA	CHC-C1C	4.63	1.49	1.35
22	A	607	CLA	OBD-CAD	4.63	1.29	1.22
22	c	510	CLA	O2D-CGD	4.64	1.45	1.33
22	b	603	CLA	CHC-C1C	4.66	1.49	1.35
22	B	604	CLA	C3C-C2C	4.66	1.46	1.36
22	b	604	CLA	C3C-C2C	4.66	1.46	1.36
22	a	604	CLA	C3C-C2C	4.67	1.46	1.36
22	c	509	CLA	OBD-CAD	4.68	1.29	1.22
22	b	607	CLA	O2D-CGD	4.68	1.45	1.33
22	C	509	CLA	OBD-CAD	4.68	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	505	CLA	O2D-CGD	4.68	1.45	1.33
23	a	606	PHO	O2D-CGD	4.68	1.45	1.33
23	A	606	PHO	O2D-CGD	4.69	1.45	1.33
22	c	502	CLA	O2D-CGD	4.69	1.45	1.33
22	B	602	CLA	O2A-CGA	4.70	1.47	1.33
22	b	602	CLA	O2A-CGA	4.70	1.47	1.33
22	A	604	CLA	C3C-C2C	4.71	1.47	1.36
22	c	505	CLA	O2D-CGD	4.71	1.45	1.33
22	B	607	CLA	O2D-CGD	4.71	1.45	1.33
22	C	502	CLA	O2D-CGD	4.73	1.45	1.33
22	B	613	CLA	C3C-C2C	4.73	1.47	1.36
22	b	613	CLA	C3C-C2C	4.75	1.47	1.36
22	b	609	CLA	O2D-CGD	4.76	1.45	1.33
22	c	512	CLA	O2D-CGD	4.76	1.45	1.33
22	C	512	CLA	O2D-CGD	4.77	1.45	1.33
22	B	609	CLA	O2D-CGD	4.77	1.45	1.33
22	C	507	CLA	O2D-CGD	4.78	1.45	1.33
22	C	502	CLA	C3C-C2C	4.79	1.47	1.36
22	b	605	CLA	C3C-C2C	4.79	1.47	1.36
22	B	615	CLA	C3C-C2C	4.79	1.47	1.36
23	A	606	PHO	C3C-C2C	4.79	1.47	1.36
22	c	502	CLA	C3C-C2C	4.80	1.47	1.36
22	C	508	CLA	O2D-CGD	4.80	1.45	1.33
22	D	401	CLA	C3C-C2C	4.81	1.47	1.36
22	b	615	CLA	C3C-C2C	4.81	1.47	1.36
22	B	612	CLA	C3B-C2B	4.81	1.46	1.40
22	d	401	CLA	C3C-C2C	4.81	1.47	1.36
23	a	606	PHO	C3C-C2C	4.82	1.47	1.36
22	c	504	CLA	C3C-C2C	4.82	1.47	1.36
22	B	605	CLA	C3C-C2C	4.82	1.47	1.36
22	c	501	CLA	C3C-C2C	4.83	1.47	1.36
22	c	508	CLA	O2D-CGD	4.83	1.45	1.33
22	C	506	CLA	O2D-CGD	4.83	1.45	1.33
22	D	402	CLA	C3C-C2C	4.83	1.47	1.36
22	c	511	CLA	O2D-CGD	4.83	1.45	1.33
22	c	507	CLA	O2D-CGD	4.84	1.45	1.33
22	C	511	CLA	O2D-CGD	4.84	1.45	1.33
22	d	402	CLA	C3C-C2C	4.85	1.47	1.36
22	C	509	CLA	O2D-CGD	4.85	1.45	1.33
22	c	506	CLA	O2D-CGD	4.85	1.45	1.33
22	b	612	CLA	C3B-C2B	4.85	1.46	1.40
22	B	617	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	C3C-C2C	4.86	1.47	1.36
22	B	610	CLA	C3C-C2C	4.86	1.47	1.36
22	b	610	CLA	C3C-C2C	4.86	1.47	1.36
22	C	501	CLA	C3C-C2C	4.86	1.47	1.36
22	c	513	CLA	O2D-CGD	4.86	1.45	1.33
22	c	509	CLA	O2D-CGD	4.87	1.45	1.33
22	b	606	CLA	C3B-C2B	4.87	1.46	1.40
22	B	614	CLA	C3C-C2C	4.88	1.47	1.36
22	C	509	CLA	C3C-C2C	4.88	1.47	1.36
22	b	617	CLA	C3C-C2C	4.89	1.47	1.36
22	C	513	CLA	O2D-CGD	4.89	1.45	1.33
22	B	606	CLA	C3B-C2B	4.91	1.46	1.40
22	c	509	CLA	C3C-C2C	4.91	1.47	1.36
22	b	614	CLA	C3C-C2C	4.91	1.47	1.36
22	b	608	CLA	C3C-C2C	4.91	1.47	1.36
23	A	605	PHO	C3C-C2C	4.92	1.47	1.36
22	b	615	CLA	C3B-C2B	4.92	1.46	1.40
22	c	511	CLA	C3C-C2C	4.92	1.47	1.36
23	a	605	PHO	C3C-C2C	4.93	1.47	1.36
22	B	608	CLA	C3C-C2C	4.94	1.47	1.36
22	c	506	CLA	C3C-C2C	4.95	1.47	1.36
33	v	201	HEM	C3D-C2D	4.95	1.52	1.37
22	C	511	CLA	C3C-C2C	4.96	1.47	1.36
22	a	607	CLA	C3C-C2C	4.96	1.47	1.36
22	B	615	CLA	C3B-C2B	4.97	1.46	1.40
22	C	506	CLA	C3C-C2C	4.98	1.47	1.36
22	C	510	CLA	C3C-C2C	4.98	1.47	1.36
22	c	510	CLA	C3C-C2C	4.98	1.47	1.36
33	V	201	HEM	C3D-C2D	4.98	1.52	1.37
22	B	609	CLA	C3C-C2C	4.98	1.47	1.36
22	b	609	CLA	C3C-C2C	4.99	1.47	1.36
22	b	602	CLA	O2D-CGD	4.99	1.46	1.33
22	A	607	CLA	C3C-C2C	5.00	1.47	1.36
22	B	602	CLA	O2D-CGD	5.00	1.46	1.33
23	a	606	PHO	CHB-C1B	5.00	1.48	1.38
23	A	606	PHO	CHB-C1B	5.00	1.48	1.38
22	D	403	CLA	C3C-C2C	5.02	1.47	1.36
22	C	505	CLA	C3C-C2C	5.02	1.47	1.36
22	c	505	CLA	C3C-C2C	5.02	1.47	1.36
22	d	403	CLA	C3C-C2C	5.03	1.47	1.36
22	b	611	CLA	C3C-C2C	5.05	1.47	1.36
22	B	605	CLA	C3B-C2B	5.06	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	C3C-C2C	5.07	1.47	1.36
22	b	607	CLA	C3C-C2C	5.07	1.47	1.36
22	a	603	CLA	C3C-C2C	5.08	1.47	1.36
22	B	611	CLA	C3C-C2C	5.08	1.47	1.36
22	B	606	CLA	C3C-C2C	5.10	1.47	1.36
22	B	607	CLA	C3C-C2C	5.10	1.47	1.36
22	b	605	CLA	C3B-C2B	5.12	1.46	1.40
22	B	602	CLA	C3C-C2C	5.13	1.47	1.36
22	C	507	CLA	C3C-C2C	5.13	1.47	1.36
22	A	603	CLA	C3C-C2C	5.14	1.47	1.36
22	c	502	CLA	C3B-C2B	5.14	1.46	1.40
22	b	602	CLA	C3C-C2C	5.15	1.47	1.36
22	b	610	CLA	C3B-C2B	5.16	1.46	1.40
22	B	616	CLA	C3C-C2C	5.16	1.47	1.36
22	c	507	CLA	C3C-C2C	5.16	1.48	1.36
22	C	502	CLA	C3B-C2B	5.16	1.46	1.40
22	b	616	CLA	C3C-C2C	5.16	1.48	1.36
22	c	503	CLA	C3C-C2C	5.19	1.48	1.36
22	B	611	CLA	C3B-C2B	5.22	1.47	1.40
23	a	605	PHO	CHB-C1B	5.23	1.49	1.38
22	B	610	CLA	C3B-C2B	5.23	1.47	1.40
22	a	604	CLA	C3B-C2B	5.23	1.47	1.40
23	A	605	PHO	CHB-C1B	5.24	1.49	1.38
22	C	503	CLA	C3C-C2C	5.24	1.48	1.36
22	B	616	CLA	C3B-C2B	5.25	1.47	1.40
22	b	611	CLA	C3B-C2B	5.26	1.47	1.40
22	D	402	CLA	C3B-C2B	5.27	1.47	1.40
22	b	616	CLA	C3B-C2B	5.27	1.47	1.40
22	d	402	CLA	C3B-C2B	5.27	1.47	1.40
33	f	101	HEM	C3D-C2D	5.27	1.53	1.37
22	c	513	CLA	C3C-C2C	5.27	1.48	1.36
33	F	101	HEM	C3D-C2D	5.28	1.53	1.37
22	C	512	CLA	C3C-C2C	5.29	1.48	1.36
22	A	604	CLA	C3B-C2B	5.30	1.47	1.40
22	B	603	CLA	C3C-C2C	5.31	1.48	1.36
22	C	513	CLA	C3C-C2C	5.31	1.48	1.36
22	c	512	CLA	C3C-C2C	5.31	1.48	1.36
22	C	509	CLA	C3B-C2B	5.31	1.47	1.40
22	B	614	CLA	C3B-C2B	5.34	1.47	1.40
22	b	603	CLA	C3C-C2C	5.35	1.48	1.36
22	C	508	CLA	C3C-C2C	5.35	1.48	1.36
22	b	614	CLA	C3B-C2B	5.36	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	C3B-C2B	5.37	1.47	1.40
22	c	508	CLA	C3C-C2C	5.39	1.48	1.36
22	C	511	CLA	C3B-C2B	5.39	1.47	1.40
22	c	509	CLA	C3B-C2B	5.44	1.47	1.40
22	b	602	CLA	C3B-C2B	5.45	1.47	1.40
22	B	608	CLA	C3B-C2B	5.45	1.47	1.40
22	b	608	CLA	C3B-C2B	5.46	1.47	1.40
22	C	510	CLA	C3B-C2B	5.47	1.47	1.40
22	B	602	CLA	C3B-C2B	5.48	1.47	1.40
22	b	604	CLA	C3B-C2B	5.49	1.47	1.40
22	c	510	CLA	C3B-C2B	5.50	1.47	1.40
22	B	604	CLA	C3B-C2B	5.50	1.47	1.40
22	B	609	CLA	C3B-C2B	5.51	1.47	1.40
22	b	609	CLA	C3B-C2B	5.53	1.47	1.40
22	C	506	CLA	C3B-C2B	5.53	1.47	1.40
22	c	506	CLA	C3B-C2B	5.53	1.47	1.40
22	a	603	CLA	C3B-C2B	5.54	1.47	1.40
22	A	603	CLA	C3B-C2B	5.56	1.47	1.40
22	b	607	CLA	C3B-C2B	5.57	1.47	1.40
22	a	607	CLA	C3B-C2B	5.58	1.47	1.40
22	A	607	CLA	C3B-C2B	5.61	1.47	1.40
22	B	607	CLA	C3B-C2B	5.61	1.47	1.40
22	d	401	CLA	C3B-C2B	5.62	1.47	1.40
23	a	605	PHO	C3B-C2B	5.65	1.47	1.37
22	b	613	CLA	C3B-C2B	5.65	1.47	1.40
22	d	403	CLA	C3B-C2B	5.66	1.47	1.40
22	D	401	CLA	C3B-C2B	5.67	1.47	1.40
22	C	505	CLA	C3B-C2B	5.67	1.47	1.40
23	A	605	PHO	C3B-C2B	5.68	1.47	1.37
22	B	613	CLA	C3B-C2B	5.70	1.47	1.40
22	c	505	CLA	C3B-C2B	5.70	1.47	1.40
22	D	403	CLA	C3B-C2B	5.71	1.47	1.40
22	C	504	CLA	C3B-C2B	5.73	1.47	1.40
22	c	504	CLA	C3B-C2B	5.77	1.47	1.40
22	C	512	CLA	C3B-C2B	5.80	1.47	1.40
22	c	512	CLA	C3B-C2B	5.84	1.47	1.40
22	C	501	CLA	C3B-C2B	5.86	1.47	1.40
22	c	501	CLA	C3B-C2B	5.87	1.47	1.40
23	a	606	PHO	C3B-C2B	5.98	1.48	1.37
23	A	606	PHO	C3B-C2B	5.98	1.48	1.37
22	C	508	CLA	C3B-C2B	6.01	1.48	1.40
22	C	503	CLA	C3B-C2B	6.03	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	C3B-C2B	6.04	1.48	1.40
22	B	617	CLA	C3B-C2B	6.05	1.48	1.40
22	c	508	CLA	C3B-C2B	6.07	1.48	1.40
22	b	617	CLA	C3B-C2B	6.12	1.48	1.40
22	B	603	CLA	C3B-C2B	6.18	1.48	1.40
22	b	603	CLA	C3B-C2B	6.19	1.48	1.40
22	C	513	CLA	C3B-C2B	6.34	1.48	1.40
22	c	513	CLA	C3B-C2B	6.36	1.48	1.40
22	c	507	CLA	C3B-C2B	6.62	1.48	1.40
22	C	507	CLA	C3B-C2B	6.62	1.48	1.40

All (2184) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	102	BCR	C36-C18-C17	-10.18	108.08	122.89
24	t	101	BCR	C36-C18-C17	-10.18	108.09	122.89
24	D	404	BCR	C30-C25-C26	-9.49	109.80	122.50
24	d	404	BCR	C30-C25-C26	-9.48	109.82	122.50
24	a	608	BCR	C37-C22-C21	-9.38	109.26	122.89
24	A	608	BCR	C37-C22-C21	-9.34	109.31	122.89
24	B	619	BCR	C36-C18-C19	-8.47	104.24	118.08
24	b	618	BCR	C36-C18-C19	-8.46	104.25	118.08
24	k	101	BCR	C33-C5-C4	-8.39	97.25	113.47
24	K	101	BCR	C33-C5-C4	-8.38	97.27	113.47
24	B	618	BCR	C36-C18-C17	-8.35	110.75	122.89
24	T	101	BCR	C36-C18-C17	-8.33	110.77	122.89
24	A	608	BCR	C36-C18-C17	-7.92	111.38	122.89
24	a	608	BCR	C36-C18-C17	-7.88	111.43	122.89
24	b	618	BCR	C30-C25-C26	-7.53	112.43	122.50
24	B	619	BCR	C30-C25-C26	-7.52	112.43	122.50
24	a	608	BCR	C35-C13-C14	-7.52	111.95	122.89
24	A	608	BCR	C35-C13-C14	-7.52	111.95	122.89
24	T	101	BCR	C35-C13-C12	-7.42	105.96	118.08
24	B	618	BCR	C35-C13-C12	-7.40	105.99	118.08
24	C	514	BCR	C38-C26-C27	-7.32	99.32	113.47
24	c	514	BCR	C38-C26-C27	-7.29	99.37	113.47
24	H	101	BCR	C37-C22-C21	-7.21	112.40	122.89
24	h	101	BCR	C37-C22-C21	-7.17	112.47	122.89
24	B	618	BCR	C36-C18-C19	-7.05	106.56	118.08
24	T	101	BCR	C36-C18-C19	-7.04	106.57	118.08
24	K	101	BCR	C37-C22-C21	-6.95	112.78	122.89
24	k	101	BCR	C37-C22-C21	-6.90	112.85	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	622	BCR	C36-C18-C17	-6.83	112.95	122.89
24	b	622	BCR	C36-C18-C17	-6.83	112.95	122.89
33	F	101	HEM	CBD-CAD-C3D	-6.79	100.56	112.47
33	f	101	HEM	CBD-CAD-C3D	-6.77	100.60	112.47
24	a	608	BCR	C38-C26-C27	-6.73	100.45	113.47
24	A	608	BCR	C38-C26-C27	-6.72	100.48	113.47
24	H	101	BCR	C36-C18-C19	-6.60	107.29	118.08
24	h	101	BCR	C36-C18-C19	-6.60	107.29	118.08
24	K	101	BCR	C36-C18-C19	-6.60	107.29	118.08
24	c	514	BCR	C36-C18-C17	-6.55	113.36	122.89
24	C	514	BCR	C36-C18-C17	-6.54	113.38	122.89
24	k	101	BCR	C36-C18-C19	-6.53	107.41	118.08
24	k	102	BCR	C36-C18-C19	-6.40	107.62	118.08
24	K	102	BCR	C36-C18-C19	-6.37	107.68	118.08
24	B	618	BCR	C34-C9-C10	-6.33	113.69	122.89
24	T	101	BCR	C34-C9-C10	-6.31	113.71	122.89
24	K	102	BCR	C37-C22-C21	-6.23	113.83	122.89
24	k	102	BCR	C37-C22-C21	-6.21	113.85	122.89
24	H	101	BCR	C30-C25-C26	-6.08	114.37	122.50
24	h	101	BCR	C30-C25-C26	-6.03	114.43	122.50
24	k	101	BCR	C36-C18-C17	-5.94	114.24	122.89
24	k	101	BCR	C30-C25-C26	-5.92	114.57	122.50
24	K	101	BCR	C30-C25-C26	-5.91	114.59	122.50
24	K	101	BCR	C36-C18-C17	-5.91	114.29	122.89
24	b	618	BCR	C38-C26-C27	-5.76	102.34	113.47
24	B	619	BCR	C38-C26-C27	-5.75	102.35	113.47
24	H	101	BCR	C34-C9-C10	-5.72	114.58	122.89
24	h	101	BCR	C33-C5-C4	-5.72	102.42	113.47
24	d	404	BCR	C39-C30-C29	-5.71	88.70	108.75
24	D	404	BCR	C39-C30-C29	-5.71	88.71	108.75
24	H	101	BCR	C33-C5-C4	-5.70	102.44	113.47
24	K	102	BCR	C36-C18-C17	-5.70	114.59	122.89
24	h	101	BCR	C34-C9-C10	-5.69	114.62	122.89
24	k	102	BCR	C36-C18-C17	-5.67	114.65	122.89
24	B	619	BCR	C37-C22-C21	-5.61	114.73	122.89
24	b	618	BCR	C37-C22-C21	-5.60	114.74	122.89
24	b	618	BCR	C36-C18-C17	-5.59	114.75	122.89
24	B	619	BCR	C36-C18-C17	-5.58	114.77	122.89
24	B	619	BCR	C35-C13-C14	-5.57	114.80	122.89
24	b	618	BCR	C35-C13-C14	-5.55	114.82	122.89
24	B	618	BCR	C38-C26-C27	-5.51	102.81	113.47
24	a	608	BCR	C30-C25-C26	-5.51	115.13	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	608	BCR	C30-C25-C26	-5.51	115.13	122.50
24	T	101	BCR	C38-C26-C27	-5.49	102.86	113.47
33	V	201	HEM	CBD-CAD-C3D	-5.48	102.86	112.47
33	v	201	HEM	CBD-CAD-C3D	-5.47	102.87	112.47
24	t	101	BCR	C33-C5-C4	-5.32	103.19	113.47
24	T	102	BCR	C33-C5-C4	-5.30	103.22	113.47
24	D	404	BCR	C36-C18-C17	-5.20	115.33	122.89
24	d	404	BCR	C36-C18-C17	-5.17	115.36	122.89
24	H	101	BCR	C35-C13-C12	-5.06	109.81	118.08
24	h	101	BCR	C35-C13-C12	-5.05	109.82	118.08
24	C	515	BCR	C37-C22-C21	-5.05	115.54	122.89
24	t	101	BCR	C37-C22-C23	-5.05	109.83	118.08
24	K	102	BCR	C35-C13-C14	-5.02	115.59	122.89
24	C	515	BCR	C35-C13-C12	-5.02	109.88	118.08
24	c	515	BCR	C35-C13-C12	-5.00	109.90	118.08
24	k	102	BCR	C35-C13-C14	-5.00	115.61	122.89
24	T	102	BCR	C37-C22-C23	-5.00	109.90	118.08
24	c	515	BCR	C37-C22-C21	-4.96	115.67	122.89
24	D	404	BCR	C34-C9-C10	-4.94	115.70	122.89
24	d	404	BCR	C34-C9-C10	-4.93	115.72	122.89
24	k	101	BCR	C34-C9-C10	-4.92	115.74	122.89
24	c	514	BCR	C33-C5-C4	-4.91	103.97	113.47
24	K	101	BCR	C34-C9-C10	-4.91	115.75	122.89
22	d	402	CLA	C1C-C2C-C3C	-4.91	101.49	106.93
22	D	402	CLA	C1C-C2C-C3C	-4.90	101.49	106.93
24	C	514	BCR	C33-C5-C4	-4.90	103.99	113.47
24	c	515	BCR	C38-C26-C27	-4.88	104.03	113.47
24	C	515	BCR	C38-C26-C27	-4.88	104.04	113.47
24	C	515	BCR	C36-C18-C19	-4.82	110.20	118.08
24	B	622	BCR	C33-C5-C4	-4.81	104.18	113.47
24	b	622	BCR	C33-C5-C4	-4.80	104.19	113.47
24	B	622	BCR	C38-C26-C27	-4.79	104.20	113.47
24	c	515	BCR	C36-C18-C19	-4.79	110.25	118.08
24	b	622	BCR	C38-C26-C27	-4.78	104.24	113.47
24	k	101	BCR	C35-C13-C14	-4.74	116.00	122.89
24	K	101	BCR	C35-C13-C14	-4.73	116.01	122.89
24	c	515	BCR	C36-C18-C17	-4.69	116.06	122.89
24	C	515	BCR	C36-C18-C17	-4.66	116.12	122.89
22	A	604	CLA	C1C-C2C-C3C	-4.65	101.78	106.93
22	a	604	CLA	C1C-C2C-C3C	-4.62	101.81	106.93
24	a	608	BCR	C36-C18-C19	-4.61	110.54	118.08
24	A	608	BCR	C36-C18-C19	-4.61	110.55	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	619	BCR	C33-C5-C4	-4.60	104.58	113.47
24	b	618	BCR	C33-C5-C4	-4.58	104.62	113.47
24	D	404	BCR	C33-C5-C4	-4.54	104.68	113.47
23	A	606	PHO	C4C-C3C-C2C	-4.53	101.87	106.80
24	c	514	BCR	C30-C25-C26	-4.52	116.45	122.50
23	a	606	PHO	C4C-C3C-C2C	-4.52	101.88	106.80
24	k	102	BCR	C35-C13-C12	-4.52	110.70	118.08
24	K	102	BCR	C35-C13-C12	-4.51	110.71	118.08
24	K	101	BCR	C1-C6-C5	-4.51	116.46	122.50
24	k	101	BCR	C1-C6-C5	-4.51	116.47	122.50
23	a	605	PHO	C3D-C2D-C1D	-4.51	98.37	105.76
24	d	404	BCR	C33-C5-C4	-4.50	104.78	113.47
24	C	514	BCR	C30-C25-C26	-4.49	116.49	122.50
24	T	101	BCR	C30-C25-C26	-4.47	116.51	122.50
23	A	605	PHO	C3D-C2D-C1D	-4.47	98.43	105.76
24	B	618	BCR	C30-C25-C26	-4.44	116.55	122.50
24	c	514	BCR	C35-C13-C12	-4.44	110.83	118.08
22	b	604	CLA	C1C-C2C-C3C	-4.43	102.01	106.93
24	C	514	BCR	C35-C13-C12	-4.43	110.84	118.08
22	B	604	CLA	C1C-C2C-C3C	-4.42	102.03	106.93
24	C	515	BCR	C31-C1-C2	-4.40	93.32	108.75
24	C	515	BCR	C35-C13-C14	-4.40	116.50	122.89
24	c	515	BCR	C31-C1-C2	-4.39	93.32	108.75
24	c	515	BCR	C35-C13-C14	-4.39	116.51	122.89
24	c	514	BCR	C32-C1-C2	-4.37	93.42	108.75
24	B	619	BCR	C40-C30-C29	-4.36	93.43	108.75
24	T	102	BCR	C34-C9-C8	-4.36	110.96	118.08
24	b	618	BCR	C40-C30-C29	-4.36	93.44	108.75
24	C	514	BCR	C32-C1-C2	-4.36	93.45	108.75
22	B	605	CLA	C1C-C2C-C3C	-4.35	102.11	106.93
24	t	101	BCR	C34-C9-C8	-4.35	110.98	118.08
22	b	605	CLA	C1C-C2C-C3C	-4.35	102.11	106.93
24	T	102	BCR	C30-C25-C26	-4.33	116.71	122.50
24	t	101	BCR	C30-C25-C26	-4.32	116.72	122.50
24	d	404	BCR	C35-C13-C12	-4.32	111.02	118.08
24	D	404	BCR	C35-C13-C12	-4.31	111.03	118.08
23	A	606	PHO	C3D-C2D-C1D	-4.30	98.71	105.76
24	T	101	BCR	C37-C22-C23	-4.29	111.06	118.08
22	C	504	CLA	C1C-C2C-C3C	-4.28	102.18	106.93
24	d	404	BCR	C36-C18-C19	-4.27	111.10	118.08
23	a	606	PHO	C3D-C2D-C1D	-4.27	98.76	105.76
24	B	618	BCR	C37-C22-C23	-4.26	111.11	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	622	BCR	C35-C13-C14	-4.26	116.70	122.89
24	D	404	BCR	C36-C18-C19	-4.25	111.13	118.08
23	a	605	PHO	C4C-C3C-C2C	-4.25	102.17	106.80
24	B	622	BCR	C35-C13-C14	-4.24	116.73	122.89
24	H	101	BCR	C35-C13-C14	-4.23	116.73	122.89
22	c	504	CLA	C1C-C2C-C3C	-4.23	102.24	106.93
24	h	101	BCR	C35-C13-C14	-4.23	116.73	122.89
23	A	605	PHO	C4C-C3C-C2C	-4.23	102.20	106.80
24	d	404	BCR	C38-C26-C27	-4.21	105.33	113.47
24	D	404	BCR	C38-C26-C27	-4.21	105.34	113.47
24	b	622	BCR	C30-C25-C26	-4.19	116.89	122.50
22	B	609	CLA	C1C-C2C-C3C	-4.17	102.30	106.93
22	b	609	CLA	C1C-C2C-C3C	-4.16	102.32	106.93
24	B	622	BCR	C30-C25-C26	-4.14	116.96	122.50
24	K	101	BCR	C38-C26-C27	-4.09	105.56	113.47
24	k	101	BCR	C38-C26-C27	-4.09	105.57	113.47
24	k	102	BCR	C30-C25-C26	-4.07	117.06	122.50
22	c	509	CLA	C1C-C2C-C3C	-4.06	102.42	106.93
22	c	501	CLA	O2D-CGD-O1D	-4.06	115.22	123.77
22	A	607	CLA	C1C-C2C-C3C	-4.06	102.43	106.93
22	C	501	CLA	O2D-CGD-O1D	-4.05	115.23	123.77
22	a	607	CLA	C1C-C2C-C3C	-4.05	102.44	106.93
24	K	102	BCR	C30-C25-C26	-4.04	117.09	122.50
22	B	608	CLA	C1C-C2C-C3C	-4.04	102.45	106.93
24	C	515	BCR	C33-C5-C4	-4.04	105.67	113.47
24	c	515	BCR	C33-C5-C4	-4.03	105.67	113.47
24	c	514	BCR	C36-C18-C19	-4.03	111.49	118.08
24	C	514	BCR	C36-C18-C19	-4.02	111.51	118.08
22	C	509	CLA	C1C-C2C-C3C	-4.02	102.47	106.93
22	b	614	CLA	C1C-C2C-C3C	-4.02	102.48	106.93
22	B	614	CLA	C1C-C2C-C3C	-4.01	102.48	106.93
22	b	608	CLA	C1C-C2C-C3C	-3.99	102.51	106.93
24	T	102	BCR	C35-C13-C14	-3.97	117.11	122.89
24	T	101	BCR	C35-C13-C14	-3.97	117.11	122.89
24	B	618	BCR	C35-C13-C14	-3.96	117.13	122.89
24	t	101	BCR	C35-C13-C14	-3.95	117.14	122.89
24	b	618	BCR	C35-C13-C12	-3.94	111.64	118.08
24	h	101	BCR	C38-C26-C27	-3.93	105.87	113.47
22	c	501	CLA	C1C-C2C-C3C	-3.93	102.57	106.93
24	H	101	BCR	C38-C26-C27	-3.93	105.88	113.47
22	C	501	CLA	C1C-C2C-C3C	-3.92	102.58	106.93
24	B	619	BCR	C35-C13-C12	-3.92	111.67	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	607	CLA	O2D-CGD-O1D	-3.90	115.56	123.77
22	B	607	CLA	O2D-CGD-O1D	-3.89	115.58	123.77
22	c	507	CLA	C1C-C2C-C3C	-3.89	102.62	106.93
24	D	404	BCR	C32-C1-C2	-3.88	95.11	108.75
24	d	404	BCR	C32-C1-C2	-3.87	95.15	108.75
22	C	507	CLA	C1C-C2C-C3C	-3.87	102.64	106.93
24	h	101	BCR	C36-C18-C17	-3.83	117.31	122.89
24	H	101	BCR	C36-C18-C17	-3.83	117.31	122.89
24	T	102	BCR	C37-C22-C21	-3.81	117.34	122.89
24	k	102	BCR	C38-C26-C27	-3.81	106.10	113.47
24	K	102	BCR	C38-C26-C27	-3.80	106.12	113.47
24	t	101	BCR	C37-C22-C21	-3.80	117.36	122.89
22	d	403	CLA	C1C-C2C-C3C	-3.78	102.74	106.93
22	C	503	CLA	C1C-C2C-C3C	-3.76	102.76	106.93
22	b	602	CLA	C1C-C2C-C3C	-3.76	102.76	106.93
22	D	403	CLA	C1C-C2C-C3C	-3.75	102.77	106.93
22	B	607	CLA	O1D-CGD-CBD	-3.75	118.80	124.64
22	B	607	CLA	C1C-C2C-C3C	-3.75	102.77	106.93
22	b	607	CLA	O1D-CGD-CBD	-3.74	118.81	124.64
22	B	602	CLA	C1C-C2C-C3C	-3.74	102.78	106.93
22	C	506	CLA	C1C-C2C-C3C	-3.73	102.80	106.93
22	c	503	CLA	C1C-C2C-C3C	-3.73	102.80	106.93
22	c	510	CLA	C1C-C2C-C3C	-3.72	102.81	106.93
22	b	607	CLA	C1C-C2C-C3C	-3.71	102.81	106.93
22	c	513	CLA	C1C-C2C-C3C	-3.69	102.84	106.93
22	C	513	CLA	C1C-C2C-C3C	-3.68	102.85	106.93
22	C	511	CLA	C1C-C2C-C3C	-3.68	102.85	106.93
22	C	510	CLA	C1C-C2C-C3C	-3.67	102.86	106.93
22	c	506	CLA	C1C-C2C-C3C	-3.67	102.87	106.93
22	b	610	CLA	C1C-C2C-C3C	-3.66	102.87	106.93
24	d	404	BCR	C37-C22-C21	-3.66	117.56	122.89
22	B	610	CLA	C1C-C2C-C3C	-3.65	102.88	106.93
22	c	511	CLA	C1C-C2C-C3C	-3.65	102.88	106.93
24	D	404	BCR	C37-C22-C21	-3.63	117.61	122.89
24	K	102	BCR	C33-C5-C4	-3.62	106.47	113.47
22	c	508	CLA	C1C-C2C-C3C	-3.62	102.91	106.93
22	b	615	CLA	C1C-C2C-C3C	-3.62	102.92	106.93
22	B	615	CLA	C1C-C2C-C3C	-3.61	102.92	106.93
24	k	102	BCR	C33-C5-C4	-3.61	106.49	113.47
22	A	603	CLA	C1C-C2C-C3C	-3.60	102.94	106.93
24	D	404	BCR	C1-C6-C5	-3.59	117.69	122.50
24	d	404	BCR	C1-C6-C5	-3.57	117.72	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	508	CLA	C1C-C2C-C3C	-3.57	102.97	106.93
22	a	603	CLA	C1C-C2C-C3C	-3.57	102.97	106.93
24	c	514	BCR	C37-C22-C21	-3.55	117.73	122.89
24	C	514	BCR	C37-C22-C21	-3.54	117.75	122.89
22	B	616	CLA	C1C-C2C-C3C	-3.53	103.01	106.93
24	d	404	BCR	C35-C13-C14	-3.53	117.75	122.89
24	D	404	BCR	C35-C13-C14	-3.52	117.76	122.89
22	b	616	CLA	C1C-C2C-C3C	-3.51	103.04	106.93
25	A	609	SQD	C1-C2-C3	-3.46	103.11	109.98
22	C	512	CLA	C1C-C2C-C3C	-3.46	103.09	106.93
22	c	512	CLA	C1C-C2C-C3C	-3.46	103.09	106.93
22	b	609	CLA	O1D-CGD-CBD	-3.46	119.25	124.64
25	a	609	SQD	C1-C2-C3	-3.46	103.12	109.98
24	a	608	BCR	C35-C13-C12	-3.45	112.45	118.08
24	A	608	BCR	C35-C13-C12	-3.44	112.46	118.08
22	B	612	CLA	C1C-C2C-C3C	-3.44	103.12	106.93
22	b	612	CLA	C1C-C2C-C3C	-3.41	103.15	106.93
22	B	609	CLA	O1D-CGD-CBD	-3.41	119.33	124.64
22	C	505	CLA	C1C-C2C-C3C	-3.41	103.15	106.93
22	b	603	CLA	C1C-C2C-C3C	-3.41	103.15	106.93
24	a	608	BCR	C33-C5-C4	-3.40	106.89	113.47
22	c	505	CLA	C1C-C2C-C3C	-3.40	103.16	106.93
24	b	618	BCR	C37-C22-C23	-3.40	112.53	118.08
22	C	502	CLA	C1C-C2C-C3C	-3.40	103.17	106.93
24	A	608	BCR	C33-C5-C4	-3.39	106.91	113.47
22	C	507	CLA	O1D-CGD-CBD	-3.39	119.36	124.64
24	B	619	BCR	C37-C22-C23	-3.38	112.56	118.08
22	c	502	CLA	C1C-C2C-C3C	-3.37	103.19	106.93
22	B	603	CLA	C1C-C2C-C3C	-3.37	103.20	106.93
22	c	507	CLA	O1D-CGD-CBD	-3.36	119.41	124.64
23	a	605	PHO	C4D-ND-C1D	-3.36	100.83	106.99
22	B	611	CLA	C1C-C2C-C3C	-3.35	103.22	106.93
23	A	605	PHO	C4D-ND-C1D	-3.35	100.86	106.99
22	b	611	CLA	C1C-C2C-C3C	-3.34	103.22	106.93
24	A	608	BCR	C34-C9-C8	-3.33	112.64	118.08
24	T	102	BCR	C36-C18-C19	-3.33	112.64	118.08
22	b	606	CLA	C1C-C2C-C3C	-3.32	103.25	106.93
22	D	401	CLA	C3B-CAB-CBB	-3.30	119.75	126.40
22	d	401	CLA	C3B-CAB-CBB	-3.30	119.76	126.40
24	a	608	BCR	C34-C9-C8	-3.29	112.70	118.08
22	B	606	CLA	C1C-C2C-C3C	-3.29	103.28	106.93
24	t	101	BCR	C36-C18-C19	-3.29	112.71	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	102	BCR	C35-C13-C12	-3.26	112.75	118.08
24	t	101	BCR	C35-C13-C12	-3.26	112.76	118.08
22	d	401	CLA	C1C-C2C-C3C	-3.25	103.32	106.93
31	C	518	DGD	O3G-C3G-C2G	-3.25	103.25	110.99
22	B	604	CLA	O2D-CGD-O1D	-3.25	116.94	123.77
22	B	617	CLA	O1D-CGD-CBD	-3.24	119.59	124.64
22	D	401	CLA	C1C-C2C-C3C	-3.24	103.34	106.93
31	c	518	DGD	O3G-C3G-C2G	-3.23	103.30	110.99
22	b	617	CLA	O1D-CGD-CBD	-3.23	119.61	124.64
22	b	617	CLA	C4C-C3C-C2C	-3.23	101.78	106.94
22	B	617	CLA	C4C-C3C-C2C	-3.21	101.80	106.94
28	A	613	PL9	C32-C33-C34	-3.19	120.71	127.75
22	b	604	CLA	O2D-CGD-O1D	-3.18	117.07	123.77
28	a	613	PL9	C32-C33-C34	-3.18	120.73	127.75
22	B	606	CLA	C4C-C3C-C2C	-3.18	101.86	106.94
22	b	602	CLA	C3B-CAB-CBB	-3.17	120.01	126.40
22	B	602	CLA	C3B-CAB-CBB	-3.17	120.03	126.40
22	c	501	CLA	C3B-CAB-CBB	-3.16	120.04	126.40
24	h	101	BCR	C39-C30-C29	-3.15	97.68	108.75
22	C	501	CLA	C3B-CAB-CBB	-3.15	120.06	126.40
24	H	101	BCR	C39-C30-C29	-3.15	97.69	108.75
22	b	602	CLA	O1D-CGD-CBD	-3.14	119.75	124.64
22	b	606	CLA	C4C-C3C-C2C	-3.14	101.92	106.94
22	B	613	CLA	C1C-C2C-C3C	-3.13	103.46	106.93
22	B	602	CLA	O1D-CGD-CBD	-3.13	119.77	124.64
22	d	401	CLA	C4C-C3C-C2C	-3.13	101.94	106.94
22	b	613	CLA	C1C-C2C-C3C	-3.12	103.47	106.93
23	A	606	PHO	C4D-ND-C1D	-3.11	101.29	106.99
22	D	401	CLA	C4C-C3C-C2C	-3.11	101.96	106.94
24	C	514	BCR	C39-C30-C29	-3.11	97.83	108.75
24	K	102	BCR	C31-C1-C2	-3.11	97.84	108.75
24	c	514	BCR	C39-C30-C29	-3.11	97.85	108.75
24	k	102	BCR	C31-C1-C2	-3.10	97.85	108.75
24	c	515	BCR	C30-C25-C26	-3.09	118.36	122.50
23	a	606	PHO	C4D-ND-C1D	-3.09	101.34	106.99
22	b	615	CLA	O2D-CGD-O1D	-3.09	117.27	123.77
24	B	619	BCR	C34-C9-C8	-3.09	113.04	118.08
24	C	515	BCR	C30-C25-C26	-3.09	118.37	122.50
24	b	618	BCR	C34-C9-C8	-3.08	113.04	118.08
22	B	611	CLA	C4C-C3C-C2C	-3.08	102.02	106.94
22	b	611	CLA	C4C-C3C-C2C	-3.06	102.05	106.94
24	B	619	BCR	C34-C9-C10	-3.06	118.44	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	615	CLA	O2D-CGD-O1D	-3.06	117.33	123.77
24	B	622	BCR	C34-C9-C8	-3.05	113.10	118.08
22	D	401	CLA	O2D-CGD-O1D	-3.04	117.36	123.77
24	B	622	BCR	C36-C18-C19	-3.04	113.11	118.08
24	b	622	BCR	C36-C18-C19	-3.04	113.12	118.08
24	b	618	BCR	C34-C9-C10	-3.04	118.47	122.89
24	b	622	BCR	C34-C9-C8	-3.03	113.13	118.08
22	d	401	CLA	O2D-CGD-O1D	-3.03	117.40	123.77
23	a	605	PHO	C1C-C2C-C3C	-3.02	102.95	106.43
24	b	618	BCR	C1-C6-C5	-3.01	118.48	122.50
22	b	616	CLA	C4C-C3C-C2C	-3.00	102.14	106.94
22	B	616	CLA	C4C-C3C-C2C	-3.00	102.14	106.94
22	C	506	CLA	C3B-CAB-CBB	-3.00	120.37	126.40
24	B	619	BCR	C1-C6-C5	-2.99	118.49	122.50
22	c	506	CLA	C3B-CAB-CBB	-2.99	120.38	126.40
23	A	605	PHO	C1C-C2C-C3C	-2.99	102.98	106.43
22	D	402	CLA	CBC-CAC-C3C	-2.99	103.29	112.38
22	C	508	CLA	C4C-C3C-C2C	-2.98	102.18	106.94
22	d	402	CLA	CBC-CAC-C3C	-2.97	103.34	112.38
22	c	508	CLA	C4C-C3C-C2C	-2.97	102.19	106.94
24	k	101	BCR	C39-C30-C29	-2.97	98.34	108.75
22	B	612	CLA	C4C-C3C-C2C	-2.96	102.20	106.94
24	K	101	BCR	C39-C30-C29	-2.96	98.35	108.75
22	b	612	CLA	C4C-C3C-C2C	-2.96	102.21	106.94
24	B	618	BCR	C39-C30-C29	-2.95	98.40	108.75
24	T	101	BCR	C39-C30-C29	-2.94	98.42	108.75
22	c	513	CLA	O2D-CGD-O1D	-2.93	117.61	123.77
24	K	102	BCR	C34-C9-C10	-2.91	118.66	122.89
22	b	613	CLA	C4C-C3C-C2C	-2.90	102.30	106.94
22	C	513	CLA	O2D-CGD-O1D	-2.90	117.67	123.77
22	c	502	CLA	C4C-C3C-C2C	-2.89	102.32	106.94
22	B	613	CLA	C4C-C3C-C2C	-2.88	102.33	106.94
24	k	102	BCR	C34-C9-C10	-2.88	118.70	122.89
25	A	609	SQD	C45-O47-C7	-2.88	110.80	117.91
24	B	622	BCR	C35-C13-C12	-2.87	113.38	118.08
24	C	515	BCR	C34-C9-C8	-2.87	113.38	118.08
22	c	510	CLA	O1D-CGD-CBD	-2.87	120.17	124.64
24	c	515	BCR	C34-C9-C8	-2.87	113.39	118.08
25	a	609	SQD	C45-O47-C7	-2.87	110.82	117.91
24	b	622	BCR	C35-C13-C12	-2.87	113.40	118.08
32	D	405	LHG	O8-C23-O10	-2.86	116.00	123.51
32	d	405	LHG	O8-C23-O10	-2.86	116.02	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	502	CLA	C4C-C3C-C2C	-2.86	102.37	106.94
22	C	507	CLA	CBC-CAC-C3C	-2.86	103.71	112.38
22	c	507	CLA	CBC-CAC-C3C	-2.85	103.72	112.38
24	B	622	BCR	C37-C22-C21	-2.85	118.74	122.89
22	c	502	CLA	C3B-CAB-CBB	-2.84	120.68	126.40
22	C	510	CLA	O1D-CGD-CBD	-2.84	120.22	124.64
22	C	502	CLA	C3B-CAB-CBB	-2.84	120.69	126.40
28	A	613	PL9	C37-C38-C39	-2.84	121.49	127.75
22	c	511	CLA	C4C-C3C-C2C	-2.84	102.40	106.94
22	c	506	CLA	C4C-C3C-C2C	-2.84	102.41	106.94
25	l	101	SQD	C1-O5-C5	-2.83	108.18	113.74
22	C	511	CLA	C4C-C3C-C2C	-2.83	102.41	106.94
22	C	506	CLA	C4C-C3C-C2C	-2.83	102.42	106.94
24	b	622	BCR	C37-C22-C21	-2.83	118.78	122.89
22	B	610	CLA	C4C-C3C-C2C	-2.82	102.43	106.94
28	a	613	PL9	C37-C38-C39	-2.82	121.52	127.75
24	A	608	BCR	C34-C9-C10	-2.81	118.80	122.89
24	B	622	BCR	C1-C6-C5	-2.81	118.74	122.50
24	a	608	BCR	C34-C9-C10	-2.81	118.80	122.89
22	b	608	CLA	CBC-CAC-C3C	-2.81	103.85	112.38
22	B	608	CLA	CBC-CAC-C3C	-2.81	103.86	112.38
22	c	512	CLA	O1D-CGD-CBD	-2.80	120.28	124.64
25	L	101	SQD	C1-O5-C5	-2.80	108.26	113.74
22	b	617	CLA	C1C-C2C-C3C	-2.80	103.83	106.93
22	b	610	CLA	C4C-C3C-C2C	-2.79	102.47	106.94
22	B	617	CLA	O2D-CGD-O1D	-2.79	117.90	123.77
24	b	622	BCR	C1-C6-C5	-2.79	118.77	122.50
22	B	617	CLA	C1C-C2C-C3C	-2.78	103.85	106.93
22	b	617	CLA	O2D-CGD-O1D	-2.78	117.92	123.77
22	C	512	CLA	O1D-CGD-CBD	-2.78	120.32	124.64
22	B	603	CLA	C4C-C3C-C2C	-2.77	102.52	106.94
23	A	605	PHO	O1D-CGD-CBD	-2.76	120.34	124.64
22	b	603	CLA	C4C-C3C-C2C	-2.76	102.53	106.94
24	T	101	BCR	C37-C22-C21	-2.76	118.88	122.89
24	B	618	BCR	C37-C22-C21	-2.75	118.89	122.89
22	B	615	CLA	C4C-C3C-C2C	-2.75	102.55	106.94
22	C	513	CLA	C4C-C3C-C2C	-2.75	102.55	106.94
22	c	512	CLA	C4C-C3C-C2C	-2.75	102.55	106.94
22	C	506	CLA	O1D-CGD-CBD	-2.75	120.36	124.64
23	a	605	PHO	O1D-CGD-CBD	-2.75	120.37	124.64
22	c	505	CLA	C4C-C3C-C2C	-2.74	102.55	106.94
22	b	615	CLA	C4C-C3C-C2C	-2.74	102.56	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	h	102	DGD	O1G-C1A-O1A	-2.74	116.33	123.51
22	C	505	CLA	C4C-C3C-C2C	-2.73	102.58	106.94
22	C	512	CLA	C4C-C3C-C2C	-2.73	102.58	106.94
31	H	102	DGD	O1G-C1A-O1A	-2.72	116.38	123.51
24	k	101	BCR	C35-C13-C12	-2.71	113.65	118.08
22	c	506	CLA	O1D-CGD-CBD	-2.71	120.42	124.64
22	c	513	CLA	C4C-C3C-C2C	-2.71	102.61	106.94
22	d	403	CLA	C4C-C3C-C2C	-2.70	102.63	106.94
22	B	609	CLA	O2D-CGD-O1D	-2.70	118.09	123.77
24	K	101	BCR	C35-C13-C12	-2.69	113.68	118.08
22	b	604	CLA	O1D-CGD-CBD	-2.69	120.45	124.64
31	C	516	DGD	O3G-C3G-C2G	-2.69	104.59	110.99
23	A	606	PHO	CHD-C1D-ND	-2.68	119.80	124.67
22	b	609	CLA	O2D-CGD-O1D	-2.68	118.13	123.77
31	c	516	DGD	O3G-C3G-C2G	-2.68	104.61	110.99
22	D	403	CLA	C4C-C3C-C2C	-2.68	102.66	106.94
22	c	503	CLA	C4C-C3C-C2C	-2.67	102.67	106.94
23	a	606	PHO	CHD-C1D-ND	-2.67	119.82	124.67
22	A	603	CLA	C4C-C3C-C2C	-2.67	102.67	106.94
22	b	608	CLA	O1D-CGD-CBD	-2.67	120.49	124.64
22	C	503	CLA	C4C-C3C-C2C	-2.67	102.68	106.94
22	c	504	CLA	O2D-CGD-O1D	-2.67	118.16	123.77
25	a	609	SQD	C44-O6-C1	-2.66	108.25	113.81
25	A	609	SQD	C44-O6-C1	-2.66	108.25	113.81
22	c	509	CLA	C4C-C3C-C2C	-2.66	102.69	106.94
22	C	509	CLA	C4C-C3C-C2C	-2.66	102.69	106.94
22	C	504	CLA	O2D-CGD-O1D	-2.65	118.19	123.77
22	C	510	CLA	CHD-C4C-C3C	-2.65	120.82	124.91
22	B	611	CLA	O2D-CGD-O1D	-2.65	118.19	123.77
23	a	606	PHO	O1D-CGD-CBD	-2.65	120.52	124.64
22	b	607	CLA	C4C-C3C-C2C	-2.64	102.71	106.94
22	a	603	CLA	C4C-C3C-C2C	-2.64	102.71	106.94
22	B	608	CLA	O1D-CGD-CBD	-2.64	120.53	124.64
22	B	604	CLA	O1D-CGD-CBD	-2.64	120.53	124.64
22	b	611	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
22	b	615	CLA	CBC-CAC-C3C	-2.64	104.37	112.38
22	B	615	CLA	CBC-CAC-C3C	-2.64	104.37	112.38
23	A	606	PHO	O1D-CGD-CBD	-2.64	120.54	124.64
22	c	506	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
24	k	102	BCR	C37-C22-C23	-2.63	113.78	118.08
23	a	605	PHO	CHD-C1D-ND	-2.63	119.90	124.67
24	K	102	BCR	C37-C22-C23	-2.63	113.79	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	510	CLA	CHD-C4C-C3C	-2.63	120.86	124.91
22	b	607	CLA	C3B-CAB-CBB	-2.63	121.12	126.40
22	b	609	CLA	C4C-C3C-C2C	-2.63	102.74	106.94
22	b	616	CLA	C3B-CAB-CBB	-2.62	121.12	126.40
22	B	607	CLA	C3B-CAB-CBB	-2.62	121.12	126.40
23	A	605	PHO	CHD-C1D-ND	-2.62	119.91	124.67
22	B	609	CLA	C4C-C3C-C2C	-2.62	102.76	106.94
24	T	102	BCR	C32-C1-C2	-2.62	99.57	108.75
22	B	607	CLA	C4C-C3C-C2C	-2.62	102.76	106.94
22	B	605	CLA	C4C-C3C-C2C	-2.61	102.76	106.94
22	B	616	CLA	C3B-CAB-CBB	-2.61	121.15	126.40
24	t	101	BCR	C32-C1-C2	-2.61	99.60	108.75
22	C	506	CLA	O2D-CGD-O1D	-2.61	118.28	123.77
33	F	101	HEM	CBA-CAA-C2A	-2.59	107.93	112.49
33	v	201	HEM	C3B-CAB-CBB	-2.59	121.18	126.40
33	f	101	HEM	CBA-CAA-C2A	-2.59	107.94	112.49
33	V	201	HEM	C3B-CAB-CBB	-2.59	121.19	126.40
22	C	510	CLA	C4C-C3C-C2C	-2.59	102.80	106.94
22	B	603	CLA	O2D-CGD-O1D	-2.58	118.33	123.77
22	c	505	CLA	C3B-CAB-CBB	-2.58	121.21	126.40
24	H	101	BCR	C32-C1-C31	-2.58	100.06	108.36
22	A	604	CLA	O1D-CGD-CBD	-2.58	120.63	124.64
22	b	605	CLA	C4C-C3C-C2C	-2.58	102.82	106.94
24	h	101	BCR	C32-C1-C31	-2.57	100.07	108.36
22	b	614	CLA	C4C-C3C-C2C	-2.57	102.83	106.94
22	C	505	CLA	O1D-CGD-CBD	-2.57	120.64	124.64
22	a	604	CLA	O1D-CGD-CBD	-2.57	120.64	124.64
22	c	505	CLA	O1D-CGD-CBD	-2.57	120.64	124.64
22	C	508	CLA	O1D-CGD-CBD	-2.57	120.64	124.64
22	B	602	CLA	C4C-C3C-C2C	-2.56	102.84	106.94
22	C	502	CLA	O2D-CGD-O1D	-2.56	118.38	123.77
22	B	612	CLA	CHD-C4C-C3C	-2.56	120.96	124.91
22	c	508	CLA	O1D-CGD-CBD	-2.56	120.66	124.64
22	C	505	CLA	C3B-CAB-CBB	-2.55	121.26	126.40
22	b	612	CLA	CHD-C4C-C3C	-2.55	120.97	124.91
22	b	603	CLA	O2D-CGD-O1D	-2.55	118.40	123.77
22	c	510	CLA	C4C-C3C-C2C	-2.55	102.86	106.94
24	C	515	BCR	C1-C6-C5	-2.55	119.09	122.50
22	B	615	CLA	O1D-CGD-CBD	-2.55	120.67	124.64
22	c	502	CLA	O2D-CGD-O1D	-2.55	118.40	123.77
22	b	602	CLA	C4C-C3C-C2C	-2.55	102.87	106.94
25	a	609	SQD	C1-O5-C5	-2.55	108.75	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	615	CLA	O1D-CGD-CBD	-2.54	120.68	124.64
22	B	614	CLA	C4C-C3C-C2C	-2.54	102.88	106.94
24	c	515	BCR	C1-C6-C5	-2.54	119.10	122.50
25	A	609	SQD	C1-O5-C5	-2.52	108.80	113.74
24	B	618	BCR	C1-C6-C5	-2.51	119.14	122.50
28	d	408	PL9	C27-C28-C29	-2.51	122.22	127.75
24	T	101	BCR	C1-C6-C5	-2.50	119.15	122.50
24	t	101	BCR	C1-C6-C5	-2.50	119.16	122.50
28	D	408	PL9	C27-C28-C29	-2.50	122.24	127.75
22	C	504	CLA	C3B-CAB-CBB	-2.50	121.38	126.40
22	b	614	CLA	CHD-C4C-C3C	-2.49	121.06	124.91
22	c	504	CLA	C3B-CAB-CBB	-2.49	121.39	126.40
24	T	102	BCR	C1-C6-C5	-2.49	119.17	122.50
24	k	102	BCR	C34-C9-C8	-2.49	114.02	118.08
22	d	401	CLA	CHD-C4C-C3C	-2.48	121.08	124.91
22	b	613	CLA	O1D-CGD-CBD	-2.48	120.78	124.64
22	A	607	CLA	C4C-C3C-C2C	-2.48	102.98	106.94
22	B	614	CLA	CHD-C4C-C3C	-2.47	121.10	124.91
24	K	102	BCR	C34-C9-C8	-2.46	114.05	118.08
22	a	607	CLA	C4C-C3C-C2C	-2.46	103.00	106.94
22	B	613	CLA	O1D-CGD-CBD	-2.46	120.81	124.64
22	D	401	CLA	CHD-C4C-C3C	-2.46	121.11	124.91
22	d	403	CLA	O1D-CGD-CBD	-2.46	120.81	124.64
22	C	511	CLA	O2D-CGD-O1D	-2.46	118.59	123.77
22	c	511	CLA	O2D-CGD-O1D	-2.45	118.61	123.77
22	D	403	CLA	O1D-CGD-CBD	-2.45	120.83	124.64
24	B	622	BCR	C37-C22-C23	-2.45	114.08	118.08
22	C	509	CLA	O1D-CGD-CBD	-2.44	120.83	124.64
22	C	512	CLA	C3B-CAB-CBB	-2.44	121.48	126.40
22	c	512	CLA	C3B-CAB-CBB	-2.44	121.48	126.40
22	a	604	CLA	CBC-CAC-C3C	-2.44	104.97	112.38
22	b	604	CLA	C4C-C3C-C2C	-2.44	103.05	106.94
22	A	607	CLA	O1D-CGD-CBD	-2.43	120.85	124.64
22	b	608	CLA	C4C-C3C-C2C	-2.43	103.05	106.94
24	c	514	BCR	C40-C30-C29	-2.43	100.22	108.75
24	b	622	BCR	C37-C22-C23	-2.43	114.11	118.08
22	A	604	CLA	CBC-CAC-C3C	-2.42	105.02	112.38
23	a	606	PHO	C3B-C2B-C1B	-2.42	100.98	106.36
22	B	608	CLA	C4C-C3C-C2C	-2.42	103.07	106.94
24	C	514	BCR	C40-C30-C29	-2.42	100.25	108.75
23	A	606	PHO	C3B-C2B-C1B	-2.42	100.99	106.36
22	b	602	CLA	C4-C3-C2	-2.42	118.90	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C4C-C3C-C2C	-2.42	103.08	106.94
22	a	607	CLA	O1D-CGD-CBD	-2.42	120.88	124.64
22	B	610	CLA	O2D-CGD-O1D	-2.42	118.69	123.77
22	B	602	CLA	C4-C3-C2	-2.41	118.91	123.58
22	b	610	CLA	O2D-CGD-O1D	-2.41	118.70	123.77
22	B	612	CLA	O2D-CGD-O1D	-2.41	118.70	123.77
22	C	507	CLA	C4C-C3C-C2C	-2.41	103.09	106.94
22	b	612	CLA	O2D-CGD-O1D	-2.40	118.71	123.77
22	c	507	CLA	C4C-C3C-C2C	-2.40	103.10	106.94
22	c	509	CLA	O1D-CGD-CBD	-2.40	120.90	124.64
22	c	503	CLA	C3B-CAB-CBB	-2.40	121.58	126.40
22	C	503	CLA	C3B-CAB-CBB	-2.40	121.58	126.40
22	C	501	CLA	O1D-CGD-CBD	-2.39	120.91	124.64
24	K	102	BCR	C1-C6-C5	-2.39	119.30	122.50
22	d	403	CLA	O2D-CGD-O1D	-2.39	118.74	123.77
22	c	501	CLA	O1D-CGD-CBD	-2.39	120.93	124.64
24	k	102	BCR	C1-C6-C5	-2.39	119.31	122.50
22	D	403	CLA	O2D-CGD-O1D	-2.38	118.77	123.77
22	C	512	CLA	O2D-CGD-O1D	-2.37	118.77	123.77
22	a	603	CLA	C3B-CAB-CBB	-2.37	121.63	126.40
22	c	509	CLA	O2D-CGD-O1D	-2.37	118.78	123.77
22	a	603	CLA	O2D-CGD-O1D	-2.37	118.79	123.77
22	A	603	CLA	O2D-CGD-O1D	-2.37	118.79	123.77
22	A	603	CLA	C3B-CAB-CBB	-2.35	121.67	126.40
22	C	509	CLA	O2D-CGD-O1D	-2.35	118.82	123.77
22	c	512	CLA	O2D-CGD-O1D	-2.35	118.83	123.77
24	B	618	BCR	C33-C5-C4	-2.35	108.94	113.47
24	T	101	BCR	C33-C5-C4	-2.34	108.95	113.47
24	h	101	BCR	C29-C28-C27	-2.34	105.51	111.42
22	d	402	CLA	CHD-C4C-C3C	-2.33	121.31	124.91
22	D	402	CLA	CHD-C4C-C3C	-2.33	121.31	124.91
22	D	402	CLA	C3B-CAB-CBB	-2.33	121.71	126.40
29	D	406	LMG	O8-C28-O10	-2.32	117.44	123.51
24	H	101	BCR	C29-C28-C27	-2.31	105.56	111.42
29	d	406	LMG	O8-C28-O10	-2.31	117.44	123.51
22	d	402	CLA	C3B-CAB-CBB	-2.31	121.75	126.40
22	C	501	CLA	C4C-C3C-C2C	-2.30	103.26	106.94
33	v	201	HEM	C3C-CAC-CBC	-2.30	121.77	126.40
29	c	519	LMG	O1-C7-C8	-2.29	105.53	110.99
29	C	519	LMG	O1-C7-C8	-2.29	105.53	110.99
22	C	501	CLA	CBC-CAC-C3C	-2.29	105.43	112.38
22	B	602	CLA	O2D-CGD-O1D	-2.29	118.95	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	501	CLA	CBC-CAC-C3C	-2.29	105.43	112.38
33	V	201	HEM	C3C-CAC-CBC	-2.29	121.80	126.40
22	B	614	CLA	O2D-CGD-O1D	-2.29	118.95	123.77
22	b	614	CLA	O2D-CGD-O1D	-2.28	118.96	123.77
22	c	501	CLA	C4C-C3C-C2C	-2.28	103.29	106.94
22	b	606	CLA	O2A-CGA-O1A	-2.28	117.53	123.51
22	b	602	CLA	O2D-CGD-O1D	-2.27	118.99	123.77
24	h	101	BCR	C40-C30-C29	-2.27	100.78	108.75
24	H	101	BCR	C40-C30-C29	-2.27	100.78	108.75
22	B	606	CLA	O2A-CGA-O1A	-2.27	117.57	123.51
24	t	101	BCR	C40-C30-C39	-2.27	101.07	108.36
24	T	102	BCR	C40-C30-C39	-2.26	101.09	108.36
22	d	402	CLA	CHC-C1C-C2C	-2.25	120.06	126.31
24	a	608	BCR	C28-C27-C26	-2.25	110.13	113.87
22	d	402	CLA	O1D-CGD-CBD	-2.25	121.14	124.64
22	D	402	CLA	O1D-CGD-CBD	-2.25	121.14	124.64
22	D	402	CLA	CHC-C1C-C2C	-2.24	120.09	126.31
24	A	608	BCR	C28-C27-C26	-2.24	110.16	113.87
22	A	604	CLA	O2D-CGD-O1D	-2.24	119.06	123.77
23	a	606	PHO	C1C-C2C-C3C	-2.24	103.85	106.43
28	d	408	PL9	C7-C8-C9	-2.24	122.90	126.70
22	a	604	CLA	O2D-CGD-O1D	-2.23	119.07	123.77
28	D	408	PL9	C7-C8-C9	-2.23	122.91	126.70
22	C	512	CLA	CBA-CAA-C2A	-2.23	108.22	113.96
22	b	604	CLA	O2A-CGA-O1A	-2.23	117.67	123.51
31	c	517	DGD	O2G-C1B-O1B	-2.23	117.62	123.67
22	c	512	CLA	CBA-CAA-C2A	-2.22	108.22	113.96
31	C	517	DGD	O2G-C1B-O1B	-2.22	117.62	123.67
22	B	604	CLA	O2A-CGA-O1A	-2.22	117.69	123.51
22	b	609	CLA	C11-C12-C13	-2.22	108.60	115.46
22	B	609	CLA	C11-C12-C13	-2.21	108.62	115.46
22	c	503	CLA	O1D-CGD-CBD	-2.21	121.20	124.64
22	A	604	CLA	C4C-C3C-C2C	-2.21	103.41	106.94
23	A	606	PHO	C1C-C2C-C3C	-2.20	103.89	106.43
23	a	605	PHO	C3B-C2B-C1B	-2.20	101.47	106.36
23	A	606	PHO	O2D-CGD-O1D	-2.20	119.14	123.77
23	A	605	PHO	C3B-C2B-C1B	-2.20	101.48	106.36
22	a	604	CLA	C4C-C3C-C2C	-2.20	103.43	106.94
22	C	503	CLA	O1D-CGD-CBD	-2.20	121.22	124.64
24	A	608	BCR	C37-C22-C23	-2.20	114.49	118.08
24	D	404	BCR	C37-C22-C23	-2.20	114.49	118.08
23	A	606	PHO	CBA-CAA-C2A	-2.18	108.33	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	606	PHO	CBA-CAA-C2A	-2.18	108.34	113.96
23	a	606	PHO	O2D-CGD-O1D	-2.18	119.18	123.77
24	a	608	BCR	C37-C22-C23	-2.18	114.52	118.08
22	c	502	CLA	CHD-C4C-C3C	-2.17	121.56	124.91
22	c	504	CLA	C4C-C3C-C2C	-2.17	103.47	106.94
23	a	605	PHO	C1C-NC-C4C	-2.17	102.37	106.50
22	C	504	CLA	C4C-C3C-C2C	-2.17	103.47	106.94
22	D	402	CLA	C4C-C3C-C2C	-2.16	103.48	106.94
24	d	404	BCR	C37-C22-C23	-2.16	114.55	118.08
22	d	402	CLA	C4C-C3C-C2C	-2.16	103.48	106.94
22	b	617	CLA	C4-C3-C2	-2.16	119.39	123.58
22	C	502	CLA	CHD-C4C-C3C	-2.16	121.57	124.91
22	D	401	CLA	CAA-CBA-CGA	-2.16	107.03	113.28
22	C	507	CLA	C3B-CAB-CBB	-2.16	122.06	126.40
22	B	617	CLA	C4-C3-C2	-2.15	119.42	123.58
22	a	607	CLA	C3B-CAB-CBB	-2.15	122.07	126.40
22	d	401	CLA	CAA-CBA-CGA	-2.15	107.06	113.28
23	A	605	PHO	C1C-NC-C4C	-2.15	102.41	106.50
22	c	507	CLA	C3B-CAB-CBB	-2.15	122.08	126.40
22	b	605	CLA	C3B-CAB-CBB	-2.15	122.08	126.40
22	A	607	CLA	C3B-CAB-CBB	-2.14	122.08	126.40
22	b	608	CLA	C3B-CAB-CBB	-2.14	122.09	126.40
22	B	617	CLA	CHD-C4C-C3C	-2.14	121.60	124.91
28	A	613	PL9	C17-C18-C19	-2.14	123.02	127.75
24	t	101	BCR	C31-C1-C2	-2.14	101.23	108.75
22	B	605	CLA	C3B-CAB-CBB	-2.14	122.09	126.40
22	C	510	CLA	O2D-CGD-O1D	-2.14	119.27	123.77
22	B	614	CLA	CBC-CAC-C3C	-2.14	105.89	112.38
22	b	614	CLA	CBC-CAC-C3C	-2.14	105.89	112.38
24	T	102	BCR	C31-C1-C2	-2.14	101.25	108.75
24	c	515	BCR	C37-C22-C23	-2.13	114.60	118.08
29	c	519	LMG	O8-C28-O10	-2.13	117.93	123.51
22	b	617	CLA	CHD-C4C-C3C	-2.13	121.62	124.91
25	l	102	SQD	O5-C1-C2	-2.13	105.86	110.28
24	C	515	BCR	C37-C22-C23	-2.12	114.61	118.08
22	C	513	CLA	C3B-CAB-CBB	-2.12	122.13	126.40
28	a	613	PL9	C17-C18-C19	-2.12	123.07	127.75
22	B	608	CLA	C3B-CAB-CBB	-2.12	122.14	126.40
29	C	519	LMG	O8-C28-O10	-2.12	117.96	123.51
31	c	516	DGD	C3G-C2G-C1G	-2.12	107.15	112.08
22	c	513	CLA	C3B-CAB-CBB	-2.11	122.15	126.40
22	B	612	CLA	CBC-CAC-C3C	-2.11	105.97	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	t	101	BCR	C38-C26-C27	-2.11	109.39	113.47
25	b	621	SQD	O5-C1-C2	-2.11	105.89	110.28
22	c	509	CLA	C3B-CAB-CBB	-2.11	122.16	126.40
22	b	606	CLA	CHD-C4C-C3C	-2.11	121.66	124.91
25	d	411	SQD	O48-C23-O10	-2.11	117.99	123.51
31	C	516	DGD	C3G-C2G-C1G	-2.10	107.18	112.08
32	E	101	LHG	O8-C23-O10	-2.10	118.00	123.51
22	B	607	CLA	C6-C5-C3	-2.10	108.99	112.76
22	c	510	CLA	O2D-CGD-O1D	-2.10	119.35	123.77
25	D	411	SQD	O48-C23-O10	-2.10	118.01	123.51
22	b	612	CLA	CBC-CAC-C3C	-2.10	106.02	112.38
32	L	102	LHG	C6-C5-C4	-2.09	107.20	112.08
22	B	606	CLA	CHD-C4C-C3C	-2.09	121.68	124.91
25	A	609	SQD	O48-C23-O10	-2.09	118.03	123.51
29	B	620	LMG	O7-C10-O9	-2.09	117.99	123.67
22	C	509	CLA	C3B-CAB-CBB	-2.09	122.20	126.40
24	b	618	BCR	C29-C28-C27	-2.08	106.14	111.42
22	b	609	CLA	C2A-C3A-C4A	-2.08	99.70	101.84
32	e	101	LHG	O8-C23-O10	-2.08	118.06	123.51
25	a	609	SQD	O48-C23-O10	-2.08	118.06	123.51
22	b	606	CLA	O2D-CGD-O1D	-2.08	119.40	123.77
25	a	609	SQD	O9-S-O7	-2.07	108.10	113.96
22	B	606	CLA	O2D-CGD-O1D	-2.07	119.41	123.77
32	l	103	LHG	C6-C5-C4	-2.07	107.25	112.08
24	T	102	BCR	C38-C26-C27	-2.07	109.47	113.47
22	b	613	CLA	O2D-CGD-O1D	-2.07	119.41	123.77
22	b	607	CLA	C6-C5-C3	-2.07	109.05	112.76
22	B	613	CLA	O2D-CGD-O1D	-2.07	119.42	123.77
25	A	609	SQD	O9-S-O7	-2.07	108.13	113.96
29	b	619	LMG	O7-C10-O9	-2.06	118.05	123.67
24	B	619	BCR	C29-C28-C27	-2.06	106.19	111.42
22	B	616	CLA	O2D-CGD-O1D	-2.06	119.43	123.77
22	B	609	CLA	C2A-C3A-C4A	-2.06	99.73	101.84
22	b	616	CLA	O2D-CGD-O1D	-2.06	119.44	123.77
25	A	609	SQD	O5-C1-C2	-2.05	106.01	110.28
24	b	618	BCR	C32-C1-C6	-2.05	107.19	110.33
31	H	102	DGD	O3G-C3G-C2G	-2.05	106.11	110.99
25	a	609	SQD	O5-C1-C2	-2.05	106.02	110.28
31	h	102	DGD	O3G-C3G-C2G	-2.05	106.11	110.99
24	H	101	BCR	C1-C6-C5	-2.05	119.76	122.50
22	c	501	CLA	C6-C5-C3	-2.04	109.09	112.76
22	b	604	CLA	CHD-C4C-C3C	-2.04	121.75	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	621	SQD	O9-S-O7	-2.04	108.19	113.96
22	B	604	CLA	CHD-C4C-C3C	-2.04	121.76	124.91
22	C	501	CLA	C6-C5-C3	-2.04	109.10	112.76
23	a	605	PHO	CHC-C1C-C2C	-2.04	120.79	125.52
22	b	609	CLA	C11-C10-C8	-2.04	109.16	115.46
28	D	408	PL9	C31-C32-C33	-2.03	106.27	111.61
25	d	411	SQD	O9-S-O7	-2.03	108.22	113.96
24	a	608	BCR	C32-C1-C2	-2.03	101.61	108.75
24	A	608	BCR	C32-C1-C2	-2.03	101.61	108.75
24	B	619	BCR	C32-C1-C6	-2.03	107.23	110.33
23	A	605	PHO	CBA-CAA-C2A	-2.03	108.72	113.96
23	a	605	PHO	CBA-CAA-C2A	-2.03	108.72	113.96
22	B	616	CLA	C11-C10-C8	-2.03	109.18	115.46
22	b	609	CLA	C3B-CAB-CBB	-2.03	122.32	126.40
22	b	609	CLA	O2A-CGA-O1A	-2.03	118.20	123.51
25	l	102	SQD	O9-S-O7	-2.03	108.24	113.96
22	B	609	CLA	C11-C10-C8	-2.02	109.19	115.46
22	c	509	CLA	O2A-CGA-O1A	-2.02	118.20	123.51
22	B	611	CLA	CAA-CBA-CGA	-2.02	107.43	113.28
22	b	610	CLA	O1D-CGD-CBD	-2.02	121.49	124.64
24	h	101	BCR	C1-C6-C5	-2.02	119.80	122.50
22	d	401	CLA	C5-C3-C2	-2.02	117.22	120.98
22	D	401	CLA	C5-C3-C2	-2.02	117.22	120.98
25	D	411	SQD	O9-S-O7	-2.02	108.26	113.96
22	C	511	CLA	C3B-CAB-CBB	-2.02	122.34	126.40
22	b	611	CLA	CAA-CBA-CGA	-2.01	107.45	113.28
22	B	610	CLA	O1D-CGD-CBD	-2.01	121.50	124.64
23	A	605	PHO	CHC-C1C-C2C	-2.01	120.85	125.52
22	B	609	CLA	C3B-CAB-CBB	-2.01	122.35	126.40
22	C	509	CLA	O2A-CGA-O1A	-2.01	118.23	123.51
22	b	605	CLA	O2D-CGD-O1D	-2.01	119.53	123.77
28	d	408	PL9	C31-C32-C33	-2.01	106.33	111.61
22	b	616	CLA	C11-C10-C8	-2.01	109.24	115.46
22	B	617	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
22	B	609	CLA	O2A-CGA-O1A	-2.01	118.25	123.51
22	B	606	CLA	C3B-CAB-CBB	-2.01	122.36	126.40
22	B	605	CLA	O2D-CGD-O1D	-2.01	119.55	123.77
22	c	511	CLA	C3B-CAB-CBB	-2.00	122.37	126.40
22	b	606	CLA	C3B-CAB-CBB	-2.00	122.37	126.40
22	C	503	CLA	CED-O2D-CGD	2.00	120.72	115.97
22	b	605	CLA	CAC-C3C-C4C	2.00	127.77	124.82
29	d	406	LMG	O8-C28-C29	2.00	118.01	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	406	LMG	O8-C28-C29	2.00	118.02	111.85
22	B	602	CLA	C4-C3-C5	2.00	118.42	115.37
32	D	409	LHG	O4-P-O5	2.01	123.00	112.56
22	c	503	CLA	CED-O2D-CGD	2.01	120.74	115.97
22	c	509	CLA	CMB-C2B-C3B	2.01	129.02	125.09
22	B	609	CLA	C4A-NA-C1A	2.01	108.93	106.38
22	C	509	CLA	CMB-C2B-C3B	2.01	129.03	125.09
22	D	402	CLA	C4A-NA-C1A	2.01	108.93	106.38
22	c	508	CLA	CAC-C3C-C4C	2.02	127.80	124.82
22	b	611	CLA	CMB-C2B-C3B	2.02	129.05	125.09
24	B	619	BCR	C28-C29-C30	2.03	122.15	114.77
24	b	618	BCR	C28-C29-C30	2.03	122.15	114.77
24	t	101	BCR	C3-C2-C1	2.03	122.16	114.77
24	k	102	BCR	C1-C6-C7	2.03	121.77	115.96
24	T	102	BCR	C3-C2-C1	2.03	122.17	114.77
22	B	605	CLA	CAC-C3C-C4C	2.03	127.82	124.82
22	b	609	CLA	C4A-NA-C1A	2.04	108.96	106.38
22	B	603	CLA	CMC-C2C-C1C	2.04	128.02	125.00
24	K	102	BCR	C1-C6-C7	2.04	121.78	115.96
22	B	615	CLA	O2A-CGA-CBA	2.04	118.13	111.85
22	c	501	CLA	CMB-C2B-C3B	2.04	129.08	125.09
22	B	603	CLA	O2A-CGA-CBA	2.05	118.14	111.85
31	C	517	DGD	O1G-C1A-C2A	2.05	118.15	111.85
22	C	501	CLA	CMB-C2B-C3B	2.05	129.09	125.09
22	b	602	CLA	C4-C3-C5	2.05	118.49	115.37
28	D	408	PL9	C20-C19-C21	2.05	118.49	115.37
22	B	611	CLA	CMB-C2B-C3B	2.05	129.10	125.09
31	c	517	DGD	O1G-C1A-C2A	2.05	118.17	111.85
22	b	603	CLA	O2A-CGA-CBA	2.05	118.17	111.85
22	c	511	CLA	CED-O2D-CGD	2.06	120.85	115.97
22	C	511	CLA	CED-O2D-CGD	2.06	120.85	115.97
29	z	101	LMG	C9-O8-C28	2.06	122.27	117.12
22	b	615	CLA	O2A-CGA-CBA	2.06	118.18	111.85
22	b	616	CLA	CMB-C2B-C3B	2.06	129.12	125.09
22	b	615	CLA	CED-O2D-CGD	2.07	120.88	115.97
22	B	615	CLA	CMB-C2B-C3B	2.07	129.13	125.09
29	Z	101	LMG	C9-O8-C28	2.07	122.30	117.12
22	B	616	CLA	CMB-C2B-C3B	2.07	129.14	125.09
22	B	615	CLA	CED-O2D-CGD	2.07	120.89	115.97
22	c	506	CLA	O2A-CGA-CBA	2.08	118.24	111.85
22	B	608	CLA	CMB-C2B-C3B	2.08	129.15	125.09
22	c	507	CLA	CED-O2D-CGD	2.08	120.91	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	d	408	PL9	C20-C19-C21	2.08	118.54	115.37
25	D	411	SQD	C3-C4-C5	2.08	113.93	110.23
22	b	615	CLA	CMB-C2B-C3B	2.08	129.16	125.09
22	b	610	CLA	CMB-C2B-C3B	2.09	129.17	125.09
22	C	506	CLA	O2A-CGA-CBA	2.09	118.27	111.85
22	b	603	CLA	CMC-C2C-C1C	2.09	128.09	125.00
22	C	512	CLA	CAC-C3C-C4C	2.09	127.90	124.82
22	a	604	CLA	CED-O2D-CGD	2.09	120.93	115.97
22	B	602	CLA	CMB-C2B-C3B	2.09	129.17	125.09
22	B	617	CLA	CED-O2D-CGD	2.09	120.94	115.97
22	B	612	CLA	CMB-C2B-C3B	2.09	129.18	125.09
22	b	606	CLA	CMC-C2C-C1C	2.09	128.10	125.00
22	b	602	CLA	CMB-C2B-C3B	2.10	129.19	125.09
22	A	604	CLA	CED-O2D-CGD	2.10	120.95	115.97
22	C	507	CLA	CED-O2D-CGD	2.10	120.95	115.97
22	c	513	CLA	CAC-C3C-C4C	2.10	127.92	124.82
22	b	608	CLA	CMB-C2B-C3B	2.10	129.20	125.09
22	b	617	CLA	CED-O2D-CGD	2.10	120.96	115.97
25	d	411	SQD	C3-C4-C5	2.10	113.97	110.23
22	d	401	CLA	CED-O2D-CGD	2.10	120.96	115.97
22	D	401	CLA	CED-O2D-CGD	2.10	120.97	115.97
31	h	102	DGD	O6E-C5E-C6E	2.10	111.83	106.38
22	B	610	CLA	CMB-C2B-C3B	2.11	129.21	125.09
22	c	512	CLA	CAC-C3C-C4C	2.11	127.93	124.82
31	H	102	DGD	O6E-C5E-C6E	2.11	111.85	106.38
22	B	616	CLA	CED-O2D-CGD	2.11	120.99	115.97
22	c	511	CLA	CAC-C3C-C4C	2.12	127.94	124.82
22	C	511	CLA	CAC-C3C-C4C	2.12	127.94	124.82
22	b	616	CLA	CED-O2D-CGD	2.12	121.00	115.97
24	t	101	BCR	C40-C30-C25	2.13	113.58	110.33
22	b	616	CLA	CMC-C2C-C1C	2.13	128.15	125.00
22	b	612	CLA	CMB-C2B-C3B	2.13	129.25	125.09
22	c	510	CLA	CAC-C3C-C4C	2.13	127.96	124.82
24	a	608	BCR	C2-C1-C6	2.13	113.65	110.48
22	b	607	CLA	CMC-C2C-C1C	2.13	128.16	125.00
23	a	606	PHO	CMB-C2B-C1B	2.13	128.47	125.06
22	b	610	CLA	CMC-C2C-C1C	2.14	128.16	125.00
24	C	515	BCR	C28-C27-C26	2.14	117.41	113.87
24	T	102	BCR	C40-C30-C25	2.14	113.60	110.33
22	B	609	CLA	CMC-C2C-C1C	2.14	128.17	125.00
22	C	513	CLA	CAC-C3C-C4C	2.14	127.98	124.82
24	c	515	BCR	C28-C27-C26	2.15	117.42	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	610	CLA	CMC-C2C-C1C	2.15	128.18	125.00
22	C	510	CLA	CAC-C3C-C4C	2.15	127.99	124.82
22	B	607	CLA	CMC-C2C-C1C	2.15	128.18	125.00
23	a	606	PHO	C3D-C4D-ND	2.15	116.09	109.76
22	b	604	CLA	O2A-CGA-CBA	2.15	118.46	111.85
22	B	616	CLA	CMC-C2C-C1C	2.15	128.18	125.00
22	B	606	CLA	CMC-C2C-C1C	2.15	128.18	125.00
24	A	608	BCR	C2-C1-C6	2.15	113.68	110.48
24	D	404	BCR	C38-C26-C25	2.16	126.92	124.62
22	B	604	CLA	O2A-CGA-CBA	2.16	118.50	111.85
22	b	609	CLA	CMC-C2C-C1C	2.16	128.20	125.00
23	A	606	PHO	C3D-C4D-ND	2.16	116.14	109.76
23	A	605	PHO	C3D-C4D-ND	2.16	116.14	109.76
23	A	605	PHO	CMB-C2B-C1B	2.16	128.52	125.06
23	A	606	PHO	CMB-C2B-C1B	2.16	128.52	125.06
22	A	603	CLA	O2A-CGA-CBA	2.16	118.51	111.85
24	d	404	BCR	C38-C26-C25	2.17	126.93	124.62
22	B	606	CLA	CED-O2D-CGD	2.17	121.12	115.97
32	D	407	LHG	O7-C7-C8	2.17	116.09	111.53
22	c	511	CLA	CMC-C2C-C1C	2.17	128.21	125.00
22	b	606	CLA	CED-O2D-CGD	2.17	121.12	115.97
32	d	409	LHG	O8-C23-C24	2.17	118.53	111.85
32	d	407	LHG	O7-C7-C8	2.17	116.11	111.53
32	D	409	LHG	O8-C23-C24	2.17	118.54	111.85
22	B	603	CLA	CED-O2D-CGD	2.17	121.14	115.97
22	a	603	CLA	O2A-CGA-CBA	2.18	118.54	111.85
22	b	603	CLA	CED-O2D-CGD	2.18	121.14	115.97
22	B	613	CLA	O2A-CGA-CBA	2.18	118.55	111.85
24	K	101	BCR	C30-C25-C24	2.18	122.18	115.96
24	T	101	BCR	C2-C3-C4	2.18	116.95	111.42
23	a	605	PHO	C3D-C4D-ND	2.18	116.20	109.76
22	C	512	CLA	CMC-C2C-C1C	2.18	128.24	125.00
23	a	605	PHO	CMB-C2B-C1B	2.19	128.56	125.06
22	c	510	CLA	C4-C3-C5	2.19	118.70	115.37
22	b	613	CLA	O2A-CGA-CBA	2.19	118.59	111.85
24	k	101	BCR	C30-C25-C24	2.19	122.22	115.96
22	C	510	CLA	C4-C3-C5	2.19	118.71	115.37
24	B	618	BCR	C2-C3-C4	2.20	116.99	111.42
22	C	511	CLA	CMC-C2C-C1C	2.20	128.26	125.00
22	D	401	CLA	O2A-CGA-CBA	2.20	118.63	111.85
22	A	607	CLA	CMB-C2B-C3B	2.21	129.40	125.09
22	C	506	CLA	CMB-C2B-C3B	2.21	129.40	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	CMB-C2B-C3B	2.21	129.40	125.09
22	d	401	CLA	O2A-CGA-CBA	2.21	118.65	111.85
22	c	512	CLA	CMC-C2C-C1C	2.21	128.28	125.00
22	a	607	CLA	CMB-C2B-C3B	2.22	129.43	125.09
24	d	404	BCR	C24-C25-C26	2.23	126.53	121.36
22	b	605	CLA	CMC-C2C-C1C	2.23	128.30	125.00
22	a	607	CLA	CAC-C3C-C4C	2.23	128.11	124.82
24	D	404	BCR	C24-C25-C26	2.23	126.53	121.36
22	C	509	CLA	C4-C3-C5	2.23	118.77	115.37
22	c	506	CLA	CAC-C3C-C4C	2.23	128.12	124.82
22	b	610	CLA	CED-O2D-CGD	2.24	121.28	115.97
22	B	610	CLA	CED-O2D-CGD	2.24	121.28	115.97
22	c	509	CLA	C4-C3-C5	2.24	118.78	115.37
29	D	406	LMG	O7-C10-C11	2.24	116.26	111.53
24	a	608	BCR	C4-C5-C6	2.25	125.20	122.73
22	c	507	CLA	O2A-CGA-CBA	2.25	118.77	111.85
22	C	507	CLA	O2A-CGA-CBA	2.25	118.77	111.85
29	d	406	LMG	O7-C10-C11	2.25	116.27	111.53
24	H	101	BCR	C28-C29-C30	2.25	122.97	114.77
22	B	617	CLA	C4-C3-C5	2.26	118.81	115.37
24	h	101	BCR	C28-C29-C30	2.26	122.99	114.77
24	b	622	BCR	C1-C6-C7	2.26	122.42	115.96
24	B	622	BCR	C1-C6-C7	2.26	122.42	115.96
22	B	605	CLA	CMC-C2C-C1C	2.26	128.35	125.00
22	D	403	CLA	CMB-C2B-C3B	2.26	129.52	125.09
22	d	403	CLA	CMB-C2B-C3B	2.27	129.52	125.09
23	a	606	PHO	C4D-C3D-CAD	2.27	109.81	105.61
22	A	607	CLA	CAC-C3C-C4C	2.27	128.17	124.82
22	C	506	CLA	CAC-C3C-C4C	2.27	128.17	124.82
22	b	614	CLA	CMB-C2B-C3B	2.27	129.52	125.09
24	A	608	BCR	C4-C5-C6	2.27	125.23	122.73
22	b	617	CLA	C4-C3-C5	2.27	118.83	115.37
22	C	509	CLA	CAC-C3C-C4C	2.27	128.17	124.82
23	A	606	PHO	C4D-C3D-CAD	2.27	109.82	105.61
31	D	410	DGD	O6E-C5E-C6E	2.28	112.28	106.38
22	B	605	CLA	O2A-CGA-CBA	2.28	118.86	111.85
25	b	601	SQD	C3-C4-C5	2.28	114.29	110.23
22	C	510	CLA	O2A-CGA-CBA	2.28	118.86	111.85
31	d	410	DGD	O6E-C5E-C6E	2.28	112.29	106.38
22	B	614	CLA	CMC-C2C-C1C	2.28	128.38	125.00
22	B	614	CLA	CMB-C2B-C3B	2.28	129.55	125.09
22	b	605	CLA	O2A-CGA-CBA	2.28	118.88	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	609	SQD	O48-C23-C24	2.28	118.88	111.85
22	c	510	CLA	O2A-CGA-CBA	2.29	118.88	111.85
25	a	609	SQD	O48-C23-C24	2.29	118.89	111.85
22	c	505	CLA	CED-O2D-CGD	2.29	121.41	115.97
22	C	505	CLA	CED-O2D-CGD	2.29	121.42	115.97
25	B	601	SQD	C3-C4-C5	2.29	114.32	110.23
22	A	607	CLA	O2A-CGA-CBA	2.30	118.93	111.85
22	c	509	CLA	CAC-C3C-C4C	2.31	128.22	124.82
25	B	601	SQD	O8-S-C6	2.31	109.78	104.99
22	b	614	CLA	CMC-C2C-C1C	2.31	128.42	125.00
22	D	403	CLA	CAC-C3C-C4C	2.31	128.23	124.82
24	H	101	BCR	C30-C25-C24	2.31	122.57	115.96
24	h	101	BCR	C30-C25-C24	2.31	122.57	115.96
22	a	607	CLA	O2A-CGA-CBA	2.32	118.97	111.85
25	b	601	SQD	O8-S-C6	2.32	109.81	104.99
22	b	609	CLA	CAC-C3C-C4C	2.32	128.24	124.82
23	a	606	PHO	CED-O2D-CGD	2.32	121.48	115.97
22	a	603	CLA	CMC-C2C-C1C	2.32	128.44	125.00
22	c	512	CLA	CED-O2D-CGD	2.33	121.50	115.97
31	d	410	DGD	O6D-C5D-C6D	2.33	111.43	106.61
23	A	606	PHO	CED-O2D-CGD	2.33	121.51	115.97
32	D	407	LHG	O8-C23-C24	2.33	119.03	111.85
32	d	407	LHG	O8-C23-C24	2.34	119.03	111.85
22	C	512	CLA	CED-O2D-CGD	2.34	121.52	115.97
22	c	501	CLA	C4-C3-C5	2.34	118.94	115.37
22	d	403	CLA	CAC-C3C-C4C	2.34	128.28	124.82
23	A	605	PHO	C4D-C3D-CAD	2.34	109.95	105.61
22	C	501	CLA	C4-C3-C5	2.35	118.94	115.37
22	B	609	CLA	CAC-C3C-C4C	2.35	128.29	124.82
22	A	603	CLA	CMC-C2C-C1C	2.36	128.49	125.00
29	A	614	LMG	O8-C28-C29	2.36	119.11	111.85
22	C	501	CLA	CAC-C3C-C4C	2.36	128.31	124.82
31	D	410	DGD	O6D-C5D-C6D	2.37	111.50	106.61
22	b	612	CLA	CAC-C3C-C4C	2.37	128.31	124.82
29	a	614	LMG	O8-C28-C29	2.37	119.15	111.85
22	B	614	CLA	O2A-CGA-CBA	2.38	119.16	111.85
22	c	501	CLA	CAC-C3C-C4C	2.38	128.33	124.82
22	b	614	CLA	O2A-CGA-CBA	2.38	119.17	111.85
23	a	605	PHO	C4D-C3D-CAD	2.38	110.02	105.61
22	B	612	CLA	CAC-C3C-C4C	2.39	128.35	124.82
24	d	404	BCR	C30-C25-C24	2.39	122.80	115.96
24	D	404	BCR	C30-C25-C24	2.40	122.80	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	D	401	CLA	CAC-C3C-C4C	2.40	128.36	124.82
22	C	505	CLA	CMB-C2B-C3B	2.40	129.79	125.09
22	c	505	CLA	CMB-C2B-C3B	2.41	129.80	125.09
25	l	101	SQD	O8-S-C6	2.41	110.00	104.99
22	a	603	CLA	CAC-C3C-C4C	2.41	128.38	124.82
25	L	101	SQD	O8-S-C6	2.42	110.01	104.99
22	B	609	CLA	C4-C3-C5	2.42	119.06	115.37
24	b	622	BCR	C32-C1-C6	2.43	114.04	110.33
22	b	609	CLA	C4-C3-C5	2.43	119.07	115.37
22	c	513	CLA	O2A-CGA-CBA	2.43	119.33	111.85
22	a	603	CLA	C4-C3-C5	2.43	119.08	115.37
22	C	513	CLA	O2A-CGA-CBA	2.43	119.34	111.85
22	B	607	CLA	O2A-CGA-CBA	2.44	119.34	111.85
22	b	607	CLA	O2A-CGA-CBA	2.44	119.34	111.85
22	C	508	CLA	CMB-C2B-C3B	2.44	129.86	125.09
22	d	402	CLA	CMB-C2B-C3B	2.44	129.86	125.09
22	a	607	CLA	CED-O2D-CGD	2.44	121.77	115.97
22	D	402	CLA	CMC-C2C-C1C	2.44	128.62	125.00
22	B	615	CLA	CMC-C2C-C1C	2.45	128.62	125.00
22	d	402	CLA	CAC-C3C-C4C	2.45	128.43	124.82
22	D	402	CLA	CAC-C3C-C4C	2.45	128.43	124.82
22	d	401	CLA	CAC-C3C-C4C	2.45	128.43	124.82
22	c	504	CLA	CMC-C2C-C1C	2.45	128.63	125.00
22	A	607	CLA	CED-O2D-CGD	2.45	121.79	115.97
22	A	603	CLA	CAC-C3C-C4C	2.45	128.44	124.82
22	c	508	CLA	CMB-C2B-C3B	2.45	129.88	125.09
22	c	506	CLA	CMC-C2C-C1C	2.45	128.63	125.00
28	D	408	PL9	C10-C9-C11	2.45	119.11	115.37
22	d	402	CLA	CMC-C2C-C1C	2.45	128.64	125.00
24	B	622	BCR	C32-C1-C6	2.46	114.09	110.33
28	d	408	PL9	C10-C9-C11	2.46	119.12	115.37
22	D	402	CLA	CMB-C2B-C3B	2.47	129.91	125.09
22	c	512	CLA	O2A-CGA-CBA	2.47	119.45	111.85
24	b	622	BCR	C38-C26-C25	2.47	127.25	124.62
22	D	403	CLA	CED-O2D-CGD	2.47	121.84	115.97
22	b	615	CLA	CMC-C2C-C1C	2.48	128.67	125.00
22	C	506	CLA	CMC-C2C-C1C	2.48	128.67	125.00
22	c	510	CLA	CMB-C2B-C3B	2.48	129.93	125.09
24	c	515	BCR	C23-C24-C25	2.48	134.45	127.24
22	d	403	CLA	CED-O2D-CGD	2.48	121.87	115.97
22	C	510	CLA	CMB-C2B-C3B	2.48	129.94	125.09
22	A	603	CLA	C4-C3-C5	2.49	119.16	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	CMC-C2C-C1C	2.49	128.69	125.00
22	d	401	CLA	C4A-NA-C1A	2.49	109.54	106.38
22	c	507	CLA	CMB-C2B-C3B	2.50	129.97	125.09
22	C	512	CLA	O2A-CGA-CBA	2.50	119.53	111.85
24	C	515	BCR	C23-C24-C25	2.50	134.51	127.24
22	A	603	CLA	C4A-NA-C1A	2.51	109.56	106.38
22	C	507	CLA	CMB-C2B-C3B	2.51	130.00	125.09
24	b	622	BCR	C23-C24-C25	2.51	134.53	127.24
22	C	509	CLA	O2A-CGA-CBA	2.51	119.58	111.85
24	b	622	BCR	C40-C30-C25	2.51	114.17	110.33
24	B	622	BCR	C23-C24-C25	2.51	134.54	127.24
24	B	622	BCR	C40-C30-C25	2.51	114.17	110.33
22	c	509	CLA	O2A-CGA-CBA	2.52	119.59	111.85
28	d	408	PL9	C35-C34-C36	2.52	119.21	115.37
24	t	101	BCR	C31-C1-C6	2.52	114.18	110.33
24	B	622	BCR	C38-C26-C25	2.52	127.31	124.62
22	c	507	CLA	CMC-C2C-C1C	2.52	128.74	125.00
28	D	408	PL9	C35-C34-C36	2.53	119.23	115.37
32	d	405	LHG	O7-C7-C8	2.53	116.87	111.53
29	C	520	LMG	O8-C28-C29	2.54	119.66	111.85
22	b	617	CLA	CMB-C2B-C3B	2.54	130.06	125.09
22	c	512	CLA	CMB-C2B-C3B	2.54	130.06	125.09
29	c	520	LMG	O8-C28-C29	2.54	119.67	111.85
22	C	507	CLA	CMC-C2C-C1C	2.54	128.77	125.00
22	C	502	CLA	CMC-C2C-C1C	2.54	128.77	125.00
22	B	617	CLA	CMB-C2B-C3B	2.55	130.07	125.09
22	a	603	CLA	C4A-NA-C1A	2.55	109.61	106.38
24	B	619	BCR	C1-C6-C7	2.55	123.24	115.96
22	D	401	CLA	C4A-NA-C1A	2.55	109.61	106.38
25	b	621	SQD	C4-C3-C2	2.55	115.48	110.79
28	A	613	PL9	C45-C44-C46	2.55	119.26	115.37
22	C	512	CLA	CMB-C2B-C3B	2.56	130.09	125.09
32	D	405	LHG	O7-C7-C8	2.56	116.92	111.53
22	c	502	CLA	CMC-C2C-C1C	2.56	128.79	125.00
24	b	618	BCR	C1-C6-C7	2.56	123.28	115.96
24	T	102	BCR	C31-C1-C6	2.56	114.25	110.33
25	l	102	SQD	C4-C3-C2	2.56	115.51	110.79
28	a	613	PL9	C45-C44-C46	2.57	119.28	115.37
24	k	102	BCR	C33-C5-C6	2.57	127.36	124.62
22	c	503	CLA	CMC-C2C-C1C	2.59	128.84	125.00
24	K	101	BCR	C28-C27-C26	2.59	118.17	113.87
24	k	101	BCR	C28-C27-C26	2.60	118.17	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	102	BCR	C33-C5-C6	2.60	127.39	124.62
22	c	505	CLA	CAC-C3C-C4C	2.60	128.66	124.82
22	C	505	CLA	CAC-C3C-C4C	2.60	128.66	124.82
22	c	504	CLA	CAC-C3C-C4C	2.60	128.66	124.82
22	B	613	CLA	CED-O2D-CGD	2.61	122.17	115.97
22	b	604	CLA	CMB-C2B-C3B	2.61	130.19	125.09
22	c	513	CLA	C4-C3-C5	2.61	119.35	115.37
22	C	503	CLA	CMC-C2C-C1C	2.62	128.88	125.00
22	C	504	CLA	CAC-C3C-C4C	2.62	128.68	124.82
24	H	101	BCR	C39-C30-C25	2.62	114.33	110.33
22	A	607	CLA	CMC-C2C-C1C	2.62	128.88	125.00
22	B	613	CLA	CMC-C2C-C1C	2.62	128.88	125.00
24	h	101	BCR	C39-C30-C25	2.62	114.34	110.33
22	a	607	CLA	CMC-C2C-C1C	2.62	128.89	125.00
22	b	613	CLA	CED-O2D-CGD	2.63	122.21	115.97
22	d	401	CLA	CMC-C2C-C1C	2.63	128.89	125.00
22	B	604	CLA	CMB-C2B-C3B	2.63	130.23	125.09
22	C	513	CLA	C4-C3-C5	2.63	119.38	115.37
22	D	401	CLA	CMC-C2C-C1C	2.64	128.91	125.00
31	C	518	DGD	O1G-C1A-C2A	2.64	119.98	111.85
31	c	518	DGD	O1G-C1A-C2A	2.65	119.99	111.85
24	C	514	BCR	C3-C4-C5	2.65	118.26	113.87
31	D	410	DGD	O1G-C1A-C2A	2.65	120.01	111.85
31	d	410	DGD	O1G-C1A-C2A	2.65	120.01	111.85
24	c	514	BCR	C3-C4-C5	2.66	118.27	113.87
23	A	605	PHO	CAC-C3C-C4C	2.66	128.28	125.21
22	c	501	CLA	CMC-C2C-C1C	2.66	128.94	125.00
24	c	515	BCR	C4-C5-C6	2.67	125.67	122.73
24	a	608	BCR	C29-C30-C25	2.67	114.45	110.48
22	B	602	CLA	C3B-C4B-NB	2.67	112.66	109.21
22	B	615	CLA	CAC-C3C-C4C	2.67	128.77	124.82
22	b	615	CLA	CAC-C3C-C4C	2.67	128.77	124.82
22	b	613	CLA	CMC-C2C-C1C	2.67	128.96	125.00
23	a	605	PHO	CAC-C3C-C4C	2.68	128.30	125.21
24	C	515	BCR	C4-C5-C6	2.68	125.68	122.73
22	C	513	CLA	CMB-C2B-C3B	2.68	130.33	125.09
24	A	608	BCR	C29-C30-C25	2.69	114.48	110.48
22	b	617	CLA	O2A-CGA-CBA	2.70	120.15	111.85
22	c	506	CLA	C3B-C4B-NB	2.70	112.70	109.21
22	C	501	CLA	CMC-C2C-C1C	2.70	129.00	125.00
22	b	602	CLA	C3B-C4B-NB	2.70	112.70	109.21
22	d	403	CLA	C4-C3-C5	2.70	119.49	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	BCR	C39-C30-C25	2.71	114.47	110.33
24	K	102	BCR	C29-C30-C25	2.71	114.51	110.48
22	c	513	CLA	CMB-C2B-C3B	2.71	130.39	125.09
22	C	506	CLA	C3B-C4B-NB	2.71	112.72	109.21
22	C	513	CLA	C3B-C4B-NB	2.71	112.72	109.21
28	A	613	PL9	C10-C9-C11	2.72	119.52	115.37
24	b	622	BCR	C3-C4-C5	2.72	118.38	113.87
24	B	622	BCR	C3-C4-C5	2.72	118.38	113.87
22	B	617	CLA	O2A-CGA-CBA	2.73	120.24	111.85
22	b	611	CLA	O2A-CGA-CBA	2.73	120.24	111.85
22	B	611	CLA	C4-C3-C5	2.73	119.52	115.37
24	C	514	BCR	C39-C30-C25	2.73	114.50	110.33
22	b	606	CLA	C3B-C4B-NB	2.73	112.74	109.21
22	B	611	CLA	O2A-CGA-CBA	2.73	120.25	111.85
22	c	513	CLA	C3B-C4B-NB	2.73	112.74	109.21
22	b	611	CLA	C4-C3-C5	2.74	119.54	115.37
22	D	403	CLA	C4-C3-C5	2.74	119.54	115.37
28	a	613	PL9	C10-C9-C11	2.74	119.55	115.37
22	b	603	CLA	CMB-C2B-C3B	2.74	130.45	125.09
22	B	603	CLA	CMB-C2B-C3B	2.74	130.45	125.09
22	b	609	CLA	O2A-CGA-CBA	2.75	120.30	111.85
22	C	513	CLA	CMC-C2C-C1C	2.75	129.07	125.00
22	C	510	CLA	CMC-C2C-C1C	2.75	129.07	125.00
22	C	504	CLA	CMB-C2B-C3B	2.75	130.47	125.09
24	k	102	BCR	C29-C30-C25	2.75	114.57	110.48
24	d	404	BCR	C2-C1-C6	2.75	114.58	110.48
22	c	513	CLA	CMC-C2C-C1C	2.75	129.08	125.00
22	B	609	CLA	O2A-CGA-CBA	2.76	120.33	111.85
22	c	504	CLA	CMB-C2B-C3B	2.76	130.48	125.09
22	B	614	CLA	C4-C3-C5	2.76	119.57	115.37
22	c	503	CLA	C3B-C4B-NB	2.76	112.78	109.21
24	a	608	BCR	C8-C7-C6	2.76	135.27	127.24
29	b	619	LMG	O8-C28-C29	2.78	120.40	111.85
22	B	606	CLA	C3B-C4B-NB	2.78	112.80	109.21
22	b	614	CLA	C4-C3-C5	2.78	119.61	115.37
22	c	510	CLA	CMC-C2C-C1C	2.78	129.13	125.00
25	b	621	SQD	O48-C23-C24	2.79	120.42	111.85
22	c	512	CLA	C3B-C4B-NB	2.79	112.81	109.21
24	A	608	BCR	C8-C7-C6	2.79	135.34	127.24
22	C	503	CLA	C3B-C4B-NB	2.79	112.82	109.21
24	D	404	BCR	C2-C1-C6	2.79	114.64	110.48
25	L	101	SQD	O48-C23-C24	2.80	120.46	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	l	102	SQD	O48-C23-C24	2.80	120.46	111.85
29	B	620	LMG	O8-C28-C29	2.80	120.47	111.85
25	l	101	SQD	O48-C23-C24	2.80	120.47	111.85
22	C	512	CLA	C3B-C4B-NB	2.81	112.84	109.21
22	B	616	CLA	C4-C3-C5	2.82	119.66	115.37
22	b	616	CLA	C4-C3-C5	2.82	119.67	115.37
24	B	622	BCR	C29-C30-C25	2.82	114.68	110.48
22	C	502	CLA	C4-C3-C5	2.82	119.67	115.37
22	C	511	CLA	C4-C3-C5	2.83	119.68	115.37
22	c	502	CLA	C4-C3-C5	2.83	119.68	115.37
24	b	622	BCR	C29-C30-C25	2.84	114.70	110.48
22	c	511	CLA	C4-C3-C5	2.84	119.70	115.37
22	C	507	CLA	C3B-C4B-NB	2.86	112.91	109.21
22	b	610	CLA	CAC-C3C-C4C	2.87	129.05	124.82
22	a	604	CLA	CAC-C3C-C4C	2.87	129.05	124.82
22	c	503	CLA	C4-C3-C5	2.87	119.74	115.37
22	c	505	CLA	C3B-C4B-NB	2.87	112.92	109.21
22	B	613	CLA	CMB-C2B-C3B	2.88	130.71	125.09
22	c	507	CLA	C3B-C4B-NB	2.88	112.93	109.21
22	C	503	CLA	C4-C3-C5	2.88	119.76	115.37
22	B	610	CLA	CAC-C3C-C4C	2.88	129.07	124.82
22	D	401	CLA	C4-C3-C5	2.88	119.76	115.37
22	b	613	CLA	CMB-C2B-C3B	2.89	130.73	125.09
24	t	101	BCR	C30-C25-C24	2.89	124.22	115.96
24	T	102	BCR	C30-C25-C24	2.89	124.22	115.96
22	C	505	CLA	C3B-C4B-NB	2.89	112.95	109.21
28	A	613	PL9	C53-C6-C1	2.90	120.83	114.66
22	b	609	CLA	CMB-C2B-C3B	2.90	130.76	125.09
22	A	604	CLA	CAC-C3C-C4C	2.90	129.10	124.82
22	B	609	CLA	CMB-C2B-C3B	2.90	130.76	125.09
28	a	613	PL9	C53-C6-C1	2.91	120.85	114.66
22	B	603	CLA	C4A-NA-C1A	2.92	110.08	106.38
22	d	401	CLA	C4-C3-C5	2.92	119.82	115.37
25	A	609	SQD	O8-S-C6	2.93	111.07	104.99
22	B	613	CLA	C3B-C4B-NB	2.93	113.00	109.21
22	B	617	CLA	CAC-C3C-C4C	2.93	129.15	124.82
24	T	101	BCR	C39-C30-C25	2.93	114.81	110.33
22	b	602	CLA	CMC-C2C-C1C	2.93	129.34	125.00
22	C	502	CLA	CAC-C3C-C4C	2.94	129.16	124.82
28	A	613	PL9	C40-C39-C41	2.94	119.84	115.37
22	b	617	CLA	CAC-C3C-C4C	2.94	129.16	124.82
22	b	613	CLA	C3B-C4B-NB	2.94	113.01	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	404	BCR	C3-C2-C1	2.94	125.48	114.77
22	B	602	CLA	CMC-C2C-C1C	2.95	129.37	125.00
22	c	502	CLA	CAC-C3C-C4C	2.95	129.17	124.82
25	a	609	SQD	O8-S-C6	2.95	111.12	104.99
31	H	102	DGD	O1G-C1A-C2A	2.96	120.95	111.85
24	d	404	BCR	C3-C2-C1	2.96	125.54	114.77
28	a	613	PL9	C40-C39-C41	2.96	119.88	115.37
22	b	603	CLA	C4A-NA-C1A	2.96	110.14	106.38
31	h	102	DGD	O1G-C1A-C2A	2.96	120.97	111.85
22	c	508	CLA	C4-C3-C5	2.96	119.89	115.37
24	T	102	BCR	C39-C30-C25	2.97	114.87	110.33
28	D	408	PL9	C53-C6-C1	2.97	120.98	114.66
22	B	605	CLA	C4-C3-C5	2.98	119.91	115.37
22	C	508	CLA	C4-C3-C5	2.98	119.92	115.37
31	h	102	DGD	O2G-C1B-C2B	2.99	117.82	111.53
22	a	604	CLA	C4A-NA-C1A	2.99	110.17	106.38
28	A	613	PL9	C35-C34-C36	2.99	119.92	115.37
28	d	408	PL9	C53-C6-C1	2.99	121.02	114.66
31	H	102	DGD	O2G-C1B-C2B	2.99	117.84	111.53
29	C	519	LMG	O8-C28-C29	3.00	121.07	111.85
24	B	618	BCR	C39-C30-C25	3.00	114.91	110.33
22	A	604	CLA	C4A-NA-C1A	3.00	110.19	106.38
29	c	519	LMG	O8-C28-C29	3.00	121.09	111.85
22	B	603	CLA	C3B-C4B-NB	3.01	113.10	109.21
28	a	613	PL9	C35-C34-C36	3.01	119.95	115.37
24	t	101	BCR	C39-C30-C25	3.01	114.93	110.33
25	b	601	SQD	O48-C23-C24	3.01	121.12	111.85
22	B	608	CLA	CED-O2D-CGD	3.02	123.14	115.97
25	D	411	SQD	O48-C23-C24	3.02	121.14	111.85
22	b	605	CLA	C4-C3-C5	3.02	119.97	115.37
22	b	608	CLA	CED-O2D-CGD	3.02	123.14	115.97
22	b	604	CLA	C4A-NA-C1A	3.02	110.21	106.38
25	B	601	SQD	O48-C23-C24	3.02	121.15	111.85
22	c	501	CLA	C3B-C4B-NB	3.02	113.12	109.21
24	C	515	BCR	C27-C26-C25	3.03	126.06	122.73
25	d	411	SQD	O48-C23-C24	3.03	121.18	111.85
24	c	515	BCR	C27-C26-C25	3.04	126.07	122.73
22	C	501	CLA	C3B-C4B-NB	3.04	113.14	109.21
22	B	604	CLA	C4A-NA-C1A	3.04	110.24	106.38
24	A	608	BCR	C33-C5-C6	3.04	127.86	124.62
32	e	101	LHG	O8-C23-C24	3.05	121.23	111.85
22	b	602	CLA	O2A-CGA-CBA	3.05	121.23	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	C3B-C4B-NB	3.05	113.15	109.21
22	B	602	CLA	O2A-CGA-CBA	3.06	121.27	111.85
22	b	608	CLA	C4A-NA-C1A	3.06	110.27	106.38
32	E	101	LHG	O8-C23-C24	3.07	121.28	111.85
22	C	502	CLA	C4A-NA-C1A	3.07	110.27	106.38
22	B	608	CLA	C4-C3-C5	3.08	120.06	115.37
22	b	613	CLA	CAC-C3C-C4C	3.08	129.37	124.82
24	a	608	BCR	C31-C1-C6	3.08	115.04	110.33
24	a	608	BCR	C33-C5-C6	3.08	127.91	124.62
22	c	502	CLA	C4A-NA-C1A	3.09	110.29	106.38
22	c	505	CLA	CMC-C2C-C1C	3.09	129.57	125.00
24	a	608	BCR	C30-C25-C24	3.09	124.78	115.96
24	k	102	BCR	C40-C30-C25	3.09	115.05	110.33
22	C	505	CLA	CMC-C2C-C1C	3.09	129.58	125.00
22	d	402	CLA	C4-C3-C5	3.09	120.08	115.37
22	b	608	CLA	C4-C3-C5	3.09	120.08	115.37
22	D	401	CLA	CMB-C2B-C3B	3.09	131.14	125.09
22	d	401	CLA	CMB-C2B-C3B	3.09	131.14	125.09
24	K	102	BCR	C40-C30-C25	3.09	115.06	110.33
24	A	608	BCR	C31-C1-C6	3.09	115.06	110.33
22	B	608	CLA	C4A-NA-C1A	3.09	110.31	106.38
24	b	618	BCR	C4-C5-C6	3.09	126.13	122.73
22	B	613	CLA	CAC-C3C-C4C	3.10	129.39	124.82
28	a	613	PL9	C15-C14-C16	3.10	120.09	115.37
28	A	613	PL9	C25-C24-C26	3.10	120.10	115.37
22	B	615	CLA	C4A-NA-C1A	3.10	110.32	106.38
24	A	608	BCR	C30-C25-C24	3.10	124.83	115.96
24	K	102	BCR	C4-C5-C6	3.11	126.15	122.73
28	A	613	PL9	C15-C14-C16	3.11	120.11	115.37
22	D	402	CLA	C4-C3-C5	3.11	120.11	115.37
24	B	619	BCR	C4-C5-C6	3.11	126.15	122.73
24	k	102	BCR	C4-C5-C6	3.12	126.16	122.73
22	b	615	CLA	C4A-NA-C1A	3.12	110.33	106.38
22	b	606	CLA	C4A-NA-C1A	3.12	110.34	106.38
22	a	607	CLA	C4A-NA-C1A	3.12	110.34	106.38
22	A	607	CLA	C4A-NA-C1A	3.12	110.34	106.38
22	b	612	CLA	CMC-C2C-C1C	3.13	129.64	125.00
22	b	607	CLA	C4-C3-C5	3.13	120.14	115.37
28	a	613	PL9	C25-C24-C26	3.14	120.15	115.37
22	B	606	CLA	C4A-NA-C1A	3.15	110.37	106.38
22	B	607	CLA	C4-C3-C5	3.15	120.17	115.37
22	B	612	CLA	CMC-C2C-C1C	3.15	129.67	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	607	CLA	C3B-C4B-NB	3.16	113.30	109.21
22	a	604	CLA	CMC-C2C-C1C	3.17	129.69	125.00
32	l	103	LHG	O7-C7-C8	3.17	118.20	111.53
28	a	613	PL9	C30-C29-C31	3.17	120.20	115.37
32	L	102	LHG	O7-C7-C8	3.17	118.21	111.53
22	b	607	CLA	C3B-C4B-NB	3.18	113.32	109.21
22	A	604	CLA	CMC-C2C-C1C	3.19	129.73	125.00
28	A	613	PL9	C30-C29-C31	3.21	120.25	115.37
22	A	604	CLA	CMB-C2B-C3B	3.21	131.36	125.09
22	a	604	CLA	CMB-C2B-C3B	3.21	131.37	125.09
22	c	503	CLA	CMB-C2B-C3B	3.22	131.39	125.09
32	d	409	LHG	O7-C7-C8	3.23	118.32	111.53
23	A	606	PHO	C2C-C1C-NC	3.23	114.61	109.81
22	c	502	CLA	C3B-C4B-NB	3.23	113.38	109.21
22	C	502	CLA	C3B-C4B-NB	3.24	113.39	109.21
24	b	618	BCR	C38-C26-C25	3.24	128.07	124.62
23	a	606	PHO	C2C-C1C-NC	3.24	114.63	109.81
24	B	619	BCR	C38-C26-C25	3.24	128.08	124.62
22	b	617	CLA	C4A-NA-C1A	3.25	110.50	106.38
32	D	409	LHG	O7-C7-C8	3.25	118.38	111.53
22	b	617	CLA	C3B-C4B-NB	3.26	113.42	109.21
22	B	604	CLA	C4-C3-C5	3.26	120.34	115.37
22	C	503	CLA	CMB-C2B-C3B	3.26	131.47	125.09
22	B	617	CLA	C4A-NA-C1A	3.27	110.52	106.38
22	c	504	CLA	C4-C3-C5	3.27	120.35	115.37
22	b	614	CLA	O2D-CGD-CBD	3.27	115.94	111.22
22	C	504	CLA	C4-C3-C5	3.28	120.37	115.37
22	B	614	CLA	O2D-CGD-CBD	3.28	115.95	111.22
22	b	604	CLA	C4-C3-C5	3.28	120.37	115.37
22	B	605	CLA	CED-O2D-CGD	3.28	123.77	115.97
22	b	605	CLA	CED-O2D-CGD	3.29	123.78	115.97
22	B	617	CLA	C3B-C4B-NB	3.31	113.49	109.21
22	b	611	CLA	C4A-NA-C1A	3.33	110.60	106.38
24	a	608	BCR	C40-C30-C25	3.33	115.42	110.33
22	c	507	CLA	C4-C3-C5	3.34	120.45	115.37
22	B	611	CLA	C4A-NA-C1A	3.34	110.61	106.38
24	A	608	BCR	C40-C30-C25	3.34	115.44	110.33
22	C	507	CLA	C4-C3-C5	3.35	120.47	115.37
29	A	614	LMG	O7-C10-C11	3.35	118.58	111.53
29	A	614	LMG	O1-C1-C2	3.35	112.12	108.00
29	a	614	LMG	O7-C10-C11	3.35	118.59	111.53
22	C	506	CLA	C4-C3-C5	3.36	120.48	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	612	CLA	C3B-C4B-NB	3.36	113.56	109.21
22	c	506	CLA	C4-C3-C5	3.36	120.49	115.37
22	a	604	CLA	C4-C3-C5	3.37	120.51	115.37
22	A	604	CLA	C4-C3-C5	3.38	120.52	115.37
22	B	604	CLA	CMC-C2C-C1C	3.38	130.01	125.00
29	a	614	LMG	O1-C1-C2	3.38	112.16	108.00
24	h	101	BCR	C23-C24-C25	3.38	137.06	127.24
24	B	618	BCR	C32-C1-C6	3.38	115.50	110.33
24	H	101	BCR	C23-C24-C25	3.38	137.07	127.24
24	T	101	BCR	C4-C5-C6	3.39	126.46	122.73
22	b	607	CLA	C4A-NA-C1A	3.39	110.69	106.38
24	T	101	BCR	C32-C1-C6	3.40	115.53	110.33
22	C	501	CLA	C4A-NA-C1A	3.40	110.69	106.38
24	B	618	BCR	C4-C5-C6	3.40	126.47	122.73
22	c	508	CLA	C4A-NA-C1A	3.40	110.70	106.38
22	B	603	CLA	C4-C3-C5	3.40	120.56	115.37
22	c	503	CLA	C4A-NA-C1A	3.41	110.71	106.38
22	B	616	CLA	C3B-C4B-NB	3.41	113.62	109.21
23	A	605	PHO	C2B-C1B-NB	3.41	114.89	109.81
22	c	501	CLA	C4A-NA-C1A	3.41	110.71	106.38
32	D	405	LHG	O8-C23-C24	3.42	122.36	111.85
32	d	405	LHG	O8-C23-C24	3.42	122.36	111.85
23	a	605	PHO	C2B-C1B-NB	3.42	114.90	109.81
24	k	102	BCR	C31-C1-C6	3.42	115.56	110.33
22	C	503	CLA	C4A-NA-C1A	3.43	110.73	106.38
24	K	102	BCR	C31-C1-C6	3.43	115.57	110.33
22	b	603	CLA	C4-C3-C5	3.43	120.59	115.37
22	B	607	CLA	C4A-NA-C1A	3.43	110.73	106.38
23	A	606	PHO	C4-C3-C5	3.43	120.60	115.37
22	b	604	CLA	CMC-C2C-C1C	3.44	130.10	125.00
22	C	508	CLA	C4A-NA-C1A	3.44	110.74	106.38
22	a	603	CLA	CMB-C2B-C3B	3.44	131.82	125.09
25	b	601	SQD	O47-C7-C8	3.44	118.79	111.53
22	b	614	CLA	C4A-NA-C1A	3.45	110.75	106.38
25	B	601	SQD	O47-C7-C8	3.45	118.80	111.53
22	b	612	CLA	C3B-C4B-NB	3.45	113.68	109.21
25	l	101	SQD	O9-S-C6	3.46	109.36	106.92
22	B	611	CLA	C3B-C4B-NB	3.46	113.69	109.21
22	b	611	CLA	C3B-C4B-NB	3.47	113.69	109.21
22	B	614	CLA	C4A-NA-C1A	3.47	110.78	106.38
22	A	603	CLA	CMB-C2B-C3B	3.47	131.87	125.09
22	b	616	CLA	C3B-C4B-NB	3.47	113.70	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	606	PHO	C4-C3-C5	3.47	120.66	115.37
25	L	101	SQD	O9-S-C6	3.48	109.37	106.92
24	k	101	BCR	C2-C1-C6	3.50	115.68	110.48
22	b	612	CLA	C4A-NA-C1A	3.50	110.82	106.38
22	B	614	CLA	C3B-C4B-NB	3.50	113.74	109.21
24	K	102	BCR	C24-C23-C22	3.50	131.50	126.21
24	K	101	BCR	C2-C1-C6	3.50	115.69	110.48
24	k	102	BCR	C24-C23-C22	3.50	131.50	126.21
22	b	614	CLA	C3B-C4B-NB	3.50	113.74	109.21
22	B	608	CLA	O2D-CGD-CBD	3.51	116.28	111.22
22	b	613	CLA	C4-C3-C5	3.51	120.72	115.37
22	C	512	CLA	C4A-NA-C1A	3.52	110.84	106.38
22	b	615	CLA	C3B-C4B-NB	3.52	113.76	109.21
22	B	612	CLA	C4A-NA-C1A	3.52	110.85	106.38
22	b	608	CLA	O2D-CGD-CBD	3.52	116.30	111.22
22	b	610	CLA	C4A-NA-C1A	3.52	110.85	106.38
22	D	403	CLA	C3B-C4B-NB	3.53	113.77	109.21
31	d	410	DGD	O5D-C1E-C2E	3.53	112.34	108.00
22	B	615	CLA	C3B-C4B-NB	3.53	113.77	109.21
22	c	512	CLA	C4A-NA-C1A	3.53	110.86	106.38
22	b	610	CLA	C3B-C4B-NB	3.54	113.78	109.21
24	c	515	BCR	C40-C30-C25	3.54	115.74	110.33
22	d	403	CLA	C3B-C4B-NB	3.54	113.79	109.21
22	B	613	CLA	C4-C3-C5	3.55	120.77	115.37
22	B	610	CLA	C3B-C4B-NB	3.55	113.79	109.21
24	C	515	BCR	C40-C30-C25	3.55	115.76	110.33
22	B	610	CLA	C4A-NA-C1A	3.56	110.89	106.38
31	D	410	DGD	O5D-C1E-C2E	3.56	112.38	108.00
22	D	403	CLA	C4A-NA-C1A	3.58	110.92	106.38
22	D	401	CLA	C3B-C4B-NB	3.58	113.83	109.21
22	C	508	CLA	C3B-C4B-NB	3.58	113.83	109.21
22	c	512	CLA	C4-C3-C5	3.58	120.82	115.37
22	d	401	CLA	C3B-C4B-NB	3.58	113.84	109.21
22	c	510	CLA	C4A-NA-C1A	3.59	110.94	106.38
23	A	606	PHO	C4A-NA-C1A	3.59	110.92	108.22
22	c	508	CLA	C3B-C4B-NB	3.59	113.85	109.21
22	c	505	CLA	C4A-NA-C1A	3.59	110.94	106.38
22	C	512	CLA	C4-C3-C5	3.60	120.86	115.37
22	C	510	CLA	C4A-NA-C1A	3.60	110.95	106.38
24	T	101	BCR	C8-C7-C6	3.60	137.71	127.24
22	d	403	CLA	C4A-NA-C1A	3.60	110.95	106.38
22	c	511	CLA	C3B-C4B-NB	3.61	113.87	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	504	CLA	C3B-C4B-NB	3.61	113.87	109.21
23	A	606	PHO	C3C-C4C-NC	3.61	116.00	110.31
23	a	606	PHO	C3C-C4C-NC	3.61	116.00	110.31
24	B	618	BCR	C8-C7-C6	3.63	137.77	127.24
22	C	509	CLA	C3B-C4B-NB	3.63	113.90	109.21
23	a	606	PHO	C4A-NA-C1A	3.64	110.96	108.22
22	c	509	CLA	C3B-C4B-NB	3.64	113.92	109.21
22	C	505	CLA	C4A-NA-C1A	3.65	111.01	106.38
22	C	511	CLA	C3B-C4B-NB	3.65	113.93	109.21
22	B	605	CLA	C3B-C4B-NB	3.65	113.93	109.21
22	B	613	CLA	C4A-NA-C1A	3.66	111.02	106.38
24	H	101	BCR	C24-C23-C22	3.66	131.74	126.21
22	C	506	CLA	C4A-NA-C1A	3.67	111.03	106.38
22	b	605	CLA	C3B-C4B-NB	3.67	113.95	109.21
22	c	504	CLA	C3B-C4B-NB	3.67	113.96	109.21
24	h	101	BCR	C24-C23-C22	3.68	131.77	126.21
22	c	506	CLA	C4A-NA-C1A	3.69	111.06	106.38
22	b	613	CLA	C4A-NA-C1A	3.69	111.06	106.38
22	B	615	CLA	C4-C3-C5	3.73	121.05	115.37
22	a	607	CLA	C3B-C4B-NB	3.73	114.03	109.21
24	B	618	BCR	C23-C24-C25	3.73	138.07	127.24
22	D	402	CLA	C3B-C4B-NB	3.73	114.03	109.21
22	b	615	CLA	C4-C3-C5	3.73	121.06	115.37
24	T	101	BCR	C23-C24-C25	3.73	138.08	127.24
23	A	606	PHO	C2B-C1B-NB	3.73	115.37	109.81
22	A	607	CLA	C3B-C4B-NB	3.74	114.04	109.21
23	a	606	PHO	C2B-C1B-NB	3.74	115.37	109.81
22	d	402	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	k	102	BCR	C2-C1-C6	3.76	116.07	110.48
22	c	509	CLA	C4A-NA-C1A	3.76	111.15	106.38
31	c	517	DGD	O2G-C1B-C2B	3.77	119.47	111.53
22	C	504	CLA	C4A-NA-C1A	3.77	111.17	106.38
22	C	509	CLA	C4A-NA-C1A	3.78	111.17	106.38
24	K	102	BCR	C2-C1-C6	3.78	116.11	110.48
24	C	515	BCR	C33-C5-C6	3.79	128.66	124.62
24	c	515	BCR	C33-C5-C6	3.79	128.66	124.62
23	a	606	PHO	C2D-C1D-ND	3.79	115.46	109.81
31	C	517	DGD	O2G-C1B-C2B	3.79	119.52	111.53
25	b	621	SQD	C3-C4-C5	3.80	117.01	110.23
25	l	102	SQD	C3-C4-C5	3.80	117.01	110.23
22	c	504	CLA	C4A-NA-C1A	3.80	111.20	106.38
25	L	101	SQD	O47-C7-C8	3.80	119.54	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	411	SQD	O47-C7-C8	3.81	119.55	111.53
25	D	411	SQD	O47-C7-C8	3.81	119.56	111.53
22	c	513	CLA	C4A-NA-C1A	3.81	111.22	106.38
22	a	603	CLA	O2D-CGD-CBD	3.81	116.72	111.22
25	l	101	SQD	O47-C7-C8	3.82	119.57	111.53
23	A	606	PHO	C2D-C1D-ND	3.82	115.50	109.81
24	A	608	BCR	C23-C24-C25	3.82	138.34	127.24
22	A	603	CLA	O2D-CGD-CBD	3.83	116.74	111.22
24	a	608	BCR	C23-C24-C25	3.84	138.38	127.24
24	k	102	BCR	C32-C1-C6	3.85	116.21	110.33
29	c	519	LMG	O7-C10-C11	3.85	119.64	111.53
22	C	513	CLA	C4A-NA-C1A	3.85	111.27	106.38
24	c	515	BCR	C8-C9-C10	3.85	125.17	118.95
22	B	602	CLA	C4A-NA-C1A	3.86	111.28	106.38
22	b	602	CLA	C4A-NA-C1A	3.86	111.28	106.38
22	A	607	CLA	C4-C3-C5	3.87	121.26	115.37
24	b	622	BCR	C8-C9-C10	3.87	125.19	118.95
23	A	606	PHO	CAC-C3C-C4C	3.87	129.68	125.21
23	a	606	PHO	CAC-C3C-C4C	3.87	129.68	125.21
22	b	616	CLA	O2D-CGD-CBD	3.87	116.80	111.22
24	B	622	BCR	C8-C9-C10	3.87	125.19	118.95
24	K	102	BCR	C32-C1-C6	3.87	116.25	110.33
22	A	603	CLA	C3B-C4B-NB	3.88	114.22	109.21
24	h	101	BCR	C4-C5-C6	3.88	127.00	122.73
29	C	519	LMG	O7-C10-C11	3.88	119.71	111.53
24	C	515	BCR	C8-C9-C10	3.88	125.22	118.95
22	C	510	CLA	C3B-C4B-NB	3.89	114.23	109.21
22	a	607	CLA	C4-C3-C5	3.89	121.29	115.37
24	H	101	BCR	C8-C7-C6	3.89	138.54	127.24
22	c	510	CLA	C3B-C4B-NB	3.90	114.25	109.21
22	a	603	CLA	C3B-C4B-NB	3.90	114.25	109.21
29	c	520	LMG	O7-C10-C11	3.90	119.74	111.53
23	A	605	PHO	C3C-C4C-NC	3.90	116.46	110.31
24	h	101	BCR	C8-C7-C6	3.90	138.58	127.24
22	B	616	CLA	O2D-CGD-CBD	3.91	116.86	111.22
24	H	101	BCR	C4-C5-C6	3.92	127.04	122.73
23	A	605	PHO	C4A-NA-C1A	3.93	111.18	108.22
29	C	520	LMG	O7-C10-C11	3.93	119.81	111.53
23	a	605	PHO	C3C-C4C-NC	3.94	116.52	110.31
22	b	616	CLA	C4A-NA-C1A	3.94	111.38	106.38
24	c	515	BCR	C2-C1-C6	3.94	116.35	110.48
22	B	616	CLA	C4A-NA-C1A	3.95	111.39	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	BCR	C23-C24-C25	3.96	138.73	127.24
24	C	515	BCR	C2-C1-C6	3.96	116.38	110.48
28	A	613	PL9	C20-C19-C21	3.97	121.41	115.37
24	C	514	BCR	C23-C24-C25	3.97	138.78	127.24
29	b	619	LMG	O7-C10-C11	3.98	119.91	111.53
24	T	102	BCR	C23-C24-C25	3.98	138.80	127.24
29	B	620	LMG	O7-C10-C11	3.99	119.93	111.53
24	c	514	BCR	C23-C22-C21	3.99	125.39	118.95
23	a	605	PHO	C4A-NA-C1A	3.99	111.22	108.22
24	t	101	BCR	C23-C24-C25	3.99	138.83	127.24
22	D	401	CLA	O2D-CGD-CBD	3.99	116.98	111.22
22	d	401	CLA	O2D-CGD-CBD	3.99	116.98	111.22
28	a	613	PL9	C20-C19-C21	3.99	121.45	115.37
22	D	403	CLA	O2D-CGD-CBD	4.00	116.99	111.22
24	C	514	BCR	C23-C22-C21	4.00	125.40	118.95
24	k	102	BCR	C27-C26-C25	4.02	127.15	122.73
25	l	102	SQD	O47-C7-C8	4.02	120.01	111.53
24	K	102	BCR	C27-C26-C25	4.03	127.16	122.73
22	d	403	CLA	O2D-CGD-CBD	4.03	117.04	111.22
25	b	621	SQD	O47-C7-C8	4.04	120.03	111.53
32	e	101	LHG	O7-C7-C8	4.05	120.06	111.53
32	E	101	LHG	O7-C7-C8	4.05	120.07	111.53
28	d	408	PL9	C40-C39-C41	4.08	121.58	115.37
24	B	619	BCR	C8-C7-C6	4.09	139.13	127.24
24	b	618	BCR	C8-C7-C6	4.10	139.13	127.24
23	A	605	PHO	C2C-C1C-NC	4.10	115.91	109.81
22	b	605	CLA	C4A-NA-C1A	4.10	111.58	106.38
28	D	408	PL9	C40-C39-C41	4.12	121.64	115.37
23	a	605	PHO	C2C-C1C-NC	4.12	115.95	109.81
24	T	102	BCR	C33-C5-C6	4.13	129.02	124.62
22	B	605	CLA	C4A-NA-C1A	4.14	111.63	106.38
22	C	504	CLA	C3C-C4C-NC	4.15	114.42	110.21
22	c	504	CLA	C3C-C4C-NC	4.16	114.42	110.21
25	B	601	SQD	O6-C1-C2	4.17	113.13	108.00
22	b	608	CLA	C3B-C4B-NB	4.17	114.60	109.21
24	d	404	BCR	C23-C24-C25	4.17	139.35	127.24
25	b	601	SQD	O6-C1-C2	4.18	113.14	108.00
24	D	404	BCR	C23-C24-C25	4.18	139.37	127.24
24	t	101	BCR	C33-C5-C6	4.18	129.08	124.62
22	B	604	CLA	C3B-C4B-NB	4.19	114.63	109.21
22	B	608	CLA	C3B-C4B-NB	4.20	114.64	109.21
22	b	604	CLA	C3B-C4B-NB	4.20	114.64	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	101	BCR	C38-C26-C25	4.21	129.11	124.62
24	T	102	BCR	C8-C7-C6	4.24	139.55	127.24
24	t	101	BCR	C8-C7-C6	4.24	139.56	127.24
24	B	618	BCR	C38-C26-C25	4.25	129.15	124.62
22	b	606	CLA	C4-C3-C5	4.26	121.86	115.37
23	A	605	PHO	C2D-C1D-ND	4.26	116.16	109.81
22	B	606	CLA	C4-C3-C5	4.27	121.87	115.37
22	B	609	CLA	C3B-C4B-NB	4.28	114.74	109.21
24	T	101	BCR	C29-C30-C25	4.29	116.87	110.48
23	a	605	PHO	C2D-C1D-ND	4.30	116.21	109.81
24	B	618	BCR	C29-C30-C25	4.30	116.88	110.48
22	b	609	CLA	C3B-C4B-NB	4.30	114.77	109.21
24	b	618	BCR	C33-C5-C6	4.31	129.22	124.62
24	T	102	BCR	C2-C1-C6	4.33	116.93	110.48
31	c	516	DGD	O2G-C1B-C2B	4.33	120.66	111.53
24	B	619	BCR	C33-C5-C6	4.34	129.24	124.62
24	t	101	BCR	C2-C1-C6	4.35	116.96	110.48
31	C	516	DGD	O2G-C1B-C2B	4.36	120.71	111.53
22	c	507	CLA	C4A-NA-C1A	4.40	111.96	106.38
22	C	511	CLA	C4A-NA-C1A	4.41	111.98	106.38
24	h	101	BCR	C27-C26-C25	4.41	127.58	122.73
25	a	609	SQD	O47-C7-C8	4.43	120.86	111.53
25	A	609	SQD	O47-C7-C8	4.43	120.86	111.53
22	a	604	CLA	C3B-C4B-NB	4.43	114.94	109.21
22	c	511	CLA	C4A-NA-C1A	4.43	112.01	106.38
24	H	101	BCR	C27-C26-C25	4.44	127.61	122.73
22	C	507	CLA	C4A-NA-C1A	4.44	112.02	106.38
22	A	604	CLA	C3B-C4B-NB	4.47	114.99	109.21
22	B	605	CLA	O2D-CGD-CBD	4.48	117.68	111.22
24	k	101	BCR	C23-C24-C25	4.49	140.28	127.24
24	K	101	BCR	C23-C24-C25	4.50	140.29	127.24
22	b	605	CLA	O2D-CGD-CBD	4.50	117.71	111.22
22	B	611	CLA	O2D-CGD-CBD	4.51	117.72	111.22
22	b	611	CLA	O2D-CGD-CBD	4.52	117.74	111.22
24	T	102	BCR	C29-C30-C25	4.52	117.21	110.48
24	b	622	BCR	C23-C22-C21	4.54	126.27	118.95
24	t	101	BCR	C29-C30-C25	4.54	117.23	110.48
25	b	621	SQD	O9-S-C6	4.54	110.12	106.92
24	t	101	BCR	C4-C5-C6	4.55	127.73	122.73
24	d	404	BCR	C27-C26-C25	4.55	127.74	122.73
25	l	102	SQD	O9-S-C6	4.56	110.13	106.92
24	D	404	BCR	C27-C26-C25	4.56	127.74	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	t	101	BCR	C27-C26-C25	4.56	127.75	122.73
24	T	102	BCR	C27-C26-C25	4.56	127.75	122.73
24	B	622	BCR	C23-C22-C21	4.57	126.32	118.95
24	T	102	BCR	C4-C5-C6	4.57	127.76	122.73
22	b	608	CLA	C3C-C4C-NC	4.59	114.86	110.21
22	b	607	CLA	O2D-CGD-CBD	4.60	117.85	111.22
24	C	514	BCR	C32-C1-C6	4.60	117.36	110.33
22	C	501	CLA	C3C-C4C-NC	4.60	114.88	110.21
22	B	607	CLA	O2D-CGD-CBD	4.61	117.86	111.22
31	D	410	DGD	O2G-C1B-C2B	4.61	121.25	111.53
24	c	514	BCR	C32-C1-C6	4.61	117.38	110.33
31	d	410	DGD	O2G-C1B-C2B	4.62	121.27	111.53
22	c	501	CLA	C3C-C4C-NC	4.63	114.90	110.21
22	B	608	CLA	C3C-C4C-NC	4.65	114.92	110.21
24	d	404	BCR	C8-C7-C6	4.69	140.85	127.24
24	D	404	BCR	C8-C7-C6	4.69	140.87	127.24
22	c	510	CLA	O2D-CGD-CBD	4.69	117.99	111.22
22	C	503	CLA	O2D-CGD-CBD	4.70	118.00	111.22
22	C	510	CLA	O2D-CGD-CBD	4.71	118.01	111.22
24	H	101	BCR	C28-C27-C26	4.71	121.68	113.87
24	b	618	BCR	C2-C1-C6	4.71	117.50	110.48
24	h	101	BCR	C28-C27-C26	4.72	121.70	113.87
24	K	101	BCR	C27-C26-C25	4.73	127.93	122.73
24	B	619	BCR	C2-C1-C6	4.73	117.52	110.48
22	C	507	CLA	C3C-C4C-NC	4.73	115.00	110.21
22	c	503	CLA	O2D-CGD-CBD	4.74	118.05	111.22
22	B	606	CLA	O2D-CGD-CBD	4.74	118.06	111.22
24	k	101	BCR	C27-C26-C25	4.75	127.95	122.73
22	b	606	CLA	O2D-CGD-CBD	4.75	118.08	111.22
29	Z	101	LMG	O7-C10-C11	4.78	121.60	111.53
29	z	101	LMG	O7-C10-C11	4.78	121.60	111.53
22	c	507	CLA	C3C-C4C-NC	4.80	115.08	110.21
24	T	101	BCR	C27-C26-C25	4.81	128.03	122.73
22	D	403	CLA	C3C-C4C-NC	4.82	115.09	110.21
24	B	618	BCR	C27-C26-C25	4.83	128.04	122.73
22	d	403	CLA	C3C-C4C-NC	4.86	115.13	110.21
24	d	404	BCR	C7-C8-C9	4.86	133.56	126.21
24	d	404	BCR	C8-C9-C10	4.87	126.80	118.95
24	D	404	BCR	C7-C8-C9	4.87	133.57	126.21
22	b	617	CLA	O2D-CGD-CBD	4.89	118.27	111.22
22	B	603	CLA	O2D-CGD-CBD	4.89	118.28	111.22
24	D	404	BCR	C8-C9-C10	4.91	126.87	118.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	603	CLA	O2D-CGD-CBD	4.92	118.31	111.22
22	c	513	CLA	C3C-C4C-NC	4.92	115.19	110.21
22	b	615	CLA	C3C-C4C-NC	4.92	115.20	110.21
24	T	102	BCR	C24-C23-C22	4.93	133.65	126.21
22	B	615	CLA	C3C-C4C-NC	4.93	115.20	110.21
22	B	617	CLA	O2D-CGD-CBD	4.93	118.33	111.22
22	a	607	CLA	C3C-C4C-NC	4.93	115.20	110.21
22	B	602	CLA	C3C-C4C-NC	4.94	115.22	110.21
24	c	515	BCR	C38-C26-C25	4.94	129.89	124.62
24	k	101	BCR	C23-C22-C21	4.94	126.93	118.95
24	C	515	BCR	C38-C26-C25	4.95	129.90	124.62
22	A	607	CLA	C3C-C4C-NC	4.96	115.24	110.21
24	k	102	BCR	C23-C24-C25	4.96	141.65	127.24
24	K	102	BCR	C23-C24-C25	4.97	141.66	127.24
24	K	101	BCR	C23-C22-C21	4.97	126.96	118.95
22	C	513	CLA	C3C-C4C-NC	4.97	115.25	110.21
22	C	512	CLA	C3C-C4C-NC	4.97	115.25	110.21
24	t	101	BCR	C24-C23-C22	4.98	133.73	126.21
24	C	515	BCR	C8-C7-C6	4.99	141.72	127.24
22	b	603	CLA	C3C-C4C-NC	5.00	115.28	110.21
24	c	515	BCR	C8-C7-C6	5.00	141.77	127.24
22	b	602	CLA	C3C-C4C-NC	5.01	115.28	110.21
29	Z	101	LMG	O1-C1-C2	5.01	114.17	108.00
22	c	512	CLA	C3C-C4C-NC	5.02	115.29	110.21
22	c	510	CLA	C3C-C4C-NC	5.02	115.30	110.21
23	a	606	PHO	O2D-CGD-CBD	5.02	118.47	111.22
23	A	606	PHO	O2D-CGD-CBD	5.03	118.48	111.22
22	C	502	CLA	O2D-CGD-CBD	5.03	118.48	111.22
24	C	514	BCR	C2-C1-C6	5.04	117.97	110.48
22	c	502	CLA	O2D-CGD-CBD	5.04	118.49	111.22
24	K	101	BCR	C8-C7-C6	5.04	141.87	127.24
22	C	510	CLA	C3C-C4C-NC	5.04	115.31	110.21
24	k	101	BCR	C8-C7-C6	5.05	141.91	127.24
22	B	603	CLA	C3C-C4C-NC	5.06	115.33	110.21
29	z	101	LMG	O1-C1-C2	5.06	114.22	108.00
24	c	514	BCR	C2-C1-C6	5.07	118.02	110.48
22	B	607	CLA	C3C-C4C-NC	5.09	115.36	110.21
22	b	607	CLA	C3C-C4C-NC	5.10	115.38	110.21
24	d	404	BCR	C24-C23-C22	5.11	133.93	126.21
22	C	508	CLA	C3C-C4C-NC	5.11	115.39	110.21
22	a	607	CLA	O2D-CGD-CBD	5.12	118.60	111.22
22	C	511	CLA	O2D-CGD-CBD	5.13	118.61	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	K	101	BCR	C8-C9-C10	5.14	127.24	118.95
22	c	511	CLA	O2D-CGD-CBD	5.15	118.65	111.22
22	c	508	CLA	C3C-C4C-NC	5.15	115.43	110.21
24	k	101	BCR	C8-C9-C10	5.15	127.26	118.95
24	C	515	BCR	C29-C30-C25	5.16	118.15	110.48
24	D	404	BCR	C24-C23-C22	5.16	134.00	126.21
24	B	618	BCR	C2-C1-C6	5.16	118.16	110.48
22	A	607	CLA	O2D-CGD-CBD	5.16	118.67	111.22
24	k	102	BCR	C8-C9-C10	5.17	127.28	118.95
24	c	515	BCR	C29-C30-C25	5.17	118.17	110.48
24	K	102	BCR	C8-C9-C10	5.17	127.29	118.95
24	T	101	BCR	C2-C1-C6	5.18	118.18	110.48
22	c	503	CLA	C3C-C4C-NC	5.21	115.49	110.21
22	B	614	CLA	C3C-C4C-NC	5.21	115.49	110.21
22	C	509	CLA	C3C-C4C-NC	5.22	115.50	110.21
22	C	503	CLA	C3C-C4C-NC	5.22	115.50	110.21
24	h	101	BCR	C29-C30-C25	5.22	118.25	110.48
22	C	505	CLA	C3C-C4C-NC	5.22	115.50	110.21
24	A	608	BCR	C24-C23-C22	5.23	134.11	126.21
22	c	505	CLA	C3C-C4C-NC	5.23	115.51	110.21
23	A	605	PHO	O2D-CGD-CBD	5.23	118.77	111.22
24	B	622	BCR	C27-C26-C25	5.24	128.49	122.73
23	a	605	PHO	O2D-CGD-CBD	5.25	118.79	111.22
24	a	608	BCR	C24-C23-C22	5.25	134.14	126.21
24	b	622	BCR	C27-C26-C25	5.26	128.51	122.73
22	c	509	CLA	C3C-C4C-NC	5.26	115.54	110.21
22	b	612	CLA	O2D-CGD-CBD	5.26	118.81	111.22
22	b	614	CLA	C3C-C4C-NC	5.27	115.55	110.21
25	d	411	SQD	O9-S-C6	5.27	110.63	106.92
22	a	604	CLA	C3C-C4C-NC	5.27	115.55	110.21
25	D	411	SQD	O9-S-C6	5.27	110.64	106.92
24	H	101	BCR	C29-C30-C25	5.27	118.33	110.48
22	B	612	CLA	O2D-CGD-CBD	5.27	118.83	111.22
22	A	604	CLA	C3C-C4C-NC	5.30	115.58	110.21
22	b	610	CLA	C3C-C4C-NC	5.32	115.60	110.21
22	C	502	CLA	C3C-C4C-NC	5.34	115.62	110.21
22	c	511	CLA	C3C-C4C-NC	5.36	115.64	110.21
22	C	511	CLA	C3C-C4C-NC	5.36	115.64	110.21
24	b	618	BCR	C40-C30-C25	5.36	118.53	110.33
22	b	611	CLA	C3C-C4C-NC	5.37	115.65	110.21
25	d	411	SQD	O7-S-C6	5.37	110.70	106.92
24	B	619	BCR	C40-C30-C25	5.38	118.55	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	502	CLA	C3C-C4C-NC	5.38	115.66	110.21
25	D	411	SQD	O7-S-C6	5.39	110.72	106.92
22	C	513	CLA	O2D-CGD-CBD	5.39	118.99	111.22
22	B	611	CLA	C3C-C4C-NC	5.39	115.67	110.21
22	c	513	CLA	O2D-CGD-CBD	5.39	119.00	111.22
22	a	603	CLA	C3C-C4C-NC	5.41	115.69	110.21
22	c	507	CLA	O2D-CGD-CBD	5.41	119.03	111.22
22	B	610	CLA	C3C-C4C-NC	5.42	115.70	110.21
22	b	609	CLA	C3C-C4C-NC	5.42	115.71	110.21
22	C	507	CLA	O2D-CGD-CBD	5.43	119.06	111.22
24	c	514	BCR	C8-C7-C6	5.45	143.05	127.24
22	b	613	CLA	C3C-C4C-NC	5.45	115.73	110.21
22	A	603	CLA	C3C-C4C-NC	5.45	115.73	110.21
24	C	514	BCR	C8-C7-C6	5.46	143.11	127.24
22	d	402	CLA	O2D-CGD-CBD	5.47	119.11	111.22
22	B	613	CLA	C3C-C4C-NC	5.48	115.76	110.21
22	B	609	CLA	C3C-C4C-NC	5.49	115.77	110.21
22	c	506	CLA	C3C-C4C-NC	5.49	115.78	110.21
22	B	604	CLA	C3C-C4C-NC	5.49	115.78	110.21
22	D	402	CLA	O2D-CGD-CBD	5.50	119.15	111.22
25	D	411	SQD	O6-C1-C2	5.50	114.77	108.00
24	d	404	BCR	C23-C22-C21	5.51	127.83	118.95
25	d	411	SQD	O6-C1-C2	5.51	114.78	108.00
24	D	404	BCR	C23-C22-C21	5.51	127.84	118.95
22	b	604	CLA	C3C-C4C-NC	5.52	115.80	110.21
24	H	101	BCR	C33-C5-C6	5.53	130.52	124.62
22	C	506	CLA	C3C-C4C-NC	5.54	115.82	110.21
24	k	101	BCR	C24-C23-C22	5.54	134.58	126.21
24	c	514	BCR	C12-C13-C14	5.54	127.88	118.95
24	C	514	BCR	C12-C13-C14	5.56	127.91	118.95
24	C	514	BCR	C29-C30-C25	5.56	118.75	110.48
22	C	505	CLA	O2D-CGD-CBD	5.56	119.24	111.22
24	K	101	BCR	C24-C23-C22	5.56	134.61	126.21
24	c	514	BCR	C29-C30-C25	5.57	118.76	110.48
22	c	505	CLA	O2D-CGD-CBD	5.57	119.25	111.22
24	h	101	BCR	C33-C5-C6	5.59	130.58	124.62
22	b	610	CLA	O2D-CGD-CBD	5.61	119.31	111.22
22	B	610	CLA	O2D-CGD-CBD	5.61	119.31	111.22
25	l	102	SQD	O6-C1-C2	5.62	114.92	108.00
22	c	508	CLA	O2D-CGD-CBD	5.65	119.36	111.22
22	d	402	CLA	C3C-C4C-NC	5.67	115.95	110.21
22	C	508	CLA	O2D-CGD-CBD	5.67	119.40	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	621	SQD	O6-C1-C2	5.67	114.98	108.00
24	B	622	BCR	C2-C1-C6	5.69	118.95	110.48
22	D	402	CLA	C3C-C4C-NC	5.70	115.98	110.21
24	b	622	BCR	C2-C1-C6	5.70	118.96	110.48
22	b	616	CLA	C3C-C4C-NC	5.71	116.00	110.21
22	B	616	CLA	C3C-C4C-NC	5.73	116.01	110.21
22	B	615	CLA	O2D-CGD-CBD	5.75	119.52	111.22
25	B	601	SQD	O9-S-C6	5.76	110.98	106.92
22	b	615	CLA	O2D-CGD-CBD	5.76	119.53	111.22
25	b	601	SQD	O9-S-C6	5.78	111.00	106.92
24	C	515	BCR	C7-C8-C9	5.80	134.97	126.21
24	c	515	BCR	C7-C8-C9	5.81	134.99	126.21
22	c	509	CLA	O2D-CGD-CBD	5.82	119.62	111.22
22	C	509	CLA	O2D-CGD-CBD	5.85	119.66	111.22
22	B	613	CLA	O2D-CGD-CBD	5.86	119.68	111.22
24	b	618	BCR	C29-C30-C25	5.88	119.23	110.48
24	B	619	BCR	C29-C30-C25	5.88	119.23	110.48
22	b	613	CLA	O2D-CGD-CBD	5.88	119.71	111.22
24	t	101	BCR	C8-C9-C10	5.89	128.44	118.95
24	k	102	BCR	C8-C7-C6	5.91	144.40	127.24
22	B	617	CLA	C3C-C4C-NC	5.91	116.20	110.21
24	b	618	BCR	C8-C9-C10	5.91	128.48	118.95
24	a	608	BCR	C8-C9-C10	5.92	128.49	118.95
24	K	102	BCR	C8-C7-C6	5.92	144.44	127.24
22	b	617	CLA	C3C-C4C-NC	5.93	116.22	110.21
24	T	102	BCR	C8-C9-C10	5.93	128.51	118.95
24	B	619	BCR	C8-C9-C10	5.94	128.53	118.95
22	B	609	CLA	O2D-CGD-CBD	5.96	119.82	111.22
24	b	618	BCR	C23-C24-C25	5.96	144.55	127.24
24	B	619	BCR	C23-C24-C25	5.96	144.56	127.24
24	A	608	BCR	C8-C9-C10	5.96	128.57	118.95
22	b	609	CLA	O2D-CGD-CBD	5.97	119.84	111.22
22	b	605	CLA	C3C-C4C-NC	5.98	116.27	110.21
22	a	604	CLA	O2D-CGD-CBD	5.99	119.86	111.22
22	A	604	CLA	O2D-CGD-CBD	6.00	119.88	111.22
22	b	606	CLA	C3C-C4C-NC	6.01	116.30	110.21
22	c	513	CLA	C2C-C1C-NC	6.01	114.36	110.22
24	T	101	BCR	C7-C8-C9	6.02	135.30	126.21
25	l	101	SQD	O6-C1-C2	6.03	115.42	108.00
24	b	618	BCR	C11-C12-C13	6.03	144.01	126.34
24	B	619	BCR	C11-C12-C13	6.03	144.01	126.34
22	c	504	CLA	O2D-CGD-CBD	6.04	119.94	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	604	CLA	O2D-CGD-CBD	6.05	119.94	111.22
24	B	618	BCR	C7-C8-C9	6.05	135.35	126.21
22	C	504	CLA	O2D-CGD-CBD	6.05	119.95	111.22
22	B	606	CLA	C3C-C4C-NC	6.05	116.34	110.21
22	D	401	CLA	C3C-C4C-NC	6.06	116.35	110.21
22	C	513	CLA	C2C-C1C-NC	6.06	114.39	110.22
22	B	605	CLA	C3C-C4C-NC	6.07	116.36	110.21
22	B	604	CLA	O2D-CGD-CBD	6.07	119.98	111.22
24	b	622	BCR	C24-C23-C22	6.08	135.39	126.21
24	c	514	BCR	C38-C26-C25	6.08	131.10	124.62
25	L	101	SQD	O6-C1-C2	6.09	115.49	108.00
24	B	622	BCR	C24-C23-C22	6.11	135.44	126.21
24	c	514	BCR	C24-C23-C22	6.11	135.44	126.21
22	d	401	CLA	C3C-C4C-NC	6.11	116.40	110.21
24	C	514	BCR	C38-C26-C25	6.12	131.15	124.62
24	C	514	BCR	C24-C23-C22	6.14	135.48	126.21
22	B	603	CLA	C2C-C1C-NC	6.14	114.45	110.22
25	a	609	SQD	O6-C1-C2	6.17	115.59	108.00
24	c	514	BCR	C27-C26-C25	6.18	129.53	122.73
25	A	609	SQD	O6-C1-C2	6.18	115.61	108.00
24	C	514	BCR	C27-C26-C25	6.19	129.53	122.73
22	C	512	CLA	C2C-C1C-NC	6.19	114.48	110.22
25	l	101	SQD	O7-S-C6	6.20	111.29	106.92
22	b	603	CLA	C2C-C1C-NC	6.21	114.49	110.22
22	B	612	CLA	C3C-C4C-NC	6.21	116.50	110.21
24	B	619	BCR	C27-C26-C25	6.21	129.56	122.73
22	b	612	CLA	C3C-C4C-NC	6.21	116.50	110.21
24	b	618	BCR	C27-C26-C25	6.23	129.58	122.73
22	c	512	CLA	C2C-C1C-NC	6.25	114.52	110.22
25	L	101	SQD	O7-S-C6	6.26	111.33	106.92
24	c	515	BCR	C23-C22-C21	6.28	129.09	118.95
24	c	515	BCR	C31-C1-C6	6.32	119.98	110.33
24	d	404	BCR	C4-C5-C6	6.32	129.69	122.73
22	C	506	CLA	O2D-CGD-CBD	6.33	120.35	111.22
22	c	506	CLA	O2D-CGD-CBD	6.33	120.35	111.22
24	B	618	BCR	C23-C22-C21	6.33	129.16	118.95
22	c	512	CLA	O2D-CGD-CBD	6.34	120.37	111.22
24	C	515	BCR	C23-C22-C21	6.34	129.18	118.95
24	h	101	BCR	C8-C9-C10	6.34	129.18	118.95
24	C	515	BCR	C31-C1-C6	6.35	120.03	110.33
22	C	512	CLA	O2D-CGD-CBD	6.35	120.39	111.22
24	D	404	BCR	C4-C5-C6	6.35	129.72	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	H	101	BCR	C8-C9-C10	6.36	129.20	118.95
24	T	101	BCR	C23-C22-C21	6.38	129.23	118.95
22	B	602	CLA	C2C-C1C-NC	6.38	114.61	110.22
24	k	101	BCR	C4-C5-C6	6.39	129.76	122.73
24	K	101	BCR	C4-C5-C6	6.41	129.78	122.73
22	b	602	CLA	C2C-C1C-NC	6.41	114.63	110.22
24	b	622	BCR	C8-C7-C6	6.48	146.04	127.24
24	B	622	BCR	C8-C7-C6	6.48	146.06	127.24
25	l	102	SQD	O7-S-C6	6.52	111.51	106.92
25	b	621	SQD	O7-S-C6	6.58	111.56	106.92
24	c	515	BCR	C24-C23-C22	6.58	136.15	126.21
22	c	503	CLA	C2C-C1C-NC	6.60	114.76	110.22
22	C	503	CLA	C2C-C1C-NC	6.62	114.77	110.22
24	C	515	BCR	C24-C23-C22	6.63	136.22	126.21
24	C	514	BCR	C33-C5-C6	6.66	131.72	124.62
22	c	507	CLA	C2C-C1C-NC	6.66	114.81	110.22
22	B	617	CLA	C2C-C1C-NC	6.70	114.83	110.22
24	H	101	BCR	C32-C1-C6	6.71	120.59	110.33
24	h	101	BCR	C32-C1-C6	6.72	120.60	110.33
24	c	514	BCR	C33-C5-C6	6.74	131.80	124.62
24	K	101	BCR	C29-C30-C25	6.74	120.51	110.48
24	k	101	BCR	C29-C30-C25	6.74	120.51	110.48
22	C	507	CLA	C2C-C1C-NC	6.77	114.88	110.22
24	B	622	BCR	C12-C13-C14	6.78	129.89	118.95
24	b	622	BCR	C12-C13-C14	6.79	129.91	118.95
22	D	403	CLA	C2C-C1C-NC	6.80	114.90	110.22
22	b	617	CLA	C2C-C1C-NC	6.84	114.92	110.22
22	d	403	CLA	C2C-C1C-NC	6.86	114.94	110.22
22	b	616	CLA	C2C-C1C-NC	6.90	114.97	110.22
24	t	101	BCR	C12-C13-C14	6.91	130.10	118.95
22	b	611	CLA	C2C-C1C-NC	6.92	114.98	110.22
22	B	611	CLA	C2C-C1C-NC	6.92	114.98	110.22
24	T	102	BCR	C12-C13-C14	6.94	130.14	118.95
22	B	613	CLA	C2C-C1C-NC	6.94	115.00	110.22
24	B	618	BCR	C24-C23-C22	6.94	136.70	126.21
22	b	602	CLA	O2D-CGD-CBD	6.96	121.27	111.22
22	C	508	CLA	C2C-C1C-NC	6.96	115.01	110.22
22	B	616	CLA	C2C-C1C-NC	6.97	115.02	110.22
22	B	602	CLA	O2D-CGD-CBD	6.97	121.28	111.22
22	b	613	CLA	C2C-C1C-NC	6.99	115.03	110.22
24	T	101	BCR	C24-C23-C22	6.99	136.77	126.21
22	c	511	CLA	C2C-C1C-NC	7.00	115.03	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	502	CLA	C2C-C1C-NC	7.00	115.03	110.22
22	c	502	CLA	C2C-C1C-NC	7.00	115.03	110.22
22	C	511	CLA	C2C-C1C-NC	7.01	115.04	110.22
22	c	508	CLA	C2C-C1C-NC	7.03	115.05	110.22
22	C	505	CLA	C2C-C1C-NC	7.04	115.06	110.22
22	B	607	CLA	C2C-C1C-NC	7.05	115.07	110.22
24	K	101	BCR	C12-C13-C14	7.05	130.31	118.95
22	c	505	CLA	C2C-C1C-NC	7.05	115.07	110.22
22	b	607	CLA	C2C-C1C-NC	7.06	115.08	110.22
24	k	101	BCR	C12-C13-C14	7.07	130.35	118.95
23	A	605	PHO	CMD-C2D-C1D	7.13	136.46	125.06
22	b	606	CLA	C2C-C1C-NC	7.14	115.13	110.22
22	B	606	CLA	C2C-C1C-NC	7.15	115.14	110.22
22	c	501	CLA	C2C-C1C-NC	7.16	115.14	110.22
23	a	605	PHO	CMD-C2D-C1D	7.16	136.51	125.06
22	a	603	CLA	C2C-C1C-NC	7.19	115.16	110.22
22	A	603	CLA	C2C-C1C-NC	7.19	115.17	110.22
22	C	501	CLA	C2C-C1C-NC	7.20	115.17	110.22
25	a	609	SQD	O9-S-C6	7.28	112.05	106.92
25	A	609	SQD	O9-S-C6	7.29	112.06	106.92
24	D	404	BCR	C10-C11-C12	7.29	145.61	123.11
23	a	606	PHO	CMD-C2D-C1D	7.30	136.73	125.06
24	d	404	BCR	C10-C11-C12	7.30	145.65	123.11
23	A	606	PHO	CMD-C2D-C1D	7.33	136.78	125.06
22	C	501	CLA	O2D-CGD-CBD	7.39	121.89	111.22
22	c	501	CLA	O2D-CGD-CBD	7.40	121.90	111.22
22	c	506	CLA	C2C-C1C-NC	7.42	115.32	110.22
22	C	506	CLA	C2C-C1C-NC	7.45	115.34	110.22
22	C	510	CLA	C2C-C1C-NC	7.47	115.36	110.22
24	T	101	BCR	C8-C9-C10	7.47	131.00	118.95
24	B	618	BCR	C8-C9-C10	7.50	131.05	118.95
22	B	614	CLA	C2C-C1C-NC	7.52	115.40	110.22
22	c	510	CLA	C2C-C1C-NC	7.53	115.40	110.22
22	B	615	CLA	C2C-C1C-NC	7.55	115.42	110.22
22	b	615	CLA	C2C-C1C-NC	7.56	115.42	110.22
22	b	614	CLA	C2C-C1C-NC	7.56	115.42	110.22
24	D	404	BCR	C12-C13-C14	7.59	131.20	118.95
24	K	101	BCR	C7-C8-C9	7.59	137.68	126.21
24	d	404	BCR	C12-C13-C14	7.61	131.23	118.95
24	k	101	BCR	C7-C8-C9	7.63	137.74	126.21
22	b	608	CLA	C2C-C1C-NC	7.65	115.48	110.22
24	B	622	BCR	C33-C5-C6	7.69	132.82	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	622	BCR	C33-C5-C6	7.72	132.84	124.62
22	B	608	CLA	C2C-C1C-NC	7.74	115.54	110.22
22	D	401	CLA	C2C-C1C-NC	7.75	115.55	110.22
22	d	401	CLA	C2C-C1C-NC	7.75	115.55	110.22
22	c	504	CLA	C2C-C1C-NC	7.78	115.57	110.22
22	b	612	CLA	C2C-C1C-NC	7.78	115.57	110.22
22	C	504	CLA	C2C-C1C-NC	7.81	115.59	110.22
24	K	101	BCR	C33-C5-C6	7.81	132.95	124.62
22	B	612	CLA	C2C-C1C-NC	7.82	115.60	110.22
24	H	101	BCR	C7-C8-C9	7.83	138.04	126.21
22	b	610	CLA	C2C-C1C-NC	7.84	115.61	110.22
24	h	101	BCR	C7-C8-C9	7.85	138.06	126.21
24	b	618	BCR	C7-C8-C9	7.86	138.08	126.21
22	C	509	CLA	C2C-C1C-NC	7.86	115.62	110.22
24	k	101	BCR	C33-C5-C6	7.86	132.99	124.62
22	B	610	CLA	C2C-C1C-NC	7.87	115.63	110.22
24	B	619	BCR	C7-C8-C9	7.87	138.10	126.21
22	c	509	CLA	C2C-C1C-NC	7.87	115.64	110.22
22	A	607	CLA	C2C-C1C-NC	7.88	115.64	110.22
22	a	607	CLA	C2C-C1C-NC	7.91	115.66	110.22
24	a	608	BCR	C7-C8-C9	7.91	138.16	126.21
24	b	618	BCR	C10-C11-C12	7.91	147.54	123.11
24	B	619	BCR	C10-C11-C12	7.92	147.56	123.11
24	k	102	BCR	C23-C22-C21	7.96	131.78	118.95
24	K	102	BCR	C23-C22-C21	7.96	131.79	118.95
24	K	101	BCR	C10-C11-C12	7.96	147.69	123.11
24	k	101	BCR	C10-C11-C12	7.98	147.73	123.11
24	A	608	BCR	C7-C8-C9	7.99	138.29	126.21
24	K	101	BCR	C11-C12-C13	8.02	149.85	126.34
24	k	101	BCR	C11-C12-C13	8.03	149.87	126.34
22	B	604	CLA	C2C-C1C-NC	8.05	115.75	110.22
24	c	514	BCR	C11-C10-C9	8.11	139.01	127.22
24	C	514	BCR	C11-C10-C9	8.12	139.02	127.22
22	b	604	CLA	C2C-C1C-NC	8.18	115.85	110.22
24	c	515	BCR	C11-C12-C13	8.19	150.34	126.34
24	a	608	BCR	C20-C19-C18	8.20	150.38	126.34
24	B	618	BCR	C15-C14-C13	8.20	139.15	127.22
24	C	515	BCR	C11-C12-C13	8.21	150.40	126.34
24	T	101	BCR	C15-C14-C13	8.21	139.15	127.22
24	A	608	BCR	C20-C19-C18	8.22	150.43	126.34
24	h	101	BCR	C23-C22-C21	8.31	132.36	118.95
24	H	101	BCR	C23-C22-C21	8.31	132.36	118.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	102	BCR	C23-C22-C21	8.35	132.41	118.95
24	t	101	BCR	C23-C22-C21	8.38	132.46	118.95
24	B	619	BCR	C23-C22-C21	8.51	132.67	118.95
24	b	618	BCR	C23-C22-C21	8.52	132.69	118.95
24	d	404	BCR	C29-C30-C25	8.58	123.25	110.48
24	D	404	BCR	C29-C30-C25	8.61	123.29	110.48
24	B	619	BCR	C24-C23-C22	8.65	139.28	126.21
24	D	404	BCR	C32-C1-C6	8.67	123.58	110.33
24	d	404	BCR	C32-C1-C6	8.67	123.58	110.33
24	b	618	BCR	C24-C23-C22	8.69	139.34	126.21
24	B	618	BCR	C10-C11-C12	8.75	150.12	123.11
24	T	101	BCR	C10-C11-C12	8.76	150.14	123.11
22	B	609	CLA	C2C-C1C-NC	8.80	116.28	110.22
24	k	102	BCR	C11-C10-C9	8.80	140.02	127.22
22	b	609	CLA	C2C-C1C-NC	8.81	116.28	110.22
24	K	102	BCR	C11-C10-C9	8.82	140.04	127.22
22	b	605	CLA	C2C-C1C-NC	8.86	116.31	110.22
22	B	605	CLA	C2C-C1C-NC	8.89	116.33	110.22
24	b	622	BCR	C7-C8-C9	8.89	139.64	126.21
24	H	101	BCR	C11-C12-C13	8.90	152.42	126.34
24	h	101	BCR	C11-C12-C13	8.90	152.44	126.34
24	B	622	BCR	C7-C8-C9	8.91	139.67	126.21
22	A	604	CLA	C2C-C1C-NC	8.94	116.37	110.22
22	a	604	CLA	C2C-C1C-NC	8.95	116.38	110.22
24	t	101	BCR	C20-C19-C18	8.98	152.66	126.34
24	h	101	BCR	C12-C13-C14	8.99	133.44	118.95
24	H	101	BCR	C12-C13-C14	9.00	133.46	118.95
24	T	102	BCR	C20-C19-C18	9.00	152.73	126.34
24	B	618	BCR	C11-C12-C13	9.02	152.77	126.34
24	T	101	BCR	C11-C12-C13	9.02	152.78	126.34
24	D	404	BCR	C11-C12-C13	9.03	152.80	126.34
24	B	619	BCR	C12-C13-C14	9.04	133.52	118.95
24	d	404	BCR	C19-C18-C17	9.04	133.53	118.95
24	D	404	BCR	C19-C18-C17	9.04	133.53	118.95
24	d	404	BCR	C11-C12-C13	9.04	152.85	126.34
24	b	618	BCR	C12-C13-C14	9.05	133.54	118.95
24	c	515	BCR	C12-C13-C14	9.08	133.59	118.95
24	C	515	BCR	C12-C13-C14	9.10	133.63	118.95
24	C	515	BCR	C19-C18-C17	9.13	133.68	118.95
24	c	515	BCR	C19-C18-C17	9.14	133.68	118.95
24	k	102	BCR	C12-C13-C14	9.14	133.69	118.95
24	K	102	BCR	C12-C13-C14	9.15	133.71	118.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	404	BCR	C20-C19-C18	9.15	153.17	126.34
24	D	404	BCR	C20-C19-C18	9.15	153.17	126.34
24	b	622	BCR	C19-C18-C17	9.29	133.93	118.95
24	B	622	BCR	C19-C18-C17	9.29	133.93	118.95
24	t	101	BCR	C7-C8-C9	9.31	140.28	126.21
24	T	102	BCR	C7-C8-C9	9.31	140.28	126.21
24	k	102	BCR	C7-C8-C9	9.32	140.29	126.21
24	K	102	BCR	C7-C8-C9	9.33	140.31	126.21
24	A	608	BCR	C11-C12-C13	9.36	153.78	126.34
24	a	608	BCR	C11-C12-C13	9.37	153.80	126.34
22	D	402	CLA	C2C-C1C-NC	9.53	116.77	110.22
22	d	402	CLA	C2C-C1C-NC	9.54	116.78	110.22
24	c	514	BCR	C15-C14-C13	9.58	141.15	127.22
24	C	514	BCR	C15-C14-C13	9.59	141.16	127.22
24	H	101	BCR	C10-C11-C12	9.61	152.78	123.11
24	h	101	BCR	C10-C11-C12	9.63	152.83	123.11
24	b	622	BCR	C15-C14-C13	9.71	141.34	127.22
24	B	622	BCR	C15-C14-C13	9.71	141.34	127.22
24	t	101	BCR	C11-C12-C13	9.71	154.81	126.34
24	T	102	BCR	C11-C12-C13	9.72	154.83	126.34
24	c	514	BCR	C7-C8-C9	9.72	140.90	126.21
24	a	608	BCR	C10-C11-C12	9.75	153.22	123.11
24	A	608	BCR	C10-C11-C12	9.76	153.24	123.11
24	C	514	BCR	C7-C8-C9	9.78	140.99	126.21
24	C	514	BCR	C19-C18-C17	10.02	135.11	118.95
24	c	514	BCR	C19-C18-C17	10.04	135.15	118.95
24	A	608	BCR	C27-C26-C25	10.11	133.84	122.73
24	a	608	BCR	C27-C26-C25	10.15	133.90	122.73
24	t	101	BCR	C15-C14-C13	10.16	141.99	127.22
24	C	514	BCR	C11-C12-C13	10.18	156.18	126.34
24	c	514	BCR	C11-C12-C13	10.18	156.18	126.34
24	h	101	BCR	C19-C18-C17	10.20	135.40	118.95
24	H	101	BCR	C19-C18-C17	10.20	135.40	118.95
24	T	102	BCR	C15-C14-C13	10.22	142.07	127.22
24	d	404	BCR	C11-C10-C9	10.24	142.10	127.22
24	D	404	BCR	C11-C10-C9	10.27	142.15	127.22
24	C	515	BCR	C10-C11-C12	10.27	154.81	123.11
24	B	619	BCR	C20-C19-C18	10.27	156.44	126.34
24	c	515	BCR	C10-C11-C12	10.28	154.85	123.11
24	t	101	BCR	C10-C11-C12	10.29	154.86	123.11
24	b	618	BCR	C20-C19-C18	10.29	156.50	126.34
24	T	101	BCR	C20-C19-C18	10.31	156.55	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	T	102	BCR	C10-C11-C12	10.31	154.93	123.11
24	B	622	BCR	C21-C20-C19	10.31	154.94	123.11
24	B	618	BCR	C20-C19-C18	10.32	156.58	126.34
24	A	608	BCR	C12-C13-C14	10.32	135.59	118.95
24	a	608	BCR	C12-C13-C14	10.33	135.60	118.95
24	B	622	BCR	C20-C19-C18	10.33	156.61	126.34
24	b	622	BCR	C21-C20-C19	10.33	155.00	123.11
24	b	622	BCR	C20-C19-C18	10.34	156.64	126.34
24	D	404	BCR	C15-C14-C13	10.42	142.36	127.22
24	d	404	BCR	C15-C14-C13	10.45	142.41	127.22
24	h	101	BCR	C20-C19-C18	10.47	157.02	126.34
24	H	101	BCR	C20-C19-C18	10.47	157.04	126.34
24	A	608	BCR	C23-C22-C21	10.55	135.96	118.95
24	a	608	BCR	C23-C22-C21	10.57	135.99	118.95
24	A	608	BCR	C15-C14-C13	10.64	142.68	127.22
24	a	608	BCR	C15-C14-C13	10.66	142.71	127.22
24	k	101	BCR	C20-C19-C18	10.71	157.72	126.34
24	K	101	BCR	C20-C19-C18	10.73	157.79	126.34
24	K	102	BCR	C11-C12-C13	10.86	158.18	126.34
24	k	102	BCR	C11-C12-C13	10.87	158.21	126.34
24	T	101	BCR	C11-C10-C9	10.88	143.03	127.22
24	B	618	BCR	C11-C10-C9	10.89	143.05	127.22
24	K	102	BCR	C10-C11-C12	10.95	156.90	123.11
24	k	102	BCR	C10-C11-C12	10.96	156.93	123.11
24	B	622	BCR	C11-C12-C13	11.09	158.86	126.34
24	b	622	BCR	C11-C12-C13	11.12	158.93	126.34
24	B	618	BCR	C12-C13-C14	11.12	136.88	118.95
24	T	101	BCR	C12-C13-C14	11.15	136.92	118.95
24	K	101	BCR	C15-C14-C13	11.21	143.51	127.22
24	a	608	BCR	C11-C10-C9	11.22	143.54	127.22
24	k	101	BCR	C15-C14-C13	11.23	143.54	127.22
24	A	608	BCR	C11-C10-C9	11.26	143.59	127.22
24	c	515	BCR	C15-C14-C13	11.35	143.72	127.22
24	C	515	BCR	C15-C14-C13	11.36	143.73	127.22
24	h	101	BCR	C15-C14-C13	11.36	143.73	127.22
24	T	101	BCR	C21-C20-C19	11.36	158.19	123.11
24	B	618	BCR	C21-C20-C19	11.37	158.22	123.11
24	H	101	BCR	C15-C14-C13	11.38	143.76	127.22
24	K	102	BCR	C19-C18-C17	11.65	137.73	118.95
24	k	102	BCR	C19-C18-C17	11.65	137.73	118.95
24	K	102	BCR	C20-C19-C18	11.75	160.78	126.34
24	k	102	BCR	C20-C19-C18	11.77	160.84	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	608	BCR	C19-C18-C17	11.83	138.03	118.95
24	c	515	BCR	C20-C19-C18	11.85	161.08	126.34
24	A	608	BCR	C19-C18-C17	11.86	138.07	118.95
24	C	515	BCR	C20-C19-C18	11.87	161.13	126.34
24	B	622	BCR	C10-C11-C12	11.92	159.90	123.11
24	b	622	BCR	C10-C11-C12	11.93	159.94	123.11
24	k	101	BCR	C19-C18-C17	12.03	138.34	118.95
24	K	101	BCR	C19-C18-C17	12.07	138.41	118.95
24	C	514	BCR	C10-C11-C12	12.09	160.44	123.11
24	c	514	BCR	C10-C11-C12	12.10	160.46	123.11
24	B	622	BCR	C11-C10-C9	12.11	144.82	127.22
24	b	622	BCR	C11-C10-C9	12.12	144.84	127.22
24	c	514	BCR	C20-C19-C18	12.18	162.03	126.34
24	C	514	BCR	C20-C19-C18	12.18	162.05	126.34
24	t	101	BCR	C11-C10-C9	12.37	145.20	127.22
24	T	102	BCR	C11-C10-C9	12.45	145.32	127.22
24	t	101	BCR	C19-C18-C17	12.56	139.20	118.95
24	T	102	BCR	C19-C18-C17	12.61	139.28	118.95
24	K	101	BCR	C11-C10-C9	12.84	145.88	127.22
24	D	404	BCR	C21-C20-C19	12.84	162.75	123.11
24	k	101	BCR	C11-C10-C9	12.84	145.89	127.22
24	d	404	BCR	C21-C20-C19	12.84	162.76	123.11
24	a	608	BCR	C21-C20-C19	12.87	162.84	123.11
24	A	608	BCR	C21-C20-C19	12.89	162.90	123.11
24	b	618	BCR	C11-C10-C9	13.12	146.29	127.22
24	B	619	BCR	C11-C10-C9	13.14	146.32	127.22
24	b	618	BCR	C15-C14-C13	13.36	146.65	127.22
24	B	619	BCR	C15-C14-C13	13.37	146.66	127.22
24	t	101	BCR	C21-C20-C19	13.49	164.76	123.11
24	B	618	BCR	C16-C15-C14	13.50	152.35	123.23
24	T	102	BCR	C21-C20-C19	13.51	164.81	123.11
24	T	101	BCR	C16-C15-C14	13.52	152.40	123.23
24	h	101	BCR	C11-C10-C9	13.63	147.04	127.22
24	H	101	BCR	C11-C10-C9	13.64	147.04	127.22
24	B	619	BCR	C19-C18-C17	13.67	140.99	118.95
24	b	618	BCR	C19-C18-C17	13.67	141.00	118.95
24	B	622	BCR	C20-C21-C22	13.79	147.26	127.22
24	b	622	BCR	C20-C21-C22	13.79	147.27	127.22
24	k	102	BCR	C21-C20-C19	13.90	166.03	123.11
24	K	102	BCR	C21-C20-C19	13.91	166.04	123.11
24	k	102	BCR	C15-C14-C13	13.96	147.51	127.22
24	K	102	BCR	C15-C14-C13	13.96	147.51	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	608	BCR	C16-C15-C14	13.99	153.41	123.23
24	a	608	BCR	C16-C15-C14	14.00	153.43	123.23
24	C	515	BCR	C11-C10-C9	14.26	147.96	127.22
24	c	515	BCR	C11-C10-C9	14.27	147.97	127.22
24	T	101	BCR	C19-C18-C17	14.70	142.66	118.95
24	B	618	BCR	C19-C18-C17	14.73	142.69	118.95
24	B	619	BCR	C21-C20-C19	14.79	168.76	123.11
24	b	618	BCR	C21-C20-C19	14.81	168.82	123.11
24	k	101	BCR	C21-C20-C19	14.81	168.83	123.11
24	K	101	BCR	C21-C20-C19	14.81	168.84	123.11
24	H	101	BCR	C21-C20-C19	15.16	169.92	123.11
24	h	101	BCR	C21-C20-C19	15.16	169.92	123.11
24	B	619	BCR	C16-C15-C14	15.17	155.96	123.23
24	b	618	BCR	C16-C15-C14	15.17	155.97	123.23
24	B	619	BCR	C15-C16-C17	15.33	156.31	123.23
24	b	618	BCR	C15-C16-C17	15.34	156.33	123.23
24	h	101	BCR	C16-C15-C14	15.38	156.42	123.23
24	H	101	BCR	C16-C15-C14	15.41	156.47	123.23
24	K	101	BCR	C16-C15-C14	15.83	157.37	123.23
24	k	101	BCR	C16-C15-C14	15.84	157.39	123.23
24	c	515	BCR	C21-C20-C19	16.50	174.04	123.11
24	C	515	BCR	C21-C20-C19	16.51	174.06	123.11
24	b	622	BCR	C16-C17-C18	16.97	151.88	127.22
24	B	622	BCR	C16-C17-C18	16.99	151.91	127.22
24	c	514	BCR	C21-C20-C19	17.14	176.01	123.11
24	C	514	BCR	C21-C20-C19	17.15	176.07	123.11
24	a	608	BCR	C15-C16-C17	17.32	160.60	123.23
24	A	608	BCR	C15-C16-C17	17.34	160.63	123.23
24	t	101	BCR	C16-C15-C14	17.58	161.15	123.23
24	T	102	BCR	C16-C15-C14	17.59	161.18	123.23
24	T	101	BCR	C20-C21-C22	17.78	153.07	127.22
24	B	618	BCR	C20-C21-C22	17.78	153.07	127.22
24	K	102	BCR	C16-C15-C14	18.34	162.80	123.23
24	k	102	BCR	C16-C15-C14	18.37	162.86	123.23
24	k	102	BCR	C16-C17-C18	18.44	154.02	127.22
24	K	102	BCR	C16-C17-C18	18.45	154.04	127.22
24	B	618	BCR	C15-C16-C17	18.79	163.77	123.23
24	T	101	BCR	C15-C16-C17	18.83	163.86	123.23
24	d	404	BCR	C16-C15-C14	19.27	164.81	123.23
24	D	404	BCR	C16-C15-C14	19.28	164.82	123.23
24	b	622	BCR	C16-C15-C14	19.43	165.14	123.23
24	B	622	BCR	C16-C15-C14	19.44	165.18	123.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	k	101	BCR	C15-C16-C17	19.77	165.89	123.23
24	K	101	BCR	C15-C16-C17	19.77	165.89	123.23
24	C	514	BCR	C16-C15-C14	19.78	165.91	123.23
24	c	514	BCR	C16-C15-C14	19.80	165.94	123.23
24	b	622	BCR	C15-C16-C17	20.19	166.79	123.23
24	H	101	BCR	C16-C17-C18	20.21	156.59	127.22
24	h	101	BCR	C16-C17-C18	20.22	156.61	127.22
24	B	622	BCR	C15-C16-C17	20.22	166.85	123.23
24	c	515	BCR	C16-C17-C18	20.30	156.72	127.22
24	C	515	BCR	C16-C17-C18	20.30	156.73	127.22
24	b	618	BCR	C16-C17-C18	20.31	156.74	127.22
24	B	619	BCR	C16-C17-C18	20.31	156.75	127.22
24	k	102	BCR	C20-C21-C22	20.61	157.18	127.22
24	K	102	BCR	C20-C21-C22	20.65	157.25	127.22
24	c	515	BCR	C16-C15-C14	20.80	168.10	123.23
24	C	515	BCR	C16-C15-C14	20.82	168.15	123.23
24	a	608	BCR	C16-C17-C18	21.19	158.03	127.22
24	A	608	BCR	C16-C17-C18	21.21	158.06	127.22
24	K	102	BCR	C15-C16-C17	21.35	169.28	123.23
24	k	102	BCR	C15-C16-C17	21.37	169.34	123.23
24	B	619	BCR	C20-C21-C22	21.58	158.59	127.22
24	b	618	BCR	C20-C21-C22	21.58	158.60	127.22
24	D	404	BCR	C16-C17-C18	21.97	159.15	127.22
24	d	404	BCR	C16-C17-C18	21.97	159.16	127.22
24	D	404	BCR	C20-C21-C22	22.12	159.38	127.22
24	d	404	BCR	C20-C21-C22	22.14	159.41	127.22
24	d	404	BCR	C15-C16-C17	22.15	171.02	123.23
24	D	404	BCR	C15-C16-C17	22.17	171.05	123.23
24	c	515	BCR	C15-C16-C17	22.59	171.97	123.23
24	C	515	BCR	C15-C16-C17	22.62	172.04	123.23
24	c	514	BCR	C20-C21-C22	22.69	160.21	127.22
24	C	514	BCR	C20-C21-C22	22.71	160.23	127.22
24	K	101	BCR	C16-C17-C18	22.95	160.59	127.22
24	k	101	BCR	C16-C17-C18	22.97	160.61	127.22
24	B	618	BCR	C16-C17-C18	23.81	161.83	127.22
24	T	101	BCR	C16-C17-C18	23.82	161.85	127.22
24	H	101	BCR	C15-C16-C17	24.14	175.32	123.23
24	h	101	BCR	C15-C16-C17	24.15	175.33	123.23
24	T	102	BCR	C15-C16-C17	24.18	175.40	123.23
24	t	101	BCR	C15-C16-C17	24.20	175.44	123.23
24	C	514	BCR	C16-C17-C18	24.67	163.08	127.22
24	c	514	BCR	C16-C17-C18	24.69	163.11	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	608	BCR	C20-C21-C22	24.76	163.21	127.22
24	a	608	BCR	C20-C21-C22	24.76	163.21	127.22
24	T	102	BCR	C16-C17-C18	25.03	163.60	127.22
24	t	101	BCR	C16-C17-C18	25.03	163.61	127.22
24	k	101	BCR	C20-C21-C22	25.14	163.77	127.22
24	K	101	BCR	C20-C21-C22	25.17	163.81	127.22
24	c	515	BCR	C20-C21-C22	25.26	163.95	127.22
24	C	515	BCR	C20-C21-C22	25.33	164.04	127.22
24	C	514	BCR	C15-C16-C17	25.54	178.33	123.23
24	c	514	BCR	C15-C16-C17	25.59	178.43	123.23
24	t	101	BCR	C20-C21-C22	26.15	165.24	127.22
24	T	102	BCR	C20-C21-C22	26.17	165.27	127.22
24	h	101	BCR	C20-C21-C22	26.48	165.71	127.22
24	H	101	BCR	C20-C21-C22	26.49	165.72	127.22

All (166) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	B	617	CLA	NC
22	B	617	CLA	ND
22	B	617	CLA	NA
22	c	513	CLA	NC
22	c	513	CLA	NA
22	A	607	CLA	NC
22	d	402	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	c	502	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	602	CLA	ND
22	b	602	CLA	NA
22	D	403	CLA	NC
22	D	403	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	NA
22	B	609	CLA	NC

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Mol	Chain	Res	Type	Atom
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	C	505	CLA	ND
22	A	603	CLA	NC
22	A	603	CLA	ND
22	A	603	CLA	NA
22	C	501	CLA	NC
22	C	501	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	613	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	B	602	CLA	ND
22	B	602	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND

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Mol	Chain	Res	Type	Atom
22	c	507	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	B	616	CLA	NC
22	B	616	CLA	ND
22	B	616	CLA	NA
22	D	401	CLA	ND
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	d	401	CLA	ND
22	c	501	CLA	NC
22	c	501	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	b	604	CLA	NC
22	b	604	CLA	ND
22	b	604	CLA	NA
22	C	513	CLA	NC
22	C	513	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	a	603	CLA	NC
22	a	603	CLA	ND
22	a	603	CLA	NA
22	D	402	CLA	NA
22	C	502	CLA	NA

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Mol	Chain	Res	Type	Atom
22	b	607	CLA	NC
22	b	607	CLA	NA
22	a	604	CLA	NC
22	a	604	CLA	NA
22	c	505	CLA	ND
22	b	603	CLA	NC
22	b	603	CLA	ND
22	b	603	CLA	NA
22	b	609	CLA	NC
22	A	604	CLA	NC
22	A	604	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	NA
22	C	512	CLA	ND
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	B	613	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	c	512	CLA	NC
22	c	512	CLA	NA
22	c	512	CLA	ND
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	d	403	CLA	NC
22	d	403	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
22	B	604	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	a	607	CLA	NC
22	C	511	CLA	NC
22	C	511	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	z	101	LMG	C7-O1-C1-O6
29	Z	101	LMG	C7-O1-C1-O6

There are no ring outliers.

62 monomers are involved in 148 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	603	CLA	5	0
22	A	604	CLA	3	0
23	A	605	PHO	2	0
23	A	606	PHO	4	0
22	A	607	CLA	2	0
24	A	608	BCR	1	0
25	A	609	SQD	2	0
28	A	613	PL9	8	0
29	A	614	LMG	3	0
25	B	601	SQD	4	0
22	B	603	CLA	1	0
22	B	604	CLA	2	0
22	B	605	CLA	2	0
22	B	606	CLA	5	0
22	B	607	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	609	CLA	2	0
22	B	611	CLA	4	0
22	B	612	CLA	2	0
22	B	613	CLA	3	0
22	B	614	CLA	5	0
22	B	615	CLA	3	0
22	B	616	CLA	2	0
22	B	617	CLA	4	0
24	B	618	BCR	3	0
24	B	619	BCR	1	0
29	B	620	LMG	3	0
24	B	622	BCR	4	0
22	C	501	CLA	2	0
22	C	502	CLA	3	0
22	C	503	CLA	3	0
22	C	504	CLA	1	0
22	C	505	CLA	2	0
22	C	506	CLA	4	0
22	C	507	CLA	1	0
22	C	508	CLA	3	0
22	C	509	CLA	2	0
22	C	510	CLA	6	0
22	C	511	CLA	2	0
22	C	512	CLA	3	0
22	C	513	CLA	1	0
31	C	516	DGD	2	0
31	C	517	DGD	2	0
31	C	518	DGD	1	0
29	C	519	LMG	1	0
22	D	401	CLA	1	0
22	D	402	CLA	4	0
22	D	403	CLA	3	0
24	D	404	BCR	3	0
29	D	406	LMG	2	0
32	D	409	LHG	13	0
31	D	410	DGD	3	0
32	E	101	LHG	2	0
33	F	101	HEM	1	0
24	H	101	BCR	1	0
31	H	102	DGD	1	0
24	K	102	BCR	1	0
25	L	101	SQD	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	L	102	LHG	1	0
24	T	101	BCR	7	0
24	T	102	BCR	2	0
33	V	201	HEM	9	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%)	0.59	21 (6%) 23 22	16, 22, 43, 53	0
1	a	334/334 (100%)	0.60	26 (7%) 16 17	16, 22, 43, 53	0
2	B	504/504 (100%)	0.47	32 (6%) 23 22	18, 27, 49, 70	0
2	b	504/504 (100%)	0.76	70 (13%) 4 8	18, 27, 49, 70	0
3	C	451/461 (97%)	0.64	43 (9%) 10 13	21, 31, 44, 56	0
3	c	451/461 (97%)	0.52	39 (8%) 13 16	21, 31, 44, 56	0
4	D	342/342 (100%)	0.78	33 (9%) 10 13	17, 23, 39, 61	0
4	d	342/342 (100%)	0.70	24 (7%) 19 20	17, 23, 39, 61	0
5	E	81/81 (100%)	0.82	10 (12%) 5 9	27, 40, 57, 63	0
5	e	81/81 (100%)	0.42	9 (11%) 7 11	27, 40, 57, 63	0
6	F	34/34 (100%)	0.36	1 (2%) 55 49	28, 33, 58, 61	0
6	f	34/34 (100%)	-0.00	0 100 100	28, 33, 58, 61	0
7	H	65/65 (100%)	0.65	9 (13%) 4 8	23, 34, 40, 58	0
7	h	65/65 (100%)	1.42	18 (27%) 1 4	23, 34, 40, 58	0
8	I	38/38 (100%)	0.54	5 (13%) 4 8	30, 34, 65, 68	0
8	i	38/38 (100%)	0.08	3 (7%) 15 17	30, 34, 65, 68	0
9	J	38/40 (95%)	0.56	3 (7%) 15 17	26, 37, 68, 72	0
9	j	38/40 (95%)	-0.14	0 100 100	26, 37, 68, 72	0
10	K	37/37 (100%)	0.52	2 (5%) 29 29	33, 38, 45, 47	0
10	k	37/37 (100%)	0.60	4 (10%) 8 11	33, 38, 45, 47	0
11	L	37/37 (100%)	0.60	2 (5%) 29 29	17, 22, 50, 59	0
11	l	37/37 (100%)	0.59	3 (8%) 15 17	17, 22, 50, 59	0
12	M	34/34 (100%)	1.02	6 (17%) 2 6	21, 23, 36, 52	0
12	m	34/34 (100%)	0.74	3 (8%) 12 15	21, 23, 36, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	0.38	8 (3%) 50 44	18, 32, 55, 71	0
13	o	243/243 (100%)	0.56	14 (5%) 26 25	18, 32, 55, 71	0
14	T	30/30 (100%)	0.87	3 (10%) 9 12	19, 23, 44, 52	0
14	t	30/30 (100%)	0.85	1 (3%) 50 44	19, 23, 44, 52	0
15	U	97/97 (100%)	0.30	2 (2%) 67 61	23, 30, 48, 50	0
15	u	97/97 (100%)	0.55	6 (6%) 24 23	23, 30, 48, 50	0
16	V	137/137 (100%)	0.22	2 (1%) 76 70	23, 28, 39, 48	0
16	v	137/137 (100%)	0.38	6 (4%) 38 35	23, 28, 39, 48	0
17	X	39/39 (100%)	0.99	7 (17%) 2 6	33, 40, 66, 68	0
17	x	39/39 (100%)	1.00	7 (17%) 2 6	33, 40, 66, 68	0
18	Y	29/29 (100%)	0.69	3 (10%) 9 12	42, 48, 75, 77	0
18	y	29/29 (100%)	0.29	0 100 100	42, 48, 75, 77	0
19	Z	62/62 (100%)	0.48	2 (3%) 51 45	39, 48, 68, 72	0
19	z	62/62 (100%)	0.69	7 (11%) 7 10	39, 48, 68, 72	0
All	All	5264/5288 (99%)	0.59	434 (8%) 14 16	16, 29, 51, 77	0

All (434) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	X	2	THR	7.2
4	D	59	TYR	6.8
9	J	3	SER	6.5
4	D	56	THR	5.7
4	d	136	VAL	5.4
4	D	136	VAL	5.4
1	a	140	ARG	5.4
2	b	270	PRO	5.3
1	a	138	GLY	5.2
3	C	24	THR	5.1
2	b	499	VAL	5.1
4	d	59	TYR	5.1
2	b	262	THR	5.0
17	x	2	THR	5.0
3	C	256	PRO	5.0
4	d	135	LEU	4.9
7	H	56	ASP	4.8
3	C	265	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	a	139	MET	4.8
3	c	146	PHE	4.7
4	d	107	LEU	4.6
3	c	198	VAL	4.6
2	b	187	PRO	4.6
4	d	106	GLN	4.6
2	b	435	GLU	4.5
1	a	245	THR	4.5
3	C	137	PRO	4.5
4	D	106	GLN	4.5
2	b	131	PRO	4.4
3	C	264	PHE	4.4
2	b	500	GLY	4.4
12	M	2	GLU	4.3
7	h	23	PRO	4.3
3	C	138	GLU	4.2
3	c	228	ASN	4.2
3	C	97	TRP	4.2
6	F	12	SER	4.2
2	B	136	PRO	4.1
4	D	135	LEU	4.1
5	E	49	THR	4.1
2	b	71	VAL	4.1
7	H	55	LEU	4.1
2	b	261	ALA	4.1
4	D	55	VAL	4.1
3	c	86	LEU	4.1
17	X	40	SER	4.1
1	A	245	THR	4.0
3	c	197	ARG	4.0
19	z	62	VAL	4.0
7	h	55	LEU	4.0
4	D	137	GLY	3.9
17	x	40	SER	3.9
3	C	266	TRP	3.9
19	Z	1	MET	3.9
2	b	361	ALA	3.9
4	d	137	GLY	3.9
2	b	188	ASP	3.8
3	C	25	ASN	3.8
4	d	264	LYS	3.8
2	b	267	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
16	v	21	LEU	3.7
1	a	246	TYR	3.7
1	A	11	ALA	3.7
3	c	127	PHE	3.7
3	C	146	PHE	3.6
2	b	70	GLY	3.6
3	C	400	PRO	3.6
15	U	8	GLU	3.6
1	A	317	TRP	3.6
1	A	262	TYR	3.6
4	d	29	PHE	3.6
17	x	3	ILE	3.6
4	D	107	LEU	3.5
19	z	61	VAL	3.5
2	b	190	PHE	3.5
2	b	229	LEU	3.5
19	z	1	MET	3.5
2	b	218	LEU	3.5
3	C	263	ALA	3.5
4	d	221	THR	3.5
3	c	373	ASN	3.5
19	z	23	VAL	3.5
3	C	457	LYS	3.5
7	h	54	ILE	3.5
2	B	43	ALA	3.5
13	o	243	ILE	3.4
4	D	27	PHE	3.4
2	B	499	VAL	3.4
1	A	139	MET	3.4
1	A	137	LEU	3.4
5	e	84	LYS	3.4
7	h	56	ASP	3.4
18	Y	46	LEU	3.3
4	d	54	PHE	3.3
2	B	367	PRO	3.3
7	h	27	THR	3.3
2	B	183	PRO	3.3
4	D	93	TRP	3.3
7	h	53	LEU	3.3
13	O	243	ILE	3.3
2	B	362	PHE	3.2
17	x	38	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	b	133	LEU	3.2
3	c	457	LYS	3.2
18	Y	43	ARG	3.2
1	a	137	LEU	3.2
4	D	32	TRP	3.2
7	H	65	LEU	3.2
2	b	219	VAL	3.2
3	c	264	PHE	3.2
4	D	54	PHE	3.1
5	e	55	TYR	3.1
17	X	3	ILE	3.1
10	k	18	PHE	3.1
2	b	72	THR	3.1
3	C	127	PHE	3.1
2	b	87	ASP	3.1
8	i	38	GLU	3.1
13	O	169	ASP	3.1
2	b	305	ILE	3.1
2	b	123	PHE	3.1
8	I	25	SER	3.1
1	A	12	ASN	3.1
4	D	264	LYS	3.1
2	b	119	ASP	3.1
4	d	98	GLN	3.0
2	B	44	THR	3.0
2	B	378	LYS	3.0
3	c	400	PRO	3.0
3	C	452	ALA	3.0
2	B	187	PRO	3.0
4	d	28	VAL	3.0
1	A	306	VAL	3.0
4	D	12	ARG	3.0
2	B	368	VAL	3.0
2	b	217	ILE	3.0
2	B	500	GLY	3.0
2	B	262	THR	3.0
7	h	2	ALA	3.0
3	c	422	PRO	3.0
1	A	246	TYR	3.0
2	b	497	GLN	3.0
8	i	37	LEU	3.0
4	d	11	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	b	356	VAL	3.0
1	a	257	ARG	3.0
1	a	268	SER	3.0
3	c	291	TRP	3.0
4	d	138	VAL	3.0
3	C	147	PHE	2.9
15	u	66	GLY	2.9
2	B	309	LEU	2.9
2	B	69	LEU	2.9
16	v	3	LEU	2.9
17	X	38	GLN	2.9
13	o	129	THR	2.9
7	h	26	GLY	2.9
2	b	302	TRP	2.9
1	A	265	PHE	2.9
16	v	120	LEU	2.9
3	c	336	GLY	2.9
1	A	257	ARG	2.9
3	c	112	PHE	2.9
5	E	70	PHE	2.9
2	b	343	HIS	2.9
4	D	333	ASP	2.9
3	C	255	THR	2.9
15	u	56	GLU	2.9
2	b	264	PRO	2.8
3	C	399	ALA	2.8
19	z	24	PRO	2.8
3	c	69	LEU	2.8
4	D	96	GLU	2.8
7	h	47	GLU	2.8
5	E	47	PHE	2.8
12	M	1	MET	2.8
8	I	30	ARG	2.8
1	a	240	GLY	2.8
5	e	56	TYR	2.8
15	u	103	TYR	2.8
3	C	268	GLY	2.8
10	K	32	PHE	2.8
2	B	347	ARG	2.8
13	o	181	GLU	2.8
2	B	366	PHE	2.8
3	C	199	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	a	244	GLU	2.8
3	c	200	THR	2.8
4	D	103	ARG	2.8
4	d	56	THR	2.7
7	h	14	LEU	2.7
2	B	306	PRO	2.7
3	c	134	ILE	2.7
7	H	66	GLY	2.7
9	J	5	GLY	2.7
3	c	181	PHE	2.7
19	z	27	TYR	2.7
12	M	3	VAL	2.7
2	B	70	GLY	2.7
2	b	490	GLN	2.7
4	D	95	PRO	2.7
19	Z	35	ARG	2.7
4	d	262	SER	2.7
2	b	16	PRO	2.7
3	C	139	THR	2.7
13	o	190	PHE	2.7
3	c	296	VAL	2.7
8	I	32	PRO	2.7
5	e	66	VAL	2.7
4	d	108	GLY	2.6
2	B	305	ILE	2.6
3	C	99	VAL	2.6
2	B	498	LYS	2.6
17	x	39	ARG	2.6
2	b	491	VAL	2.6
2	B	229	LEU	2.6
19	z	40	ILE	2.6
2	B	166	MET	2.6
4	d	23	LYS	2.6
3	c	147	PHE	2.6
1	A	261	GLN	2.6
15	U	32	ILE	2.6
1	a	74	GLY	2.6
2	b	494	GLY	2.6
3	C	204	LEU	2.6
2	B	87	ASP	2.6
3	c	458	GLY	2.6
13	o	87	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	81	MET	2.6
2	b	318	ASN	2.6
3	C	202	PRO	2.6
3	c	199	ILE	2.6
2	b	268	PHE	2.6
14	T	30	THR	2.6
3	C	267	SER	2.6
3	c	143	TYR	2.6
8	i	36	ASP	2.6
1	a	223	LEU	2.6
2	B	185	TRP	2.5
2	b	234	ILE	2.5
15	u	8	GLU	2.5
4	D	110	LEU	2.5
3	c	81	MET	2.5
3	c	227	VAL	2.5
2	b	220	ARG	2.5
3	C	365	TRP	2.5
17	X	34	ILE	2.5
1	A	268	SER	2.5
2	b	317	ASN	2.5
13	O	164	LEU	2.5
13	o	184	ARG	2.5
4	D	180	ARG	2.5
3	c	238	ILE	2.5
2	b	392	PHE	2.5
2	b	438	ASN	2.5
4	d	32	TRP	2.5
1	A	219	VAL	2.5
1	a	239	PHE	2.5
11	l	33	SER	2.5
2	B	195	PRO	2.5
1	a	250	ALA	2.4
2	B	497	GLN	2.4
2	b	353	GLU	2.4
2	b	443	PHE	2.4
12	m	7	GLY	2.4
1	a	222	SER	2.4
1	a	317	TRP	2.4
15	u	101	GLY	2.4
5	e	54	SER	2.4
2	b	447	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	362	PHE	2.4
4	D	60	THR	2.4
2	B	71	VAL	2.4
2	b	120	LEU	2.4
5	e	64	PRO	2.4
1	A	244	GLU	2.4
2	b	195	PRO	2.4
5	e	57	ALA	2.4
2	b	183	PRO	2.4
7	H	57	GLY	2.4
5	E	64	PRO	2.4
5	E	84	LYS	2.4
8	I	24	LEU	2.4
7	h	22	ALA	2.4
13	o	211	ILE	2.4
13	O	120	PHE	2.3
1	a	224	ILE	2.3
5	e	60	GLN	2.3
13	O	20	PRO	2.3
16	v	116	ALA	2.3
2	B	77	GLY	2.3
4	D	138	VAL	2.3
2	B	490	GLN	2.3
7	h	65	LEU	2.3
1	a	141	PRO	2.3
3	c	456	GLU	2.3
17	X	39	ARG	2.3
12	m	33	GLN	2.3
17	x	37	VAL	2.3
1	a	76	ASN	2.3
1	a	306	VAL	2.3
2	b	189	GLY	2.3
3	C	296	VAL	2.3
4	D	25	ASP	2.3
1	A	85	SER	2.3
7	h	3	ARG	2.3
2	b	122	LEU	2.3
7	H	53	LEU	2.3
4	d	60	THR	2.3
2	b	274	GLN	2.3
5	E	17	VAL	2.3
3	C	203	THR	2.3

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Mol	Chain	Res	Type	RSRZ
10	K	11	LEU	2.3
3	C	23	ALA	2.3
1	A	143	ILE	2.2
2	B	505	ARG	2.2
4	D	28	VAL	2.2
4	D	300	SER	2.2
7	h	24	GLY	2.2
13	o	42	ARG	2.2
2	b	306	PRO	2.2
2	b	182	ALA	2.2
2	b	369	ILE	2.2
3	C	200	THR	2.2
2	b	309	LEU	2.2
3	c	263	ALA	2.2
3	c	82	TYR	2.2
7	H	47	GLU	2.2
3	C	336	GLY	2.2
3	C	234	VAL	2.2
12	M	4	ASN	2.2
3	c	149	TYR	2.2
11	L	33	SER	2.2
4	d	292	ASN	2.2
3	C	238	ILE	2.2
3	c	203	THR	2.2
5	E	18	ARG	2.2
5	E	22	ILE	2.2
4	d	308	ASP	2.2
5	E	12	ASP	2.2
14	T	2	GLU	2.2
7	h	20	LYS	2.2
1	a	80	GLY	2.2
2	b	84	THR	2.2
11	l	8	GLN	2.2
2	b	185	TRP	2.2
2	b	436	THR	2.2
12	M	5	GLN	2.2
13	o	150	SER	2.2
7	H	64	ALA	2.2
7	H	54	ILE	2.2
3	C	72	LEU	2.2
13	O	87	VAL	2.2
13	O	154	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
7	h	28	THR	2.2
13	o	40	ILE	2.2
14	t	3	THR	2.2
1	A	304	HIS	2.2
2	b	132	ALA	2.2
3	C	466	VAL	2.2
3	c	249	ILE	2.2
4	D	350	ASN	2.2
4	d	341	PHE	2.2
5	E	5	THR	2.2
3	C	291	TRP	2.2
18	Y	45	ASN	2.2
7	h	48	ILE	2.2
3	C	213	LEU	2.1
9	J	4	GLU	2.1
1	a	247	ASN	2.1
2	b	367	PRO	2.1
10	k	21	LEU	2.1
1	a	75	ASN	2.1
11	l	1	MET	2.1
3	C	124	VAL	2.1
7	h	66	GLY	2.1
3	C	86	LEU	2.1
17	x	36	LYS	2.1
1	a	340	PRO	2.1
15	u	77	GLU	2.1
12	M	7	GLY	2.1
14	T	3	THR	2.1
3	C	95	LEU	2.1
13	O	76	THR	2.1
2	b	445	THR	2.1
2	b	420	TYR	2.1
2	b	428	GLU	2.1
4	D	307	GLU	2.1
4	D	79	SER	2.1
4	D	308	ASP	2.1
4	d	35	ILE	2.1
2	b	192	PRO	2.1
3	C	269	GLU	2.1
3	c	292	PHE	2.1
12	m	4	ASN	2.1
2	b	344	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	89	LEU	2.1
17	X	36	LYS	2.1
3	C	111	PHE	2.1
10	k	15	TYR	2.1
13	o	101	ILE	2.1
4	D	23	LYS	2.1
3	c	230	LEU	2.1
1	a	79	THR	2.1
2	b	284	ILE	2.1
16	v	90	GLU	2.1
2	B	379	ALA	2.1
1	a	236	GLY	2.0
3	c	243	ILE	2.0
16	V	125	ILE	2.0
3	c	447	ARG	2.0
13	o	140	THR	2.0
8	I	37	LEU	2.0
13	o	176	GLN	2.0
1	A	194	MET	2.0
2	b	85	GLY	2.0
2	b	311	PHE	2.0
3	c	372	PRO	2.0
13	o	112	GLY	2.0
2	b	304	ALA	2.0
16	V	120	LEU	2.0
2	b	231	MET	2.0
10	k	14	ALA	2.0
11	L	2	GLU	2.0
3	c	256	PRO	2.0
1	A	206	PHE	2.0
2	b	194	ASN	2.0
3	c	120	ILE	2.0
4	D	29	PHE	2.0
2	B	421	ALA	2.0
1	A	220	THR	2.0
16	v	10	VAL	2.0
5	e	37	PHE	2.0
4	D	30	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
24	BCR	K	102	40/40	0.81	2.30	11.02	29,33,37,37	0
28	PL9	A	613	55/55	0.34	1.95	7.12	52,69,78,78	0
24	BCR	k	102	40/40	0.70	2.17	6.57	29,33,37,37	0
29	LMG	Z	101	37/55	0.33	1.65	6.14	55,84,88,88	0
24	BCR	D	404	40/40	0.40	1.52	6.09	25,30,48,49	0
22	CLA	c	501	65/65	0.72	1.66	6.07	29,32,44,46	0
24	BCR	c	514	40/40	0.72	1.69	5.47	37,43,47,47	0
24	BCR	C	515	40/40	0.73	1.99	5.43	30,37,40,41	0
29	LMG	c	520	51/55	0.21	1.84	5.31	43,76,81,82	0
24	BCR	K	101	40/40	0.61	1.39	5.10	34,38,39,39	0
25	SQD	D	411	43/54	0.66	1.27	5.06	67,74,78,79	0
29	LMG	C	519	51/55	0.42	0.86	5.03	31,57,72,73	0
24	BCR	c	515	40/40	0.79	1.59	4.80	30,37,40,41	0
28	PL9	a	613	55/55	0.27	1.47	4.75	52,69,78,78	0
24	BCR	d	404	40/40	0.33	1.17	4.66	25,30,48,49	0
24	BCR	C	514	40/40	0.76	1.48	4.52	37,43,47,47	0
22	CLA	a	607	65/65	0.76	0.81	4.40	21,24,71,72	0
23	PHO	A	606	64/64	0.82	1.13	4.35	19,22,28,32	0
22	CLA	C	509	65/65	0.93	1.30	4.34	29,32,46,47	0
22	CLA	c	509	65/65	0.82	1.18	4.33	29,32,46,47	0
24	BCR	T	102	40/40	0.41	1.10	4.26	27,33,39,39	0
22	CLA	c	507	65/65	0.76	1.38	4.23	29,33,52,53	0
22	CLA	B	603	65/65	0.83	1.15	4.22	23,26,32,32	0
31	DGD	D	410	62/66	0.48	1.24	4.16	77,89,103,103	0
22	CLA	c	503	65/65	0.82	1.11	4.03	27,31,35,36	0
22	CLA	C	501	65/65	0.79	1.23	3.99	29,32,44,46	0
22	CLA	c	512	65/65	0.66	1.58	3.98	37,41,62,63	0
29	LMG	c	519	51/55	0.83	0.67	3.92	31,57,72,73	0
22	CLA	D	401	65/65	0.84	0.95	3.87	13,18,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	BCR	k	101	40/40	0.29	1.14	3.87	34,38,39,39	0
22	CLA	b	604	65/65	0.88	1.30	3.78	18,22,31,35	0
25	SQD	d	411	43/54	0.61	0.90	3.75	67,74,78,79	0
29	LMG	z	101	37/55	0.26	1.48	3.65	55,84,88,88	0
31	DGD	H	102	62/66	0.85	1.00	3.58	26,32,38,40	0
22	CLA	d	401	65/65	0.90	0.84	3.51	13,18,34,35	0
22	CLA	c	510	65/65	0.86	0.86	3.49	24,28,35,37	0
22	CLA	C	512	65/65	0.70	1.33	3.45	37,41,62,63	0
22	CLA	A	607	65/65	0.82	0.78	3.43	21,24,71,72	0
22	CLA	D	403	65/65	0.70	1.20	3.42	24,27,65,67	0
29	LMG	C	520	51/55	0.31	1.35	3.39	43,76,81,82	0
22	CLA	b	603	65/65	0.83	1.17	3.28	23,26,32,32	0
33	HEM	f	101	43/43	0.91	0.69	3.22	39,42,45,47	0
22	CLA	d	403	65/65	0.74	1.19	3.12	24,27,65,67	0
29	LMG	a	614	51/55	0.68	0.80	3.11	53,59,64,65	0
22	CLA	a	604	65/65	0.57	0.86	3.09	19,21,63,65	0
32	LHG	E	101	42/49	0.55	1.29	3.06	69,83,86,86	0
24	BCR	A	608	40/40	0.45	0.70	3.00	22,27,32,32	0
22	CLA	A	604	65/65	0.75	1.01	2.96	19,21,63,65	0
22	CLA	C	511	65/65	0.91	1.24	2.83	29,34,37,38	0
22	CLA	B	613	65/65	0.87	0.73	2.75	20,24,30,31	0
22	CLA	c	502	65/65	0.68	0.96	2.71	24,26,39,42	0
29	LMG	A	614	51/55	0.63	0.84	2.68	53,59,64,65	0
23	PHO	a	606	64/64	0.82	0.79	2.60	19,22,28,32	0
32	LHG	D	409	49/49	0.75	0.75	2.59	26,33,62,64	0
22	CLA	B	604	65/65	0.88	1.04	2.57	18,22,31,35	0
25	SQD	a	609	54/54	0.64	0.53	2.49	49,57,66,67	0
29	LMG	D	406	51/55	0.78	0.79	2.48	26,35,65,67	0
22	CLA	C	507	65/65	0.70	1.33	2.45	29,33,52,53	0
22	CLA	b	616	65/65	0.81	1.25	2.42	25,27,45,46	0
31	DGD	h	102	62/66	0.82	0.90	2.41	26,32,38,40	0
22	CLA	b	605	65/65	0.82	0.79	2.40	19,22,50,51	0
24	BCR	t	101	40/40	0.47	0.63	2.37	27,33,39,39	0
22	CLA	b	602	65/65	0.61	1.48	2.36	32,41,66,66	0
22	CLA	b	610	65/65	0.86	1.10	2.24	23,28,31,32	0
22	CLA	c	506	65/65	0.85	0.93	2.23	31,38,74,75	0
22	CLA	B	611	65/65	0.90	0.99	2.22	21,25,32,37	0
22	CLA	B	610	65/65	0.90	0.83	2.21	23,28,31,32	0
22	CLA	c	505	65/65	0.87	0.82	2.21	28,30,44,45	0
27	BCT	a	612	4/4	0.93	1.21	2.14	39,39,40,42	0
22	CLA	B	609	65/65	0.81	0.88	2.08	20,24,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	b	609	65/65	0.83	1.02	2.04	20,24,31,31	0
33	HEM	v	201	43/43	0.92	0.72	1.98	23,24,27,29	0
22	CLA	B	606	65/65	0.83	0.84	1.92	19,23,34,35	0
22	CLA	B	616	65/65	0.78	0.74	1.87	25,27,45,46	0
22	CLA	C	508	65/65	0.73	0.74	1.87	25,29,54,58	0
22	CLA	b	606	65/65	0.78	0.84	1.84	19,23,34,35	0
22	CLA	B	605	65/65	0.89	0.57	1.83	19,22,50,51	0
24	BCR	h	101	40/40	0.81	1.32	1.82	26,33,42,42	0
22	CLA	b	613	65/65	0.86	0.75	1.82	20,24,30,31	0
22	CLA	b	611	65/65	0.84	0.94	1.76	21,25,32,37	0
22	CLA	C	504	65/65	0.81	0.70	1.70	25,28,54,54	0
22	CLA	a	603	65/65	0.73	0.60	1.69	15,19,25,34	0
22	CLA	c	511	65/65	0.83	0.88	1.68	29,34,37,38	0
26	CL	a	610	1/1	0.57	0.55	1.68	24,24,24,24	0
24	BCR	H	101	40/40	0.67	1.32	1.66	26,33,42,42	0
33	HEM	V	201	43/43	0.91	0.69	1.65	23,24,27,29	0
31	DGD	d	410	62/66	0.53	0.76	1.65	77,89,103,103	0
27	BCT	A	612	4/4	0.88	1.02	1.63	39,39,40,42	0
22	CLA	c	508	65/65	0.87	0.60	1.60	25,29,54,58	0
33	HEM	F	101	43/43	0.89	0.79	1.56	39,42,45,47	0
22	CLA	C	510	65/65	0.83	0.81	1.55	24,28,35,37	0
22	CLA	C	513	65/65	0.66	1.10	1.52	39,45,64,64	0
22	CLA	c	513	65/65	0.68	1.02	1.49	39,45,64,64	0
22	CLA	C	502	65/65	0.86	0.79	1.47	24,26,39,42	0
22	CLA	b	617	65/65	0.67	0.91	1.45	22,29,77,78	0
22	CLA	C	505	65/65	0.90	0.90	1.44	28,30,44,45	0
25	SQD	A	609	54/54	0.65	0.63	1.42	49,57,66,67	0
22	CLA	A	603	65/65	0.77	0.67	1.41	15,19,25,34	0
22	CLA	B	602	65/65	0.62	1.02	1.37	32,41,66,66	0
22	CLA	b	607	65/65	0.51	0.88	1.34	24,28,40,41	0
31	DGD	C	518	62/66	0.75	0.64	1.25	22,31,52,56	0
31	DGD	C	516	62/66	0.85	0.58	1.25	23,33,61,62	0
23	PHO	A	605	64/64	0.77	0.59	1.22	16,21,25,26	0
22	CLA	C	506	65/65	0.76	0.97	1.21	31,38,74,75	0
22	CLA	C	503	65/65	0.90	0.80	1.13	27,31,35,36	0
32	LHG	d	409	49/49	0.77	0.71	1.09	26,33,62,64	0
24	BCR	a	608	40/40	0.39	0.47	1.07	22,27,32,32	0
32	LHG	e	101	42/49	0.52	0.61	1.06	69,83,86,86	0
31	DGD	c	518	62/66	0.81	0.53	1.02	22,31,52,56	0
23	PHO	a	605	64/64	0.81	0.52	0.99	16,21,25,26	0
24	BCR	b	618	40/40	0.75	0.41	0.98	21,28,40,40	0
25	SQD	b	601	54/54	0.73	0.49	0.84	50,63,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	LHG	D	407	49/49	0.81	0.49	0.82	24,28,37,40	0
22	CLA	B	617	65/65	0.69	0.51	0.78	22,29,77,78	0
28	PL9	D	408	55/55	0.70	0.51	0.75	19,23,29,32	0
29	LMG	d	406	51/55	0.76	0.50	0.75	26,35,65,67	0
22	CLA	B	607	65/65	0.61	0.62	0.70	24,28,40,41	0
22	CLA	B	612	65/65	0.85	0.44	0.61	19,21,32,34	0
31	DGD	C	517	62/66	0.82	0.54	0.59	23,35,62,63	0
31	DGD	c	516	62/66	0.87	0.55	0.51	23,33,61,62	0
22	CLA	D	402	65/65	0.78	0.53	0.49	14,18,29,35	0
22	CLA	c	504	65/65	0.91	0.51	0.46	25,28,54,54	0
22	CLA	b	612	65/65	0.77	0.43	0.27	19,21,32,34	0
20	OEX	a	601	10/10	0.93	0.41	0.19	22,23,26,26	0
22	CLA	b	614	65/65	0.73	0.45	0.13	19,22,45,47	0
24	BCR	T	101	40/40	0.79	0.40	0.07	23,27,28,29	0
24	BCR	b	622	40/40	0.69	0.48	0.02	25,37,44,45	0
31	DGD	c	517	62/66	0.89	0.40	-0.02	23,35,62,63	0
25	SQD	L	101	54/54	0.77	0.41	-0.04	57,69,84,85	0
22	CLA	d	402	65/65	0.78	0.47	-0.06	14,18,29,35	0
22	CLA	b	608	65/65	0.87	0.43	-0.09	17,20,32,34	0
25	SQD	b	621	54/54	0.77	0.40	-0.12	58,66,80,80	0
32	LHG	d	405	49/49	0.81	0.44	-0.13	29,34,41,41	0
26	CL	a	611	1/1	0.91	0.37	-0.22	21,21,21,21	0
34	MG	j	101	1/1	0.71	0.30	-0.25	27,27,27,27	0
28	PL9	d	408	55/55	0.78	0.40	-0.38	19,23,29,32	0
32	LHG	d	407	49/49	0.80	0.37	-0.39	24,28,37,40	0
22	CLA	b	615	65/65	0.67	0.44	-0.40	20,24,60,61	0
22	CLA	B	608	65/65	0.91	0.41	-0.51	17,20,32,34	0
22	CLA	B	614	65/65	0.91	0.38	-0.52	19,22,45,47	0
26	CL	A	610	1/1	0.80	0.45	-0.57	24,24,24,24	0
20	OEX	A	601	10/10	0.92	0.40	-0.57	22,23,26,26	0
29	LMG	b	619	51/55	0.67	0.38	-0.58	29,39,51,54	0
32	LHG	D	405	49/49	0.76	0.38	-0.62	29,34,41,41	0
32	LHG	L	102	49/49	0.84	0.35	-0.64	23,31,43,44	0
32	LHG	l	103	49/49	0.86	0.33	-0.73	23,31,43,44	0
29	LMG	B	620	51/55	0.58	0.38	-0.80	29,39,51,54	0
25	SQD	l	101	54/54	0.82	0.32	-0.82	57,69,84,85	0
25	SQD	l	102	54/54	0.82	0.32	-0.82	58,66,80,80	0
24	BCR	B	618	40/40	0.82	0.30	-0.85	23,27,28,29	0
22	CLA	B	615	65/65	0.74	0.38	-0.86	20,24,60,61	0
25	SQD	B	601	54/54	0.73	0.35	-0.86	50,63,68,68	0
24	BCR	B	622	40/40	0.67	0.43	-0.91	25,37,44,45	0
26	CL	A	611	1/1	0.85	0.35	-1.00	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	MG	J	101	1/1	0.87	0.11	-1.31	27,27,27,27	0
21	FE2	A	602	1/1	0.96	0.16	-1.50	26,26,26,26	0
30	CA	o	301	1/1	0.95	0.28	-1.83	49,49,49,49	0
24	BCR	B	619	40/40	0.73	0.31	-1.99	21,28,40,40	0
21	FE2	a	602	1/1	0.83	0.35	-1.99	26,26,26,26	0
30	CA	O	301	1/1	0.93	0.14	-2.63	49,49,49,49	0
30	CA	f	102	1/1	0.28	0.73	-	56,56,56,56	0
26	CL	U	201	1/1	0.02	0.17	-	50,50,50,50	0
30	CA	B	621	1/1	0.25	0.73	-	76,76,76,76	0
26	CL	u	201	1/1	0.03	0.36	-	50,50,50,50	0
30	CA	F	102	1/1	0.70	0.50	-	56,56,56,56	0
30	CA	b	620	1/1	0.53	1.24	-	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.