Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:52 PM GMT

PDB ID	:	4PBU
Title	:	Serial Time-resolved crystallography of Photosystem II using a femtosecond X-ray laser The S1 state
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.A.; 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	:	2014-04-13
Resolution	:	5.00 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:

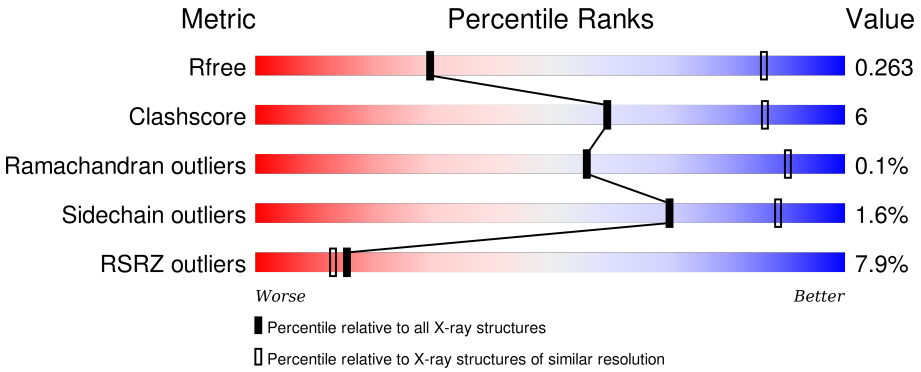
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135

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 5.00 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	1119 (6.22-3.60)
Clashscore	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)
RSRZ outliers	91569	1122 (6.22-3.60)

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	4% 85% 15%
1	a	334	8% 99%

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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)	:	trunk26865

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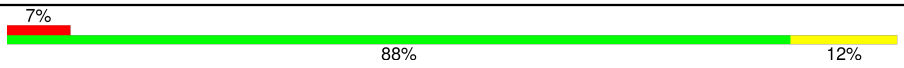
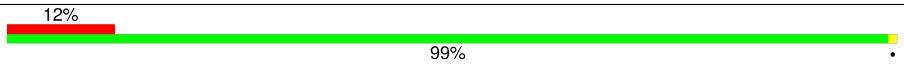
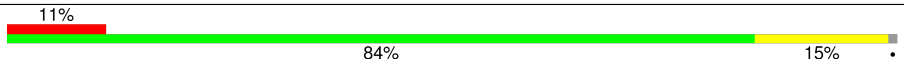
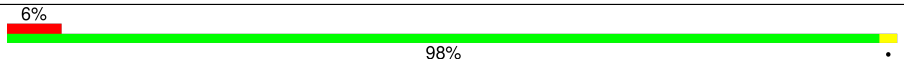
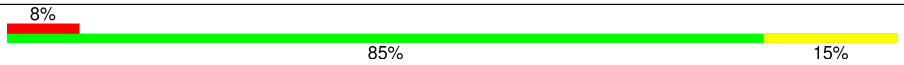
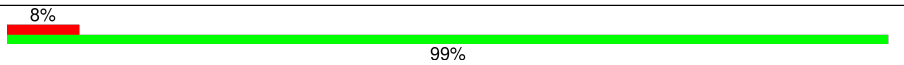
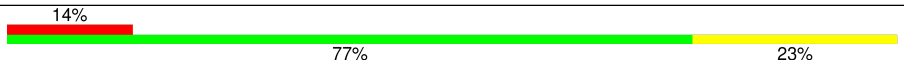
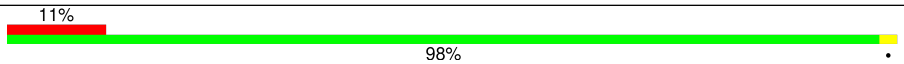
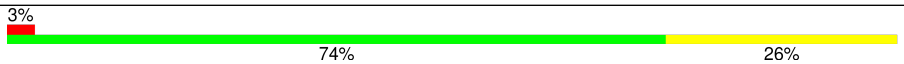
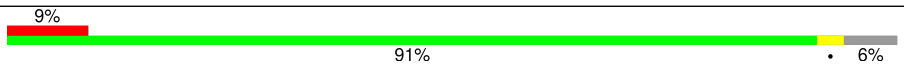
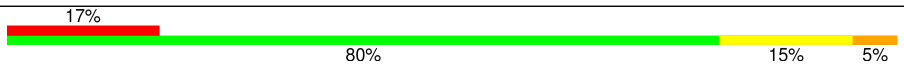
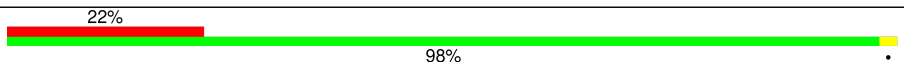
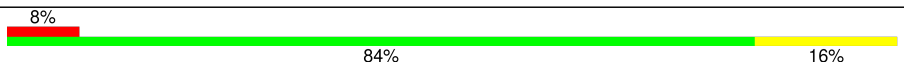
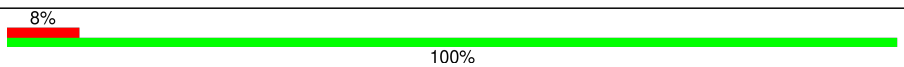
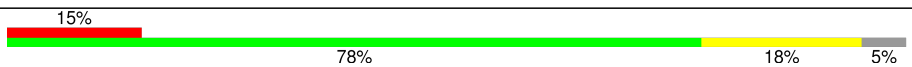
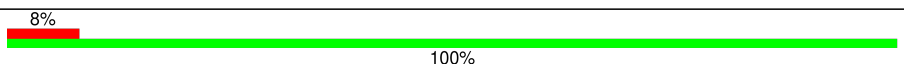
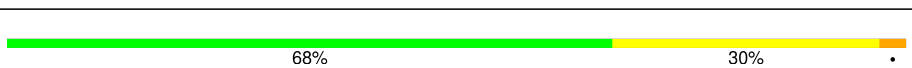
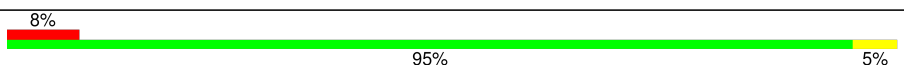
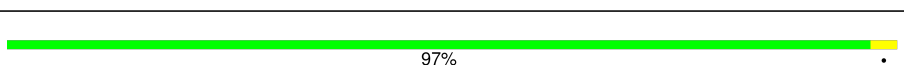
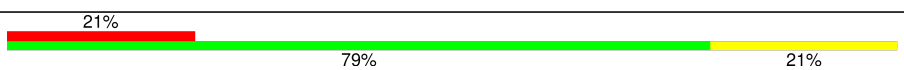
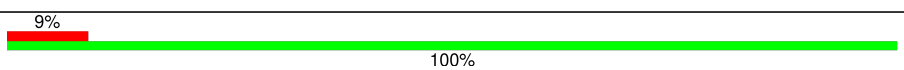
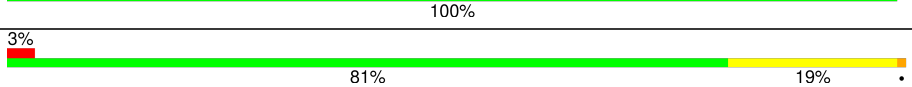
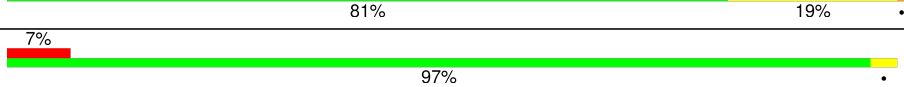
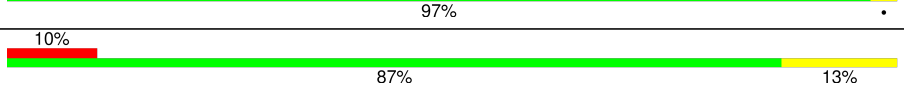
Mol	Chain	Length	Quality of chain
2	B	504	
2	b	504	
3	C	455	
3	c	455	
4	D	342	
4	d	342	
5	E	81	
5	e	81	
6	F	34	
6	f	34	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	34	
12	m	34	
13	O	243	
13	o	243	
14	T	30	

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Mol	Chain	Length	Quality of chain
14	t	30	10% 93% 7%
15	U	97	2% 81% 19%
15	u	97	3% 99%
16	V	137	% 85% 15%
16	v	137	7% 98%
17	Y	29	7% 59% 41%
17	y	29	97%
18	X	39	21% 85% 15%
18	x	39	15% 97%
19	Z	62	5% 87% 11%
19	z	62	8% 95% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	A	603	-	-	-	X
22	CL	a	404	-	-	-	X
23	BCT	A	605	-	-	-	X
23	BCT	a	414	-	-	-	X
24	CLA	A	606	X	-	-	X
24	CLA	A	607	X	-	-	X
24	CLA	A	609	X	-	-	X
24	CLA	A	614	X	-	-	X
24	CLA	B	602	X	-	-	X
24	CLA	B	603	X	-	-	X
24	CLA	B	604	X	-	-	X
24	CLA	B	605	X	-	-	X
24	CLA	B	606	X	-	-	X
24	CLA	B	607	X	-	-	X
24	CLA	B	608	X	-	-	X
24	CLA	B	609	X	-	-	X
24	CLA	B	610	X	-	-	X
24	CLA	B	611	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	612	X	-	-	X
24	CLA	B	613	X	-	-	X
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	X
24	CLA	B	617	X	-	-	X
24	CLA	C	501	X	-	-	X
24	CLA	C	502	X	-	-	X
24	CLA	C	503	X	-	-	X
24	CLA	C	504	X	-	-	X
24	CLA	C	505	X	-	-	X
24	CLA	C	506	X	-	-	X
24	CLA	C	507	X	-	-	X
24	CLA	C	508	X	-	-	X
24	CLA	C	509	X	-	-	X
24	CLA	C	510	X	-	-	X
24	CLA	C	511	X	-	-	X
24	CLA	C	512	X	-	-	X
24	CLA	C	513	X	-	-	X
24	CLA	D	402	X	-	-	X
24	CLA	D	403	X	-	-	X
24	CLA	a	406	X	-	-	X
24	CLA	a	407	X	-	-	X
24	CLA	a	408	X	-	-	X
24	CLA	b	602	X	-	-	X
24	CLA	b	603	X	-	-	X
24	CLA	b	604	X	-	-	X
24	CLA	b	605	X	-	-	X
24	CLA	b	606	X	-	-	X
24	CLA	b	607	X	-	-	X
24	CLA	b	608	X	-	-	X
24	CLA	b	609	X	-	-	X
24	CLA	b	610	-	-	-	X
24	CLA	b	611	X	-	-	X
24	CLA	b	612	X	-	-	X
24	CLA	b	613	X	-	-	X
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	X
24	CLA	b	617	X	-	-	X
24	CLA	c	902	X	-	-	X
24	CLA	c	903	X	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	904	X	-	-	X
24	CLA	c	905	X	-	-	X
24	CLA	c	906	X	-	-	X
24	CLA	c	907	X	-	-	X
24	CLA	c	908	X	-	-	X
24	CLA	c	909	X	-	-	X
24	CLA	c	910	X	-	-	X
24	CLA	c	911	X	-	-	X
24	CLA	c	912	X	-	-	X
24	CLA	c	913	X	-	-	X
24	CLA	c	914	X	-	-	X
24	CLA	d	401	X	-	-	X
24	CLA	d	403	X	-	-	X
24	CLA	d	404	X	-	-	X
25	PHO	A	608	-	-	-	X
25	PHO	D	401	-	-	-	X
25	PHO	a	412	-	-	-	X
25	PHO	d	402	-	-	-	X
26	BCR	A	610	-	-	-	X
26	BCR	B	620	-	-	-	X
26	BCR	C	514	-	-	-	X
26	BCR	C	515	-	-	-	X
26	BCR	D	404	-	-	-	X
26	BCR	H	101	-	-	-	X
26	BCR	K	101	-	-	-	X
26	BCR	T	101	-	-	-	X
26	BCR	T	102	-	-	-	X
26	BCR	Y	101	-	-	-	X
26	BCR	a	409	-	-	-	X
26	BCR	b	618	-	-	-	X
26	BCR	b	619	-	-	-	X
26	BCR	c	915	-	-	-	X
26	BCR	c	918	-	-	-	X
26	BCR	f	101	-	-	-	X
26	BCR	h	101	-	-	-	X
26	BCR	k	101	-	-	-	X
26	BCR	k	102	-	-	-	X
27	PL9	A	611	-	-	-	X
27	PL9	D	405	-	-	-	X
27	PL9	a	410	-	-	-	X
27	PL9	d	405	-	-	-	X
28	SQD	A	612	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	SQD	A	613	-	-	-	X
28	SQD	F	101	-	-	-	X
28	SQD	a	411	-	-	-	X
28	SQD	d	407	-	-	-	X
28	SQD	l	101	-	-	-	X
29	LHG	A	615	-	-	-	X
29	LHG	D	408	-	-	-	X
29	LHG	D	409	-	-	X	X
29	LHG	a	413	-	-	-	X
29	LHG	d	410	-	-	-	X
30	CA	c	901	-	-	-	X
31	DGD	C	516	-	-	-	X
31	DGD	C	517	-	-	-	X
31	DGD	C	518	-	-	-	X
31	DGD	D	406	-	-	-	X
31	DGD	H	102	-	-	-	X
31	DGD	c	916	-	-	-	X
31	DGD	c	917	-	-	-	X
31	DGD	d	406	-	-	-	X
31	DGD	h	102	-	-	-	X
31	DGD	j	101	-	-	-	X
32	HEM	E	101	-	-	-	X
32	HEM	V	202	-	-	-	X
32	HEM	e	101	-	-	-	X
32	HEM	v	202	-	-	-	X

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48924 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem Q(B) protein 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 core light harvesting protein.

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	d	341	Total	C	N	O	S	0	0	0
			2717	1800	444	461	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	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	40	Total	C	N	O	S	0	0	0
			288	192	44	49	3			

- 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	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

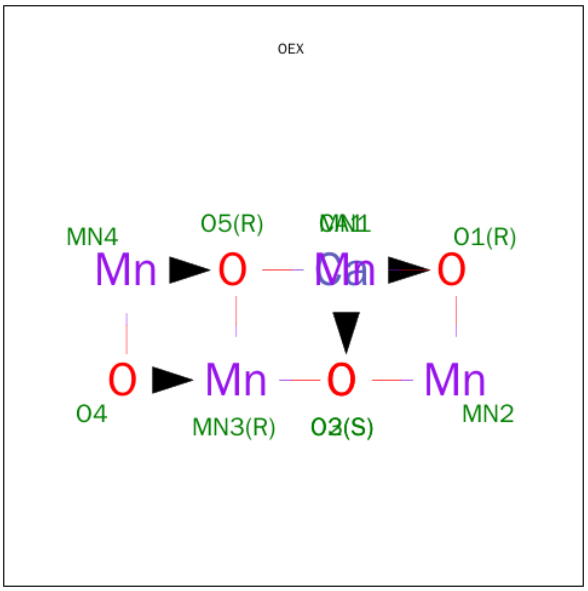
- Molecule 18 is a protein called Photosystem II reaction center X protein.

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

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

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

- 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 10 1 4 5	0	0
20	a	1	Total Ca Mn O 10 1 4 5	0	0

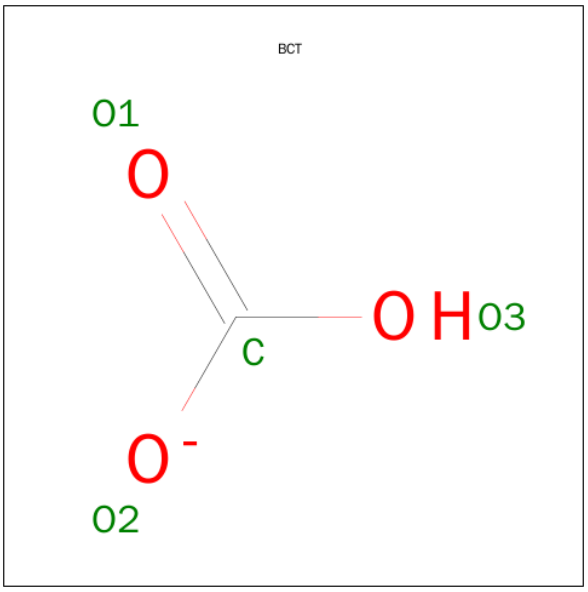
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

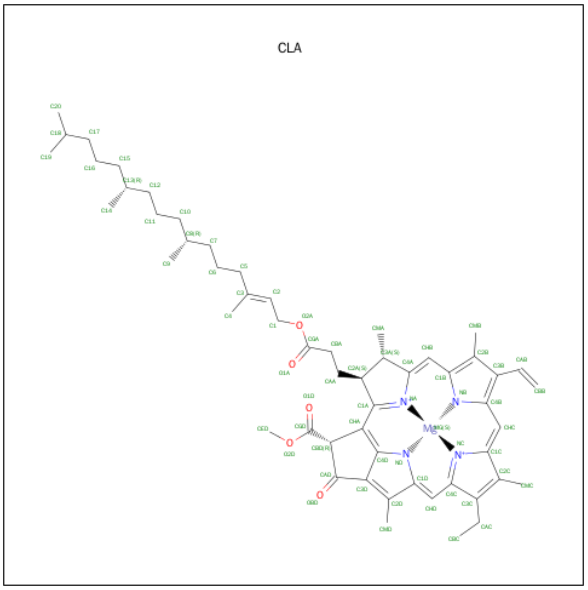
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 2 2	0	0
22	A	2	Total Cl 2 2	0	0
22	v	1	Total Cl 1 1	0	0
22	V	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

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



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

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

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

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

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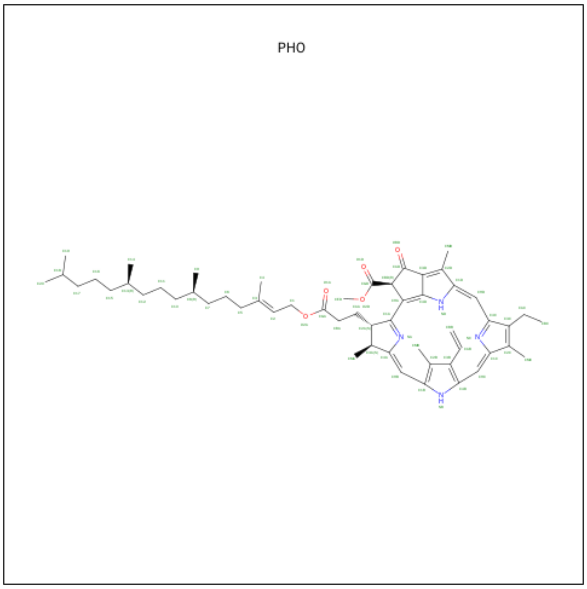
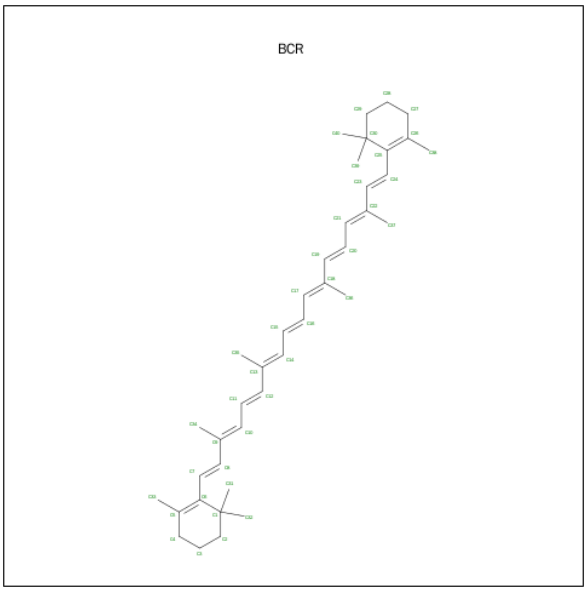
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



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

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



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

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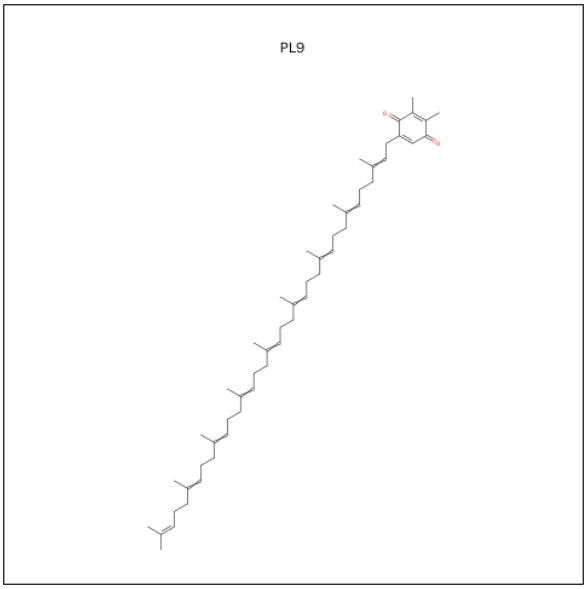
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	b	1	Total C 40 40	0	0
26	b	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	c	1	Total C 40 40	0	0
26	f	1	Total C 40 40	0	0
26	h	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0
26	k	1	Total C 40 40	0	0

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



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

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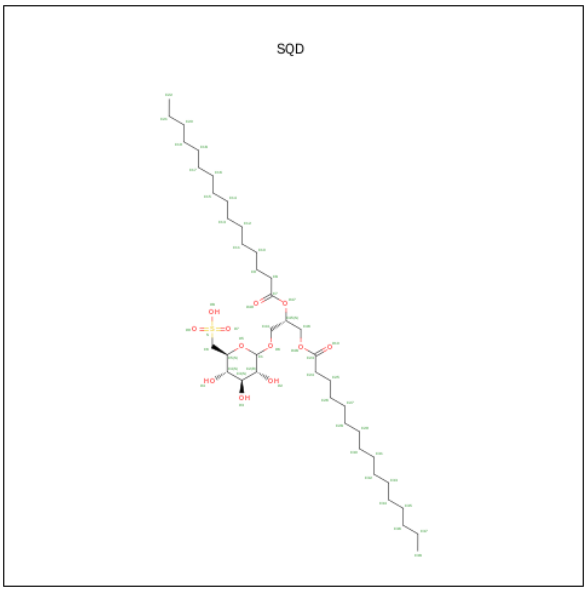
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

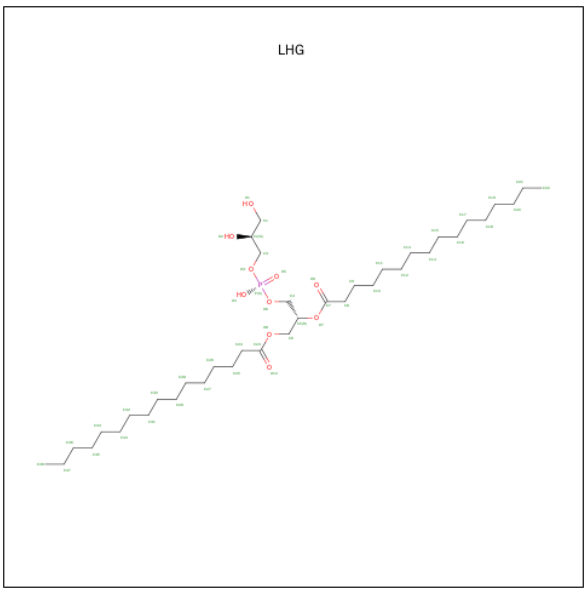
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O S 54 41 12 1	0	0
28	A	1	Total C O S 54 41 12 1	0	0
28	F	1	Total C O S 43 30 12 1	0	0
28	L	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	a	1	Total C O S 54 41 12 1	0	0
28	d	1	Total C O S 43 30 12 1	0	0
28	l	1	Total C O S 54 41 12 1	0	0

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			42	31	10	1		
29	B	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	D	1	Total	C	O	P	0	0
			49	38	10	1		
29	a	1	Total	C	O	P	0	0
			42	31	10	1		
29	b	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		
29	d	1	Total	C	O	P	0	0
			49	38	10	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	B	1	Total	Ca	0	0
			1	1		

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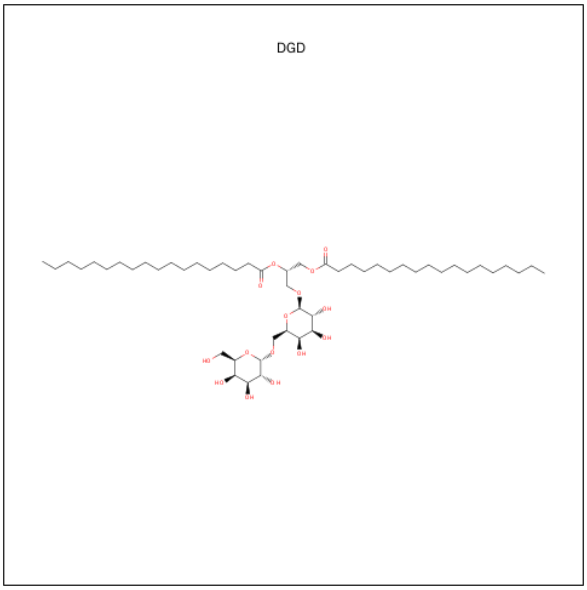
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	c	1	Total Ca 1 1	0	0
30	F	1	Total Ca 1 1	0	0
30	o	1	Total Ca 1 1	0	0
30	O	1	Total Ca 1 1	0	0
30	b	1	Total Ca 1 1	0	0
30	f	1	Total Ca 1 1	0	0

- 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	D	1	Total C O 62 47 15	0	0
31	H	1	Total C O 62 47 15	0	0

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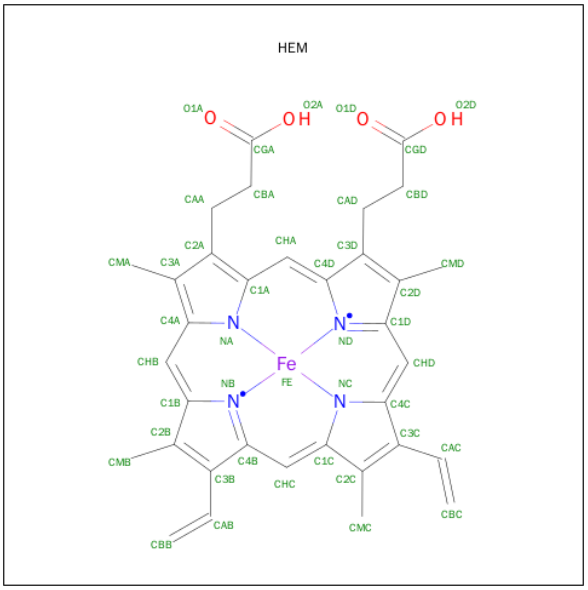
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	c	1	Total C O 62 47 15	0	0
31	c	1	Total C O 62 47 15	0	0
31	d	1	Total C O 62 47 15	0	0
31	h	1	Total C O 62 47 15	0	0
31	j	1	Total C O 62 47 15	0	0

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



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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

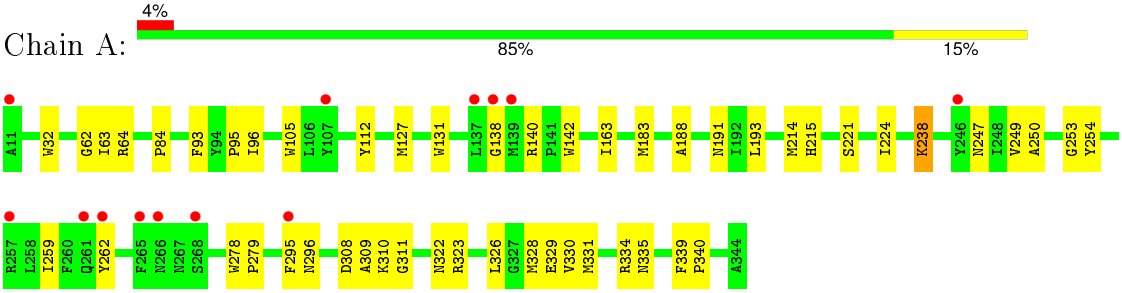
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	j	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

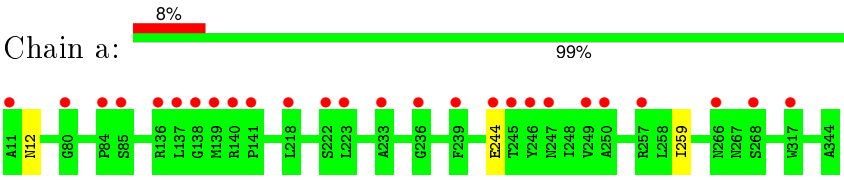
• Molecule 1: Photosystem Q(B) protein 1

Chain A:



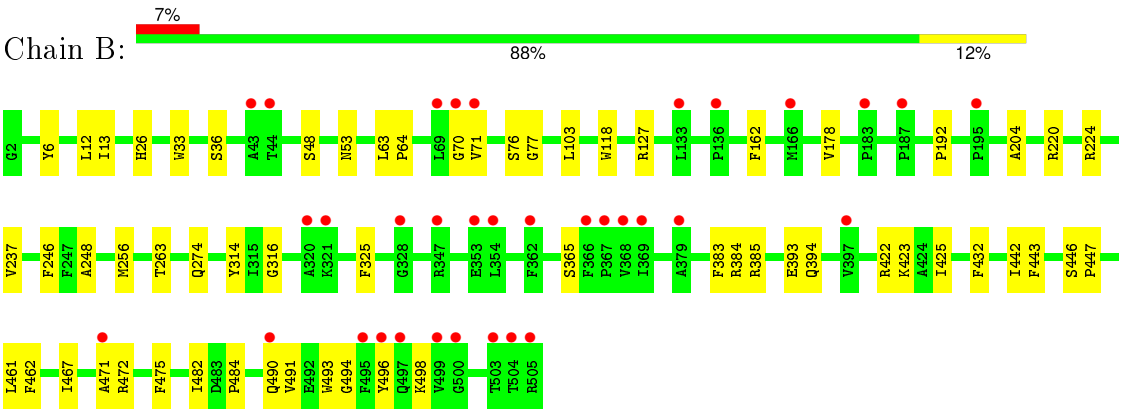
• Molecule 1: Photosystem Q(B) protein 1

Chain a:



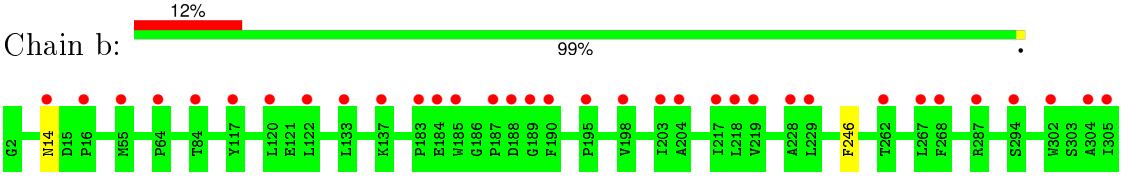
• Molecule 2: Photosystem II core light harvesting protein

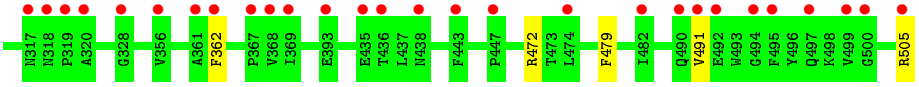
Chain B:



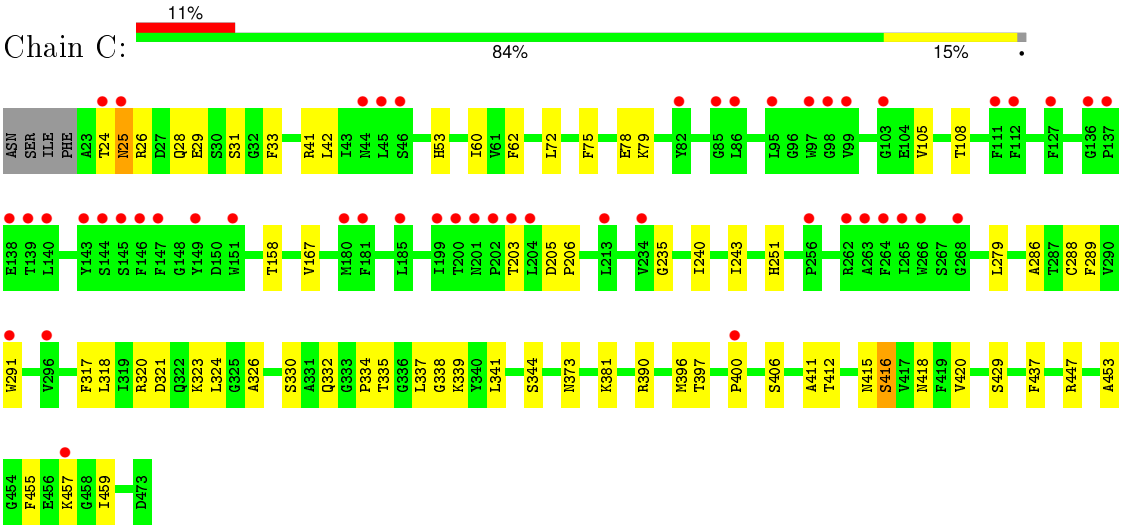
• Molecule 2: Photosystem II core light harvesting protein

Chain b:

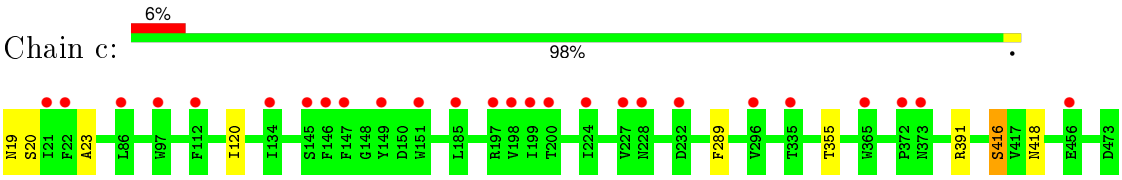




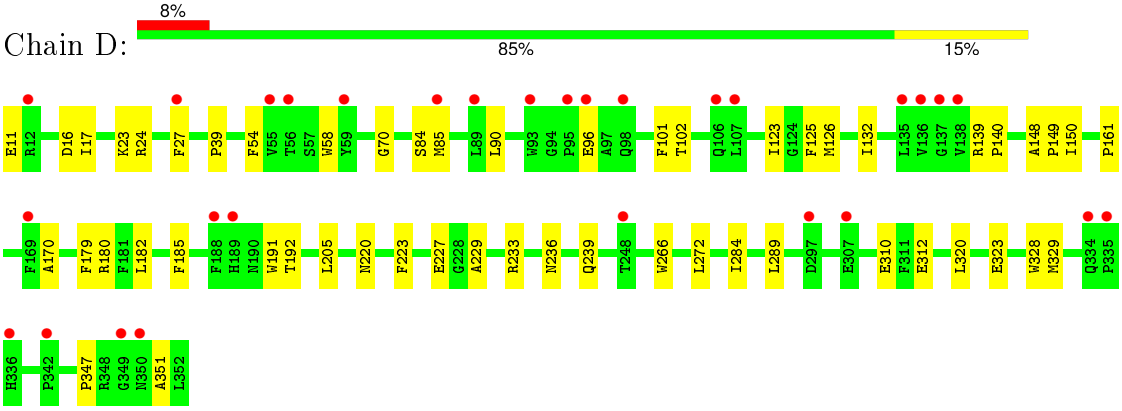
• Molecule 3: Photosystem II CP43 protein



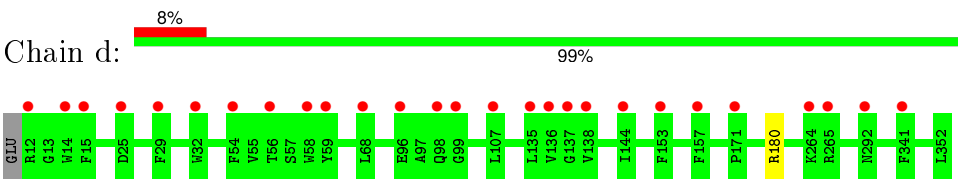
• Molecule 3: Photosystem II CP43 protein



• Molecule 4: Photosystem II D2 protein

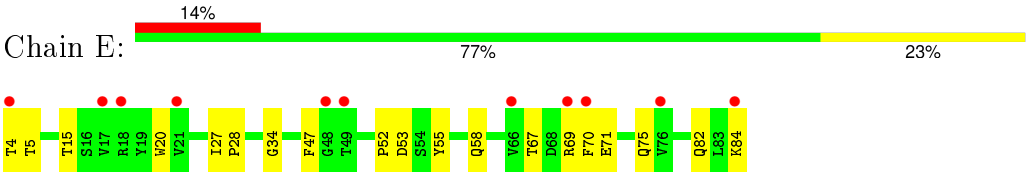


• Molecule 4: Photosystem II D2 protein



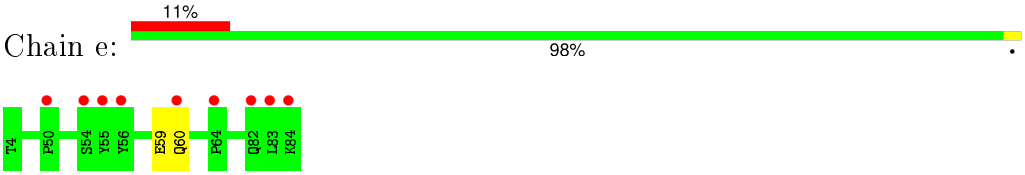
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



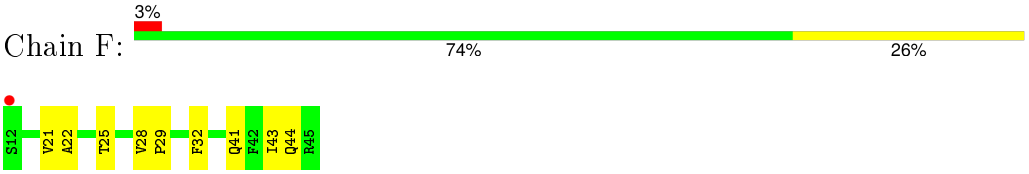
• Molecule 5: Cytochrome b559 subunit alpha

Chain e:



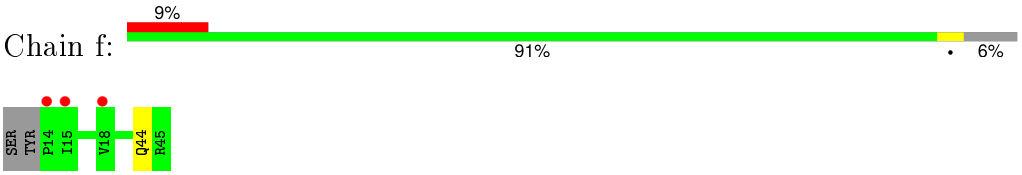
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



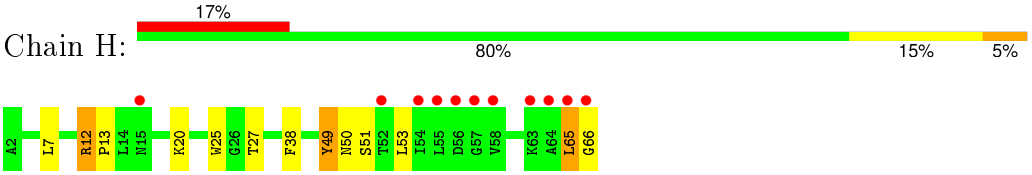
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



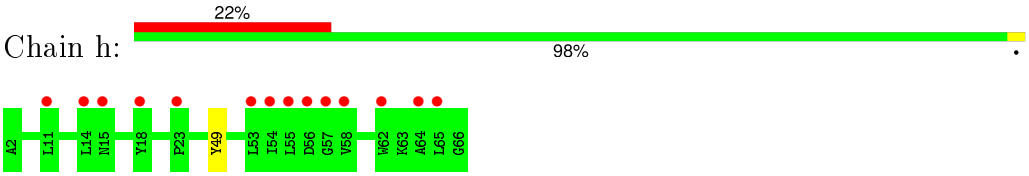
• Molecule 7: Photosystem II reaction center protein H

Chain H:



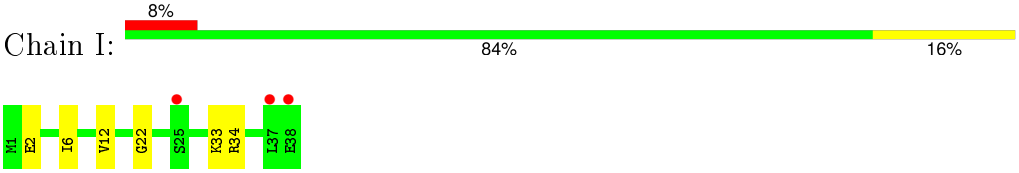
• Molecule 7: Photosystem II reaction center protein H

Chain h:



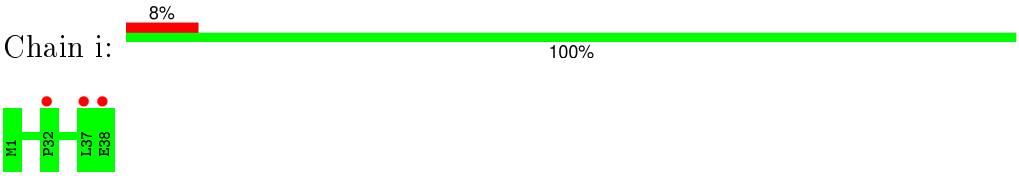
• Molecule 8: Photosystem II reaction center protein I

Chain I:



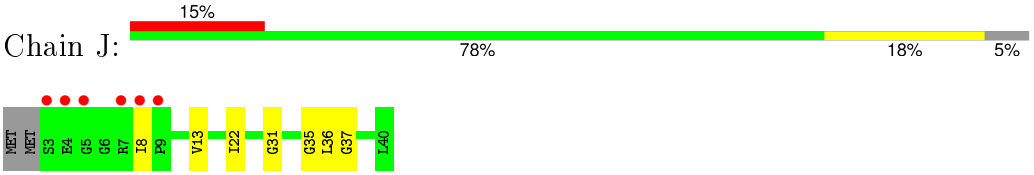
• Molecule 8: Photosystem II reaction center protein I

Chain i:



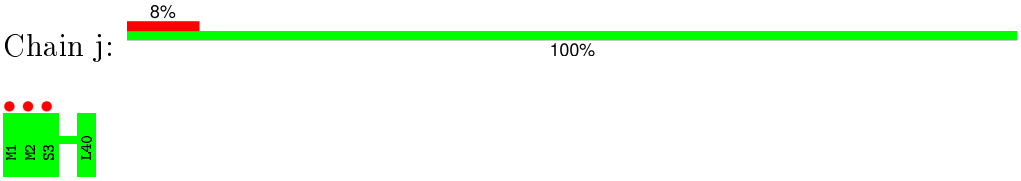
• Molecule 9: Photosystem II reaction center protein J

Chain J:



• Molecule 9: Photosystem II reaction center protein J

Chain j:

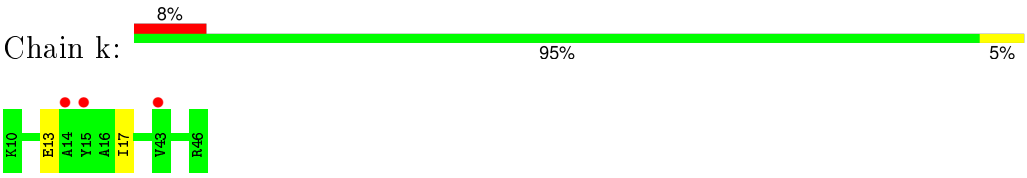


• Molecule 10: Photosystem II reaction center protein K

Chain K:

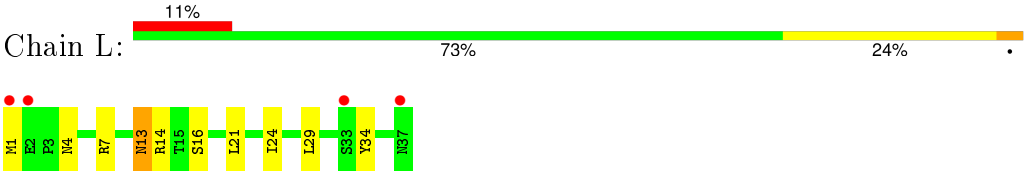
• Molecule 10: Photosystem II reaction center protein K

Chain k:



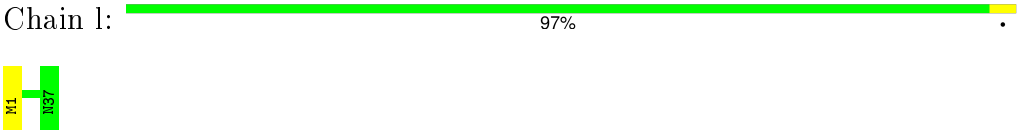
• Molecule 11: Photosystem II reaction center protein L

Chain L:



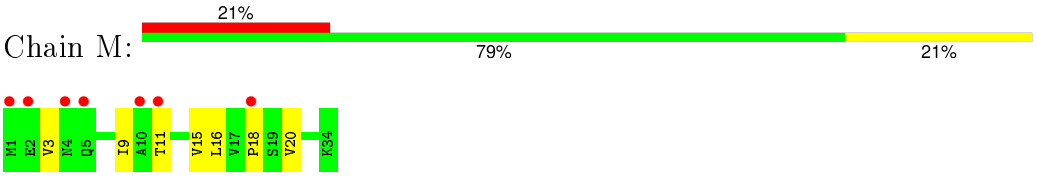
• Molecule 11: Photosystem II reaction center protein L

Chain l:



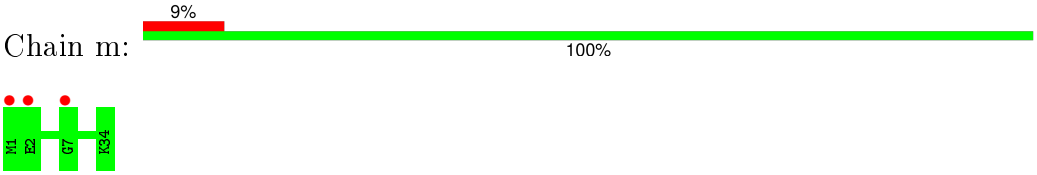
• Molecule 12: Photosystem II reaction center protein M

Chain M:



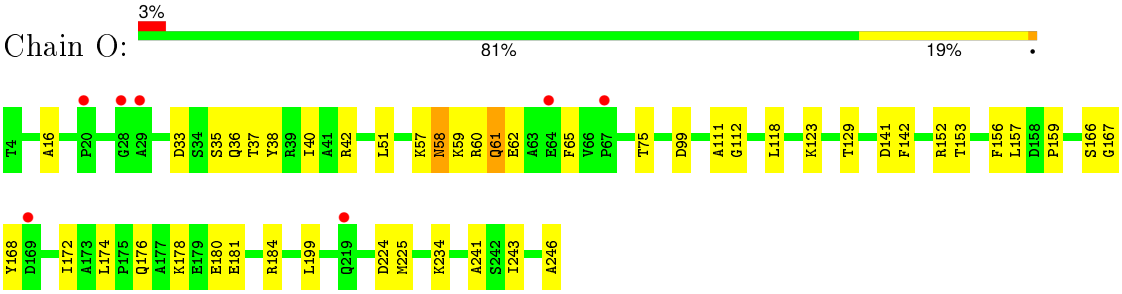
• Molecule 12: Photosystem II reaction center protein M

Chain m:



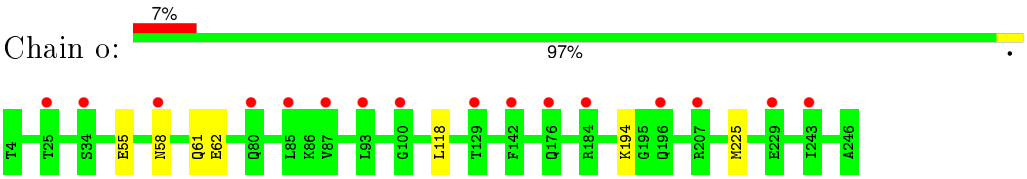
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



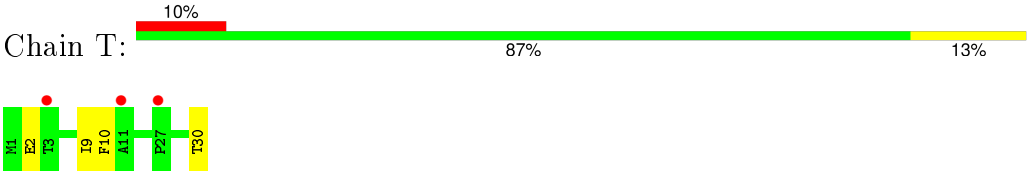
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



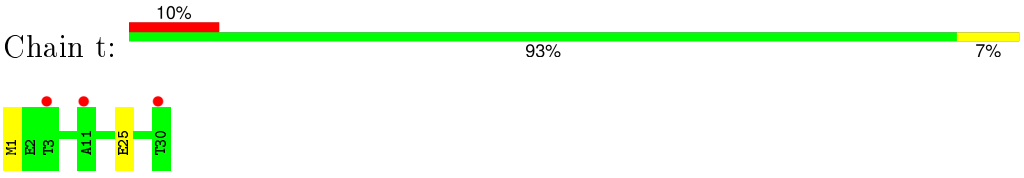
• Molecule 14: Photosystem II reaction center protein T

Chain T:



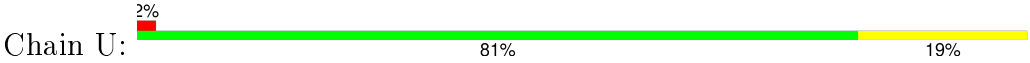
• Molecule 14: Photosystem II reaction center protein T

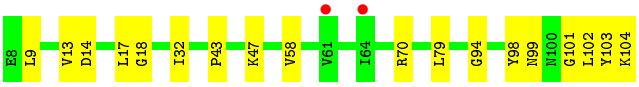
Chain t:



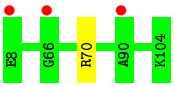
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

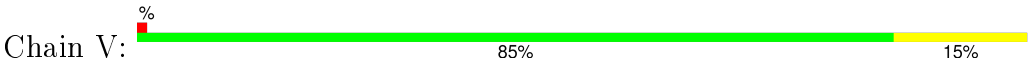


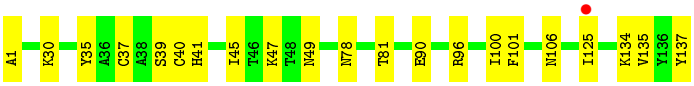


• Molecule 15: Photosystem II 12 kDa extrinsic protein

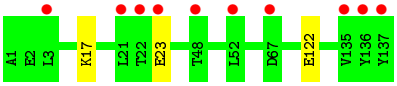


• Molecule 16: Cytochrome c-550

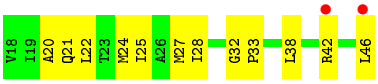




• Molecule 16: Cytochrome c-550

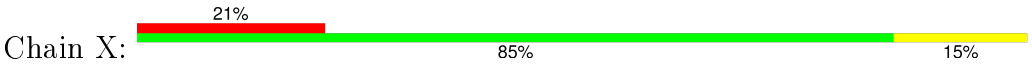


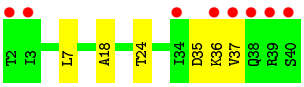
• Molecule 17: Photosystem II reaction center protein Ycf12



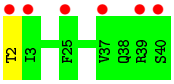
• Molecule 17: Photosystem II reaction center protein Ycf12

• Molecule 18: Photosystem II reaction center X protein



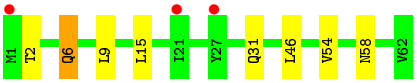


• Molecule 18: Photosystem II reaction center X protein



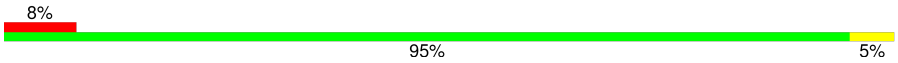
• Molecule 19: Photosystem II reaction center protein Z

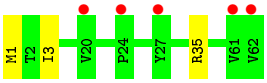
Chain Z:



• 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	133.25Å 226.26Å 307.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.64 – 5.00 100.64 – 5.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.64-5.00) 100.0 (100.64-5.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.261 , 0.262 0.259 , 0.263	Depositor DCC
R_{free} test set	2055 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	285.1	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 40956 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	48924	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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, BCR, SQD

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	0.52	0/2705	0.55	0/3689
1	a	0.51	0/2705	0.54	0/3689
2	B	0.50	0/4109	0.54	0/5600
2	b	0.49	0/4109	0.53	0/5600
3	C	0.47	0/3599	0.51	0/4900
3	c	0.44	0/3633	0.50	0/4946
4	D	0.53	0/2821	0.55	0/3844
4	d	0.49	0/2812	0.53	0/3832
5	E	0.43	0/681	0.51	0/928
5	e	0.42	0/681	0.50	0/928
6	F	0.49	0/284	0.45	0/387
6	f	0.47	0/265	0.44	0/360
7	H	0.47	0/524	0.50	0/713
7	h	0.44	0/524	0.49	0/713
8	I	0.47	0/319	0.51	0/429
8	i	0.46	0/319	0.47	0/429
9	J	0.46	0/278	0.43	0/376
9	j	0.39	0/294	0.45	0/396
10	K	0.43	0/303	0.50	0/416
10	k	0.43	0/303	0.51	0/416
11	L	0.55	0/311	0.51	0/422
11	l	0.54	0/311	0.52	0/422
12	M	0.47	0/270	0.58	0/367
12	m	0.49	0/270	0.52	0/367
13	O	0.45	0/1896	0.58	0/2571
13	o	0.43	0/1896	0.56	0/2571
14	T	0.54	0/265	0.52	0/359
14	t	0.55	0/265	0.52	0/359
15	U	0.46	0/785	0.55	0/1064
15	u	0.45	0/785	0.55	0/1064
16	V	0.47	0/1085	0.53	0/1473
16	v	0.42	0/1085	0.52	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
17	Y	0.41	0/216	0.45	0/289
17	y	0.35	0/216	0.52	0/289
18	X	0.43	0/290	0.46	0/392
18	x	0.42	0/290	0.48	0/392
19	Z	0.41	0/490	0.45	0/669
19	z	0.40	0/490	0.47	0/669
All	All	0.48	0/42484	0.53	0/57803

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (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	64	0
1	a	2620	0	2517	0	0
2	B	3969	0	3828	85	0
2	b	3969	0	3828	0	0
3	C	3486	0	3407	73	0
3	c	3519	0	3437	0	23
4	D	2726	0	2627	69	0
4	d	2717	0	2621	0	0
5	E	662	0	648	18	0
5	e	662	0	648	0	0
6	F	275	0	282	6	0
6	f	257	0	269	0	0
7	H	511	0	532	14	0
7	h	511	0	532	0	0
8	I	312	0	329	6	0
8	i	312	0	329	0	0
9	J	272	0	279	7	0
9	j	288	0	300	0	0
10	K	293	0	305	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	k	293	0	305	0	0
11	L	304	0	316	11	0
11	l	304	0	316	0	0
12	M	267	0	289	9	0
12	m	267	0	289	0	0
13	O	1865	0	1838	48	23
13	o	1865	0	1838	0	0
14	T	256	0	262	5	0
14	t	256	0	262	0	0
15	U	774	0	773	32	0
15	u	774	0	773	0	0
16	V	1064	0	1073	34	0
16	v	1064	0	1075	0	0
17	Y	215	0	246	11	0
17	y	215	0	246	0	0
18	X	287	0	317	7	0
18	x	287	0	317	0	0
19	Z	479	0	516	4	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	2	0	0	0	0
22	V	1	0	0	0	0
22	a	2	0	0	0	0
22	v	1	0	0	0	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	48	0
24	C	845	0	936	43	0
24	D	130	0	144	6	0
24	a	195	0	216	0	0
24	b	1040	0	1152	0	0
24	c	845	0	936	0	0
24	d	195	0	216	0	0
25	A	64	0	74	4	0
25	D	64	0	74	4	0
25	a	64	0	74	0	0
25	d	64	0	74	0	0
26	A	40	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	B	160	0	188	9	0
26	C	80	0	93	0	0
26	D	40	0	48	2	0
26	H	40	0	46	2	0
26	K	40	0	46	5	0
26	T	80	0	94	2	0
26	Y	40	0	47	1	0
26	a	40	0	48	0	0
26	b	80	0	92	0	0
26	c	80	0	95	0	0
26	f	40	0	46	0	0
26	h	40	0	46	0	0
26	k	80	0	90	0	0
27	A	55	0	80	9	0
27	D	55	0	80	2	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	108	0	156	6	0
28	F	43	0	53	0	0
28	L	54	0	78	10	0
28	a	108	0	156	0	0
28	d	43	0	53	0	0
28	l	54	0	78	0	0
29	A	42	0	57	3	0
29	B	49	0	74	3	0
29	D	147	0	222	28	0
29	a	42	0	57	0	0
29	b	49	0	74	0	0
29	d	147	0	222	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	c	1	0	0	0	0
30	f	1	0	0	0	0
30	o	1	0	0	0	0
31	C	186	0	246	6	0
31	D	62	0	82	4	0
31	H	62	0	82	3	0
31	c	124	0	164	0	0
31	d	62	0	82	0	0
31	h	62	0	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	j	62	0	82	0	0
32	E	43	0	30	0	0
32	V	43	0	30	9	0
32	e	43	0	30	0	0
32	v	43	0	30	0	0
33	j	1	0	0	0	0
All	All	48924	0	49705	447	23

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

All (447) 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	32:V:202:HEM:HAB	1.52	1.49
16:V:40:CYS:SG	32:V:202:HEM:HAC	1.56	1.46
16:V:37:CYS:SG	32:V:202:HEM:CAB	2.03	1.46
16:V:40:CYS:SG	32:V:202:HEM:CAC	2.03	1.44
1:A:214:MET:HG2	27:A:611:PL9:H102	1.20	1.18
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.02	1.14
1:A:253:GLY:HA3	2:B:491:VAL:HG12	3.10	1.11
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.09	0.98
10:K:17:ILE:H	10:K:17:ILE:HD13	1.29	0.97
29:D:409:LHG:H372	29:D:409:LHG:H132	1.48	0.92
24:C:510:CLA:H43	29:D:409:LHG:H383	1.53	0.91
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.35	0.90
24:C:510:CLA:C4	29:D:409:LHG:H383	2.03	0.88
1:A:214:MET:HG2	27:A:611:PL9:C10	2.02	0.88
3:C:457:LYS:NZ	4:D:227:GLU:O	2.26	0.88
2:B:393:GLU:HB3	15:U:18:GLY:CA	2.22	0.84
2:B:162:PHE:O	24:B:607:CLA:HHD	2.39	0.84
4:D:233:ARG:HH11	4:D:233:ARG:HG2	4.50	0.84
29:D:409:LHG:H352	29:D:409:LHG:H151	1.59	0.82
6:F:41:GLN:OE1	9:J:31:GLY:HA3	1.96	0.82
2:B:383:PHE:CE2	13:O:167:GLY:HA2	2.38	0.82
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.61	0.82
1:A:250:ALA:CA	2:B:491:VAL:HG11	2.96	0.81
5:E:67:THR:H	5:E:75:GLN:HE22	2.53	0.81
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.63	0.80
2:B:442:ILE:HD11	13:O:174:LEU:HD23	1.98	0.77
2:B:442:ILE:HD11	13:O:174:LEU:CD2	2.43	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.68	0.76
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.73	0.75
13:O:156:PHE:HB3	13:O:225:MET:CE	4.48	0.74
1:A:340:PRO:HD3	15:U:103:TYR:CZ	2.23	0.74
24:C:508:CLA:H92	29:D:409:LHG:H371	1.69	0.73
13:O:57:LYS:O	13:O:58:ASN:HB2	1.87	0.73
3:C:381:LYS:NZ	13:O:99:ASP:OD2	2.20	0.73
31:C:518:DGD:HBH2	29:D:409:LHG:H223	1.70	0.72
29:D:409:LHG:H112	29:D:409:LHG:H382	1.71	0.72
24:A:614:CLA:HBB1	24:A:614:CLA:HMB1	1.71	0.72
1:A:340:PRO:HB3	15:U:103:TYR:CG	2.26	0.71
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.87	0.70
4:D:351:ALA:HA	15:U:101:GLY:O	1.92	0.70
3:C:344:SER:O	13:O:75:THR:HG22	1.92	0.70
24:A:606:CLA:HMB1	24:A:606:CLA:HBB1	1.73	0.69
1:A:334:ARG:HG3	13:O:157:LEU:HB2	1.73	0.69
4:D:24:ARG:HH12	18:X:35:ASP:CG	2.99	0.69
13:O:156:PHE:HB3	13:O:225:MET:HE1	4.28	0.69
3:C:447:ARG:NH2	4:D:229:ALA:HB1	2.27	0.68
3:C:321:ASP:OD2	15:U:99:ASN:HB2	1.92	0.68
24:B:612:CLA:H142	29:B:621:LHG:H361	1.76	0.68
16:V:37:CYS:SG	32:V:202:HEM:C3B	2.85	0.68
25:D:401:PHO:HBB1	25:D:401:PHO:HMB1	1.76	0.68
24:C:508:CLA:HBB1	24:C:508:CLA:HMB1	1.75	0.68
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.24	0.67
1:A:250:ALA:HA	2:B:491:VAL:CG1	2.94	0.67
1:A:253:GLY:HA3	2:B:491:VAL:CG1	3.30	0.67
1:A:214:MET:CG	27:A:611:PL9:H102	2.12	0.67
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.75	0.67
24:B:612:CLA:HMB1	24:B:612:CLA:HBB1	1.76	0.67
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.77	0.67
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.77	0.66
16:V:40:CYS:SG	32:V:202:HEM:CBC	2.81	0.65
2:B:462:PHE:CZ	24:B:614:CLA:HMB3	2.49	0.65
24:B:617:CLA:HMB1	24:B:617:CLA:HBB1	1.79	0.65
1:A:247:ASN:HB3	2:B:482:ILE:HD11	1.94	0.65
2:B:462:PHE:CE2	24:B:614:CLA:HMB3	2.38	0.65
16:V:40:CYS:SG	32:V:202:HEM:C3C	2.90	0.64
2:B:385:ARG:NE	15:U:14:ASP:OD1	2.26	0.64
1:A:296:ASN:HB2	3:C:400:PRO:O	2.04	0.63
3:C:72:LEU:HD11	3:C:108:THR:HB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ASP:HB2	5:E:52:PRO:O	1.98	0.63
28:L:101:SQD:H462	28:L:101:SQD:H1	1.79	0.63
27:A:611:PL9:H403	6:F:22:ALA:HB2	1.80	0.63
1:A:183:MET:HA	24:A:606:CLA:HMD2	1.81	0.63
2:B:383:PHE:O	13:O:166:SER:HA	2.12	0.62
29:D:409:LHG:H112	29:D:409:LHG:C38	2.30	0.61
24:C:510:CLA:H41	29:D:409:LHG:H383	1.81	0.61
2:B:393:GLU:HB3	15:U:18:GLY:HA3	1.83	0.61
10:K:35:LEU:HD13	17:Y:32:GLY:HA3	2.40	0.61
5:E:53:ASP:HA	16:V:1:ALA:O	2.40	0.60
10:K:17:ILE:HD13	10:K:17:ILE:N	2.08	0.60
3:C:167:VAL:HG21	24:C:512:CLA:HHB	1.84	0.60
25:A:608:PHO:HMB1	25:A:608:PHO:HBB1	1.84	0.60
5:E:53:ASP:O	16:V:1:ALA:N	2.39	0.59
11:L:13:ASN:ND2	11:L:16:SER:H	2.01	0.59
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.33	0.59
24:B:611:CLA:HBB1	24:B:611:CLA:HHC	1.85	0.59
1:A:326:LEU:HD22	16:V:134:LYS:HB2	2.08	0.59
4:D:24:ARG:NH1	18:X:35:ASP:OD2	4.44	0.59
3:C:324:LEU:HB3	15:U:32:ILE:HD13	1.85	0.59
3:C:381:LYS:CE	13:O:99:ASP:OD2	2.51	0.58
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.85	0.58
2:B:314:TYR:OH	13:O:176:GLN:NE2	2.53	0.58
28:A:612:SQD:H291	24:C:508:CLA:H71	1.84	0.58
1:A:326:LEU:CD2	16:V:134:LYS:HB2	2.59	0.58
4:D:85:MET:CE	4:D:96:GLU:HG2	2.49	0.58
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.89	0.58
5:E:69:ARG:NH2	7:H:50:ASN:O	2.33	0.58
2:B:467:ILE:HG13	4:D:126:MET:CE	2.34	0.57
24:B:609:CLA:HMB1	4:D:126:MET:HB3	1.86	0.57
29:D:409:LHG:H372	29:D:409:LHG:C13	2.29	0.57
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	1.86	0.57
2:B:237:VAL:HG12	24:B:613:CLA:HMD1	1.98	0.57
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.40	0.57
12:M:20:VAL:CG2	12:M:20:VAL:HG11	2.72	0.56
11:L:21:LEU:HD13	28:L:101:SQD:H312	3.46	0.56
24:B:616:CLA:H2	24:B:617:CLA:CBB	2.48	0.56
1:A:322:ASN:OD1	3:C:412:THR:HA	2.14	0.56
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.53	0.56
1:A:331:MET:SD	4:D:347:PRO:HB2	2.64	0.56
1:A:309:ALA:HB3	16:V:1:ALA:O	2.14	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:21:LEU:HD13	17:Y:24:MET:CE	5.44	0.56
26:B:619:BCR:H381	26:B:622:BCR:H341	1.87	0.56
1:A:63:ILE:HB	3:C:335:THR:HG21	1.87	0.56
3:C:390:ARG:HD2	16:V:101:PHE:CZ	2.41	0.56
10:K:17:ILE:H	10:K:17:ILE:CD1	2.00	0.55
4:D:236:ASN:O	4:D:239:GLN:HG2	2.34	0.55
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.04	0.55
13:O:42:ARG:O	13:O:241:ALA:HA	2.15	0.55
3:C:323:LYS:O	15:U:47:LYS:HD2	2.06	0.55
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.89	0.55
28:A:612:SQD:H383	9:J:22:ILE:HD11	1.89	0.55
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.00	0.54
3:C:33:PHE:CE1	4:D:229:ALA:HB3	2.57	0.54
3:C:41:ARG:NH1	24:C:511:CLA:HMD1	2.22	0.54
1:A:340:PRO:HD3	15:U:103:TYR:CE1	2.42	0.54
4:D:323:GLU:HB3	13:O:168:TYR:OH	2.17	0.54
3:C:459:ILE:H	4:D:223:PHE:HA	2.04	0.54
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.38	0.53
26:D:404:BCR:H313	31:D:406:DGD:HA91	1.89	0.53
2:B:394:GLN:HG3	15:U:17:LEU:O	2.08	0.53
28:A:612:SQD:H321	24:C:508:CLA:H193	1.91	0.53
4:D:312:GLU:HB2	13:O:159:PRO:CG	2.38	0.53
2:B:26:HIS:HB2	24:B:613:CLA:HMB2	1.89	0.53
5:E:15:THR:HB	9:J:8:ILE:O	2.08	0.53
24:D:403:CLA:H121	18:X:18:ALA:HB2	1.90	0.53
7:H:65:LEU:HD12	7:H:66:GLY:H	1.73	0.53
4:D:233:ARG:CG	4:D:233:ARG:HH11	4.04	0.53
2:B:393:GLU:HB3	15:U:18:GLY:HA2	2.19	0.53
10:K:21:LEU:HD13	17:Y:24:MET:HE2	5.86	0.53
2:B:475:PHE:CD1	4:D:140:PRO:HG3	2.44	0.52
1:A:310:LYS:NZ	5:E:58:GLN:O	2.78	0.52
24:C:504:CLA:H201	29:D:409:LHG:H342	1.90	0.52
24:C:513:CLA:HMB1	24:C:513:CLA:HBB1	1.91	0.52
24:C:503:CLA:HBB1	24:C:503:CLA:HMB1	1.91	0.52
13:O:40:ILE:HG12	13:O:243:ILE:HD13	1.92	0.52
19:Z:2:THR:O	19:Z:6:GLN:HB2	2.51	0.52
3:C:396:MET:HE1	16:V:47:LYS:O	2.29	0.52
2:B:48:SER:O	13:O:57:LYS:HE3	52.36	0.52
4:D:351:ALA:N	15:U:101:GLY:O	2.57	0.52
1:A:253:GLY:CA	2:B:491:VAL:HG12	4.00	0.52
2:B:446:SER:HB2	2:B:447:PRO:CD	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:ALA:HB2	15:U:98:TYR:CB	2.40	0.52
24:B:603:CLA:H161	31:H:102:DGD:HAW1	1.92	0.52
24:C:506:CLA:HBB1	24:C:506:CLA:HMB1	1.91	0.51
24:B:609:CLA:HBB2	4:D:150:ILE:HD13	1.93	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
1:A:340:PRO:HG3	3:C:317:PHE:CZ	2.50	0.51
3:C:334:PRO:HA	13:O:153:THR:OG1	2.15	0.51
2:B:248:ALA:HA	24:B:604:CLA:H42	1.92	0.51
2:B:76:SER:O	13:O:111:ALA:HA	62.53	0.51
2:B:493:TRP:HB3	5:E:5:THR:HG23	1.93	0.51
13:O:58:ASN:HA	13:O:60:ARG:HH21	1.81	0.51
24:B:603:CLA:HMD2	7:H:38:PHE:HZ	1.76	0.51
2:B:383:PHE:CD1	13:O:166:SER:OG	2.94	0.50
13:O:184:ARG:HA	15:U:9:LEU:CD1	2.41	0.50
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.93	0.50
2:B:442:ILE:CD1	13:O:174:LEU:HD23	2.68	0.50
2:B:325:PHE:CG	11:L:34:TYR:HB3	2.46	0.50
24:C:504:CLA:H191	29:D:409:LHG:H341	1.91	0.50
2:B:443:PHE:CE1	13:O:176:GLN:HG3	2.59	0.50
2:B:467:ILE:HG13	4:D:126:MET:HE2	1.92	0.50
24:A:606:CLA:CBD	24:A:614:CLA:HAC2	2.42	0.50
29:D:409:LHG:H132	29:D:409:LHG:C37	2.33	0.50
24:B:603:CLA:HMD2	7:H:38:PHE:CZ	2.47	0.50
3:C:437:PHE:CZ	24:C:510:CLA:HMB3	2.47	0.50
3:C:390:ARG:HD3	16:V:100:ILE:HD12	2.25	0.50
1:A:311:GLY:HA3	16:V:125:ILE:HG21	1.99	0.50
1:A:334:ARG:HD3	4:D:320:LEU:HD13	1.98	0.50
3:C:326:ALA:HA	15:U:98:TYR:CD2	2.46	0.50
11:L:13:ASN:C	11:L:13:ASN:HD22	2.15	0.49
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.47	0.49
16:V:37:CYS:SG	32:V:202:HEM:CBB	2.88	0.49
1:A:334:ARG:HB2	13:O:157:LEU:HD12	1.94	0.49
3:C:339:LYS:NZ	15:U:99:ASN:O	2.58	0.49
7:H:38:PHE:HB2	26:H:101:BCR:C10	2.59	0.49
3:C:390:ARG:HD3	16:V:90:GLU:O	2.13	0.49
1:A:238:LYS:HD2	14:T:30:THR:HG21	4.13	0.49
27:A:611:PL9:H503	18:X:24:THR:HG21	1.94	0.49
2:B:36:SER:OG	26:B:619:BCR:H362	2.12	0.49
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.47	0.49
2:B:383:PHE:CE2	13:O:167:GLY:CA	3.15	0.49
3:C:60:ILE:HG22	24:C:503:CLA:HHD	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:422:ARG:O	2:B:425:ILE:HG12	2.13	0.49
1:A:329:GLU:OE1	16:V:134:LYS:NZ	2.41	0.49
4:D:272:LEU:C	4:D:272:LEU:HD23	2.40	0.49
29:D:409:LHG:C11	29:D:409:LHG:H382	2.42	0.49
24:B:604:CLA:HAB	24:B:606:CLA:H171	1.95	0.48
11:L:13:ASN:HD22	11:L:16:SER:H	1.60	0.48
1:A:224:ILE:HG23	2:B:484:PRO:HA	2.23	0.48
3:C:324:LEU:HD22	15:U:32:ILE:HD13	1.96	0.48
2:B:471:ALA:HB1	4:D:140:PRO:HG2	1.94	0.48
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.13	0.48
28:A:613:SQD:H252	26:B:619:BCR:H373	53.37	0.48
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.07	0.48
1:A:330:VAL:HG21	4:D:328:TRP:CE2	2.62	0.48
17:Y:22:LEU:HA	17:Y:25:ILE:HD12	7.06	0.48
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.36	0.48
28:L:101:SQD:H462	28:L:101:SQD:C1	2.41	0.48
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.48
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.48
3:C:373:ASN:ND2	13:O:16:ALA:HA	2.59	0.48
3:C:324:LEU:HD13	15:U:32:ILE:HG21	1.96	0.48
1:A:221:SER:HA	4:D:139:ARG:HB2	2.12	0.48
1:A:334:ARG:NH2	13:O:159:PRO:HA	2.28	0.48
2:B:385:ARG:HB2	15:U:13:VAL:HG11	1.95	0.48
2:B:498:LYS:HA	4:D:24:ARG:HA	2.15	0.47
1:A:335:ASN:ND2	13:O:156:PHE:CE1	3.14	0.47
2:B:127:ARG:NH1	2:B:127:ARG:HG3	2.12	0.47
11:L:14:ARG:HD3	28:L:101:SQD:H241	2.58	0.47
24:C:501:CLA:H42	24:C:502:CLA:HMD1	1.94	0.47
24:B:610:CLA:HMD1	7:H:27:THR:HB	1.96	0.47
2:B:365:SER:HB3	13:O:172:ILE:HD12	2.12	0.47
4:D:328:TRP:CZ3	16:V:135:VAL:HA	2.61	0.47
28:L:101:SQD:C46	28:L:101:SQD:H1	2.68	0.47
5:E:34:GLY:HA3	6:F:32:PHE:O	2.15	0.47
3:C:437:PHE:CE2	24:C:510:CLA:HMB3	2.50	0.47
24:C:508:CLA:O1D	29:D:409:LHG:HC2	2.15	0.47
3:C:78:GLU:OE2	16:V:106:ASN:ND2	2.48	0.47
25:D:401:PHO:HHD	25:D:401:PHO:HBC2	1.97	0.47
2:B:237:VAL:HG11	24:B:611:CLA:H201	2.16	0.47
3:C:62:PHE:CE2	26:K:101:BCR:H331	10.95	0.47
2:B:365:SER:CB	13:O:172:ILE:HD12	2.58	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)
3:C:288:CYS:SG	31:C:516:DGD:HB32	2.55	0.47
3:C:415:ASN:O	3:C:416:SER:HB2	2.14	0.47
24:C:504:CLA:H202	29:D:409:LHG:H172	1.97	0.47
2:B:467:ILE:HG13	4:D:126:MET:HE1	1.97	0.47
4:D:123:ILE:HD11	31:H:102:DGD:HAH1	3.50	0.47
2:B:385:ARG:HE	15:U:14:ASP:CG	2.15	0.47
24:B:605:CLA:H43	24:B:606:CLA:H2	2.01	0.47
3:C:33:PHE:CE1	4:D:229:ALA:CB	3.15	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.46
10:K:31:LEU:HB3	26:K:101:BCR:C15	11.44	0.46
27:D:405:PL9:H411	11:L:29:LEU:HD23	2.03	0.46
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	2.18	0.46
4:D:84:SER:O	5:E:69:ARG:HB2	2.28	0.46
1:A:295:PHE:HD1	3:C:291:TRP:CD2	2.41	0.46
15:U:43:PRO:HD3	16:V:81:THR:HB	1.97	0.46
26:B:620:BCR:H24C	26:B:620:BCR:H371	1.78	0.46
3:C:25:ASN:HD21	3:C:31:SER:HA	1.79	0.46
4:D:192:THR:HG23	24:D:403:CLA:HBC2	40.85	0.46
24:B:616:CLA:H161	7:H:7:LEU:HD21	3.35	0.46
17:Y:20:ALA:O	17:Y:24:MET:HG2	2.36	0.46
3:C:429:SER:HB3	31:C:517:DGD:HBT2	1.98	0.46
3:C:453:ALA:O	8:I:33:LYS:HB3	2.16	0.46
24:A:606:CLA:CAD	24:A:614:CLA:HAC2	2.45	0.46
24:B:603:CLA:HBB1	24:B:603:CLA:HMB1	2.28	0.46
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.98	0.46
1:A:127:MET:CE	24:C:505:CLA:HBB1	2.45	0.46
3:C:332:GLN:O	15:U:94:GLY:HA2	2.16	0.46
4:D:85:MET:HE1	4:D:96:GLU:HG2	2.11	0.46
3:C:79:LYS:HD2	16:V:35:TYR:CE1	2.97	0.46
13:O:129:THR:HA	13:O:141:ASP:O	2.33	0.46
3:C:397:THR:HG21	16:V:40:CYS:SG	2.79	0.46
24:A:607:CLA:HMD3	4:D:182:LEU:HD11	1.98	0.46
26:B:618:BCR:H371	26:B:618:BCR:H24C	1.83	0.46
29:A:615:LHG:HC12	4:D:27:PHE:CD2	2.51	0.46
2:B:77:GLY:C	13:O:111:ALA:HB1	63.97	0.46
15:U:43:PRO:CD	16:V:81:THR:HB	2.46	0.46
2:B:384:ARG:NH1	15:U:102:LEU:HG	2.51	0.46
25:A:608:PHO:HAB	4:D:205:LEU:HD13	1.98	0.46
24:B:609:CLA:HBB1	24:B:609:CLA:HMB1	1.97	0.46
2:B:224:ARG:NH1	4:D:16:ASP:OD1	2.42	0.46
12:M:11:THR:CG2	14:T:9:ILE:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:ILE:O	9:J:35:GLY:HA3	2.34	0.45
3:C:381:LYS:HE3	13:O:99:ASP:OD2	2.14	0.45
1:A:64:ARG:O	13:O:152:ARG:NH1	2.45	0.45
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.03	0.45
2:B:498:LYS:HE3	4:D:23:LYS:HB2	2.00	0.45
24:A:609:CLA:H122	24:A:609:CLA:H162	1.76	0.45
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.04	0.45
13:O:156:PHE:HB3	13:O:225:MET:HE2	5.20	0.45
4:D:54:PHE:HB3	5:E:47:PHE:CD2	2.57	0.45
4:D:58:TRP:CD2	5:E:55:TYR:HD1	2.35	0.45
1:A:191:ASN:HB2	3:C:411:ALA:HB1	2.04	0.45
29:B:621:LHG:HC81	29:D:407:LHG:O9	2.16	0.45
11:L:24:ILE:HG13	12:M:18:PRO:HB2	1.98	0.45
12:M:3:VAL:HG11	14:T:2:GLU:CG	2.41	0.45
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.49	0.45
27:A:611:PL9:H502	4:D:39:PRO:HG3	1.99	0.45
3:C:28:GLN:NE2	4:D:233:ARG:NE	2.95	0.45
24:C:504:CLA:H191	29:D:409:LHG:C34	2.47	0.45
4:D:266:TRP:CD1	29:D:409:LHG:HC31	29.62	0.45
24:B:611:CLA:OBD	24:B:611:CLA:H152	2.17	0.45
5:E:70:PHE:HZ	7:H:51:SER:HB3	1.81	0.45
2:B:432:PHE:O	13:O:178:LYS:NZ	2.60	0.45
24:C:508:CLA:CBC	29:D:409:LHG:H341	2.47	0.45
12:M:20:VAL:HG11	12:M:20:VAL:HG22	3.05	0.45
2:B:6:TYR:OH	29:D:408:LHG:HC2	9.97	0.45
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.05	0.45
12:M:20:VAL:HG11	12:M:20:VAL:HG21	2.53	0.45
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.70	0.45
1:A:323:ARG:HD3	16:V:137:TYR:OXT	2.43	0.45
8:I:33:LYS:HB3	8:I:34:ARG:H	1.50	0.45
4:D:70:GLY:O	9:J:37:GLY:HA3	2.16	0.45
24:B:612:CLA:HMD1	29:D:407:LHG:O7	2.17	0.45
4:D:233:ARG:HG2	4:D:233:ARG:NH1	4.71	0.45
3:C:318:LEU:C	3:C:318:LEU:HD23	2.43	0.45
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.99	0.44
1:A:215:HIS:HA	27:A:611:PL9:O1	2.17	0.44
2:B:127:ARG:CG	2:B:127:ARG:HH11	2.18	0.44
24:B:607:CLA:H161	24:B:607:CLA:H192	3.85	0.44
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.98	0.44
10:K:17:ILE:N	10:K:17:ILE:CD1	2.76	0.44
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:GLY:HA3	5:E:4:THR:O	2.16	0.44
5:E:20:TRP:HZ2	9:J:13:VAL:HG13	1.83	0.44
1:A:262:TYR:CE2	29:A:615:LHG:HC31	2.52	0.44
4:D:101:PHE:HB3	31:D:406:DGD:HG2	2.04	0.44
3:C:459:ILE:HB	4:D:223:PHE:CD1	2.74	0.44
1:A:311:GLY:C	16:V:125:ILE:CG2	3.05	0.44
5:E:82:GLN:C	5:E:84:LYS:H	2.21	0.44
4:D:233:ARG:CG	4:D:233:ARG:NH1	4.33	0.44
24:C:510:CLA:H192	24:C:510:CLA:HBC3	1.99	0.44
2:B:393:GLU:HB3	15:U:18:GLY:N	2.45	0.44
24:B:607:CLA:H72	26:B:619:BCR:H311	25.84	0.44
4:D:17:ILE:HD12	18:X:36:LYS:HE3	1.99	0.44
28:A:612:SQD:O7	3:C:28:GLN:NE2	2.37	0.44
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	1.99	0.44
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.54	0.44
1:A:138:GLY:HA2	3:C:455:PHE:CZ	2.53	0.44
1:A:215:HIS:ND1	27:A:611:PL9:O1	2.47	0.43
26:B:619:BCR:H371	26:B:619:BCR:H24C	1.92	0.43
24:A:607:CLA:HBB1	24:A:607:CLA:HMB1	2.00	0.43
2:B:461:LEU:HD22	29:D:407:LHG:H301	1.99	0.43
1:A:323:ARG:NH1	16:V:135:VAL:O	2.76	0.43
24:C:508:CLA:OBD	29:D:409:LHG:HC31	2.19	0.43
24:D:403:CLA:HBB1	24:D:403:CLA:HMB1	2.00	0.43
19:Z:15:LEU:HD22	19:Z:46:LEU:HD23	2.77	0.43
29:A:615:LHG:HC12	4:D:27:PHE:HD2	1.84	0.43
4:D:185:PHE:CD2	24:D:403:CLA:HMD3	29.98	0.43
1:A:163:ILE:HD11	31:C:516:DGD:HA22	2.01	0.43
10:K:46:ARG:NH2	17:Y:46:LEU:OXT	4.66	0.43
13:O:58:ASN:HA	13:O:60:ARG:NH2	2.33	0.43
5:E:52:PRO:HG3	9:J:36:LEU:HD21	2.44	0.43
28:L:101:SQD:H382	12:M:15:VAL:CG1	2.74	0.43
1:A:32:TRP:CD2	8:I:22:GLY:HA3	2.54	0.43
13:O:61:GLN:HG2	13:O:62:GLU:N	4.41	0.43
4:D:125:PHE:CE2	25:D:401:PHO:HBD	2.54	0.43
3:C:339:LYS:NZ	15:U:94:GLY:O	2.49	0.43
2:B:13:ILE:HG12	24:B:613:CLA:HAC2	2.00	0.43
24:B:606:CLA:H41	24:B:606:CLA:H62	1.77	0.43
4:D:85:MET:HE3	4:D:96:GLU:HG2	2.07	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.23	0.43
24:C:510:CLA:HBB1	24:C:510:CLA:HMB1	2.01	0.43
10:K:10:LYS:N	10:K:10:LYS:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:615:CLA:H62	24:B:615:CLA:H41	2.52	0.43
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.51	0.43
24:B:612:CLA:H112	29:B:621:LHG:H342	2.01	0.43
8:I:33:LYS:HA	8:I:33:LYS:HD3	3.63	0.43
24:C:506:CLA:H122	24:C:506:CLA:H162	1.72	0.42
28:L:101:SQD:H341	28:L:101:SQD:H311	1.81	0.42
16:V:37:CYS:CB	32:V:202:HEM:HAB	2.44	0.42
31:C:518:DGD:CGB	29:D:409:LHG:H202	2.49	0.42
1:A:254:TYR:CD2	4:D:132:ILE:HG22	4.66	0.42
2:B:71:VAL:HG23	24:B:607:CLA:HMA2	2.01	0.42
26:D:404:BCR:HC22	31:D:406:DGD:HA72	2.00	0.42
11:L:14:ARG:HH12	28:L:101:SQD:H3	1.85	0.42
24:C:511:CLA:HMB2	26:K:101:BCR:H382	2.02	0.42
26:B:618:BCR:H381	26:T:101:BCR:H341	41.94	0.42
7:H:53:LEU:CD1	18:X:7:LEU:HA	2.69	0.42
3:C:397:THR:HB	16:V:39:SER:O	2.32	0.42
15:U:104:LYS:HG3	16:V:45:ILE:CG2	2.49	0.42
4:D:310:GLU:HG3	13:O:224:ASP:OD2	2.20	0.42
25:A:608:PHO:ND	25:A:608:PHO:NC	2.68	0.42
3:C:26:ARG:HH21	17:Y:46:LEU:C	2.87	0.42
13:O:59:LYS:HD2	13:O:61:GLN:CG	2.50	0.42
1:A:249:VAL:HG12	2:B:491:VAL:HG23	2.00	0.42
1:A:323:ARG:HB3	4:D:329:MET:HA	2.03	0.42
1:A:142:TRP:HZ2	3:C:447:ARG:HB2	2.03	0.42
3:C:53:HIS:CB	24:C:512:CLA:HMD1	2.49	0.42
4:D:102:THR:OG1	31:D:406:DGD:HG31	2.19	0.42
2:B:256:MET:HA	2:B:263:THR:HG21	2.19	0.42
6:F:21:VAL:O	6:F:25:THR:HG23	2.39	0.42
10:K:34:ALA:HB1	26:K:101:BCR:C20	14.03	0.42
26:H:101:BCR:H371	26:H:101:BCR:H24C	1.81	0.42
26:T:101:BCR:H371	26:T:101:BCR:H24C	1.89	0.42
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.23	0.42
8:I:2:GLU:O	8:I:6:ILE:HG12	4.16	0.42
3:C:205:ASP:HA	3:C:206:PRO:HD3	1.90	0.42
4:D:185:PHE:CG	24:D:402:CLA:HMD3	2.55	0.42
2:B:274:GLN:HG2	31:H:102:DGD:O5E	2.20	0.42
24:B:605:CLA:H161	24:B:605:CLA:H141	1.93	0.41
24:B:606:CLA:H122	24:B:611:CLA:HMA2	2.13	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
3:C:406:SER:HA	3:C:420:VAL:HG23	2.03	0.41
31:C:518:DGD:HBN2	29:D:409:LHG:H202	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D:405:PL9:H512	14:T:10:PHE:HB2	2.03	0.41
3:C:447:ARG:HH21	4:D:229:ALA:HB1	1.91	0.41
24:C:502:CLA:H61	24:C:512:CLA:H42	2.03	0.41
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	2.12	0.41
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.51	0.41
24:B:614:CLA:H162	24:B:614:CLA:H121	1.89	0.41
24:A:609:CLA:C1B	8:I:12:VAL:HG22	2.50	0.41
2:B:204:ALA:CB	24:B:603:CLA:HAB	2.50	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.58	0.41
27:A:611:PL9:C22	25:D:401:PHO:HMA2	2.51	0.41
4:D:351:ALA:CA	15:U:101:GLY:O	2.64	0.41
28:L:101:SQD:H381	12:M:16:LEU:HD23	2.03	0.41
3:C:330:SER:O	13:O:123:LYS:NZ	2.43	0.41
3:C:29:GLU:H	3:C:29:GLU:CD	2.22	0.41
3:C:320:ARG:HD2	16:V:49:ASN:CG	2.57	0.41
4:D:185:PHE:CG	24:D:403:CLA:HMD3	29.94	0.41
2:B:33:TRP:CD1	26:B:622:BCR:H381	2.55	0.41
24:B:610:CLA:HMB2	24:B:611:CLA:C2B	2.62	0.41
3:C:158:THR:O	3:C:251:HIS:HB3	2.28	0.41
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.94	0.41
29:D:409:LHG:H302	29:D:409:LHG:H332	1.88	0.41
2:B:127:ARG:NH1	2:B:127:ARG:CG	2.81	0.41
2:B:220:ARG:HG3	7:H:20:LYS:HD3	2.03	0.41
1:A:62:GLY:O	3:C:337:LEU:HD11	2.25	0.41
25:A:608:PHO:H161	24:A:614:CLA:HMB3	2.03	0.41
24:C:504:CLA:HAC2	10:K:26:PRO:O	2.20	0.41
3:C:243:ILE:HG22	24:C:506:CLA:HMC1	2.03	0.41
24:C:507:CLA:H41	24:C:507:CLA:H61	1.93	0.41
11:L:7:ARG:HD2	28:L:101:SQD:O8	30.78	0.41
24:B:611:CLA:CBB	24:B:611:CLA:HHC	2.50	0.41
1:A:193:LEU:HD13	4:D:179:PHE:HB3	2.14	0.41
24:B:607:CLA:HBB1	24:B:607:CLA:HMB1	2.03	0.41
16:V:41:HIS:HA	16:V:45:ILE:O	2.31	0.41
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.10	0.41
24:B:607:CLA:H122	24:B:607:CLA:H162	3.81	0.40
2:B:385:ARG:HB2	15:U:13:VAL:CG1	2.51	0.40
24:B:612:CLA:HBC1	29:D:407:LHG:H321	2.03	0.40
2:B:76:SER:OG	13:O:112:GLY:HA2	56.32	0.40
17:Y:33:PRO:HD3	26:Y:101:BCR:C16	2.51	0.40
28:A:612:SQD:H321	24:C:508:CLA:C19	2.51	0.40
3:C:324:LEU:O	15:U:98:TYR:HE1	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:SER:HB2	3:C:41:ARG:HG2	2.17	0.40
3:C:338:GLY:HA3	3:C:341:LEU:O	2.21	0.40
10:K:28:ILE:HG12	17:Y:28:ILE:HG21	2.19	0.40
3:C:286:ALA:HB2	24:C:502:CLA:CMD	2.51	0.40
4:D:323:GLU:CD	13:O:172:ILE:HD11	2.42	0.40
2:B:118:TRP:CZ2	11:L:4:ASN:HA	2.56	0.40
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.56	0.40
24:A:609:CLA:H202	24:C:506:CLA:H101	2.02	0.40
2:B:192:PRO:HB3	7:H:49:TYR:CE2	2.57	0.40
13:O:180:GLU:CD	13:O:180:GLU:H	2.24	0.40

All (23) 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)
13:O:37:THR:O	3:c:19:ASN:CG[2_455]	0.56	1.64
13:O:37:THR:O	3:c:19:ASN:ND2[2_455]	0.91	1.29
13:O:36:GLN:NE2	3:c:19:ASN:CA[2_455]	0.99	1.21
13:O:37:THR:N	3:c:19:ASN:OD1[2_455]	1.04	1.16
13:O:36:GLN:NE2	3:c:19:ASN:C[2_455]	1.05	1.15
13:O:35:SER:O	3:c:20:SER:OG[2_455]	1.43	0.77
13:O:36:GLN:NE2	3:c:19:ASN:N[2_455]	1.56	0.64
13:O:37:THR:C	3:c:19:ASN:OD1[2_455]	1.59	0.61
13:O:37:THR:O	3:c:19:ASN:CB[2_455]	1.60	0.60
13:O:37:THR:O	3:c:19:ASN:OD1[2_455]	1.73	0.47
13:O:36:GLN:OE1	3:c:20:SER:N[2_455]	1.77	0.43
13:O:36:GLN:CA	3:c:20:SER:CB[2_455]	1.77	0.43
13:O:36:GLN:CD	3:c:19:ASN:N[2_455]	1.89	0.31
13:O:36:GLN:C	3:c:19:ASN:OD1[2_455]	1.94	0.26
13:O:36:GLN:CD	3:c:19:ASN:C[2_455]	1.97	0.23
13:O:36:GLN:OE1	3:c:20:SER:O[2_455]	2.03	0.17
13:O:35:SER:C	3:c:20:SER:OG[2_455]	2.06	0.14
13:O:37:THR:CA	3:c:19:ASN:CG[2_455]	2.09	0.11
13:O:38:TYR:N	3:c:19:ASN:ND2[2_455]	2.12	0.08
13:O:33:ASP:OD2	3:c:23:ALA:CA[2_455]	2.14	0.06
13:O:246:ALA:OXT	3:c:19:ASN:CB[2_455]	2.14	0.06
13:O:36:GLN:NE2	3:c:19:ASN:CB[2_455]	2.17	0.03
13:O:35:SER:O	3:c:20:SER:CB[2_455]	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%)	325 (98%)	6 (2%)	1 (0%)	46	83
2	B	502/504 (100%)	496 (99%)	6 (1%)	0	100	100
2	b	502/504 (100%)	492 (98%)	10 (2%)	0	100	100
3	C	449/455 (99%)	440 (98%)	8 (2%)	1 (0%)	52	86
3	c	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	52	86
4	D	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
4	d	339/342 (99%)	333 (98%)	6 (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	30/34 (88%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	58 (92%)	5 (8%)	0	100	100
7	h	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	36/40 (90%)	36 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	o	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	39 80
14	T	28/30 (93%)	27 (96%)	1 (4%)	0	100 100
14	t	28/30 (93%)	28 (100%)	0	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%)	130 (96%)	5 (4%)	0	100 100
17	Y	27/29 (93%)	27 (100%)	0	0	100 100
17	y	27/29 (93%)	26 (96%)	1 (4%)	0	100 100
18	X	37/39 (95%)	36 (97%)	1 (3%)	0	100 100
18	x	37/39 (95%)	35 (95%)	2 (5%)	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	5191/5276 (98%)	5072 (98%)	113 (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%)	268 (100%)	1 (0%)	93 96
1	a	269/269 (100%)	267 (99%)	2 (1%)	88 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	402/402 (100%)	399 (99%)	3 (1%)	88 94
2	b	402/402 (100%)	395 (98%)	7 (2%)	68 88
3	C	352/356 (99%)	348 (99%)	4 (1%)	80 91
3	c	356/356 (100%)	350 (98%)	6 (2%)	68 88
4	D	277/277 (100%)	274 (99%)	3 (1%)	80 91
4	d	276/277 (100%)	275 (100%)	1 (0%)	93 96
5	E	72/72 (100%)	71 (99%)	1 (1%)	74 89
5	e	72/72 (100%)	70 (97%)	2 (3%)	51 79
6	F	28/28 (100%)	27 (96%)	1 (4%)	42 75
6	f	26/28 (93%)	25 (96%)	1 (4%)	40 74
7	H	54/54 (100%)	51 (94%)	3 (6%)	26 65
7	h	54/54 (100%)	53 (98%)	1 (2%)	65 86
8	I	35/35 (100%)	35 (100%)	0	100 100
8	i	35/35 (100%)	35 (100%)	0	100 100
9	J	26/28 (93%)	26 (100%)	0	100 100
9	j	28/28 (100%)	28 (100%)	0	100 100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20 59
10	k	30/30 (100%)	28 (93%)	2 (7%)	20 59
11	L	35/35 (100%)	33 (94%)	2 (6%)	25 64
11	l	35/35 (100%)	34 (97%)	1 (3%)	50 79
12	M	31/31 (100%)	30 (97%)	1 (3%)	46 77
12	m	31/31 (100%)	31 (100%)	0	100 100
13	O	206/206 (100%)	202 (98%)	4 (2%)	65 86
13	o	206/206 (100%)	200 (97%)	6 (3%)	50 79
14	T	27/27 (100%)	27 (100%)	0	100 100
14	t	27/27 (100%)	25 (93%)	2 (7%)	17 55
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%)	114 (97%)	3 (3%)	54 81
17	Y	22/22 (100%)	21 (96%)	1 (4%)	34 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	y	22/22 (100%)	21 (96%)	1 (4%)	34 70
18	X	32/32 (100%)	32 (100%)	0	100 100
18	x	32/32 (100%)	31 (97%)	1 (3%)	47 78
19	Z	52/52 (100%)	50 (96%)	2 (4%)	40 74
19	z	52/52 (100%)	49 (94%)	3 (6%)	25 63
All	All	4305/4314 (100%)	4235 (98%)	70 (2%)	70 88

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	238	LYS
2	B	53	ASN
2	B	246	PHE
2	B	472	ARG
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
5	E	71	GLU
6	F	44	GLN
7	H	12	ARG
7	H	49	TYR
7	H	65	LEU
10	K	13	GLU
10	K	17	ILE
11	L	1	MET
11	L	13	ASN
12	M	9	ILE
13	O	61	GLN
13	O	118	LEU
13	O	181	GLU
13	O	234	LYS
15	U	70	ARG
16	V	30	LYS
17	Y	27	MET
19	Z	6	GLN
19	Z	31	GLN

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Mol	Chain	Res	Type
1	a	12	ASN
1	a	244	GLU
2	b	14	ASN
2	b	246	PHE
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
2	b	491	VAL
2	b	505	ARG
3	c	120	ILE
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	416	SER
3	c	418	ASN
4	d	180	ARG
5	e	59	GLU
5	e	60	GLN
6	f	44	GLN
7	h	49	TYR
10	k	13	GLU
10	k	17	ILE
11	l	1	MET
13	o	55	GLU
13	o	61	GLN
13	o	62	GLU
13	o	118	LEU
13	o	194	LYS
13	o	225	MET
14	t	1	MET
14	t	25	GLU
15	u	70	ARG
16	v	17	LYS
16	v	23	GLU
16	v	122	GLU
17	y	42	ARG
18	x	2	THR
19	z	1	MET
19	z	3	ILE
19	z	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
2	B	53	ASN
2	B	281	GLN
2	B	331	ASN
3	C	25	ASN
3	C	373	ASN
4	D	83	ASN
4	D	332	GLN
6	F	44	GLN
10	K	40	GLN
11	L	13	ASN
13	O	82	GLN
13	O	124	ASN
13	O	147	ASN
16	V	34	GLN
19	Z	58	ASN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	331	ASN
3	c	28	GLN
3	c	201	ASN
3	c	373	ASN
4	d	83	ASN
4	d	332	GLN
5	e	75	GLN
13	o	61	GLN
13	o	82	GLN
13	o	124	ASN
13	o	147	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 152 ligands modelled in this entry, 16 are monoatomic - leaving 136 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	-
23	BCT	A	605	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	606	-	55,73,73	1.80	10 (18%)	61,113,113	1.76	14 (22%)
24	CLA	A	607	-	55,73,73	1.72	10 (18%)	61,113,113	2.07	16 (26%)
25	PHO	A	608	-	67,69,69	1.88	14 (20%)	84,99,99	1.97	20 (23%)
24	CLA	A	609	-	55,73,73	1.84	10 (18%)	61,113,113	1.89	16 (26%)
26	BCR	A	610	-	41,41,41	3.66	14 (34%)	56,56,56	7.57	38 (67%)
27	PL9	A	611	-	55,55,55	0.71	2 (3%)	68,69,69	1.64	13 (19%)
28	SQD	A	612	-	53,54,54	1.33	3 (5%)	61,65,65	1.67	10 (16%)
28	SQD	A	613	-	53,54,54	1.36	3 (5%)	61,65,65	1.33	5 (8%)
24	CLA	A	614	-	55,73,73	1.74	10 (18%)	61,113,113	2.06	16 (26%)
29	LHG	A	615	-	41,41,48	1.01	2 (4%)	42,47,54	1.10	3 (7%)
24	CLA	B	602	-	55,73,73	1.90	11 (20%)	61,113,113	1.90	14 (22%)
24	CLA	B	603	-	55,73,73	1.89	11 (20%)	61,113,113	1.69	11 (18%)
24	CLA	B	604	-	55,73,73	1.82	10 (18%)	61,113,113	2.02	15 (24%)
24	CLA	B	605	-	55,73,73	1.71	10 (18%)	61,113,113	1.96	15 (24%)
24	CLA	B	606	-	55,73,73	1.76	10 (18%)	61,113,113	1.79	14 (22%)
24	CLA	B	607	-	55,73,73	1.85	11 (20%)	61,113,113	1.90	12 (19%)
24	CLA	B	608	-	55,73,73	1.78	10 (18%)	61,113,113	1.81	13 (21%)
24	CLA	B	609	-	55,73,73	1.77	10 (18%)	61,113,113	2.04	17 (27%)
24	CLA	B	610	-	55,73,73	1.78	10 (18%)	61,113,113	1.84	13 (21%)
24	CLA	B	611	-	55,73,73	1.81	10 (18%)	61,113,113	1.77	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	612	-	55,73,73	1.66	10 (18%)	61,113,113	1.84	13 (21%)
24	CLA	B	613	-	55,73,73	1.81	11 (20%)	61,113,113	1.87	15 (24%)
24	CLA	B	614	-	55,73,73	1.79	11 (20%)	61,113,113	1.74	15 (24%)
24	CLA	B	615	-	55,73,73	1.77	11 (20%)	61,113,113	1.91	15 (24%)
24	CLA	B	616	-	55,73,73	1.82	11 (20%)	61,113,113	1.69	11 (18%)
24	CLA	B	617	-	55,73,73	1.85	10 (18%)	61,113,113	1.82	17 (27%)
26	BCR	B	618	-	41,41,41	3.60	14 (34%)	56,56,56	7.30	38 (67%)
26	BCR	B	619	-	41,41,41	3.60	14 (34%)	56,56,56	7.55	41 (73%)
26	BCR	B	620	-	41,41,41	3.67	14 (34%)	56,56,56	8.19	41 (73%)
29	LHG	B	621	-	48,48,48	0.86	2 (4%)	49,54,54	1.00	2 (4%)
26	BCR	B	622	-	41,41,41	3.73	15 (36%)	56,56,56	7.41	34 (60%)
24	CLA	C	501	-	55,73,73	1.85	11 (20%)	61,113,113	1.98	14 (22%)
24	CLA	C	502	-	55,73,73	1.79	10 (18%)	61,113,113	1.79	14 (22%)
24	CLA	C	503	-	55,73,73	1.87	11 (20%)	61,113,113	1.71	12 (19%)
24	CLA	C	504	-	55,73,73	1.83	10 (18%)	61,113,113	1.93	13 (21%)
24	CLA	C	505	-	55,73,73	1.85	12 (21%)	61,113,113	1.78	13 (21%)
24	CLA	C	506	-	55,73,73	1.87	11 (20%)	61,113,113	1.89	15 (24%)
24	CLA	C	507	-	55,73,73	1.93	11 (20%)	61,113,113	1.88	14 (22%)
24	CLA	C	508	-	55,73,73	1.92	12 (21%)	61,113,113	1.80	11 (18%)
24	CLA	C	509	-	55,73,73	1.85	12 (21%)	61,113,113	1.91	16 (26%)
24	CLA	C	510	-	55,73,73	1.82	11 (20%)	61,113,113	1.85	15 (24%)
24	CLA	C	511	3	55,73,73	1.86	11 (20%)	61,113,113	1.78	11 (18%)
24	CLA	C	512	-	55,73,73	1.90	12 (21%)	61,113,113	1.83	15 (24%)
24	CLA	C	513	-	55,73,73	1.95	11 (20%)	61,113,113	1.69	13 (21%)
26	BCR	C	514	-	41,41,41	3.80	15 (36%)	56,56,56	8.21	35 (62%)
26	BCR	C	515	-	41,41,41	3.76	14 (34%)	56,56,56	8.00	39 (69%)
31	DGD	C	516	-	63,63,67	0.84	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	0.76	3 (4%)	77,77,81	0.91	3 (3%)
25	PHO	D	401	-	67,69,69	1.98	15 (22%)	84,99,99	1.97	21 (25%)
24	CLA	D	402	-	55,73,73	1.79	10 (18%)	61,113,113	1.87	18 (29%)
24	CLA	D	403	-	55,73,73	1.86	12 (21%)	61,113,113	1.73	12 (19%)
26	BCR	D	404	-	41,41,41	3.75	14 (34%)	56,56,56	7.56	41 (73%)
27	PL9	D	405	-	55,55,55	0.82	1 (1%)	68,69,69	1.42	9 (13%)
31	DGD	D	406	-	63,63,67	0.96	4 (6%)	77,77,81	1.07	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LHG	D	407	-	48,48,48	0.84	2 (4%)	49,54,54	1.01	3 (6%)
29	LHG	D	408	-	48,48,48	0.87	2 (4%)	49,54,54	0.86	2 (4%)
29	LHG	D	409	-	48,48,48	0.91	2 (4%)	49,54,54	0.90	2 (4%)
32	HEM	E	101	5,6	30,50,50	2.21	8 (26%)	24,82,82	2.44	9 (37%)
28	SQD	F	101	-	42,43,54	1.54	3 (7%)	50,54,65	1.66	7 (14%)
26	BCR	H	101	-	41,41,41	3.74	14 (34%)	56,56,56	8.04	40 (71%)
31	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	0.94	6 (7%)
26	BCR	K	101	-	41,41,41	3.70	14 (34%)	56,56,56	7.54	41 (73%)
28	SQD	L	101	-	53,54,54	1.35	4 (7%)	61,65,65	1.61	8 (13%)
26	BCR	T	101	-	41,41,41	3.74	14 (34%)	56,56,56	6.87	38 (67%)
26	BCR	T	102	-	41,41,41	3.62	15 (36%)	56,56,56	7.04	38 (67%)
32	HEM	V	202	16	30,50,50	2.26	9 (30%)	24,82,82	2.41	9 (37%)
26	BCR	Y	101	-	41,41,41	3.78	14 (34%)	56,56,56	7.85	36 (64%)
20	OEX	a	401	1,3	0,15,15	0.00	-	0,32,32	0.00	-
28	SQD	a	402	-	53,54,54	1.38	3 (5%)	61,65,65	1.33	5 (8%)
24	CLA	a	406	-	55,73,73	1.75	10 (18%)	61,113,113	1.86	14 (22%)
24	CLA	a	407	-	55,73,73	1.72	10 (18%)	61,113,113	1.97	16 (26%)
24	CLA	a	408	-	55,73,73	1.84	10 (18%)	61,113,113	1.91	16 (26%)
26	BCR	a	409	-	41,41,41	3.59	14 (34%)	56,56,56	7.59	36 (64%)
27	PL9	a	410	-	55,55,55	0.71	2 (3%)	68,69,69	1.61	16 (23%)
28	SQD	a	411	-	53,54,54	1.33	3 (5%)	61,65,65	1.73	9 (14%)
25	PHO	a	412	-	67,69,69	2.01	15 (22%)	84,99,99	1.97	19 (22%)
29	LHG	a	413	-	41,41,48	1.02	2 (4%)	42,47,54	0.93	2 (4%)
23	BCT	a	414	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	b	602	-	55,73,73	1.95	11 (20%)	61,113,113	1.84	14 (22%)
24	CLA	b	603	-	55,73,73	1.86	11 (20%)	61,113,113	1.71	12 (19%)
24	CLA	b	604	-	55,73,73	1.79	10 (18%)	61,113,113	1.99	18 (29%)
24	CLA	b	605	-	55,73,73	1.77	11 (20%)	61,113,113	1.96	17 (27%)
24	CLA	b	606	-	55,73,73	1.72	11 (20%)	61,113,113	1.98	15 (24%)
24	CLA	b	607	-	55,73,73	1.89	11 (20%)	61,113,113	1.85	13 (21%)
24	CLA	b	608	-	55,73,73	1.82	10 (18%)	61,113,113	1.83	15 (24%)
24	CLA	b	609	-	55,73,73	1.84	11 (20%)	61,113,113	1.87	14 (22%)
24	CLA	b	610	-	55,73,73	1.88	12 (21%)	61,113,113	1.81	12 (19%)
24	CLA	b	611	-	55,73,73	1.84	12 (21%)	61,113,113	1.71	10 (16%)
24	CLA	b	612	-	55,73,73	1.78	10 (18%)	61,113,113	1.81	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	b	613	-	55,73,73	1.78	10 (18%)	61,113,113	1.90	14 (22%)
24	CLA	b	614	-	55,73,73	1.83	11 (20%)	61,113,113	1.81	13 (21%)
24	CLA	b	615	-	55,73,73	1.78	11 (20%)	61,113,113	2.03	19 (31%)
24	CLA	b	616	-	55,73,73	1.83	10 (18%)	61,113,113	1.83	15 (24%)
24	CLA	b	617	-	55,73,73	1.88	11 (20%)	61,113,113	1.88	16 (26%)
26	BCR	b	618	-	41,41,41	3.65	14 (34%)	56,56,56	7.79	41 (73%)
26	BCR	b	619	-	41,41,41	3.75	15 (36%)	56,56,56	8.34	40 (71%)
29	LHG	b	620	-	48,48,48	0.87	2 (4%)	49,54,54	1.00	2 (4%)
24	CLA	c	902	-	55,73,73	1.87	12 (21%)	61,113,113	1.92	12 (19%)
24	CLA	c	903	-	55,73,73	1.84	11 (20%)	61,113,113	1.86	13 (21%)
24	CLA	c	904	-	55,73,73	1.88	12 (21%)	61,113,113	1.66	14 (22%)
24	CLA	c	905	-	55,73,73	1.88	12 (21%)	61,113,113	1.85	14 (22%)
24	CLA	c	906	-	55,73,73	1.86	11 (20%)	61,113,113	1.80	16 (26%)
24	CLA	c	907	-	55,73,73	1.87	11 (20%)	61,113,113	1.71	11 (18%)
24	CLA	c	908	-	55,73,73	1.87	11 (20%)	61,113,113	1.93	12 (19%)
24	CLA	c	909	-	55,73,73	1.84	13 (23%)	61,113,113	1.69	10 (16%)
24	CLA	c	910	-	55,73,73	1.89	11 (20%)	61,113,113	1.91	14 (22%)
24	CLA	c	911	-	55,73,73	1.84	10 (18%)	61,113,113	1.78	14 (22%)
24	CLA	c	912	3	55,73,73	1.89	11 (20%)	61,113,113	1.78	12 (19%)
24	CLA	c	913	-	55,73,73	1.90	12 (21%)	61,113,113	1.85	13 (21%)
24	CLA	c	914	-	55,73,73	1.96	12 (21%)	61,113,113	1.70	13 (21%)
26	BCR	c	915	-	41,41,41	3.73	15 (36%)	56,56,56	8.32	40 (71%)
31	DGD	c	916	-	63,63,67	0.83	2 (3%)	77,77,81	0.91	3 (3%)
31	DGD	c	917	-	63,63,67	0.85	2 (3%)	77,77,81	0.81	2 (2%)
26	BCR	c	918	-	41,41,41	3.56	15 (36%)	56,56,56	7.37	36 (64%)
24	CLA	d	401	-	55,73,73	1.75	10 (18%)	61,113,113	1.86	14 (22%)
25	PHO	d	402	-	67,69,69	1.92	14 (20%)	84,99,99	1.90	19 (22%)
24	CLA	d	403	-	55,73,73	1.76	11 (20%)	61,113,113	1.92	16 (26%)
24	CLA	d	404	-	55,73,73	1.88	12 (21%)	61,113,113	1.82	13 (21%)
27	PL9	d	405	-	55,55,55	0.85	3 (5%)	68,69,69	1.39	11 (16%)
31	DGD	d	406	-	63,63,67	0.93	3 (4%)	77,77,81	0.98	3 (3%)
28	SQD	d	407	-	42,43,54	1.57	3 (7%)	50,54,65	1.59	7 (14%)
29	LHG	d	408	-	48,48,48	0.87	2 (4%)	49,54,54	0.98	4 (8%)
29	LHG	d	409	-	48,48,48	0.82	2 (4%)	49,54,54	0.92	3 (6%)
29	LHG	d	410	-	48,48,48	0.89	2 (4%)	49,54,54	0.96	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	HEM	e	101	5,6	30,50,50	2.14	9 (30%)	24,82,82	2.48	9 (37%)
26	BCR	f	101	-	41,41,41	3.77	15 (36%)	56,56,56	7.74	47 (83%)
26	BCR	h	101	-	41,41,41	3.73	14 (34%)	56,56,56	8.15	41 (73%)
31	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	0.86	3 (3%)
31	DGD	j	101	-	63,63,67	0.85	3 (4%)	77,77,81	0.88	3 (3%)
26	BCR	k	101	-	41,41,41	3.82	14 (34%)	56,56,56	8.29	42 (75%)
26	BCR	k	102	-	41,41,41	3.74	14 (34%)	56,56,56	8.23	42 (75%)
28	SQD	l	101	-	53,54,54	1.30	4 (7%)	61,65,65	1.51	6 (9%)
32	HEM	v	202	16	30,50,50	2.27	11 (36%)	24,82,82	2.43	10 (41%)

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
23	BCT	A	605	21	-	0/0/0/0	0/0/0/0
24	CLA	A	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	607	-	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	A	608	-	-	0/53/103/103	0/1/6/6
24	CLA	A	609	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	A	610	-	-	0/29/63/63	0/2/2/2
27	PL9	A	611	-	-	0/53/73/73	0/1/1/1
28	SQD	A	612	-	-	0/49/69/69	0/1/1/1
28	SQD	A	613	-	-	0/49/69/69	0/1/1/1
24	CLA	A	614	-	1/1/20/25	0/37/135/135	0/0/9/9
29	LHG	A	615	-	-	0/46/46/53	0/0/0/0
24	CLA	B	602	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	612	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
29	LHG	B	621	-	-	0/53/53/53	0/0/0/0
26	BCR	B	622	-	-	0/29/63/63	0/2/2/2
24	CLA	C	501	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	502	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
26	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
25	PHO	D	401	-	-	0/53/103/103	0/1/6/6
24	CLA	D	402	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	D	403	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	D	404	-	-	0/29/63/63	0/2/2/2
27	PL9	D	405	-	-	0/53/73/73	0/1/1/1
31	DGD	D	406	-	-	0/51/91/95	0/2/2/2
29	LHG	D	407	-	-	0/53/53/53	0/0/0/0
29	LHG	D	408	-	-	0/53/53/53	0/0/0/0
29	LHG	D	409	-	-	0/53/53/53	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HEM	E	101	5,6	-	0/10/54/54	0/0/8/8
28	SQD	F	101	-	-	0/38/58/69	0/1/1/1
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	DGD	H	102	-	-	0/51/91/95	0/2/2/2
26	BCR	K	101	-	-	0/29/63/63	0/2/2/2
28	SQD	L	101	-	-	0/49/69/69	0/1/1/1
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
26	BCR	T	102	-	-	0/29/63/63	0/2/2/2
32	HEM	V	202	16	-	0/10/54/54	0/0/8/8
26	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
20	OEX	a	401	1,3	-	0/0/68/68	0/0/6/6
28	SQD	a	402	-	-	0/49/69/69	0/1/1/1
24	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	a	407	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	a	408	-	1/1/20/25	0/37/135/135	0/0/9/9
26	BCR	a	409	-	-	0/29/63/63	0/2/2/2
27	PL9	a	410	-	-	0/53/73/73	0/1/1/1
28	SQD	a	411	-	-	0/49/69/69	0/1/1/1
25	PHO	a	412	-	-	0/53/103/103	0/1/6/6
29	LHG	a	413	-	-	0/46/46/53	0/0/0/0
23	BCT	a	414	21	-	0/0/0/0	0/0/0/0
24	CLA	b	602	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	-	-	0/37/135/135	0/0/9/9
24	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
29	LHG	b	620	-	-	0/53/53/53	0/0/0/0
24	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	903	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	905	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	906	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	907	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	908	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	912	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	c	913	-	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	914	-	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	c	915	-	-	0/29/63/63	0/2/2/2
31	DGD	c	916	-	-	0/51/91/95	0/2/2/2
31	DGD	c	917	-	-	0/51/91/95	0/2/2/2
26	BCR	c	918	-	-	0/29/63/63	0/2/2/2
24	CLA	d	401	-	1/1/20/25	0/37/135/135	0/0/9/9
25	PHO	d	402	-	-	0/53/103/103	0/1/6/6
24	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	d	404	-	1/1/20/25	0/37/135/135	0/0/9/9
27	PL9	d	405	-	-	0/53/73/73	0/1/1/1
31	DGD	d	406	-	-	0/51/91/95	0/2/2/2
28	SQD	d	407	-	-	0/38/58/69	0/1/1/1
29	LHG	d	408	-	-	0/53/53/53	0/0/0/0
29	LHG	d	409	-	-	0/53/53/53	0/0/0/0
29	LHG	d	410	-	-	0/53/53/53	0/0/0/0
32	HEM	e	101	5,6	-	0/10/54/54	0/0/8/8
26	BCR	f	101	-	-	0/29/63/63	0/2/2/2
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
31	DGD	h	102	-	-	0/51/91/95	0/2/2/2
31	DGD	j	101	-	-	0/51/91/95	0/2/2/2
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	BCR	k	102	-	-	0/29/63/63	0/2/2/2
28	SQD	l	101	-	-	0/49/69/69	0/1/1/1
32	HEM	v	202	16	-	0/10/54/54	0/0/8/8

All (1250) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	918	BCR	C8-C9	-8.63	1.26	1.45
26	b	619	BCR	C8-C9	-8.58	1.26	1.45
26	B	622	BCR	C8-C9	-8.53	1.27	1.45
26	C	514	BCR	C8-C9	-8.51	1.27	1.45
26	C	514	BCR	C12-C13	-8.48	1.27	1.45
26	c	915	BCR	C8-C9	-8.47	1.27	1.45
26	D	404	BCR	C8-C9	-8.42	1.27	1.45
26	c	918	BCR	C12-C13	-8.42	1.27	1.45
26	K	101	BCR	C8-C9	-8.41	1.27	1.45
26	h	101	BCR	C8-C9	-8.41	1.27	1.45
26	k	101	BCR	C8-C9	-8.40	1.27	1.45
26	f	101	BCR	C8-C9	-8.38	1.27	1.45
26	H	101	BCR	C19-C18	-8.38	1.27	1.45
26	T	101	BCR	C8-C9	-8.36	1.27	1.45
26	f	101	BCR	C19-C18	-8.36	1.27	1.45
26	k	101	BCR	C12-C13	-8.35	1.27	1.45
26	C	515	BCR	C8-C9	-8.34	1.27	1.45
26	Y	101	BCR	C8-C9	-8.33	1.27	1.45
26	h	101	BCR	C19-C18	-8.32	1.27	1.45
26	k	101	BCR	C19-C18	-8.31	1.27	1.45
26	Y	101	BCR	C19-C18	-8.29	1.27	1.45
26	k	102	BCR	C8-C9	-8.28	1.27	1.45
26	B	620	BCR	C8-C9	-8.26	1.27	1.45
26	k	102	BCR	C19-C18	-8.25	1.27	1.45
26	Y	101	BCR	C12-C13	-8.25	1.27	1.45
26	B	622	BCR	C12-C13	-8.22	1.27	1.45
26	C	514	BCR	C19-C18	-8.22	1.27	1.45
26	T	101	BCR	C12-C13	-8.22	1.27	1.45
26	B	620	BCR	C12-C13	-8.22	1.27	1.45
26	c	918	BCR	C19-C18	-8.21	1.27	1.45
26	k	102	BCR	C12-C13	-8.20	1.27	1.45
26	C	515	BCR	C19-C18	-8.20	1.27	1.45
26	B	618	BCR	C8-C9	-8.19	1.27	1.45
26	H	101	BCR	C12-C13	-8.19	1.27	1.45
26	H	101	BCR	C8-C9	-8.18	1.27	1.45
26	b	618	BCR	C8-C9	-8.17	1.27	1.45
26	b	619	BCR	C12-C13	-8.16	1.27	1.45
26	D	404	BCR	C19-C18	-8.16	1.27	1.45
26	B	619	BCR	C8-C9	-8.16	1.27	1.45
26	b	619	BCR	C19-C18	-8.16	1.27	1.45
26	C	515	BCR	C12-C13	-8.15	1.27	1.45
26	T	102	BCR	C8-C9	-8.13	1.27	1.45
26	K	101	BCR	C19-C18	-8.13	1.27	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	610	BCR	C8-C9	-8.12	1.27	1.45
26	c	915	BCR	C19-C18	-8.12	1.27	1.45
26	b	618	BCR	C12-C13	-8.11	1.27	1.45
26	c	915	BCR	C12-C13	-8.09	1.28	1.45
26	h	101	BCR	C12-C13	-8.08	1.28	1.45
26	T	101	BCR	C19-C18	-8.08	1.28	1.45
26	D	404	BCR	C12-C13	-8.06	1.28	1.45
26	B	622	BCR	C19-C18	-8.05	1.28	1.45
26	f	101	BCR	C12-C13	-8.03	1.28	1.45
26	B	619	BCR	C19-C18	-8.02	1.28	1.45
26	T	102	BCR	C19-C18	-8.01	1.28	1.45
26	K	101	BCR	C12-C13	-8.00	1.28	1.45
26	B	618	BCR	C12-C13	-7.99	1.28	1.45
26	T	102	BCR	C12-C13	-7.96	1.28	1.45
26	A	610	BCR	C12-C13	-7.96	1.28	1.45
26	A	610	BCR	C19-C18	-7.94	1.28	1.45
26	a	409	BCR	C8-C9	-7.93	1.28	1.45
26	B	620	BCR	C19-C18	-7.90	1.28	1.45
26	B	619	BCR	C12-C13	-7.89	1.28	1.45
26	a	409	BCR	C12-C13	-7.88	1.28	1.45
26	b	618	BCR	C19-C18	-7.85	1.28	1.45
26	a	409	BCR	C19-C18	-7.83	1.28	1.45
26	B	618	BCR	C19-C18	-7.77	1.28	1.45
26	k	101	BCR	C20-C21	-7.77	1.19	1.43
26	f	101	BCR	C20-C21	-7.73	1.19	1.43
26	Y	101	BCR	C20-C21	-7.68	1.19	1.43
26	D	404	BCR	C20-C21	-7.64	1.20	1.43
26	k	102	BCR	C20-C21	-7.63	1.20	1.43
26	C	514	BCR	C20-C21	-7.62	1.20	1.43
26	k	101	BCR	C16-C17	-7.62	1.20	1.43
26	C	515	BCR	C20-C21	-7.60	1.20	1.43
26	H	101	BCR	C20-C21	-7.60	1.20	1.43
26	f	101	BCR	C16-C17	-7.60	1.20	1.43
26	C	514	BCR	C16-C17	-7.59	1.20	1.43
26	Y	101	BCR	C16-C17	-7.59	1.20	1.43
26	C	515	BCR	C16-C17	-7.56	1.20	1.43
26	h	101	BCR	C20-C21	-7.56	1.20	1.43
26	b	619	BCR	C20-C21	-7.55	1.20	1.43
26	c	915	BCR	C20-C21	-7.53	1.20	1.43
32	v	202	HEM	C3B-C4B	-7.52	1.45	1.51
26	K	101	BCR	C20-C21	-7.52	1.20	1.43
26	h	101	BCR	C16-C17	-7.51	1.20	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H	101	BCR	C16-C17	-7.50	1.20	1.43
26	k	102	BCR	C16-C17	-7.49	1.20	1.43
26	b	619	BCR	C16-C17	-7.48	1.20	1.43
26	T	101	BCR	C16-C17	-7.46	1.20	1.43
26	c	915	BCR	C16-C17	-7.45	1.20	1.43
26	B	622	BCR	C16-C17	-7.45	1.20	1.43
26	D	404	BCR	C16-C17	-7.45	1.20	1.43
26	T	101	BCR	C20-C21	-7.44	1.20	1.43
26	A	610	BCR	C20-C21	-7.43	1.20	1.43
26	B	620	BCR	C16-C17	-7.40	1.20	1.43
26	B	619	BCR	C20-C21	-7.39	1.20	1.43
26	A	610	BCR	C16-C17	-7.39	1.20	1.43
26	b	618	BCR	C20-C21	-7.38	1.20	1.43
26	K	101	BCR	C16-C17	-7.37	1.20	1.43
28	d	407	SQD	C6-S	-7.36	1.67	1.77
26	B	622	BCR	C20-C21	-7.35	1.20	1.43
26	T	102	BCR	C16-C17	-7.34	1.20	1.43
26	a	409	BCR	C16-C17	-7.34	1.21	1.43
26	c	918	BCR	C20-C21	-7.32	1.21	1.43
26	B	620	BCR	C20-C21	-7.32	1.21	1.43
26	B	618	BCR	C20-C21	-7.32	1.21	1.43
28	A	612	SQD	C6-S	-7.28	1.67	1.77
26	B	618	BCR	C16-C17	-7.27	1.21	1.43
26	T	102	BCR	C20-C21	-7.27	1.21	1.43
26	b	618	BCR	C16-C17	-7.26	1.21	1.43
26	B	619	BCR	C16-C17	-7.22	1.21	1.43
32	V	202	HEM	C3B-C4B	-7.22	1.45	1.51
28	a	411	SQD	C6-S	-7.21	1.67	1.77
28	a	402	SQD	C6-S	-7.21	1.67	1.77
26	a	409	BCR	C20-C21	-7.15	1.21	1.43
28	A	613	SQD	C6-S	-7.13	1.67	1.77
32	E	101	HEM	C3B-C4B	-7.08	1.45	1.51
28	F	101	SQD	C6-S	-6.98	1.67	1.77
28	L	101	SQD	C6-S	-6.66	1.68	1.77
26	k	101	BCR	C21-C22	-6.64	1.27	1.35
26	c	918	BCR	C21-C22	-6.50	1.27	1.35
28	l	101	SQD	C6-S	-6.48	1.68	1.77
26	H	101	BCR	C21-C22	-6.35	1.27	1.35
26	C	515	BCR	C21-C22	-6.33	1.27	1.35
26	f	101	BCR	C21-C22	-6.30	1.27	1.35
26	D	404	BCR	C21-C22	-6.29	1.27	1.35
26	T	101	BCR	C21-C22	-6.26	1.27	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	915	BCR	C17-C18	-6.25	1.27	1.35
26	Y	101	BCR	C21-C22	-6.25	1.27	1.35
26	h	101	BCR	C21-C22	-6.24	1.27	1.35
26	b	619	BCR	C21-C22	-6.24	1.27	1.35
26	K	101	BCR	C21-C22	-6.22	1.27	1.35
26	C	514	BCR	C17-C18	-6.21	1.27	1.35
26	B	622	BCR	C21-C22	-6.20	1.27	1.35
26	Y	101	BCR	C17-C18	-6.20	1.27	1.35
26	k	101	BCR	C17-C18	-6.18	1.27	1.35
26	f	101	BCR	C17-C18	-6.17	1.27	1.35
26	C	514	BCR	C21-C22	-6.16	1.27	1.35
26	k	102	BCR	C17-C18	-6.12	1.27	1.35
32	e	101	HEM	C3B-C4B	-6.11	1.46	1.51
26	B	619	BCR	C21-C22	-6.09	1.27	1.35
26	b	618	BCR	C17-C18	-6.09	1.27	1.35
26	B	622	BCR	C17-C18	-6.08	1.27	1.35
26	D	404	BCR	C17-C18	-6.04	1.27	1.35
26	B	620	BCR	C21-C22	-6.03	1.27	1.35
26	C	515	BCR	C17-C18	-6.03	1.27	1.35
26	c	915	BCR	C21-C22	-6.00	1.27	1.35
26	b	619	BCR	C17-C18	-5.99	1.27	1.35
26	h	101	BCR	C17-C18	-5.99	1.27	1.35
26	T	101	BCR	C17-C18	-5.98	1.27	1.35
26	T	101	BCR	C16-C15	-5.95	1.19	1.35
26	A	610	BCR	C17-C18	-5.94	1.27	1.35
26	b	619	BCR	C16-C15	-5.94	1.19	1.35
26	C	514	BCR	C16-C15	-5.94	1.19	1.35
26	c	915	BCR	C16-C15	-5.92	1.20	1.35
26	B	618	BCR	C21-C22	-5.90	1.28	1.35
26	k	102	BCR	C21-C22	-5.86	1.28	1.35
26	K	101	BCR	C17-C18	-5.86	1.28	1.35
26	C	515	BCR	C16-C15	-5.84	1.20	1.35
26	k	101	BCR	C16-C15	-5.84	1.20	1.35
26	H	101	BCR	C17-C18	-5.84	1.28	1.35
26	A	610	BCR	C21-C22	-5.83	1.28	1.35
26	k	102	BCR	C16-C15	-5.83	1.20	1.35
26	f	101	BCR	C16-C15	-5.83	1.20	1.35
26	B	622	BCR	C16-C15	-5.83	1.20	1.35
26	b	618	BCR	C21-C22	-5.82	1.28	1.35
26	Y	101	BCR	C16-C15	-5.80	1.20	1.35
26	A	610	BCR	C16-C15	-5.79	1.20	1.35
26	a	409	BCR	C17-C18	-5.75	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	K	101	BCR	C16-C15	-5.74	1.20	1.35
26	h	101	BCR	C16-C15	-5.73	1.20	1.35
26	D	404	BCR	C16-C15	-5.73	1.20	1.35
26	B	620	BCR	C16-C15	-5.72	1.20	1.35
26	B	618	BCR	C16-C15	-5.72	1.20	1.35
26	T	102	BCR	C16-C15	-5.71	1.20	1.35
26	H	101	BCR	C16-C15	-5.70	1.20	1.35
26	B	620	BCR	C17-C18	-5.69	1.28	1.35
26	T	102	BCR	C17-C18	-5.66	1.28	1.35
26	c	918	BCR	C17-C18	-5.65	1.28	1.35
26	a	409	BCR	C16-C15	-5.65	1.20	1.35
26	b	618	BCR	C16-C15	-5.61	1.20	1.35
26	a	409	BCR	C21-C22	-5.61	1.28	1.35
26	T	102	BCR	C21-C22	-5.58	1.28	1.35
26	Y	101	BCR	C11-C12	-5.58	1.19	1.34
26	C	514	BCR	C11-C12	-5.57	1.19	1.34
26	A	610	BCR	C20-C19	-5.56	1.19	1.34
26	k	101	BCR	C11-C12	-5.54	1.20	1.34
26	k	101	BCR	C20-C19	-5.51	1.20	1.34
26	C	515	BCR	C20-C19	-5.50	1.20	1.34
26	k	102	BCR	C20-C19	-5.50	1.20	1.34
26	H	101	BCR	C20-C19	-5.50	1.20	1.34
26	c	918	BCR	C11-C12	-5.49	1.20	1.34
26	B	618	BCR	C17-C18	-5.49	1.28	1.35
26	D	404	BCR	C20-C19	-5.48	1.20	1.34
26	Y	101	BCR	C20-C19	-5.47	1.20	1.34
26	B	620	BCR	C11-C12	-5.47	1.20	1.34
26	T	101	BCR	C11-C12	-5.47	1.20	1.34
26	f	101	BCR	C20-C19	-5.47	1.20	1.34
26	b	619	BCR	C11-C12	-5.45	1.20	1.34
26	C	514	BCR	C20-C19	-5.45	1.20	1.34
26	k	102	BCR	C11-C12	-5.43	1.20	1.34
26	c	915	BCR	C20-C19	-5.43	1.20	1.34
26	B	622	BCR	C11-C12	-5.42	1.20	1.34
32	V	202	HEM	C3D-C4D	-5.42	1.44	1.51
26	D	404	BCR	C11-C12	-5.42	1.20	1.34
26	c	918	BCR	C11-C10	-5.40	1.27	1.43
26	f	101	BCR	C11-C12	-5.39	1.20	1.34
26	B	622	BCR	C20-C19	-5.36	1.20	1.34
26	h	101	BCR	C20-C19	-5.36	1.20	1.34
26	T	101	BCR	C20-C19	-5.36	1.20	1.34
26	C	515	BCR	C11-C12	-5.36	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	H	101	BCR	C11-C10	-5.36	1.27	1.43
26	C	514	BCR	C11-C10	-5.36	1.27	1.43
26	T	102	BCR	C11-C12	-5.34	1.20	1.34
26	D	404	BCR	C11-C10	-5.34	1.27	1.43
26	K	101	BCR	C11-C12	-5.33	1.20	1.34
26	h	101	BCR	C11-C12	-5.33	1.20	1.34
26	B	619	BCR	C17-C18	-5.32	1.28	1.35
26	K	101	BCR	C20-C19	-5.32	1.20	1.34
26	b	618	BCR	C11-C12	-5.32	1.20	1.34
26	c	915	BCR	C11-C12	-5.32	1.20	1.34
26	H	101	BCR	C11-C12	-5.31	1.20	1.34
26	c	918	BCR	C15-C14	-5.31	1.27	1.43
26	B	619	BCR	C16-C15	-5.30	1.21	1.35
26	C	515	BCR	C11-C10	-5.29	1.27	1.43
26	B	620	BCR	C20-C19	-5.29	1.20	1.34
26	k	101	BCR	C11-C10	-5.29	1.27	1.43
26	a	409	BCR	C11-C12	-5.28	1.20	1.34
26	b	619	BCR	C11-C10	-5.26	1.27	1.43
26	B	622	BCR	C11-C10	-5.25	1.27	1.43
26	B	619	BCR	C20-C19	-5.25	1.20	1.34
26	k	101	BCR	C15-C14	-5.24	1.27	1.43
26	T	101	BCR	C11-C10	-5.23	1.27	1.43
26	k	102	BCR	C11-C10	-5.23	1.27	1.43
26	T	101	BCR	C15-C14	-5.22	1.27	1.43
26	Y	101	BCR	C11-C10	-5.22	1.27	1.43
26	f	101	BCR	C15-C14	-5.21	1.27	1.43
26	b	619	BCR	C20-C19	-5.21	1.20	1.34
26	C	514	BCR	C15-C14	-5.21	1.27	1.43
26	k	102	BCR	C15-C14	-5.21	1.27	1.43
26	B	619	BCR	C11-C12	-5.20	1.20	1.34
26	f	101	BCR	C11-C10	-5.19	1.27	1.43
26	A	610	BCR	C11-C10	-5.18	1.27	1.43
26	C	515	BCR	C15-C14	-5.17	1.27	1.43
26	H	101	BCR	C15-C14	-5.16	1.27	1.43
26	B	618	BCR	C11-C12	-5.16	1.21	1.34
26	Y	101	BCR	C15-C14	-5.14	1.27	1.43
26	c	915	BCR	C11-C10	-5.13	1.27	1.43
26	K	101	BCR	C11-C10	-5.13	1.27	1.43
26	h	101	BCR	C11-C10	-5.13	1.27	1.43
26	h	101	BCR	C15-C14	-5.13	1.27	1.43
26	B	620	BCR	C11-C10	-5.12	1.27	1.43
26	A	610	BCR	C11-C12	-5.12	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	618	BCR	C11-C10	-5.12	1.27	1.43
26	T	102	BCR	C20-C19	-5.11	1.21	1.34
26	B	618	BCR	C11-C10	-5.10	1.27	1.43
26	T	102	BCR	C11-C10	-5.10	1.27	1.43
26	b	619	BCR	C15-C14	-5.10	1.27	1.43
26	D	404	BCR	C15-C14	-5.10	1.27	1.43
26	B	622	BCR	C15-C14	-5.09	1.27	1.43
26	b	618	BCR	C20-C19	-5.09	1.21	1.34
26	B	620	BCR	C15-C14	-5.07	1.28	1.43
26	a	409	BCR	C11-C10	-5.07	1.28	1.43
26	a	409	BCR	C20-C19	-5.06	1.21	1.34
26	K	101	BCR	C15-C14	-5.04	1.28	1.43
26	c	915	BCR	C15-C14	-5.03	1.28	1.43
26	B	619	BCR	C11-C10	-5.02	1.28	1.43
26	A	610	BCR	C15-C14	-5.01	1.28	1.43
26	a	409	BCR	C15-C14	-4.99	1.28	1.43
32	v	202	HEM	C3D-C4D	-4.96	1.45	1.51
26	c	918	BCR	C20-C19	-4.96	1.21	1.34
32	e	101	HEM	C3D-C4D	-4.95	1.45	1.51
26	T	102	BCR	C15-C14	-4.94	1.28	1.43
26	B	618	BCR	C20-C19	-4.91	1.21	1.34
26	b	618	BCR	C15-C14	-4.88	1.28	1.43
26	B	619	BCR	C15-C14	-4.85	1.28	1.43
26	B	618	BCR	C15-C14	-4.82	1.28	1.43
32	E	101	HEM	C3D-C4D	-4.76	1.45	1.51
26	c	918	BCR	C23-C22	-4.74	1.35	1.45
26	C	515	BCR	C23-C22	-4.73	1.35	1.45
26	T	101	BCR	C23-C22	-4.72	1.35	1.45
26	k	101	BCR	C23-C22	-4.69	1.35	1.45
26	h	101	BCR	C23-C22	-4.67	1.35	1.45
26	b	618	BCR	C23-C22	-4.67	1.35	1.45
26	D	404	BCR	C23-C22	-4.65	1.35	1.45
26	k	102	BCR	C23-C22	-4.63	1.35	1.45
26	Y	101	BCR	C23-C22	-4.63	1.35	1.45
26	K	101	BCR	C23-C22	-4.60	1.35	1.45
26	B	618	BCR	C23-C22	-4.59	1.35	1.45
26	C	514	BCR	C23-C22	-4.59	1.35	1.45
26	a	409	BCR	C23-C22	-4.57	1.35	1.45
26	f	101	BCR	C23-C22	-4.54	1.35	1.45
26	H	101	BCR	C23-C22	-4.54	1.35	1.45
26	b	619	BCR	C23-C22	-4.44	1.36	1.45
26	c	915	BCR	C23-C22	-4.44	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C23-C22	-4.40	1.36	1.45
26	B	620	BCR	C23-C22	-4.35	1.36	1.45
25	a	412	PHO	C1A-NA	-4.32	1.27	1.37
26	T	102	BCR	C23-C22	-4.31	1.36	1.45
26	c	918	BCR	C16-C17	-4.31	1.30	1.43
26	B	622	BCR	C23-C22	-4.25	1.36	1.45
26	A	610	BCR	C23-C22	-4.25	1.36	1.45
25	D	401	PHO	C1A-NA	-4.06	1.28	1.37
25	A	608	PHO	C1A-NA	-3.92	1.28	1.37
25	d	402	PHO	C1A-NA	-3.87	1.28	1.37
32	E	101	HEM	C2C-C1C	-3.84	1.45	1.52
32	V	202	HEM	C2C-C1C	-3.68	1.45	1.52
32	e	101	HEM	C2C-C1C	-3.66	1.45	1.52
32	v	202	HEM	C2C-C1C	-3.51	1.45	1.52
26	c	918	BCR	C16-C15	-3.22	1.27	1.35
25	D	401	PHO	CHB-C4A	-3.00	1.34	1.40
25	a	412	PHO	C3D-C4D	-2.91	1.34	1.43
25	a	412	PHO	CHB-C4A	-2.84	1.35	1.40
25	A	608	PHO	CHB-C4A	-2.81	1.35	1.40
25	D	401	PHO	C3D-C4D	-2.80	1.34	1.43
25	d	402	PHO	CHB-C4A	-2.80	1.35	1.40
26	c	918	BCR	C24-C25	-2.71	1.35	1.45
25	A	608	PHO	C3D-C4D	-2.71	1.35	1.43
26	K	101	BCR	C24-C25	-2.62	1.35	1.45
26	C	515	BCR	C24-C25	-2.61	1.36	1.45
26	C	514	BCR	C24-C25	-2.60	1.36	1.45
26	H	101	BCR	C24-C25	-2.58	1.36	1.45
26	k	101	BCR	C24-C25	-2.57	1.36	1.45
26	h	101	BCR	C24-C25	-2.57	1.36	1.45
26	Y	101	BCR	C24-C25	-2.56	1.36	1.45
26	B	618	BCR	C24-C25	-2.56	1.36	1.45
26	c	915	BCR	C24-C25	-2.55	1.36	1.45
26	k	102	BCR	C24-C25	-2.54	1.36	1.45
26	T	102	BCR	C24-C25	-2.53	1.36	1.45
26	b	619	BCR	C24-C25	-2.53	1.36	1.45
26	B	620	BCR	C24-C25	-2.53	1.36	1.45
26	A	610	BCR	C24-C25	-2.52	1.36	1.45
25	d	402	PHO	C3D-C4D	-2.52	1.35	1.43
26	B	622	BCR	C24-C25	-2.52	1.36	1.45
26	D	404	BCR	C24-C25	-2.52	1.36	1.45
26	b	618	BCR	C24-C25	-2.49	1.36	1.45
26	f	101	BCR	C24-C25	-2.47	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	101	BCR	C24-C25	-2.46	1.36	1.45
26	B	619	BCR	C24-C25	-2.35	1.36	1.45
24	B	615	CLA	C1C-NC	-2.34	1.33	1.37
26	a	409	BCR	C24-C25	-2.31	1.37	1.45
32	v	202	HEM	C2D-C1D	-2.25	1.44	1.51
32	v	202	HEM	C2B-C1B	-2.23	1.44	1.51
26	B	622	BCR	C8-C7	-2.22	1.26	1.33
24	c	909	CLA	C1C-NC	-2.20	1.34	1.37
24	C	509	CLA	C4C-NC	-2.19	1.34	1.37
31	j	101	DGD	O2G-C2G	-2.16	1.41	1.46
26	T	102	BCR	C8-C7	-2.15	1.26	1.33
32	E	101	HEM	C2D-C1D	-2.11	1.45	1.51
32	V	202	HEM	C2D-C1D	-2.09	1.45	1.51
24	c	909	CLA	C4C-NC	-2.06	1.34	1.37
26	c	915	BCR	C8-C7	-2.05	1.26	1.33
26	c	918	BCR	C8-C7	-2.05	1.26	1.33
26	C	514	BCR	C8-C7	-2.04	1.26	1.33
26	b	619	BCR	C8-C7	-2.04	1.27	1.33
24	c	902	CLA	C4C-NC	-2.02	1.34	1.37
31	C	518	DGD	O2G-C2G	-2.02	1.41	1.46
26	f	101	BCR	C8-C7	-2.01	1.27	1.33
27	a	410	PL9	C2-C3	2.00	1.39	1.34
31	D	406	DGD	O3G-C1D	2.01	1.43	1.40
28	l	101	SQD	O6-C1	2.01	1.43	1.40
24	c	905	CLA	C4C-C3C	2.01	1.48	1.45
24	C	505	CLA	C4C-C3C	2.01	1.48	1.45
24	c	913	CLA	C4C-C3C	2.02	1.48	1.45
24	B	613	CLA	C1C-C2C	2.02	1.48	1.44
24	c	912	CLA	C1C-C2C	2.02	1.48	1.44
24	c	902	CLA	C1C-C2C	2.03	1.48	1.44
32	V	202	HEM	CMA-C3A	2.03	1.55	1.51
32	v	202	HEM	C4C-NC	2.04	1.38	1.36
24	b	609	CLA	C1C-C2C	2.05	1.48	1.44
24	b	614	CLA	C1C-C2C	2.05	1.48	1.44
24	c	904	CLA	C4C-C3C	2.06	1.48	1.45
24	D	403	CLA	C4C-C3C	2.06	1.48	1.45
28	L	101	SQD	O6-C1	2.07	1.43	1.40
24	c	914	CLA	C4C-C3C	2.07	1.48	1.45
24	C	508	CLA	C1C-C2C	2.07	1.48	1.44
24	b	606	CLA	C1C-C2C	2.08	1.48	1.44
32	E	101	HEM	C3C-CAC	2.08	1.55	1.51
24	C	509	CLA	C4C-C3C	2.08	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	d	406	DGD	O5D-C1E	2.08	1.43	1.40
25	D	401	PHO	C3B-C4B	2.09	1.48	1.43
31	D	406	DGD	O5D-C1E	2.10	1.43	1.40
24	b	615	CLA	C1C-C2C	2.10	1.48	1.44
24	C	511	CLA	C1C-C2C	2.11	1.48	1.44
24	c	903	CLA	C1C-C2C	2.12	1.48	1.44
27	d	405	PL9	C2-C3	2.12	1.40	1.34
24	d	403	CLA	C1C-C2C	2.12	1.48	1.44
24	C	512	CLA	C4C-C3C	2.13	1.48	1.45
24	C	510	CLA	C1C-C2C	2.14	1.48	1.44
24	b	610	CLA	C1C-C2C	2.14	1.48	1.44
27	d	405	PL9	C7-C3	2.16	1.53	1.51
24	C	508	CLA	C4C-C3C	2.17	1.48	1.45
24	B	616	CLA	C1C-C2C	2.17	1.48	1.44
24	B	607	CLA	C1C-C2C	2.17	1.48	1.44
24	b	603	CLA	C1C-C2C	2.17	1.48	1.44
24	b	611	CLA	C1C-C2C	2.18	1.49	1.44
24	C	505	CLA	C1C-C2C	2.18	1.49	1.44
24	B	614	CLA	C1C-C2C	2.19	1.49	1.44
24	b	610	CLA	C4C-C3C	2.19	1.49	1.45
32	e	101	HEM	C3C-CAC	2.20	1.55	1.51
24	d	404	CLA	C1C-C2C	2.20	1.49	1.44
27	A	611	PL9	C2-C3	2.20	1.40	1.34
24	D	403	CLA	C1C-C2C	2.20	1.49	1.44
31	h	102	DGD	O5D-C1E	2.21	1.44	1.40
25	a	412	PHO	C3B-C4B	2.22	1.48	1.43
24	B	603	CLA	C1C-C2C	2.22	1.49	1.44
24	c	909	CLA	C1C-C2C	2.24	1.49	1.44
24	b	605	CLA	C1C-C2C	2.25	1.49	1.44
24	d	404	CLA	C4C-C3C	2.25	1.49	1.45
24	c	913	CLA	C1C-C2C	2.26	1.49	1.44
24	b	607	CLA	C1C-C2C	2.27	1.49	1.44
24	C	501	CLA	C1C-C2C	2.27	1.49	1.44
24	b	613	CLA	CHD-C4C	2.28	1.46	1.41
24	C	506	CLA	C1C-C2C	2.28	1.49	1.44
32	e	101	HEM	C3B-CAB	2.28	1.55	1.51
24	d	403	CLA	CHD-C4C	2.28	1.46	1.41
24	b	611	CLA	C4C-C3C	2.29	1.49	1.45
32	e	101	HEM	FE-NB	2.30	2.09	1.97
24	c	907	CLA	C1C-C2C	2.31	1.49	1.44
32	E	101	HEM	FE-ND	2.31	2.09	1.97
32	E	101	HEM	C3B-CAB	2.32	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	V	202	HEM	FE-ND	2.32	2.09	1.97
24	b	617	CLA	C1C-C2C	2.35	1.49	1.44
24	c	909	CLA	CHD-C4C	2.36	1.46	1.41
32	e	101	HEM	FE-ND	2.37	2.10	1.97
24	c	910	CLA	C1C-C2C	2.37	1.49	1.44
32	V	202	HEM	C3C-CAC	2.37	1.55	1.51
27	D	405	PL9	C6-C5	2.38	1.49	1.35
24	c	905	CLA	C1C-C2C	2.40	1.49	1.44
27	d	405	PL9	C6-C5	2.41	1.49	1.35
24	B	606	CLA	CHD-C4C	2.41	1.46	1.41
32	v	202	HEM	FE-NC	2.43	2.05	1.95
24	C	512	CLA	C1C-C2C	2.45	1.49	1.44
27	A	611	PL9	C6-C5	2.45	1.49	1.35
24	A	614	CLA	CHD-C4C	2.45	1.46	1.41
24	C	513	CLA	C1C-C2C	2.45	1.49	1.44
27	a	410	PL9	C6-C5	2.46	1.49	1.35
24	b	605	CLA	CHD-C4C	2.46	1.46	1.41
24	B	605	CLA	C3D-C2D	2.47	1.46	1.40
24	c	906	CLA	C1C-C2C	2.47	1.49	1.44
31	H	102	DGD	O5D-C1E	2.47	1.44	1.40
24	c	904	CLA	C1C-C2C	2.47	1.49	1.44
24	a	406	CLA	C3D-C2D	2.48	1.46	1.40
32	v	202	HEM	C1C-NC	2.49	1.39	1.36
24	b	606	CLA	C3D-C2D	2.49	1.46	1.40
24	D	402	CLA	C3D-C2D	2.49	1.46	1.40
24	c	910	CLA	CHD-C4C	2.49	1.47	1.41
24	c	911	CLA	C3D-C2D	2.50	1.46	1.40
32	V	202	HEM	C1C-NC	2.50	1.39	1.36
24	c	907	CLA	C3D-C2D	2.50	1.46	1.40
24	C	507	CLA	C1C-C2C	2.50	1.49	1.44
32	v	202	HEM	C3C-CAC	2.51	1.56	1.51
24	B	609	CLA	C4B-CHC	2.51	1.46	1.39
24	A	607	CLA	C4B-CHC	2.52	1.46	1.39
24	a	407	CLA	CHD-C4C	2.52	1.47	1.41
24	b	614	CLA	CHD-C4C	2.52	1.47	1.41
24	B	602	CLA	C3D-C2D	2.52	1.46	1.40
24	D	402	CLA	CHD-C4C	2.52	1.47	1.41
24	b	617	CLA	CHD-C4C	2.53	1.47	1.41
24	B	610	CLA	CHD-C4C	2.53	1.47	1.41
24	B	612	CLA	CHD-C4C	2.54	1.47	1.41
24	c	914	CLA	C1C-C2C	2.54	1.49	1.44
32	v	202	HEM	C3B-CAB	2.54	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	e	101	HEM	C1C-NC	2.55	1.39	1.36
24	B	602	CLA	C1C-C2C	2.55	1.49	1.44
24	a	406	CLA	CHD-C4C	2.55	1.47	1.41
24	C	502	CLA	CHD-C4C	2.56	1.47	1.41
32	V	202	HEM	C3B-CAB	2.56	1.56	1.51
24	a	406	CLA	C4B-CHC	2.57	1.46	1.39
24	b	605	CLA	C4B-CHC	2.57	1.46	1.39
24	c	908	CLA	C1C-C2C	2.57	1.49	1.44
24	b	604	CLA	C4B-CHC	2.57	1.46	1.39
24	d	401	CLA	CHD-C4C	2.58	1.47	1.41
24	b	611	CLA	C3D-C2D	2.58	1.46	1.40
24	b	606	CLA	CHD-C4C	2.59	1.47	1.41
24	c	902	CLA	C3D-C2D	2.59	1.46	1.40
24	b	612	CLA	C4B-CHC	2.61	1.47	1.39
24	B	617	CLA	CHD-C4C	2.61	1.47	1.41
24	b	612	CLA	CHD-C4C	2.61	1.47	1.41
24	B	604	CLA	CHD-C4C	2.62	1.47	1.41
24	B	612	CLA	C3D-C2D	2.62	1.46	1.40
25	D	401	PHO	CHD-C4C	2.62	1.46	1.40
24	c	905	CLA	CHD-C4C	2.62	1.47	1.41
24	B	605	CLA	C4B-CHC	2.64	1.47	1.39
24	B	607	CLA	C3D-C2D	2.64	1.46	1.40
24	d	401	CLA	C3D-C2D	2.64	1.46	1.40
24	C	503	CLA	C3D-C2D	2.64	1.46	1.40
24	B	615	CLA	C4B-CHC	2.65	1.47	1.39
24	C	503	CLA	C1C-C2C	2.66	1.49	1.44
25	A	608	PHO	C3D-C2D	2.66	1.46	1.38
24	c	910	CLA	C3D-C2D	2.66	1.46	1.40
24	b	609	CLA	C3D-C2D	2.66	1.46	1.40
24	B	613	CLA	C3D-C2D	2.66	1.46	1.40
25	A	608	PHO	CHC-C4B	2.68	1.47	1.40
24	C	506	CLA	C3D-C2D	2.68	1.46	1.40
24	C	509	CLA	C3D-C2D	2.68	1.46	1.40
24	c	903	CLA	CHD-C4C	2.69	1.47	1.41
24	B	611	CLA	CHD-C4C	2.69	1.47	1.41
32	v	202	HEM	FE-ND	2.69	2.11	1.97
24	C	504	CLA	C4B-CHC	2.69	1.47	1.39
24	B	615	CLA	CHD-C4C	2.69	1.47	1.41
24	b	615	CLA	C3D-C2D	2.70	1.46	1.40
24	A	609	CLA	C3D-C2D	2.70	1.46	1.40
24	C	502	CLA	C3D-C2D	2.70	1.46	1.40
24	b	602	CLA	C1C-C2C	2.71	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	605	CLA	C3D-C2D	2.71	1.46	1.40
24	b	604	CLA	C3D-C2D	2.71	1.46	1.40
24	b	614	CLA	C3D-C2D	2.72	1.46	1.40
24	a	408	CLA	C4B-CHC	2.72	1.47	1.39
24	A	609	CLA	CHD-C4C	2.72	1.47	1.41
24	B	615	CLA	C3D-C2D	2.72	1.46	1.40
24	A	606	CLA	C3D-C2D	2.73	1.46	1.40
24	c	904	CLA	C3D-C2D	2.73	1.46	1.40
24	c	906	CLA	C3D-C2D	2.73	1.46	1.40
24	b	604	CLA	CHD-C4C	2.73	1.47	1.41
24	C	510	CLA	C3D-C2D	2.73	1.46	1.40
24	B	608	CLA	C4B-CHC	2.74	1.47	1.39
24	b	603	CLA	C3D-C2D	2.74	1.46	1.40
25	a	412	PHO	CHD-C4C	2.75	1.47	1.40
24	d	403	CLA	C3D-C2D	2.75	1.46	1.40
24	c	913	CLA	C3D-C2D	2.75	1.46	1.40
24	B	608	CLA	C3D-C2D	2.75	1.46	1.40
24	a	408	CLA	C3D-C2D	2.76	1.46	1.40
24	d	401	CLA	C4B-CHC	2.76	1.47	1.39
24	C	510	CLA	C4B-CHC	2.77	1.47	1.39
24	C	507	CLA	C3D-C2D	2.77	1.46	1.40
24	B	606	CLA	C3D-C2D	2.77	1.46	1.40
24	A	607	CLA	CHD-C4C	2.77	1.47	1.41
24	B	609	CLA	CHD-C4C	2.78	1.47	1.41
24	C	505	CLA	C3D-C2D	2.78	1.46	1.40
24	a	408	CLA	CHD-C4C	2.78	1.47	1.41
24	b	616	CLA	CHD-C4C	2.80	1.47	1.41
24	C	509	CLA	C4B-CHC	2.80	1.47	1.39
24	B	605	CLA	CHD-C4C	2.80	1.47	1.41
24	B	616	CLA	C3D-C2D	2.81	1.46	1.40
24	b	602	CLA	C3D-C2D	2.81	1.46	1.40
24	c	904	CLA	CHD-C4C	2.81	1.47	1.41
24	b	613	CLA	C3D-C2D	2.81	1.46	1.40
24	a	407	CLA	C4B-CHC	2.81	1.47	1.39
24	b	611	CLA	CHD-C4C	2.82	1.47	1.41
24	B	609	CLA	C3D-C2D	2.82	1.46	1.40
24	b	608	CLA	CHD-C4C	2.82	1.47	1.41
24	C	508	CLA	CHD-C4C	2.82	1.47	1.41
24	B	604	CLA	C4B-CHC	2.82	1.47	1.39
24	c	903	CLA	C3D-C2D	2.82	1.46	1.40
24	D	403	CLA	C3D-C2D	2.83	1.46	1.40
24	C	509	CLA	CHD-C4C	2.83	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C3D-C2D	2.83	1.46	1.40
24	b	608	CLA	C4B-CHC	2.83	1.47	1.39
25	A	608	PHO	CHD-C4C	2.83	1.47	1.40
24	B	614	CLA	CHD-C4C	2.83	1.47	1.41
24	b	606	CLA	C4B-CHC	2.84	1.47	1.39
24	b	609	CLA	CHD-C4C	2.84	1.47	1.41
24	b	615	CLA	CHD-C4C	2.84	1.47	1.41
24	c	911	CLA	CHD-C4C	2.84	1.47	1.41
24	b	616	CLA	C4B-CHC	2.85	1.47	1.39
24	c	903	CLA	C4B-CHC	2.85	1.47	1.39
24	A	614	CLA	C4B-CHC	2.85	1.47	1.39
24	A	614	CLA	C1B-CHB	2.86	1.47	1.39
24	B	610	CLA	C3D-C2D	2.86	1.47	1.40
24	b	610	CLA	C4B-CHC	2.86	1.47	1.39
24	B	606	CLA	C4B-CHC	2.87	1.47	1.39
24	c	905	CLA	C3D-C2D	2.87	1.47	1.40
24	B	616	CLA	C4B-CHC	2.87	1.47	1.39
24	A	614	CLA	C3D-C2D	2.87	1.47	1.40
24	d	403	CLA	C4B-CHC	2.87	1.47	1.39
24	b	614	CLA	C4B-CHC	2.87	1.47	1.39
25	A	608	PHO	OBD-CAD	2.87	1.27	1.22
24	c	912	CLA	C3D-C2D	2.87	1.47	1.40
24	A	607	CLA	C1B-CHB	2.88	1.47	1.39
24	d	403	CLA	C1B-CHB	2.88	1.47	1.39
24	B	611	CLA	C3D-C2D	2.88	1.47	1.40
24	C	501	CLA	C3D-C2D	2.88	1.47	1.40
24	A	606	CLA	CHD-C4C	2.88	1.47	1.41
24	c	908	CLA	CHD-C4C	2.88	1.48	1.41
24	c	910	CLA	C4B-CHC	2.89	1.47	1.39
24	c	913	CLA	CHD-C4C	2.90	1.48	1.41
24	a	407	CLA	C3D-C2D	2.90	1.47	1.40
24	c	914	CLA	C3D-C2D	2.90	1.47	1.40
24	a	406	CLA	C1B-CHB	2.90	1.47	1.39
24	B	612	CLA	C4B-CHC	2.90	1.47	1.39
24	b	610	CLA	C3D-C2D	2.91	1.47	1.40
24	c	908	CLA	C3D-C2D	2.91	1.47	1.40
24	A	607	CLA	C3D-C2D	2.91	1.47	1.40
24	c	912	CLA	C4B-CHC	2.91	1.47	1.39
24	b	612	CLA	C3D-C2D	2.92	1.47	1.40
24	c	909	CLA	C3D-C2D	2.92	1.47	1.40
24	c	907	CLA	C4B-CHC	2.92	1.47	1.39
24	c	902	CLA	CHD-C4C	2.92	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	CHD-C4C	2.92	1.48	1.41
24	C	512	CLA	C3D-C2D	2.92	1.47	1.40
24	C	511	CLA	CHD-C4C	2.93	1.48	1.41
24	B	610	CLA	C4B-CHC	2.93	1.47	1.39
24	C	513	CLA	CHD-C4C	2.93	1.48	1.41
24	b	615	CLA	C4B-CHC	2.93	1.47	1.39
24	b	613	CLA	C4B-CHC	2.93	1.47	1.39
24	D	402	CLA	C1B-CHB	2.93	1.47	1.39
24	B	607	CLA	CHD-C4C	2.94	1.48	1.41
24	B	614	CLA	C3D-C2D	2.94	1.47	1.40
24	C	502	CLA	C4B-CHC	2.94	1.47	1.39
24	C	504	CLA	C3D-C2D	2.94	1.47	1.40
24	B	616	CLA	CHD-C4C	2.94	1.48	1.41
24	C	507	CLA	CHD-C4C	2.95	1.48	1.41
24	B	614	CLA	C4B-CHC	2.95	1.48	1.39
24	c	905	CLA	C4B-CHC	2.96	1.48	1.39
24	C	511	CLA	C4B-CHC	2.96	1.48	1.39
24	B	602	CLA	CHD-C4C	2.96	1.48	1.41
24	B	604	CLA	C3D-C2D	2.97	1.47	1.40
24	D	403	CLA	CHD-C4C	2.97	1.48	1.41
24	c	909	CLA	C4B-CHC	2.97	1.48	1.39
25	D	401	PHO	C3D-C2D	2.98	1.46	1.38
24	B	617	CLA	C4B-CHC	2.98	1.48	1.39
24	D	402	CLA	C4B-CHC	2.98	1.48	1.39
24	c	902	CLA	C4B-CHC	2.98	1.48	1.39
24	C	511	CLA	C3D-C2D	2.99	1.47	1.40
24	C	505	CLA	CHD-C4C	2.99	1.48	1.41
24	b	610	CLA	CHD-C4C	2.99	1.48	1.41
24	B	613	CLA	C4B-CHC	2.99	1.48	1.39
25	a	412	PHO	CHC-C4B	3.00	1.47	1.40
24	B	609	CLA	C1B-CHB	3.00	1.48	1.39
25	d	402	PHO	CHC-C4B	3.00	1.47	1.40
29	D	407	LHG	O7-C7	3.01	1.43	1.34
24	C	503	CLA	CHD-C4C	3.01	1.48	1.41
24	b	616	CLA	C3D-C2D	3.01	1.47	1.40
24	c	911	CLA	C4B-CHC	3.01	1.48	1.39
24	b	609	CLA	C4B-CHC	3.01	1.48	1.39
24	b	617	CLA	C3D-C2D	3.01	1.47	1.40
24	c	912	CLA	CHD-C4C	3.01	1.48	1.41
24	C	513	CLA	C3D-C2D	3.01	1.47	1.40
25	d	402	PHO	OBD-CAD	3.01	1.27	1.22
24	b	607	CLA	CHD-C4C	3.01	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	CHD-C4C	3.02	1.48	1.41
24	d	404	CLA	C4B-CHC	3.02	1.48	1.39
24	d	404	CLA	C3D-C2D	3.02	1.47	1.40
24	B	603	CLA	CHD-C4C	3.02	1.48	1.41
24	C	512	CLA	C4B-CHC	3.02	1.48	1.39
24	B	613	CLA	CHD-C4C	3.03	1.48	1.41
24	B	608	CLA	CHD-C4C	3.03	1.48	1.41
24	B	617	CLA	C3D-C2D	3.04	1.47	1.40
24	C	508	CLA	C4B-CHC	3.04	1.48	1.39
24	A	606	CLA	C4B-CHC	3.05	1.48	1.39
24	C	506	CLA	C4B-CHC	3.05	1.48	1.39
25	a	412	PHO	C3D-C2D	3.05	1.47	1.38
32	e	101	HEM	FE-NC	3.06	2.07	1.95
24	b	603	CLA	C4B-CHC	3.07	1.48	1.39
24	B	607	CLA	C4B-CHC	3.07	1.48	1.39
24	B	611	CLA	C4B-CHC	3.07	1.48	1.39
24	D	403	CLA	C4B-CHC	3.08	1.48	1.39
24	c	907	CLA	CHD-C4C	3.08	1.48	1.41
24	B	603	CLA	C3D-C2D	3.09	1.47	1.40
25	d	402	PHO	C3D-C2D	3.09	1.47	1.38
24	B	612	CLA	C1B-CHB	3.09	1.48	1.39
24	C	508	CLA	C3D-C2D	3.10	1.47	1.40
24	A	609	CLA	C4B-CHC	3.10	1.48	1.39
24	c	906	CLA	CHD-C4C	3.11	1.48	1.41
24	d	404	CLA	CHD-C4C	3.12	1.48	1.41
24	b	606	CLA	C1B-CHB	3.12	1.48	1.39
24	C	507	CLA	C4B-CHC	3.12	1.48	1.39
24	B	602	CLA	C1B-CHB	3.12	1.48	1.39
24	b	602	CLA	CHD-C4C	3.13	1.48	1.41
25	D	401	PHO	CHC-C4B	3.13	1.48	1.40
24	b	611	CLA	C1B-CHB	3.14	1.48	1.39
24	c	906	CLA	C4B-CHC	3.14	1.48	1.39
24	C	501	CLA	C4B-CHC	3.14	1.48	1.39
25	a	412	PHO	OBD-CAD	3.14	1.28	1.22
24	b	617	CLA	C4B-CHC	3.15	1.48	1.39
24	C	512	CLA	CHD-C4C	3.15	1.48	1.41
24	b	607	CLA	C4B-CHC	3.15	1.48	1.39
24	C	509	CLA	C1B-CHB	3.16	1.48	1.39
24	C	502	CLA	C1B-CHB	3.17	1.48	1.39
24	C	503	CLA	C1B-CHB	3.17	1.48	1.39
24	C	501	CLA	CHD-C4C	3.17	1.48	1.41
24	A	606	CLA	C1B-CHB	3.17	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	913	CLA	C4B-CHC	3.18	1.48	1.39
24	B	608	CLA	O2A-CGA	3.18	1.42	1.33
24	c	914	CLA	CHD-C4C	3.18	1.48	1.41
24	b	616	CLA	C1B-CHB	3.18	1.48	1.39
24	B	603	CLA	C4B-CHC	3.18	1.48	1.39
24	B	611	CLA	C1B-CHB	3.19	1.48	1.39
24	d	404	CLA	C1B-CHB	3.19	1.48	1.39
31	C	518	DGD	O2G-C1B	3.20	1.43	1.34
24	b	604	CLA	C1B-CHB	3.20	1.48	1.39
24	b	611	CLA	C4B-CHC	3.20	1.48	1.39
24	B	617	CLA	C1B-CHB	3.21	1.48	1.39
24	c	910	CLA	C1B-CHB	3.21	1.48	1.39
24	c	908	CLA	C4B-CHC	3.22	1.48	1.39
24	b	614	CLA	C1B-CHB	3.23	1.48	1.39
24	C	505	CLA	C4B-CHC	3.23	1.48	1.39
24	b	603	CLA	CHD-C4C	3.23	1.48	1.41
24	B	616	CLA	C1B-CHB	3.24	1.48	1.39
24	c	914	CLA	C4B-CHC	3.25	1.48	1.39
24	c	905	CLA	C1B-CHB	3.27	1.48	1.39
24	c	904	CLA	C4B-CHC	3.27	1.48	1.39
24	C	501	CLA	C1B-CHB	3.28	1.48	1.39
24	C	503	CLA	C4B-CHC	3.28	1.48	1.39
24	c	911	CLA	C1B-CHB	3.28	1.48	1.39
24	b	617	CLA	C1B-CHB	3.29	1.48	1.39
24	c	907	CLA	C1B-CHB	3.29	1.48	1.39
24	B	604	CLA	C1B-CHB	3.31	1.49	1.39
24	B	610	CLA	C1B-CHB	3.31	1.49	1.39
24	d	401	CLA	C1B-CHB	3.31	1.49	1.39
24	b	603	CLA	C1B-CHB	3.32	1.49	1.39
24	a	407	CLA	C1B-CHB	3.32	1.49	1.39
24	B	613	CLA	C1B-CHB	3.32	1.49	1.39
24	C	504	CLA	CHD-C4C	3.33	1.49	1.41
24	c	909	CLA	C1B-CHB	3.33	1.49	1.39
24	C	513	CLA	C4B-CHC	3.33	1.49	1.39
25	d	402	PHO	CHD-C4C	3.34	1.48	1.40
31	c	917	DGD	O2G-C1B	3.35	1.44	1.34
24	b	615	CLA	C1B-CHB	3.35	1.49	1.39
24	b	608	CLA	C3D-C2D	3.35	1.48	1.40
24	B	612	CLA	O2A-CGA	3.36	1.43	1.33
24	B	603	CLA	O2A-CGA	3.36	1.43	1.33
24	B	605	CLA	C1B-CHB	3.36	1.49	1.39
29	d	409	LHG	O7-C7	3.37	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	C1B-CHB	3.37	1.49	1.39
24	a	408	CLA	C1B-CHB	3.38	1.49	1.39
24	A	606	CLA	O2A-CGA	3.38	1.43	1.33
25	d	402	PHO	O2A-CGA	3.39	1.43	1.33
24	c	903	CLA	C1B-CHB	3.39	1.49	1.39
24	b	602	CLA	C1B-CHB	3.39	1.49	1.39
31	j	101	DGD	O2G-C1B	3.41	1.44	1.34
24	C	508	CLA	C1B-CHB	3.41	1.49	1.39
24	C	507	CLA	C1B-CHB	3.42	1.49	1.39
24	C	504	CLA	C1B-CHB	3.42	1.49	1.39
31	c	916	DGD	O2G-C1B	3.42	1.44	1.34
24	c	914	CLA	C1B-CHB	3.44	1.49	1.39
24	b	605	CLA	C1B-CHB	3.44	1.49	1.39
24	C	503	CLA	OBD-CAD	3.45	1.27	1.22
24	C	512	CLA	C1B-CHB	3.46	1.49	1.39
24	C	513	CLA	C1B-CHB	3.46	1.49	1.39
24	A	609	CLA	C1B-CHB	3.46	1.49	1.39
24	B	607	CLA	C1B-CHB	3.46	1.49	1.39
24	B	605	CLA	OBD-CAD	3.46	1.27	1.22
24	B	615	CLA	C1B-CHB	3.47	1.49	1.39
24	c	904	CLA	C1B-CHB	3.47	1.49	1.39
24	c	913	CLA	C1B-CHB	3.47	1.49	1.39
24	C	505	CLA	C1B-CHB	3.48	1.49	1.39
24	B	602	CLA	C4B-CHC	3.48	1.49	1.39
29	d	408	LHG	O7-C7	3.48	1.44	1.34
24	b	608	CLA	O2A-CGA	3.49	1.43	1.33
24	C	511	CLA	C1B-CHB	3.50	1.49	1.39
24	b	613	CLA	C1B-CHB	3.50	1.49	1.39
24	c	906	CLA	C1B-CHB	3.50	1.49	1.39
24	a	406	CLA	CHC-C1C	3.51	1.46	1.35
24	b	602	CLA	C4B-CHC	3.51	1.49	1.39
24	b	607	CLA	C1B-CHB	3.52	1.49	1.39
24	c	912	CLA	C1B-CHB	3.52	1.49	1.39
24	b	606	CLA	O2A-CGA	3.52	1.43	1.33
25	D	401	PHO	OBD-CAD	3.53	1.28	1.22
29	d	409	LHG	O8-C23	3.53	1.44	1.33
24	B	603	CLA	C1B-CHB	3.53	1.49	1.39
24	B	606	CLA	C1B-CHB	3.54	1.49	1.39
24	B	614	CLA	C1B-CHB	3.54	1.49	1.39
29	b	620	LHG	O7-C7	3.54	1.44	1.34
24	C	506	CLA	C1B-CHB	3.54	1.49	1.39
24	b	606	CLA	OBD-CAD	3.55	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	408	LHG	O7-C7	3.55	1.44	1.34
24	b	610	CLA	C1B-CHB	3.55	1.49	1.39
31	C	517	DGD	O2G-C1B	3.56	1.44	1.34
24	b	608	CLA	C1B-CHB	3.57	1.49	1.39
24	a	407	CLA	OBD-CAD	3.57	1.27	1.22
24	B	608	CLA	C1B-CHB	3.58	1.49	1.39
24	c	908	CLA	C1B-CHB	3.59	1.49	1.39
24	C	510	CLA	C1B-CHB	3.59	1.49	1.39
24	B	614	CLA	O2A-CGA	3.59	1.44	1.33
24	b	611	CLA	O2A-CGA	3.59	1.44	1.33
25	D	401	PHO	O2A-CGA	3.60	1.44	1.33
24	B	613	CLA	O2A-CGA	3.60	1.44	1.33
29	d	410	LHG	O7-C7	3.60	1.45	1.34
29	B	621	LHG	O7-C7	3.61	1.45	1.34
24	D	403	CLA	C1B-CHB	3.62	1.49	1.39
24	c	902	CLA	C1B-CHB	3.64	1.49	1.39
24	B	606	CLA	O2A-CGA	3.64	1.44	1.33
31	H	102	DGD	O2G-C1B	3.64	1.45	1.34
24	b	604	CLA	O2A-CGA	3.65	1.44	1.33
29	D	409	LHG	O7-C7	3.66	1.45	1.34
24	b	612	CLA	C1B-CHB	3.67	1.50	1.39
24	B	609	CLA	CHC-C1C	3.68	1.46	1.35
24	A	614	CLA	CHC-C1C	3.68	1.46	1.35
24	b	605	CLA	O2A-CGA	3.68	1.44	1.33
24	a	406	CLA	O2A-CGA	3.69	1.44	1.33
24	B	605	CLA	O2A-CGA	3.69	1.44	1.33
24	d	403	CLA	OBD-CAD	3.69	1.28	1.22
24	D	402	CLA	CHC-C1C	3.69	1.46	1.35
25	A	608	PHO	CHD-C1D	3.69	1.45	1.38
24	b	616	CLA	O2A-CGA	3.71	1.44	1.33
24	c	904	CLA	O2A-CGA	3.71	1.44	1.33
31	C	516	DGD	O2G-C1B	3.71	1.45	1.34
25	a	412	PHO	O2A-CGA	3.73	1.44	1.33
24	B	612	CLA	OBD-CAD	3.73	1.28	1.22
24	A	607	CLA	O2A-CGA	3.74	1.44	1.33
31	h	102	DGD	O2G-C1B	3.74	1.45	1.34
24	B	612	CLA	CHC-C1C	3.74	1.47	1.35
24	c	904	CLA	OBD-CAD	3.74	1.28	1.22
24	c	903	CLA	O2A-CGA	3.74	1.44	1.33
24	b	612	CLA	OBD-CAD	3.74	1.28	1.22
24	b	615	CLA	CHC-C1C	3.75	1.47	1.35
24	B	614	CLA	OBD-CAD	3.75	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	O2A-CGA	3.76	1.44	1.33
24	B	611	CLA	O2A-CGA	3.76	1.44	1.33
24	B	605	CLA	CHC-C1C	3.77	1.47	1.35
24	C	505	CLA	O2A-CGA	3.78	1.44	1.33
24	A	607	CLA	CHC-C1C	3.78	1.47	1.35
24	d	403	CLA	O2D-CGD	3.79	1.42	1.33
31	C	516	DGD	O1G-C1A	3.79	1.44	1.33
29	d	410	LHG	O8-C23	3.80	1.44	1.33
24	C	510	CLA	CHC-C1C	3.80	1.47	1.35
28	a	411	SQD	O47-C7	3.80	1.45	1.34
24	a	407	CLA	O2A-CGA	3.82	1.44	1.33
24	B	609	CLA	O2A-CGA	3.82	1.44	1.33
24	c	905	CLA	O2A-CGA	3.82	1.44	1.33
24	c	909	CLA	O2A-CGA	3.82	1.44	1.33
24	C	512	CLA	OBD-CAD	3.82	1.28	1.22
31	c	916	DGD	O1G-C1A	3.82	1.44	1.33
25	A	608	PHO	O2A-CGA	3.82	1.44	1.33
24	d	401	CLA	OBD-CAD	3.83	1.28	1.22
29	D	408	LHG	O8-C23	3.83	1.44	1.33
24	C	510	CLA	O2A-CGA	3.84	1.44	1.33
31	H	102	DGD	O1G-C1A	3.84	1.44	1.33
24	b	615	CLA	OBD-CAD	3.84	1.28	1.22
31	C	518	DGD	O1G-C1A	3.84	1.44	1.33
29	D	407	LHG	O8-C23	3.85	1.44	1.33
24	A	614	CLA	O2A-CGA	3.85	1.44	1.33
24	b	603	CLA	O2A-CGA	3.86	1.44	1.33
24	b	608	CLA	OBD-CAD	3.86	1.28	1.22
24	b	613	CLA	O2A-CGA	3.86	1.45	1.33
24	a	407	CLA	CHC-C1C	3.86	1.47	1.35
28	A	612	SQD	O47-C7	3.87	1.45	1.34
28	A	612	SQD	O48-C23	3.88	1.45	1.33
24	b	612	CLA	O2A-CGA	3.88	1.45	1.33
31	j	101	DGD	O1G-C1A	3.88	1.45	1.33
24	C	504	CLA	O2A-CGA	3.88	1.45	1.33
24	C	508	CLA	O2A-CGA	3.89	1.45	1.33
29	d	408	LHG	O8-C23	3.89	1.45	1.33
24	B	609	CLA	OBD-CAD	3.89	1.28	1.22
24	B	608	CLA	OBD-CAD	3.89	1.28	1.22
29	B	621	LHG	O8-C23	3.89	1.45	1.33
24	B	615	CLA	OBD-CAD	3.90	1.28	1.22
24	c	909	CLA	OBD-CAD	3.90	1.28	1.22
29	b	620	LHG	O8-C23	3.90	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	O2A-CGA	3.91	1.45	1.33
24	B	604	CLA	CHC-C1C	3.92	1.47	1.35
32	E	101	HEM	FE-NC	3.92	2.11	1.95
24	c	910	CLA	CHC-C1C	3.92	1.47	1.35
24	C	502	CLA	O2A-CGA	3.92	1.45	1.33
31	h	102	DGD	O1G-C1A	3.93	1.45	1.33
24	d	403	CLA	CHC-C1C	3.93	1.47	1.35
24	b	605	CLA	OBD-CAD	3.94	1.28	1.22
24	C	501	CLA	O2A-CGA	3.94	1.45	1.33
24	B	615	CLA	O2A-CGA	3.94	1.45	1.33
24	B	613	CLA	OBD-CAD	3.94	1.28	1.22
24	c	906	CLA	O2A-CGA	3.94	1.45	1.33
24	B	606	CLA	OBD-CAD	3.94	1.28	1.22
24	d	401	CLA	O2D-CGD	3.95	1.43	1.33
24	b	610	CLA	O2A-CGA	3.95	1.45	1.33
24	c	911	CLA	CHC-C1C	3.95	1.47	1.35
24	C	504	CLA	CHC-C1C	3.95	1.47	1.35
24	c	909	CLA	CHC-C1C	3.96	1.47	1.35
24	c	907	CLA	CHC-C1C	3.96	1.47	1.35
24	c	903	CLA	CHC-C1C	3.97	1.47	1.35
24	C	509	CLA	CHC-C1C	3.97	1.47	1.35
24	c	902	CLA	CHC-C1C	3.97	1.47	1.35
24	c	911	CLA	O2A-CGA	3.97	1.45	1.33
29	A	615	LHG	O7-C7	3.98	1.46	1.34
24	c	913	CLA	OBD-CAD	3.98	1.28	1.22
24	c	910	CLA	O2A-CGA	3.98	1.45	1.33
28	l	101	SQD	O48-C23	3.98	1.45	1.33
24	b	607	CLA	O2A-CGA	3.98	1.45	1.33
24	B	607	CLA	O2A-CGA	3.99	1.45	1.33
24	c	905	CLA	CHC-C1C	3.99	1.47	1.35
24	B	616	CLA	O2A-CGA	3.99	1.45	1.33
24	B	611	CLA	OBD-CAD	3.99	1.28	1.22
24	B	608	CLA	CHC-C1C	4.00	1.47	1.35
24	b	616	CLA	CHC-C1C	4.00	1.47	1.35
29	D	409	LHG	O8-C23	4.00	1.45	1.33
24	b	614	CLA	CHC-C1C	4.00	1.47	1.35
24	C	511	CLA	CHC-C1C	4.01	1.47	1.35
24	B	610	CLA	O2A-CGA	4.01	1.45	1.33
31	C	517	DGD	O1G-C1A	4.01	1.45	1.33
24	B	616	CLA	OBD-CAD	4.01	1.28	1.22
24	c	907	CLA	OBD-CAD	4.01	1.28	1.22
24	C	511	CLA	O2A-CGA	4.02	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	CLA	CHC-C1C	4.02	1.47	1.35
24	d	401	CLA	O2A-CGA	4.02	1.45	1.33
24	b	617	CLA	OBD-CAD	4.02	1.28	1.22
24	d	401	CLA	CHC-C1C	4.02	1.47	1.35
24	B	616	CLA	CHC-C1C	4.02	1.47	1.35
24	c	908	CLA	CHC-C1C	4.02	1.47	1.35
24	C	506	CLA	OBD-CAD	4.02	1.28	1.22
24	D	403	CLA	O2A-CGA	4.03	1.45	1.33
24	B	617	CLA	CHC-C1C	4.03	1.48	1.35
24	D	403	CLA	OBD-CAD	4.03	1.28	1.22
28	A	613	SQD	O47-C7	4.03	1.46	1.34
24	c	912	CLA	O2A-CGA	4.03	1.45	1.33
24	B	610	CLA	CHC-C1C	4.04	1.48	1.35
24	b	609	CLA	CHC-C1C	4.04	1.48	1.35
24	b	613	CLA	CHC-C1C	4.04	1.48	1.35
24	A	614	CLA	O2D-CGD	4.04	1.43	1.33
24	A	606	CLA	CHC-C1C	4.04	1.48	1.35
24	C	507	CLA	OBD-CAD	4.04	1.28	1.22
24	C	508	CLA	OBD-CAD	4.04	1.28	1.22
24	b	604	CLA	CHC-C1C	4.04	1.48	1.35
24	b	605	CLA	CHC-C1C	4.05	1.48	1.35
24	C	513	CLA	O2A-CGA	4.05	1.45	1.33
24	b	614	CLA	O2A-CGA	4.05	1.45	1.33
24	c	907	CLA	O2A-CGA	4.06	1.45	1.33
24	b	611	CLA	CHC-C1C	4.06	1.48	1.35
24	A	609	CLA	O2A-CGA	4.06	1.45	1.33
24	B	615	CLA	CHC-C1C	4.06	1.48	1.35
24	C	503	CLA	O2A-CGA	4.07	1.45	1.33
31	c	917	DGD	O1G-C1A	4.07	1.45	1.33
24	d	404	CLA	CHC-C1C	4.07	1.48	1.35
24	b	607	CLA	OBD-CAD	4.08	1.28	1.22
29	a	413	LHG	O7-C7	4.08	1.46	1.34
24	b	616	CLA	OBD-CAD	4.08	1.28	1.22
24	b	603	CLA	O2D-CGD	4.09	1.43	1.33
28	a	411	SQD	O48-C23	4.09	1.45	1.33
24	b	606	CLA	CHC-C1C	4.09	1.48	1.35
24	C	505	CLA	OBD-CAD	4.09	1.28	1.22
24	D	403	CLA	CHC-C1C	4.10	1.48	1.35
24	b	607	CLA	CHC-C1C	4.11	1.48	1.35
24	B	614	CLA	CHC-C1C	4.11	1.48	1.35
24	b	612	CLA	CHC-C1C	4.11	1.48	1.35
24	A	609	CLA	CHC-C1C	4.11	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	OBD-CAD	4.11	1.28	1.22
24	C	505	CLA	CHC-C1C	4.12	1.48	1.35
24	C	512	CLA	O2A-CGA	4.12	1.45	1.33
24	C	502	CLA	OBD-CAD	4.12	1.28	1.22
28	l	101	SQD	O47-C7	4.12	1.46	1.34
24	B	611	CLA	CHC-C1C	4.12	1.48	1.35
24	C	508	CLA	CHC-C1C	4.13	1.48	1.35
24	C	509	CLA	O2A-CGA	4.13	1.45	1.33
24	B	610	CLA	OBD-CAD	4.13	1.28	1.22
24	C	507	CLA	O2A-CGA	4.13	1.45	1.33
24	d	404	CLA	OBD-CAD	4.14	1.28	1.22
28	a	402	SQD	O47-C7	4.15	1.46	1.34
24	c	902	CLA	OBD-CAD	4.15	1.28	1.22
24	c	908	CLA	OBD-CAD	4.15	1.28	1.22
24	d	404	CLA	O2A-CGA	4.15	1.45	1.33
24	C	501	CLA	OBD-CAD	4.15	1.28	1.22
24	D	402	CLA	O2A-CGA	4.15	1.45	1.33
24	C	506	CLA	CHC-C1C	4.15	1.48	1.35
24	B	607	CLA	CHC-C1C	4.16	1.48	1.35
24	a	408	CLA	O2A-CGA	4.16	1.45	1.33
24	C	504	CLA	OBD-CAD	4.17	1.28	1.22
24	B	602	CLA	OBD-CAD	4.17	1.28	1.22
24	B	617	CLA	O2A-CGA	4.17	1.45	1.33
28	L	101	SQD	O47-C7	4.17	1.46	1.34
24	B	606	CLA	CHC-C1C	4.19	1.48	1.35
24	c	902	CLA	O2A-CGA	4.19	1.45	1.33
28	d	407	SQD	O47-C7	4.19	1.46	1.34
24	C	501	CLA	CHC-C1C	4.20	1.48	1.35
24	c	913	CLA	CHC-C1C	4.20	1.48	1.35
24	A	609	CLA	O2D-CGD	4.20	1.43	1.33
24	A	607	CLA	OBD-CAD	4.20	1.28	1.22
24	c	912	CLA	CHC-C1C	4.20	1.48	1.35
31	d	406	DGD	O1G-C1A	4.20	1.46	1.33
24	c	908	CLA	O2A-CGA	4.21	1.46	1.33
24	b	602	CLA	OBD-CAD	4.21	1.28	1.22
24	C	506	CLA	O2A-CGA	4.21	1.46	1.33
24	C	513	CLA	OBD-CAD	4.21	1.28	1.22
31	d	406	DGD	O2G-C1B	4.22	1.46	1.34
24	B	603	CLA	O2D-CGD	4.22	1.44	1.33
24	C	513	CLA	CHC-C1C	4.22	1.48	1.35
24	B	602	CLA	CHC-C1C	4.23	1.48	1.35
28	F	101	SQD	O47-C7	4.23	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	CHC-C1C	4.23	1.48	1.35
24	c	914	CLA	O2A-CGA	4.24	1.46	1.33
24	C	507	CLA	CHC-C1C	4.24	1.48	1.35
24	d	403	CLA	O2A-CGA	4.24	1.46	1.33
24	c	905	CLA	OBD-CAD	4.24	1.28	1.22
29	a	413	LHG	O8-C23	4.25	1.46	1.33
31	D	406	DGD	O2G-C1B	4.25	1.47	1.34
24	B	605	CLA	O2D-CGD	4.25	1.44	1.33
24	c	906	CLA	CHC-C1C	4.25	1.48	1.35
24	b	617	CLA	CHC-C1C	4.25	1.48	1.35
24	b	610	CLA	CHC-C1C	4.25	1.48	1.35
24	a	408	CLA	OBD-CAD	4.26	1.28	1.22
24	c	904	CLA	CHC-C1C	4.27	1.48	1.35
24	C	512	CLA	CHC-C1C	4.27	1.48	1.35
24	b	615	CLA	O2A-CGA	4.27	1.46	1.33
24	b	604	CLA	OBD-CAD	4.27	1.28	1.22
24	b	608	CLA	CHC-C1C	4.28	1.48	1.35
24	B	607	CLA	OBD-CAD	4.28	1.28	1.22
28	L	101	SQD	O48-C23	4.28	1.46	1.33
24	B	603	CLA	OBD-CAD	4.29	1.28	1.22
24	c	906	CLA	OBD-CAD	4.29	1.28	1.22
24	c	908	CLA	O2D-CGD	4.29	1.44	1.33
25	d	402	PHO	CHD-C1D	4.29	1.47	1.38
24	B	604	CLA	OBD-CAD	4.29	1.28	1.22
24	B	610	CLA	O2D-CGD	4.29	1.44	1.33
24	b	603	CLA	CHC-C1C	4.29	1.48	1.35
28	d	407	SQD	O48-C23	4.30	1.46	1.33
24	C	511	CLA	OBD-CAD	4.30	1.28	1.22
24	C	502	CLA	CHC-C1C	4.30	1.48	1.35
24	b	617	CLA	O2A-CGA	4.30	1.46	1.33
24	B	614	CLA	O2D-CGD	4.31	1.44	1.33
24	c	911	CLA	OBD-CAD	4.32	1.28	1.22
24	D	402	CLA	OBD-CAD	4.32	1.28	1.22
24	c	906	CLA	O2D-CGD	4.32	1.44	1.33
28	A	613	SQD	O48-C23	4.33	1.46	1.33
24	B	613	CLA	CHC-C1C	4.33	1.48	1.35
25	A	608	PHO	CHC-C1C	4.33	1.47	1.38
24	B	612	CLA	O2D-CGD	4.33	1.44	1.33
24	c	913	CLA	O2A-CGA	4.33	1.46	1.33
24	c	914	CLA	CHC-C1C	4.35	1.49	1.35
24	A	606	CLA	OBD-CAD	4.35	1.29	1.22
28	a	402	SQD	O48-C23	4.35	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	615	LHG	O8-C23	4.35	1.46	1.33
24	c	912	CLA	OBD-CAD	4.36	1.29	1.22
24	c	903	CLA	OBD-CAD	4.36	1.29	1.22
25	a	412	PHO	CHD-C1D	4.36	1.47	1.38
24	B	611	CLA	O2D-CGD	4.36	1.44	1.33
24	c	914	CLA	OBD-CAD	4.37	1.29	1.22
24	B	617	CLA	OBD-CAD	4.37	1.29	1.22
24	b	609	CLA	OBD-CAD	4.39	1.29	1.22
25	A	608	PHO	O2D-CGD	4.39	1.44	1.33
31	D	406	DGD	O1G-C1A	4.40	1.46	1.33
24	B	603	CLA	CHC-C1C	4.40	1.49	1.35
24	a	407	CLA	C3B-C2B	4.41	1.46	1.40
24	b	611	CLA	OBD-CAD	4.43	1.29	1.22
25	D	401	PHO	CHD-C1D	4.44	1.47	1.38
28	F	101	SQD	O48-C23	4.45	1.46	1.33
24	d	404	CLA	O2D-CGD	4.45	1.44	1.33
24	A	614	CLA	OBD-CAD	4.45	1.29	1.22
24	b	602	CLA	CHC-C1C	4.45	1.49	1.35
24	a	406	CLA	O2D-CGD	4.45	1.44	1.33
24	A	607	CLA	O2D-CGD	4.45	1.44	1.33
25	d	402	PHO	CHC-C1C	4.46	1.47	1.38
24	b	610	CLA	OBD-CAD	4.47	1.29	1.22
24	D	402	CLA	O2D-CGD	4.47	1.44	1.33
24	C	501	CLA	O2D-CGD	4.48	1.44	1.33
24	D	403	CLA	O2D-CGD	4.49	1.44	1.33
24	C	504	CLA	O2D-CGD	4.49	1.44	1.33
24	C	510	CLA	OBD-CAD	4.50	1.29	1.22
24	b	614	CLA	OBD-CAD	4.52	1.29	1.22
24	b	606	CLA	C3B-C2B	4.53	1.46	1.40
24	B	608	CLA	O2D-CGD	4.54	1.44	1.33
24	C	503	CLA	O2D-CGD	4.55	1.44	1.33
24	C	509	CLA	OBD-CAD	4.55	1.29	1.22
24	b	605	CLA	O2D-CGD	4.56	1.44	1.33
24	a	408	CLA	O2D-CGD	4.56	1.44	1.33
24	b	609	CLA	O2D-CGD	4.57	1.44	1.33
24	b	603	CLA	OBD-CAD	4.57	1.29	1.22
24	c	902	CLA	O2D-CGD	4.57	1.44	1.33
24	b	602	CLA	O2A-CGA	4.58	1.47	1.33
24	b	615	CLA	O2D-CGD	4.58	1.44	1.33
24	B	615	CLA	O2D-CGD	4.60	1.44	1.33
24	B	602	CLA	O2A-CGA	4.61	1.47	1.33
24	A	609	CLA	OBD-CAD	4.61	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	612	CLA	C3C-C2C	4.62	1.46	1.36
24	b	612	CLA	O2D-CGD	4.63	1.45	1.33
24	B	613	CLA	O2D-CGD	4.63	1.45	1.33
24	b	613	CLA	O2D-CGD	4.63	1.45	1.33
25	D	401	PHO	CHC-C1C	4.64	1.47	1.38
24	b	612	CLA	C3C-C2C	4.66	1.46	1.36
24	B	604	CLA	O2D-CGD	4.66	1.45	1.33
24	c	904	CLA	O2D-CGD	4.66	1.45	1.33
24	B	606	CLA	O2D-CGD	4.67	1.45	1.33
24	a	407	CLA	O2D-CGD	4.67	1.45	1.33
24	C	510	CLA	O2D-CGD	4.68	1.45	1.33
24	A	606	CLA	O2D-CGD	4.68	1.45	1.33
24	B	616	CLA	O2D-CGD	4.69	1.45	1.33
24	b	608	CLA	O2D-CGD	4.70	1.45	1.33
24	B	617	CLA	O2D-CGD	4.70	1.45	1.33
24	a	406	CLA	OBD-CAD	4.71	1.29	1.22
24	B	607	CLA	O2D-CGD	4.71	1.45	1.33
24	B	612	CLA	C3B-C2B	4.71	1.46	1.40
24	B	604	CLA	C3C-C2C	4.73	1.46	1.36
24	C	505	CLA	O2D-CGD	4.73	1.45	1.33
24	A	607	CLA	C3C-C2C	4.73	1.46	1.36
24	B	606	CLA	C3B-C2B	4.74	1.46	1.40
25	D	401	PHO	O2D-CGD	4.74	1.45	1.33
25	d	402	PHO	O2D-CGD	4.76	1.45	1.33
24	C	502	CLA	O2D-CGD	4.78	1.45	1.33
24	b	615	CLA	C3C-C2C	4.79	1.47	1.36
24	b	614	CLA	O2D-CGD	4.79	1.45	1.33
24	B	613	CLA	C3C-C2C	4.79	1.47	1.36
24	B	615	CLA	C3C-C2C	4.79	1.47	1.36
24	c	903	CLA	C3C-C2C	4.80	1.47	1.36
24	b	611	CLA	O2D-CGD	4.80	1.45	1.33
24	B	609	CLA	O2D-CGD	4.81	1.45	1.33
24	c	910	CLA	O2D-CGD	4.81	1.45	1.33
24	a	406	CLA	C3C-C2C	4.81	1.47	1.36
25	a	412	PHO	O2D-CGD	4.82	1.45	1.33
24	C	512	CLA	O2D-CGD	4.82	1.45	1.33
24	b	604	CLA	O2D-CGD	4.82	1.45	1.33
24	C	502	CLA	C3C-C2C	4.82	1.47	1.36
24	C	507	CLA	O2D-CGD	4.83	1.45	1.33
24	A	614	CLA	C3C-C2C	4.83	1.47	1.36
25	D	401	PHO	C3C-C2C	4.83	1.47	1.36
24	c	906	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	C3B-C2B	4.85	1.46	1.40
24	B	615	CLA	C3B-C2B	4.86	1.46	1.40
24	C	511	CLA	O2D-CGD	4.86	1.45	1.33
24	B	605	CLA	C3B-C2B	4.87	1.46	1.40
24	C	508	CLA	O2D-CGD	4.87	1.45	1.33
24	b	607	CLA	O2D-CGD	4.87	1.45	1.33
24	b	617	CLA	C3C-C2C	4.88	1.47	1.36
24	b	606	CLA	C3C-C2C	4.88	1.47	1.36
24	c	912	CLA	O2D-CGD	4.88	1.45	1.33
24	b	617	CLA	O2D-CGD	4.88	1.45	1.33
24	C	504	CLA	C3C-C2C	4.88	1.47	1.36
24	b	616	CLA	C3C-C2C	4.88	1.47	1.36
24	c	911	CLA	O2D-CGD	4.88	1.45	1.33
24	b	616	CLA	O2D-CGD	4.88	1.45	1.33
24	B	610	CLA	C3C-C2C	4.89	1.47	1.36
24	B	605	CLA	C3C-C2C	4.89	1.47	1.36
24	C	506	CLA	O2D-CGD	4.89	1.45	1.33
24	C	509	CLA	O2D-CGD	4.90	1.45	1.33
24	C	501	CLA	C3C-C2C	4.91	1.47	1.36
25	A	608	PHO	C3C-C2C	4.91	1.47	1.36
24	C	513	CLA	O2D-CGD	4.91	1.45	1.33
24	D	402	CLA	C3C-C2C	4.91	1.47	1.36
24	c	902	CLA	C3C-C2C	4.92	1.47	1.36
24	b	614	CLA	C3C-C2C	4.92	1.47	1.36
24	a	407	CLA	C3C-C2C	4.93	1.47	1.36
24	c	910	CLA	C3C-C2C	4.93	1.47	1.36
24	a	408	CLA	C3C-C2C	4.93	1.47	1.36
24	c	913	CLA	O2D-CGD	4.93	1.45	1.33
25	d	402	PHO	CHB-C1B	4.93	1.48	1.38
24	B	614	CLA	C3C-C2C	4.93	1.47	1.36
24	C	509	CLA	C3C-C2C	4.93	1.47	1.36
24	c	903	CLA	O2D-CGD	4.95	1.45	1.33
24	B	617	CLA	C3C-C2C	4.96	1.47	1.36
24	C	506	CLA	C3C-C2C	4.96	1.47	1.36
24	c	905	CLA	O2D-CGD	4.97	1.45	1.33
24	b	613	CLA	C3B-C2B	4.97	1.46	1.40
24	b	606	CLA	O2D-CGD	4.98	1.45	1.33
24	C	511	CLA	C3C-C2C	4.98	1.47	1.36
24	d	403	CLA	C3C-C2C	4.99	1.47	1.36
24	c	909	CLA	O2D-CGD	4.99	1.45	1.33
24	B	608	CLA	C3C-C2C	4.99	1.47	1.36
24	A	609	CLA	C3C-C2C	5.00	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	O2D-CGD	5.00	1.46	1.33
24	C	502	CLA	C3B-C2B	5.00	1.46	1.40
24	b	609	CLA	C3C-C2C	5.00	1.47	1.36
24	B	609	CLA	C3C-C2C	5.00	1.47	1.36
24	b	605	CLA	C3B-C2B	5.01	1.46	1.40
24	b	605	CLA	C3C-C2C	5.01	1.47	1.36
24	B	616	CLA	C3B-C2B	5.01	1.46	1.40
24	b	613	CLA	C3C-C2C	5.02	1.47	1.36
24	b	610	CLA	O2D-CGD	5.02	1.46	1.33
24	c	914	CLA	O2D-CGD	5.02	1.46	1.33
25	a	412	PHO	C3C-C2C	5.04	1.47	1.36
24	b	604	CLA	C3C-C2C	5.04	1.47	1.36
24	c	907	CLA	O2D-CGD	5.04	1.46	1.33
24	D	403	CLA	C3C-C2C	5.04	1.47	1.36
24	c	911	CLA	C3C-C2C	5.04	1.47	1.36
24	C	505	CLA	C3C-C2C	5.06	1.47	1.36
24	C	510	CLA	C3C-C2C	5.06	1.47	1.36
24	A	607	CLA	C3B-C2B	5.06	1.47	1.40
25	D	401	PHO	CHB-C1B	5.07	1.48	1.38
24	b	610	CLA	C3C-C2C	5.07	1.47	1.36
24	b	610	CLA	C3B-C2B	5.07	1.47	1.40
24	B	606	CLA	C3C-C2C	5.07	1.47	1.36
25	d	402	PHO	C3B-C2B	5.07	1.47	1.36
24	c	912	CLA	C3C-C2C	5.08	1.47	1.36
24	B	610	CLA	C3B-C2B	5.08	1.47	1.40
24	b	602	CLA	C3C-C2C	5.08	1.47	1.36
24	d	401	CLA	C3B-C2B	5.12	1.47	1.40
24	B	602	CLA	C3C-C2C	5.12	1.47	1.36
24	B	611	CLA	C3C-C2C	5.12	1.47	1.36
24	A	614	CLA	C3B-C2B	5.12	1.47	1.40
25	a	412	PHO	C3B-C2B	5.12	1.47	1.36
24	B	611	CLA	C3B-C2B	5.12	1.47	1.40
24	B	607	CLA	C3C-C2C	5.13	1.47	1.36
24	b	608	CLA	C3B-C2B	5.13	1.47	1.40
24	c	909	CLA	C3B-C2B	5.13	1.47	1.40
24	A	606	CLA	C3C-C2C	5.15	1.47	1.36
24	b	615	CLA	C3B-C2B	5.15	1.47	1.40
25	d	402	PHO	C3C-C2C	5.15	1.47	1.36
24	b	607	CLA	C3C-C2C	5.17	1.47	1.36
24	C	511	CLA	C3B-C2B	5.17	1.47	1.40
24	d	401	CLA	C3C-C2C	5.17	1.47	1.36
24	B	616	CLA	C3C-C2C	5.19	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	C3C-C2C	5.19	1.47	1.36
24	c	907	CLA	C3C-C2C	5.20	1.47	1.36
24	B	602	CLA	C3B-C2B	5.21	1.47	1.40
24	C	507	CLA	C3C-C2C	5.21	1.48	1.36
24	B	614	CLA	C3B-C2B	5.23	1.47	1.40
24	c	904	CLA	C3C-C2C	5.23	1.48	1.36
24	c	910	CLA	OBD-CAD	5.23	1.30	1.22
24	b	602	CLA	O2D-CGD	5.23	1.46	1.33
24	c	909	CLA	C3C-C2C	5.24	1.48	1.36
25	a	412	PHO	CHC-C1C	5.24	1.48	1.38
24	C	509	CLA	C3B-C2B	5.24	1.47	1.40
24	a	406	CLA	C3B-C2B	5.25	1.47	1.40
25	A	608	PHO	C3B-C2B	5.25	1.47	1.36
24	b	604	CLA	C3B-C2B	5.26	1.47	1.40
24	b	608	CLA	C3C-C2C	5.27	1.48	1.36
24	c	908	CLA	C3C-C2C	5.27	1.48	1.36
24	C	510	CLA	C3B-C2B	5.28	1.47	1.40
24	b	611	CLA	C3C-C2C	5.28	1.48	1.36
24	C	513	CLA	C3C-C2C	5.28	1.48	1.36
24	B	608	CLA	C3B-C2B	5.30	1.47	1.40
24	b	603	CLA	C3C-C2C	5.31	1.48	1.36
24	C	503	CLA	C3C-C2C	5.32	1.48	1.36
24	C	512	CLA	C3C-C2C	5.33	1.48	1.36
24	A	606	CLA	C3B-C2B	5.33	1.47	1.40
24	B	604	CLA	C3B-C2B	5.33	1.47	1.40
24	c	913	CLA	C3C-C2C	5.34	1.48	1.36
24	b	614	CLA	C3B-C2B	5.36	1.47	1.40
24	C	506	CLA	C3B-C2B	5.37	1.47	1.40
24	B	603	CLA	C3C-C2C	5.38	1.48	1.36
24	B	607	CLA	C3B-C2B	5.39	1.47	1.40
24	B	609	CLA	C3B-C2B	5.39	1.47	1.40
24	c	905	CLA	C3C-C2C	5.40	1.48	1.36
24	c	914	CLA	C3C-C2C	5.41	1.48	1.36
24	A	609	CLA	C3B-C2B	5.41	1.47	1.40
25	A	608	PHO	CHB-C1B	5.42	1.49	1.38
24	c	905	CLA	C3B-C2B	5.45	1.47	1.40
24	D	403	CLA	C3B-C2B	5.45	1.47	1.40
24	C	508	CLA	C3C-C2C	5.46	1.48	1.36
24	d	403	CLA	C3B-C2B	5.47	1.47	1.40
24	c	913	CLA	C3B-C2B	5.49	1.47	1.40
24	b	602	CLA	C3B-C2B	5.50	1.47	1.40
24	c	911	CLA	C3B-C2B	5.51	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	908	CLA	C3B-C2B	5.51	1.47	1.40
24	b	609	CLA	C3B-C2B	5.52	1.47	1.40
24	D	402	CLA	C3B-C2B	5.53	1.47	1.40
25	D	401	PHO	C3B-C2B	5.54	1.48	1.36
24	C	505	CLA	C3B-C2B	5.55	1.47	1.40
24	C	504	CLA	C3B-C2B	5.58	1.47	1.40
24	a	408	CLA	C3B-C2B	5.58	1.47	1.40
24	B	613	CLA	C3B-C2B	5.59	1.47	1.40
24	b	603	CLA	C3B-C2B	5.59	1.47	1.40
24	c	907	CLA	C3B-C2B	5.61	1.47	1.40
24	b	612	CLA	C3B-C2B	5.62	1.47	1.40
24	c	903	CLA	C3B-C2B	5.66	1.47	1.40
24	c	910	CLA	C3B-C2B	5.66	1.47	1.40
24	b	616	CLA	C3B-C2B	5.67	1.47	1.40
24	C	512	CLA	C3B-C2B	5.67	1.47	1.40
24	C	501	CLA	C3B-C2B	5.71	1.47	1.40
25	a	412	PHO	CHB-C1B	5.72	1.49	1.38
24	b	607	CLA	C3B-C2B	5.72	1.47	1.40
24	d	404	CLA	C3B-C2B	5.75	1.47	1.40
24	c	904	CLA	C3B-C2B	5.76	1.47	1.40
24	c	906	CLA	C3B-C2B	5.76	1.47	1.40
24	c	914	CLA	C3B-C2B	5.79	1.47	1.40
24	b	617	CLA	C3B-C2B	5.82	1.48	1.40
24	c	902	CLA	C3B-C2B	5.85	1.48	1.40
24	C	503	CLA	C3B-C2B	5.85	1.48	1.40
24	B	617	CLA	C3B-C2B	5.86	1.48	1.40
24	C	508	CLA	C3B-C2B	5.88	1.48	1.40
24	c	912	CLA	C3B-C2B	5.94	1.48	1.40
24	B	603	CLA	C3B-C2B	5.97	1.48	1.40
24	C	513	CLA	C3B-C2B	6.18	1.48	1.40
24	C	507	CLA	C3B-C2B	6.36	1.48	1.40

All (2127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	620	BCR	C36-C18-C17	-10.02	108.10	122.90
26	A	610	BCR	C37-C22-C21	-9.26	109.22	122.90
26	D	404	BCR	C30-C25-C26	-8.76	109.80	122.66
26	Y	101	BCR	C33-C5-C4	-8.54	97.23	113.43
26	B	619	BCR	C36-C18-C19	-8.30	104.28	118.10
26	B	618	BCR	C36-C18-C17	-8.23	110.75	122.90
26	b	618	BCR	C36-C18-C17	-8.06	111.00	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	618	BCR	C36-C18-C19	-7.89	104.96	118.10
26	A	610	BCR	C36-C18-C17	-7.85	111.31	122.90
26	T	102	BCR	C36-C18-C17	-7.71	111.51	122.90
26	b	619	BCR	C36-C18-C17	-7.47	111.87	122.90
26	C	514	BCR	C38-C26-C27	-7.43	99.34	113.43
26	A	610	BCR	C35-C13-C14	-7.42	111.94	122.90
26	f	101	BCR	C30-C25-C26	-7.37	111.84	122.66
26	k	102	BCR	C37-C22-C21	-7.27	112.16	122.90
26	B	618	BCR	C35-C13-C12	-7.26	106.01	118.10
26	a	409	BCR	C36-C18-C17	-7.22	112.24	122.90
26	k	101	BCR	C36-C18-C19	-7.21	106.10	118.10
26	H	101	BCR	C37-C22-C21	-7.06	112.47	122.90
26	a	409	BCR	C37-C22-C21	-7.05	112.49	122.90
26	k	101	BCR	C33-C5-C4	-7.04	100.08	113.43
26	B	619	BCR	C30-C25-C26	-6.96	112.44	122.66
26	B	618	BCR	C36-C18-C19	-6.92	106.57	118.10
26	Y	101	BCR	C37-C22-C21	-6.82	112.83	122.90
26	A	610	BCR	C38-C26-C27	-6.80	100.53	113.43
26	k	102	BCR	C36-C18-C17	-6.79	112.88	122.90
26	T	101	BCR	C36-C18-C17	-6.76	112.91	122.90
26	H	101	BCR	C36-C18-C19	-6.49	107.30	118.10
26	Y	101	BCR	C36-C18-C19	-6.48	107.32	118.10
26	C	514	BCR	C36-C18-C17	-6.46	113.36	122.90
26	b	619	BCR	C37-C22-C21	-6.44	113.39	122.90
26	f	101	BCR	C36-C18-C19	-6.40	107.44	118.10
26	k	102	BCR	C38-C26-C27	-6.40	101.30	113.43
26	B	622	BCR	C36-C18-C17	-6.38	113.48	122.90
26	h	101	BCR	C36-C18-C17	-6.38	113.48	122.90
26	b	619	BCR	C33-C5-C4	-6.30	101.48	113.43
26	K	101	BCR	C36-C18-C19	-6.24	107.70	118.10
26	B	618	BCR	C34-C9-C10	-6.22	113.72	122.90
26	T	102	BCR	C35-C13-C14	-6.21	113.72	122.90
26	K	101	BCR	C37-C22-C21	-6.14	113.83	122.90
26	c	915	BCR	C36-C18-C17	-6.07	113.93	122.90
26	b	618	BCR	C38-C26-C27	-6.07	101.92	113.43
26	f	101	BCR	C37-C22-C21	-5.85	114.26	122.90
26	B	619	BCR	C38-C26-C27	-5.84	102.35	113.43
26	H	101	BCR	C33-C5-C4	-5.81	102.40	113.43
26	Y	101	BCR	C36-C18-C17	-5.81	114.32	122.90
26	b	618	BCR	C35-C13-C14	-5.75	114.41	122.90
26	b	618	BCR	C33-C5-C4	-5.71	102.61	113.43
26	a	409	BCR	C35-C13-C14	-5.68	114.51	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	622	BCR	C37-C22-C21	-5.67	114.52	122.90
26	H	101	BCR	C34-C9-C10	-5.67	114.53	122.90
26	T	102	BCR	C38-C26-C27	-5.64	102.74	113.43
26	K	101	BCR	C36-C18-C17	-5.62	114.59	122.90
26	D	404	BCR	C39-C30-C29	-5.62	88.67	108.79
26	b	619	BCR	C38-C26-C27	-5.62	102.78	113.43
26	B	618	BCR	C38-C26-C27	-5.59	102.84	113.43
26	k	102	BCR	C33-C5-C4	-5.58	102.84	113.43
26	H	101	BCR	C30-C25-C26	-5.58	114.46	122.66
26	a	409	BCR	C37-C22-C23	-5.56	108.84	118.10
26	B	619	BCR	C37-C22-C21	-5.54	114.72	122.90
26	Y	101	BCR	C30-C25-C26	-5.51	114.57	122.66
26	k	101	BCR	C37-C22-C21	-5.49	114.79	122.90
26	B	619	BCR	C36-C18-C17	-5.49	114.79	122.90
26	B	619	BCR	C35-C13-C14	-5.47	114.82	122.90
26	c	918	BCR	C38-C26-C27	-5.45	103.09	113.43
26	h	101	BCR	C37-C22-C21	-5.44	114.87	122.90
26	f	101	BCR	C36-C18-C17	-5.43	114.88	122.90
26	k	101	BCR	C38-C26-C27	-5.42	103.14	113.43
26	f	101	BCR	C39-C30-C29	-5.41	89.41	108.79
26	B	620	BCR	C33-C5-C4	-5.41	103.18	113.43
26	b	618	BCR	C37-C22-C21	-5.27	115.11	122.90
26	b	618	BCR	C30-C25-C26	-5.22	114.99	122.66
26	B	622	BCR	C33-C5-C4	-5.19	103.59	113.43
26	A	610	BCR	C30-C25-C26	-5.16	115.08	122.66
26	D	404	BCR	C36-C18-C17	-5.10	115.36	122.90
26	k	101	BCR	C36-C18-C17	-5.08	115.39	122.90
26	b	618	BCR	C34-C9-C8	-5.02	109.74	118.10
26	C	514	BCR	C33-C5-C4	-5.00	103.95	113.43
26	f	101	BCR	C38-C26-C27	-5.00	103.95	113.43
26	c	915	BCR	C37-C22-C21	-4.98	115.55	122.90
26	H	101	BCR	C35-C13-C12	-4.98	109.81	118.10
26	B	620	BCR	C37-C22-C23	-4.95	109.86	118.10
26	K	101	BCR	C35-C13-C14	-4.95	115.59	122.90
26	b	618	BCR	C37-C22-C23	-4.94	109.87	118.10
26	C	515	BCR	C38-C26-C27	-4.94	104.06	113.43
26	C	515	BCR	C35-C13-C12	-4.93	109.89	118.10
26	C	515	BCR	C37-C22-C21	-4.90	115.66	122.90
26	T	101	BCR	C33-C5-C4	-4.90	104.15	113.43
26	b	619	BCR	C36-C18-C19	-4.87	109.98	118.10
26	Y	101	BCR	C34-C9-C10	-4.87	115.71	122.90
26	T	101	BCR	C38-C26-C27	-4.85	104.23	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	409	BCR	C30-C25-C26	-4.85	115.54	122.66
26	D	404	BCR	C34-C9-C10	-4.83	115.77	122.90
26	b	618	BCR	C35-C13-C12	-4.81	110.09	118.10
26	k	101	BCR	C35-C13-C14	-4.77	115.86	122.90
26	C	515	BCR	C36-C18-C19	-4.74	110.21	118.10
26	Y	101	BCR	C35-C13-C14	-4.72	115.92	122.90
27	a	410	PL9	C7-C3-C2	-4.70	119.52	123.42
26	c	918	BCR	C37-C22-C21	-4.69	115.97	122.90
26	c	918	BCR	C33-C5-C4	-4.67	104.57	113.43
26	h	101	BCR	C38-C26-C27	-4.65	104.61	113.43
26	B	619	BCR	C33-C5-C4	-4.64	104.63	113.43
26	h	101	BCR	C34-C9-C10	-4.64	116.05	122.90
26	B	622	BCR	C36-C18-C19	-4.62	110.40	118.10
26	C	515	BCR	C36-C18-C17	-4.61	116.09	122.90
25	A	608	PHO	C3D-C2D-C1D	-4.60	98.38	105.77
26	D	404	BCR	C33-C5-C4	-4.57	104.77	113.43
26	b	619	BCR	C39-C30-C29	-4.52	92.59	108.79
24	A	614	CLA	C1C-C2C-C3C	-4.51	101.52	106.91
26	A	610	BCR	C36-C18-C19	-4.49	110.61	118.10
26	a	409	BCR	C36-C18-C19	-4.49	110.63	118.10
32	E	101	HEM	CBD-CAD-C3D	-4.43	100.67	113.55
26	K	101	BCR	C35-C13-C12	-4.41	110.75	118.10
26	a	409	BCR	C35-C13-C12	-4.41	110.76	118.10
26	h	101	BCR	C33-C5-C4	-4.39	105.10	113.43
26	k	102	BCR	C36-C18-C19	-4.39	110.79	118.10
26	C	514	BCR	C35-C13-C12	-4.38	110.80	118.10
25	D	401	PHO	C4C-C3C-C2C	-4.37	101.94	106.81
25	D	401	PHO	C3D-C2D-C1D	-4.36	98.77	105.77
26	k	101	BCR	C30-C25-C26	-4.35	116.27	122.66
26	C	515	BCR	C35-C13-C14	-4.35	116.47	122.90
26	f	101	BCR	C32-C1-C2	-4.35	93.21	108.79
26	T	102	BCR	C36-C18-C19	-4.33	110.88	118.10
26	k	101	BCR	C1-C6-C5	-4.33	116.30	122.66
26	C	515	BCR	C31-C1-C2	-4.33	93.28	108.79
24	A	607	CLA	C1C-C2C-C3C	-4.31	101.75	106.91
26	T	102	BCR	C39-C30-C29	-4.29	93.41	108.79
26	C	514	BCR	C32-C1-C2	-4.29	93.44	108.79
26	B	619	BCR	C40-C30-C29	-4.29	93.44	108.79
26	c	915	BCR	C35-C13-C14	-4.29	116.57	122.90
26	D	404	BCR	C38-C26-C27	-4.28	105.31	113.43
26	B	620	BCR	C34-C9-C8	-4.26	111.00	118.10
26	D	404	BCR	C35-C13-C12	-4.26	111.01	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	618	BCR	C37-C22-C23	-4.24	111.04	118.10
26	Y	101	BCR	C1-C6-C5	-4.22	116.46	122.66
26	C	514	BCR	C30-C25-C26	-4.21	116.47	122.66
25	a	412	PHO	C3D-C2D-C1D	-4.21	99.02	105.77
26	B	618	BCR	C30-C25-C26	-4.20	116.50	122.66
26	H	101	BCR	C35-C13-C14	-4.19	116.71	122.90
26	T	101	BCR	C35-C13-C14	-4.19	116.71	122.90
26	Y	101	BCR	C38-C26-C27	-4.18	105.50	113.43
24	C	501	CLA	O2D-CGD-O1D	-4.17	115.17	123.79
26	D	404	BCR	C36-C18-C19	-4.17	111.15	118.10
26	h	101	BCR	C30-C25-C26	-4.17	116.54	122.66
24	B	607	CLA	O1D-CGD-CBD	-4.15	118.68	124.62
24	d	401	CLA	C1C-C2C-C3C	-4.14	101.95	106.91
25	d	402	PHO	C3D-C2D-C1D	-4.13	99.15	105.77
26	C	515	BCR	C33-C5-C4	-4.11	105.64	113.43
26	h	101	BCR	C39-C30-C29	-4.11	94.08	108.79
26	f	101	BCR	C34-C9-C10	-4.10	116.84	122.90
26	c	918	BCR	C36-C18-C17	-4.10	116.85	122.90
25	A	608	PHO	C4C-C3C-C2C	-4.10	102.24	106.81
26	c	915	BCR	C30-C25-C26	-4.06	116.70	122.66
24	B	604	CLA	C1C-C2C-C3C	-4.05	102.06	106.91
26	B	620	BCR	C30-C25-C26	-4.05	116.71	122.66
24	c	902	CLA	C1C-C2C-C3C	-4.04	102.08	106.91
25	a	412	PHO	C4C-C3C-C2C	-4.01	102.33	106.81
24	C	504	CLA	C1C-C2C-C3C	-4.01	102.11	106.91
24	B	605	CLA	C1C-C2C-C3C	-4.00	102.13	106.91
24	a	407	CLA	C1C-C2C-C3C	-3.99	102.13	106.91
26	b	619	BCR	C35-C13-C14	-3.99	117.00	122.90
26	H	101	BCR	C38-C26-C27	-3.99	105.87	113.43
26	k	102	BCR	C35-C13-C14	-3.98	117.02	122.90
24	B	607	CLA	O2D-CGD-O1D	-3.98	115.57	123.79
26	C	514	BCR	C36-C18-C19	-3.96	111.51	118.10
26	h	101	BCR	C35-C13-C12	-3.95	111.52	118.10
26	B	620	BCR	C35-C13-C14	-3.94	117.09	122.90
26	B	618	BCR	C35-C13-C14	-3.93	117.09	122.90
24	b	604	CLA	C1C-C2C-C3C	-3.93	102.21	106.91
26	T	101	BCR	C30-C25-C26	-3.92	116.90	122.66
24	d	403	CLA	C1C-C2C-C3C	-3.92	102.22	106.91
24	b	617	CLA	O1D-CGD-CBD	-3.90	119.03	124.62
26	K	101	BCR	C38-C26-C27	-3.88	106.07	113.43
26	B	619	BCR	C35-C13-C12	-3.87	111.66	118.10
24	d	404	CLA	C1C-C2C-C3C	-3.87	102.28	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406	CLA	C1C-C2C-C3C	-3.84	102.32	106.91
24	B	609	CLA	C1C-C2C-C3C	-3.83	102.33	106.91
26	h	101	BCR	C1-C6-C5	-3.82	117.05	122.66
24	b	607	CLA	O1D-CGD-CBD	-3.82	119.15	124.62
26	T	102	BCR	C37-C22-C23	-3.81	111.75	118.10
26	H	101	BCR	C36-C18-C17	-3.81	117.27	122.90
26	D	404	BCR	C32-C1-C2	-3.80	95.17	108.79
26	K	101	BCR	C30-C25-C26	-3.79	117.09	122.66
32	v	202	HEM	CBD-CAD-C3D	-3.77	102.57	113.55
24	C	509	CLA	C1C-C2C-C3C	-3.76	102.41	106.91
24	c	908	CLA	C1C-C2C-C3C	-3.75	102.42	106.91
24	A	609	CLA	C1C-C2C-C3C	-3.75	102.42	106.91
24	B	609	CLA	O1D-CGD-CBD	-3.73	119.28	124.62
26	T	102	BCR	C35-C13-C12	-3.73	111.90	118.10
26	k	102	BCR	C35-C13-C12	-3.72	111.91	118.10
26	B	620	BCR	C37-C22-C21	-3.71	117.42	122.90
24	B	608	CLA	C1C-C2C-C3C	-3.71	102.47	106.91
26	c	915	BCR	C33-C5-C4	-3.71	106.39	113.43
26	f	101	BCR	C35-C13-C14	-3.71	117.42	122.90
26	c	915	BCR	C1-C6-C5	-3.71	117.22	122.66
25	d	402	PHO	C4C-C3C-C2C	-3.70	102.68	106.81
26	B	622	BCR	C35-C13-C14	-3.70	117.44	122.90
24	b	615	CLA	C1C-C2C-C3C	-3.70	102.49	106.91
24	B	614	CLA	C1C-C2C-C3C	-3.69	102.50	106.91
32	V	202	HEM	CBD-CAD-C3D	-3.66	102.91	113.55
24	c	913	CLA	C3B-CAB-CBB	-3.65	118.85	126.32
24	C	507	CLA	O1D-CGD-CBD	-3.64	119.40	124.62
24	C	501	CLA	C1C-C2C-C3C	-3.64	102.56	106.91
26	K	101	BCR	C33-C5-C4	-3.64	106.53	113.43
26	b	619	BCR	C30-C25-C26	-3.63	117.32	122.66
26	a	409	BCR	C34-C9-C8	-3.63	112.05	118.10
26	D	404	BCR	C37-C22-C21	-3.63	117.54	122.90
24	d	404	CLA	O1D-CGD-CBD	-3.60	119.46	124.62
24	b	602	CLA	O1D-CGD-CBD	-3.60	119.46	124.62
24	C	507	CLA	C1C-C2C-C3C	-3.59	102.62	106.91
26	c	915	BCR	C38-C26-C27	-3.57	106.66	113.43
26	c	915	BCR	C34-C9-C8	-3.56	112.17	118.10
26	k	101	BCR	C34-C9-C8	-3.55	112.19	118.10
24	c	905	CLA	C1C-C2C-C3C	-3.54	102.68	106.91
26	c	915	BCR	C31-C1-C2	-3.53	96.15	108.79
32	e	101	HEM	CBD-CAD-C3D	-3.52	103.30	113.55
24	b	609	CLA	C1C-C2C-C3C	-3.51	102.71	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	405	PL9	C7-C3-C2	-3.51	120.51	123.42
24	b	604	CLA	O2D-CGD-O1D	-3.51	116.55	123.79
24	a	408	CLA	C1C-C2C-C3C	-3.50	102.73	106.91
24	b	607	CLA	O2D-CGD-O1D	-3.49	116.58	123.79
24	b	607	CLA	C1C-C2C-C3C	-3.49	102.73	106.91
24	c	902	CLA	O2D-CGD-O1D	-3.49	116.58	123.79
28	a	411	SQD	C1-C2-C3	-3.49	103.10	109.97
24	c	911	CLA	C1C-C2C-C3C	-3.49	102.74	106.91
24	B	617	CLA	O1D-CGD-CBD	-3.48	119.63	124.62
26	D	404	BCR	C35-C13-C14	-3.48	117.76	122.90
26	h	101	BCR	C35-C13-C14	-3.48	117.76	122.90
24	C	503	CLA	C1C-C2C-C3C	-3.47	102.75	106.91
26	C	514	BCR	C37-C22-C21	-3.47	117.77	122.90
24	c	913	CLA	C1C-C2C-C3C	-3.47	102.76	106.91
28	A	612	SQD	C1-C2-C3	-3.47	103.14	109.97
24	D	403	CLA	C1C-C2C-C3C	-3.46	102.77	106.91
26	A	610	BCR	C33-C5-C4	-3.45	106.88	113.43
26	c	915	BCR	C36-C18-C19	-3.45	112.36	118.10
24	b	605	CLA	C1C-C2C-C3C	-3.44	102.79	106.91
24	a	407	CLA	C3B-CAB-CBB	-3.44	119.28	126.32
24	B	602	CLA	C1C-C2C-C3C	-3.44	102.80	106.91
24	B	602	CLA	O1D-CGD-CBD	-3.43	119.71	124.62
26	a	409	BCR	C33-C5-C4	-3.42	106.94	113.43
24	B	607	CLA	C1C-C2C-C3C	-3.42	102.82	106.91
24	C	510	CLA	C1C-C2C-C3C	-3.41	102.83	106.91
24	b	613	CLA	C4C-C3C-C2C	-3.41	101.41	106.94
26	A	610	BCR	C35-C13-C12	-3.40	112.44	118.10
25	A	608	PHO	C4D-ND-C1D	-3.40	100.82	107.05
26	T	102	BCR	C30-C25-C26	-3.39	117.68	122.66
26	b	619	BCR	C35-C13-C12	-3.39	112.46	118.10
24	C	506	CLA	C1C-C2C-C3C	-3.39	102.86	106.91
26	D	404	BCR	C1-C6-C5	-3.38	117.69	122.66
26	f	101	BCR	C40-C30-C29	-3.38	96.67	108.79
24	c	910	CLA	C1C-C2C-C3C	-3.38	102.86	106.91
24	b	606	CLA	C1C-C2C-C3C	-3.38	102.87	106.91
26	b	618	BCR	C40-C30-C29	-3.38	96.69	108.79
26	h	101	BCR	C36-C18-C19	-3.37	112.48	118.10
24	B	610	CLA	C1C-C2C-C3C	-3.37	102.88	106.91
24	C	508	CLA	C1C-C2C-C3C	-3.36	102.89	106.91
24	b	614	CLA	C1C-C2C-C3C	-3.35	102.90	106.91
24	C	511	CLA	C1C-C2C-C3C	-3.35	102.90	106.91
24	c	908	CLA	O2D-CGD-O1D	-3.35	116.88	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f	101	BCR	C33-C5-C4	-3.34	107.09	113.43
26	a	409	BCR	C38-C26-C27	-3.34	107.10	113.43
24	c	908	CLA	O1D-CGD-CBD	-3.33	119.84	124.62
26	B	619	BCR	C37-C22-C23	-3.33	112.55	118.10
24	C	513	CLA	C1C-C2C-C3C	-3.33	102.93	106.91
24	b	616	CLA	C1C-C2C-C3C	-3.31	102.94	106.91
24	c	914	CLA	C1C-C2C-C3C	-3.31	102.95	106.91
24	A	614	CLA	C1C-NC-C4C	-3.31	102.25	106.27
26	T	102	BCR	C37-C22-C21	-3.30	118.02	122.90
24	c	909	CLA	C4C-C3C-C2C	-3.30	101.59	106.94
26	T	102	BCR	C1-C6-C5	-3.29	117.83	122.66
24	B	604	CLA	O2D-CGD-O1D	-3.29	117.00	123.79
24	B	615	CLA	C1C-C2C-C3C	-3.28	102.98	106.91
26	B	620	BCR	C36-C18-C19	-3.27	112.65	118.10
24	c	907	CLA	C1C-C2C-C3C	-3.26	103.01	106.91
24	A	606	CLA	C1C-C2C-C3C	-3.26	103.01	106.91
24	B	616	CLA	C1C-C2C-C3C	-3.25	103.02	106.91
24	b	603	CLA	C1C-C2C-C3C	-3.25	103.02	106.91
24	c	905	CLA	O1D-CGD-CBD	-3.25	119.97	124.62
31	C	518	DGD	O3G-C3G-C2G	-3.25	103.26	110.99
25	a	412	PHO	O2D-CGD-O1D	-3.25	117.09	123.79
27	A	611	PL9	C32-C33-C34	-3.25	120.70	127.76
24	D	402	CLA	C3B-CAB-CBB	-3.22	119.73	126.32
24	b	610	CLA	C1C-C2C-C3C	-3.21	103.06	106.91
24	b	617	CLA	C4C-C3C-C2C	-3.21	101.73	106.94
26	A	610	BCR	C34-C9-C8	-3.21	112.75	118.10
24	c	904	CLA	C1C-C2C-C3C	-3.21	103.07	106.91
24	B	617	CLA	C4C-C3C-C2C	-3.20	101.75	106.94
25	a	412	PHO	C4D-ND-C1D	-3.20	101.19	107.05
24	c	912	CLA	C1C-C2C-C3C	-3.18	103.10	106.91
26	k	101	BCR	C39-C30-C29	-3.18	97.40	108.79
24	b	611	CLA	C1C-C2C-C3C	-3.18	103.11	106.91
26	B	622	BCR	C35-C13-C12	-3.18	112.81	118.10
24	b	602	CLA	C1C-C2C-C3C	-3.17	103.11	106.91
24	B	612	CLA	C1C-C2C-C3C	-3.17	103.11	106.91
24	C	512	CLA	C1C-C2C-C3C	-3.17	103.12	106.91
26	b	618	BCR	C1-C6-C5	-3.16	118.01	122.66
24	b	612	CLA	C1C-C2C-C3C	-3.16	103.13	106.91
24	B	615	CLA	O2D-CGD-O1D	-3.16	117.28	123.79
24	C	505	CLA	C1C-C2C-C3C	-3.15	103.14	106.91
26	B	620	BCR	C35-C13-C12	-3.15	112.86	118.10
26	c	915	BCR	C35-C13-C12	-3.14	112.87	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	401	PHO	C4D-ND-C1D	-3.14	101.28	107.05
24	B	603	CLA	C1C-C2C-C3C	-3.13	103.16	106.91
24	C	502	CLA	C1C-C2C-C3C	-3.13	103.16	106.91
24	B	602	CLA	C3B-CAB-CBB	-3.13	119.91	126.32
24	c	910	CLA	O1D-CGD-CBD	-3.13	120.14	124.62
24	B	605	CLA	C1C-NC-C4C	-3.12	102.48	106.27
24	B	606	CLA	C4C-C3C-C2C	-3.11	101.90	106.94
24	c	909	CLA	C1C-C2C-C3C	-3.11	103.19	106.91
26	k	101	BCR	C35-C13-C12	-3.10	112.94	118.10
26	H	101	BCR	C39-C30-C29	-3.10	97.69	108.79
24	B	611	CLA	C1C-C2C-C3C	-3.10	103.20	106.91
24	D	402	CLA	O2D-CGD-O1D	-3.08	117.43	123.79
26	b	619	BCR	C34-C9-C8	-3.08	112.98	118.10
24	d	403	CLA	O2D-CGD-O1D	-3.07	117.44	123.79
26	K	101	BCR	C31-C1-C2	-3.07	97.79	108.79
24	D	402	CLA	C1C-C2C-C3C	-3.07	103.24	106.91
24	C	510	CLA	O1D-CGD-CBD	-3.07	120.22	124.62
24	C	501	CLA	C3B-CAB-CBB	-3.07	120.05	126.32
24	b	615	CLA	O2D-CGD-O1D	-3.06	117.46	123.79
24	D	402	CLA	C4C-C3C-C2C	-3.06	101.98	106.94
24	b	608	CLA	C1C-C2C-C3C	-3.05	103.25	106.91
26	B	619	BCR	C34-C9-C8	-3.05	113.02	118.10
26	k	102	BCR	C30-C25-C26	-3.05	118.19	122.66
24	B	606	CLA	C1C-C2C-C3C	-3.04	103.27	106.91
26	C	514	BCR	C39-C30-C29	-3.04	97.89	108.79
24	c	903	CLA	O1D-CGD-CBD	-3.03	120.28	124.62
24	c	903	CLA	C1C-C2C-C3C	-3.02	103.29	106.91
26	B	619	BCR	C34-C9-C10	-3.01	118.46	122.90
24	B	612	CLA	C1C-NC-C4C	-3.01	102.61	106.27
25	d	402	PHO	C1C-C2C-C3C	-3.00	102.91	106.50
24	B	611	CLA	C4C-C3C-C2C	-3.00	102.08	106.94
24	C	512	CLA	O1D-CGD-CBD	-3.00	120.33	124.62
24	c	913	CLA	O1D-CGD-CBD	-3.00	120.33	124.62
26	T	101	BCR	C34-C9-C8	-2.99	113.12	118.10
24	b	605	CLA	C4C-C3C-C2C	-2.98	102.10	106.94
24	b	610	CLA	C3B-CAB-CBB	-2.98	120.21	126.32
26	T	101	BCR	C36-C18-C19	-2.98	113.13	118.10
24	A	614	CLA	CBC-CAC-C3C	-2.98	103.30	112.39
24	C	506	CLA	O1D-CGD-CBD	-2.96	120.38	124.62
25	A	608	PHO	O1D-CGD-CBD	-2.96	120.38	124.62
27	a	410	PL9	C37-C38-C39	-2.96	121.33	127.76
24	c	910	CLA	C4C-C3C-C2C	-2.95	102.15	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	608	PHO	C1C-C2C-C3C	-2.95	102.97	106.50
24	C	513	CLA	O2D-CGD-O1D	-2.95	117.70	123.79
24	c	903	CLA	C4C-C3C-C2C	-2.95	102.16	106.94
24	c	906	CLA	C1C-C2C-C3C	-2.94	103.39	106.91
26	Y	101	BCR	C39-C30-C29	-2.94	98.25	108.79
24	C	508	CLA	C4C-C3C-C2C	-2.93	102.18	106.94
24	B	616	CLA	C4C-C3C-C2C	-2.93	102.18	106.94
24	b	616	CLA	C3B-CAB-CBB	-2.93	120.32	126.32
28	A	612	SQD	C45-O47-C7	-2.93	110.86	117.89
24	C	506	CLA	C3B-CAB-CBB	-2.91	120.37	126.32
26	c	918	BCR	C39-C30-C29	-2.90	98.38	108.79
26	c	918	BCR	C36-C18-C19	-2.90	113.27	118.10
26	C	515	BCR	C30-C25-C26	-2.90	118.40	122.66
26	B	618	BCR	C39-C30-C29	-2.90	98.41	108.79
27	A	611	PL9	C37-C38-C39	-2.90	121.46	127.76
24	b	614	CLA	C4C-C3C-C2C	-2.90	102.24	106.94
24	B	612	CLA	C4C-C3C-C2C	-2.89	102.25	106.94
26	T	102	BCR	C34-C9-C8	-2.89	113.28	118.10
24	B	604	CLA	O1D-CGD-CBD	-2.89	120.48	124.62
24	B	608	CLA	O1D-CGD-CBD	-2.88	120.49	124.62
29	D	407	LHG	O8-C23-O10	-2.88	116.06	123.49
26	B	619	BCR	C1-C6-C5	-2.88	118.43	122.66
24	b	611	CLA	C4C-C3C-C2C	-2.88	102.27	106.94
24	D	402	CLA	C1C-NC-C4C	-2.88	102.77	106.27
24	B	613	CLA	C4C-C3C-C2C	-2.88	102.28	106.94
24	B	613	CLA	C1C-C2C-C3C	-2.87	103.48	106.91
25	D	401	PHO	O1D-CGD-CBD	-2.87	120.52	124.62
32	v	202	HEM	C3B-CAB-CBB	-2.86	120.06	124.46
26	c	915	BCR	C37-C22-C23	-2.86	113.33	118.10
24	b	608	CLA	C4C-C3C-C2C	-2.86	102.30	106.94
24	a	407	CLA	O1D-CGD-CBD	-2.86	120.53	124.62
28	a	411	SQD	C1-O5-C5	-2.86	108.20	113.75
24	a	407	CLA	C1C-NC-C4C	-2.85	102.80	106.27
24	B	617	CLA	O2D-CGD-O1D	-2.85	117.90	123.79
26	C	515	BCR	C34-C9-C8	-2.85	113.35	118.10
24	b	604	CLA	C5-C3-C2	-2.85	115.65	121.05
24	C	507	CLA	CBC-CAC-C3C	-2.84	103.72	112.39
26	f	101	BCR	C34-C9-C8	-2.84	113.38	118.10
28	l	101	SQD	C1-O5-C5	-2.83	108.25	113.75
26	T	101	BCR	C35-C13-C12	-2.83	113.39	118.10
26	B	622	BCR	C31-C1-C2	-2.82	98.68	108.79
24	c	906	CLA	O1D-CGD-CBD	-2.82	120.58	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	603	CLA	O2D-CGD-O1D	-2.82	117.97	123.79
26	K	101	BCR	C34-C9-C10	-2.82	118.73	122.90
24	C	502	CLA	C4C-C3C-C2C	-2.82	102.37	106.94
24	A	607	CLA	O1D-CGD-CBD	-2.82	120.59	124.62
24	C	511	CLA	C4C-C3C-C2C	-2.81	102.38	106.94
28	d	407	SQD	C44-O6-C1	-2.81	107.91	113.82
24	c	904	CLA	C4C-C3C-C2C	-2.81	102.39	106.94
24	b	606	CLA	C4C-C3C-C2C	-2.80	102.39	106.94
24	A	607	CLA	C1C-NC-C4C	-2.80	102.86	106.27
24	b	602	CLA	O2D-CGD-O1D	-2.79	118.02	123.79
24	C	505	CLA	O1D-CGD-CBD	-2.79	120.62	124.62
24	b	610	CLA	C4C-C3C-C2C	-2.79	102.41	106.94
26	B	622	BCR	C1-C6-C5	-2.79	118.56	122.66
27	a	410	PL9	C32-C33-C34	-2.79	121.70	127.76
24	C	506	CLA	C4C-C3C-C2C	-2.79	102.42	106.94
25	d	402	PHO	CHD-C1D-ND	-2.79	119.46	124.66
26	c	918	BCR	C1-C6-C5	-2.78	118.57	122.66
24	B	608	CLA	CBC-CAC-C3C	-2.78	103.90	112.39
26	A	610	BCR	C34-C9-C10	-2.78	118.80	122.90
24	B	609	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
24	C	508	CLA	O1D-CGD-CBD	-2.78	120.64	124.62
26	T	101	BCR	C37-C22-C21	-2.78	118.80	122.90
24	c	905	CLA	C4C-C3C-C2C	-2.77	102.44	106.94
24	b	602	CLA	C3B-CAB-CBB	-2.77	120.64	126.32
25	a	412	PHO	CHD-C1D-ND	-2.77	119.49	124.66
24	C	502	CLA	C3B-CAB-CBB	-2.77	120.65	126.32
24	c	907	CLA	C4C-C3C-C2C	-2.76	102.46	106.94
24	d	401	CLA	CBC-CAC-C3C	-2.76	103.96	112.39
24	a	408	CLA	O1D-CGD-CBD	-2.76	120.67	124.62
31	H	102	DGD	O1G-C1A-O1A	-2.75	116.38	123.49
27	A	611	PL9	C7-C3-C2	-2.75	121.13	123.42
24	d	401	CLA	C1C-NC-C4C	-2.75	102.92	106.27
25	d	402	PHO	C4D-ND-C1D	-2.75	102.00	107.05
26	B	618	BCR	C37-C22-C21	-2.75	118.84	122.90
24	B	609	CLA	C1C-NC-C4C	-2.75	102.92	106.27
24	B	610	CLA	C4C-C3C-C2C	-2.75	102.48	106.94
28	a	411	SQD	O5-C1-C2	-2.75	104.64	110.28
24	B	603	CLA	C4C-C3C-C2C	-2.75	102.49	106.94
25	d	402	PHO	O1D-CGD-CBD	-2.74	120.70	124.62
24	a	408	CLA	C4C-C3C-C2C	-2.74	102.50	106.94
24	c	906	CLA	C4C-C3C-C2C	-2.73	102.52	106.94
24	B	615	CLA	O1D-CGD-CBD	-2.73	120.71	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	605	CLA	O1D-CGD-CBD	-2.73	120.72	124.62
24	b	606	CLA	O1D-CGD-CBD	-2.72	120.72	124.62
24	c	914	CLA	C3B-CAB-CBB	-2.72	120.75	126.32
24	C	512	CLA	C4C-C3C-C2C	-2.72	102.53	106.94
24	c	912	CLA	C4C-C3C-C2C	-2.71	102.54	106.94
24	b	610	CLA	O1D-CGD-CBD	-2.71	120.74	124.62
24	b	613	CLA	C1C-NC-C4C	-2.71	102.97	106.27
24	b	617	CLA	C1C-C2C-C3C	-2.71	103.67	106.91
24	c	911	CLA	O1D-CGD-CBD	-2.71	120.74	124.62
24	B	611	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
24	c	906	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
24	a	406	CLA	C1C-NC-C4C	-2.70	102.98	106.27
25	d	402	PHO	O2D-CGD-O1D	-2.70	118.21	123.79
24	b	605	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
26	b	619	BCR	C1-C6-C5	-2.69	118.70	122.66
24	B	615	CLA	C4C-C3C-C2C	-2.69	102.58	106.94
24	d	403	CLA	C1C-NC-C4C	-2.69	103.00	106.27
24	C	504	CLA	O2D-CGD-O1D	-2.69	118.24	123.79
24	c	911	CLA	C4C-C3C-C2C	-2.69	102.58	106.94
24	C	513	CLA	C4C-C3C-C2C	-2.68	102.59	106.94
24	a	408	CLA	C1C-NC-C4C	-2.68	103.01	106.27
24	D	403	CLA	O1D-CGD-CBD	-2.68	120.78	124.62
24	d	401	CLA	CHD-C4C-C3C	-2.68	120.80	124.94
31	C	516	DGD	O3G-C3G-C2G	-2.68	104.61	110.99
24	C	510	CLA	CHD-C4C-C3C	-2.67	120.81	124.94
24	C	505	CLA	C4C-C3C-C2C	-2.67	102.61	106.94
24	b	606	CLA	C1C-NC-C4C	-2.67	103.02	106.27
24	a	406	CLA	C4C-C3C-C2C	-2.66	102.62	106.94
24	a	406	CLA	O2D-CGD-O1D	-2.66	118.29	123.79
24	A	606	CLA	C4C-C3C-C2C	-2.66	102.62	106.94
24	b	613	CLA	C1C-C2C-C3C	-2.66	103.73	106.91
24	b	616	CLA	O2D-CGD-O1D	-2.65	118.31	123.79
24	C	503	CLA	C4C-C3C-C2C	-2.65	102.64	106.94
24	C	506	CLA	O2D-CGD-O1D	-2.65	118.32	123.79
24	c	913	CLA	C4C-C3C-C2C	-2.65	102.65	106.94
24	b	609	CLA	O2D-CGD-O1D	-2.65	118.33	123.79
26	f	101	BCR	C37-C22-C23	-2.64	113.69	118.10
24	D	403	CLA	C4C-C3C-C2C	-2.64	102.65	106.94
26	Y	101	BCR	C35-C13-C12	-2.64	113.70	118.10
24	C	509	CLA	O1D-CGD-CBD	-2.64	120.84	124.62
24	B	613	CLA	O1D-CGD-CBD	-2.64	120.84	124.62
24	a	407	CLA	C4C-C3C-C2C	-2.64	102.67	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	609	CLA	O1D-CGD-CBD	-2.63	120.85	124.62
24	b	614	CLA	C1C-NC-C4C	-2.63	103.07	106.27
27	d	405	PL9	C36-C37-C38	-2.63	104.80	111.69
28	A	612	SQD	C44-O6-C1	-2.63	108.30	113.82
24	B	615	CLA	CBC-CAC-C3C	-2.62	104.38	112.39
26	T	101	BCR	C1-C6-C5	-2.62	118.81	122.66
24	c	914	CLA	C4C-C3C-C2C	-2.62	102.69	106.94
24	b	609	CLA	C4C-C3C-C2C	-2.62	102.70	106.94
24	B	603	CLA	O2D-CGD-O1D	-2.61	118.39	123.79
24	B	605	CLA	C4C-C3C-C2C	-2.61	102.71	106.94
24	B	607	CLA	C4C-C3C-C2C	-2.61	102.71	106.94
24	C	509	CLA	C4C-C3C-C2C	-2.61	102.71	106.94
26	T	102	BCR	C34-C9-C10	-2.61	119.05	122.90
24	C	502	CLA	O2D-CGD-O1D	-2.60	118.41	123.79
25	D	401	PHO	CHD-C1D-ND	-2.60	119.80	124.66
24	b	616	CLA	C4C-C3C-C2C	-2.60	102.72	106.94
26	c	918	BCR	C30-C25-C26	-2.60	118.85	122.66
24	b	612	CLA	C4C-C3C-C2C	-2.60	102.73	106.94
24	B	612	CLA	CHD-C4C-C3C	-2.59	120.93	124.94
26	H	101	BCR	C32-C1-C31	-2.59	100.06	108.37
26	K	101	BCR	C37-C22-C23	-2.59	113.79	118.10
24	b	602	CLA	C4C-C3C-C2C	-2.59	102.74	106.94
26	h	101	BCR	C37-C22-C23	-2.59	113.79	118.10
28	a	411	SQD	C44-O6-C1	-2.58	108.40	113.82
24	B	609	CLA	C4C-C3C-C2C	-2.58	102.76	106.94
32	E	101	HEM	CBA-CAA-C2A	-2.57	107.92	112.53
24	d	403	CLA	C4C-C3C-C2C	-2.56	102.78	106.94
24	B	607	CLA	C3B-CAB-CBB	-2.56	121.08	126.32
24	C	510	CLA	C4C-C3C-C2C	-2.56	102.79	106.94
26	B	620	BCR	C32-C1-C2	-2.56	99.62	108.79
24	c	912	CLA	O2D-CGD-O1D	-2.56	118.51	123.79
27	D	405	PL9	C27-C28-C29	-2.55	122.21	127.76
25	A	608	PHO	CHD-C1D-ND	-2.55	119.89	124.66
24	c	908	CLA	C4C-C3C-C2C	-2.55	102.81	106.94
28	A	612	SQD	C1-O5-C5	-2.54	108.81	113.75
24	B	614	CLA	C4C-C3C-C2C	-2.54	102.82	106.94
24	B	617	CLA	C1C-C2C-C3C	-2.54	103.87	106.91
24	b	613	CLA	O2D-CGD-O1D	-2.54	118.55	123.79
24	C	501	CLA	O1D-CGD-CBD	-2.53	120.99	124.62
24	b	614	CLA	CHD-C4C-C3C	-2.53	121.03	124.94
24	C	511	CLA	O2D-CGD-O1D	-2.53	118.57	123.79
24	b	607	CLA	C4C-C3C-C2C	-2.52	102.85	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	402	CLA	CHD-C4C-C3C	-2.52	121.05	124.94
24	B	616	CLA	C3B-CAB-CBB	-2.52	121.16	126.32
26	f	101	BCR	C35-C13-C12	-2.52	113.91	118.10
24	a	407	CLA	CBC-CAC-C3C	-2.51	104.72	112.39
32	e	101	HEM	CBA-CAA-C2A	-2.51	108.03	112.53
24	b	605	CLA	C3B-CAB-CBB	-2.51	121.18	126.32
24	B	610	CLA	O2D-CGD-O1D	-2.51	118.61	123.79
24	b	612	CLA	O2D-CGD-O1D	-2.50	118.62	123.79
26	k	102	BCR	C31-C1-C2	-2.50	99.84	108.79
24	c	910	CLA	O2D-CGD-O1D	-2.50	118.63	123.79
24	B	614	CLA	CHD-C4C-C3C	-2.50	121.08	124.94
24	b	612	CLA	CBC-CAC-C3C	-2.50	104.77	112.39
26	B	622	BCR	C30-C25-C26	-2.49	119.01	122.66
24	B	602	CLA	C4C-C3C-C2C	-2.48	102.91	106.94
24	B	604	CLA	C1C-NC-C4C	-2.48	103.25	106.27
24	b	603	CLA	C4C-C3C-C2C	-2.48	102.92	106.94
24	C	505	CLA	C3B-CAB-CBB	-2.47	121.26	126.32
31	c	916	DGD	O3G-C3G-C2G	-2.47	105.12	110.99
24	B	617	CLA	C1C-NC-C4C	-2.47	103.27	106.27
26	k	101	BCR	C31-C1-C2	-2.47	99.96	108.79
26	T	102	BCR	C33-C5-C6	-2.46	122.19	124.61
24	B	612	CLA	O2D-CGD-O1D	-2.46	118.71	123.79
24	A	614	CLA	O1D-CGD-CBD	-2.46	121.10	124.62
27	a	410	PL9	C42-C43-C44	-2.46	122.42	127.76
25	D	401	PHO	C3B-C2B-C1B	-2.45	101.02	106.33
26	k	102	BCR	C34-C9-C10	-2.45	119.28	122.90
24	c	914	CLA	O2D-CGD-O1D	-2.45	118.73	123.79
26	K	101	BCR	C34-C9-C8	-2.45	114.02	118.10
24	c	904	CLA	O1D-CGD-CBD	-2.45	121.12	124.62
27	a	410	PL9	C22-C23-C24	-2.44	122.46	127.76
26	c	915	BCR	C40-C30-C29	-2.44	100.05	108.79
26	C	515	BCR	C1-C6-C5	-2.44	119.08	122.66
24	A	606	CLA	O2D-CGD-O1D	-2.43	118.77	123.79
24	A	609	CLA	C4C-C3C-C2C	-2.43	103.00	106.94
24	b	604	CLA	C1C-NC-C4C	-2.43	103.32	106.27
26	b	619	BCR	C32-C1-C2	-2.43	100.10	108.79
24	A	607	CLA	CBC-CAC-C3C	-2.42	104.99	112.39
24	b	605	CLA	C1C-NC-C4C	-2.42	103.32	106.27
24	c	903	CLA	O2D-CGD-O1D	-2.42	118.79	123.79
24	D	403	CLA	O2D-CGD-O1D	-2.42	118.79	123.79
24	B	608	CLA	C4C-C3C-C2C	-2.42	103.02	106.94
24	C	512	CLA	O2D-CGD-O1D	-2.42	118.80	123.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	604	CLA	O1D-CGD-CBD	-2.42	121.16	124.62
24	B	604	CLA	C4C-C3C-C2C	-2.41	103.03	106.94
24	a	408	CLA	C3B-CAB-CBB	-2.41	121.38	126.32
24	C	504	CLA	C3B-CAB-CBB	-2.40	121.40	126.32
24	c	907	CLA	O1D-CGD-CBD	-2.40	121.18	124.62
26	T	101	BCR	C37-C22-C23	-2.40	114.10	118.10
24	d	403	CLA	C3B-CAB-CBB	-2.40	121.41	126.32
24	b	613	CLA	CHD-C4C-C3C	-2.40	121.23	124.94
26	k	102	BCR	C39-C30-C29	-2.40	100.20	108.79
24	d	404	CLA	O2D-CGD-O1D	-2.40	118.84	123.79
26	B	620	BCR	C1-C6-C5	-2.39	119.15	122.66
26	h	101	BCR	C40-C30-C39	-2.39	100.71	108.37
24	a	408	CLA	CHD-C4C-C3C	-2.39	121.25	124.94
26	B	618	BCR	C1-C6-C5	-2.38	119.16	122.66
26	H	101	BCR	C29-C28-C27	-2.38	105.53	111.53
26	C	514	BCR	C40-C30-C29	-2.38	100.26	108.79
24	A	614	CLA	CHC-C1C-C2C	-2.38	120.09	126.35
24	C	509	CLA	O2D-CGD-O1D	-2.38	118.88	123.79
24	B	606	CLA	C1C-NC-C4C	-2.38	103.38	106.27
24	C	507	CLA	C4C-C3C-C2C	-2.37	103.09	106.94
24	b	615	CLA	O1D-CGD-CBD	-2.37	121.22	124.62
24	b	616	CLA	O1D-CGD-CBD	-2.37	121.23	124.62
25	a	412	PHO	C1C-C2C-C3C	-2.37	103.67	106.50
24	C	503	CLA	O1D-CGD-CBD	-2.37	121.23	124.62
24	b	609	CLA	O1D-CGD-CBD	-2.36	121.24	124.62
24	C	512	CLA	C3B-CAB-CBB	-2.36	121.49	126.32
24	b	615	CLA	C4C-C3C-C2C	-2.36	103.11	106.94
24	b	612	CLA	C1C-NC-C4C	-2.36	103.40	106.27
24	B	614	CLA	O2D-CGD-O1D	-2.35	118.93	123.79
24	B	602	CLA	C4-C3-C2	-2.35	118.90	123.50
26	B	618	BCR	C33-C5-C4	-2.34	108.99	113.43
24	A	606	CLA	C1C-NC-C4C	-2.34	103.42	106.27
24	d	401	CLA	C4C-C3C-C2C	-2.34	103.15	106.94
24	C	503	CLA	C3B-CAB-CBB	-2.33	121.55	126.32
24	B	610	CLA	C1C-NC-C4C	-2.33	103.44	106.27
26	b	619	BCR	C37-C22-C23	-2.33	114.22	118.10
24	c	902	CLA	C4C-C3C-C2C	-2.33	103.17	106.94
26	A	610	BCR	C28-C27-C26	-2.33	110.18	113.87
24	b	617	CLA	CHD-C4C-C3C	-2.32	121.36	124.94
27	a	410	PL9	C27-C28-C29	-2.32	122.72	127.76
24	b	606	CLA	O2D-CGD-O1D	-2.32	119.01	123.79
24	b	604	CLA	C4C-C3C-C2C	-2.32	103.19	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	CBC-CAC-C3C	-2.31	105.33	112.39
25	a	412	PHO	C3B-C2B-C1B	-2.30	101.34	106.33
24	B	602	CLA	O2D-CGD-O1D	-2.30	119.04	123.79
24	A	606	CLA	C3B-CAB-CBB	-2.30	121.61	126.32
24	a	406	CLA	CHC-C1C-C2C	-2.30	120.31	126.35
31	C	517	DGD	O2G-C1B-O1B	-2.29	117.52	123.67
24	B	606	CLA	O2A-CGA-O1A	-2.29	117.57	123.49
24	A	614	CLA	CHD-C4C-C3C	-2.29	121.40	124.94
24	c	913	CLA	O2D-CGD-O1D	-2.29	119.06	123.79
24	c	912	CLA	C3B-CAB-CBB	-2.29	121.63	126.32
24	d	403	CLA	CHD-C4C-C3C	-2.29	121.40	124.94
24	b	608	CLA	C3B-CAB-CBB	-2.29	121.64	126.32
24	C	501	CLA	CBC-CAC-C3C	-2.28	105.43	112.39
24	b	607	CLA	C3B-CAB-CBB	-2.28	121.66	126.32
25	A	608	PHO	C3B-C2B-C1B	-2.28	101.40	106.33
26	B	620	BCR	C40-C30-C39	-2.27	101.08	108.37
24	b	606	CLA	OBD-CAD-C3D	-2.27	123.72	128.35
24	d	401	CLA	C3B-CAB-CBB	-2.27	121.67	126.32
24	b	615	CLA	O2A-CGA-O1A	-2.27	117.64	123.49
24	C	501	CLA	C4C-C3C-C2C	-2.27	103.26	106.94
24	b	617	CLA	C1C-NC-C4C	-2.27	103.51	106.27
24	A	607	CLA	O2D-CGD-O1D	-2.26	119.12	123.79
24	d	404	CLA	C3B-CAB-CBB	-2.26	121.69	126.32
24	B	613	CLA	C1C-NC-C4C	-2.26	103.52	106.27
24	b	604	CLA	C3B-CAB-CBB	-2.26	121.70	126.32
25	D	401	PHO	C1C-C2C-C3C	-2.26	103.80	106.50
26	K	101	BCR	C1-C6-C5	-2.25	119.35	122.66
24	B	604	CLA	O2A-CGA-O1A	-2.25	117.69	123.49
27	D	405	PL9	C7-C8-C9	-2.25	122.89	126.70
24	c	905	CLA	C3B-CAB-CBB	-2.24	121.73	126.32
26	f	101	BCR	C1-C6-C5	-2.24	119.37	122.66
25	d	402	PHO	C3B-C2B-C1B	-2.24	101.48	106.33
24	c	902	CLA	CBC-CAC-C3C	-2.24	105.56	112.39
31	h	102	DGD	O1G-C1A-O1A	-2.23	117.73	123.49
26	H	101	BCR	C40-C30-C29	-2.23	100.79	108.79
26	B	622	BCR	C38-C26-C27	-2.23	109.20	113.43
25	D	401	PHO	O2D-CGD-O1D	-2.23	119.19	123.79
24	b	606	CLA	CHD-C4C-C3C	-2.22	121.51	124.94
31	j	101	DGD	O1G-C1A-O1A	-2.22	117.77	123.49
24	b	605	CLA	O2A-CGA-O1A	-2.22	117.77	123.49
24	b	614	CLA	O2D-CGD-O1D	-2.21	119.22	123.79
29	d	408	LHG	O8-C23-O10	-2.21	117.79	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	908	CLA	CBC-CAC-C3C	-2.21	105.66	112.39
24	A	614	CLA	C3B-CAB-CBB	-2.19	121.84	126.32
26	a	409	BCR	C1-C6-C5	-2.19	119.45	122.66
28	a	411	SQD	C45-O47-C7	-2.18	112.65	117.89
26	T	102	BCR	C31-C1-C2	-2.18	100.97	108.79
24	b	608	CLA	O1D-CGD-CBD	-2.18	121.50	124.62
26	b	618	BCR	C40-C30-C39	-2.18	101.39	108.37
24	c	904	CLA	C3B-CAB-CBB	-2.18	121.86	126.32
24	C	510	CLA	O2D-CGD-O1D	-2.18	119.29	123.79
24	b	615	CLA	C3B-CAB-CBB	-2.18	121.86	126.32
27	d	405	PL9	C7-C8-C9	-2.18	123.01	126.70
26	a	409	BCR	C38-C26-C25	-2.18	122.47	124.61
24	b	615	CLA	C1C-NC-C4C	-2.17	103.62	106.27
27	a	410	PL9	C17-C18-C19	-2.17	123.04	127.76
24	C	502	CLA	CHD-C4C-C3C	-2.17	121.59	124.94
24	b	615	CLA	C4-C3-C2	-2.16	119.25	123.50
24	B	610	CLA	O1D-CGD-CBD	-2.16	121.52	124.62
24	d	404	CLA	C4C-C3C-C2C	-2.16	103.43	106.94
24	A	607	CLA	C4C-C3C-C2C	-2.16	103.43	106.94
26	a	409	BCR	C31-C1-C2	-2.16	101.05	108.79
24	C	510	CLA	C1C-NC-C4C	-2.16	103.64	106.27
26	C	515	BCR	C37-C22-C23	-2.15	114.52	118.10
24	B	613	CLA	O2D-CGD-O1D	-2.15	119.35	123.79
27	A	611	PL9	C17-C18-C19	-2.15	123.09	127.76
28	F	101	SQD	O48-C23-O10	-2.15	117.95	123.49
24	B	616	CLA	O2D-CGD-O1D	-2.15	119.36	123.79
24	c	902	CLA	C3B-CAB-CBB	-2.15	121.93	126.32
24	c	911	CLA	C4-C3-C2	-2.14	119.29	123.50
24	B	617	CLA	CHD-C4C-C3C	-2.14	121.63	124.94
24	b	603	CLA	C3B-CAB-CBB	-2.14	121.94	126.32
24	C	506	CLA	C1C-NC-C4C	-2.14	103.67	106.27
24	c	910	CLA	C1C-NC-C4C	-2.14	103.67	106.27
28	L	101	SQD	O5-C1-C2	-2.14	105.89	110.28
24	b	617	CLA	O2D-CGD-O1D	-2.14	119.38	123.79
24	B	614	CLA	CBC-CAC-C3C	-2.13	105.88	112.39
24	c	906	CLA	C3B-CAB-CBB	-2.13	121.96	126.32
24	D	402	CLA	CAA-CBA-CGA	-2.13	107.08	113.32
29	d	409	LHG	O8-C23-O10	-2.13	118.00	123.49
24	b	608	CLA	C1C-NC-C4C	-2.13	103.68	106.27
26	B	619	BCR	C29-C28-C27	-2.13	106.17	111.53
24	A	609	CLA	C1C-NC-C4C	-2.13	103.68	106.27
29	A	615	LHG	O8-C23-O10	-2.12	118.01	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C31-C1-C2	-2.12	101.18	108.79
24	C	505	CLA	C1C-NC-C4C	-2.12	103.69	106.27
25	A	608	PHO	CHC-C1C-C2C	-2.12	120.81	125.61
26	D	404	BCR	C37-C22-C23	-2.12	114.57	118.10
24	A	614	CLA	C4C-C3C-C2C	-2.12	103.50	106.94
27	d	405	PL9	C22-C23-C24	-2.12	123.16	127.76
26	A	610	BCR	C37-C22-C23	-2.11	114.58	118.10
26	B	620	BCR	C38-C26-C27	-2.11	109.43	113.43
32	V	202	HEM	C3B-CAB-CBB	-2.11	121.23	124.46
31	C	516	DGD	C3G-C2G-C1G	-2.11	107.14	112.07
25	A	608	PHO	C1C-NC-C4C	-2.11	102.35	106.51
26	f	101	BCR	C31-C1-C2	-2.10	101.25	108.79
24	B	606	CLA	O2D-CGD-O1D	-2.10	119.45	123.79
24	b	604	CLA	O2A-CGA-O1A	-2.10	118.07	123.49
31	c	916	DGD	C2G-O2G-C1B	-2.10	112.85	117.89
24	B	612	CLA	CBC-CAC-C3C	-2.10	105.99	112.39
24	C	504	CLA	C4C-C3C-C2C	-2.10	103.54	106.94
32	v	202	HEM	C3B-C4B-NB	-2.09	107.62	111.63
24	b	610	CLA	C1C-NC-C4C	-2.09	103.72	106.27
28	A	612	SQD	O48-C23-O10	-2.09	118.09	123.49
28	A	612	SQD	O5-C1-C2	-2.09	105.98	110.28
24	a	406	CLA	C7-C6-C5	-2.09	106.88	113.06
24	C	509	CLA	C1C-NC-C4C	-2.09	103.73	106.27
24	A	609	CLA	C3B-CAB-CBB	-2.09	122.05	126.32
29	B	621	LHG	C6-C5-C4	-2.08	107.20	112.07
24	b	609	CLA	O2A-CGA-O1A	-2.08	118.13	123.49
24	C	507	CLA	C3B-CAB-CBB	-2.08	122.07	126.32
24	B	606	CLA	CHD-C4C-C3C	-2.07	121.74	124.94
24	B	608	CLA	C3B-CAB-CBB	-2.07	122.08	126.32
24	C	504	CLA	O1D-CGD-CBD	-2.07	121.65	124.62
26	k	102	BCR	C37-C22-C23	-2.07	114.65	118.10
24	d	403	CLA	OBD-CAD-C3D	-2.07	124.13	128.35
26	k	102	BCR	C34-C9-C8	-2.07	114.65	118.10
24	c	911	CLA	O2D-CGD-O1D	-2.07	119.52	123.79
24	b	612	CLA	C3B-CAB-CBB	-2.07	122.08	126.32
24	B	609	CLA	O2A-CGA-O1A	-2.07	118.16	123.49
24	B	609	CLA	C11-C12-C13	-2.07	108.64	115.49
24	B	609	CLA	CHC-C1C-C2C	-2.06	120.92	126.35
27	d	405	PL9	C42-C43-C44	-2.06	123.27	127.76
31	H	102	DGD	O3G-C3G-C2G	-2.06	106.08	110.99
24	D	402	CLA	C5-C3-C2	-2.06	117.14	121.05
24	b	608	CLA	CHD-C4C-C3C	-2.06	121.76	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	915	BCR	C39-C30-C29	-2.06	101.42	108.79
27	D	405	PL9	C31-C32-C33	-2.06	106.30	111.69
24	B	617	CLA	C4-C3-C2	-2.06	119.46	123.50
24	B	605	CLA	C3B-CAB-CBB	-2.05	122.12	126.32
24	B	604	CLA	CHD-C4C-C3C	-2.05	121.77	124.94
24	C	502	CLA	C1C-NC-C4C	-2.05	103.78	106.27
24	d	403	CLA	C5-C3-C2	-2.05	117.16	121.05
24	c	906	CLA	CBC-CAC-C3C	-2.05	106.14	112.39
24	b	606	CLA	C5-C3-C2	-2.05	117.17	121.05
24	C	513	CLA	C3B-CAB-CBB	-2.05	122.13	126.32
24	c	904	CLA	O2D-CGD-O1D	-2.05	119.56	123.79
24	b	610	CLA	C7-C6-C5	-2.04	107.03	113.06
26	c	918	BCR	C31-C1-C2	-2.04	101.47	108.79
24	B	617	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
24	C	509	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
32	E	101	HEM	CAA-C2A-C1A	-2.04	124.79	127.01
24	B	614	CLA	C1C-NC-C4C	-2.04	103.79	106.27
24	c	905	CLA	C7-C6-C5	-2.03	107.06	113.06
24	C	502	CLA	O1D-CGD-CBD	-2.03	121.71	124.62
24	a	407	CLA	CHC-C1C-C2C	-2.03	121.01	126.35
24	B	605	CLA	O2D-CGD-O1D	-2.03	119.60	123.79
24	B	606	CLA	O1D-CGD-CBD	-2.03	121.71	124.62
24	C	509	CLA	C3B-CAB-CBB	-2.03	122.17	126.32
25	d	402	PHO	CBA-CAA-C2A	-2.03	108.01	113.73
24	b	604	CLA	CBC-CAC-C3C	-2.03	106.20	112.39
24	A	607	CLA	CHC-C1C-C2C	-2.03	121.02	126.35
31	D	406	DGD	O2G-C1B-O1B	-2.02	118.24	123.67
24	B	611	CLA	CAA-CBA-CGA	-2.02	107.40	113.32
24	b	616	CLA	C1C-NC-C4C	-2.02	103.81	106.27
24	c	909	CLA	O1D-CGD-CBD	-2.02	121.73	124.62
26	B	619	BCR	C32-C1-C6	-2.02	107.14	110.30
24	B	605	CLA	O2A-CGA-O1A	-2.01	118.29	123.49
24	B	614	CLA	O2A-CGA-O1A	-2.01	118.29	123.49
24	c	905	CLA	C5-C3-C2	-2.01	117.23	121.05
31	H	102	DGD	C3E-C4E-C5E	-2.01	106.69	110.20
24	B	611	CLA	O2A-CGA-O1A	-2.01	118.30	123.49
26	A	610	BCR	C32-C1-C2	-2.01	101.59	108.79
24	d	404	CLA	CBC-CAC-C3C	-2.01	106.27	112.39
31	C	518	DGD	O1G-C1A-O1A	-2.00	118.32	123.49
24	C	509	CLA	CHC-C1C-C2C	-2.00	121.08	126.35
24	b	615	CLA	CMC-C2C-C1C	2.01	128.13	125.02
24	B	609	CLA	C4A-NA-C1A	2.01	108.95	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	CHB-C4A-NA	2.01	127.29	124.51
26	a	409	BCR	C4-C5-C6	2.01	125.34	122.78
24	c	903	CLA	CMC-C2C-C1C	2.01	128.13	125.02
24	A	614	CLA	C4A-NA-C1A	2.01	108.96	106.36
25	A	608	PHO	C3D-C4D-ND	2.02	116.15	109.65
24	B	609	CLA	CMC-C2C-C1C	2.02	128.15	125.02
24	b	611	CLA	CAC-C3C-C4C	2.02	127.77	124.83
26	D	404	BCR	C3-C4-C5	2.03	117.08	113.87
24	B	610	CLA	CMC-C2C-C1C	2.03	128.16	125.02
24	c	913	CLA	CED-O2D-CGD	2.03	120.75	115.99
26	c	915	BCR	C4-C5-C6	2.03	125.37	122.78
24	B	606	CLA	CMC-C2C-C1C	2.03	128.16	125.02
24	C	501	CLA	CMB-C2B-C3B	2.03	129.06	125.09
24	B	602	CLA	C4-C3-C5	2.03	118.51	115.41
24	B	611	CLA	CAC-C3C-C4C	2.03	127.78	124.83
25	a	412	PHO	O2A-CGA-CBA	2.03	118.10	111.90
24	C	503	CLA	CED-O2D-CGD	2.04	120.76	115.99
24	c	904	CLA	CMC-C2C-C1C	2.04	128.17	125.02
25	D	401	PHO	C3D-C4D-ND	2.04	116.22	109.65
24	B	615	CLA	O2A-CGA-CBA	2.04	118.11	111.90
24	a	407	CLA	CMC-C2C-C1C	2.04	128.18	125.02
24	c	904	CLA	CAC-C3C-C4C	2.04	127.79	124.83
32	e	101	HEM	C2D-C3D-C4D	2.04	104.96	101.50
24	c	911	CLA	CMC-C2C-C1C	2.04	128.18	125.02
24	C	509	CLA	CMB-C2B-C3B	2.05	129.09	125.09
31	C	517	DGD	O1G-C1A-C2A	2.05	118.13	111.90
27	D	405	PL9	C20-C19-C21	2.05	118.54	115.41
24	B	603	CLA	O2A-CGA-CBA	2.05	118.15	111.90
24	c	912	CLA	CMC-C2C-C1C	2.05	128.19	125.02
24	B	605	CLA	CAC-C3C-C4C	2.05	127.81	124.83
24	B	610	CLA	CMB-C2B-C3B	2.06	129.11	125.09
24	c	906	CLA	C4-C3-C5	2.06	118.55	115.41
24	B	607	CLA	CMC-C2C-C1C	2.06	128.20	125.02
24	B	608	CLA	CMB-C2B-C3B	2.06	129.12	125.09
24	b	610	CLA	CMC-C2C-C1C	2.06	128.21	125.02
24	C	508	CLA	C1D-CHD-C4C	2.06	125.72	122.60
24	B	611	CLA	CMB-C2B-C3B	2.06	129.12	125.09
24	C	511	CLA	CMC-C2C-C1C	2.06	128.21	125.02
24	d	401	CLA	CMC-C2C-C1C	2.07	128.22	125.02
24	C	508	CLA	CAC-C3C-C4C	2.07	127.83	124.83
26	f	101	BCR	C24-C25-C26	2.07	126.11	121.37
24	b	612	CLA	CMB-C2B-C3B	2.07	129.14	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	913	CLA	CMC-C2C-C1C	2.07	128.23	125.02
26	b	618	BCR	C31-C1-C6	2.08	113.56	110.30
29	b	620	LHG	O8-C23-C24	2.08	118.23	111.90
24	C	512	CLA	CMC-C2C-C1C	2.08	128.24	125.02
24	c	907	CLA	O2A-CGA-CBA	2.08	118.24	111.90
24	B	616	CLA	CMB-C2B-C3B	2.08	129.16	125.09
24	C	511	CLA	CED-O2D-CGD	2.08	120.88	115.99
24	A	609	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	c	906	CLA	O2A-CGA-CBA	2.09	118.26	111.90
24	b	607	CLA	CAC-C3C-C4C	2.09	127.86	124.83
24	c	911	CLA	CAC-C3C-C4C	2.09	127.86	124.83
24	B	615	CLA	CED-O2D-CGD	2.09	120.89	115.99
24	a	406	CLA	O2A-CGA-CBA	2.09	118.28	111.90
24	d	401	CLA	CED-O2D-CGD	2.10	120.90	115.99
29	d	410	LHG	O4-P-O5	2.10	123.88	112.53
24	B	615	CLA	CMB-C2B-C3B	2.10	129.19	125.09
26	B	620	BCR	C40-C30-C25	2.10	113.60	110.30
26	K	101	BCR	C1-C6-C7	2.10	121.71	115.82
24	D	402	CLA	CED-O2D-CGD	2.11	120.93	115.99
24	C	506	CLA	O2A-CGA-CBA	2.11	118.32	111.90
24	B	617	CLA	CED-O2D-CGD	2.11	120.93	115.99
24	B	602	CLA	CMB-C2B-C3B	2.11	129.22	125.09
24	b	603	CLA	CED-O2D-CGD	2.11	120.94	115.99
29	D	408	LHG	O7-C7-C8	2.11	116.12	111.53
24	A	607	CLA	CED-O2D-CGD	2.11	120.95	115.99
26	A	610	BCR	C2-C1-C6	2.11	113.71	110.36
24	d	404	CLA	CMC-C2C-C1C	2.12	128.29	125.02
24	C	512	CLA	CAC-C3C-C4C	2.12	127.91	124.83
25	D	401	PHO	CMB-C2B-C1B	2.12	128.51	125.06
24	b	616	CLA	O2A-CGA-CBA	2.12	118.37	111.90
26	c	915	BCR	C39-C30-C25	2.12	113.63	110.30
24	B	612	CLA	CMB-C2B-C3B	2.12	129.24	125.09
28	d	407	SQD	O47-C45-C46	2.13	115.85	108.36
26	B	618	BCR	C2-C3-C4	2.13	116.90	111.53
24	a	407	CLA	O2A-CGA-CBA	2.13	118.39	111.90
24	b	604	CLA	CAC-C3C-C4C	2.13	127.93	124.83
24	C	513	CLA	CAC-C3C-C4C	2.13	127.93	124.83
24	b	602	CLA	CMB-C2B-C3B	2.13	129.26	125.09
24	c	905	CLA	CMC-C2C-C1C	2.14	128.32	125.02
24	C	507	CLA	CED-O2D-CGD	2.14	121.00	115.99
24	b	611	CLA	CMB-C2B-C3B	2.14	129.27	125.09
24	b	609	CLA	CAC-C3C-C4C	2.14	127.93	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	CED-O2D-CGD	2.14	121.01	115.99
24	C	511	CLA	CAC-C3C-C4C	2.14	127.94	124.83
28	F	101	SQD	C3-C4-C5	2.14	113.93	110.20
24	c	904	CLA	O2A-CGA-CBA	2.14	118.43	111.90
24	B	604	CLA	O2A-CGA-CBA	2.15	118.44	111.90
24	C	510	CLA	CAC-C3C-C4C	2.15	127.94	124.83
25	A	608	PHO	CMB-C2B-C1B	2.15	128.56	125.06
25	d	402	PHO	CMC-C2C-C1C	2.15	128.56	125.06
24	b	607	CLA	CMB-C2B-C3B	2.15	129.30	125.09
31	H	102	DGD	O6E-C5E-C6E	2.16	111.81	106.36
26	f	101	BCR	C30-C25-C24	2.16	121.87	115.82
24	c	909	CLA	CAC-C3C-C2C	2.16	131.30	127.51
24	b	617	CLA	C4-C3-C5	2.16	118.71	115.41
24	B	606	CLA	CED-O2D-CGD	2.17	121.07	115.99
24	C	510	CLA	C4-C3-C5	2.17	118.72	115.41
24	a	407	CLA	CED-O2D-CGD	2.17	121.09	115.99
24	C	509	CLA	C4-C3-C5	2.18	118.73	115.41
24	b	614	CLA	C4-C3-C5	2.18	118.73	115.41
24	A	606	CLA	O2A-CGA-CBA	2.18	118.54	111.90
24	a	408	CLA	CED-O2D-CGD	2.18	121.10	115.99
24	c	902	CLA	O2A-CGA-CBA	2.18	118.54	111.90
24	b	604	CLA	O2A-CGA-CBA	2.18	118.55	111.90
26	b	618	BCR	C1-C6-C7	2.19	121.95	115.82
29	D	409	LHG	O8-C23-C24	2.19	118.57	111.90
24	c	912	CLA	O2A-CGA-CBA	2.19	118.57	111.90
24	B	613	CLA	O2A-CGA-CBA	2.19	118.58	111.90
24	A	609	CLA	CMB-C2B-C3B	2.19	129.38	125.09
26	k	101	BCR	C30-C25-C24	2.19	121.96	115.82
24	c	914	CLA	CED-O2D-CGD	2.19	121.13	115.99
26	K	101	BCR	C38-C26-C25	2.20	126.77	124.61
26	H	101	BCR	C28-C29-C30	2.20	122.98	114.83
24	B	603	CLA	CED-O2D-CGD	2.20	121.15	115.99
24	c	909	CLA	CED-O2D-CGD	2.21	121.16	115.99
26	h	101	BCR	C28-C29-C30	2.21	123.00	114.83
24	B	614	CLA	CMC-C2C-C1C	2.21	128.44	125.02
24	C	506	CLA	CMB-C2B-C3B	2.21	129.41	125.09
26	k	101	BCR	C1-C6-C7	2.21	122.00	115.82
24	B	605	CLA	CMC-C2C-C1C	2.21	128.44	125.02
27	d	405	PL9	C10-C9-C11	2.22	118.80	115.41
24	a	406	CLA	C4A-NA-C1A	2.22	109.23	106.36
24	A	606	CLA	CMC-C2C-C1C	2.22	128.46	125.02
26	C	515	BCR	C28-C27-C26	2.22	117.39	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	907	CLA	CMC-C2C-C1C	2.22	128.46	125.02
24	b	602	CLA	CED-O2D-CGD	2.22	121.20	115.99
24	D	402	CLA	O2A-CGA-CBA	2.23	118.69	111.90
24	B	617	CLA	C4-C3-C5	2.23	118.81	115.41
24	b	617	CLA	CMC-C2C-C1C	2.23	128.48	125.02
24	b	609	CLA	O2A-CGA-CBA	2.24	118.71	111.90
27	a	410	PL9	C15-C14-C16	2.24	118.83	115.41
24	d	401	CLA	CMB-C2B-C3B	2.25	129.48	125.09
24	b	609	CLA	CMC-C2C-C1C	2.25	128.50	125.02
26	D	404	BCR	C24-C25-C26	2.25	126.53	121.37
24	C	507	CLA	O2A-CGA-CBA	2.25	118.76	111.90
31	j	101	DGD	O2G-C1B-C2B	2.25	116.42	111.53
29	d	409	LHG	O7-C7-C8	2.25	116.42	111.53
24	b	607	CLA	O2A-CGA-CBA	2.26	118.78	111.90
27	d	405	PL9	C25-C24-C26	2.26	118.86	115.41
24	C	506	CLA	CAC-C3C-C4C	2.27	128.12	124.83
24	C	501	CLA	C4-C3-C5	2.27	118.87	115.41
24	D	403	CLA	CMB-C2B-C3B	2.27	129.53	125.09
24	c	910	CLA	O2A-CGA-CBA	2.27	118.82	111.90
24	b	604	CLA	C4A-NA-C1A	2.27	109.30	106.36
26	Y	101	BCR	C30-C25-C24	2.28	122.19	115.82
24	B	610	CLA	CED-O2D-CGD	2.28	121.33	115.99
24	b	614	CLA	CMB-C2B-C3B	2.28	129.54	125.09
24	b	608	CLA	CMC-C2C-C1C	2.28	128.55	125.02
26	C	515	BCR	C4-C5-C6	2.28	125.69	122.78
24	B	605	CLA	O2A-CGA-CBA	2.28	118.86	111.90
24	c	903	CLA	O2A-CGA-CBA	2.28	118.86	111.90
24	b	605	CLA	CMB-C2B-C3B	2.29	129.56	125.09
24	c	910	CLA	CED-O2D-CGD	2.29	121.36	115.99
24	c	912	CLA	CMB-C2B-C3B	2.29	129.57	125.09
24	d	403	CLA	CMC-C2C-C1C	2.29	128.57	125.02
25	a	412	PHO	CAC-C3C-C4C	2.30	127.84	125.16
28	A	612	SQD	O48-C23-C24	2.30	118.90	111.90
24	C	505	CLA	CED-O2D-CGD	2.30	121.38	115.99
24	C	506	CLA	CMC-C2C-C1C	2.30	128.58	125.02
24	c	911	CLA	O2A-CGA-CBA	2.30	118.91	111.90
25	d	402	PHO	C4D-C3D-CAD	2.30	109.65	105.51
24	B	615	CLA	CMC-C2C-C1C	2.30	128.59	125.02
24	C	509	CLA	CAC-C3C-C4C	2.31	128.18	124.83
24	b	613	CLA	CED-O2D-CGD	2.31	121.40	115.99
24	A	609	CLA	CAC-C3C-C4C	2.31	128.18	124.83
24	b	608	CLA	CMB-C2B-C3B	2.31	129.61	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	d	405	PL9	C35-C34-C36	2.31	118.94	115.41
24	d	404	CLA	CMB-C2B-C3B	2.32	129.62	125.09
24	C	510	CLA	O2A-CGA-CBA	2.32	118.97	111.90
24	A	609	CLA	O2A-CGA-CBA	2.32	118.97	111.90
24	c	902	CLA	CMC-C2C-C1C	2.32	128.61	125.02
24	B	614	CLA	CMB-C2B-C3B	2.32	129.63	125.09
24	C	512	CLA	CED-O2D-CGD	2.32	121.44	115.99
24	d	403	CLA	O2A-CGA-CBA	2.33	119.01	111.90
28	A	613	SQD	C3-C4-C5	2.34	114.27	110.20
24	b	614	CLA	CAC-C3C-C4C	2.34	128.23	124.83
29	d	408	LHG	C6-O8-C23	2.34	123.41	116.85
31	D	406	DGD	O6E-C5E-C6E	2.35	112.28	106.36
26	T	101	BCR	C1-C6-C7	2.35	122.39	115.82
25	D	401	PHO	CED-O2D-CGD	2.35	121.50	115.99
24	c	914	CLA	C4-C3-C5	2.35	119.00	115.41
24	c	911	CLA	CMB-C2B-C3B	2.35	129.69	125.09
26	D	404	BCR	C38-C26-C25	2.35	126.92	124.61
24	c	905	CLA	CAC-C3C-C4C	2.35	128.25	124.83
24	b	602	CLA	C3B-C4B-NB	2.35	112.25	109.21
24	c	906	CLA	CED-O2D-CGD	2.36	121.52	115.99
24	A	614	CLA	CMC-C2C-C1C	2.36	128.67	125.02
31	D	406	DGD	O6D-C5D-C6D	2.36	111.43	106.61
24	c	907	CLA	C4-C3-C5	2.36	119.01	115.41
24	B	609	CLA	CAC-C3C-C4C	2.36	128.26	124.83
24	D	403	CLA	CAC-C3C-C4C	2.36	128.26	124.83
31	c	917	DGD	O1G-C1A-C2A	2.36	119.10	111.90
24	C	504	CLA	CMC-C2C-C1C	2.37	128.68	125.02
26	k	101	BCR	C3-C4-C5	2.37	117.62	113.87
24	B	611	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	C	515	BCR	C23-C24-C25	2.37	134.44	127.32
24	b	612	CLA	CAC-C3C-C4C	2.38	128.28	124.83
29	D	408	LHG	O8-C23-C24	2.38	119.16	111.90
26	T	101	BCR	C32-C1-C6	2.38	114.04	110.30
24	c	903	CLA	CMB-C2B-C3B	2.38	129.75	125.09
32	v	202	HEM	C3B-C4B-CHC	2.38	126.52	123.16
24	c	903	CLA	C4-C3-C5	2.39	119.05	115.41
29	d	409	LHG	O8-C23-C24	2.39	119.17	111.90
24	b	611	CLA	O2A-CGA-CBA	2.39	119.18	111.90
24	a	408	CLA	O2A-CGA-CBA	2.39	119.18	111.90
27	a	410	PL9	C10-C9-C11	2.39	119.06	115.41
27	a	410	PL9	C45-C44-C46	2.39	119.06	115.41
24	a	407	CLA	C4A-NA-C1A	2.40	109.45	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	910	CLA	CMB-C2B-C3B	2.40	129.77	125.09
26	B	622	BCR	C27-C26-C25	2.40	125.83	122.78
27	a	410	PL9	C53-C6-C1	2.40	120.67	114.94
24	B	612	CLA	CAC-C3C-C4C	2.40	128.32	124.83
24	A	606	CLA	C4-C3-C5	2.40	119.08	115.41
24	b	615	CLA	CAC-C3C-C4C	2.41	128.32	124.83
24	B	614	CLA	O2A-CGA-CBA	2.41	119.23	111.90
26	T	101	BCR	C23-C24-C25	2.41	134.55	127.32
25	a	412	PHO	CMB-C2B-C1B	2.41	128.98	125.06
26	H	101	BCR	C30-C25-C24	2.41	122.56	115.82
24	B	609	CLA	C4-C3-C5	2.41	119.09	115.41
24	C	501	CLA	CAC-C3C-C4C	2.41	128.33	124.83
24	C	502	CLA	CMC-C2C-C1C	2.41	128.76	125.02
24	A	606	CLA	C4A-NA-C1A	2.42	109.49	106.36
26	f	101	BCR	C3-C2-C1	2.42	123.80	114.83
24	C	505	CLA	CMB-C2B-C3B	2.42	129.83	125.09
24	b	615	CLA	CHB-C4A-NA	2.42	127.86	124.51
24	A	614	CLA	CAC-C3C-C4C	2.43	128.35	124.83
24	c	914	CLA	C3B-C4B-NB	2.43	112.35	109.21
24	C	507	CLA	CMC-C2C-C1C	2.43	128.78	125.02
24	a	406	CLA	C4-C3-C5	2.43	119.13	115.41
24	A	609	CLA	CED-O2D-CGD	2.44	121.70	115.99
24	B	607	CLA	O2A-CGA-CBA	2.44	119.33	111.90
26	T	101	BCR	C40-C30-C25	2.44	114.13	110.30
25	D	401	PHO	C4D-C3D-CAD	2.44	109.90	105.51
26	b	619	BCR	C28-C27-C26	2.44	117.75	113.87
26	k	102	BCR	C30-C25-C24	2.44	122.66	115.82
27	d	405	PL9	C20-C19-C21	2.45	119.15	115.41
24	C	513	CLA	O2A-CGA-CBA	2.45	119.37	111.90
24	b	605	CLA	C4-C3-C5	2.45	119.15	115.41
24	C	508	CLA	CMB-C2B-C3B	2.45	129.89	125.09
24	c	910	CLA	CMC-C2C-C1C	2.45	128.82	125.02
26	B	622	BCR	C1-C6-C7	2.45	122.69	115.82
24	b	605	CLA	CED-O2D-CGD	2.46	121.75	115.99
24	A	609	CLA	CMC-C2C-C1C	2.46	128.82	125.02
27	D	405	PL9	C10-C9-C11	2.46	119.16	115.41
26	B	620	BCR	C31-C1-C6	2.46	114.16	110.30
24	D	402	CLA	C4A-NA-C1A	2.47	109.55	106.36
26	k	101	BCR	C32-C1-C6	2.47	114.17	110.30
24	c	903	CLA	CAC-C3C-C4C	2.47	128.41	124.83
29	D	407	LHG	O7-C7-C8	2.47	116.90	111.53
24	b	616	CLA	CAC-C3C-C4C	2.47	128.42	124.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	614	CLA	CMB-C2B-C3B	2.48	129.93	125.09
24	b	614	CLA	O2A-CGA-CBA	2.48	119.45	111.90
24	D	402	CLA	CAC-C3C-C4C	2.48	128.43	124.83
27	A	611	PL9	C53-C6-C1	2.48	120.86	114.94
24	b	602	CLA	C4-C3-C5	2.48	119.20	115.41
29	d	410	LHG	O8-C23-C24	2.48	119.46	111.90
24	A	606	CLA	CAC-C3C-C4C	2.48	128.44	124.83
26	k	101	BCR	C28-C27-C26	2.49	117.81	113.87
32	V	202	HEM	C3B-C4B-CHC	2.49	126.67	123.16
25	A	608	PHO	C4D-C3D-CAD	2.49	109.99	105.51
24	b	617	CLA	CED-O2D-CGD	2.49	121.83	115.99
27	d	405	PL9	C53-C6-C1	2.49	120.89	114.94
24	D	403	CLA	CED-O2D-CGD	2.49	121.83	115.99
24	C	512	CLA	O2A-CGA-CBA	2.49	119.49	111.90
27	D	405	PL9	C35-C34-C36	2.49	119.21	115.41
24	a	408	CLA	CAC-C3C-C4C	2.49	128.45	124.83
26	h	101	BCR	C30-C25-C24	2.49	122.80	115.82
24	C	510	CLA	CMB-C2B-C3B	2.50	129.97	125.09
26	D	404	BCR	C30-C25-C24	2.50	122.81	115.82
24	c	914	CLA	CMC-C2C-C1C	2.50	128.89	125.02
24	b	613	CLA	O2A-CGA-CBA	2.50	119.53	111.90
24	b	611	CLA	C4-C3-C5	2.50	119.23	115.41
24	b	603	CLA	O2A-CGA-CBA	2.51	119.53	111.90
24	B	613	CLA	CMC-C2C-C1C	2.51	128.90	125.02
29	a	413	LHG	O8-C23-C24	2.51	119.54	111.90
24	C	507	CLA	CMB-C2B-C3B	2.51	130.00	125.09
24	c	908	CLA	CMC-C2C-C1C	2.51	128.91	125.02
24	b	608	CLA	CED-O2D-CGD	2.52	121.89	115.99
27	d	405	PL9	C15-C14-C16	2.52	119.25	115.41
24	C	509	CLA	O2A-CGA-CBA	2.52	119.58	111.90
32	E	101	HEM	C2D-C3D-C4D	2.52	105.78	101.50
24	d	404	CLA	C4-C3-C5	2.53	119.27	115.41
24	C	503	CLA	CMC-C2C-C1C	2.53	128.93	125.02
24	c	913	CLA	O2A-CGA-CBA	2.53	119.60	111.90
24	b	613	CLA	CMC-C2C-C1C	2.53	128.93	125.02
28	L	101	SQD	C4-C3-C2	2.54	115.52	110.79
24	D	402	CLA	CMC-C2C-C1C	2.54	128.94	125.02
24	b	606	CLA	C4A-NA-C1A	2.54	109.64	106.36
24	C	512	CLA	CMB-C2B-C3B	2.55	130.07	125.09
27	D	405	PL9	C53-C6-C1	2.55	121.03	114.94
24	b	603	CLA	C4A-NA-C1A	2.55	109.66	106.36
24	B	617	CLA	CMB-C2B-C3B	2.56	130.09	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	411	SQD	O48-C23-C24	2.56	119.69	111.90
24	C	501	CLA	CMC-C2C-C1C	2.56	128.99	125.02
27	A	611	PL9	C45-C44-C46	2.57	119.33	115.41
26	H	101	BCR	C39-C30-C25	2.57	114.33	110.30
25	a	412	PHO	C4D-C3D-CAD	2.57	110.13	105.51
24	C	513	CLA	CMC-C2C-C1C	2.57	129.00	125.02
26	C	515	BCR	C27-C26-C25	2.57	126.06	122.78
24	c	908	CLA	O2A-CGA-CBA	2.58	119.77	111.90
24	d	403	CLA	C4A-NA-C1A	2.59	109.70	106.36
24	C	513	CLA	C4-C3-C5	2.59	119.37	115.41
24	a	408	CLA	CMB-C2B-C3B	2.59	130.16	125.09
26	c	918	BCR	C8-C9-C10	2.60	123.17	118.98
24	B	604	CLA	CMB-C2B-C3B	2.60	130.18	125.09
26	K	101	BCR	C4-C5-C6	2.61	126.11	122.78
24	b	605	CLA	O2A-CGA-CBA	2.61	119.86	111.90
24	c	914	CLA	O2A-CGA-CBA	2.61	119.86	111.90
24	b	616	CLA	C4-C3-C5	2.62	119.41	115.41
24	a	408	CLA	C4-C3-C5	2.62	119.41	115.41
26	c	918	BCR	C40-C30-C25	2.63	114.43	110.30
26	A	610	BCR	C29-C30-C25	2.63	114.53	110.36
32	E	101	HEM	CMD-C2D-C3D	2.64	126.01	114.35
26	c	918	BCR	C27-C26-C25	2.64	126.14	122.78
26	B	619	BCR	C4-C5-C6	2.64	126.14	122.78
24	C	505	CLA	CAC-C3C-C4C	2.64	128.67	124.83
24	B	613	CLA	CED-O2D-CGD	2.64	122.19	115.99
24	b	615	CLA	CED-O2D-CGD	2.65	122.20	115.99
26	A	610	BCR	C8-C7-C6	2.65	135.27	127.32
26	C	514	BCR	C39-C30-C25	2.65	114.45	110.30
24	a	406	CLA	CMB-C2B-C3B	2.65	130.27	125.09
31	C	518	DGD	O1G-C1A-C2A	2.65	119.98	111.90
24	C	504	CLA	CAC-C3C-C4C	2.65	128.68	124.83
24	c	905	CLA	CMB-C2B-C3B	2.65	130.28	125.09
31	D	406	DGD	O1G-C1A-C2A	2.65	119.98	111.90
24	B	602	CLA	C3B-C4B-NB	2.65	112.64	109.21
24	b	612	CLA	CMC-C2C-C1C	2.66	129.13	125.02
26	T	101	BCR	C38-C26-C25	2.66	127.22	124.61
25	d	402	PHO	CAC-C3C-C4C	2.66	128.27	125.16
25	A	608	PHO	CAC-C3C-C4C	2.66	128.27	125.16
24	c	904	CLA	CMB-C2B-C3B	2.67	130.31	125.09
24	c	906	CLA	CMC-C2C-C1C	2.67	129.15	125.02
26	D	404	BCR	C2-C1-C6	2.67	114.59	110.36
26	B	619	BCR	C1-C6-C7	2.67	123.30	115.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	602	CLA	CMC-C2C-C1C	2.67	129.15	125.02
24	C	510	CLA	CMC-C2C-C1C	2.67	129.15	125.02
26	K	101	BCR	C29-C30-C25	2.67	114.59	110.36
24	c	906	CLA	CAC-C3C-C4C	2.67	128.71	124.83
31	c	917	DGD	O2G-C1B-C2B	2.68	117.34	111.53
24	d	403	CLA	CMB-C2B-C3B	2.68	130.33	125.09
31	d	406	DGD	O1G-C1A-C2A	2.69	120.09	111.90
24	B	615	CLA	CAC-C3C-C4C	2.70	128.74	124.83
26	Y	101	BCR	C28-C27-C26	2.70	118.15	113.87
24	D	403	CLA	C4-C3-C5	2.70	119.53	115.41
24	C	513	CLA	CMB-C2B-C3B	2.70	130.37	125.09
24	C	506	CLA	C3B-C4B-NB	2.70	112.70	109.21
28	a	402	SQD	C3-C4-C5	2.70	114.91	110.20
24	d	401	CLA	C4A-NA-C1A	2.70	109.85	106.36
24	c	913	CLA	C3B-C4B-NB	2.70	112.71	109.21
24	B	614	CLA	C4-C3-C5	2.71	119.54	115.41
24	b	609	CLA	C4-C3-C5	2.71	119.55	115.41
28	d	407	SQD	O48-C23-C24	2.71	120.16	111.90
24	B	617	CLA	O2A-CGA-CBA	2.71	120.17	111.90
31	h	102	DGD	O1G-C1A-C2A	2.72	120.18	111.90
26	b	618	BCR	C2-C1-C6	2.72	114.66	110.36
24	b	615	CLA	O2A-CGA-CBA	2.72	120.18	111.90
26	T	101	BCR	C29-C30-C25	2.72	114.67	110.36
24	b	608	CLA	CAC-C3C-C4C	2.72	128.78	124.83
24	B	611	CLA	O2A-CGA-CBA	2.72	120.20	111.90
24	B	611	CLA	C4-C3-C5	2.73	119.58	115.41
24	B	606	CLA	C3B-C4B-NB	2.73	112.75	109.21
24	C	513	CLA	C3B-C4B-NB	2.73	112.75	109.21
31	j	101	DGD	O1G-C1A-C2A	2.74	120.24	111.90
24	C	512	CLA	C3B-C4B-NB	2.75	112.76	109.21
27	A	611	PL9	C10-C9-C11	2.75	119.60	115.41
24	B	602	CLA	CMC-C2C-C1C	2.75	129.28	125.02
24	a	408	CLA	CMC-C2C-C1C	2.75	129.28	125.02
24	b	617	CLA	O2A-CGA-CBA	2.75	120.29	111.90
24	B	603	CLA	CMB-C2B-C3B	2.76	130.48	125.09
24	b	609	CLA	C4A-NA-C1A	2.76	109.92	106.36
24	B	616	CLA	C4-C3-C5	2.76	119.63	115.41
24	B	609	CLA	O2A-CGA-CBA	2.76	120.32	111.90
26	C	514	BCR	C3-C4-C5	2.77	118.26	113.87
24	C	504	CLA	CMB-C2B-C3B	2.78	130.52	125.09
24	c	907	CLA	CED-O2D-CGD	2.78	122.52	115.99
24	C	503	CLA	C3B-C4B-NB	2.79	112.82	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	502	CLA	C4-C3-C5	2.80	119.68	115.41
28	L	101	SQD	O48-C23-C24	2.80	120.42	111.90
26	K	101	BCR	C33-C5-C6	2.81	127.36	124.61
24	a	407	CLA	CAC-C3C-C4C	2.81	128.91	124.83
28	l	101	SQD	O48-C23-C24	2.81	120.47	111.90
24	b	604	CLA	CMC-C2C-C1C	2.82	129.38	125.02
24	C	503	CLA	C4-C3-C5	2.82	119.72	115.41
24	C	511	CLA	C4-C3-C5	2.82	119.72	115.41
31	d	406	DGD	O5D-C1E-C2E	2.82	111.61	108.04
28	l	101	SQD	O9-S-C6	2.83	109.33	106.94
24	d	401	CLA	C4-C3-C5	2.83	119.73	115.41
24	C	507	CLA	C3B-C4B-NB	2.84	112.88	109.21
24	C	505	CLA	C3B-C4B-NB	2.84	112.89	109.21
28	d	407	SQD	O7-S-C6	2.84	109.34	106.94
26	T	101	BCR	C3-C4-C5	2.85	118.38	113.87
26	k	102	BCR	C4-C5-C6	2.85	126.41	122.78
24	c	914	CLA	CMB-C2B-C3B	2.86	130.67	125.09
24	B	609	CLA	CMB-C2B-C3B	2.86	130.69	125.09
24	c	906	CLA	CMB-C2B-C3B	2.86	130.69	125.09
24	b	616	CLA	CMB-C2B-C3B	2.87	130.69	125.09
24	D	402	CLA	C4-C3-C5	2.87	119.78	115.41
26	B	618	BCR	C4-C5-C6	2.87	126.44	122.78
24	B	613	CLA	CMB-C2B-C3B	2.87	130.70	125.09
24	B	610	CLA	CAC-C3C-C4C	2.87	129.00	124.83
27	A	611	PL9	C40-C39-C41	2.88	119.80	115.41
24	b	617	CLA	CAC-C3C-C4C	2.88	129.01	124.83
24	c	913	CLA	C4-C3-C5	2.88	119.80	115.41
27	a	410	PL9	C40-C39-C41	2.88	119.81	115.41
31	H	102	DGD	O2G-C1B-C2B	2.88	117.79	111.53
28	a	402	SQD	O48-C23-C24	2.88	120.69	111.90
27	a	410	PL9	C30-C29-C31	2.89	119.81	115.41
26	D	404	BCR	C3-C2-C1	2.89	125.52	114.83
32	V	202	HEM	CMD-C2D-C3D	2.89	127.12	114.35
26	f	101	BCR	C28-C27-C26	2.89	118.45	113.87
26	B	620	BCR	C39-C30-C25	2.89	114.83	110.30
24	c	911	CLA	C4-C3-C5	2.90	119.83	115.41
32	e	101	HEM	CMD-C2D-C3D	2.90	127.19	114.35
24	b	606	CLA	C3B-C4B-NB	2.90	112.96	109.21
26	b	618	BCR	C32-C1-C6	2.90	114.86	110.30
24	b	604	CLA	CMB-C2B-C3B	2.91	130.77	125.09
24	B	603	CLA	C4A-NA-C1A	2.91	110.12	106.36
29	d	408	LHG	O8-C23-C24	2.91	120.77	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	a	410	PL9	C20-C19-C21	2.92	119.86	115.41
24	B	613	CLA	C3B-C4B-NB	2.92	112.98	109.21
24	c	904	CLA	C3B-C4B-NB	2.92	112.99	109.21
26	B	618	BCR	C39-C30-C25	2.93	114.89	110.30
26	k	102	BCR	C29-C30-C25	2.93	115.00	110.36
24	c	909	CLA	C4-C3-C5	2.93	119.88	115.41
32	V	202	HEM	C2D-C3D-C4D	2.93	106.47	101.50
32	v	202	HEM	CMD-C2D-C3D	2.93	127.31	114.35
32	e	101	HEM	C3B-C4B-CHC	2.93	127.29	123.16
24	C	505	CLA	CMC-C2C-C1C	2.94	129.57	125.02
29	d	408	LHG	O7-C7-C8	2.94	117.92	111.53
24	A	607	CLA	CAC-C3C-C4C	2.94	129.10	124.83
27	a	410	PL9	C35-C34-C36	2.94	119.90	115.41
24	C	508	CLA	C4-C3-C5	2.95	119.91	115.41
26	f	101	BCR	C3-C4-C5	2.96	118.56	113.87
24	c	904	CLA	C4-C3-C5	2.96	119.92	115.41
24	B	612	CLA	CMC-C2C-C1C	2.96	129.60	125.02
24	b	610	CLA	CAC-C3C-C4C	2.96	129.13	124.83
24	c	908	CLA	C3B-C4B-NB	2.96	113.04	109.21
24	b	603	CLA	C3B-C4B-NB	2.97	113.05	109.21
27	A	611	PL9	C35-C34-C36	2.97	119.94	115.41
24	c	906	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	B	605	CLA	C4-C3-C5	2.98	119.95	115.41
25	D	401	PHO	C4A-NA-C1A	2.98	110.87	108.21
24	b	606	CLA	CAC-C3C-C4C	2.98	129.15	124.83
31	H	102	DGD	O1G-C1A-C2A	2.98	120.98	111.90
24	a	408	CLA	C4A-NA-C1A	2.98	110.21	106.36
24	B	617	CLA	CAC-C3C-C4C	2.98	129.16	124.83
24	C	501	CLA	C3B-C4B-NB	2.99	113.07	109.21
25	a	412	PHO	C4A-NA-C1A	2.99	110.88	108.21
24	C	502	CLA	C4A-NA-C1A	3.00	110.23	106.36
24	A	607	CLA	C4A-NA-C1A	3.00	110.23	106.36
24	B	603	CLA	C3B-C4B-NB	3.00	113.09	109.21
24	C	502	CLA	CAC-C3C-C4C	3.01	129.20	124.83
24	b	616	CLA	CMC-C2C-C1C	3.02	129.69	125.02
28	A	613	SQD	O48-C23-C24	3.02	121.10	111.90
24	b	605	CLA	CMC-C2C-C1C	3.02	129.70	125.02
28	F	101	SQD	O48-C23-C24	3.02	121.11	111.90
24	B	604	CLA	C4A-NA-C1A	3.03	110.27	106.36
26	K	101	BCR	C40-C30-C25	3.03	115.05	110.30
26	B	620	BCR	C30-C25-C24	3.03	124.30	115.82
24	d	404	CLA	C4A-NA-C1A	3.03	110.27	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	916	DGD	O2G-C1B-C2B	3.03	118.11	111.53
24	b	603	CLA	C4-C3-C5	3.04	120.05	115.41
24	B	608	CLA	C4A-NA-C1A	3.04	110.29	106.36
24	B	606	CLA	C4A-NA-C1A	3.04	110.29	106.36
26	k	101	BCR	C23-C24-C25	3.04	136.45	127.32
24	B	608	CLA	C4-C3-C5	3.04	120.05	115.41
26	A	610	BCR	C31-C1-C6	3.04	115.07	110.30
24	a	407	CLA	C4-C3-C5	3.05	120.06	115.41
26	h	101	BCR	C27-C26-C25	3.05	126.67	122.78
32	v	202	HEM	C2D-C3D-C4D	3.05	106.67	101.50
24	A	607	CLA	CMC-C2C-C1C	3.05	129.74	125.02
29	B	621	LHG	O7-C7-C8	3.05	118.16	111.53
24	b	607	CLA	C4-C3-C5	3.06	120.08	115.41
24	B	608	CLA	CED-O2D-CGD	3.06	123.17	115.99
29	A	615	LHG	O8-C23-C24	3.06	121.24	111.90
24	D	402	CLA	CMB-C2B-C3B	3.06	131.08	125.09
25	a	412	PHO	C2C-C1C-NC	3.07	114.33	109.73
25	d	402	PHO	C4A-NA-C1A	3.07	110.95	108.21
27	A	611	PL9	C15-C14-C16	3.07	120.10	115.41
24	A	609	CLA	C4A-NA-C1A	3.07	110.33	106.36
24	b	609	CLA	CMB-C2B-C3B	3.07	131.10	125.09
24	B	602	CLA	O2A-CGA-CBA	3.08	121.28	111.90
24	B	615	CLA	C4A-NA-C1A	3.09	110.35	106.36
24	b	607	CLA	C3B-C4B-NB	3.09	113.21	109.21
24	c	910	CLA	C4-C3-C5	3.09	120.13	115.41
24	b	611	CLA	C3B-C4B-NB	3.10	113.21	109.21
24	A	614	CLA	C4-C3-C5	3.10	120.14	115.41
24	B	607	CLA	C4-C3-C5	3.10	120.14	115.41
26	k	101	BCR	C8-C9-C10	3.11	124.00	118.98
24	c	907	CLA	C4A-NA-C1A	3.12	110.39	106.36
27	A	611	PL9	C25-C24-C26	3.12	120.17	115.41
29	D	409	LHG	O7-C7-C8	3.12	118.32	111.53
27	A	611	PL9	C30-C29-C31	3.13	120.18	115.41
24	a	406	CLA	O2D-CGD-CBD	3.13	115.59	111.30
24	b	610	CLA	C3B-C4B-NB	3.13	113.26	109.21
24	c	902	CLA	C4-C3-C5	3.14	120.20	115.41
25	a	412	PHO	C3C-C4C-NC	3.14	115.31	110.24
31	h	102	DGD	O2G-C1B-C2B	3.14	118.36	111.53
24	c	911	CLA	C4A-NA-C1A	3.16	110.44	106.36
26	a	409	BCR	C33-C5-C6	3.17	127.72	124.61
26	f	101	BCR	C4-C5-C6	3.17	126.82	122.78
26	k	102	BCR	C31-C1-C6	3.17	115.28	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	CAC-C3C-C4C	3.17	129.44	124.83
24	b	610	CLA	C4A-NA-C1A	3.18	110.47	106.36
24	c	914	CLA	C4A-NA-C1A	3.18	110.47	106.36
24	B	607	CLA	C3B-C4B-NB	3.18	113.32	109.21
24	c	908	CLA	C4-C3-C5	3.19	120.27	115.41
26	c	918	BCR	C12-C13-C14	3.19	124.12	118.98
24	c	912	CLA	C3B-C4B-NB	3.19	113.34	109.21
25	a	412	PHO	C4-C3-C5	3.19	120.28	115.41
24	C	503	CLA	CMB-C2B-C3B	3.21	131.36	125.09
24	A	607	CLA	CMB-C2B-C3B	3.21	131.36	125.09
24	B	617	CLA	C4A-NA-C1A	3.21	110.51	106.36
24	b	605	CLA	CAC-C3C-C4C	3.22	129.51	124.83
24	C	504	CLA	C4-C3-C5	3.22	120.33	115.41
26	c	918	BCR	C39-C30-C25	3.23	115.37	110.30
26	A	610	BCR	C30-C25-C24	3.23	124.87	115.82
24	B	604	CLA	C4-C3-C5	3.23	120.35	115.41
24	C	502	CLA	C3B-C4B-NB	3.24	113.39	109.21
29	a	413	LHG	O7-C7-C8	3.24	118.57	111.53
26	c	918	BCR	C32-C1-C6	3.24	115.38	110.30
24	c	912	CLA	C4-C3-C5	3.25	120.37	115.41
26	A	610	BCR	C40-C30-C25	3.25	115.40	110.30
26	H	101	BCR	C23-C24-C25	3.25	137.09	127.32
25	D	401	PHO	C2C-C1C-NC	3.26	114.61	109.73
25	a	412	PHO	C2B-C1B-NB	3.27	114.63	109.73
24	B	604	CLA	CMC-C2C-C1C	3.27	130.08	125.02
24	b	606	CLA	CMC-C2C-C1C	3.27	130.09	125.02
24	b	617	CLA	C3B-C4B-NB	3.28	113.45	109.21
24	C	507	CLA	C4-C3-C5	3.29	120.43	115.41
24	B	617	CLA	C3B-C4B-NB	3.29	113.46	109.21
24	c	905	CLA	C4A-NA-C1A	3.30	110.62	106.36
26	b	619	BCR	C27-C26-C25	3.30	126.99	122.78
29	d	410	LHG	O7-C7-C8	3.31	118.71	111.53
24	b	617	CLA	CMB-C2B-C3B	3.31	131.56	125.09
24	B	605	CLA	CED-O2D-CGD	3.31	123.76	115.99
24	b	617	CLA	C4A-NA-C1A	3.32	110.65	106.36
26	B	618	BCR	C32-C1-C6	3.32	115.51	110.30
24	b	616	CLA	C3B-C4B-NB	3.32	113.51	109.21
27	a	410	PL9	C25-C24-C26	3.33	120.49	115.41
26	H	101	BCR	C4-C5-C6	3.33	127.02	122.78
24	A	607	CLA	C4-C3-C5	3.33	120.49	115.41
24	b	613	CLA	C4-C3-C5	3.33	120.49	115.41
26	b	618	BCR	C38-C26-C25	3.33	127.88	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	402	SQD	O6-C1-C2	3.34	112.26	108.04
26	Y	101	BCR	C2-C1-C6	3.34	115.66	110.36
28	A	613	SQD	O47-C7-C8	3.34	118.80	111.53
24	B	611	CLA	C4A-NA-C1A	3.35	110.69	106.36
25	d	402	PHO	C2B-C1B-NB	3.35	114.75	109.73
24	C	508	CLA	C4A-NA-C1A	3.35	110.69	106.36
24	C	506	CLA	C4-C3-C5	3.35	120.53	115.41
25	A	608	PHO	C4A-NA-C1A	3.36	111.21	108.21
26	A	610	BCR	C33-C5-C6	3.37	127.91	124.61
26	K	101	BCR	C31-C1-C6	3.37	115.59	110.30
24	b	613	CLA	CAC-C3C-C4C	3.37	129.73	124.83
24	C	503	CLA	C4A-NA-C1A	3.38	110.73	106.36
26	b	619	BCR	C4-C5-C6	3.38	127.09	122.78
24	b	602	CLA	O2A-CGA-CBA	3.39	122.24	111.90
24	B	614	CLA	C4A-NA-C1A	3.40	110.75	106.36
24	c	909	CLA	C4A-NA-C1A	3.40	110.75	106.36
26	c	918	BCR	C4-C5-C6	3.40	127.11	122.78
24	B	607	CLA	C4A-NA-C1A	3.40	110.76	106.36
24	b	613	CLA	C3B-C4B-NB	3.40	113.61	109.21
24	C	501	CLA	C4A-NA-C1A	3.41	110.77	106.36
24	B	603	CLA	C4-C3-C5	3.41	120.61	115.41
24	c	907	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	c	905	CLA	C3B-C4B-NB	3.42	113.63	109.21
29	D	407	LHG	O8-C23-C24	3.43	122.34	111.90
24	B	612	CLA	C3B-C4B-NB	3.43	113.65	109.21
24	b	605	CLA	C3B-C4B-NB	3.43	113.65	109.21
24	B	614	CLA	O2D-CGD-CBD	3.44	116.01	111.30
25	D	401	PHO	C4-C3-C5	3.44	120.66	115.41
26	K	101	BCR	C27-C26-C25	3.44	127.16	122.78
24	B	612	CLA	C4A-NA-C1A	3.44	110.81	106.36
24	C	512	CLA	C4A-NA-C1A	3.44	110.81	106.36
24	b	603	CLA	CMB-C2B-C3B	3.44	131.82	125.09
31	D	406	DGD	O5D-C1E-C2E	3.45	112.39	108.04
24	b	614	CLA	C4A-NA-C1A	3.45	110.83	106.36
24	B	611	CLA	C3B-C4B-NB	3.45	113.68	109.21
24	B	616	CLA	C3B-C4B-NB	3.46	113.68	109.21
26	C	515	BCR	C40-C30-C25	3.47	115.74	110.30
26	K	101	BCR	C24-C23-C22	3.47	131.51	126.22
26	c	915	BCR	C8-C7-C6	3.47	137.75	127.32
24	A	606	CLA	CMB-C2B-C3B	3.48	131.89	125.09
26	f	101	BCR	C27-C26-C25	3.48	127.22	122.78
26	B	618	BCR	C8-C7-C6	3.48	137.78	127.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	909	CLA	C3B-C4B-NB	3.48	113.71	109.21
24	b	612	CLA	C3B-C4B-NB	3.49	113.72	109.21
24	B	613	CLA	C4-C3-C5	3.49	120.73	115.41
25	A	608	PHO	C2B-C1B-NB	3.49	114.96	109.73
24	B	614	CLA	C3B-C4B-NB	3.49	113.72	109.21
24	D	403	CLA	C4A-NA-C1A	3.50	110.88	106.36
26	b	618	BCR	C8-C7-C6	3.50	137.83	127.32
24	b	608	CLA	C4A-NA-C1A	3.50	110.89	106.36
24	C	512	CLA	C4-C3-C5	3.51	120.77	115.41
24	B	610	CLA	C4A-NA-C1A	3.51	110.90	106.36
24	B	615	CLA	C3B-C4B-NB	3.52	113.76	109.21
24	b	608	CLA	C3B-C4B-NB	3.52	113.76	109.21
24	b	602	CLA	C4A-NA-C1A	3.52	110.91	106.36
24	c	911	CLA	C3B-C4B-NB	3.52	113.77	109.21
25	d	402	PHO	C3C-C4C-NC	3.53	115.94	110.24
24	B	610	CLA	C3B-C4B-NB	3.54	113.78	109.21
25	D	401	PHO	C3C-C4C-NC	3.54	115.97	110.24
26	B	619	BCR	C38-C26-C25	3.56	128.10	124.61
24	b	611	CLA	C4A-NA-C1A	3.56	110.96	106.36
26	h	101	BCR	C2-C1-C6	3.56	116.01	110.36
24	C	508	CLA	C3B-C4B-NB	3.57	113.82	109.21
24	D	403	CLA	C3B-C4B-NB	3.57	113.83	109.21
26	b	619	BCR	C2-C1-C6	3.57	116.02	110.36
24	b	615	CLA	C4A-NA-C1A	3.57	110.98	106.36
24	C	510	CLA	C4A-NA-C1A	3.58	110.99	106.36
24	C	511	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	B	613	CLA	C4A-NA-C1A	3.59	111.00	106.36
26	B	622	BCR	C3-C4-C5	3.59	119.56	113.87
26	B	618	BCR	C23-C24-C25	3.59	138.11	127.32
24	C	505	CLA	C4A-NA-C1A	3.59	111.01	106.36
26	K	101	BCR	C2-C1-C6	3.59	116.05	110.36
24	C	509	CLA	C3B-C4B-NB	3.60	113.86	109.21
24	c	910	CLA	C3B-C4B-NB	3.60	113.86	109.21
24	D	402	CLA	C3B-C4B-NB	3.60	113.87	109.21
26	c	918	BCR	C23-C22-C21	3.61	124.80	118.98
28	a	402	SQD	O47-C7-C8	3.61	119.37	111.53
24	c	902	CLA	C3B-C4B-NB	3.62	113.89	109.21
24	c	903	CLA	C3B-C4B-NB	3.62	113.90	109.21
24	a	407	CLA	C3B-C4B-NB	3.63	113.90	109.21
26	k	102	BCR	C40-C30-C25	3.63	115.99	110.30
24	c	903	CLA	C4A-NA-C1A	3.64	111.07	106.36
24	C	506	CLA	C4A-NA-C1A	3.64	111.07	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	604	CLA	C3B-C4B-NB	3.64	113.92	109.21
28	l	101	SQD	O47-C7-C8	3.65	119.45	111.53
24	c	905	CLA	C4-C3-C5	3.65	120.98	115.41
24	B	605	CLA	C3B-C4B-NB	3.65	113.93	109.21
26	f	101	BCR	C2-C1-C6	3.65	116.14	110.36
24	C	504	CLA	C3B-C4B-NB	3.65	113.93	109.21
24	C	504	CLA	C4A-NA-C1A	3.65	111.08	106.36
24	B	608	CLA	O2D-CGD-CBD	3.65	116.31	111.30
24	b	609	CLA	C3B-C4B-NB	3.66	113.94	109.21
24	d	403	CLA	C4-C3-C5	3.66	121.00	115.41
24	B	615	CLA	C4-C3-C5	3.66	121.00	115.41
26	h	101	BCR	C29-C30-C25	3.67	116.17	110.36
24	c	913	CLA	C4A-NA-C1A	3.67	111.11	106.36
24	c	906	CLA	C4A-NA-C1A	3.67	111.11	106.36
26	A	610	BCR	C23-C24-C25	3.67	138.35	127.32
26	H	101	BCR	C24-C23-C22	3.67	131.81	126.22
31	C	517	DGD	O2G-C1B-C2B	3.67	119.51	111.53
24	b	615	CLA	C4-C3-C5	3.68	121.02	115.41
24	d	401	CLA	C3B-C4B-NB	3.68	113.97	109.21
24	b	607	CLA	C4A-NA-C1A	3.68	111.12	106.36
24	b	608	CLA	C4-C3-C5	3.69	121.04	115.41
28	F	101	SQD	O47-C7-C8	3.69	119.54	111.53
26	k	101	BCR	C4-C5-C6	3.69	127.48	122.78
26	f	101	BCR	C31-C1-C6	3.70	116.10	110.30
26	c	915	BCR	C33-C5-C6	3.70	128.24	124.61
24	C	509	CLA	C4A-NA-C1A	3.70	111.15	106.36
24	b	616	CLA	C4A-NA-C1A	3.71	111.15	106.36
24	c	910	CLA	C4A-NA-C1A	3.73	111.18	106.36
29	b	620	LHG	O7-C7-C8	3.73	119.63	111.53
24	A	609	CLA	C3B-C4B-NB	3.73	114.03	109.21
24	A	614	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	b	613	CLA	C4A-NA-C1A	3.74	111.20	106.36
28	L	101	SQD	O9-S-C6	3.75	110.10	106.94
26	k	102	BCR	C23-C24-C25	3.75	138.59	127.32
26	T	102	BCR	C8-C7-C6	3.75	138.59	127.32
26	H	101	BCR	C8-C7-C6	3.76	138.61	127.32
26	H	101	BCR	C27-C26-C25	3.76	127.58	122.78
24	b	612	CLA	C4A-NA-C1A	3.77	111.23	106.36
25	D	401	PHO	C2B-C1B-NB	3.77	115.38	109.73
24	B	602	CLA	C4A-NA-C1A	3.77	111.23	106.36
25	d	402	PHO	C2D-C1D-ND	3.77	115.38	109.73
24	d	403	CLA	O2D-CGD-CBD	3.77	116.47	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	918	BCR	C33-C5-C6	3.77	128.31	124.61
26	T	102	BCR	C27-C26-C25	3.78	127.59	122.78
24	b	614	CLA	C3B-C4B-NB	3.78	114.09	109.21
24	c	902	CLA	C4A-NA-C1A	3.78	111.25	106.36
24	C	513	CLA	C4A-NA-C1A	3.78	111.25	106.36
25	a	412	PHO	C2D-C1D-ND	3.78	115.40	109.73
26	C	515	BCR	C2-C1-C6	3.79	116.37	110.36
24	a	408	CLA	C3B-C4B-NB	3.79	114.12	109.21
26	a	409	BCR	C23-C24-C25	3.80	138.73	127.32
26	C	514	BCR	C23-C24-C25	3.80	138.74	127.32
24	d	404	CLA	C3B-C4B-NB	3.81	114.14	109.21
26	K	101	BCR	C32-C1-C6	3.81	116.28	110.30
26	B	620	BCR	C23-C24-C25	3.82	138.78	127.32
26	B	622	BCR	C40-C30-C25	3.83	116.31	110.30
25	D	401	PHO	C2D-C1D-ND	3.84	115.48	109.73
26	c	918	BCR	C23-C24-C25	3.84	138.85	127.32
26	b	619	BCR	C23-C24-C25	3.84	138.86	127.32
26	T	101	BCR	C8-C9-C10	3.84	125.18	118.98
25	A	608	PHO	C3C-C4C-NC	3.85	116.45	110.24
24	A	609	CLA	C4-C3-C5	3.85	121.28	115.41
26	C	515	BCR	C8-C9-C10	3.86	125.19	118.98
26	B	620	BCR	C4-C5-C6	3.86	127.71	122.78
24	A	606	CLA	C3B-C4B-NB	3.87	114.22	109.21
26	B	620	BCR	C27-C26-C25	3.88	127.72	122.78
24	C	510	CLA	C3B-C4B-NB	3.89	114.23	109.21
24	B	616	CLA	C4A-NA-C1A	3.89	111.39	106.36
26	k	101	BCR	C27-C26-C25	3.90	127.75	122.78
32	v	202	HEM	CMC-C2C-C3C	3.90	126.26	116.53
26	c	918	BCR	C29-C30-C25	3.90	116.54	110.36
26	B	622	BCR	C31-C1-C6	3.90	116.42	110.30
28	L	101	SQD	O47-C7-C8	3.90	120.01	111.53
27	A	611	PL9	C20-C19-C21	3.91	121.37	115.41
26	h	101	BCR	C32-C1-C6	3.91	116.43	110.30
28	L	101	SQD	C3-C4-C5	3.91	117.02	110.20
25	D	401	PHO	CAC-C3C-C4C	3.91	129.73	125.16
29	A	615	LHG	O7-C7-C8	3.91	120.04	111.53
24	a	406	CLA	C3B-C4B-NB	3.92	114.28	109.21
26	D	404	BCR	C27-C26-C25	3.92	127.78	122.78
24	A	606	CLA	O2D-CGD-CBD	3.92	116.68	111.30
25	d	402	PHO	C2C-C1C-NC	3.94	115.64	109.73
26	a	409	BCR	C8-C7-C6	3.94	139.16	127.32
26	T	102	BCR	C2-C1-C6	3.95	116.62	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	619	BCR	C8-C7-C6	3.95	139.19	127.32
26	b	619	BCR	C8-C9-C10	3.96	125.36	118.98
26	c	915	BCR	C29-C30-C25	3.96	116.64	110.36
26	b	618	BCR	C23-C24-C25	3.97	139.23	127.32
26	C	514	BCR	C23-C22-C21	3.97	125.38	118.98
24	c	904	CLA	C4A-NA-C1A	3.97	111.49	106.36
24	b	615	CLA	C3B-C4B-NB	3.98	114.36	109.21
24	a	406	CLA	CAC-C3C-C4C	3.99	130.63	124.83
26	T	102	BCR	C4-C5-C6	4.00	127.87	122.78
26	D	404	BCR	C23-C24-C25	4.01	139.35	127.32
27	d	405	PL9	C40-C39-C41	4.01	121.53	115.41
32	e	101	HEM	CAD-C3D-C4D	4.02	126.65	112.47
28	a	411	SQD	O47-C7-C8	4.02	120.27	111.53
24	d	403	CLA	C3B-C4B-NB	4.03	114.42	109.21
27	D	405	PL9	C40-C39-C41	4.03	121.57	115.41
24	B	616	CLA	O2D-CGD-CBD	4.04	116.84	111.30
26	T	102	BCR	C29-C30-C25	4.04	116.76	110.36
26	b	619	BCR	C32-C1-C6	4.04	116.64	110.30
24	B	605	CLA	C4A-NA-C1A	4.05	111.60	106.36
28	A	613	SQD	O6-C1-C2	4.05	113.16	108.04
26	B	620	BCR	C8-C7-C6	4.05	139.50	127.32
32	V	202	HEM	CAD-C3D-C4D	4.07	126.81	112.47
26	k	102	BCR	C27-C26-C25	4.07	127.96	122.78
26	c	915	BCR	C31-C1-C6	4.07	116.68	110.30
26	Y	101	BCR	C27-C26-C25	4.08	127.98	122.78
26	k	102	BCR	C32-C1-C6	4.09	116.71	110.30
24	D	402	CLA	O2D-CGD-CBD	4.09	116.92	111.30
26	a	409	BCR	C29-C30-C25	4.10	116.85	110.36
32	V	202	HEM	CMC-C2C-C3C	4.11	126.80	116.53
26	B	618	BCR	C27-C26-C25	4.12	128.03	122.78
26	h	101	BCR	C23-C24-C25	4.12	139.70	127.32
26	B	618	BCR	C29-C30-C25	4.14	116.91	110.36
26	C	515	BCR	C33-C5-C6	4.14	128.67	124.61
25	A	608	PHO	C2C-C1C-NC	4.15	115.94	109.73
24	c	912	CLA	C4A-NA-C1A	4.15	111.72	106.36
24	D	403	CLA	O2D-CGD-CBD	4.16	117.00	111.30
32	v	202	HEM	CAD-C3D-C2D	4.16	125.18	113.22
24	B	608	CLA	C3B-C4B-NB	4.19	114.63	109.21
26	B	620	BCR	C2-C1-C6	4.20	117.01	110.36
26	h	101	BCR	C38-C26-C25	4.20	128.73	124.61
24	B	604	CLA	C3B-C4B-NB	4.20	114.64	109.21
26	k	102	BCR	C2-C1-C6	4.21	117.02	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	619	BCR	C24-C23-C22	4.22	132.64	126.22
24	B	606	CLA	C4-C3-C5	4.23	121.86	115.41
31	d	406	DGD	O2G-C1B-C2B	4.25	120.77	111.53
24	b	605	CLA	C4A-NA-C1A	4.25	111.86	106.36
31	C	516	DGD	O2G-C1B-C2B	4.25	120.77	111.53
26	k	101	BCR	C40-C30-C25	4.27	116.99	110.30
26	b	619	BCR	C8-C7-C6	4.27	140.15	127.32
24	b	614	CLA	O2D-CGD-CBD	4.28	117.18	111.30
26	B	622	BCR	C23-C24-C25	4.29	140.21	127.32
24	b	604	CLA	C4-C3-C5	4.30	121.97	115.41
26	f	101	BCR	C38-C26-C25	4.30	128.83	124.61
24	B	609	CLA	C3B-C4B-NB	4.30	114.77	109.21
26	T	102	BCR	C23-C24-C25	4.30	140.24	127.32
28	A	612	SQD	O47-C7-C8	4.31	120.89	111.53
28	d	407	SQD	O47-C7-C8	4.31	120.90	111.53
28	F	101	SQD	O9-S-C6	4.32	110.58	106.94
24	C	507	CLA	C4A-NA-C1A	4.32	111.95	106.36
26	Y	101	BCR	C23-C24-C25	4.33	140.32	127.32
25	A	608	PHO	C2D-C1D-ND	4.34	116.23	109.73
26	B	620	BCR	C29-C30-C25	4.34	117.24	110.36
26	b	618	BCR	C4-C5-C6	4.35	128.32	122.78
24	d	401	CLA	O2D-CGD-CBD	4.35	117.27	111.30
26	c	918	BCR	C2-C1-C6	4.37	117.28	110.36
32	E	101	HEM	CMB-C2B-C3B	4.39	127.48	116.53
26	k	102	BCR	C8-C9-C10	4.40	126.07	118.98
24	C	511	CLA	C4A-NA-C1A	4.40	112.05	106.36
32	E	101	HEM	CAD-C3D-C4D	4.40	128.00	112.47
24	A	607	CLA	C3B-C4B-NB	4.42	114.92	109.21
24	c	904	CLA	O2D-CGD-CBD	4.42	117.36	111.30
26	a	409	BCR	C2-C1-C6	4.42	117.36	110.36
32	v	202	HEM	CAD-C3D-C4D	4.43	128.10	112.47
26	c	915	BCR	C2-C1-C6	4.43	117.38	110.36
32	e	101	HEM	CMB-C2B-C3B	4.44	127.60	116.53
26	c	918	BCR	C8-C7-C6	4.45	140.68	127.32
31	D	406	DGD	O2G-C1B-C2B	4.47	121.25	111.53
26	k	102	BCR	C24-C23-C22	4.50	133.07	126.22
32	E	101	HEM	CAD-C3D-C2D	4.50	126.14	113.22
26	B	622	BCR	C2-C1-C6	4.50	117.48	110.36
32	E	101	HEM	CMC-C2C-C3C	4.50	127.76	116.53
26	T	101	BCR	C23-C22-C21	4.51	126.25	118.98
26	D	404	BCR	C8-C7-C6	4.52	140.90	127.32
26	b	619	BCR	C39-C30-C25	4.52	117.39	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	e	101	HEM	CMC-C2C-C3C	4.53	127.83	116.53
26	T	101	BCR	C27-C26-C25	4.53	128.55	122.78
26	C	514	BCR	C32-C1-C6	4.53	117.41	110.30
28	F	101	SQD	O7-S-C6	4.54	110.77	106.94
24	b	606	CLA	C4-C3-C5	4.54	122.35	115.41
26	b	618	BCR	C33-C5-C6	4.55	129.07	124.61
26	c	915	BCR	C40-C30-C25	4.55	117.44	110.30
26	B	619	BCR	C2-C1-C6	4.57	117.59	110.36
32	v	202	HEM	CMB-C2B-C3B	4.57	127.94	116.53
26	k	101	BCR	C38-C26-C25	4.58	129.11	124.61
26	B	620	BCR	C33-C5-C6	4.59	129.11	124.61
26	f	101	BCR	C23-C24-C25	4.60	141.13	127.32
26	c	918	BCR	C24-C23-C22	4.60	133.22	126.22
24	c	908	CLA	C4A-NA-C1A	4.60	112.31	106.36
26	h	101	BCR	C4-C5-C6	4.60	128.65	122.78
28	d	407	SQD	O9-S-C6	4.61	110.83	106.94
26	B	618	BCR	C38-C26-C25	4.61	129.13	124.61
24	B	605	CLA	O2D-CGD-CBD	4.63	117.65	111.30
26	f	101	BCR	C24-C23-C22	4.63	133.28	126.22
32	V	202	HEM	CAD-C3D-C2D	4.66	126.62	113.22
26	B	619	BCR	C33-C5-C6	4.68	129.20	124.61
32	V	202	HEM	CMB-C2B-C3B	4.68	128.21	116.53
26	c	915	BCR	C23-C24-C25	4.68	141.38	127.32
24	B	611	CLA	O2D-CGD-CBD	4.70	117.75	111.30
24	c	909	CLA	O2D-CGD-CBD	4.72	117.78	111.30
26	k	101	BCR	C2-C1-C6	4.73	117.84	110.36
26	k	102	BCR	C39-C30-C25	4.75	117.75	110.30
26	K	101	BCR	C23-C24-C25	4.77	141.66	127.32
26	C	515	BCR	C8-C7-C6	4.80	141.73	127.32
26	C	514	BCR	C2-C1-C6	4.82	117.99	110.36
24	B	607	CLA	O2D-CGD-CBD	4.85	117.95	111.30
28	a	402	SQD	O9-S-C6	4.85	111.03	106.94
26	Y	101	BCR	C8-C7-C6	4.86	141.91	127.32
26	B	620	BCR	C24-C23-C22	4.86	133.62	126.22
26	D	404	BCR	C7-C8-C9	4.88	133.65	126.22
24	C	510	CLA	O2D-CGD-CBD	4.88	117.99	111.30
26	C	515	BCR	C29-C30-C25	4.88	118.09	110.36
26	h	101	BCR	C28-C27-C26	4.89	121.63	113.87
26	D	404	BCR	C8-C9-C10	4.89	126.87	118.98
28	A	613	SQD	O9-S-C6	4.90	111.07	106.94
26	Y	101	BCR	C23-C22-C21	4.91	126.89	118.98
26	c	915	BCR	C27-C26-C25	4.91	129.04	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	618	BCR	C2-C1-C6	4.91	118.14	110.36
26	H	101	BCR	C28-C27-C26	4.92	121.68	113.87
24	B	606	CLA	O2D-CGD-CBD	4.93	118.06	111.30
24	C	503	CLA	O2D-CGD-CBD	4.95	118.09	111.30
26	H	101	BCR	C29-C30-C25	4.98	118.25	110.36
26	b	619	BCR	C29-C30-C25	4.98	118.25	110.36
24	d	404	CLA	O2D-CGD-CBD	4.99	118.14	111.30
24	b	611	CLA	O2D-CGD-CBD	4.99	118.14	111.30
24	b	608	CLA	O2D-CGD-CBD	5.00	118.15	111.30
26	k	101	BCR	C24-C23-C22	5.01	133.85	126.22
26	a	409	BCR	C8-C9-C10	5.01	127.06	118.98
24	c	907	CLA	O2D-CGD-CBD	5.02	118.18	111.30
26	b	618	BCR	C8-C9-C10	5.03	127.08	118.98
26	D	404	BCR	C24-C23-C22	5.07	133.94	126.22
24	B	617	CLA	O2D-CGD-CBD	5.08	118.27	111.30
24	B	603	CLA	O2D-CGD-CBD	5.09	118.28	111.30
26	K	101	BCR	C8-C9-C10	5.13	127.24	118.98
26	T	102	BCR	C39-C30-C25	5.13	118.34	110.30
26	T	102	BCR	C38-C26-C25	5.14	129.66	124.61
26	A	610	BCR	C24-C23-C22	5.16	134.08	126.22
26	Y	101	BCR	C8-C9-C10	5.16	127.29	118.98
26	B	622	BCR	C8-C7-C6	5.16	142.82	127.32
26	B	619	BCR	C40-C30-C25	5.18	118.42	110.30
26	h	101	BCR	C8-C7-C6	5.19	142.90	127.32
25	D	401	PHO	O2D-CGD-CBD	5.20	118.43	111.30
24	c	911	CLA	O2D-CGD-CBD	5.20	118.43	111.30
24	b	605	CLA	O2D-CGD-CBD	5.20	118.44	111.30
28	l	101	SQD	O7-S-C6	5.22	111.34	106.94
26	C	514	BCR	C8-C7-C6	5.24	143.07	127.32
24	C	502	CLA	O2D-CGD-CBD	5.25	118.50	111.30
32	e	101	HEM	CAD-C3D-C2D	5.26	128.33	113.22
24	a	407	CLA	O2D-CGD-CBD	5.27	118.52	111.30
26	C	514	BCR	C29-C30-C25	5.27	118.70	110.36
24	c	912	CLA	O2D-CGD-CBD	5.29	118.55	111.30
24	b	602	CLA	C2C-C1C-NC	5.30	114.19	110.24
26	B	619	BCR	C27-C26-C25	5.30	129.54	122.78
26	C	514	BCR	C27-C26-C25	5.33	129.58	122.78
28	F	101	SQD	O6-C1-C2	5.34	114.78	108.04
24	A	609	CLA	O2D-CGD-CBD	5.34	118.62	111.30
28	d	407	SQD	O6-C1-C2	5.36	114.81	108.04
26	h	101	BCR	C8-C9-C10	5.37	127.63	118.98
26	C	515	BCR	C38-C26-C25	5.37	129.88	124.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	511	CLA	O2D-CGD-CBD	5.38	118.69	111.30
28	L	101	SQD	O7-S-C6	5.39	111.48	106.94
26	T	102	BCR	C8-C9-C10	5.39	127.67	118.98
26	T	102	BCR	C7-C8-C9	5.39	134.43	126.22
24	C	513	CLA	C2C-C1C-NC	5.40	114.26	110.24
28	L	101	SQD	O6-C1-C2	5.41	114.88	108.04
26	T	101	BCR	C2-C1-C6	5.42	118.94	110.36
26	D	404	BCR	C4-C5-C6	5.44	129.72	122.78
25	A	608	PHO	O2D-CGD-CBD	5.44	118.77	111.30
24	B	612	CLA	O2D-CGD-CBD	5.47	118.81	111.30
24	c	914	CLA	C2C-C1C-NC	5.48	114.32	110.24
26	Y	101	BCR	C24-C23-C22	5.48	134.57	126.22
26	D	404	BCR	C23-C22-C21	5.49	127.83	118.98
26	Y	101	BCR	C4-C5-C6	5.50	129.79	122.78
26	c	915	BCR	C8-C9-C10	5.51	127.86	118.98
24	c	902	CLA	O2D-CGD-CBD	5.52	118.87	111.30
26	k	102	BCR	C8-C7-C6	5.53	143.93	127.32
26	k	101	BCR	C8-C7-C6	5.54	143.96	127.32
26	C	514	BCR	C12-C13-C14	5.55	127.92	118.98
24	b	603	CLA	C2C-C1C-NC	5.55	114.38	110.24
24	C	513	CLA	O2D-CGD-CBD	5.57	118.94	111.30
24	b	610	CLA	O2D-CGD-CBD	5.58	118.96	111.30
26	B	619	BCR	C29-C30-C25	5.59	119.21	110.36
24	b	613	CLA	O2D-CGD-CBD	5.62	119.01	111.30
26	f	101	BCR	C40-C30-C39	5.64	126.44	108.37
24	b	607	CLA	O2D-CGD-CBD	5.65	119.06	111.30
24	B	603	CLA	C2C-C1C-NC	5.65	114.45	110.24
26	K	101	BCR	C8-C7-C6	5.69	144.39	127.32
24	C	507	CLA	O2D-CGD-CBD	5.69	119.11	111.30
24	c	906	CLA	C2C-C1C-NC	5.70	114.49	110.24
24	b	616	CLA	O2D-CGD-CBD	5.71	119.13	111.30
26	b	619	BCR	C38-C26-C25	5.72	130.22	124.61
26	k	101	BCR	C29-C30-C25	5.74	119.45	110.36
24	A	614	CLA	O2D-CGD-CBD	5.74	119.17	111.30
24	a	408	CLA	O2D-CGD-CBD	5.74	119.18	111.30
26	B	619	BCR	C23-C24-C25	5.74	144.56	127.32
24	C	512	CLA	C2C-C1C-NC	5.75	114.52	110.24
24	C	505	CLA	O2D-CGD-CBD	5.75	119.19	111.30
24	c	904	CLA	C2C-C1C-NC	5.76	114.53	110.24
26	C	515	BCR	C7-C8-C9	5.77	135.01	126.22
24	b	603	CLA	O2D-CGD-CBD	5.78	119.23	111.30
26	b	618	BCR	C27-C26-C25	5.82	130.19	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	914	CLA	O2D-CGD-CBD	5.83	119.29	111.30
24	B	602	CLA	C2C-C1C-NC	5.84	114.59	110.24
26	c	918	BCR	C15-C14-C13	5.84	135.63	127.20
26	B	620	BCR	C8-C9-C10	5.86	128.42	118.98
24	B	610	CLA	O2D-CGD-CBD	5.87	119.35	111.30
24	b	612	CLA	O2D-CGD-CBD	5.87	119.35	111.30
26	A	610	BCR	C8-C9-C10	5.88	128.45	118.98
28	l	101	SQD	O6-C1-C2	5.89	115.48	108.04
24	C	508	CLA	O2D-CGD-CBD	5.89	119.38	111.30
24	b	604	CLA	O2D-CGD-CBD	5.91	119.40	111.30
26	B	619	BCR	C8-C9-C10	5.92	128.53	118.98
24	c	908	CLA	O2D-CGD-CBD	5.93	119.43	111.30
24	b	617	CLA	C2C-C1C-NC	5.95	114.67	110.24
26	h	101	BCR	C39-C30-C25	5.96	119.64	110.30
26	B	618	BCR	C7-C8-C9	5.96	135.30	126.22
24	B	615	CLA	O2D-CGD-CBD	5.97	119.48	111.30
24	c	906	CLA	O2D-CGD-CBD	5.99	119.51	111.30
26	a	409	BCR	C27-C26-C25	5.99	130.41	122.78
26	B	619	BCR	C11-C12-C13	6.00	143.97	126.32
24	c	903	CLA	C2C-C1C-NC	6.00	114.71	110.24
26	f	101	BCR	C12-C13-C14	6.01	128.67	118.98
28	A	612	SQD	O6-C1-C2	6.03	115.65	108.04
26	T	101	BCR	C24-C23-C22	6.04	135.41	126.22
24	C	509	CLA	O2D-CGD-CBD	6.05	119.59	111.30
28	a	411	SQD	O9-S-C6	6.05	112.05	106.94
26	B	622	BCR	C23-C22-C21	6.06	128.75	118.98
26	C	514	BCR	C24-C23-C22	6.08	135.48	126.22
26	H	101	BCR	C33-C5-C6	6.08	130.57	124.61
24	c	907	CLA	C2C-C1C-NC	6.08	114.77	110.24
24	b	607	CLA	C2C-C1C-NC	6.10	114.79	110.24
24	C	503	CLA	C2C-C1C-NC	6.11	114.79	110.24
28	A	612	SQD	O9-S-C6	6.13	112.11	106.94
24	B	613	CLA	O2D-CGD-CBD	6.13	119.71	111.30
26	b	618	BCR	C29-C30-C25	6.14	120.09	110.36
24	c	912	CLA	C2C-C1C-NC	6.16	114.83	110.24
24	c	909	CLA	C2C-C1C-NC	6.19	114.85	110.24
24	c	913	CLA	C2C-C1C-NC	6.20	114.86	110.24
24	c	905	CLA	O2D-CGD-CBD	6.22	119.83	111.30
26	C	515	BCR	C31-C1-C6	6.22	120.06	110.30
24	D	403	CLA	C2C-C1C-NC	6.22	114.88	110.24
24	C	507	CLA	C2C-C1C-NC	6.23	114.88	110.24
24	A	607	CLA	O2D-CGD-CBD	6.24	119.86	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k	102	BCR	C38-C26-C25	6.24	130.73	124.61
24	B	609	CLA	O2D-CGD-CBD	6.24	119.86	111.30
24	B	616	CLA	C2C-C1C-NC	6.25	114.89	110.24
26	T	101	BCR	C8-C7-C6	6.25	146.08	127.32
24	B	617	CLA	C2C-C1C-NC	6.25	114.90	110.24
26	k	102	BCR	C33-C5-C6	6.25	130.75	124.61
24	c	910	CLA	O2D-CGD-CBD	6.26	119.89	111.30
26	k	101	BCR	C23-C22-C21	6.27	129.08	118.98
24	b	616	CLA	C2C-C1C-NC	6.27	114.91	110.24
26	c	918	BCR	C38-C26-C25	6.28	130.77	124.61
24	b	612	CLA	C2C-C1C-NC	6.29	114.92	110.24
24	C	504	CLA	O2D-CGD-CBD	6.30	119.94	111.30
24	c	905	CLA	C2C-C1C-NC	6.30	114.93	110.24
26	C	515	BCR	C23-C22-C21	6.33	129.18	118.98
24	b	611	CLA	C2C-C1C-NC	6.33	114.95	110.24
24	B	613	CLA	C2C-C1C-NC	6.34	114.96	110.24
24	B	604	CLA	O2D-CGD-CBD	6.34	120.00	111.30
24	B	611	CLA	C2C-C1C-NC	6.36	114.98	110.24
24	c	913	CLA	O2D-CGD-CBD	6.38	120.05	111.30
26	B	618	BCR	C23-C22-C21	6.39	129.27	118.98
26	H	101	BCR	C8-C9-C10	6.39	129.28	118.98
24	C	502	CLA	C2C-C1C-NC	6.41	115.01	110.24
24	C	508	CLA	C2C-C1C-NC	6.42	115.02	110.24
24	b	606	CLA	O2D-CGD-CBD	6.42	120.11	111.30
24	C	511	CLA	C2C-C1C-NC	6.43	115.03	110.24
26	Y	101	BCR	C29-C30-C25	6.45	120.58	110.36
24	b	609	CLA	C2C-C1C-NC	6.47	115.06	110.24
24	b	617	CLA	O2D-CGD-CBD	6.49	120.20	111.30
24	b	608	CLA	C2C-C1C-NC	6.49	115.08	110.24
24	B	607	CLA	C2C-C1C-NC	6.49	115.08	110.24
24	C	505	CLA	C2C-C1C-NC	6.51	115.09	110.24
26	T	102	BCR	C24-C23-C22	6.53	136.17	126.22
24	c	910	CLA	C2C-C1C-NC	6.55	115.12	110.24
24	b	613	CLA	C2C-C1C-NC	6.55	115.12	110.24
24	C	506	CLA	O2D-CGD-CBD	6.56	120.30	111.30
26	C	515	BCR	C24-C23-C22	6.56	136.21	126.22
25	d	402	PHO	CMD-C2D-C1D	6.56	135.74	125.06
24	b	609	CLA	O2D-CGD-CBD	6.56	120.30	111.30
26	H	101	BCR	C32-C1-C6	6.57	120.61	110.30
26	C	514	BCR	C38-C26-C25	6.59	131.08	124.61
24	C	512	CLA	O2D-CGD-CBD	6.59	120.34	111.30
24	B	606	CLA	C2C-C1C-NC	6.60	115.16	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f	101	BCR	C8-C7-C6	6.61	147.17	127.32
24	C	501	CLA	C2C-C1C-NC	6.64	115.18	110.24
24	c	911	CLA	C2C-C1C-NC	6.64	115.19	110.24
24	d	404	CLA	C2C-C1C-NC	6.67	115.21	110.24
24	A	606	CLA	C2C-C1C-NC	6.67	115.21	110.24
24	c	908	CLA	C2C-C1C-NC	6.68	115.21	110.24
26	B	622	BCR	C12-C13-C14	6.68	129.75	118.98
26	f	101	BCR	C8-C9-C10	6.70	129.78	118.98
24	C	506	CLA	C2C-C1C-NC	6.75	115.27	110.24
26	c	918	BCR	C19-C18-C17	6.77	129.89	118.98
26	T	101	BCR	C12-C13-C14	6.78	129.90	118.98
24	B	615	CLA	C2C-C1C-NC	6.83	115.33	110.24
24	b	615	CLA	O2D-CGD-CBD	6.84	120.68	111.30
26	T	102	BCR	C23-C22-C21	6.84	130.00	118.98
26	B	620	BCR	C12-C13-C14	6.87	130.05	118.98
24	B	614	CLA	C2C-C1C-NC	6.89	115.37	110.24
24	b	610	CLA	C2C-C1C-NC	6.93	115.41	110.24
24	C	510	CLA	C2C-C1C-NC	6.94	115.41	110.24
26	b	619	BCR	C33-C5-C6	6.94	131.42	124.61
26	B	618	BCR	C24-C23-C22	6.94	136.80	126.22
25	a	412	PHO	O2D-CGD-CBD	6.95	120.84	111.30
24	b	602	CLA	O2D-CGD-CBD	6.96	120.84	111.30
25	d	402	PHO	O2D-CGD-CBD	6.97	120.87	111.30
24	b	615	CLA	C2C-C1C-NC	6.98	115.44	110.24
24	c	903	CLA	O2D-CGD-CBD	6.99	120.89	111.30
24	b	606	CLA	C2C-C1C-NC	7.00	115.46	110.24
26	f	101	BCR	C32-C1-C6	7.03	121.32	110.30
28	a	411	SQD	O6-C1-C2	7.04	116.93	108.04
25	A	608	PHO	CMD-C2D-C1D	7.06	136.55	125.06
26	Y	101	BCR	C12-C13-C14	7.07	130.37	118.98
24	b	605	CLA	C2C-C1C-NC	7.12	115.54	110.24
26	h	101	BCR	C23-C22-C21	7.12	130.46	118.98
24	B	612	CLA	C2C-C1C-NC	7.15	115.56	110.24
24	B	608	CLA	C2C-C1C-NC	7.15	115.57	110.24
26	b	619	BCR	C12-C13-C14	7.17	130.54	118.98
24	b	614	CLA	C2C-C1C-NC	7.18	115.59	110.24
26	c	915	BCR	C12-C13-C14	7.19	130.56	118.98
24	D	402	CLA	C2C-C1C-NC	7.20	115.60	110.24
24	B	610	CLA	C2C-C1C-NC	7.21	115.61	110.24
25	D	401	PHO	CMD-C2D-C1D	7.21	136.80	125.06
24	c	902	CLA	C2C-C1C-NC	7.23	115.63	110.24
24	C	509	CLA	C2C-C1C-NC	7.24	115.63	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	609	CLA	C2C-C1C-NC	7.24	115.63	110.24
24	B	602	CLA	O2D-CGD-CBD	7.25	121.25	111.30
25	a	412	PHO	CMD-C2D-C1D	7.27	136.89	125.06
26	h	101	BCR	C12-C13-C14	7.28	130.71	118.98
24	C	504	CLA	C2C-C1C-NC	7.30	115.68	110.24
26	C	514	BCR	C33-C5-C6	7.32	131.79	124.61
26	b	618	BCR	C24-C23-C22	7.34	137.40	126.22
24	a	408	CLA	C2C-C1C-NC	7.35	115.72	110.24
26	D	404	BCR	C10-C11-C12	7.38	145.63	123.13
26	B	618	BCR	C8-C9-C10	7.43	130.96	118.98
26	b	618	BCR	C11-C12-C13	7.44	148.22	126.32
24	b	604	CLA	C2C-C1C-NC	7.48	115.81	110.24
26	k	102	BCR	C12-C13-C14	7.50	131.07	118.98
24	B	604	CLA	C2C-C1C-NC	7.52	115.84	110.24
26	c	915	BCR	C23-C22-C21	7.54	131.12	118.98
26	Y	101	BCR	C7-C8-C9	7.57	137.75	126.22
26	k	101	BCR	C12-C13-C14	7.58	131.20	118.98
26	b	618	BCR	C40-C30-C25	7.59	122.21	110.30
26	D	404	BCR	C12-C13-C14	7.60	131.23	118.98
26	f	101	BCR	C23-C22-C21	7.69	131.37	118.98
24	C	501	CLA	O2D-CGD-CBD	7.71	121.88	111.30
24	d	401	CLA	C2C-C1C-NC	7.75	116.02	110.24
26	A	610	BCR	C7-C8-C9	7.83	138.15	126.22
26	B	619	BCR	C7-C8-C9	7.83	138.15	126.22
26	H	101	BCR	C7-C8-C9	7.84	138.16	126.22
24	d	403	CLA	C2C-C1C-NC	7.85	116.09	110.24
26	B	622	BCR	C33-C5-C6	7.90	132.37	124.61
26	K	101	BCR	C23-C22-C21	7.94	131.78	118.98
24	a	407	CLA	C2C-C1C-NC	7.95	116.16	110.24
26	k	101	BCR	C33-C5-C6	7.98	132.44	124.61
26	B	619	BCR	C10-C11-C12	7.99	147.47	123.13
26	Y	101	BCR	C11-C12-C13	7.99	149.84	126.32
26	b	619	BCR	C23-C22-C21	7.99	131.86	118.98
26	Y	101	BCR	C10-C11-C12	8.07	147.74	123.13
24	B	609	CLA	C2C-C1C-NC	8.11	116.28	110.24
26	B	622	BCR	C24-C23-C22	8.11	138.58	126.22
26	C	514	BCR	C11-C10-C9	8.15	138.97	127.20
26	C	515	BCR	C11-C12-C13	8.17	150.37	126.32
26	A	610	BCR	C20-C19-C18	8.17	150.37	126.32
26	D	404	BCR	C29-C30-C25	8.18	123.32	110.36
24	B	605	CLA	C2C-C1C-NC	8.19	116.34	110.24
24	a	406	CLA	C2C-C1C-NC	8.20	116.35	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	915	BCR	C24-C23-C22	8.25	138.79	126.22
26	a	409	BCR	C20-C19-C18	8.26	150.62	126.32
26	B	618	BCR	C15-C14-C13	8.30	139.18	127.20
24	A	607	CLA	C2C-C1C-NC	8.30	116.42	110.24
26	B	620	BCR	C23-C22-C21	8.31	132.37	118.98
26	H	101	BCR	C23-C22-C21	8.33	132.40	118.98
26	k	102	BCR	C23-C22-C21	8.36	132.46	118.98
26	c	918	BCR	C11-C10-C9	8.38	139.31	127.20
26	T	101	BCR	C33-C5-C6	8.44	132.89	124.61
26	D	404	BCR	C32-C1-C6	8.46	123.56	110.30
26	B	619	BCR	C23-C22-C21	8.51	132.69	118.98
26	Y	101	BCR	C33-C5-C6	8.53	132.98	124.61
26	B	619	BCR	C24-C23-C22	8.60	139.32	126.22
26	A	610	BCR	C27-C26-C25	8.67	133.83	122.78
26	B	622	BCR	C7-C8-C9	8.78	139.60	126.22
24	A	614	CLA	C2C-C1C-NC	8.79	116.79	110.24
26	T	101	BCR	C7-C8-C9	8.83	139.67	126.22
26	B	618	BCR	C10-C11-C12	8.85	150.11	123.13
26	K	101	BCR	C11-C10-C9	8.86	140.00	127.20
26	H	101	BCR	C11-C12-C13	8.88	152.44	126.32
26	a	409	BCR	C24-C23-C22	8.93	139.83	126.22
26	c	915	BCR	C7-C8-C9	8.95	139.86	126.22
26	B	620	BCR	C20-C19-C18	8.97	152.71	126.32
26	B	618	BCR	C11-C12-C13	8.98	152.75	126.32
26	H	101	BCR	C12-C13-C14	9.00	133.48	118.98
26	D	404	BCR	C19-C18-C17	9.00	133.48	118.98
26	B	619	BCR	C12-C13-C14	9.02	133.51	118.98
26	D	404	BCR	C11-C12-C13	9.02	152.86	126.32
26	b	619	BCR	C20-C19-C18	9.02	152.88	126.32
26	D	404	BCR	C20-C19-C18	9.09	153.07	126.32
26	h	101	BCR	C7-C8-C9	9.09	140.07	126.22
26	C	515	BCR	C12-C13-C14	9.09	133.63	118.98
26	K	101	BCR	C12-C13-C14	9.11	133.66	118.98
26	C	515	BCR	C19-C18-C17	9.13	133.70	118.98
26	c	915	BCR	C19-C18-C17	9.14	133.71	118.98
26	T	102	BCR	C10-C11-C12	9.15	151.03	123.13
26	B	620	BCR	C7-C8-C9	9.18	140.20	126.22
26	f	101	BCR	C10-C11-C12	9.18	151.12	123.13
26	k	101	BCR	C11-C12-C13	9.19	153.36	126.32
26	K	101	BCR	C7-C8-C9	9.24	140.30	126.22
26	T	101	BCR	C19-C18-C17	9.29	133.95	118.98
26	a	409	BCR	C7-C8-C9	9.32	140.42	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	610	BCR	C11-C12-C13	9.32	153.76	126.32
26	f	101	BCR	C15-C14-C13	9.34	140.69	127.20
26	h	101	BCR	C19-C18-C17	9.34	134.03	118.98
26	T	102	BCR	C20-C19-C18	9.39	153.96	126.32
26	h	101	BCR	C24-C23-C22	9.43	140.59	126.22
26	T	102	BCR	C11-C10-C9	9.45	140.85	127.20
26	f	101	BCR	C29-C30-C25	9.48	125.38	110.36
26	c	915	BCR	C11-C12-C13	9.52	154.33	126.32
26	T	102	BCR	C12-C13-C14	9.56	134.38	118.98
26	b	618	BCR	C23-C22-C21	9.57	134.40	118.98
26	C	514	BCR	C7-C8-C9	9.65	140.92	126.22
26	b	618	BCR	C20-C19-C18	9.65	154.74	126.32
26	B	620	BCR	C11-C12-C13	9.67	154.77	126.32
26	C	514	BCR	C15-C14-C13	9.67	141.17	127.20
26	T	102	BCR	C11-C12-C13	9.71	154.89	126.32
26	H	101	BCR	C10-C11-C12	9.74	152.83	123.13
26	a	409	BCR	C12-C13-C14	9.77	134.72	118.98
26	T	101	BCR	C15-C14-C13	9.77	141.31	127.20
26	f	101	BCR	C11-C12-C13	9.79	155.12	126.32
26	A	610	BCR	C10-C11-C12	9.86	153.19	123.13
26	c	915	BCR	C11-C10-C9	9.88	141.46	127.20
26	b	619	BCR	C11-C12-C13	9.94	155.58	126.32
26	C	514	BCR	C19-C18-C17	10.02	135.13	118.98
26	a	409	BCR	C11-C12-C13	10.03	155.84	126.32
26	k	102	BCR	C7-C8-C9	10.04	141.51	126.22
26	h	101	BCR	C11-C12-C13	10.08	156.00	126.32
26	C	514	BCR	C11-C12-C13	10.16	156.24	126.32
26	b	618	BCR	C7-C8-C9	10.19	141.75	126.22
26	f	101	BCR	C20-C19-C18	10.20	156.34	126.32
26	H	101	BCR	C19-C18-C17	10.21	135.43	118.98
26	B	619	BCR	C20-C19-C18	10.24	156.45	126.32
26	B	620	BCR	C15-C14-C13	10.24	141.99	127.20
26	b	618	BCR	C12-C13-C14	10.25	135.50	118.98
26	B	618	BCR	C20-C19-C18	10.26	156.52	126.32
26	k	102	BCR	C11-C12-C13	10.28	156.57	126.32
26	B	622	BCR	C11-C10-C9	10.28	142.05	127.20
26	T	101	BCR	C20-C19-C18	10.30	156.63	126.32
26	D	404	BCR	C11-C10-C9	10.31	142.09	127.20
26	A	610	BCR	C12-C13-C14	10.33	135.63	118.98
26	h	101	BCR	C10-C11-C12	10.33	154.63	123.13
26	C	515	BCR	C10-C11-C12	10.38	154.78	123.13
26	B	622	BCR	C11-C12-C13	10.42	157.00	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C10-C11-C12	10.43	154.92	123.13
26	H	101	BCR	C20-C19-C18	10.44	157.04	126.32
26	T	101	BCR	C21-C20-C19	10.46	155.00	123.13
26	D	404	BCR	C15-C14-C13	10.49	142.35	127.20
26	k	101	BCR	C15-C14-C13	10.52	142.39	127.20
26	c	915	BCR	C20-C19-C18	10.52	157.28	126.32
26	A	610	BCR	C23-C22-C21	10.54	135.97	118.98
26	b	618	BCR	C10-C11-C12	10.58	155.38	123.13
26	B	622	BCR	C19-C18-C17	10.63	136.12	118.98
26	Y	101	BCR	C20-C19-C18	10.67	157.72	126.32
26	h	101	BCR	C20-C19-C18	10.71	157.85	126.32
26	a	409	BCR	C21-C20-C19	10.74	155.87	123.13
26	A	610	BCR	C15-C14-C13	10.74	142.72	127.20
26	k	102	BCR	C19-C18-C17	10.77	136.33	118.98
26	k	101	BCR	C10-C11-C12	10.79	156.01	123.13
26	K	101	BCR	C11-C12-C13	10.82	158.16	126.32
26	B	618	BCR	C11-C10-C9	10.96	143.03	127.20
26	B	622	BCR	C15-C14-C13	11.00	143.08	127.20
26	T	101	BCR	C11-C12-C13	11.06	158.86	126.32
26	K	101	BCR	C10-C11-C12	11.07	156.88	123.13
26	a	409	BCR	C23-C22-C21	11.07	136.82	118.98
26	B	618	BCR	C12-C13-C14	11.12	136.90	118.98
26	f	101	BCR	C11-C10-C9	11.16	143.31	127.20
26	c	915	BCR	C15-C14-C13	11.19	143.35	127.20
26	b	619	BCR	C7-C8-C9	11.19	143.27	126.22
26	a	409	BCR	C10-C11-C12	11.19	157.25	123.13
26	T	102	BCR	C15-C14-C13	11.23	143.41	127.20
26	a	409	BCR	C19-C18-C17	11.26	137.13	118.98
26	A	610	BCR	C11-C10-C9	11.29	143.50	127.20
26	a	409	BCR	C15-C14-C13	11.31	143.54	127.20
26	Y	101	BCR	C15-C14-C13	11.32	143.54	127.20
26	C	515	BCR	C15-C14-C13	11.45	143.73	127.20
26	b	618	BCR	C15-C14-C13	11.46	143.75	127.20
26	H	101	BCR	C15-C14-C13	11.46	143.75	127.20
26	B	618	BCR	C21-C20-C19	11.48	158.14	123.13
26	T	102	BCR	C19-C18-C17	11.56	137.60	118.98
26	T	102	BCR	C21-C20-C19	11.56	158.38	123.13
26	h	101	BCR	C11-C10-C9	11.58	143.92	127.20
26	b	618	BCR	C16-C15-C14	11.58	148.99	123.39
26	a	409	BCR	C11-C10-C9	11.58	143.92	127.20
26	f	101	BCR	C19-C18-C17	11.61	137.69	118.98
26	c	918	BCR	C7-C8-C9	11.62	143.92	126.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	101	BCR	C19-C18-C17	11.62	137.70	118.98
26	f	101	BCR	C21-C20-C19	11.65	158.65	123.13
26	K	101	BCR	C20-C19-C18	11.71	160.78	126.32
26	k	101	BCR	C11-C10-C9	11.75	144.17	127.20
26	b	619	BCR	C10-C11-C12	11.75	158.95	123.13
26	k	101	BCR	C7-C8-C9	11.79	144.18	126.22
26	C	515	BCR	C20-C19-C18	11.83	161.14	126.32
26	A	610	BCR	C19-C18-C17	11.85	138.08	118.98
26	B	622	BCR	C20-C19-C18	11.89	161.31	126.32
26	b	619	BCR	C19-C18-C17	11.89	138.15	118.98
26	Y	101	BCR	C19-C18-C17	12.03	138.37	118.98
26	T	101	BCR	C10-C11-C12	12.05	159.85	123.13
26	c	915	BCR	C10-C11-C12	12.06	159.89	123.13
26	b	618	BCR	C21-C20-C19	12.09	159.98	123.13
26	h	101	BCR	C15-C14-C13	12.09	144.66	127.20
26	k	101	BCR	C19-C18-C17	12.12	138.51	118.98
26	C	514	BCR	C20-C19-C18	12.13	162.02	126.32
26	T	101	BCR	C11-C10-C9	12.16	144.75	127.20
26	C	514	BCR	C10-C11-C12	12.26	160.49	123.13
26	k	102	BCR	C15-C14-C13	12.28	144.94	127.20
26	c	918	BCR	C20-C19-C18	12.30	162.51	126.32
26	k	102	BCR	C20-C19-C18	12.33	162.60	126.32
26	k	102	BCR	C11-C10-C9	12.51	145.27	127.20
26	B	620	BCR	C11-C10-C9	12.52	145.28	127.20
26	B	620	BCR	C19-C18-C17	12.57	139.24	118.98
26	k	102	BCR	C10-C11-C12	12.59	161.49	123.13
26	b	619	BCR	C11-C10-C9	12.59	145.38	127.20
26	b	619	BCR	C15-C14-C13	12.70	145.54	127.20
26	D	404	BCR	C21-C20-C19	12.97	162.68	123.13
26	Y	101	BCR	C11-C10-C9	13.00	145.97	127.20
26	A	610	BCR	C21-C20-C19	13.06	162.93	123.13
26	B	622	BCR	C10-C11-C12	13.10	163.06	123.13
26	B	618	BCR	C16-C15-C14	13.13	152.43	123.39
26	B	619	BCR	C11-C10-C9	13.20	146.26	127.20
26	B	622	BCR	C21-C20-C19	13.21	163.40	123.13
26	b	618	BCR	C11-C10-C9	13.30	146.41	127.20
26	k	101	BCR	C20-C19-C18	13.38	165.72	126.32
26	B	619	BCR	C15-C14-C13	13.45	146.62	127.20
26	A	610	BCR	C16-C15-C14	13.57	153.39	123.39
26	f	101	BCR	C7-C8-C9	13.57	146.90	126.22
26	B	619	BCR	C19-C18-C17	13.62	140.93	118.98
26	B	620	BCR	C21-C20-C19	13.66	164.77	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	101	BCR	C11-C10-C9	13.77	147.09	127.20
26	b	619	BCR	C16-C15-C14	13.80	153.90	123.39
26	c	918	BCR	C10-C11-C12	13.85	165.34	123.13
26	T	101	BCR	C20-C21-C22	13.89	147.25	127.20
26	K	101	BCR	C15-C14-C13	14.04	147.47	127.20
26	K	101	BCR	C21-C20-C19	14.08	166.05	123.13
26	C	515	BCR	C11-C10-C9	14.36	147.93	127.20
26	c	918	BCR	C11-C12-C13	14.52	169.06	126.32
26	B	618	BCR	C19-C18-C17	14.71	142.68	118.98
26	B	619	BCR	C16-C15-C14	14.72	155.95	123.39
26	B	619	BCR	C15-C16-C17	14.88	156.29	123.39
26	H	101	BCR	C16-C15-C14	14.93	156.40	123.39
26	B	619	BCR	C21-C20-C19	14.98	168.78	123.13
26	Y	101	BCR	C21-C20-C19	14.98	168.81	123.13
26	T	102	BCR	C16-C15-C14	15.04	156.66	123.39
26	a	409	BCR	C16-C15-C14	15.31	157.26	123.39
26	Y	101	BCR	C16-C15-C14	15.33	157.30	123.39
26	H	101	BCR	C21-C20-C19	15.35	169.92	123.13
26	b	618	BCR	C15-C16-C17	15.53	157.73	123.39
26	b	618	BCR	C19-C18-C17	15.55	144.03	118.98
26	c	918	BCR	C21-C20-C19	15.60	170.69	123.13
26	f	101	BCR	C16-C15-C14	15.89	158.53	123.39
26	k	101	BCR	C16-C15-C14	16.07	158.93	123.39
26	b	619	BCR	C21-C20-C19	16.13	172.30	123.13
26	k	101	BCR	C21-C20-C19	16.45	173.27	123.13
26	k	102	BCR	C16-C15-C14	16.54	159.97	123.39
26	C	515	BCR	C21-C20-C19	16.70	174.04	123.13
26	A	610	BCR	C15-C16-C17	16.82	160.59	123.39
26	B	622	BCR	C16-C15-C14	16.87	160.69	123.39
26	h	101	BCR	C16-C15-C14	16.89	160.74	123.39
26	B	620	BCR	C16-C15-C14	17.07	161.13	123.39
26	T	101	BCR	C16-C17-C18	17.11	151.91	127.20
26	c	915	BCR	C21-C20-C19	17.28	175.79	123.13
26	C	514	BCR	C21-C20-C19	17.37	176.07	123.13
26	k	102	BCR	C21-C20-C19	17.46	176.37	123.13
26	K	101	BCR	C16-C15-C14	17.81	162.77	123.39
26	B	618	BCR	C20-C21-C22	17.93	153.09	127.20
26	T	102	BCR	C20-C21-C22	18.21	153.50	127.20
26	B	618	BCR	C15-C16-C17	18.28	163.82	123.39
26	h	101	BCR	C21-C20-C19	18.33	179.01	123.13
26	f	101	BCR	C20-C21-C22	18.44	153.83	127.20
26	c	918	BCR	C15-C16-C17	18.50	164.31	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	619	BCR	C15-C16-C17	18.53	164.36	123.39
26	K	101	BCR	C16-C17-C18	18.58	154.03	127.20
26	T	102	BCR	C15-C16-C17	18.70	164.74	123.39
26	D	404	BCR	C16-C15-C14	18.71	164.75	123.39
26	T	101	BCR	C16-C15-C14	18.90	165.19	123.39
26	Y	101	BCR	C15-C16-C17	19.19	165.83	123.39
26	B	622	BCR	C20-C21-C22	19.21	154.95	127.20
26	C	514	BCR	C16-C15-C14	19.23	165.92	123.39
26	B	622	BCR	C15-C16-C17	19.42	166.34	123.39
26	T	101	BCR	C15-C16-C17	19.66	166.87	123.39
26	c	918	BCR	C16-C17-C18	20.07	156.18	127.20
26	C	515	BCR	C16-C15-C14	20.23	168.12	123.39
26	c	918	BCR	C20-C21-C22	20.27	156.47	127.20
26	c	915	BCR	C16-C15-C14	20.33	168.36	123.39
26	H	101	BCR	C16-C17-C18	20.36	156.60	127.20
26	B	619	BCR	C16-C17-C18	20.40	156.66	127.20
26	C	515	BCR	C16-C17-C18	20.49	156.79	127.20
26	a	409	BCR	C15-C16-C17	20.51	168.74	123.39
26	c	918	BCR	C16-C15-C14	20.72	169.20	123.39
26	K	101	BCR	C15-C16-C17	20.74	169.26	123.39
26	b	618	BCR	C20-C21-C22	20.78	157.21	127.20
26	K	101	BCR	C20-C21-C22	20.81	157.25	127.20
26	h	101	BCR	C16-C17-C18	20.88	157.36	127.20
26	T	102	BCR	C16-C17-C18	21.25	157.89	127.20
26	A	610	BCR	C16-C17-C18	21.39	158.09	127.20
26	a	409	BCR	C20-C21-C22	21.41	158.13	127.20
26	D	404	BCR	C15-C16-C17	21.54	171.03	123.39
26	f	101	BCR	C15-C16-C17	21.56	171.07	123.39
26	B	619	BCR	C20-C21-C22	21.74	158.59	127.20
26	C	515	BCR	C15-C16-C17	22.01	172.06	123.39
26	a	409	BCR	C16-C17-C18	22.02	159.01	127.20
26	D	404	BCR	C16-C17-C18	22.11	159.14	127.20
26	B	622	BCR	C16-C17-C18	22.16	159.20	127.20
26	k	101	BCR	C20-C21-C22	22.24	159.31	127.20
26	D	404	BCR	C20-C21-C22	22.28	159.38	127.20
26	k	102	BCR	C15-C16-C17	22.37	172.85	123.39
26	h	101	BCR	C15-C16-C17	22.76	173.73	123.39
26	C	514	BCR	C20-C21-C22	22.84	160.19	127.20
26	k	101	BCR	C15-C16-C17	22.93	174.09	123.39
26	c	915	BCR	C15-C16-C17	22.99	174.22	123.39
26	f	101	BCR	C16-C17-C18	23.00	160.42	127.20
26	Y	101	BCR	C16-C17-C18	23.13	160.61	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	k	102	BCR	C16-C17-C18	23.27	160.81	127.20
26	k	102	BCR	C20-C21-C22	23.29	160.84	127.20
26	H	101	BCR	C15-C16-C17	23.47	175.30	123.39
26	B	620	BCR	C15-C16-C17	23.50	175.36	123.39
26	B	618	BCR	C16-C17-C18	23.99	161.85	127.20
26	c	915	BCR	C16-C17-C18	24.81	163.03	127.20
26	C	514	BCR	C15-C16-C17	24.84	178.33	123.39
26	b	618	BCR	C16-C17-C18	24.87	163.12	127.20
26	C	514	BCR	C16-C17-C18	24.89	163.14	127.20
26	A	610	BCR	C20-C21-C22	24.98	163.28	127.20
26	b	619	BCR	C16-C17-C18	25.10	163.45	127.20
26	B	620	BCR	C16-C17-C18	25.17	163.55	127.20
26	Y	101	BCR	C20-C21-C22	25.30	163.75	127.20
26	C	515	BCR	C20-C21-C22	25.47	163.98	127.20
26	B	620	BCR	C20-C21-C22	26.31	165.20	127.20
26	h	101	BCR	C20-C21-C22	26.39	165.32	127.20
26	k	101	BCR	C16-C17-C18	26.39	165.32	127.20
26	c	915	BCR	C20-C21-C22	26.59	165.60	127.20
26	H	101	BCR	C20-C21-C22	26.65	165.69	127.20
26	b	619	BCR	C20-C21-C22	29.92	170.41	127.20

All (163) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	a	408	CLA	NC
24	b	602	CLA	NC
24	b	602	CLA	ND
24	b	602	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	614	CLA	NA
24	B	613	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	b	608	CLA	NC
24	b	608	CLA	ND
24	b	608	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	ND

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Mol	Chain	Res	Type	Atom
24	C	504	CLA	NA
24	d	404	CLA	NC
24	C	505	CLA	ND
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	c	905	CLA	NC
24	c	905	CLA	NA
24	A	614	CLA	NA
24	d	403	CLA	ND
24	d	403	CLA	NA
24	B	617	CLA	NC
24	B	617	CLA	ND
24	B	617	CLA	NA
24	c	903	CLA	NC
24	c	903	CLA	NA
24	c	912	CLA	NC
24	c	912	CLA	NA
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	D	403	CLA	NC
24	D	403	CLA	NA
24	b	609	CLA	NC
24	C	501	CLA	NC
24	C	501	CLA	NA
24	c	909	CLA	NC
24	c	909	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	B	615	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	606	CLA	NA
24	b	603	CLA	NC
24	b	603	CLA	ND
24	b	603	CLA	NA
24	B	612	CLA	NC
24	B	616	CLA	NC
24	B	616	CLA	ND
24	B	616	CLA	NA
24	A	609	CLA	NC

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Mol	Chain	Res	Type	Atom
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	616	CLA	NA
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	A	606	CLA	NC
24	A	606	CLA	ND
24	A	606	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	604	CLA	NA
24	c	913	CLA	NC
24	c	913	CLA	NA
24	c	913	CLA	ND
24	B	610	CLA	NC
24	B	610	CLA	ND
24	C	511	CLA	NC
24	C	511	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	NA
24	B	602	CLA	ND
24	B	602	CLA	NA
24	c	902	CLA	NC
24	c	902	CLA	ND
24	c	902	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	c	906	CLA	ND
24	c	906	CLA	NA
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	b	615	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	a	407	CLA	NC
24	a	407	CLA	NA

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Mol	Chain	Res	Type	Atom
24	c	904	CLA	NC
24	c	911	CLA	NC
24	c	911	CLA	ND
24	c	911	CLA	NA
24	c	914	CLA	NC
24	c	914	CLA	NA
24	a	406	CLA	NC
24	a	406	CLA	ND
24	a	406	CLA	NA
24	c	907	CLA	ND
24	c	907	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	b	611	CLA	NA
24	D	402	CLA	ND
24	b	617	CLA	NC
24	b	617	CLA	ND
24	b	617	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	NA
24	C	512	CLA	ND
24	d	401	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	B	608	CLA	NC
24	B	608	CLA	ND
24	B	608	CLA	NA
24	C	508	CLA	NC
24	C	508	CLA	NA
24	A	607	CLA	NC
24	A	607	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	NA
24	b	613	CLA	NA

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Mol	Chain	Res	Type	Atom
24	b	613	CLA	NC
24	b	613	CLA	ND
24	B	609	CLA	NC
24	C	506	CLA	NC
24	C	506	CLA	ND
24	C	506	CLA	NA
24	c	908	CLA	NC
24	c	908	CLA	ND
24	c	908	CLA	NA
24	C	502	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	B	603	CLA	NA
24	c	910	CLA	NC
24	c	910	CLA	ND
24	c	910	CLA	NA
24	b	604	CLA	NC
24	b	604	CLA	ND
24	b	604	CLA	NA

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	h	101	BCR	C21-C20-C19-C18

There are no ring outliers.

60 monomers are involved in 188 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	606	CLA	4	0
24	A	607	CLA	2	0
25	A	608	PHO	4	0
24	A	609	CLA	3	0
27	A	611	PL9	9	0
28	A	612	SQD	5	0
28	A	613	SQD	1	0
24	A	614	CLA	4	0
29	A	615	LHG	3	0
24	B	603	CLA	5	0
24	B	604	CLA	2	0
24	B	605	CLA	2	0
24	B	606	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	607	CLA	6	0
24	B	609	CLA	3	0
24	B	610	CLA	2	0
24	B	611	CLA	7	0
24	B	612	CLA	5	0
24	B	613	CLA	5	0
24	B	614	CLA	4	0
24	B	615	CLA	1	0
24	B	616	CLA	3	0
24	B	617	CLA	4	0
26	B	618	BCR	2	0
26	B	619	BCR	5	0
26	B	620	BCR	1	0
29	B	621	LHG	3	0
26	B	622	BCR	2	0
24	C	501	CLA	2	0
24	C	502	CLA	3	0
24	C	503	CLA	3	0
24	C	504	CLA	5	0
24	C	505	CLA	3	0
24	C	506	CLA	5	0
24	C	507	CLA	2	0
24	C	508	CLA	8	0
24	C	509	CLA	2	0
24	C	510	CLA	7	0
24	C	511	CLA	3	0
24	C	512	CLA	3	0
24	C	513	CLA	1	0
31	C	516	DGD	2	0
31	C	517	DGD	1	0
31	C	518	DGD	3	0
25	D	401	PHO	4	0
24	D	402	CLA	1	0
24	D	403	CLA	5	0
26	D	404	BCR	2	0
27	D	405	PL9	2	0
31	D	406	DGD	4	0
29	D	407	LHG	4	0
29	D	408	LHG	1	0
29	D	409	LHG	23	0
26	H	101	BCR	2	0
31	H	102	DGD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	K	101	BCR	5	0
28	L	101	SQD	10	0
26	T	101	BCR	2	0
32	V	202	HEM	9	0
26	Y	101	BCR	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%)	0.43	13 (3%) 43 36	16, 22, 43, 53	0
1	a	334/334 (100%)	0.50	26 (7%) 16 13	19, 24, 45, 62	0
2	B	504/504 (100%)	0.39	34 (6%) 21 16	18, 27, 49, 70	0
2	b	504/504 (100%)	0.66	62 (12%) 5 7	20, 29, 52, 93	0
3	C	451/455 (99%)	0.51	50 (11%) 7 8	21, 31, 44, 56	0
3	c	455/455 (100%)	0.34	26 (5%) 27 22	24, 34, 45, 59	0
4	D	342/342 (100%)	0.70	29 (8%) 13 12	17, 23, 39, 61	0
4	d	341/342 (99%)	0.59	27 (7%) 15 13	19, 26, 42, 59	0
5	E	81/81 (100%)	0.75	11 (13%) 4 5	27, 40, 57, 63	0
5	e	81/81 (100%)	0.42	9 (11%) 7 8	34, 45, 67, 76	0
6	F	34/34 (100%)	-0.01	1 (2%) 55 45	28, 33, 58, 61	0
6	f	32/34 (94%)	0.05	3 (9%) 11 10	30, 36, 60, 62	0
7	H	65/65 (100%)	0.79	11 (16%) 2 4	23, 34, 40, 58	0
7	h	65/65 (100%)	1.20	14 (21%) 1 3	28, 37, 48, 58	0
8	I	38/38 (100%)	0.37	3 (7%) 15 13	26, 33, 65, 68	0
8	i	38/38 (100%)	0.16	3 (7%) 15 13	29, 34, 62, 65	0
9	J	38/40 (95%)	0.64	6 (15%) 3 4	26, 37, 68, 72	0
9	j	40/40 (100%)	-0.08	3 (7%) 17 15	31, 42, 76, 80	0
10	K	37/37 (100%)	0.08	0 100 100	33, 38, 45, 47	0
10	k	37/37 (100%)	0.36	3 (8%) 15 13	38, 43, 55, 58	0
11	L	37/37 (100%)	0.62	4 (10%) 8 8	17, 22, 50, 59	0
11	l	37/37 (100%)	0.47	0 100 100	19, 22, 55, 62	0
12	M	34/34 (100%)	1.07	7 (20%) 1 3	21, 23, 36, 52	0
12	m	34/34 (100%)	0.79	3 (8%) 12 11	21, 25, 37, 53	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/243 (100%)	0.36	7 (2%) 55 45	18, 32, 55, 71	0
13	o	243/243 (100%)	0.48	16 (6%) 22 17	21, 35, 61, 72	0
14	T	30/30 (100%)	0.70	3 (10%) 9 9	19, 23, 44, 52	0
14	t	30/30 (100%)	0.78	3 (10%) 9 9	20, 24, 44, 51	0
15	U	97/97 (100%)	0.13	2 (2%) 67 58	23, 30, 48, 50	0
15	u	97/97 (100%)	0.29	3 (3%) 52 43	25, 31, 37, 47	0
16	V	137/137 (100%)	0.14	1 (0%) 89 84	23, 28, 39, 48	0
16	v	137/137 (100%)	0.25	10 (7%) 18 15	27, 37, 51, 57	0
17	Y	29/29 (100%)	0.48	2 (6%) 20 16	42, 48, 75, 77	0
17	y	29/29 (100%)	0.08	0 100 100	50, 56, 75, 76	0
18	X	39/39 (100%)	0.84	8 (20%) 1 3	33, 40, 66, 68	0
18	x	39/39 (100%)	1.17	6 (15%) 3 4	37, 43, 75, 77	0
19	Z	62/62 (100%)	0.43	3 (4%) 34 28	39, 48, 68, 72	0
19	z	62/62 (100%)	0.53	5 (8%) 15 13	53, 61, 82, 87	0
All	All	5267/5276 (99%)	0.48	417 (7%) 15 13	16, 30, 56, 93	0

All (417) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	40	SER	8.1
7	H	65	LEU	7.0
4	d	136	VAL	6.5
9	J	3	SER	6.3
4	D	59	TYR	6.3
4	D	137	GLY	6.2
4	D	136	VAL	6.2
6	f	14	PRO	6.0
1	a	138	GLY	5.8
3	C	264	PHE	5.8
3	C	138	GLU	5.6
4	D	135	LEU	5.5
1	a	139	MET	5.4
18	X	2	THR	5.3
2	b	491	VAL	5.3
18	x	3	ILE	5.2
7	H	56	ASP	5.2
4	D	107	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
18	x	2	THR	5.1
2	b	187	PRO	5.0
3	C	137	PRO	5.0
3	C	97	TRP	4.9
3	C	143	TYR	4.8
3	C	147	PHE	4.8
15	u	8	GLU	4.7
7	H	66	GLY	4.7
3	c	373	ASN	4.7
2	b	499	VAL	4.7
4	d	135	LEU	4.7
3	C	263	ALA	4.6
1	a	250	ALA	4.6
3	C	265	ILE	4.5
6	f	15	ILE	4.5
4	d	137	GLY	4.5
2	B	500	GLY	4.3
2	B	505	ARG	4.3
4	D	27	PHE	4.3
1	a	222	SER	4.3
19	z	62	VAL	4.3
1	a	137	LEU	4.3
4	D	12	ARG	4.2
4	D	106	GLN	4.2
3	C	24	THR	4.1
3	C	200	THR	4.1
13	o	25	THR	4.1
7	H	54	ILE	4.1
2	b	435	GLU	4.1
7	H	55	LEU	4.1
2	b	500	GLY	4.1
2	b	218	LEU	4.1
2	b	443	PHE	4.0
3	C	146	PHE	4.0
7	h	65	LEU	4.0
2	b	362	PHE	4.0
3	c	146	PHE	4.0
5	E	70	PHE	4.0
2	b	262	THR	3.9
2	b	219	VAL	3.9
3	c	227	VAL	3.9
12	M	1	MET	3.9

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Mol	Chain	Res	Type	RSRZ
5	e	84	LYS	3.8
16	v	21	LEU	3.8
3	c	198	VAL	3.8
5	e	55	TYR	3.8
4	d	59	TYR	3.8
3	C	99	VAL	3.8
7	h	56	ASP	3.8
1	a	247	ASN	3.8
2	b	185	TRP	3.8
3	C	203	THR	3.7
3	C	266	TRP	3.7
18	X	39	ARG	3.7
3	C	199	ILE	3.7
7	H	64	ALA	3.7
1	A	266	ASN	3.7
3	c	200	THR	3.7
1	A	137	LEU	3.7
3	C	145	SER	3.6
2	B	368	VAL	3.6
5	E	84	LYS	3.6
3	C	144	SER	3.6
9	J	4	GLU	3.6
10	k	43	VAL	3.5
9	j	2	MET	3.4
8	i	37	LEU	3.4
2	b	217	ILE	3.4
4	d	12	ARG	3.4
10	k	15	TYR	3.4
7	h	55	LEU	3.4
4	D	95	PRO	3.4
3	C	202	PRO	3.4
2	B	353	GLU	3.4
5	e	64	PRO	3.4
4	D	138	VAL	3.3
3	c	228	ASN	3.3
1	a	245	THR	3.3
4	D	96	GLU	3.3
4	d	292	ASN	3.3
2	B	367	PRO	3.2
2	b	361	ALA	3.2
2	B	43	ALA	3.2
18	X	38	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
7	h	11	LEU	3.2
4	D	350	ASN	3.2
19	z	27	TYR	3.2
2	b	305	ILE	3.2
13	o	85	LEU	3.2
4	D	169	PHE	3.2
1	A	138	GLY	3.2
3	C	151	TRP	3.2
4	d	264	LYS	3.1
1	a	317	TRP	3.1
2	b	319	PRO	3.1
1	A	261	GLN	3.1
1	a	11	ALA	3.1
19	Z	1	MET	3.1
2	B	366	PHE	3.1
13	o	142	PHE	3.1
3	C	201	ASN	3.1
2	B	362	PHE	3.1
15	U	61	VAL	3.1
2	b	304	ALA	3.1
1	a	239	PHE	3.1
4	d	107	LEU	3.1
5	E	17	VAL	3.1
2	B	499	VAL	3.1
3	c	199	ILE	3.1
2	b	318	ASN	3.1
9	J	8	ILE	3.1
2	b	447	PRO	3.1
9	j	1	MET	3.1
8	I	25	SER	3.0
2	B	369	ILE	3.0
7	h	54	ILE	3.0
1	A	11	ALA	3.0
16	v	135	VAL	3.0
11	L	37	ASN	3.0
2	B	133	LEU	3.0
2	b	356	VAL	3.0
4	d	68	LEU	3.0
2	b	133	LEU	3.0
5	e	56	TYR	3.0
18	X	37	VAL	3.0
19	z	24	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
4	d	32	TRP	3.0
3	c	147	PHE	3.0
4	D	85	MET	3.0
4	D	307	GLU	3.0
1	a	223	LEU	2.9
2	b	195	PRO	2.9
11	L	2	GLU	2.9
2	b	494	GLY	2.9
18	X	3	ILE	2.9
3	c	197	ARG	2.9
4	d	56	THR	2.9
6	F	12	SER	2.9
18	x	25	PHE	2.9
7	H	63	LYS	2.9
13	o	243	ILE	2.9
2	B	70	GLY	2.9
3	C	400	PRO	2.9
2	B	195	PRO	2.9
3	c	86	LEU	2.9
3	c	365	TRP	2.9
7	h	62	TRP	2.9
3	C	139	THR	2.9
2	b	203	ILE	2.9
3	C	111	PHE	2.9
2	b	229	LEU	2.9
1	A	262	TYR	2.8
12	M	2	GLU	2.8
2	b	188	ASP	2.8
16	v	23	GLU	2.8
13	o	80	GLN	2.8
1	a	246	TYR	2.8
2	b	482	ILE	2.8
2	b	190	PHE	2.8
2	b	189	GLY	2.8
18	x	39	ARG	2.8
2	b	367	PRO	2.8
3	c	372	PRO	2.8
17	Y	46	LEU	2.8
2	b	267	LEU	2.8
2	b	287	ARG	2.8
4	d	138	VAL	2.8
4	d	171	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	166	MET	2.8
1	a	84	PRO	2.8
1	a	140	ARG	2.8
2	B	471	ALA	2.8
16	v	48	THR	2.8
4	d	14	TRP	2.8
3	C	180	MET	2.7
2	B	320	ALA	2.7
3	c	335	THR	2.7
2	b	438	ASN	2.7
3	C	85	GLY	2.7
12	M	4	ASN	2.7
2	b	16	PRO	2.7
2	b	183	PRO	2.7
2	b	84	THR	2.7
3	c	224	ILE	2.7
13	O	64	GLU	2.7
2	B	347	ARG	2.7
4	d	29	PHE	2.7
2	B	354	LEU	2.7
3	c	134	ILE	2.7
3	c	112	PHE	2.7
4	D	188	PHE	2.7
2	B	497	GLN	2.6
3	C	46	SER	2.6
5	e	83	LEU	2.6
16	v	22	THR	2.6
2	B	44	THR	2.6
3	c	22	PHE	2.6
13	o	34	SER	2.6
2	B	503	THR	2.6
2	b	369	ILE	2.6
5	E	21	VAL	2.6
1	a	85	SER	2.6
2	B	495	PHE	2.6
7	h	18	TYR	2.6
13	O	20	PRO	2.6
8	I	38	GLU	2.6
5	e	60	GLN	2.6
5	E	18	ARG	2.6
7	h	57	GLY	2.6
8	i	32	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	71	VAL	2.6
7	H	15	ASN	2.6
3	C	291	TRP	2.6
2	b	436	THR	2.6
7	H	52	THR	2.6
2	b	368	VAL	2.5
16	v	67	ASP	2.6
4	D	336	HIS	2.5
18	X	40	SER	2.5
2	b	328	GLY	2.5
5	E	66	VAL	2.5
1	A	268	SER	2.5
9	j	3	SER	2.5
2	b	490	GLN	2.5
13	o	176	GLN	2.5
2	b	55	MET	2.5
16	V	125	ILE	2.5
2	b	302	TRP	2.5
2	b	497	GLN	2.5
9	J	7	ARG	2.5
3	C	296	VAL	2.5
13	o	100	GLY	2.5
4	D	89	LEU	2.5
3	C	185	LEU	2.5
14	T	27	PRO	2.5
3	C	112	PHE	2.5
13	o	87	VAL	2.5
5	e	50	PRO	2.5
4	d	25	ASP	2.5
3	C	149	TYR	2.5
1	a	268	SER	2.5
2	B	504	THR	2.5
5	E	4	THR	2.5
1	A	246	TYR	2.5
13	o	58	ASN	2.4
12	M	10	ALA	2.4
11	L	1	MET	2.4
15	u	66	GLY	2.4
12	m	7	GLY	2.4
1	A	295	PHE	2.4
2	B	136	PRO	2.4
4	D	56	THR	2.4

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Mol	Chain	Res	Type	RSRZ
7	H	57	GLY	2.4
1	a	136	ARG	2.4
13	O	67	PRO	2.4
2	b	120	LEU	2.4
2	b	137	LYS	2.4
3	c	21	ILE	2.4
13	o	184	ARG	2.4
2	b	228	ALA	2.4
2	B	187	PRO	2.4
8	I	37	LEU	2.4
3	c	232	ASP	2.4
19	z	61	VAL	2.4
2	b	495	PHE	2.4
2	b	317	ASN	2.4
3	C	98	GLY	2.3
3	C	127	PHE	2.3
4	d	98	GLN	2.3
3	c	456	GLU	2.3
7	h	53	LEU	2.3
13	O	219	GLN	2.3
7	h	15	ASN	2.3
7	h	64	ALA	2.3
6	f	18	VAL	2.3
4	D	248	THR	2.3
1	a	257	ARG	2.3
1	a	249	VAL	2.3
3	c	185	LEU	2.3
2	B	496	TYR	2.3
1	A	257	ARG	2.3
3	C	140	LEU	2.3
1	a	244	GLU	2.3
10	k	14	ALA	2.3
9	J	5	GLY	2.3
4	d	58	TRP	2.3
1	a	266	ASN	2.3
3	C	213	LEU	2.3
5	e	82	GLN	2.3
19	Z	21	ILE	2.3
14	t	3	THR	2.3
16	v	136	TYR	2.3
1	A	139	MET	2.3
4	D	349	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
18	X	36	LYS	2.3
3	C	268	GLY	2.3
1	A	265	PHE	2.2
2	b	505	ARG	2.2
14	t	30	THR	2.2
3	C	234	VAL	2.2
3	C	95	LEU	2.2
4	D	335	PRO	2.2
15	u	90	ALA	2.2
16	v	3	LEU	2.2
4	D	93	TRP	2.2
2	B	321	LYS	2.2
14	T	3	THR	2.2
2	b	492	GLU	2.2
13	o	229	GLU	2.2
2	b	117	TYR	2.2
2	B	69	LEU	2.2
2	b	64	PRO	2.2
2	b	198	VAL	2.2
2	b	320	ALA	2.2
13	o	129	THR	2.2
3	c	149	TYR	2.2
5	E	76	VAL	2.2
3	c	97	TRP	2.2
3	C	25	ASN	2.2
2	b	122	LEU	2.2
2	B	379	ALA	2.2
3	C	262	ARG	2.2
8	i	38	GLU	2.2
13	o	207	ARG	2.2
11	L	33	SER	2.2
16	v	137	TYR	2.2
12	M	5	GLN	2.2
2	b	184	GLU	2.2
19	z	20	VAL	2.2
4	D	334	GLN	2.2
18	X	34	ILE	2.2
2	B	397	VAL	2.2
4	d	96	GLU	2.2
13	O	29	ALA	2.2
5	E	48	GLY	2.2
12	m	2	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
12	m	1	MET	2.2
14	t	11	ALA	2.2
3	C	457	LYS	2.1
13	o	196	GLN	2.1
5	e	54	SER	2.1
4	d	341	PHE	2.1
18	x	37	VAL	2.1
13	o	93	LEU	2.1
7	H	58	VAL	2.1
3	c	151	TRP	2.1
4	D	55	VAL	2.1
5	E	49	THR	2.1
2	b	393	GLU	2.1
3	C	256	PRO	2.1
7	h	58	VAL	2.1
2	b	268	PHE	2.1
4	D	297	ASP	2.1
4	d	265	ARG	2.1
4	d	54	PHE	2.1
2	B	490	GLN	2.1
9	J	9	PRO	2.1
1	a	236	GLY	2.1
3	c	296	VAL	2.1
3	C	181	PHE	2.1
1	a	80	GLY	2.1
15	U	64	ILE	2.1
2	b	204	ALA	2.1
2	b	294	SER	2.1
7	h	23	PRO	2.1
1	a	218	LEU	2.1
2	b	474	LEU	2.1
12	M	18	PRO	2.1
7	h	14	LEU	2.1
1	a	233	ALA	2.1
4	D	342	PRO	2.1
4	d	144	ILE	2.1
1	a	141	PRO	2.0
12	M	11	THR	2.0
16	v	52	LEU	2.0
1	A	107	TYR	2.0
3	C	45	LEU	2.0
3	C	86	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
17	Y	42	ARG	2.0
5	E	69	ARG	2.0
13	O	169	ASP	2.0
4	d	153	PHE	2.0
4	d	157	PHE	2.0
2	b	14	ASN	2.0
2	B	328	GLY	2.0
3	C	82	TYR	2.0
3	c	145	SER	2.0
3	C	103	GLY	2.0
4	D	98	GLN	2.0
4	d	99	GLY	2.0
3	C	44	ASN	2.0
4	d	15	PHE	2.0
3	C	136	GLY	2.0
4	D	189	HIS	2.0
14	T	11	ALA	2.0
2	B	183	PRO	2.0
19	Z	27	TYR	2.0
13	O	28	GLY	2.0
3	C	204	LEU	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
26	BCR	K	101	40/40	0.86	1.84	9.84	29,33,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
26	BCR	Y	101	40/40	0.65	1.57	9.31	34,38,39,39	0
27	PL9	A	611	55/55	0.56	2.04	8.80	52,69,78,78	0
26	BCR	k	102	40/40	0.54	2.03	7.08	33,44,47,48	0
27	PL9	a	410	55/55	0.17	1.70	6.74	63,80,85,85	0
26	BCR	c	915	40/40	0.73	1.85	6.49	30,37,41,42	0
31	DGD	D	406	62/66	0.53	1.38	6.11	77,89,103,103	0
24	CLA	B	603	65/65	0.89	1.13	5.55	23,26,32,32	0
26	BCR	c	918	40/40	0.74	1.76	5.55	50,52,58,58	0
26	BCR	f	101	40/40	0.45	0.98	5.34	30,34,48,49	0
26	BCR	k	101	40/40	0.32	1.08	4.76	37,41,45,45	0
26	BCR	b	619	40/40	0.55	1.06	4.74	30,34,41,42	0
24	CLA	c	902	65/65	0.78	1.54	4.41	30,33,41,45	0
22	CL	a	404	1/1	0.81	0.64	4.37	28,28,28,28	0
26	BCR	C	515	40/40	0.81	1.90	4.26	30,37,40,41	0
24	CLA	c	908	65/65	0.85	1.08	4.24	28,32,50,51	0
26	BCR	D	404	40/40	0.53	0.96	4.09	25,30,48,49	0
24	CLA	c	906	65/65	0.90	0.81	3.71	28,31,44,44	0
28	SQD	F	101	43/54	0.83	0.82	3.52	67,74,78,79	0
25	PHO	D	401	64/64	0.81	0.98	3.48	19,22,28,32	0
24	CLA	b	604	65/65	0.95	1.13	3.36	23,26,35,38	0
24	CLA	a	408	65/65	0.73	0.77	3.33	20,24,75,75	0
31	DGD	H	102	62/66	0.91	1.00	3.32	26,32,38,40	0
29	LHG	a	413	42/49	0.47	0.68	3.26	95,107,110,111	0
26	BCR	C	514	40/40	0.72	1.34	3.25	37,43,47,47	0
24	CLA	b	609	65/65	0.92	1.08	3.10	22,27,38,39	0
24	CLA	c	907	65/65	0.87	0.86	3.09	30,35,64,64	0
29	LHG	D	409	49/49	0.84	0.81	3.02	26,33,62,64	0
24	CLA	A	609	65/65	0.88	0.65	3.01	21,24,71,72	0
24	CLA	d	403	65/65	0.88	0.73	2.95	18,21,38,39	0
24	CLA	c	913	65/65	0.77	1.26	2.91	38,42,62,63	0
24	CLA	b	606	65/65	0.81	0.82	2.89	21,24,32,33	0
24	CLA	b	605	65/65	0.81	0.80	2.85	20,25,53,55	0
24	CLA	B	611	65/65	0.90	0.86	2.82	21,25,32,37	0
31	DGD	d	406	62/66	0.59	0.94	2.81	80,91,105,105	0
24	CLA	c	914	65/65	0.76	1.07	2.77	46,51,73,74	0
24	CLA	D	403	65/65	0.72	1.01	2.76	24,27,65,67	0
24	CLA	D	402	65/65	0.85	0.81	2.73	13,18,34,35	0
26	BCR	A	610	40/40	0.62	0.62	2.72	22,27,32,32	0
24	CLA	C	509	65/65	0.89	1.01	2.65	29,32,46,47	0
31	DGD	h	102	62/66	0.87	0.88	2.64	29,36,43,44	0
25	PHO	a	412	64/64	0.84	0.80	2.63	20,25,30,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
24	CLA	C	512	65/65	0.74	1.36	2.61	37,41,62,63	0
24	CLA	B	613	65/65	0.88	0.57	2.60	20,24,30,31	0
24	CLA	c	910	65/65	0.86	0.86	2.59	27,30,46,46	0
24	CLA	C	507	65/65	0.81	1.31	2.57	29,33,52,53	0
24	CLA	d	404	65/65	0.81	0.84	2.56	26,31,67,68	0
24	CLA	b	603	65/65	0.87	1.05	2.56	26,29,36,37	0
26	BCR	H	101	40/40	0.66	1.44	2.55	26,33,42,42	0
24	CLA	C	501	65/65	0.88	1.01	2.54	29,32,44,46	0
29	LHG	A	615	42/49	0.63	1.14	2.51	69,83,86,86	0
24	CLA	A	607	65/65	0.79	0.85	2.51	19,21,63,65	0
24	CLA	b	616	65/65	0.80	1.17	2.47	27,30,45,46	0
24	CLA	B	610	65/65	0.90	0.84	2.46	23,28,31,32	0
24	CLA	C	508	65/65	0.82	0.71	2.40	25,29,54,58	0
24	CLA	B	604	65/65	0.89	0.87	2.39	18,22,31,35	0
24	CLA	C	511	65/65	0.93	0.93	2.38	29,34,37,38	0
24	CLA	c	911	65/65	0.92	0.66	2.38	26,30,39,40	0
24	CLA	c	903	65/65	0.77	0.82	2.27	25,28,42,45	0
24	CLA	c	904	65/65	0.84	0.86	2.25	26,37,39,40	0
24	CLA	C	510	65/65	0.90	0.69	2.25	24,28,35,37	0
28	SQD	A	612	54/54	0.65	0.83	2.17	49,57,66,67	0
24	CLA	c	909	65/65	0.90	0.59	2.14	27,29,57,60	0
26	BCR	B	620	40/40	0.59	0.55	2.09	27,33,39,39	0
24	CLA	c	912	65/65	0.87	0.78	2.05	32,37,43,44	0
24	CLA	a	407	65/65	0.63	0.75	2.00	19,23,63,65	0
24	CLA	B	609	65/65	0.85	0.92	1.92	20,24,31,31	0
24	CLA	b	610	65/65	0.93	0.88	1.91	28,31,33,36	0
23	BCT	a	414	4/4	0.97	0.94	1.78	34,34,35,37	0
24	CLA	b	602	65/65	0.68	1.23	1.75	38,46,68,68	0
24	CLA	B	606	65/65	0.83	0.72	1.72	19,23,34,35	0
29	LHG	d	410	49/49	0.87	0.71	1.72	28,34,66,67	0
24	CLA	b	617	65/65	0.61	0.93	1.65	27,33,74,75	0
24	CLA	b	607	65/65	0.60	0.59	1.59	26,30,41,42	0
26	BCR	b	618	40/40	0.73	0.43	1.58	24,28,39,39	0
24	CLA	B	602	65/65	0.62	0.91	1.49	32,41,66,66	0
24	CLA	C	504	65/65	0.80	0.66	1.45	25,28,54,54	0
24	CLA	A	606	65/65	0.86	0.65	1.45	15,19,25,34	0
28	SQD	d	407	43/54	0.69	1.01	1.42	84,90,93,94	0
32	HEM	E	101	43/43	0.93	0.70	1.41	39,42,45,47	0
24	CLA	b	613	65/65	0.84	0.64	1.41	21,26,33,35	0
26	BCR	h	101	40/40	0.78	1.18	1.39	29,37,45,45	0
32	HEM	V	202	43/43	0.90	0.56	1.38	23,24,27,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
28	SQD	a	411	54/54	0.72	0.51	1.35	50,60,75,76	0
24	CLA	b	611	65/65	0.91	0.75	1.29	25,28,34,37	0
24	CLA	B	605	65/65	0.91	0.50	1.26	19,22,50,51	0
24	CLA	a	406	65/65	0.77	0.52	1.23	18,20,28,33	0
31	DGD	C	518	62/66	0.85	0.52	1.20	22,31,52,56	0
32	HEM	e	101	43/43	0.92	0.42	1.19	43,46,52,55	0
32	HEM	v	202	43/43	0.93	0.61	1.18	28,31,34,36	0
24	CLA	C	513	65/65	0.70	1.16	1.16	39,45,64,64	0
27	PL9	D	405	55/55	0.70	0.55	1.16	19,23,29,32	0
28	SQD	A	613	54/54	0.76	0.50	1.14	50,63,68,68	0
25	PHO	d	402	64/64	0.85	0.50	1.10	18,22,24,25	0
24	CLA	C	505	65/65	0.93	0.76	1.02	28,30,44,45	0
26	BCR	a	409	40/40	0.53	0.48	1.02	21,26,29,29	0
24	CLA	C	502	65/65	0.90	0.67	1.01	24,26,39,42	0
25	PHO	A	608	64/64	0.79	0.54	0.98	16,21,25,26	0
24	CLA	B	616	65/65	0.78	0.62	0.96	25,27,45,46	0
29	LHG	D	408	49/49	0.80	0.52	0.90	24,28,37,40	0
24	CLA	C	506	65/65	0.88	0.81	0.90	31,38,74,75	0
31	DGD	j	101	62/66	0.90	0.43	0.89	25,34,52,55	0
24	CLA	c	905	65/65	0.89	0.56	0.88	28,30,55,56	0
24	CLA	C	503	65/65	0.88	0.66	0.85	27,31,35,36	0
24	CLA	B	617	65/65	0.74	0.46	0.82	22,29,77,78	0
31	DGD	C	516	62/66	0.90	0.44	0.75	23,33,61,62	0
24	CLA	B	612	65/65	0.85	0.46	0.70	19,21,32,34	0
24	CLA	A	614	65/65	0.84	0.49	0.69	14,18,29,35	0
24	CLA	b	612	65/65	0.76	0.47	0.66	20,23,37,41	0
24	CLA	B	607	65/65	0.72	0.55	0.60	24,28,40,41	0
31	DGD	C	517	62/66	0.78	0.46	0.37	23,35,62,63	0
31	DGD	c	916	62/66	0.86	0.48	0.36	24,35,60,61	0
26	BCR	T	101	40/40	0.67	0.44	0.21	25,37,44,45	0
28	SQD	a	402	54/54	0.78	0.40	0.19	51,67,75,76	0
31	DGD	c	917	62/66	0.82	0.42	0.17	28,36,64,65	0
30	CA	c	901	1/1	0.57	0.44	0.15	46,46,46,46	0
26	BCR	T	102	40/40	0.75	0.41	0.10	25,29,31,31	0
24	CLA	b	608	65/65	0.74	0.46	0.05	19,23,30,32	0
24	CLA	b	614	65/65	0.82	0.38	0.04	21,24,44,45	0
24	CLA	d	401	65/65	0.84	0.46	0.03	17,20,27,31	0
22	CL	A	603	1/1	0.79	0.42	-0.02	24,24,24,24	0
29	LHG	d	409	49/49	0.84	0.34	-0.03	23,27,38,40	0
27	PL9	d	405	55/55	0.75	0.41	-0.07	19,25,29,31	0
28	SQD	l	101	54/54	0.72	0.41	-0.07	57,69,84,85	0
23	BCT	A	605	4/4	0.96	0.46	-0.08	39,39,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
20	OEX	a	401	10/10	0.95	0.35	-0.23	25,27,28,28	0
28	SQD	L	101	54/54	0.78	0.38	-0.25	58,66,80,80	0
29	LHG	D	407	49/49	0.74	0.40	-0.36	29,34,41,41	0
29	LHG	b	620	49/49	0.85	0.33	-0.46	24,31,46,50	0
29	LHG	d	408	49/49	0.80	0.40	-0.46	29,37,41,42	0
33	MG	j	102	1/1	0.59	0.20	-0.47	34,34,34,34	0
24	CLA	B	608	65/65	0.75	0.41	-0.49	17,20,32,34	0
26	BCR	B	618	40/40	0.67	0.36	-0.50	23,27,28,29	0
24	CLA	B	615	65/65	0.78	0.40	-0.61	20,24,60,61	0
30	CA	O	301	1/1	0.88	0.19	-0.69	49,49,49,49	0
20	OEX	A	601	10/10	0.93	0.35	-0.70	22,23,26,26	0
26	BCR	B	622	40/40	0.62	0.40	-0.72	23,34,41,41	0
22	CL	A	604	1/1	0.91	0.32	-0.74	21,21,21,21	0
24	CLA	B	614	65/65	0.92	0.33	-0.76	19,22,45,47	0
29	LHG	B	621	49/49	0.90	0.31	-0.78	23,31,43,44	0
24	CLA	b	615	65/65	0.78	0.35	-0.93	22,26,65,66	0
22	CL	a	405	1/1	0.94	0.20	-1.55	26,26,26,26	0
26	BCR	B	619	40/40	0.78	0.31	-2.35	21,28,40,40	0
30	CA	o	301	1/1	0.95	0.09	-2.35	51,51,51,51	0
21	FE2	A	602	1/1	0.99	0.11	-2.56	26,26,26,26	0
30	CA	F	102	1/1	0.56	0.46	-	56,56,56,56	0
30	CA	f	102	1/1	0.20	0.38	-	58,58,58,58	0
22	CL	v	201	1/1	0.48	0.38	-	60,60,60,60	0
30	CA	B	601	1/1	0.53	0.72	-	76,76,76,76	0
30	CA	b	601	1/1	0.36	1.06	-	77,77,77,77	0
22	CL	V	201	1/1	0.69	0.15	-	50,50,50,50	0
21	FE2	a	403	1/1	0.94	0.20	-	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.