Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:47 PM GMT

PDB ID	:	4TNK
Title	:	RT XFEL structure of Photosystem II 250 microsec after the third illumination at 5.2 A resolution
Authors	:	Kern, J.; Tran, R.; Alonso-Mori, R.; Koroidov, S.; Echols, N.; Hattne, J.; Ibrahim, M.; Gul, S.; Laksmono, H.; Sierra, R.G.; Gildea, R.J.; Han, G.; Hellmich, J.; Lassalle-Kaiser, B.; Chatterjee, R.; Brewster, A.; Stan, C.A.; Gloeckner, C.; Lampe, A.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Seibert, M.M.; Koglin, J.E.; Gallo, E.; Uhlig, J.; Sokaras, D.; Weng, T.-C.; Zwart, P.H.; Skinner, D.E.; Bogan, M.J.; Messerschmidt, M.; Glatzel, P.; Williams, G.J.; Boutet, S.; Adams, P.D.; Zouni, A.; Messinger, J.; Sauter, N.K.; Bergmann, U.; Yano, J.; Yachandra, V.K.
Deposited on	:	2014-06-04
Resolution	:	5.20 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:

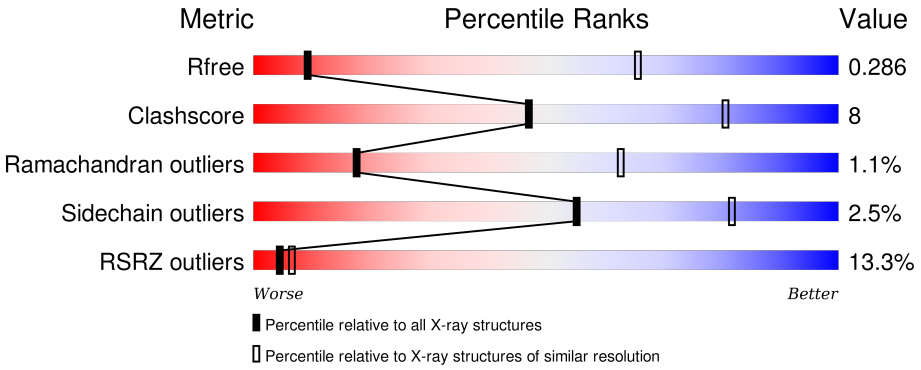
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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 5.20 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.



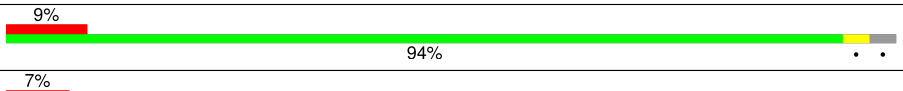
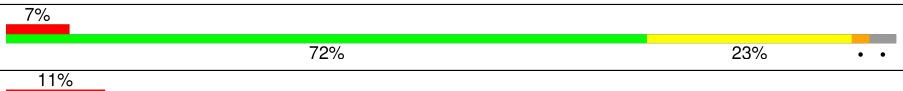
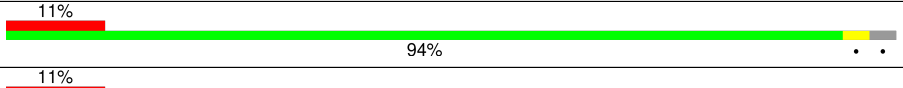
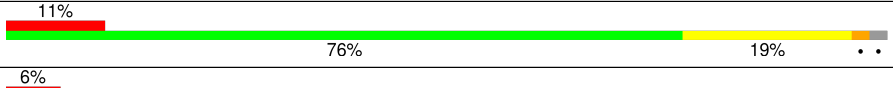
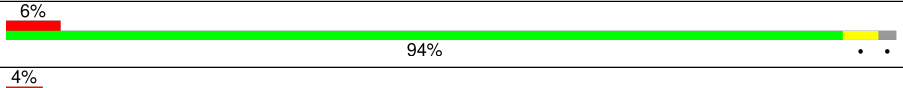
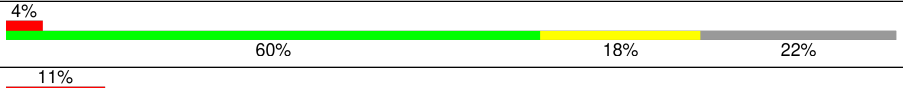
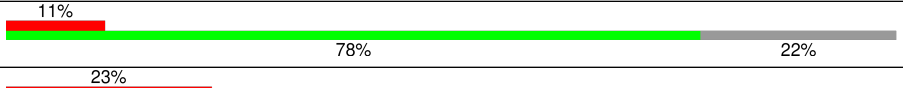
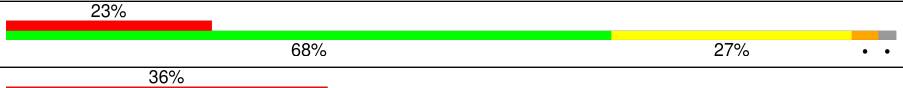
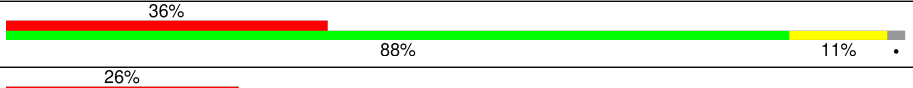
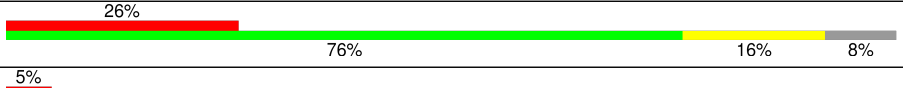
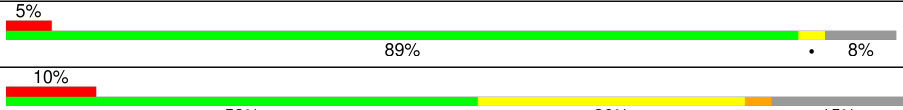
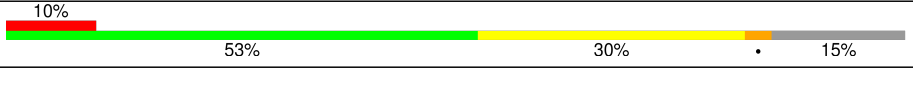
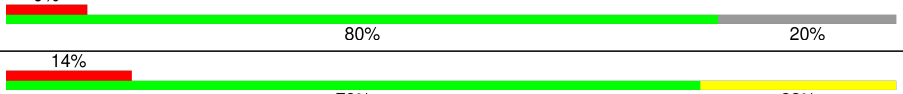
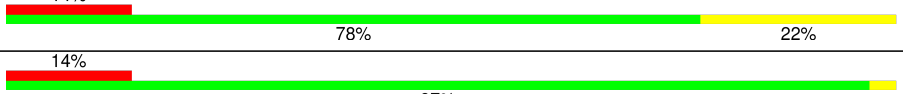
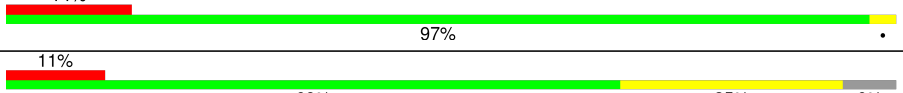
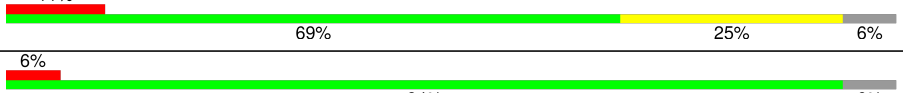
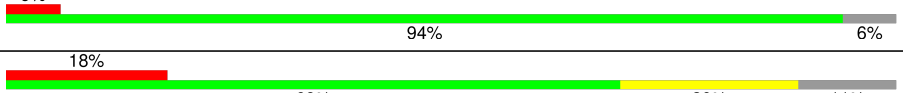
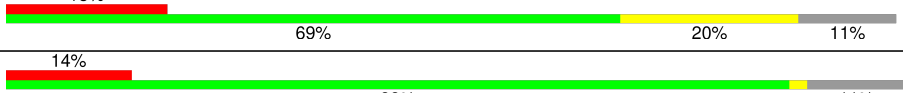
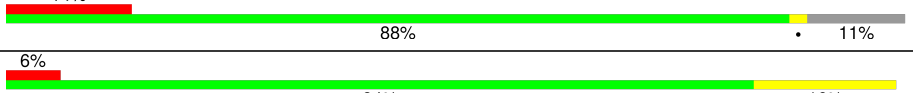
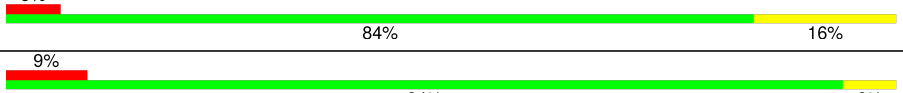
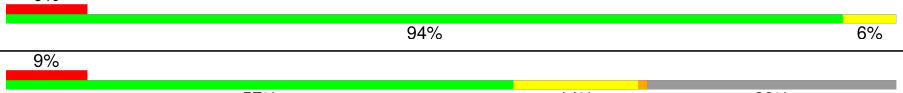
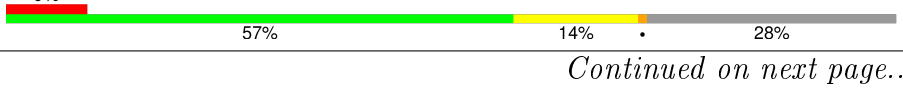
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1145 (6.80-3.60)
Clashscore	102246	1042 (6.74-3.66)
Ramachandran outliers	100387	1011 (6.76-3.62)
Sidechain outliers	100360	1158 (6.80-3.60)
RSRZ outliers	91569	1146 (6.80-3.60)

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	344	13% 70% 26%
1	a	344	20% 95%
2	B	510	10% 76% 19%
2	b	510	17% 94%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	T	32	
14	t	32	
15	U	134	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
15	u	134	16% 70% 28%
16	V	163	7% 72% 12% 16%
16	v	163	12% 83% 16%
17	g	46	4% 54% 7% 39%
17	y	46	4% 54% 7% 39%
18	X	41	17% 56% 29% 10%
18	x	41	17% 85% 5% 10%
19	G	28	100%
19	Y	28	100%
20	Z	62	2% 82% 16%
20	z	62	6% 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	CLA	A	402	X	-	-	X
22	CLA	A	403	X	-	-	X
22	CLA	A	404	X	-	-	X
22	CLA	A	406	X	-	-	X
22	CLA	B	601	X	-	-	X
22	CLA	B	602	X	-	-	X
22	CLA	B	603	X	-	-	X
22	CLA	B	604	X	-	-	X
22	CLA	B	605	X	-	-	X
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	X
22	CLA	B	608	X	-	-	X
22	CLA	B	609	X	-	-	X
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	X
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	X
22	CLA	B	614	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	615	X	-	-	X
22	CLA	C	501	X	-	-	X
22	CLA	C	502	X	-	-	X
22	CLA	C	503	X	-	-	X
22	CLA	C	504	X	-	-	X
22	CLA	C	505	X	-	-	X
22	CLA	C	506	X	-	-	X
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	X
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	X
22	CLA	C	511	X	-	-	X
22	CLA	C	512	X	-	-	X
22	CLA	C	519	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	X
22	CLA	H	101	X	-	-	X
22	CLA	a	403	X	-	-	X
22	CLA	a	404	X	-	-	X
22	CLA	a	405	X	-	-	X
22	CLA	a	406	X	-	-	X
22	CLA	b	605	X	-	-	X
22	CLA	b	606	X	-	-	X
22	CLA	b	607	X	-	-	X
22	CLA	b	608	X	-	-	X
22	CLA	b	609	X	-	-	X
22	CLA	b	610	X	-	-	X
22	CLA	b	611	X	-	-	-
22	CLA	b	612	X	-	-	X
22	CLA	b	613	X	-	-	X
22	CLA	b	614	X	-	-	X
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	X
22	CLA	b	617	X	-	-	-
22	CLA	b	618	X	-	-	-
22	CLA	b	619	X	-	-	X
22	CLA	b	620	X	-	-	X
22	CLA	c	501	X	-	-	X
22	CLA	c	502	X	-	-	X
22	CLA	c	503	X	-	-	X
22	CLA	c	504	X	-	-	X
22	CLA	c	505	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	c	506	X	-	-	X
22	CLA	c	507	X	-	-	-
22	CLA	c	508	X	-	-	X
22	CLA	c	509	X	-	-	-
22	CLA	c	510	X	-	-	X
22	CLA	c	511	X	-	-	X
22	CLA	c	512	X	-	-	X
22	CLA	c	520	X	-	-	-
22	CLA	d	405	X	-	-	X
22	CLA	d	406	X	-	-	X
23	PHO	d	401	-	-	-	X
24	PL9	A	407	-	-	-	X
24	PL9	D	405	-	-	-	X
24	PL9	J	101	-	-	-	X
24	PL9	a	407	-	-	-	X
24	PL9	d	407	-	-	-	X
24	PL9	j	101	-	-	-	X
25	BCR	A	408	-	-	-	X
25	BCR	B	616	-	-	-	X
25	BCR	B	619	-	-	-	X
25	BCR	C	513	-	-	-	X
25	BCR	C	520	-	-	-	X
25	BCR	F	102	-	-	-	X
25	BCR	H	102	-	-	-	X
25	BCR	K	101	-	-	-	X
25	BCR	b	624	-	-	-	X
25	BCR	c	513	-	-	-	X
25	BCR	c	514	-	-	-	X
25	BCR	c	521	-	-	-	X
25	BCR	g	101	-	-	-	X
25	BCR	i	101	-	-	-	X
25	BCR	x	101	-	-	-	X
25	BCR	y	101	-	-	-	X
26	DGD	A	409	-	-	-	X
26	DGD	B	626	-	-	-	X
26	DGD	C	516	-	-	-	X
26	DGD	D	407	-	-	-	X
26	DGD	a	408	-	-	-	X
26	DGD	b	601	-	-	-	X
26	DGD	d	410	-	-	-	X
28	CL	A	411	-	-	-	X
28	CL	a	410	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	OEX	A	412	-	-	-	X
29	OEX	a	411	-	-	-	X
30	SQD	A	414	-	-	-	X
30	SQD	B	622	-	-	-	X
30	SQD	B	627	-	-	-	X
30	SQD	F	103	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	b	602	-	-	-	X
30	SQD	d	403	-	-	-	X
30	SQD	f	103	-	-	-	X
31	LMG	C	517	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	b	627	-	-	-	X
31	LMG	c	518	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	m	101	-	-	-	X
32	LMT	B	624	-	-	-	X
32	LMT	B	628	-	-	-	X
32	LMT	D	408	-	-	-	X
32	LMT	I	102	-	-	-	X
32	LMT	M	102	-	-	-	X
32	LMT	b	603	-	-	-	X
32	LMT	b	629	-	-	-	X
32	LMT	d	411	-	-	-	X
32	LMT	i	103	-	-	-	X
33	BCT	d	404	-	-	-	X
34	HEM	F	101	-	-	-	X
34	HEM	V	201	-	-	-	X
34	HEM	f	101	-	-	-	X
34	HEM	v	201	-	-	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 50244 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	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			
1	a	335	Total	C	N	O	S	0	0	0
			2628	1720	432	461	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			
2	b	490	Total	C	N	O	S	0	0	0
			3850	2528	641	668	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			
3	c	447	Total	C	N	O	S	0	0	0
			3444	2256	576	599	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			
4	d	340	Total	C	N	O	S	0	0	0
			2706	1794	440	460	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			666	434	108	124			
5	e	82	Total	C	N	O	0	0	0
			666	434	108	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			282	192	46	43	1			
6	f	35	Total	C	N	O	S	0	0	0
			282	192	46	43	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
			507	338	81	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			507	338	81	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			249	170	38	40	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	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
			1845	1154	308	379	4			
13	o	243	Total	C	N	O	S	0	0	0
			1845	1154	308	379	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	32	Total	C	N	O	S	0	0	0
			275	192	40	41	2			
14	t	32	Total	C	N	O	S	0	0	0
			275	192	40	41	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
			1060	673	177	206	4			
16	v	137	Total	C	N	O	S	0	0	0
			1060	673	177	206	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	y	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			
17	g	28	Total	C	N	O	S	0	0	0
			201	134	33	31	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	37	Total	C	N	O	0	0	0
			270	182	41	47			
18	x	37	Total	C	N	O	0	0	0
			270	182	41	47			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Y	28	Total	C	N	O	0	0	0
			140	84	28	28			
19	G	28	Total	C	N	O	0	0	0
			140	84	28	28			

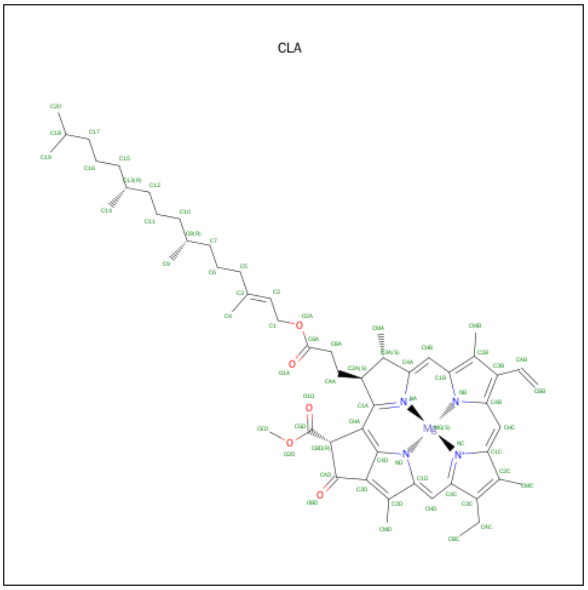
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

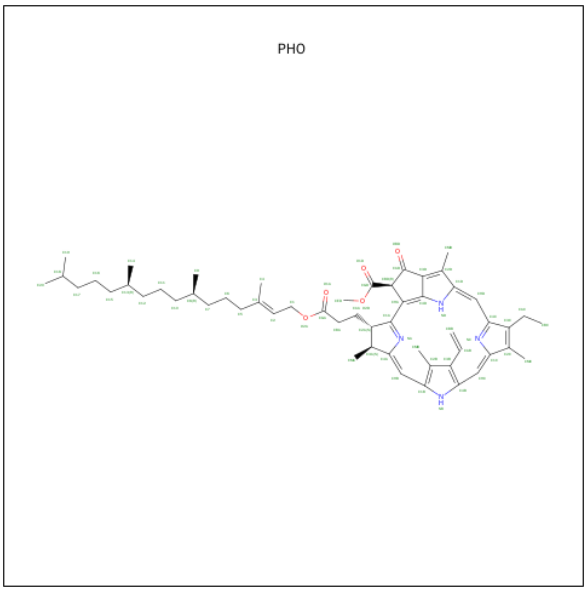
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	C	1	Total C Mg N O 65 55 1 4 5	0	0
22	D	1	Total C Mg N O 65 55 1 4 5	0	0
22	D	1	Total C Mg N O 65 55 1 4 5	0	0
22	H	1	Total C Mg N O 65 55 1 4 5	0	0
22	a	1	Total C Mg N O 65 55 1 4 5	0	0
22	a	1	Total C Mg N O 65 55 1 4 5	0	0
22	a	1	Total C Mg N O 65 55 1 4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

Continued on next page...

Continued from previous page...

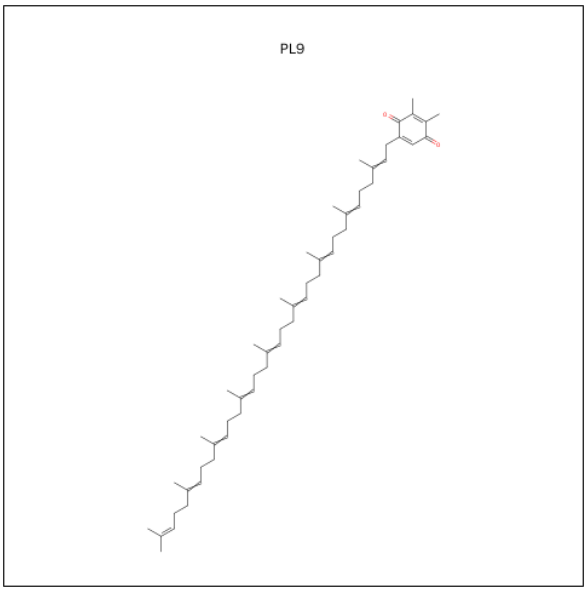
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	b	1	Total C Mg N O 65 55 1 4 5	0	0
22	b	1	Total C Mg N O 65 55 1 4 5	0	0
22	b	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4 5	0	0
22	c	1	Total C Mg N O 65 55 1 4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

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



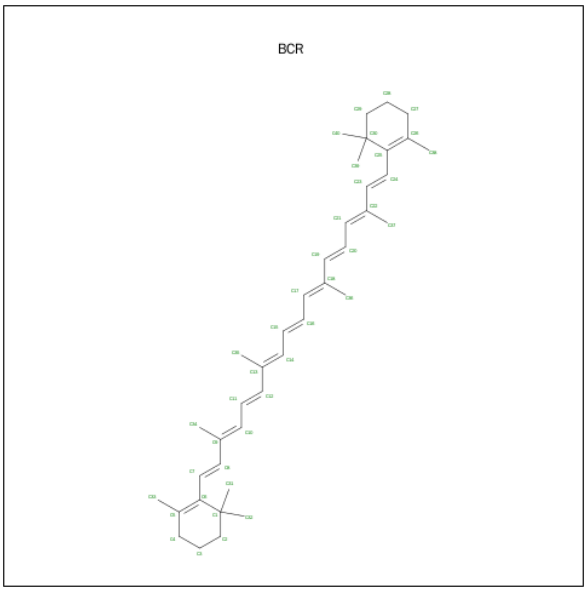
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		
23	d	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 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
24	A	1	Total C O 45 43 2	0	0
24	D	1	Total C O 55 53 2	0	0
24	J	1	Total C O 35 33 2	0	0
24	a	1	Total C O 45 43 2	0	0
24	d	1	Total C O 55 53 2	0	0
24	j	1	Total C O 35 33 2	0	0

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



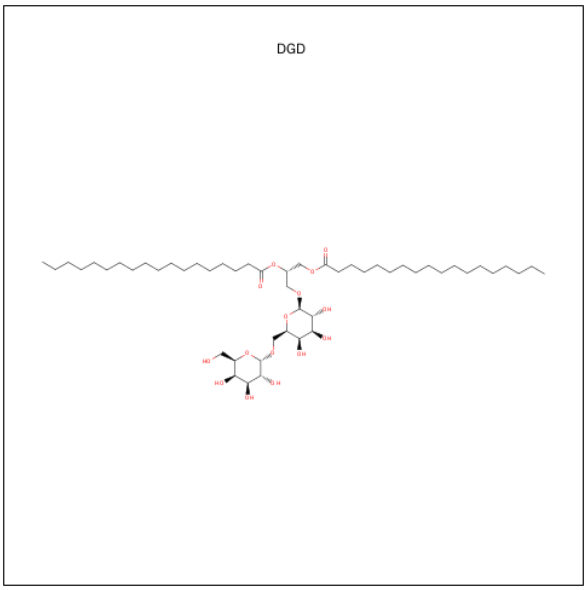
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	F	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	J	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	y	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	f	1	Total C 40 40	0	0
25	i	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	g	1	Total C 40 40	0	0
25	x	1	Total C 40 40	0	0

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



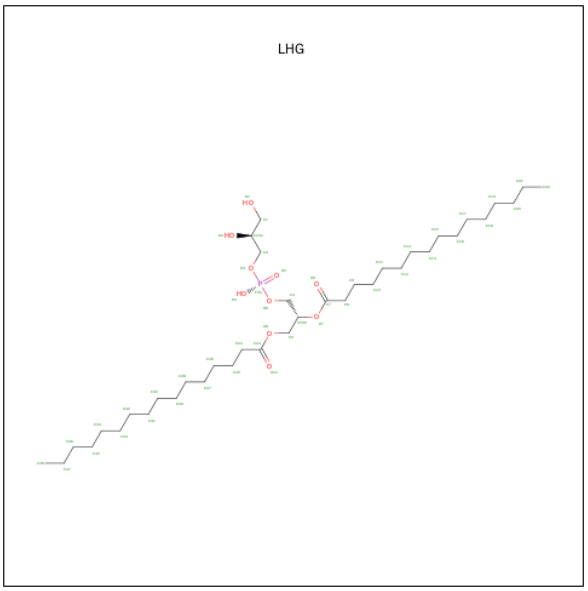
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O 56 41 15	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	B	1	Total C O 58 43 15	0	0
26	B	1	Total C O 52 37 15	0	0
26	C	1	Total C O 53 38 15	0	0
26	C	1	Total C O 62 47 15	0	0
26	C	1	Total C O 66 51 15	0	0
26	D	1	Total C O 63 48 15	0	0
26	a	1	Total C O 56 41 15	0	0
26	b	1	Total C O 52 37 15	0	0
26	b	1	Total C O 58 43 15	0	0
26	c	1	Total C O 53 38 15	0	0
26	c	1	Total C O 62 47 15	0	0
26	c	1	Total C O 66 51 15	0	0
26	d	1	Total C O 63 48 15	0	0

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).

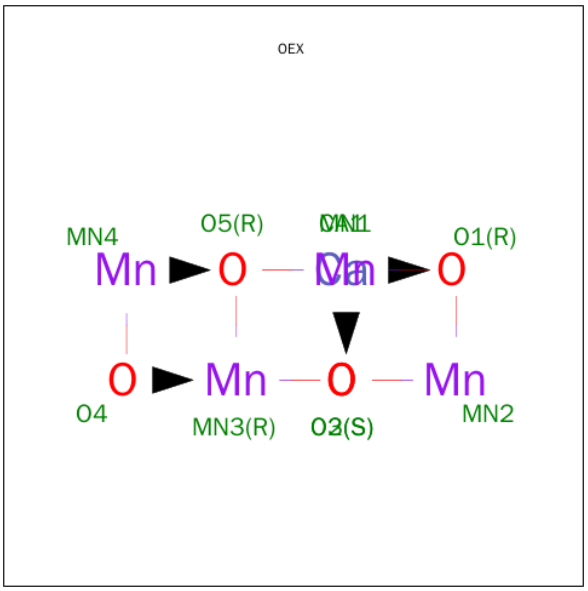


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			39	28	10	1		
27	C	1	Total	C	O	P	0	0
			37	26	10	1		
27	a	1	Total	C	O	P	0	0
			39	28	10	1		
27	c	1	Total	C	O	P	0	0
			37	26	10	1		

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

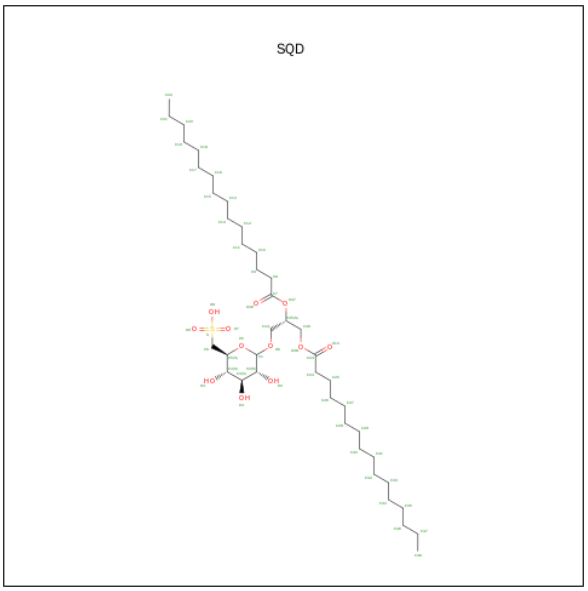
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	1	Total	Cl	0	0
			1	1		
28	a	1	Total	Cl	0	0
			1	1		

- Molecule 29 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: $CaMn_4O_5$).



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

- Molecule 30 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



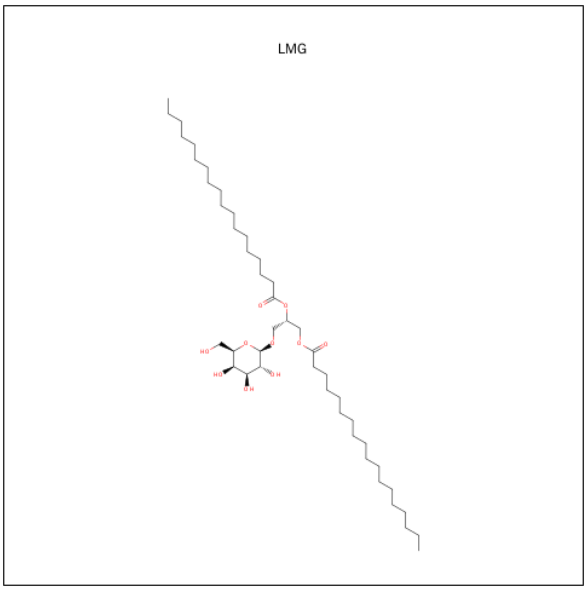
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			51	38	12	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	O	S	0	0
			54	41	12	1		
30	B	1	Total	C	O	S	0	0
			43	30	12	1		
30	B	1	Total	C	O	S	0	0
			47	34	12	1		
30	F	1	Total	C	O	S	0	0
			45	32	12	1		
30	a	1	Total	C	O	S	0	0
			54	41	12	1		
30	a	1	Total	C	O	S	0	0
			51	38	12	1		
30	b	1	Total	C	O	S	0	0
			47	34	12	1		
30	d	1	Total	C	O	S	0	0
			43	30	12	1		
30	f	1	Total	C	O	S	0	0
			45	32	12	1		

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



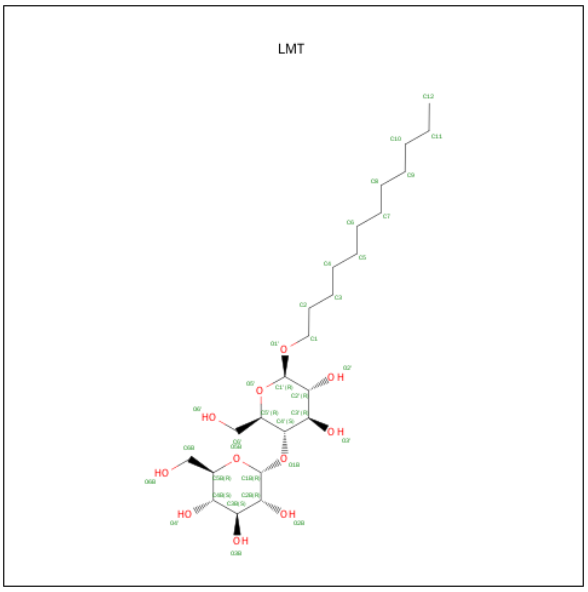
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		

Continued on next page...

Continued from previous page...

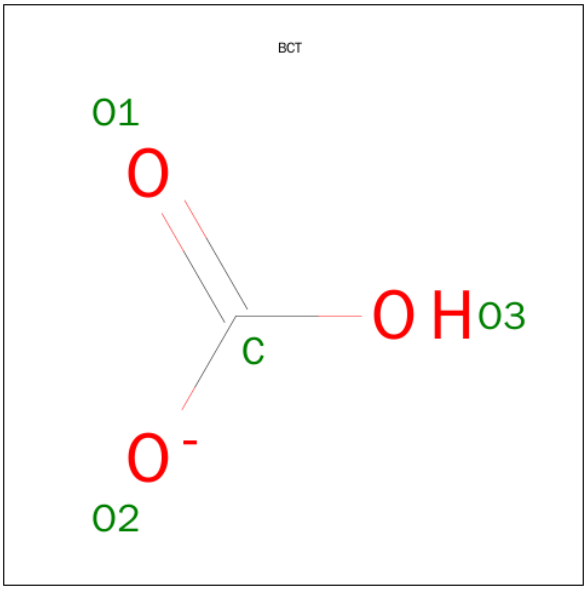
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	C	1	Total C O 45 35 10	0	0
31	C	1	Total C O 48 38 10	0	0
31	D	1	Total C O 48 38 10	0	0
31	D	1	Total C O 46 36 10	0	0
31	E	1	Total C O 44 34 10	0	0
31	I	1	Total C O 43 33 10	0	0
31	L	1	Total C O 51 41 10	0	0
31	M	1	Total C O 42 32 10	0	0
31	a	1	Total C O 42 32 10	0	0
31	b	1	Total C O 49 39 10	0	0
31	b	1	Total C O 42 32 10	0	0
31	c	1	Total C O 45 35 10	0	0
31	c	1	Total C O 48 38 10	0	0
31	d	1	Total C O 49 39 10	0	0
31	d	1	Total C O 48 38 10	0	0
31	d	1	Total C O 46 36 10	0	0
31	e	1	Total C O 44 34 10	0	0
31	i	1	Total C O 43 33 10	0	0
31	l	1	Total C O 51 41 10	0	0
31	m	1	Total C O 42 32 10	0	0

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



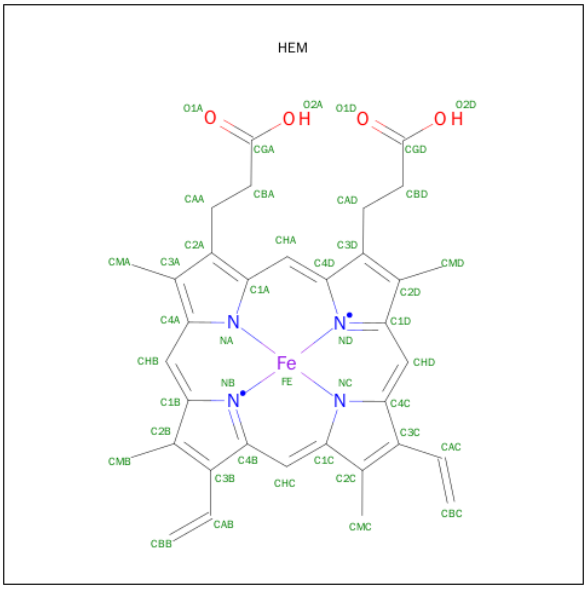
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	D	1	Total	C	O	0	0
			31	20	11		
32	I	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	b	1	Total	C	O	0	0
			35	24	11		
32	d	1	Total	C	O	0	0
			31	20	11		
32	i	1	Total	C	O	0	0
			35	24	11		

- Molecule 33 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	D	1	Total C O 4 1 3	0	0
33	d	1	Total C O 4 1 3	0	0

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



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

- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

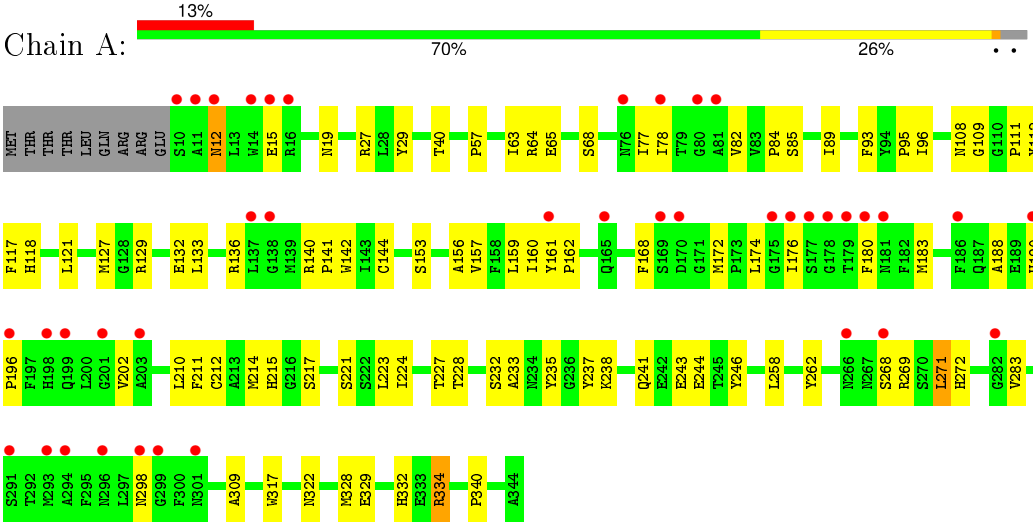
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	o	1	Total	Ca	0	0
			1	1		
35	O	1	Total	Ca	0	0
			1	1		
35	K	1	Total	Ca	0	0
			1	1		
35	k	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

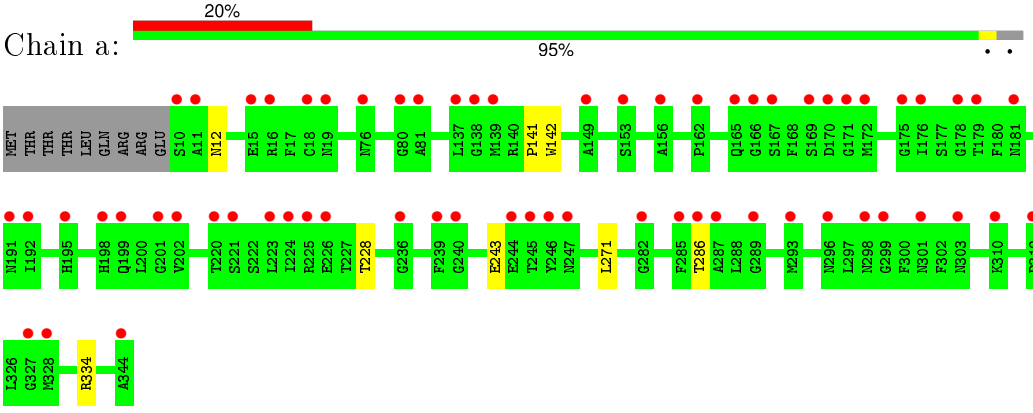
- Molecule 1: Photosystem Q(B) protein 1

Chain A:



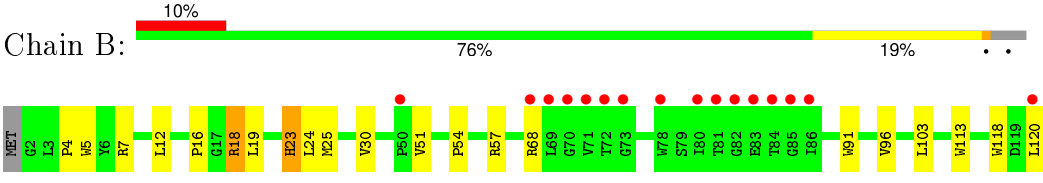
- Molecule 1: Photosystem Q(B) protein 1

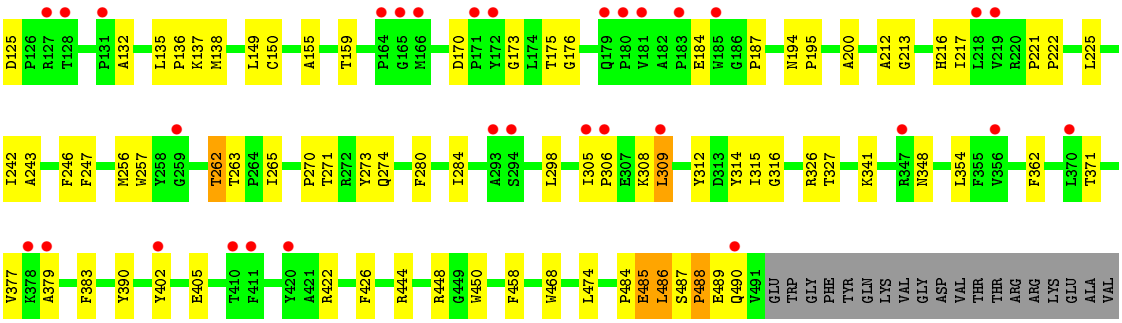
Chain a:



- Molecule 2: Photosystem II core light harvesting protein

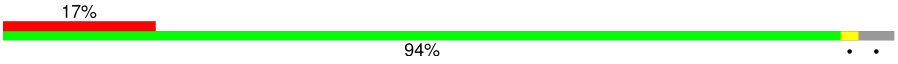
Chain B:

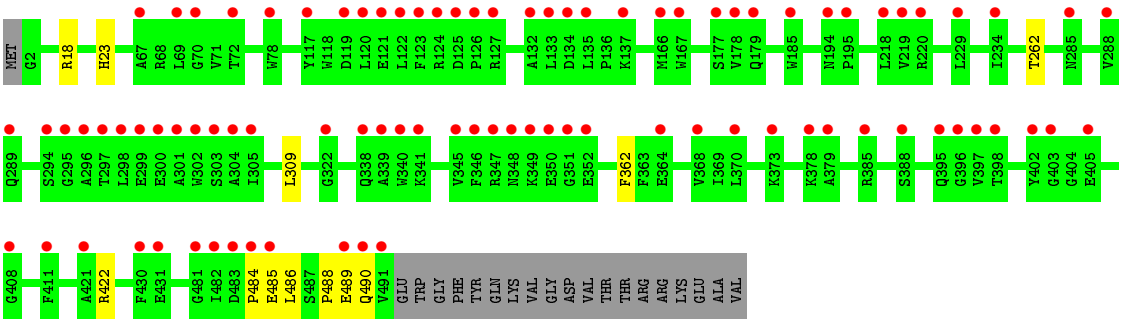




• Molecule 2: Photosystem II core light harvesting protein

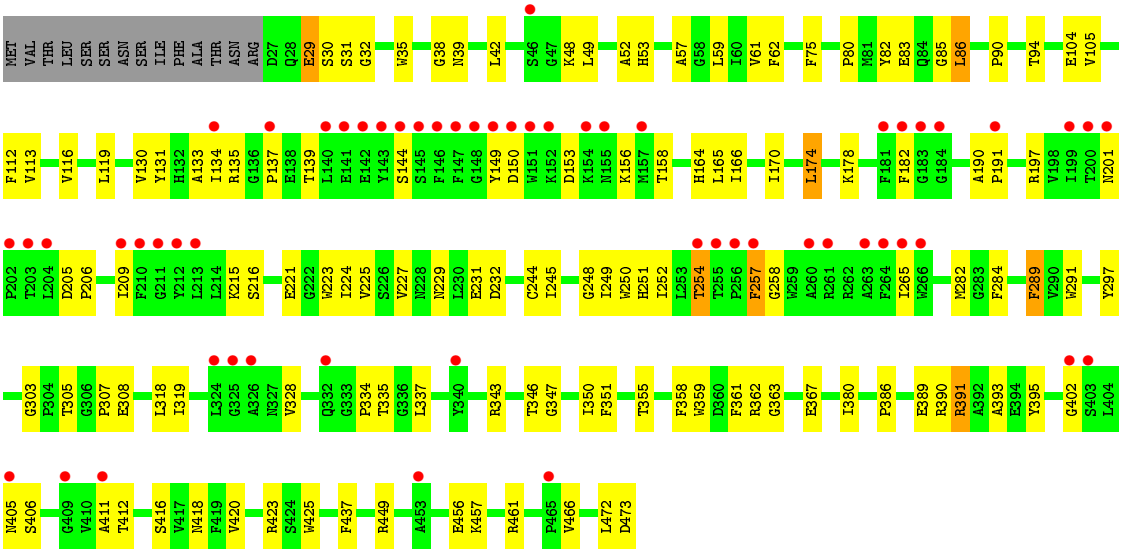
Chain b:





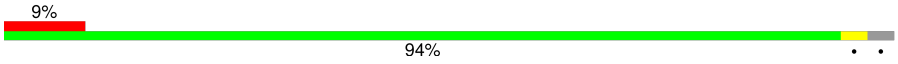
• Molecule 3: Photosystem II CP43 protein

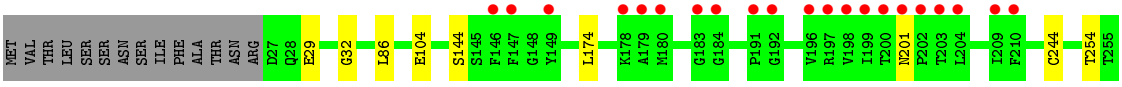
Chain C:

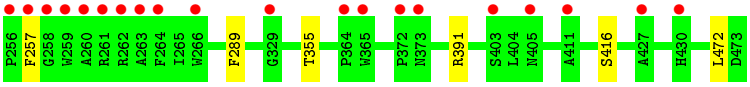


• Molecule 3: Photosystem II CP43 protein

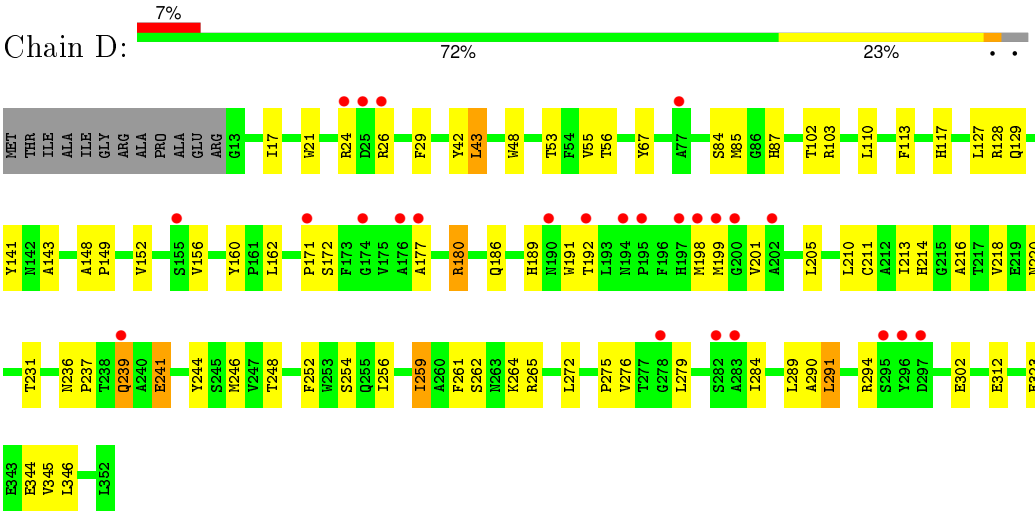
Chain c:



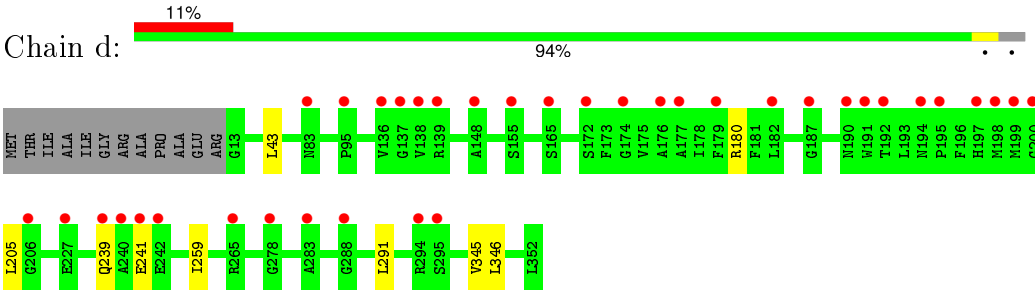




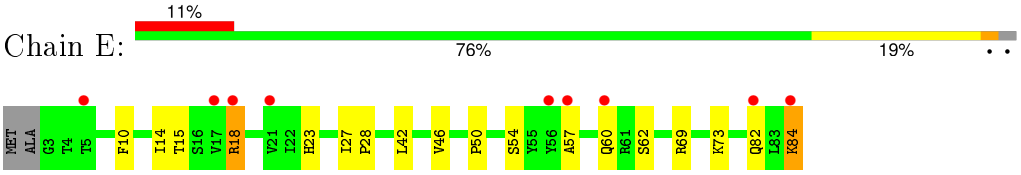
• Molecule 4: Photosystem II D2 protein



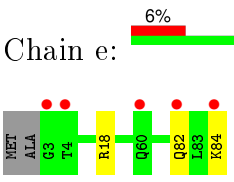
• Molecule 4: Photosystem II D2 protein



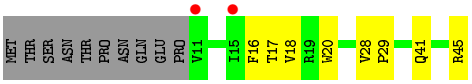
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 5: Cytochrome b559 subunit alpha

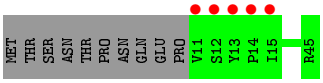


• Molecule 6: Cytochrome b559 subunit beta



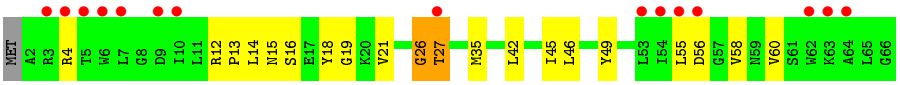
• Molecule 6: Cytochrome b559 subunit beta

Chain f:



• Molecule 7: Photosystem II reaction center protein H

Chain H:

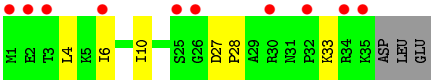


• Molecule 7: Photosystem II reaction center protein H

Chain h:

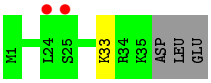
• Molecule 8: Photosystem II reaction center protein I

Chain I:



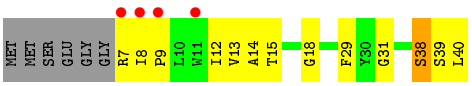
• Molecule 8: Photosystem II reaction center protein I

Chain i:



• Molecule 9: Photosystem II reaction center protein J

Chain J:

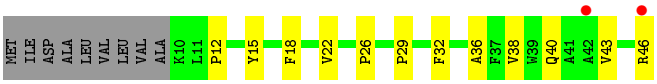


• Molecule 9: Photosystem II reaction center protein J

Chain j:

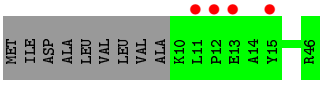
• Molecule 10: Photosystem II reaction center protein K

Chain K:



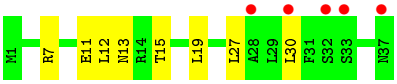
• Molecule 10: Photosystem II reaction center protein K

Chain k:



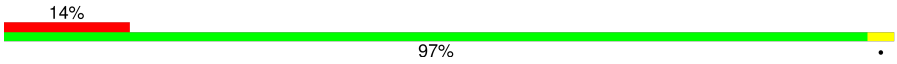
• Molecule 11: Photosystem II reaction center protein L

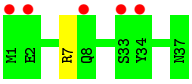
Chain L:



• Molecule 11: Photosystem II reaction center protein L

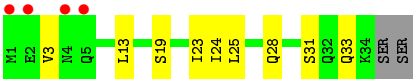
Chain l:





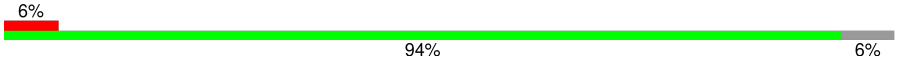
• Molecule 12: Photosystem II reaction center protein M

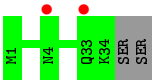
Chain M:



• Molecule 12: Photosystem II reaction center protein M

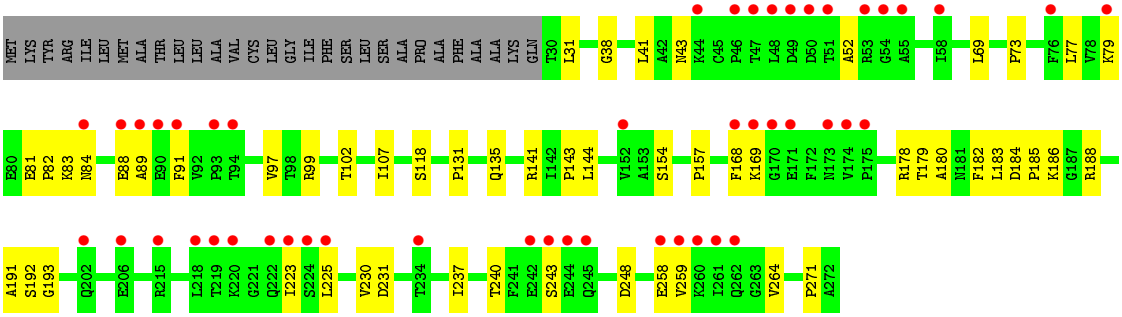
Chain m:



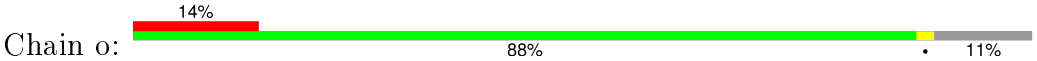


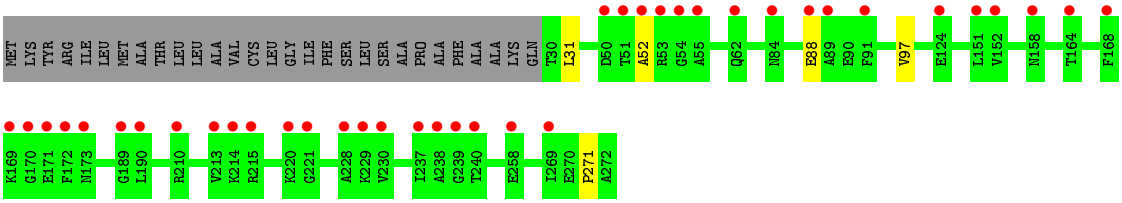
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

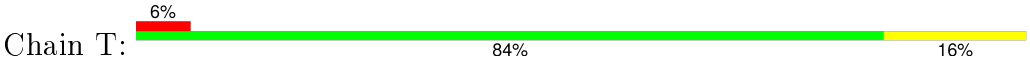


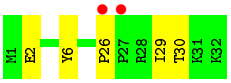
• Molecule 13: Photosystem II manganese-stabilizing polypeptide



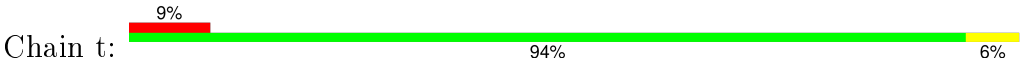


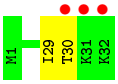
• Molecule 14: Photosystem II reaction center protein T



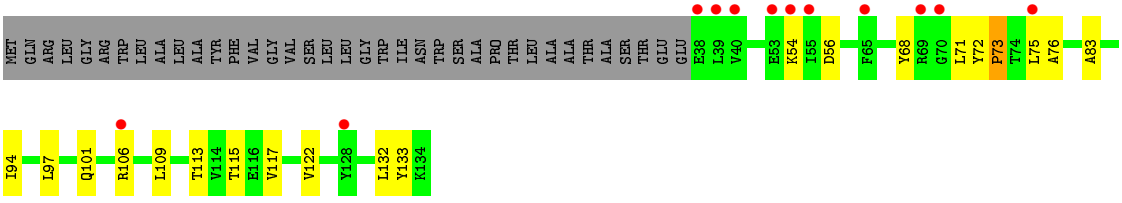


• Molecule 14: Photosystem II reaction center protein T

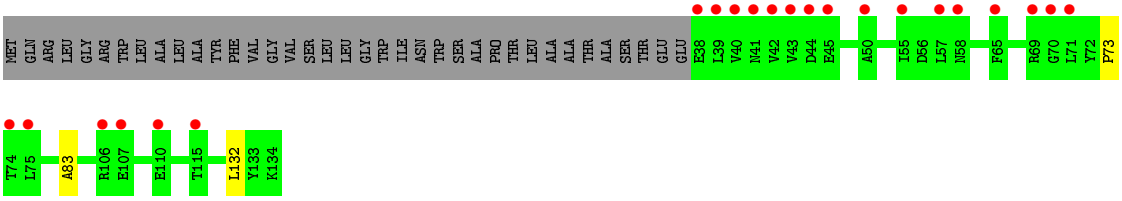




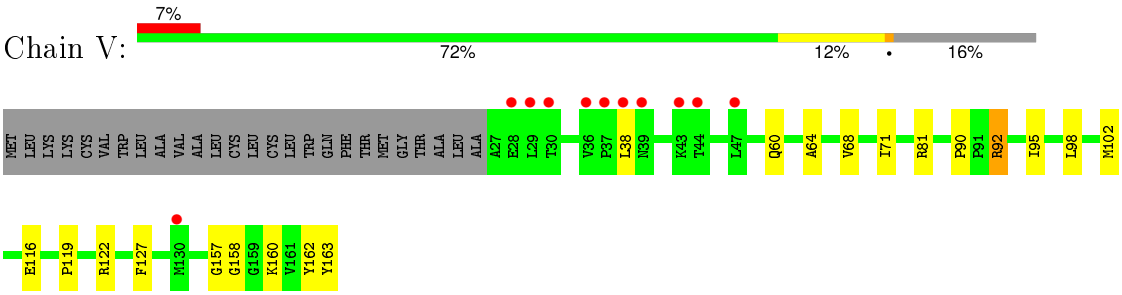
• Molecule 15: Photosystem II 12 kDa extrinsic protein



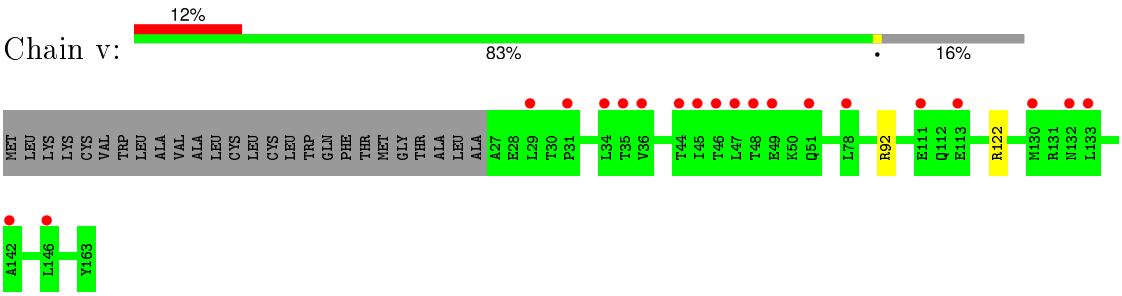
• Molecule 15: Photosystem II 12 kDa extrinsic protein



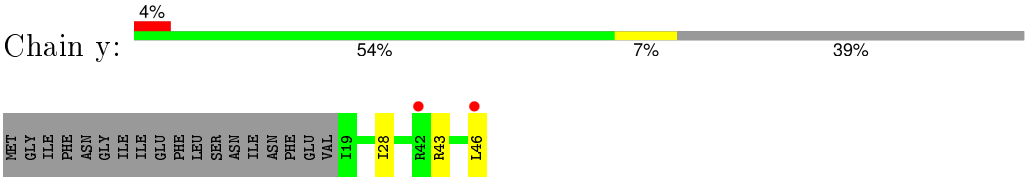
• Molecule 16: Cytochrome c-550



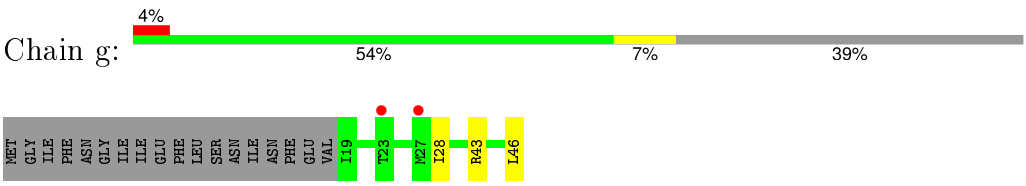
• Molecule 16: Cytochrome c-550



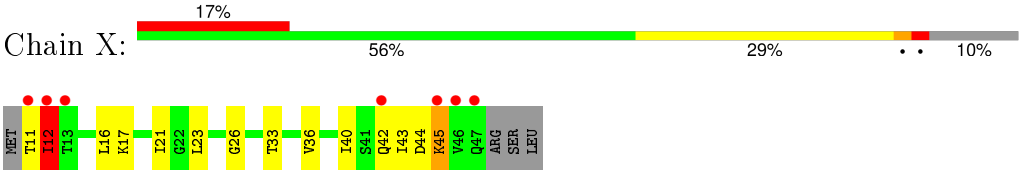
• Molecule 17: Photosystem II reaction center protein Ycf12



• Molecule 17: Photosystem II reaction center protein Ycf12

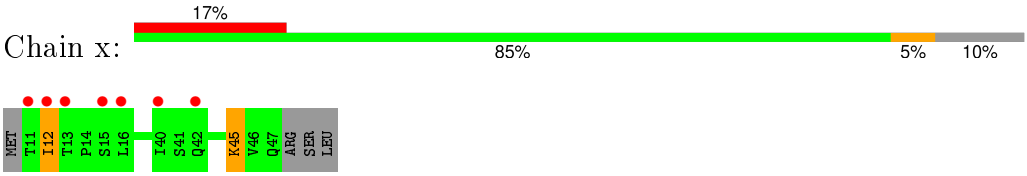


• Molecule 18: Photosystem II reaction center X protein



• Molecule 18: Photosystem II reaction center X protein

Chain x:



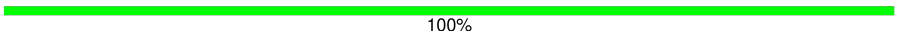
• Molecule 19: Photosystem II reaction center protein Y

Chain Y:

There are no outlier residues recorded for this chain.

• Molecule 19: Photosystem II reaction center protein Y

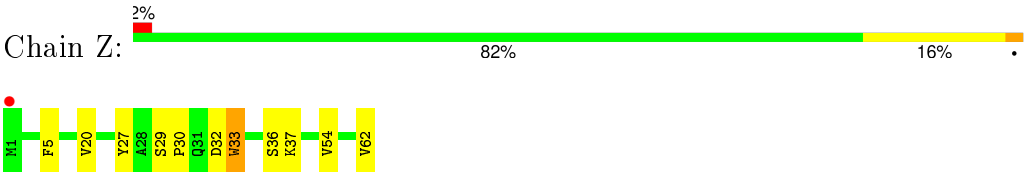
Chain G:



There are no outlier residues recorded for this chain.

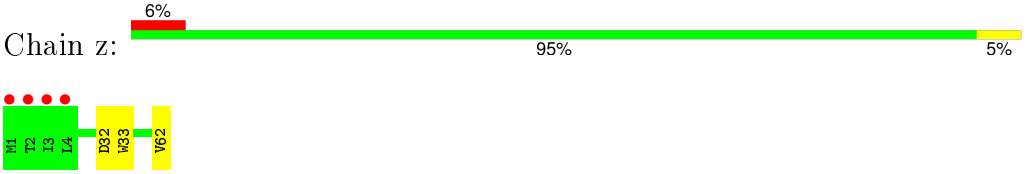
• Molecule 20: Photosystem II reaction center protein Z

Chain Z:



• Molecule 20: 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	132.62Å 229.30Å 306.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.41 – 5.20 68.41 – 5.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (68.41-5.20) 97.9 (68.41-5.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 5.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1635+SVN)	Depositor
R, R_{free}	0.271 , 0.289 0.286 , 0.286	Depositor DCC
R_{free} test set	1753 reflections (5.12%)	DCC
Wilson B-factor (Å^2)	176.5	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 157.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.33$, $< L^2 > = 0.15$	Xtriage
Outliers	0 of 35970 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	50244	wwPDB-VP
Average B, all atoms (Å^2)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, FE2, BCT, HEM, SQD, BCR, LMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.25	0/2713	0.42	0/3700
1	a	0.24	0/2713	0.42	0/3700
2	B	0.24	0/3986	0.41	0/5433
2	b	0.24	0/3986	0.41	0/5433
3	C	0.23	0/3556	0.42	0/4842
3	c	0.23	0/3556	0.42	0/4842
4	D	0.24	0/2801	0.41	0/3818
4	d	0.24	0/2801	0.41	0/3818
5	E	0.23	0/685	0.44	0/933
5	e	0.23	0/685	0.43	0/933
6	F	0.23	0/291	0.40	0/397
6	f	0.23	0/291	0.41	0/397
7	H	0.24	0/520	0.46	0/709
7	h	0.23	0/520	0.46	0/709
8	I	0.25	0/293	0.44	0/395
8	i	0.26	0/293	0.44	0/395
9	J	0.21	0/255	0.41	0/346
9	j	0.22	0/255	0.40	0/346
10	K	0.27	0/303	0.49	0/416
10	k	0.27	0/303	0.49	0/416
11	L	0.23	0/311	0.40	0/422
11	l	0.22	0/311	0.40	0/422
12	M	0.24	0/270	0.44	0/367
12	m	0.24	0/270	0.44	0/367
13	O	0.23	0/1876	0.44	0/2548
13	o	0.23	0/1876	0.44	0/2548
14	T	0.25	0/284	0.41	0/381
14	t	0.25	0/284	0.40	0/381
15	U	0.23	0/785	0.43	0/1064
15	u	0.23	0/785	0.44	0/1064
16	V	0.22	0/1081	0.42	0/1468
16	v	0.22	0/1081	0.41	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	g	0.22	0/202	0.46	0/272
17	y	0.23	0/202	0.46	0/272
18	X	0.27	0/273	0.44	0/370
18	x	0.26	0/273	0.45	0/370
20	Z	0.25	0/490	0.45	0/669
20	z	0.24	0/490	0.45	0/669
All	All	0.24	0/41950	0.42	0/57100

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	2628	0	2524	82	0
1	a	2628	0	2524	0	0
2	B	3850	0	3718	90	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	100	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	83	0
4	d	2706	0	2608	0	0
5	E	666	0	651	16	0
5	e	666	0	651	0	0
6	F	282	0	291	8	0
6	f	282	0	291	0	0
7	H	507	0	521	22	0
7	h	507	0	521	0	0
8	I	286	0	308	4	0
8	i	286	0	308	0	0
9	J	249	0	262	10	0
9	j	249	0	262	0	0
10	K	293	0	305	10	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	9	0
11	l	304	0	316	0	0
12	M	267	0	289	8	0
12	m	267	0	289	0	0
13	O	1845	0	1801	34	0
13	o	1845	0	1801	0	0
14	T	275	0	288	3	0
14	t	275	0	288	0	0
15	U	774	0	773	10	0
15	u	774	0	773	0	0
16	V	1060	0	1068	12	0
16	v	1060	0	1068	0	0
17	g	201	0	226	0	0
17	y	201	0	226	0	0
18	X	270	0	299	10	0
18	x	270	0	299	0	0
19	G	140	0	31	0	0
19	Y	140	0	31	0	0
20	Z	479	0	516	9	0
20	z	479	0	516	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	260	0	288	42	0
22	B	975	0	1080	103	0
22	C	845	0	936	45	0
22	D	130	0	144	13	0
22	H	65	0	72	11	0
22	a	260	0	288	0	0
22	b	1040	0	1152	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
23	A	64	0	74	6	0
23	D	64	0	74	12	0
23	d	128	0	148	0	0
24	A	45	0	61	6	0
24	D	55	0	80	10	0
24	J	35	0	45	0	0
24	a	45	0	61	0	0
24	d	55	0	80	0	0
24	j	35	0	45	0	0
25	A	40	0	56	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	160	0	224	13	0
25	C	80	0	112	15	0
25	F	40	0	56	3	0
25	H	40	0	56	2	0
25	J	40	0	56	3	0
25	K	40	0	56	3	0
25	b	160	0	224	0	0
25	c	120	0	168	0	0
25	f	40	0	56	0	0
25	g	40	0	56	0	0
25	i	40	0	56	0	0
25	j	40	0	56	0	0
25	x	40	0	56	0	0
25	y	40	0	56	0	0
26	A	56	0	70	1	0
26	B	110	0	136	4	0
26	C	181	0	245	18	0
26	D	63	0	87	2	0
26	a	56	0	70	0	0
26	b	110	0	136	0	0
26	c	181	0	245	0	0
26	d	63	0	87	0	0
27	A	39	0	51	2	0
27	C	37	0	44	3	0
27	a	39	0	51	0	0
27	c	37	0	44	0	0
28	A	1	0	0	0	0
28	a	1	0	0	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	105	0	147	6	0
30	B	90	0	111	3	0
30	F	45	0	54	3	0
30	a	105	0	147	0	0
30	b	47	0	61	0	0
30	d	43	0	50	0	0
30	f	45	0	54	0	0
31	B	98	0	136	6	0
31	C	93	0	126	3	0
31	D	94	0	128	15	0
31	E	44	0	58	2	0
31	I	43	0	56	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	L	51	0	72	2	0
31	M	42	0	54	3	0
31	a	42	0	54	0	0
31	b	91	0	122	0	0
31	c	93	0	126	0	0
31	d	143	0	196	0	0
31	e	44	0	58	0	0
31	i	43	0	56	0	0
31	l	51	0	72	0	0
31	m	42	0	54	0	0
32	B	140	0	184	5	0
32	D	31	0	35	0	0
32	I	35	0	46	1	0
32	M	70	0	92	0	0
32	b	140	0	184	0	0
32	d	31	0	35	0	0
32	i	35	0	46	0	0
33	D	4	0	1	0	0
33	d	4	0	1	0	0
34	F	43	0	30	5	0
34	V	43	0	30	3	0
34	f	43	0	30	0	0
34	v	43	0	30	0	0
35	K	1	0	0	0	0
35	O	1	0	0	0	0
35	k	1	0	0	0	0
35	o	1	0	0	0	0
All	All	50244	0	51374	639	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (639) 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)
3:C:39:ASN:HB2	22:C:507:CLA:HBA1	1.55	0.87
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.60	0.83
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.82
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.62	0.82
3:C:362:ARG:H	26:C:514:DGD:HE4	1.47	0.78
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:362:ARG:H	26:C:515:DGD:HE4	24.14	0.77
4:D:199:MET:HG2	24:D:405:PL9:H322	1.69	0.74
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.53	0.73
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.69	0.73
4:D:29:PHE:O	4:D:128:ARG:NH2	2.22	0.73
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.71	0.72
1:A:63:ILE:HB	3:C:335:THR:HG21	1.79	0.72
2:B:24:LEU:HD21	22:B:615:CLA:HAB	1.72	0.72
26:C:516:DGD:HAF2	22:C:519:CLA:H202	1.71	0.71
4:D:236:ASN:ND2	4:D:239:GLN:O	2.23	0.71
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.72	0.71
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.77	0.71
22:B:605:CLA:H72	25:B:619:BCR:H311	1.73	0.71
4:D:21:TRP:O	4:D:26:ARG:NH2	2.23	0.70
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.32	0.69
4:D:152:VAL:HG21	4:D:279:LEU:HD12	1.72	0.69
1:A:183:MET:HB3	22:A:402:CLA:HBC2	1.73	0.69
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.84	0.69
4:D:259:ILE:HG12	31:D:409:LMG:H292	45.22	0.69
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.74	0.68
22:C:503:CLA:H172	22:C:509:CLA:HBB2	1.74	0.68
12:M:31:SER:HA	31:M:101:LMG:HC1	1.79	0.67
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.97	0.67
3:C:297:TYR:O	3:C:423:ARG:NH2	2.28	0.67
3:C:406:SER:O	3:C:418:ASN:ND2	2.28	0.67
2:B:187:PRO:HB3	22:B:601:CLA:HMB2	1.76	0.66
6:F:17:THR:HG23	6:F:20:TRP:H	1.60	0.66
4:D:186:GLN:HB2	22:D:403:CLA:HBC1	1.77	0.66
2:B:474:LEU:O	4:D:134:ARG:NH1	2.54	0.66
3:C:165:LEU:HD21	22:C:505:CLA:HAB	1.76	0.66
22:C:506:CLA:H112	25:C:513:BCR:H362	1.76	0.65
22:A:403:CLA:H122	23:D:401:PHO:H3A	31.92	0.65
3:C:250:TRP:O	3:C:254:THR:OG1	2.13	0.65
22:C:507:CLA:HBC3	22:C:509:CLA:H92	1.79	0.65
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.65
3:C:291:TRP:O	3:C:305:THR:OG1	2.16	0.65
22:A:403:CLA:H71	22:A:404:CLA:HAB	27.47	0.65
20:Z:33:TRP:HA	20:Z:36:SER:HB3	1.80	0.64
22:B:612:CLA:H42	4:D:127:LEU:HD11	22.83	0.64
1:A:174:LEU:HD22	23:D:401:PHO:H151	37.14	0.64
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.84	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:B:622:SQD:H171	30:B:622:SQD:H301	1.79	0.64
22:B:607:CLA:HBA2	30:B:622:SQD:H101	1.81	0.63
22:A:404:CLA:H142	22:D:403:CLA:H151	1.80	0.63
22:B:607:CLA:H42	4:D:127:LEU:HD11	1.80	0.63
22:A:403:CLA:HBB1	22:A:403:CLA:HHC	2.33	0.63
22:A:402:CLA:H71	22:A:403:CLA:HAB	1.80	0.63
4:D:24:ARG:NH2	18:X:44:ASP:O	2.35	0.63
3:C:49:LEU:O	3:C:53:HIS:ND1	2.30	0.62
3:C:48:LYS:NZ	3:C:133:ALA:O	2.31	0.62
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.81	0.62
22:B:607:CLA:H193	7:H:42:LEU:HD12	10.41	0.62
1:A:15:GLU:O	1:A:19:ASN:ND2	2.34	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.84	0.62
22:B:602:CLA:H193	7:H:42:LEU:HD12	1.81	0.62
2:B:121:GLU:O	7:H:12:ARG:NH2	2.41	0.62
22:B:608:CLA:HMD1	7:H:27:THR:HB	1.82	0.61
1:A:140:ARG:NH2	27:A:410:LHG:O5	2.30	0.61
3:C:449:ARG:HE	22:C:504:CLA:HED1	1.65	0.61
22:A:404:CLA:H203	23:D:401:PHO:H71	15.37	0.61
4:D:214:HIS:ND1	24:D:405:PL9:O2	2.22	0.61
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.71	0.61
30:A:413:SQD:H172	27:C:518:LHG:H172	1.83	0.61
1:A:183:MET:HB3	22:A:403:CLA:HBC2	6.12	0.61
2:B:187:PRO:HB3	22:B:605:CLA:HMB2	29.63	0.61
2:B:149:LEU:HG	22:B:607:CLA:HBC1	22.33	0.61
4:D:216:ALA:O	4:D:220:ASN:ND2	2.35	0.61
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.86	0.61
26:B:620:DGD:HAW2	22:H:101:CLA:H152	1.83	0.60
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.83	0.60
22:A:403:CLA:HED1	24:D:405:PL9:H372	1.83	0.60
11:L:13:ASN:ND2	31:L:101:LMG:O5	2.33	0.60
1:A:329:GLU:O	1:A:332:HIS:ND1	2.32	0.60
3:C:42:LEU:HD21	22:C:510:CLA:H2A	1.83	0.60
1:A:183:MET:HA	22:A:402:CLA:HMD2	1.83	0.60
4:D:259:ILE:HG12	31:D:406:LMG:H292	1.83	0.59
31:D:406:LMG:HO5	31:D:406:LMG:HO4	1.49	0.59
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.86	0.59
1:A:227:THR:HG21	1:A:233:ALA:HA	1.84	0.59
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.96	0.59
22:B:607:CLA:C2D	22:B:609:CLA:H2	16.50	0.59
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LEU:HD22	23:A:405:PHO:H151	1.85	0.59
1:A:183:MET:HA	22:A:403:CLA:HMD2	8.57	0.58
22:B:606:CLA:HBB1	31:B:621:LMG:H341	1.84	0.58
22:B:606:CLA:HAA2	7:H:45:ILE:HD12	30.06	0.58
13:O:83:LYS:HG2	13:O:84:ASN:H	1.68	0.58
22:C:508:CLA:HBD	22:C:508:CLA:H121	1.84	0.58
34:V:201:HEM:HBB2	34:V:201:HEM:HMB1	1.85	0.58
5:E:18:ARG:NH1	34:F:101:HEM:O1A	2.37	0.58
22:B:613:CLA:HMD1	7:H:27:THR:HB	43.37	0.58
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.87	0.58
22:A:402:CLA:H122	23:A:405:PHO:H3A	1.84	0.58
2:B:327:THR:HG21	31:B:621:LMG:H111	1.85	0.58
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.89	0.57
2:B:149:LEU:HG	22:B:602:CLA:HBC1	1.85	0.57
22:C:505:CLA:HMC2	22:C:506:CLA:H102	1.87	0.57
2:B:12:LEU:HB2	22:B:611:CLA:HMC2	1.85	0.57
1:A:29:TYR:O	1:A:129:ARG:NH1	2.53	0.57
31:D:406:LMG:O6	11:L:15:THR:HG21	2.05	0.57
2:B:487:SER:N	2:B:488:PRO:HD2	2.20	0.57
30:A:413:SQD:H223	26:C:516:DGD:HAE1	1.87	0.56
3:C:164:HIS:ND1	22:C:506:CLA:OBD	2.30	0.56
1:A:217:SER:HA	4:D:272:LEU:HD12	1.89	0.56
2:B:262:THR:HG22	2:B:263:THR:HG23	1.87	0.56
3:C:361:PHE:HD1	26:C:514:DGD:HE61	1.71	0.56
22:A:403:CLA:H203	23:A:405:PHO:H71	1.87	0.56
31:D:409:LMG:H171	25:F:102:BCR:H383	1.86	0.56
22:C:501:CLA:HMB3	25:C:513:BCR:H403	1.88	0.56
27:C:518:LHG:H101	27:C:518:LHG:H271	1.87	0.56
22:B:607:CLA:H151	22:B:608:CLA:H203	1.87	0.56
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.94	0.56
30:F:103:SQD:H162	18:X:33:THR:HA	1.88	0.56
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.88	0.56
2:B:155:ALA:O	2:B:159:THR:OG1	2.18	0.56
1:A:84:PRO:HA	1:A:112:TYR:CG	2.41	0.56
1:A:153:SER:HB3	22:A:402:CLA:HED1	1.88	0.55
22:B:606:CLA:HBD	22:B:606:CLA:H2	7.91	0.55
2:B:262:THR:OG1	22:B:607:CLA:O1D	28.18	0.55
13:O:73:PRO:HG2	13:O:102:THR:HB	1.89	0.55
20:Z:33:TRP:O	20:Z:37:LYS:HB2	2.06	0.55
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.72	0.55
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:501:CLA:C2D	22:C:503:CLA:H2	2.37	0.55
12:M:25:LEU:O	12:M:28:GLN:HG3	2.07	0.55
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.89	0.55
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.57	0.55
2:B:262:THR:OG1	22:B:602:CLA:O1D	2.24	0.55
22:H:101:CLA:H2	22:H:101:CLA:HBD	1.88	0.55
22:A:404:CLA:H93	22:D:403:CLA:H152	1.89	0.55
22:B:605:CLA:H18	22:B:615:CLA:H121	1.89	0.55
22:B:607:CLA:C3D	22:B:609:CLA:H2	17.27	0.55
22:B:613:CLA:H51	25:B:616:BCR:H372	1.87	0.54
26:B:626:DGD:O2D	26:B:626:DGD:O1B	2.25	0.54
31:D:409:LMG:O6	11:L:15:THR:HG21	54.03	0.54
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.90	0.54
22:D:404:CLA:H42	18:X:26:GLY:HA3	1.89	0.54
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.94	0.54
22:C:510:CLA:HMB2	25:K:101:BCR:H382	1.89	0.54
22:B:610:CLA:H41	22:B:613:CLA:HBC3	1.90	0.54
5:E:10:PHE:N	31:E:101:LMG:O3	2.40	0.54
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.74	0.54
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.74	0.54
2:B:103:LEU:HD21	22:B:609:CLA:HMC3	27.64	0.54
22:B:612:CLA:H51	22:B:613:CLA:H101	15.99	0.54
24:D:405:PL9:H352	31:L:101:LMG:H231	1.89	0.54
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.62	0.54
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.00	0.54
2:B:256:MET:O	2:B:448:ARG:NH1	2.35	0.54
22:A:402:CLA:HBB1	22:A:402:CLA:HHC	1.89	0.54
4:D:43:LEU:HD23	4:D:117:HIS:CE1	2.44	0.54
2:B:150:CYS:HA	22:B:602:CLA:HBC2	1.90	0.53
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.96	0.53
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.42	0.53
2:B:150:CYS:HA	22:B:607:CLA:HBC2	21.60	0.53
1:A:78:ILE:O	1:A:176:ILE:HB	2.08	0.53
22:B:610:CLA:OBD	32:B:628:LMT:O6'	53.46	0.53
2:B:122:LEU:O	7:H:15:ASN:ND2	2.42	0.53
2:B:184:GLU:H	2:B:200:ALA:HB2	1.74	0.53
2:B:247:PHE:HE1	22:H:101:CLA:H101	1.73	0.53
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.89	0.53
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.53
30:B:627:SQD:H1	30:B:627:SQD:H462	1.90	0.53
25:A:408:BCR:H321	30:A:414:SQD:H321	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:THR:O	3:C:251:HIS:HB3	2.09	0.53
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.19	0.53
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.97	0.53
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.91	0.53
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.53
26:C:516:DGD:HA22	9:J:29:PHE:HE1	1.73	0.53
2:B:458:PHE:HB3	22:B:608:CLA:HBC2	29.55	0.53
31:D:409:LMG:O5	31:D:409:LMG:O4	2.96	0.53
2:B:271:THR:HB	2:B:274:GLN:HG3	1.91	0.53
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.73	0.53
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.47	0.53
25:A:408:BCR:H342	30:A:414:SQD:H311	1.91	0.52
32:B:628:LMT:H62	8:I:4:LEU:HD22	82.15	0.52
4:D:262:SER:N	31:D:409:LMG:O3	52.73	0.52
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.92	0.52
2:B:458:PHE:HB3	22:B:603:CLA:HBC2	1.91	0.52
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.92	0.52
2:B:371:THR:HG22	2:B:377:VAL:HA	1.92	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.48	0.52
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.52
3:C:85:GLY:N	26:C:515:DGD:HE4	2.24	0.52
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.92	0.52
1:A:210:LEU:HG	23:D:401:PHO:NC	2.25	0.52
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.52
22:A:404:CLA:H161	24:A:407:PL9:H253	1.91	0.52
22:B:608:CLA:HBD	22:B:609:CLA:H43	22.44	0.52
4:D:275:PRO:O	4:D:279:LEU:HD23	2.15	0.52
1:A:12:ASN:HB3	1:A:15:GLU:HB3	1.91	0.52
1:A:64:ARG:O	13:O:178:ARG:NH2	2.43	0.52
30:A:413:SQD:H311	22:C:507:CLA:H71	1.92	0.51
2:B:103:LEU:HD21	22:B:604:CLA:HMC3	1.93	0.51
3:C:85:GLY:N	26:C:516:DGD:HE4	14.14	0.51
22:D:404:CLA:H43	18:X:23:LEU:HA	1.92	0.51
22:C:504:CLA:HBA1	22:C:504:CLA:HBD	1.94	0.51
22:B:602:CLA:C2D	22:B:604:CLA:H2	2.41	0.51
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.34	0.51
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.45	0.51
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.52	0.51
6:F:45:ARG:NH2	9:J:40:LEU:O	2.42	0.51
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.93	0.51
22:B:607:CLA:H2	22:B:609:CLA:H93	26.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.03	0.51
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.80	0.51
2:B:212:ALA:HB2	22:B:608:CLA:HMC3	1.92	0.51
1:A:85:SER:HA	1:A:109:GLY:HA3	1.92	0.51
22:A:403:CLA:HBA1	22:A:403:CLA:CHA	2.41	0.51
22:B:612:CLA:H151	22:B:613:CLA:H203	17.03	0.51
1:A:224:ILE:O	4:D:265:ARG:NH2	2.46	0.51
1:A:190:HIS:O	1:A:298:ASN:HB3	2.19	0.51
4:D:85:MET:HA	5:E:69:ARG:HB3	2.00	0.51
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.49	0.51
2:B:222:PRO:HG3	7:H:27:THR:H	1.79	0.50
4:D:261:PHE:HB2	24:D:405:PL9:H522	1.93	0.50
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.92	0.50
18:X:11:THR:HG23	18:X:12:ILE:HG22	1.93	0.50
2:B:327:THR:HG22	22:B:611:CLA:H12	31.54	0.50
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.93	0.50
25:B:617:BCR:H19C	25:B:618:BCR:H363	1.92	0.50
23:D:401:PHO:H151	22:D:403:CLA:H172	1.92	0.50
25:C:513:BCR:H311	25:C:513:BCR:H343	3.34	0.50
13:O:168:PHE:HB2	13:O:225:LEU:HB2	2.02	0.50
10:K:40:GLN:HA	10:K:43:VAL:HG12	1.94	0.50
2:B:450:TRP:NE1	22:B:606:CLA:HBA1	2.27	0.50
1:A:271:LEU:HD11	24:A:407:PL9:C4	2.42	0.50
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.95	0.50
2:B:212:ALA:HB2	22:B:613:CLA:HMC3	34.89	0.50
2:B:256:MET:HA	2:B:263:THR:HG21	1.93	0.50
22:B:606:CLA:H193	11:L:27:LEU:HD11	1.92	0.50
22:C:512:CLA:HAB	25:C:520:BCR:H371	1.94	0.50
22:B:606:CLA:HBC3	25:B:618:BCR:HC8	1.94	0.50
2:B:150:CYS:HB2	22:B:607:CLA:HMC3	23.27	0.50
2:B:5:TRP:HZ3	22:B:610:CLA:H51	1.76	0.50
22:B:606:CLA:H72	7:H:46:LEU:HD13	27.36	0.49
5:E:15:THR:HG23	9:J:8:ILE:O	2.18	0.49
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.00	0.49
3:C:166:ILE:O	3:C:170:ILE:HG13	2.19	0.49
22:B:609:CLA:H202	22:B:613:CLA:HBB2	16.74	0.49
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.49
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.95	0.49
3:C:361:PHE:HD1	26:C:515:DGD:HE61	20.65	0.49
1:A:153:SER:HB3	22:A:403:CLA:HED1	17.31	0.49
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:26:PRO:O	10:K:29:PRO:HD2	2.12	0.49
22:A:404:CLA:CHA	22:A:404:CLA:HBA1	3.96	0.49
13:O:118:SER:HB3	13:O:157:PRO:HA	1.95	0.49
2:B:19:LEU:HG	2:B:23:HIS:CE1	2.48	0.49
27:A:410:LHG:H382	22:C:509:CLA:H93	1.95	0.49
22:B:612:CLA:H171	31:B:625:LMG:H401	1.95	0.49
3:C:86:LEU:HB3	3:C:90:PRO:HD3	1.94	0.49
1:A:132:GLU:O	1:A:136:ARG:HG2	2.13	0.49
3:C:284:PHE:HB3	26:C:515:DGD:HA51	19.67	0.49
31:D:406:LMG:H111	11:L:19:LEU:HD21	1.93	0.49
31:M:101:LMG:H142	31:M:101:LMG:H311	1.99	0.49
2:B:19:LEU:O	2:B:23:HIS:ND1	2.45	0.49
1:A:211:PHE:HA	1:A:214:MET:HB2	1.96	0.49
1:A:244:GLU:HG3	1:A:246:TYR:H	1.79	0.49
2:B:150:CYS:HB2	22:B:602:CLA:HMC3	1.95	0.49
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.50	0.49
22:C:501:CLA:H171	22:C:506:CLA:HMB3	1.96	0.49
4:D:48:TRP:CE2	23:D:401:PHO:H161	2.48	0.49
5:E:23:HIS:NE2	34:F:101:HEM:ND	2.63	0.49
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.94	0.49
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.43	0.48
1:A:114:LEU:O	1:A:118:HIS:ND1	2.42	0.48
22:B:612:CLA:H18	22:B:613:CLA:H192	12.16	0.48
7:H:45:ILE:HD11	22:H:101:CLA:H42	1.94	0.48
2:B:170:ASP:OD1	2:B:175:THR:N	2.53	0.48
3:C:425:TRP:CE2	22:C:519:CLA:HBA1	2.48	0.48
22:B:603:CLA:HMD2	22:B:611:CLA:H193	1.95	0.48
4:D:102:THR:OG1	26:D:407:DGD:HD62	2.13	0.48
4:D:55:VAL:HG21	4:D:110:LEU:HD12	2.01	0.48
22:A:404:CLA:HAB	22:D:403:CLA:H72	1.95	0.48
25:B:616:BCR:H333	12:M:13:LEU:HD12	1.96	0.48
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.00	0.48
22:B:605:CLA:OBD	32:B:623:LMT:O6'	2.24	0.48
2:B:120:LEU:HD13	22:B:615:CLA:HMD2	1.94	0.48
4:D:262:SER:N	31:D:406:LMG:O3	2.42	0.48
22:B:606:CLA:H41	22:B:606:CLA:H62	1.86	0.48
4:D:43:LEU:HD23	4:D:117:HIS:HE1	1.78	0.48
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.96	0.48
26:D:407:DGD:O5E	26:D:407:DGD:O4E	2.24	0.48
13:O:240:THR:HA	13:O:264:VAL:HA	2.04	0.48
3:C:284:PHE:HB3	26:C:514:DGD:HA51	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:101:CLA:H41	22:H:101:CLA:H62	1.56	0.48
13:O:230:VAL:HG12	13:O:231:ASP:H	1.77	0.48
4:D:323:GLU:HG3	4:D:326:ARG:NH2	2.28	0.48
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.07	0.48
23:A:405:PHO:H41	23:A:405:PHO:H62	1.46	0.47
2:B:96:VAL:HG22	22:B:610:CLA:HBA1	32.27	0.47
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.36	0.47
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.47	0.47
3:C:346:THR:HG21	13:O:38:GLY:HA2	2.00	0.47
22:B:602:CLA:C3D	22:B:604:CLA:H2	2.44	0.47
22:D:403:CLA:H61	22:D:403:CLA:H41	1.67	0.47
3:C:52:ALA:HA	22:C:510:CLA:HMB3	1.96	0.47
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.97	0.47
3:C:248:GLY:O	3:C:252:ILE:HG12	2.15	0.47
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.18	0.47
18:X:12:ILE:HG12	18:X:16:LEU:HD12	1.98	0.47
3:C:130:VAL:O	3:C:134:ILE:HG12	2.17	0.47
2:B:125:ASP:HB2	2:B:132:ALA:HB3	1.97	0.47
2:B:18:ARG:HD3	2:B:118:TRP:HB3	1.96	0.47
3:C:113:VAL:HG11	31:C:517:LMG:H132	1.97	0.47
22:A:403:CLA:HMA2	24:D:405:PL9:H411	1.95	0.47
3:C:391:ARG:HD2	3:C:395:TYR:CZ	2.60	0.47
13:O:135:GLN:HG2	13:O:141:ARG:HG3	2.11	0.47
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.96	0.47
2:B:68:ARG:HH22	22:B:603:CLA:HED1	1.80	0.47
15:U:75:LEU:HD21	15:U:101:GLN:HB3	1.96	0.47
22:B:603:CLA:H101	22:B:614:CLA:H2	1.97	0.47
25:B:619:BCR:H20C	25:B:619:BCR:H361	1.76	0.47
2:B:30:VAL:HG12	22:B:609:CLA:HHD	22.16	0.47
22:B:611:CLA:H193	11:L:27:LEU:HD11	26.87	0.47
1:A:298:ASN:ND2	3:C:402:GLY:O	2.48	0.47
4:D:84:SER:HB2	4:D:85:MET:HE2	1.97	0.46
3:C:319:ILE:HG21	3:C:389:GLU:HG3	2.05	0.46
2:B:5:TRP:HZ3	22:B:615:CLA:H51	35.06	0.46
3:C:245:ILE:O	3:C:249:ILE:HG12	2.18	0.46
9:J:38:SER:OG	9:J:39:SER:N	2.47	0.46
22:A:402:CLA:H3A	22:A:402:CLA:HBA1	1.53	0.46
22:B:606:CLA:H162	22:B:606:CLA:H122	4.80	0.46
22:C:508:CLA:H62	22:C:508:CLA:H92	1.71	0.46
13:O:223:ILE:HG13	13:O:243:SER:HB3	2.01	0.46
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.00	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.88	0.46
2:B:121:GLU:HG2	7:H:4:ARG:HA	2.03	0.46
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.51	0.46
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.00	0.46
2:B:213:GLY:O	2:B:217:ILE:HG13	2.14	0.46
16:V:68:VAL:O	16:V:71:ILE:HG12	2.14	0.46
22:C:512:CLA:H3A	22:C:512:CLA:HBA2	1.70	0.46
22:A:404:CLA:H161	22:A:404:CLA:H143	1.80	0.46
22:A:404:CLA:H202	22:A:404:CLA:H162	4.12	0.46
23:D:401:PHO:H62	23:D:401:PHO:H41	3.82	0.46
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.81	0.46
4:D:56:THR:HG21	5:E:50:PRO:HD3	2.02	0.46
7:H:46:LEU:HD13	22:H:101:CLA:H72	1.98	0.46
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.02	0.46
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.49	0.46
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.49	0.46
22:C:510:CLA:H61	22:C:510:CLA:H93	1.80	0.46
30:F:103:SQD:H131	18:X:36:VAL:HG11	2.00	0.46
3:C:343:ARG:NH1	3:C:347:GLY:O	2.49	0.46
3:C:456:GLU:N	3:C:456:GLU:OE1	2.48	0.46
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.55	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
22:B:609:CLA:H41	22:B:609:CLA:H62	1.95	0.45
26:C:516:DGD:HA22	9:J:29:PHE:CE1	2.50	0.45
2:B:306:PRO:HG2	2:B:309:LEU:HB2	2.03	0.45
22:B:607:CLA:H18	22:B:608:CLA:H192	1.98	0.45
3:C:166:ILE:HG23	3:C:245:ILE:HG23	2.05	0.45
3:C:59:LEU:HD13	22:C:509:CLA:HMD2	2.04	0.45
18:X:40:ILE:HA	18:X:43:ILE:HD12	1.99	0.45
3:C:386:PRO:HB3	16:V:116:GLU:HG2	1.99	0.45
25:C:513:BCR:H351	25:C:513:BCR:H15C	1.83	0.45
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.19	0.45
22:A:403:CLA:H62	22:A:403:CLA:H41	1.74	0.45
2:B:450:TRP:NE1	22:B:611:CLA:HBA1	27.87	0.45
25:B:618:BCR:H20C	25:B:618:BCR:H361	1.81	0.45
22:A:403:CLA:HAA1	24:D:405:PL9:H362	1.99	0.45
1:A:271:LEU:HD21	24:A:407:PL9:HC71	1.97	0.45
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.52	0.45
22:C:506:CLA:H92	22:C:506:CLA:H62	1.73	0.45
25:K:101:BCR:H361	25:K:101:BCR:H20C	1.77	0.45
1:A:29:TYR:CG	1:A:133:LEU:HD13	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:NH1	4:D:254:SER:O	2.48	0.45
22:B:614:CLA:H62	22:B:614:CLA:H92	1.78	0.45
22:H:101:CLA:H162	22:H:101:CLA:H122	1.55	0.45
31:D:409:LMG:H111	11:L:19:LEU:HD21	43.63	0.45
22:C:509:CLA:H61	22:C:509:CLA:H2	1.73	0.45
22:B:605:CLA:H161	22:B:605:CLA:HMD1	19.73	0.45
22:B:607:CLA:H92	22:B:607:CLA:HBB2	11.25	0.45
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.98	0.45
22:C:508:CLA:H11	22:C:508:CLA:H51	1.84	0.45
22:C:501:CLA:H193	22:C:506:CLA:H111	1.99	0.44
30:A:414:SQD:HO8	2:B:113:TRP:HE1	62.62	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.02	0.44
22:A:403:CLA:H42	24:D:405:PL9:H162	1.98	0.44
3:C:137:PRO:HB2	3:C:139:THR:O	2.18	0.44
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.52	0.44
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.98	0.44
2:B:135:LEU:HA	2:B:138:MET:HE3	2.07	0.44
1:A:202:VAL:HB	22:A:402:CLA:HMB3	1.99	0.44
22:B:608:CLA:HMC2	25:H:102:BCR:H343	1.99	0.44
31:I:101:LMG:H181	32:I:102:LMT:H42	1.98	0.44
2:B:383:PHE:N	4:D:344:GLU:O	2.37	0.44
1:A:111:PRO:O	1:A:115:ILE:HG13	2.21	0.44
26:C:516:DGD:HAW2	26:C:516:DGD:HA91	4.04	0.44
25:K:101:BCR:H343	25:K:101:BCR:H311	1.98	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.81	0.44
2:B:247:PHE:HB2	22:B:612:CLA:HBC1	22.36	0.44
25:B:616:BCR:H11C	25:B:616:BCR:H341	1.88	0.44
4:D:279:LEU:HG	23:D:401:PHO:HBC3	2.00	0.44
22:H:101:CLA:H93	22:H:101:CLA:H62	1.86	0.44
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.00	0.44
16:V:38:LEU:HD12	16:V:95:ILE:HB	2.09	0.44
3:C:350:ILE:HG21	3:C:359:TRP:HB2	2.00	0.44
9:J:14:ALA:O	9:J:18:GLY:N	2.48	0.44
13:O:79:LYS:HB3	13:O:258:GLU:HB2	2.02	0.44
1:A:258:LEU:O	4:D:128:ARG:NH1	2.52	0.44
3:C:90:PRO:O	3:C:94:THR:HG23	2.17	0.44
1:A:268:SER:O	1:A:272:HIS:ND1	2.42	0.44
2:B:135:LEU:HB2	2:B:136:PRO:HD3	2.01	0.44
2:B:247:PHE:HB2	22:B:607:CLA:HBC1	2.00	0.44
22:B:614:CLA:H172	22:B:614:CLA:H111	2.00	0.44
26:B:620:DGD:HA71	22:H:101:CLA:H193	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:12:ARG:HD3	7:H:12:ARG:O	2.18	0.44
16:V:60:GLN:HA	16:V:64:ALA:HB2	1.99	0.44
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.52	0.44
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.44
3:C:190:ALA:HA	3:C:191:PRO:HD3	1.88	0.44
3:C:437:PHE:CZ	22:C:509:CLA:HMB3	2.52	0.44
3:C:112:PHE:HE2	25:C:520:BCR:HC31	1.82	0.44
3:C:456:GLU:HG2	3:C:457:LYS:HG3	1.99	0.44
8:I:6:ILE:O	8:I:10:ILE:HG12	2.25	0.43
3:C:209:ILE:HG23	25:C:513:BCR:H382	1.99	0.43
22:B:612:CLA:H51	31:B:625:LMG:H231	1.99	0.43
26:B:620:DGD:HAT2	22:H:101:CLA:H151	2.00	0.43
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.01	0.43
3:C:42:LEU:HD13	22:C:510:CLA:HMA3	2.02	0.43
20:Z:33:TRP:O	20:Z:33:TRP:CD1	2.72	0.43
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.92	0.43
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.54	0.43
10:K:18:PHE:O	10:K:22:VAL:HG23	2.18	0.43
5:E:42:LEU:O	5:E:46:VAL:HG23	2.17	0.43
26:C:515:DGD:HA91	26:C:515:DGD:HAW2	1.75	0.43
3:C:420:VAL:H	26:C:516:DGD:HE62	11.29	0.43
25:B:616:BCR:H361	25:B:616:BCR:H20C	1.78	0.43
22:D:403:CLA:H92	22:D:403:CLA:H62	1.83	0.43
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.01	0.43
22:C:510:CLA:H141	20:Z:20:VAL:HG13	2.00	0.43
7:H:45:ILE:HD12	22:H:101:CLA:HAA2	1.99	0.43
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	2.06	0.43
1:A:93:PHE:HZ	22:A:406:CLA:HAA1	1.93	0.43
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.02	0.43
1:A:238:LYS:O	1:A:241:GLN:HG3	2.18	0.43
1:A:156:ALA:HA	1:A:160:ILE:HB	1.99	0.43
22:A:402:CLA:H51	23:A:405:PHO:C3B	2.49	0.43
22:B:602:CLA:H92	22:B:602:CLA:HBB2	2.01	0.43
3:C:29:GLU:HB2	3:C:30:SER:H	1.64	0.43
1:A:269:ARG:NH1	4:D:231:THR:HB	2.33	0.43
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.18	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.54	0.43
22:B:610:CLA:H3A	22:B:610:CLA:HBA2	3.06	0.43
23:D:401:PHO:CHB	22:D:403:CLA:H101	2.49	0.43
13:O:192:SER:OG	13:O:193:GLY:N	2.51	0.43
32:B:629:LMT:H3O2	32:B:629:LMT:H2O1	5.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:507:CLA:H172	26:C:515:DGD:HBW2	2.00	0.43
6:F:16:PHE:HB3	30:F:103:SQD:H241	2.01	0.43
1:A:317:TRP:CD1	4:D:177:ALA:HB2	2.54	0.43
2:B:280:PHE:O	2:B:284:ILE:HG13	2.18	0.43
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.53	0.43
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.00	0.43
1:A:237:TYR:OH	4:D:246:MET:HG2	2.27	0.43
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.54	0.43
20:Z:29:SER:HA	20:Z:30:PRO:HD3	1.83	0.43
25:C:513:BCR:H24C	25:C:513:BCR:H371	1.89	0.42
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.42
1:A:40:THR:HG21	1:A:121:LEU:HD23	2.01	0.42
22:B:611:CLA:H162	22:B:611:CLA:H122	1.74	0.42
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.57	0.42
2:B:194:ASN:HA	2:B:195:PRO:HD3	1.90	0.42
25:C:513:BCR:H11C	25:C:513:BCR:H341	1.90	0.42
3:C:405:ASN:HB2	26:C:516:DGD:HG31	2.01	0.42
3:C:35:TRP:CZ2	27:C:518:LHG:H261	2.54	0.42
22:A:404:CLA:H11	22:A:404:CLA:H51	4.37	0.42
1:A:322:ASN:OD1	3:C:412:THR:HA	2.22	0.42
3:C:363:GLY:O	3:C:367:GLU:HG2	2.23	0.42
22:A:403:CLA:H162	22:A:403:CLA:H202	1.76	0.42
22:B:603:CLA:HBD	22:B:604:CLA:H43	2.02	0.42
22:B:605:CLA:H3A	22:B:605:CLA:HBA2	1.23	0.42
3:C:303:GLY:O	3:C:423:ARG:NE	2.39	0.42
3:C:224:ILE:O	3:C:227:VAL:HG23	2.20	0.42
2:B:485:GLU:HG3	2:B:486:LEU:N	2.34	0.42
1:A:127:MET:HG3	1:A:144:CYS:HB2	2.02	0.42
22:C:512:CLA:HAB	25:C:520:BCR:H24C	2.00	0.42
25:C:513:BCR:H391	10:K:36:ALA:HB2	35.91	0.42
24:A:407:PL9:H351	24:A:407:PL9:H371	1.84	0.42
22:B:602:CLA:H162	22:B:602:CLA:H192	1.76	0.42
22:A:406:CLA:H162	22:A:406:CLA:H141	1.68	0.42
1:A:157:VAL:HG13	1:A:172:MET:HB3	2.07	0.42
1:A:283:VAL:O	1:A:286:THR:HG22	2.19	0.42
3:C:38:GLY:HA3	22:C:510:CLA:HMD3	2.03	0.42
25:C:513:BCR:H361	25:C:513:BCR:H20C	1.85	0.42
2:B:25:MET:HG2	25:B:616:BCR:H23C	2.00	0.42
22:B:604:CLA:H202	22:B:608:CLA:HBB2	2.01	0.42
31:D:409:LMG:HC1	31:D:409:LMG:O9	4.10	0.42
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:143:PRO:HG2	13:O:248:ASP:HB3	2.00	0.42
2:B:137:LYS:HD2	7:H:14:LEU:O	2.20	0.42
16:V:90:PRO:O	16:V:92:ARG:HD3	2.18	0.42
31:B:621:LMG:H421	4:D:284:ILE:HD13	2.01	0.42
25:H:102:BCR:H20C	25:H:102:BCR:H361	1.79	0.42
7:H:12:ARG:N	7:H:13:PRO:HD2	2.35	0.42
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.90	0.42
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.58	0.42
31:C:517:LMG:H292	31:C:517:LMG:H111	2.00	0.42
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.28	0.42
1:A:221:SER:HB2	4:D:139:ARG:O	2.19	0.42
15:U:72:TYR:O	15:U:76:ALA:HB3	2.21	0.42
13:O:154:SER:N	13:O:169:LYS:O	2.51	0.42
20:Z:5:PHE:CE1	20:Z:54:VAL:HG13	2.55	0.42
1:A:153:SER:HB2	22:A:402:CLA:H43	2.00	0.42
1:A:176:ILE:HD12	22:A:404:CLA:HED3	27.29	0.42
2:B:327:THR:HG22	22:B:606:CLA:H12	2.01	0.42
22:B:604:CLA:H62	22:B:604:CLA:H41	1.81	0.42
22:B:615:CLA:H143	22:B:615:CLA:H111	1.78	0.42
25:B:617:BCR:H15C	25:B:617:BCR:H351	1.87	0.42
25:B:618:BCR:H24C	25:B:618:BCR:H371	1.82	0.42
4:D:87:HIS:CD2	4:D:162:LEU:HD23	2.54	0.42
22:C:501:CLA:H162	22:C:501:CLA:H141	1.77	0.42
25:C:520:BCR:H371	25:C:520:BCR:H24C	1.84	0.42
2:B:91:TRP:CH2	22:B:605:CLA:H12	2.55	0.42
4:D:201:VAL:O	4:D:205:LEU:HB2	2.20	0.42
1:A:159:LEU:C	1:A:162:PRO:HD2	2.40	0.42
22:C:507:CLA:H172	26:C:516:DGD:HBW2	12.23	0.42
22:C:510:CLA:H171	20:Z:20:VAL:HA	2.10	0.42
22:B:603:CLA:H11	22:B:604:CLA:H42	2.02	0.42
1:A:191:ASN:HB2	3:C:411:ALA:HB1	2.11	0.42
16:V:158:GLY:HA3	16:V:162:TYR:CD2	2.75	0.42
23:A:405:PHO:H13	23:A:405:PHO:H102	1.86	0.41
22:B:607:CLA:CHA	22:B:607:CLA:HBA1	2.49	0.41
4:D:205:LEU:HA	4:D:205:LEU:HD12	1.84	0.41
23:D:401:PHO:H102	23:D:401:PHO:H13	4.39	0.41
4:D:252:PHE:O	4:D:256:ILE:HG22	2.23	0.41
15:U:94:ILE:HB	15:U:97:LEU:HD11	2.06	0.41
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.41
22:A:403:CLA:HED2	4:D:198:MET:SD	2.60	0.41
22:B:607:CLA:H41	22:B:607:CLA:H61	3.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:612:CLA:H161	22:B:612:CLA:H143	4.29	0.41
22:D:403:CLA:H3A	22:D:403:CLA:HBA1	1.86	0.41
4:D:236:ASN:HA	4:D:237:PRO:HD2	1.96	0.41
5:E:60:GLN:HG2	5:E:62:SER:H	1.85	0.41
3:C:80:PRO:HB2	3:C:83:GLU:HG3	2.18	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.06	0.41
31:C:521:LMG:H112	25:J:102:BCR:H373	2.02	0.41
1:A:215:HIS:HA	24:A:407:PL9:O1	2.21	0.41
2:B:242:ILE:HG12	22:B:610:CLA:HBB1	2.02	0.41
2:B:468:TRP:HH2	31:B:625:LMG:HO2	1.65	0.41
24:D:405:PL9:H13	31:D:406:LMG:H132	2.02	0.41
25:F:102:BCR:H341	25:F:102:BCR:H11C	1.94	0.41
3:C:135:ARG:HB2	20:Z:27:TYR:HB3	2.02	0.41
26:A:409:DGD:HG32	26:A:409:DGD:HD2	1.73	0.41
22:C:510:CLA:H122	10:K:32:PHE:HE1	1.86	0.41
25:A:408:BCR:H11C	25:A:408:BCR:H341	1.95	0.41
2:B:221:PRO:HA	2:B:222:PRO:HD3	1.93	0.41
4:D:148:ALA:HB1	4:D:279:LEU:HB2	2.02	0.41
31:D:406:LMG:O9	31:D:406:LMG:HC1	2.20	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.93	0.41
3:C:282:MET:HG2	22:C:501:CLA:H61	2.12	0.41
25:J:102:BCR:H351	25:J:102:BCR:H15C	1.75	0.41
22:A:403:CLA:HBA1	22:A:403:CLA:H3A	3.98	0.41
4:D:113:PHE:O	4:D:117:HIS:HB2	2.24	0.41
4:D:210:LEU:HA	4:D:213:ILE:HG22	2.07	0.41
4:D:156:VAL:HG12	4:D:171:PRO:HG3	2.02	0.41
5:E:14:ILE:HG22	9:J:13:VAL:HG11	2.08	0.41
18:X:17:LYS:O	18:X:21:ILE:HG13	2.22	0.41
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.98	0.41
22:A:403:CLA:H151	23:D:401:PHO:H72	39.38	0.41
2:B:222:PRO:HD2	2:B:225:LEU:HD12	2.15	0.41
22:B:607:CLA:H51	22:B:608:CLA:H101	2.02	0.41
22:B:612:CLA:CHA	22:B:612:CLA:HBA1	5.05	0.41
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.93	0.41
3:C:265:ILE:HD11	8:I:28:PRO:HB3	2.02	0.41
3:C:116:VAL:HG21	25:C:520:BCR:HC21	2.02	0.41
22:C:505:CLA:H161	22:C:505:CLA:H202	1.90	0.41
22:B:613:CLA:H112	22:B:613:CLA:H91	1.85	0.41
25:F:102:BCR:H15C	25:F:102:BCR:H351	1.92	0.41
5:E:10:PHE:HE1	34:F:101:HEM:HBD2	1.98	0.41
4:D:312:GLU:HB2	13:O:185:PRO:CG	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:158:GLY:HA3	16:V:162:TYR:HD2	2.03	0.41
2:B:30:VAL:HG12	22:B:604:CLA:HHD	2.02	0.41
22:B:609:CLA:H12	22:B:609:CLA:H51	1.88	0.41
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.07	0.41
5:E:50:PRO:HB3	5:E:54:SER:O	2.30	0.41
2:B:305:ILE:HA	2:B:306:PRO:HD2	1.95	0.41
4:D:342:PRO:O	4:D:345:VAL:HG12	2.23	0.41
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.31	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.41
25:J:102:BCR:H11C	25:J:102:BCR:H341	1.82	0.41
3:C:437:PHE:HZ	22:C:509:CLA:HMB3	1.86	0.41
22:B:604:CLA:H161	22:B:604:CLA:H141	1.88	0.41
22:B:614:CLA:H51	22:B:614:CLA:H12	3.14	0.41
4:D:48:TRP:CD2	23:D:401:PHO:H161	2.56	0.41
22:B:606:CLA:H61	7:H:46:LEU:HB2	31.05	0.41
32:B:624:LMT:H102	7:H:35:MET:SD	2.61	0.41
1:A:262:TYR:CZ	31:E:101:LMG:HC5	2.71	0.41
3:C:386:PRO:O	3:C:390:ARG:HG2	2.27	0.41
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.56	0.41
3:C:334:PRO:HA	13:O:179:THR:OG1	2.21	0.41
3:C:57:ALA:O	3:C:61:VAL:HG23	2.22	0.41
3:C:119:LEU:HG	25:C:513:BCR:H10C	39.47	0.41
22:B:602:CLA:H61	22:B:602:CLA:H41	1.64	0.41
1:A:334:ARG:NH1	13:O:183:LEU:O	2.66	0.41
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.03	0.41
11:L:11:GLU:HG2	11:L:12:LEU:N	2.35	0.41
12:M:19:SER:O	12:M:23:ILE:HG13	2.25	0.41
22:B:602:CLA:CBB	22:B:604:CLA:H152	2.51	0.40
22:B:606:CLA:H41	22:B:606:CLA:H93	4.04	0.40
5:E:84:LYS:HZ2	5:E:84:LYS:HB2	1.85	0.40
3:C:29:GLU:OE1	3:C:31:SER:HB2	2.34	0.40
1:A:223:LEU:HD13	4:D:265:ARG:HD3	2.16	0.40
1:A:96:ILE:HD12	22:A:406:CLA:HMD1	2.06	0.40
1:A:116:ILE:HG13	1:A:117:PHE:N	2.35	0.40
13:O:41:LEU:HD12	13:O:41:LEU:HA	1.95	0.40
2:B:222:PRO:HG3	7:H:26:GLY:HA3	2.12	0.40
4:D:261:PHE:HA	31:D:409:LMG:O2	48.82	0.40
20:Z:33:TRP:O	20:Z:33:TRP:HD1	2.05	0.40
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.57	0.40
3:C:257:PHE:HB3	3:C:258:GLY:H	1.61	0.40
2:B:212:ALA:O	2:B:216:HIS:ND1	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:24:ILE:HG21	31:M:101:LMG:H322	9.50	0.40
2:B:137:LYS:HE3	2:B:137:LYS:HB2	1.97	0.40
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.03	0.40
22:C:519:CLA:H161	22:C:519:CLA:H141	1.90	0.40
1:A:180:PHE:HA	1:A:183:MET:HE3	2.04	0.40
24:D:405:PL9:H372	11:L:30:LEU:HD13	2.03	0.40
16:V:81:ARG:NE	16:V:157:GLY:HA3	2.53	0.40
3:C:174:LEU:HD13	22:C:502:CLA:H111	2.07	0.40
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.04	0.40
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.63	0.40
22:A:403:CLA:H11	22:A:403:CLA:H51	1.85	0.40
22:A:404:CLA:HAB	22:D:403:CLA:H42	2.03	0.40
24:A:407:PL9:H301	4:D:42:TYR:HA	2.03	0.40
22:B:607:CLA:H141	22:B:607:CLA:H161	2.86	0.40
22:B:613:CLA:H112	22:B:613:CLA:H152	1.81	0.40
25:B:616:BCR:H351	25:B:616:BCR:H15C	1.88	0.40
22:C:511:CLA:H61	22:C:511:CLA:H13	2.04	0.40
15:U:106:ARG:HA	15:U:109:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	16	61
1	a	333/344 (97%)	311 (93%)	18 (5%)	4 (1%)	16	61
2	B	488/510 (96%)	451 (92%)	33 (7%)	4 (1%)	24	69
2	b	488/510 (96%)	449 (92%)	36 (7%)	3 (1%)	30	73
3	C	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	21	66
3	c	445/461 (96%)	405 (91%)	36 (8%)	4 (1%)	21	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	46 82
4	d	338/352 (96%)	316 (94%)	21 (6%)	1 (0%)	46 82
5	E	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	15 59
5	e	80/84 (95%)	76 (95%)	3 (4%)	1 (1%)	15 59
6	F	33/45 (73%)	29 (88%)	4 (12%)	0	100 100
6	f	33/45 (73%)	29 (88%)	4 (12%)	0	100 100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3 31
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	3 31
8	I	33/38 (87%)	27 (82%)	6 (18%)	0	100 100
8	i	33/38 (87%)	27 (82%)	6 (18%)	0	100 100
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 41
9	j	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5 41
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
10	k	35/46 (76%)	32 (91%)	3 (9%)	0	100 100
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	l	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
12	M	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
12	m	32/36 (89%)	29 (91%)	3 (9%)	0	100 100
13	O	241/272 (89%)	207 (86%)	31 (13%)	3 (1%)	16 61
13	o	241/272 (89%)	208 (86%)	30 (12%)	3 (1%)	16 61
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	5 40
14	t	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	5 40
15	U	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9 50
15	u	95/134 (71%)	87 (92%)	6 (6%)	2 (2%)	9 50
16	V	135/163 (83%)	123 (91%)	12 (9%)	0	100 100
16	v	135/163 (83%)	124 (92%)	11 (8%)	0	100 100
17	g	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4 37
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4 37
18	X	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 27
18	x	35/41 (85%)	31 (89%)	2 (6%)	2 (6%)	2 27
20	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11 54
All	All	5138/5618 (92%)	4677 (91%)	406 (8%)	55 (1%)	17 63

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
2	B	484	PRO
2	B	488	PRO
7	H	18	TYR
13	O	52	ALA
1	a	12	ASN
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
1	A	141	PRO
3	C	257	PHE
3	C	416	SER
14	T	30	THR
17	y	43	ARG
18	X	12	ILE
18	X	45	LYS
20	Z	32	ASP
1	a	141	PRO
3	c	257	PHE
3	c	416	SER
13	o	52	ALA
14	t	30	THR
17	g	43	ARG
18	x	12	ILE
18	x	45	LYS
20	z	32	ASP
2	B	489	GLU
3	C	32	GLY
4	D	239	GLN
7	H	26	GLY
9	J	38	SER
13	O	88	GLU
13	O	271	PRO
2	b	489	GLU
3	c	32	GLY
4	d	239	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	e	82	GLN
9	j	38	SER
13	o	88	GLU
1	A	142	TRP
1	A	334	ARG
5	E	82	GLN
1	a	334	ARG
13	o	271	PRO
15	u	73	PRO
7	H	16	SER
15	U	73	PRO
3	c	144	SER
7	h	16	SER
7	h	26	GLY
3	C	144	SER
15	U	83	ALA
1	a	142	TRP
15	u	83	ALA
2	B	176	GLY

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	271/280 (97%)	267 (98%)	4 (2%)	72 89
1	a	271/280 (97%)	267 (98%)	4 (2%)	72 89
2	B	390/407 (96%)	381 (98%)	9 (2%)	58 83
2	b	390/407 (96%)	381 (98%)	9 (2%)	58 83
3	C	347/362 (96%)	336 (97%)	11 (3%)	46 77
3	c	347/362 (96%)	336 (97%)	11 (3%)	46 77
4	D	275/283 (97%)	269 (98%)	6 (2%)	60 84
4	d	275/283 (97%)	267 (97%)	8 (3%)	50 78
5	E	72/73 (99%)	70 (97%)	2 (3%)	51 79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	e	72/73 (99%)	70 (97%)	2 (3%)	51 79
6	F	29/39 (74%)	29 (100%)	0	100 100
6	f	29/39 (74%)	29 (100%)	0	100 100
7	H	53/55 (96%)	49 (92%)	4 (8%)	17 55
7	h	53/55 (96%)	49 (92%)	4 (8%)	17 55
8	I	32/35 (91%)	31 (97%)	1 (3%)	47 78
8	i	32/35 (91%)	31 (97%)	1 (3%)	47 78
9	J	24/28 (86%)	23 (96%)	1 (4%)	36 71
9	j	24/28 (86%)	23 (96%)	1 (4%)	36 71
10	K	30/37 (81%)	30 (100%)	0	100 100
10	k	30/37 (81%)	30 (100%)	0	100 100
11	L	35/35 (100%)	34 (97%)	1 (3%)	50 78
11	l	35/35 (100%)	34 (97%)	1 (3%)	50 78
12	M	31/33 (94%)	31 (100%)	0	100 100
12	m	31/33 (94%)	31 (100%)	0	100 100
13	O	202/228 (89%)	200 (99%)	2 (1%)	82 92
13	o	202/228 (89%)	200 (99%)	2 (1%)	82 92
14	T	29/29 (100%)	28 (97%)	1 (3%)	44 76
14	t	29/29 (100%)	28 (97%)	1 (3%)	44 76
15	U	84/112 (75%)	83 (99%)	1 (1%)	78 90
15	u	84/112 (75%)	83 (99%)	1 (1%)	78 90
16	V	116/138 (84%)	114 (98%)	2 (2%)	68 88
16	v	116/138 (84%)	114 (98%)	2 (2%)	68 88
17	g	20/37 (54%)	18 (90%)	2 (10%)	9 40
17	y	20/37 (54%)	18 (90%)	2 (10%)	9 40
18	X	30/34 (88%)	28 (93%)	2 (7%)	20 59
18	x	30/34 (88%)	28 (93%)	2 (7%)	20 59
20	Z	52/52 (100%)	50 (96%)	2 (4%)	40 74
20	z	52/52 (100%)	50 (96%)	2 (4%)	40 74
All	All	4244/4594 (92%)	4140 (98%)	104 (2%)	55 82

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	THR
1	A	243	GLU
1	A	271	LEU
1	A	286	THR
2	B	18	ARG
2	B	23	HIS
2	B	262	THR
2	B	309	LEU
2	B	362	PHE
2	B	422	ARG
2	B	485	GLU
2	B	486	LEU
2	B	490	GLN
3	C	29	GLU
3	C	86	LEU
3	C	104	GLU
3	C	174	LEU
3	C	201	ASN
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	355	THR
3	C	391	ARG
3	C	472	LEU
4	D	43	LEU
4	D	180	ARG
4	D	241	GLU
4	D	259	ILE
4	D	291	LEU
4	D	346	LEU
5	E	18	ARG
5	E	84	LYS
7	H	27	THR
7	H	49	TYR
7	H	56	ASP
7	H	60	VAL
8	I	33	LYS
9	J	7	ARG
11	L	7	ARG
13	O	31	LEU
13	O	97	VAL
14	T	29	ILE
15	U	132	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	V	92	ARG
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU
18	X	12	ILE
18	X	45	LYS
20	Z	33	TRP
20	Z	62	VAL
1	a	228	THR
1	a	243	GLU
1	a	271	LEU
1	a	286	THR
2	b	18	ARG
2	b	23	HIS
2	b	262	THR
2	b	309	LEU
2	b	362	PHE
2	b	422	ARG
2	b	485	GLU
2	b	486	LEU
2	b	490	GLN
3	c	29	GLU
3	c	86	LEU
3	c	104	GLU
3	c	174	LEU
3	c	201	ASN
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	355	THR
3	c	391	ARG
3	c	472	LEU
4	d	43	LEU
4	d	180	ARG
4	d	205	LEU
4	d	241	GLU
4	d	259	ILE
4	d	291	LEU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	84	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	h	27	THR
7	h	49	TYR
7	h	56	ASP
7	h	60	VAL
8	i	33	LYS
9	j	7	ARG
11	l	7	ARG
13	o	31	LEU
13	o	97	VAL
14	t	29	ILE
15	u	132	LEU
16	v	92	ARG
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	12	ILE
18	x	45	LYS
20	z	33	TRP
20	z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	266	ASN
4	D	117	HIS
4	D	332	GLN
1	a	241	GLN
4	d	117	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 184 ligands modelled in this entry, 8 are monoatomic - leaving 176 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	$\#\|Z\|>2$
22	CLA	A	402	-	55,73,73	0.94	4 (7%)	61,113,113	1.18	6 (9%)
22	CLA	A	403	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	6 (9%)
22	CLA	A	404	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
23	PHO	A	405	-	67,69,69	1.21	8 (11%)	84,99,99	0.99	4 (4%)
22	CLA	A	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	7 (11%)
24	PL9	A	407	-	45,45,55	1.09	3 (6%)	56,57,69	1.58	11 (19%)
25	BCR	A	408	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	7 (12%)
26	DGD	A	409	-	57,57,67	0.95	0	71,71,81	1.46	9 (12%)
27	LHG	A	410	-	38,38,48	0.69	0	39,44,54	1.19	3 (7%)
29	OEX	A	412	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	A	413	-	50,51,54	0.95	3 (6%)	58,62,65	2.00	9 (15%)
30	SQD	A	414	-	53,54,54	0.94	3 (5%)	61,65,65	1.68	9 (14%)
22	CLA	B	601	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	B	602	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	9 (14%)
22	CLA	B	603	-	55,73,73	0.96	3 (5%)	61,113,113	1.25	8 (13%)
22	CLA	B	604	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	8 (13%)
22	CLA	B	605	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	6 (9%)
22	CLA	B	606	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	8 (13%)
22	CLA	B	607	-	55,73,73	0.97	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	B	608	-	55,73,73	0.98	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	B	609	-	55,73,73	0.96	3 (5%)	61,113,113	1.25	7 (11%)
22	CLA	B	610	-	55,73,73	1.02	4 (7%)	61,113,113	1.40	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	611	-	55,73,73	0.94	4 (7%)	61,113,113	1.21	8 (13%)
22	CLA	B	612	-	55,73,73	0.92	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	B	613	-	55,73,73	0.93	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	B	614	-	55,73,73	0.95	4 (7%)	61,113,113	1.22	8 (13%)
22	CLA	B	615	-	55,73,73	0.94	4 (7%)	61,113,113	1.17	6 (9%)
25	BCR	B	616	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
25	BCR	B	617	-	41,41,41	1.04	2 (4%)	56,56,56	1.38	8 (14%)
25	BCR	B	618	-	41,41,41	1.09	2 (4%)	56,56,56	1.39	11 (19%)
25	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	8 (14%)
26	DGD	B	620	-	59,59,67	0.92	0	73,73,81	1.35	6 (8%)
31	LMG	B	621	-	49,49,55	0.78	2 (4%)	57,57,63	1.32	6 (10%)
30	SQD	B	622	-	42,43,54	1.04	3 (7%)	50,54,65	1.98	10 (20%)
32	LMT	B	623	-	36,36,36	1.10	4 (11%)	47,47,47	1.04	2 (4%)
32	LMT	B	624	-	36,36,36	1.07	3 (8%)	47,47,47	1.03	2 (4%)
31	LMG	B	625	-	49,49,55	0.76	0	57,57,63	1.34	7 (12%)
26	DGD	B	626	-	53,53,67	1.05	4 (7%)	67,67,81	1.35	8 (11%)
30	SQD	B	627	-	46,47,54	1.01	3 (6%)	54,58,65	2.02	9 (16%)
32	LMT	B	628	-	36,36,36	1.09	5 (13%)	47,47,47	1.04	2 (4%)
32	LMT	B	629	-	36,36,36	1.11	4 (11%)	47,47,47	1.06	1 (2%)
22	CLA	C	501	-	55,73,73	0.96	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	C	502	-	55,73,73	0.96	4 (7%)	61,113,113	1.23	7 (11%)
22	CLA	C	503	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	7 (11%)
22	CLA	C	504	-	55,73,73	0.96	3 (5%)	61,113,113	1.25	9 (14%)
22	CLA	C	505	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	C	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	8 (13%)
22	CLA	C	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.27	7 (11%)
22	CLA	C	508	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	C	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.17	6 (9%)
22	CLA	C	510	3	55,73,73	0.94	3 (5%)	61,113,113	1.24	6 (9%)
22	CLA	C	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.22	9 (14%)
22	CLA	C	512	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	8 (13%)
25	BCR	C	513	-	41,41,41	1.08	3 (7%)	56,56,56	1.31	8 (14%)
26	DGD	C	514	-	54,54,67	0.96	2 (3%)	68,68,81	1.28	7 (10%)
26	DGD	C	515	-	63,63,67	0.91	1 (1%)	77,77,81	1.44	13 (16%)
26	DGD	C	516	-	67,67,67	0.87	2 (2%)	81,81,81	1.45	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
31	LMG	C	517	-	45,45,55	0.76	0	53,53,63	1.31	6 (11%)
27	LHG	C	518	-	36,36,48	0.70	0	37,42,54	1.29	4 (10%)
22	CLA	C	519	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	8 (13%)
25	BCR	C	520	-	41,41,41	1.06	2 (4%)	56,56,56	1.22	8 (14%)
31	LMG	C	521	-	48,48,55	0.76	0	56,56,63	1.31	5 (8%)
23	PHO	D	401	-	67,69,69	1.22	9 (13%)	84,99,99	0.99	5 (5%)
33	BCT	D	402	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	D	403	-	55,73,73	0.95	3 (5%)	61,113,113	1.18	8 (13%)
22	CLA	D	404	-	55,73,73	0.95	3 (5%)	61,113,113	1.21	7 (11%)
24	PL9	D	405	-	55,55,55	1.27	4 (7%)	68,69,69	1.61	17 (25%)
31	LMG	D	406	-	48,48,55	0.77	0	56,56,63	1.40	5 (8%)
26	DGD	D	407	-	64,64,67	0.96	2 (3%)	78,78,81	1.34	10 (12%)
32	LMT	D	408	-	32,32,36	1.15	5 (15%)	43,43,47	1.05	2 (4%)
31	LMG	D	409	-	46,46,55	0.79	2 (4%)	54,54,63	1.32	4 (7%)
31	LMG	E	101	-	44,44,55	0.75	1 (2%)	52,52,63	1.30	4 (7%)
34	HEM	F	101	5,6	30,50,50	2.13	8 (26%)	24,82,82	2.31	9 (37%)
25	BCR	F	102	-	41,41,41	1.11	2 (4%)	56,56,56	1.25	7 (12%)
30	SQD	F	103	-	44,45,54	1.03	3 (6%)	52,56,65	1.82	10 (19%)
22	CLA	H	101	-	55,73,73	0.95	3 (5%)	61,113,113	1.17	7 (11%)
25	BCR	H	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	5 (8%)
31	LMG	I	101	-	43,43,55	0.84	1 (2%)	51,51,63	1.26	4 (7%)
32	LMT	I	102	-	36,36,36	1.08	5 (13%)	47,47,47	1.11	2 (4%)
24	PL9	J	101	-	35,35,55	1.18	1 (2%)	44,45,69	1.59	6 (13%)
25	BCR	J	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.61	13 (23%)
25	BCR	K	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	10 (17%)
31	LMG	L	101	-	51,51,55	0.75	1 (1%)	59,59,63	1.35	6 (10%)
31	LMG	M	101	-	42,42,55	0.86	1 (2%)	50,50,63	1.24	4 (8%)
32	LMT	M	102	-	36,36,36	1.11	6 (16%)	47,47,47	1.05	2 (4%)
32	LMT	M	103	-	36,36,36	1.10	5 (13%)	47,47,47	1.04	3 (6%)
34	HEM	V	201	16	30,50,50	2.23	9 (30%)	24,82,82	2.23	6 (25%)
30	SQD	a	401	-	53,54,54	0.94	3 (5%)	61,65,65	1.68	9 (14%)
31	LMG	a	402	-	42,42,55	0.87	2 (4%)	50,50,63	1.23	4 (8%)
22	CLA	a	403	-	55,73,73	0.96	3 (5%)	61,113,113	1.22	6 (9%)
22	CLA	a	404	-	55,73,73	0.94	3 (5%)	61,113,113	1.20	6 (9%)
22	CLA	a	405	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	a	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	7 (11%)
24	PL9	a	407	-	45,45,55	1.14	3 (6%)	56,57,69	1.61	14 (25%)
26	DGD	a	408	-	57,57,67	0.95	0	71,71,81	1.41	9 (12%)
27	LHG	a	409	-	38,38,48	0.67	1 (2%)	39,44,54	1.21	3 (7%)
29	OEX	a	411	1,3	0,15,15	0.00	-	0,32,32	0.00	-
30	SQD	a	412	-	50,51,54	0.95	3 (6%)	58,62,65	1.97	9 (15%)
26	DGD	b	601	-	53,53,67	1.04	4 (7%)	67,67,81	1.36	8 (11%)
30	SQD	b	602	-	46,47,54	1.02	4 (8%)	54,58,65	2.05	9 (16%)
32	LMT	b	603	-	36,36,36	1.10	5 (13%)	47,47,47	1.00	1 (2%)
32	LMT	b	604	-	36,36,36	1.10	5 (13%)	47,47,47	1.07	1 (2%)
22	CLA	b	605	-	55,73,73	0.95	4 (7%)	61,113,113	1.23	8 (13%)
22	CLA	b	606	-	55,73,73	0.96	4 (7%)	61,113,113	1.19	7 (11%)
22	CLA	b	607	-	55,73,73	0.95	3 (5%)	61,113,113	1.19	8 (13%)
22	CLA	b	608	-	55,73,73	0.95	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	609	-	55,73,73	0.95	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	b	610	-	55,73,73	0.93	4 (7%)	61,113,113	1.20	6 (9%)
22	CLA	b	611	-	55,73,73	0.96	3 (5%)	61,113,113	1.15	6 (9%)
22	CLA	b	612	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	b	613	-	55,73,73	0.97	3 (5%)	61,113,113	1.18	7 (11%)
22	CLA	b	614	-	55,73,73	0.94	3 (5%)	61,113,113	1.23	8 (13%)
22	CLA	b	615	-	55,73,73	1.02	4 (7%)	61,113,113	1.37	8 (13%)
22	CLA	b	616	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	8 (13%)
22	CLA	b	617	-	55,73,73	0.93	3 (5%)	61,113,113	1.23	7 (11%)
22	CLA	b	618	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	7 (11%)
22	CLA	b	619	-	55,73,73	0.94	4 (7%)	61,113,113	1.20	9 (14%)
22	CLA	b	620	-	55,73,73	0.93	4 (7%)	61,113,113	1.16	6 (9%)
25	BCR	b	621	-	41,41,41	1.08	2 (4%)	56,56,56	1.24	6 (10%)
25	BCR	b	622	-	41,41,41	1.05	2 (4%)	56,56,56	1.37	8 (14%)
25	BCR	b	623	-	41,41,41	1.09	2 (4%)	56,56,56	1.39	11 (19%)
25	BCR	b	624	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	9 (16%)
26	DGD	b	625	-	59,59,67	0.91	0	73,73,81	1.38	7 (9%)
31	LMG	b	626	-	49,49,55	0.79	1 (2%)	57,57,63	1.34	7 (12%)
31	LMG	b	627	-	42,42,55	0.85	1 (2%)	50,50,63	1.24	4 (8%)
32	LMT	b	628	-	36,36,36	1.10	5 (13%)	47,47,47	1.04	2 (4%)
32	LMT	b	629	-	36,36,36	1.08	5 (13%)	47,47,47	1.07	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	c	501	-	55,73,73	0.96	3 (5%)	61,113,113	1.17	7 (11%)
22	CLA	c	502	-	55,73,73	0.97	4 (7%)	61,113,113	1.22	8 (13%)
22	CLA	c	503	-	55,73,73	0.95	3 (5%)	61,113,113	1.24	7 (11%)
22	CLA	c	504	-	55,73,73	0.97	3 (5%)	61,113,113	1.26	8 (13%)
22	CLA	c	505	-	55,73,73	0.94	3 (5%)	61,113,113	1.24	7 (11%)
22	CLA	c	506	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	c	507	-	55,73,73	0.95	3 (5%)	61,113,113	1.28	7 (11%)
22	CLA	c	508	-	55,73,73	0.94	3 (5%)	61,113,113	1.19	7 (11%)
22	CLA	c	509	-	55,73,73	0.96	3 (5%)	61,113,113	1.20	7 (11%)
22	CLA	c	510	3	55,73,73	0.93	3 (5%)	61,113,113	1.22	7 (11%)
22	CLA	c	511	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
22	CLA	c	512	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
25	BCR	c	513	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	11 (19%)
25	BCR	c	514	-	41,41,41	1.07	2 (4%)	56,56,56	1.32	7 (12%)
26	DGD	c	515	-	54,54,67	0.95	1 (1%)	68,68,81	1.31	8 (11%)
26	DGD	c	516	-	63,63,67	0.91	2 (3%)	77,77,81	1.45	12 (15%)
26	DGD	c	517	-	67,67,67	0.89	2 (2%)	81,81,81	1.42	10 (12%)
31	LMG	c	518	-	45,45,55	0.76	0	53,53,63	1.30	6 (11%)
27	LHG	c	519	-	36,36,48	0.74	1 (2%)	37,42,54	1.28	4 (10%)
22	CLA	c	520	-	55,73,73	0.94	3 (5%)	61,113,113	1.21	8 (13%)
25	BCR	c	521	-	41,41,41	1.05	2 (4%)	56,56,56	1.24	7 (12%)
31	LMG	c	522	-	48,48,55	0.77	1 (2%)	56,56,63	1.29	6 (10%)
23	PHO	d	401	-	67,69,69	1.19	8 (11%)	84,99,99	1.01	4 (4%)
23	PHO	d	402	-	67,69,69	1.23	8 (11%)	84,99,99	1.01	5 (5%)
30	SQD	d	403	-	42,43,54	1.03	3 (7%)	50,54,65	1.90	10 (20%)
33	BCT	d	404	21	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	d	405	-	55,73,73	0.95	4 (7%)	61,113,113	1.16	8 (13%)
22	CLA	d	406	-	55,73,73	0.95	3 (5%)	61,113,113	1.20	7 (11%)
24	PL9	d	407	-	55,55,55	1.20	4 (7%)	68,69,69	1.61	16 (23%)
31	LMG	d	408	-	49,49,55	0.76	0	57,57,63	1.35	7 (12%)
31	LMG	d	409	-	48,48,55	0.77	1 (2%)	56,56,63	1.41	4 (7%)
26	DGD	d	410	-	64,64,67	0.93	1 (1%)	78,78,81	1.38	10 (12%)
32	LMT	d	411	-	32,32,36	1.15	5 (15%)	43,43,47	1.05	2 (4%)
31	LMG	d	412	-	46,46,55	0.79	1 (2%)	54,54,63	1.30	5 (9%)
31	LMG	e	101	-	44,44,55	0.77	1 (2%)	52,52,63	1.29	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HEM	f	101	5,6	30,50,50	2.14	10 (33%)	24,82,82	2.32	10 (41%)
25	BCR	f	102	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
30	SQD	f	103	-	44,45,54	1.01	3 (6%)	52,56,65	1.83	10 (19%)
25	BCR	g	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.33	8 (14%)
25	BCR	i	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.24	6 (10%)
31	LMG	i	102	-	43,43,55	0.83	0	51,51,63	1.26	4 (7%)
32	LMT	i	103	-	36,36,36	1.07	4 (11%)	47,47,47	1.10	2 (4%)
24	PL9	j	101	-	35,35,55	1.26	2 (5%)	44,45,69	1.57	6 (13%)
25	BCR	j	102	-	41,41,41	1.03	2 (4%)	56,56,56	1.54	13 (23%)
31	LMG	l	101	-	51,51,55	0.74	1 (1%)	59,59,63	1.34	6 (10%)
31	LMG	m	101	-	42,42,55	0.86	2 (4%)	50,50,63	1.24	4 (8%)
34	HEM	v	201	16	30,50,50	2.21	11 (36%)	24,82,82	2.23	6 (25%)
25	BCR	x	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.21	5 (8%)
25	BCR	y	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.28	6 (10%)

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
22	CLA	A	402	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	PHO	A	405	-	-	0/53/103/103	0/1/6/6
22	CLA	A	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PL9	A	407	-	-	0/41/61/73	0/1/1/1
25	BCR	A	408	-	-	0/29/63/63	0/2/2/2
26	DGD	A	409	-	-	0/45/85/95	0/2/2/2
27	LHG	A	410	-	-	0/43/43/53	0/0/0/0
29	OEX	A	412	1,3	-	0/0/68/68	0/0/6/6
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
30	SQD	A	414	-	-	0/49/69/69	0/1/1/1
22	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	616	-	-	0/29/63/63	0/2/2/2
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	DGD	B	620	-	-	0/47/87/95	0/2/2/2
31	LMG	B	621	-	-	0/44/64/70	0/1/1/1
30	SQD	B	622	-	-	1/38/58/69	0/1/1/1
32	LMT	B	623	-	-	0/21/61/61	0/2/2/2
32	LMT	B	624	-	-	0/21/61/61	0/2/2/2
31	LMG	B	625	-	-	0/44/64/70	0/1/1/1
26	DGD	B	626	-	-	0/41/81/95	0/2/2/2
30	SQD	B	627	-	-	0/42/62/69	0/1/1/1
32	LMT	B	628	-	-	0/21/61/61	0/2/2/2
32	LMT	B	629	-	-	0/21/61/61	0/2/2/2
22	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	C	513	-	-	0/29/63/63	0/2/2/2
26	DGD	C	514	-	-	0/42/82/95	0/2/2/2
26	DGD	C	515	-	-	1/51/91/95	0/2/2/2
26	DGD	C	516	-	-	0/55/95/95	0/2/2/2
31	LMG	C	517	-	-	0/40/60/70	0/1/1/1
27	LHG	C	518	-	-	0/41/41/53	0/0/0/0
22	CLA	C	519	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	C	520	-	-	0/29/63/63	0/2/2/2
31	LMG	C	521	-	-	0/43/63/70	0/1/1/1
23	PHO	D	401	-	-	0/53/103/103	0/1/6/6
33	BCT	D	402	21	-	0/0/0/0	0/0/0/0
22	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	D	404	-	2/2/20/25	0/37/135/135	0/0/9/9
24	PL9	D	405	-	-	0/53/73/73	0/1/1/1
31	LMG	D	406	-	-	0/43/63/70	0/1/1/1
26	DGD	D	407	-	-	0/52/92/95	0/2/2/2
32	LMT	D	408	-	-	0/17/57/61	0/2/2/2
31	LMG	D	409	-	-	0/41/61/70	0/1/1/1
31	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/10/54/54	0/0/8/8
25	BCR	F	102	-	-	0/29/63/63	0/2/2/2
30	SQD	F	103	-	-	0/40/60/69	0/1/1/1
22	CLA	H	101	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	H	102	-	-	0/29/63/63	0/2/2/2
31	LMG	I	101	-	-	0/38/58/70	0/1/1/1
32	LMT	I	102	-	-	0/21/61/61	0/2/2/2
24	PL9	J	101	-	-	0/29/49/73	0/1/1/1
25	BCR	J	102	-	-	0/29/63/63	0/2/2/2
25	BCR	K	101	-	-	0/29/63/63	0/2/2/2
31	LMG	L	101	-	-	0/46/66/70	0/1/1/1
31	LMG	M	101	-	-	0/37/57/70	0/1/1/1
32	LMT	M	102	-	-	0/21/61/61	0/2/2/2
32	LMT	M	103	-	-	0/21/61/61	0/2/2/2
34	HEM	V	201	16	-	0/10/54/54	0/0/8/8
30	SQD	a	401	-	-	0/49/69/69	0/1/1/1
31	LMG	a	402	-	-	0/37/57/70	0/1/1/1
22	CLA	a	403	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PL9	a	407	-	-	0/41/61/73	0/1/1/1
26	DGD	a	408	-	-	0/45/85/95	0/2/2/2
27	LHG	a	409	-	-	0/43/43/53	0/0/0/0
29	OEX	a	411	1,3	-	0/0/68/68	0/0/6/6
30	SQD	a	412	-	-	0/46/66/69	0/1/1/1
26	DGD	b	601	-	-	0/41/81/95	0/2/2/2
30	SQD	b	602	-	-	0/42/62/69	0/1/1/1
32	LMT	b	603	-	-	0/21/61/61	0/2/2/2
32	LMT	b	604	-	-	0/21/61/61	0/2/2/2
22	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	621	-	-	0/29/63/63	0/2/2/2
25	BCR	b	622	-	-	0/29/63/63	0/2/2/2
25	BCR	b	623	-	-	0/29/63/63	0/2/2/2
25	BCR	b	624	-	-	0/29/63/63	0/2/2/2
26	DGD	b	625	-	-	0/47/87/95	0/2/2/2
31	LMG	b	626	-	-	0/44/64/70	0/1/1/1
31	LMG	b	627	-	-	0/37/57/70	0/1/1/1
32	LMT	b	628	-	-	0/21/61/61	0/2/2/2
32	LMT	b	629	-	-	0/21/61/61	0/2/2/2
22	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	c	513	-	-	0/29/63/63	0/2/2/2
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
26	DGD	c	515	-	-	0/42/82/95	0/2/2/2
26	DGD	c	516	-	-	1/51/91/95	0/2/2/2
26	DGD	c	517	-	-	0/55/95/95	0/2/2/2
31	LMG	c	518	-	-	0/40/60/70	0/1/1/1
27	LHG	c	519	-	-	0/41/41/53	0/0/0/0
22	CLA	c	520	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	c	521	-	-	0/29/63/63	0/2/2/2
31	LMG	c	522	-	-	0/43/63/70	0/1/1/1
23	PHO	d	401	-	-	0/53/103/103	0/1/6/6
23	PHO	d	402	-	-	0/53/103/103	0/1/6/6
30	SQD	d	403	-	-	1/38/58/69	0/1/1/1
33	BCT	d	404	21	-	0/0/0/0	0/0/0/0
22	CLA	d	405	-	3/3/20/25	0/37/135/135	0/0/9/9
22	CLA	d	406	-	2/2/20/25	0/37/135/135	0/0/9/9
24	PL9	d	407	-	-	0/53/73/73	0/1/1/1
31	LMG	d	408	-	-	0/44/64/70	0/1/1/1
31	LMG	d	409	-	-	0/43/63/70	0/1/1/1
26	DGD	d	410	-	-	0/52/92/95	0/2/2/2
32	LMT	d	411	-	-	0/17/57/61	0/2/2/2
31	LMG	d	412	-	-	0/41/61/70	0/1/1/1
31	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/10/54/54	0/0/8/8
25	BCR	f	102	-	-	0/29/63/63	0/2/2/2
30	SQD	f	103	-	-	0/40/60/69	0/1/1/1
25	BCR	g	101	-	-	0/29/63/63	0/2/2/2
25	BCR	i	101	-	-	0/29/63/63	0/2/2/2
31	LMG	i	102	-	-	0/38/58/70	0/1/1/1
32	LMT	i	103	-	-	0/21/61/61	0/2/2/2
24	PL9	j	101	-	-	0/29/49/73	0/1/1/1
25	BCR	j	102	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	l	101	-	-	0/46/66/70	0/1/1/1
31	LMG	m	101	-	-	0/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/10/54/54	0/0/8/8
25	BCR	x	101	-	-	0/29/63/63	0/2/2/2
25	BCR	y	101	-	-	0/29/63/63	0/2/2/2

All (502) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	V	201	HEM	C3B-C4B	-7.42	1.45	1.51
34	v	201	HEM	C3B-C4B	-7.17	1.45	1.51
34	F	101	HEM	C3B-C4B	-6.48	1.46	1.51
34	f	101	HEM	C3B-C4B	-6.31	1.46	1.51
24	D	405	PL9	C7-C3	-5.63	1.47	1.51
34	f	101	HEM	C3D-C4D	-5.45	1.44	1.51
34	F	101	HEM	C3D-C4D	-5.36	1.44	1.51
24	d	407	PL9	C7-C3	-5.11	1.47	1.51
24	j	101	PL9	C7-C3	-5.08	1.47	1.51
34	V	201	HEM	C3D-C4D	-4.96	1.45	1.51
34	v	201	HEM	C3D-C4D	-4.83	1.45	1.51
24	a	407	PL9	C7-C3	-4.44	1.48	1.51
24	J	101	PL9	C7-C3	-4.38	1.48	1.51
34	V	201	HEM	C2C-C1C	-4.01	1.45	1.52
24	A	407	PL9	C7-C3	-4.00	1.48	1.51
34	v	201	HEM	C2C-C1C	-3.76	1.45	1.52
34	F	101	HEM	C2C-C1C	-3.72	1.45	1.52
22	b	615	CLA	CMB-C2B	-3.68	1.44	1.51
22	B	610	CLA	CMB-C2B	-3.68	1.44	1.51
34	f	101	HEM	C2C-C1C	-3.65	1.45	1.52
25	F	102	BCR	C1-C6	-3.51	1.48	1.53
25	H	102	BCR	C1-C6	-3.49	1.48	1.53
25	x	101	BCR	C1-C6	-3.45	1.48	1.53
25	f	102	BCR	C1-C6	-3.43	1.48	1.53
25	g	101	BCR	C30-C25	-3.34	1.49	1.53
25	B	616	BCR	C1-C6	-3.34	1.49	1.53
25	y	101	BCR	C1-C6	-3.28	1.49	1.53
25	b	621	BCR	C1-C6	-3.28	1.49	1.53
25	C	513	BCR	C1-C6	-3.23	1.49	1.53
25	c	514	BCR	C1-C6	-3.22	1.49	1.53
25	b	623	BCR	C30-C25	-3.22	1.49	1.53
25	y	101	BCR	C30-C25	-3.21	1.49	1.53
25	J	102	BCR	C30-C25	-3.21	1.49	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	101	BCR	C1-C6	-3.20	1.49	1.53
25	b	622	BCR	C1-C6	-3.19	1.49	1.53
25	B	618	BCR	C30-C25	-3.16	1.49	1.53
25	j	102	BCR	C30-C25	-3.15	1.49	1.53
25	c	513	BCR	C1-C6	-3.14	1.49	1.53
25	b	624	BCR	C30-C25	-3.14	1.49	1.53
25	K	101	BCR	C1-C6	-3.13	1.49	1.53
25	C	520	BCR	C30-C25	-3.13	1.49	1.53
25	F	102	BCR	C30-C25	-3.09	1.49	1.53
25	B	619	BCR	C30-C25	-3.09	1.49	1.53
25	B	616	BCR	C30-C25	-3.06	1.49	1.53
25	i	101	BCR	C1-C6	-3.05	1.49	1.53
25	A	408	BCR	C30-C25	-3.03	1.49	1.53
25	b	624	BCR	C1-C6	-3.03	1.49	1.53
25	c	521	BCR	C30-C25	-3.02	1.49	1.53
25	B	617	BCR	C1-C6	-3.01	1.49	1.53
25	i	101	BCR	C30-C25	-3.00	1.49	1.53
25	f	102	BCR	C30-C25	-3.00	1.49	1.53
25	B	619	BCR	C1-C6	-2.99	1.49	1.53
25	B	618	BCR	C1-C6	-2.98	1.49	1.53
25	b	621	BCR	C30-C25	-2.97	1.49	1.53
25	A	408	BCR	C1-C6	-2.97	1.49	1.53
25	b	623	BCR	C1-C6	-2.97	1.49	1.53
25	C	513	BCR	C30-C25	-2.94	1.49	1.53
25	K	101	BCR	C30-C25	-2.91	1.49	1.53
25	C	520	BCR	C1-C6	-2.88	1.49	1.53
25	c	521	BCR	C1-C6	-2.80	1.49	1.53
25	c	514	BCR	C30-C25	-2.80	1.49	1.53
25	H	102	BCR	C30-C25	-2.80	1.49	1.53
25	x	101	BCR	C30-C25	-2.78	1.49	1.53
25	c	513	BCR	C30-C25	-2.77	1.49	1.53
24	D	405	PL9	C3-C4	-2.75	1.44	1.49
22	C	507	CLA	CMB-C2B	-2.69	1.46	1.51
26	C	514	DGD	O2G-C2G	-2.68	1.39	1.46
22	B	611	CLA	CMD-C2D	-2.67	1.45	1.51
22	c	507	CLA	CMB-C2B	-2.66	1.46	1.51
25	B	617	BCR	C30-C25	-2.66	1.50	1.53
25	b	622	BCR	C30-C25	-2.63	1.50	1.53
25	j	102	BCR	C1-C6	-2.62	1.50	1.53
25	J	102	BCR	C1-C6	-2.60	1.50	1.53
22	B	607	CLA	CMB-C2B	-2.60	1.46	1.51
22	B	603	CLA	CMB-C2B	-2.58	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	403	CLA	CMB-C2B	-2.57	1.46	1.51
22	b	616	CLA	CMD-C2D	-2.56	1.46	1.51
22	b	612	CLA	CMB-C2B	-2.56	1.46	1.51
32	b	629	LMT	O3'-C3'	-2.56	1.36	1.43
22	A	403	CLA	CMB-C2B	-2.55	1.46	1.51
22	A	406	CLA	CMB-C2B	-2.55	1.46	1.51
22	C	501	CLA	CMB-C2B	-2.54	1.46	1.51
22	b	609	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	609	CLA	CMB-C2B	-2.53	1.46	1.51
22	C	504	CLA	CMB-C2B	-2.53	1.46	1.51
22	C	509	CLA	CMB-C2B	-2.53	1.46	1.51
22	a	406	CLA	CMB-C2B	-2.53	1.46	1.51
22	B	605	CLA	CMB-C2B	-2.52	1.46	1.51
22	H	101	CLA	CMB-C2B	-2.52	1.46	1.51
22	C	512	CLA	CMB-C2B	-2.52	1.46	1.51
22	C	503	CLA	CMB-C2B	-2.52	1.46	1.51
22	A	402	CLA	CMB-C2B	-2.52	1.46	1.51
32	b	603	LMT	O3'-C3'	-2.52	1.36	1.43
22	C	502	CLA	CMB-C2B	-2.51	1.46	1.51
32	d	411	LMT	O3'-C3'	-2.51	1.36	1.43
22	B	601	CLA	CMB-C2B	-2.51	1.46	1.51
32	M	103	LMT	O3'-C3'	-2.51	1.36	1.43
22	c	504	CLA	CMB-C2B	-2.51	1.46	1.51
22	a	404	CLA	CMB-C2B	-2.51	1.46	1.51
22	c	504	CLA	CMD-C2D	-2.51	1.46	1.51
22	b	614	CLA	CMB-C2B	-2.51	1.46	1.51
22	c	501	CLA	CMB-C2B	-2.50	1.46	1.51
32	b	628	LMT	O3'-C3'	-2.50	1.37	1.43
24	d	407	PL9	C3-C4	-2.50	1.45	1.49
32	B	624	LMT	O3'-C3'	-2.50	1.37	1.43
22	c	520	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	618	CLA	CMB-C2B	-2.50	1.46	1.51
22	c	502	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	605	CLA	CMB-C2B	-2.50	1.46	1.51
22	c	509	CLA	CMD-C2D	-2.50	1.46	1.51
22	b	611	CLA	CMB-C2B	-2.50	1.46	1.51
22	C	508	CLA	CMB-C2B	-2.50	1.46	1.51
22	b	608	CLA	CMB-C2B	-2.49	1.46	1.51
22	C	519	CLA	CMB-C2B	-2.49	1.46	1.51
22	B	606	CLA	CMB-C2B	-2.49	1.46	1.51
32	B	623	LMT	O3'-C3'	-2.49	1.37	1.43
22	B	608	CLA	CMB-C2B	-2.49	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	CMB-C2B	-2.48	1.46	1.51
22	B	604	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.48	1.46	1.51
22	b	613	CLA	CMB-C2B	-2.48	1.46	1.51
22	c	509	CLA	CMB-C2B	-2.48	1.46	1.51
32	M	102	LMT	O3'-C3'	-2.48	1.37	1.43
32	D	408	LMT	O3'-C3'	-2.48	1.37	1.43
22	d	406	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	503	CLA	CMB-C2B	-2.47	1.46	1.51
22	c	508	CLA	CMB-C2B	-2.47	1.46	1.51
22	C	505	CLA	CMB-C2B	-2.47	1.46	1.51
32	I	102	LMT	O3'-C3'	-2.46	1.37	1.43
22	D	404	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	504	CLA	CMD-C2D	-2.46	1.46	1.51
22	c	512	CLA	CMB-C2B	-2.46	1.46	1.51
22	C	506	CLA	CMB-C2B	-2.46	1.46	1.51
22	A	404	CLA	CMB-C2B	-2.46	1.46	1.51
22	B	614	CLA	CMB-C2B	-2.45	1.46	1.51
22	a	405	CLA	CMB-C2B	-2.45	1.46	1.51
22	B	602	CLA	CMB-C2B	-2.45	1.46	1.51
32	B	628	LMT	O3'-C3'	-2.45	1.37	1.43
22	C	509	CLA	CMD-C2D	-2.44	1.46	1.51
22	C	510	CLA	CMB-C2B	-2.44	1.46	1.51
22	c	506	CLA	CMB-C2B	-2.44	1.46	1.51
22	b	612	CLA	CMD-C2D	-2.44	1.46	1.51
32	i	103	LMT	O3'-C3'	-2.43	1.37	1.43
22	C	511	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	607	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	617	CLA	CMB-C2B	-2.43	1.46	1.51
22	c	510	CLA	CMB-C2B	-2.43	1.46	1.51
22	b	610	CLA	CMB-C2B	-2.43	1.46	1.51
22	B	607	CLA	CMD-C2D	-2.42	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.42	1.46	1.51
22	B	612	CLA	CMB-C2B	-2.41	1.46	1.51
22	B	611	CLA	CMB-C2B	-2.41	1.46	1.51
22	d	405	CLA	CMB-C2B	-2.41	1.46	1.51
22	b	619	CLA	CMB-C2B	-2.41	1.46	1.51
22	D	403	CLA	CMB-C2B	-2.41	1.46	1.51
22	c	511	CLA	CMB-C2B	-2.40	1.46	1.51
22	B	603	CLA	CMD-C2D	-2.40	1.46	1.51
22	D	403	CLA	CMD-C2D	-2.39	1.46	1.51
22	b	616	CLA	CMB-C2B	-2.39	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	CMD-C2D	-2.38	1.46	1.51
22	A	404	CLA	CMD-C2D	-2.36	1.46	1.51
22	b	620	CLA	CMB-C2B	-2.36	1.46	1.51
22	a	403	CLA	CMD-C2D	-2.36	1.46	1.51
22	B	613	CLA	CMB-C2B	-2.35	1.46	1.51
32	B	629	LMT	O3'-C3'	-2.35	1.37	1.43
32	b	604	LMT	O3'-C3'	-2.35	1.37	1.43
22	b	608	CLA	CMD-C2D	-2.35	1.46	1.51
24	A	407	PL9	C3-C4	-2.35	1.45	1.49
22	A	402	CLA	CMD-C2D	-2.33	1.46	1.51
24	a	407	PL9	C3-C4	-2.33	1.45	1.49
32	I	102	LMT	O2'-C2'	-2.33	1.37	1.43
22	a	405	CLA	CMD-C2D	-2.33	1.46	1.51
22	C	508	CLA	CMD-C2D	-2.33	1.46	1.51
22	a	404	CLA	CMD-C2D	-2.33	1.46	1.51
22	b	620	CLA	CMD-C2D	-2.32	1.46	1.51
22	B	606	CLA	CMD-C2D	-2.32	1.46	1.51
22	b	605	CLA	CMD-C2D	-2.32	1.46	1.51
22	B	601	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	614	CLA	CMD-C2D	-2.31	1.46	1.51
22	c	503	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	615	CLA	CMD-C2D	-2.31	1.46	1.51
22	B	604	CLA	CMD-C2D	-2.30	1.46	1.51
22	A	403	CLA	CMD-C2D	-2.30	1.46	1.51
22	B	602	CLA	CMD-C2D	-2.30	1.46	1.51
22	b	613	CLA	CMD-C2D	-2.29	1.46	1.51
22	b	617	CLA	CMD-C2D	-2.29	1.46	1.51
22	b	611	CLA	CMD-C2D	-2.29	1.46	1.51
22	c	508	CLA	CMD-C2D	-2.29	1.46	1.51
22	c	505	CLA	CMD-C2D	-2.29	1.46	1.51
24	a	407	PL9	C53-C6	-2.29	1.46	1.50
22	c	507	CLA	CMD-C2D	-2.28	1.46	1.51
22	C	505	CLA	CMD-C2D	-2.28	1.46	1.51
32	B	629	LMT	O3B-C3B	-2.27	1.37	1.43
23	D	401	PHO	C1C-NC	-2.27	1.33	1.38
22	C	511	CLA	CMD-C2D	-2.27	1.46	1.51
23	d	402	PHO	C1C-NC	-2.27	1.33	1.38
22	B	608	CLA	CMD-C2D	-2.27	1.46	1.51
22	c	502	CLA	CMD-C2D	-2.27	1.46	1.51
22	c	511	CLA	CMD-C2D	-2.27	1.46	1.51
23	d	401	PHO	C1C-NC	-2.27	1.33	1.38
22	C	502	CLA	CMD-C2D	-2.26	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	619	CLA	CMD-C2D	-2.26	1.46	1.51
22	B	605	CLA	CMD-C2D	-2.26	1.46	1.51
22	C	503	CLA	CMD-C2D	-2.26	1.46	1.51
22	b	610	CLA	CMD-C2D	-2.26	1.46	1.51
22	A	406	CLA	CMD-C2D	-2.26	1.46	1.51
22	c	520	CLA	CMD-C2D	-2.26	1.46	1.51
32	D	408	LMT	O3B-C3B	-2.26	1.37	1.43
32	b	604	LMT	O3B-C3B	-2.26	1.37	1.43
22	b	606	CLA	CMD-C2D	-2.26	1.46	1.51
22	C	507	CLA	CMD-C2D	-2.25	1.46	1.51
22	H	101	CLA	CMD-C2D	-2.25	1.46	1.51
22	B	613	CLA	CMD-C2D	-2.25	1.46	1.51
22	a	406	CLA	CMD-C2D	-2.25	1.46	1.51
23	A	405	PHO	C1C-NC	-2.25	1.33	1.38
32	M	103	LMT	O3B-C3B	-2.25	1.37	1.43
32	b	629	LMT	O3B-C3B	-2.25	1.37	1.43
32	i	103	LMT	O2'-C2'	-2.25	1.37	1.43
22	c	512	CLA	CMD-C2D	-2.25	1.46	1.51
22	b	609	CLA	CMD-C2D	-2.24	1.46	1.51
22	b	607	CLA	CMD-C2D	-2.24	1.46	1.51
22	b	614	CLA	CMD-C2D	-2.24	1.46	1.51
22	C	519	CLA	CMD-C2D	-2.24	1.46	1.51
22	B	612	CLA	CMD-C2D	-2.24	1.46	1.51
32	B	623	LMT	O2'-C2'	-2.24	1.37	1.43
22	B	610	CLA	C3B-C2B	-2.23	1.37	1.40
31	D	409	LMG	O7-C8	-2.23	1.40	1.46
24	j	101	PL9	C3-C4	-2.23	1.45	1.49
32	b	603	LMT	O3B-C3B	-2.23	1.37	1.43
34	F	101	HEM	C2B-C1B	-2.23	1.44	1.51
32	B	629	LMT	O2'-C2'	-2.23	1.37	1.43
22	c	506	CLA	CMD-C2D	-2.22	1.46	1.51
22	d	406	CLA	CMD-C2D	-2.22	1.46	1.51
32	B	628	LMT	O2B-C2B	-2.22	1.37	1.43
22	C	506	CLA	CMD-C2D	-2.22	1.46	1.51
22	B	609	CLA	CMD-C2D	-2.22	1.46	1.51
32	b	628	LMT	O3B-C3B	-2.21	1.37	1.43
22	c	501	CLA	CMD-C2D	-2.21	1.46	1.51
25	g	101	BCR	C33-C5	-2.21	1.47	1.51
22	b	615	CLA	C3B-C2B	-2.21	1.37	1.40
32	I	102	LMT	O3B-C3B	-2.21	1.37	1.43
32	B	624	LMT	O3B-C3B	-2.21	1.37	1.43
24	A	407	PL9	C53-C6	-2.21	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	603	LMT	O2'-C2'	-2.20	1.37	1.43
32	d	411	LMT	O3B-C3B	-2.20	1.37	1.43
22	b	618	CLA	CMD-C2D	-2.20	1.46	1.51
32	M	102	LMT	O3B-C3B	-2.20	1.37	1.43
32	b	628	LMT	O2'-C2'	-2.20	1.37	1.43
22	c	510	CLA	CMD-C2D	-2.19	1.46	1.51
32	B	628	LMT	O3B-C3B	-2.19	1.37	1.43
32	i	103	LMT	O2B-C2B	-2.19	1.37	1.43
22	C	510	CLA	CMD-C2D	-2.19	1.46	1.51
22	D	404	CLA	CMD-C2D	-2.19	1.46	1.51
22	C	512	CLA	CMD-C2D	-2.19	1.46	1.51
22	B	610	CLA	CMD-C2D	-2.19	1.46	1.51
32	i	103	LMT	O3B-C3B	-2.19	1.37	1.43
22	C	501	CLA	CMD-C2D	-2.18	1.46	1.51
32	I	102	LMT	O2B-C2B	-2.17	1.37	1.43
32	b	628	LMT	O2B-C2B	-2.17	1.37	1.43
32	M	102	LMT	O2'-C2'	-2.17	1.37	1.43
32	B	624	LMT	O2'-C2'	-2.17	1.37	1.43
32	b	629	LMT	O2'-C2'	-2.17	1.37	1.43
32	b	604	LMT	O2'-C2'	-2.16	1.37	1.43
32	B	623	LMT	O3B-C3B	-2.16	1.37	1.43
22	b	615	CLA	CMD-C2D	-2.15	1.46	1.51
32	D	408	LMT	O2B-C2B	-2.15	1.37	1.43
25	y	101	BCR	C33-C5	-2.15	1.47	1.51
32	M	103	LMT	O2'-C2'	-2.15	1.37	1.43
24	D	405	PL9	C6-C1	-2.15	1.44	1.48
34	f	101	HEM	C2B-C1B	-2.14	1.44	1.51
26	C	514	DGD	O1G-C1G	-2.14	1.40	1.45
32	B	629	LMT	O2B-C2B	-2.14	1.37	1.43
32	b	603	LMT	O2B-C2B	-2.14	1.37	1.43
32	B	628	LMT	O2'-C2'	-2.13	1.37	1.43
30	b	602	SQD	O2-C2	-2.13	1.37	1.43
27	a	409	LHG	O7-C5	-2.12	1.41	1.46
32	M	103	LMT	O2B-C2B	-2.12	1.37	1.43
32	B	623	LMT	O2B-C2B	-2.12	1.37	1.43
32	d	411	LMT	O2B-C2B	-2.10	1.37	1.43
22	B	615	CLA	CMC-C2C	-2.10	1.46	1.50
30	B	627	SQD	O2-C2	-2.10	1.37	1.43
27	c	519	LHG	O7-C5	-2.09	1.41	1.46
30	a	412	SQD	O2-C2	-2.09	1.38	1.43
30	A	413	SQD	O2-C2	-2.09	1.38	1.43
23	d	401	PHO	CMC-C2C	-2.09	1.46	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	604	LMT	O2B-C2B	-2.09	1.38	1.43
23	D	401	PHO	CMC-C2C	-2.09	1.46	1.50
26	D	407	DGD	O5D-C6D	-2.09	1.39	1.43
22	b	620	CLA	CMC-C2C	-2.09	1.46	1.50
24	d	407	PL9	C53-C6	-2.08	1.46	1.50
32	d	411	LMT	O4'-C4B	-2.08	1.38	1.43
32	d	411	LMT	O2'-C2'	-2.08	1.38	1.43
34	V	201	HEM	C2D-C1D	-2.08	1.45	1.51
26	c	515	DGD	O2G-C2G	-2.07	1.41	1.46
30	A	414	SQD	O3-C3	-2.07	1.38	1.43
32	D	408	LMT	O4'-C4B	-2.07	1.38	1.43
32	b	629	LMT	O4'-C4B	-2.07	1.38	1.43
22	C	502	CLA	CMC-C2C	-2.07	1.46	1.50
32	M	102	LMT	O2B-C2B	-2.07	1.38	1.43
26	c	516	DGD	O2G-C2G	-2.07	1.41	1.46
32	I	102	LMT	O4'-C4B	-2.06	1.38	1.43
23	d	402	PHO	CMC-C2C	-2.06	1.46	1.50
34	f	101	HEM	C2D-C1D	-2.06	1.45	1.51
22	b	606	CLA	CMC-C2C	-2.06	1.46	1.50
30	a	401	SQD	O3-C3	-2.05	1.38	1.43
30	F	103	SQD	O2-C2	-2.04	1.38	1.43
32	b	629	LMT	O2B-C2B	-2.04	1.38	1.43
32	B	628	LMT	O4'-C4B	-2.04	1.38	1.43
32	b	604	LMT	O4'-C4B	-2.04	1.38	1.43
32	b	603	LMT	O4'-C4B	-2.04	1.38	1.43
32	D	408	LMT	O2'-C2'	-2.04	1.38	1.43
22	b	605	CLA	CMC-C2C	-2.04	1.46	1.50
31	a	402	LMG	O7-C8	-2.04	1.41	1.46
23	d	401	PHO	CMB-C2B	-2.04	1.46	1.50
22	c	502	CLA	CMC-C2C	-2.03	1.46	1.50
23	A	405	PHO	CMC-C2C	-2.03	1.46	1.50
26	c	516	DGD	O5D-C6D	-2.03	1.40	1.43
24	D	405	PL9	C53-C6	-2.03	1.46	1.50
24	d	407	PL9	C31-C29	-2.03	1.46	1.51
22	A	402	CLA	CMC-C2C	-2.03	1.46	1.50
22	d	405	CLA	CMC-C2C	-2.03	1.46	1.50
34	v	201	HEM	C2D-C1D	-2.02	1.45	1.51
34	F	101	HEM	C2D-C1D	-2.02	1.45	1.51
32	M	103	LMT	O4'-C4B	-2.02	1.38	1.43
30	f	103	SQD	O2-C2	-2.02	1.38	1.43
22	B	611	CLA	CMC-C2C	-2.02	1.46	1.50
32	M	102	LMT	O4'-C4B	-2.01	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	b	628	LMT	O4'-C4B	-2.01	1.38	1.43
30	B	622	SQD	O2-C2	-2.01	1.38	1.43
22	B	614	CLA	CMC-C2C	-2.01	1.46	1.50
30	b	602	SQD	O3-C3	-2.01	1.38	1.43
23	D	401	PHO	CMD-C2D	-2.01	1.46	1.50
26	C	515	DGD	O2G-C2G	-2.01	1.41	1.46
22	b	610	CLA	CMC-C2C	-2.00	1.46	1.50
30	d	403	SQD	O2-C2	-2.00	1.38	1.43
25	C	513	BCR	C38-C26	-2.00	1.47	1.51
32	M	102	LMT	O1'-C1'	-2.00	1.36	1.40
22	b	619	CLA	CMC-C2C	-2.00	1.46	1.50
34	V	201	HEM	C1C-NC	2.01	1.38	1.36
31	B	621	LMG	C7-C8	2.01	1.56	1.50
31	c	522	LMG	C7-C8	2.02	1.56	1.50
34	f	101	HEM	C3B-CAB	2.03	1.55	1.51
31	M	101	LMG	C7-C8	2.04	1.56	1.50
23	d	401	PHO	C4C-C3C	2.04	1.49	1.45
31	d	409	LMG	C7-C8	2.04	1.56	1.50
34	f	101	HEM	C1C-NC	2.05	1.38	1.36
34	F	101	HEM	FE-NC	2.05	2.03	1.95
31	E	101	LMG	C7-C8	2.06	1.56	1.50
23	D	401	PHO	C4C-C3C	2.07	1.49	1.45
26	d	410	DGD	C1D-C2D	2.09	1.58	1.52
34	v	201	HEM	C1C-NC	2.09	1.38	1.36
31	m	101	LMG	C4-C5	2.10	1.57	1.53
31	d	412	LMG	C7-C8	2.11	1.56	1.50
26	B	626	DGD	C1G-C2G	2.12	1.56	1.50
26	C	516	DGD	C3G-C2G	2.12	1.56	1.50
31	e	101	LMG	C7-C8	2.12	1.56	1.50
26	C	516	DGD	C1G-C2G	2.13	1.56	1.50
31	a	402	LMG	C4-C5	2.14	1.57	1.53
22	B	610	CLA	CHC-C1C	2.15	1.42	1.35
23	D	401	PHO	CHD-C1D	2.15	1.43	1.38
31	D	409	LMG	C7-C8	2.16	1.56	1.50
26	c	517	DGD	C3G-C2G	2.17	1.56	1.50
31	m	101	LMG	C7-C8	2.19	1.56	1.50
22	b	615	CLA	CHC-C1C	2.19	1.42	1.35
34	v	201	HEM	C3C-CAC	2.20	1.55	1.51
34	V	201	HEM	C3C-CAC	2.20	1.55	1.51
23	A	405	PHO	CHD-C1D	2.21	1.43	1.38
31	L	101	LMG	C7-C8	2.21	1.57	1.50
34	V	201	HEM	C4C-NC	2.22	1.38	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	517	DGD	C1G-C2G	2.23	1.57	1.50
34	F	101	HEM	C3C-CAC	2.23	1.55	1.51
23	d	401	PHO	C1A-NA	2.23	1.42	1.37
34	v	201	HEM	FE-NB	2.23	2.09	1.97
23	d	402	PHO	C1A-NA	2.24	1.42	1.37
26	b	601	DGD	C4D-C5D	2.24	1.57	1.53
26	b	601	DGD	C1G-C2G	2.24	1.57	1.50
23	A	405	PHO	C4C-C3C	2.24	1.49	1.45
31	b	627	LMG	C4-C5	2.25	1.57	1.53
31	I	101	LMG	C4-C5	2.25	1.57	1.53
23	D	401	PHO	C1A-NA	2.26	1.42	1.37
34	v	201	HEM	C3B-CAB	2.27	1.55	1.51
26	D	407	DGD	C1G-C2G	2.27	1.57	1.50
23	A	405	PHO	C1A-NA	2.27	1.42	1.37
31	B	621	LMG	C4-C5	2.28	1.57	1.53
31	l	101	LMG	C7-C8	2.29	1.57	1.50
26	b	601	DGD	C3G-C2G	2.29	1.57	1.50
22	a	404	CLA	CHC-C1C	2.30	1.42	1.35
34	V	201	HEM	C3B-CAB	2.30	1.55	1.51
23	d	402	PHO	C4C-C3C	2.30	1.49	1.45
34	v	201	HEM	C4C-NC	2.31	1.38	1.36
34	f	101	HEM	C3C-CAC	2.33	1.55	1.51
26	B	626	DGD	C3G-C2G	2.33	1.57	1.50
22	B	611	CLA	CHC-C1C	2.36	1.42	1.35
22	b	620	CLA	CHC-C1C	2.36	1.42	1.35
22	B	615	CLA	CHC-C1C	2.38	1.42	1.35
22	C	504	CLA	CHC-C1C	2.38	1.42	1.35
22	c	504	CLA	CHC-C1C	2.39	1.42	1.35
22	b	609	CLA	CHC-C1C	2.39	1.42	1.35
22	B	601	CLA	CHC-C1C	2.39	1.42	1.35
22	C	506	CLA	CHC-C1C	2.40	1.42	1.35
22	b	611	CLA	CHC-C1C	2.40	1.42	1.35
22	A	402	CLA	CHC-C1C	2.41	1.42	1.35
23	d	402	PHO	CHD-C1D	2.41	1.43	1.38
22	C	507	CLA	CHC-C1C	2.41	1.42	1.35
26	B	626	DGD	C4D-C5D	2.41	1.58	1.53
22	c	520	CLA	CHC-C1C	2.41	1.42	1.35
31	b	626	LMG	C4-C5	2.41	1.58	1.53
22	b	605	CLA	CHC-C1C	2.41	1.42	1.35
22	C	503	CLA	CHC-C1C	2.42	1.42	1.35
22	C	508	CLA	CHC-C1C	2.42	1.42	1.35
22	C	510	CLA	CHC-C1C	2.42	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	CHC-C1C	2.42	1.42	1.35
22	b	614	CLA	CHC-C1C	2.42	1.42	1.35
22	C	501	CLA	CHC-C1C	2.43	1.42	1.35
22	A	406	CLA	CHC-C1C	2.43	1.42	1.35
22	B	606	CLA	CHC-C1C	2.43	1.42	1.35
22	a	403	CLA	CHC-C1C	2.44	1.42	1.35
22	D	403	CLA	CHC-C1C	2.44	1.43	1.35
22	b	619	CLA	CHC-C1C	2.45	1.43	1.35
22	B	605	CLA	CHC-C1C	2.45	1.43	1.35
22	C	519	CLA	CHC-C1C	2.45	1.43	1.35
22	B	609	CLA	CHC-C1C	2.45	1.43	1.35
34	v	201	HEM	FE-NC	2.45	2.05	1.95
22	C	505	CLA	CHC-C1C	2.45	1.43	1.35
22	b	616	CLA	CHC-C1C	2.45	1.43	1.35
22	c	501	CLA	CHC-C1C	2.46	1.43	1.35
22	A	403	CLA	CHC-C1C	2.46	1.43	1.35
22	B	614	CLA	CHC-C1C	2.46	1.43	1.35
22	B	604	CLA	CHC-C1C	2.46	1.43	1.35
22	b	617	CLA	CHC-C1C	2.46	1.43	1.35
34	f	101	HEM	FE-ND	2.46	2.10	1.97
22	c	508	CLA	CHC-C1C	2.46	1.43	1.35
22	A	404	CLA	CHC-C1C	2.46	1.43	1.35
22	C	509	CLA	CHC-C1C	2.47	1.43	1.35
22	c	510	CLA	CHC-C1C	2.47	1.43	1.35
22	c	503	CLA	CHC-C1C	2.47	1.43	1.35
22	B	612	CLA	CHC-C1C	2.47	1.43	1.35
22	a	406	CLA	CHC-C1C	2.47	1.43	1.35
22	C	512	CLA	CHC-C1C	2.47	1.43	1.35
22	C	502	CLA	CHC-C1C	2.48	1.43	1.35
22	d	405	CLA	CHC-C1C	2.48	1.43	1.35
22	D	404	CLA	CHC-C1C	2.48	1.43	1.35
22	B	602	CLA	CHC-C1C	2.49	1.43	1.35
22	c	505	CLA	CHC-C1C	2.49	1.43	1.35
22	c	506	CLA	CHC-C1C	2.49	1.43	1.35
22	c	507	CLA	CHC-C1C	2.49	1.43	1.35
22	b	608	CLA	CHC-C1C	2.49	1.43	1.35
34	V	201	HEM	FE-ND	2.50	2.10	1.97
22	B	603	CLA	CHC-C1C	2.51	1.43	1.35
22	c	509	CLA	CHC-C1C	2.51	1.43	1.35
23	d	401	PHO	C4C-NC	2.51	1.42	1.37
22	a	405	CLA	CHC-C1C	2.52	1.43	1.35
22	c	511	CLA	CHC-C1C	2.53	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	CHC-C1C	2.53	1.43	1.35
23	D	401	PHO	C4C-NC	2.53	1.42	1.37
22	b	618	CLA	CHC-C1C	2.53	1.43	1.35
22	c	502	CLA	CHC-C1C	2.54	1.43	1.35
22	d	406	CLA	CHC-C1C	2.54	1.43	1.35
34	f	101	HEM	FE-NC	2.55	2.05	1.95
22	b	607	CLA	CHC-C1C	2.56	1.43	1.35
34	v	201	HEM	FE-ND	2.56	2.11	1.97
22	B	607	CLA	CHC-C1C	2.56	1.43	1.35
23	d	402	PHO	C4C-NC	2.56	1.42	1.37
22	c	512	CLA	CHC-C1C	2.56	1.43	1.35
23	A	405	PHO	C4C-NC	2.57	1.42	1.37
22	H	101	CLA	CHC-C1C	2.57	1.43	1.35
22	B	613	CLA	CHC-C1C	2.59	1.43	1.35
22	b	612	CLA	CHC-C1C	2.60	1.43	1.35
22	b	606	CLA	CHC-C1C	2.61	1.43	1.35
34	F	101	HEM	FE-ND	2.61	2.11	1.97
30	f	103	SQD	O47-C7	2.61	1.42	1.34
22	b	613	CLA	CHC-C1C	2.62	1.43	1.35
22	B	608	CLA	CHC-C1C	2.67	1.43	1.35
30	b	602	SQD	O47-C7	2.69	1.42	1.34
30	B	627	SQD	O47-C7	2.70	1.42	1.34
30	F	103	SQD	O47-C7	2.70	1.42	1.34
30	A	413	SQD	O47-C7	2.71	1.42	1.34
26	B	626	DGD	C1E-C2E	2.71	1.60	1.52
23	d	401	PHO	CHC-C1C	2.72	1.44	1.38
30	a	401	SQD	O47-C7	2.72	1.42	1.34
30	A	414	SQD	O47-C7	2.73	1.42	1.34
30	a	412	SQD	O47-C7	2.73	1.42	1.34
30	d	403	SQD	O47-C7	2.74	1.42	1.34
26	b	601	DGD	C1E-C2E	2.75	1.60	1.52
30	B	622	SQD	O47-C7	2.77	1.42	1.34
23	A	405	PHO	CHC-C1C	2.81	1.44	1.38
23	d	401	PHO	C3B-C4B	2.90	1.49	1.43
23	A	405	PHO	C3B-C4B	2.91	1.49	1.43
30	A	413	SQD	O48-C23	2.97	1.42	1.33
23	D	401	PHO	CHC-C1C	2.99	1.44	1.38
23	d	402	PHO	CHC-C1C	2.99	1.44	1.38
30	d	403	SQD	O48-C23	2.99	1.42	1.33
30	f	103	SQD	O48-C23	3.03	1.42	1.33
30	a	412	SQD	O48-C23	3.04	1.42	1.33
30	A	414	SQD	O48-C23	3.05	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	F	103	SQD	O48-C23	3.05	1.42	1.33
30	a	401	SQD	O48-C23	3.07	1.42	1.33
23	d	402	PHO	C3B-C4B	3.09	1.50	1.43
30	B	627	SQD	O48-C23	3.11	1.42	1.33
23	D	401	PHO	C3B-C4B	3.11	1.50	1.43
30	B	622	SQD	O48-C23	3.11	1.42	1.33
30	b	602	SQD	O48-C23	3.20	1.43	1.33

All (1200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	J	101	PL9	C7-C3-C2	-6.25	118.23	123.42
24	j	101	PL9	C7-C3-C2	-6.08	118.37	123.42
24	d	407	PL9	C7-C3-C2	-5.88	118.54	123.42
24	D	405	PL9	C7-C3-C2	-5.78	118.62	123.42
24	a	407	PL9	C7-C3-C2	-5.76	118.64	123.42
24	A	407	PL9	C7-C3-C2	-5.60	118.78	123.42
22	B	610	CLA	CMB-C2B-C1B	-5.07	119.98	128.36
22	b	615	CLA	CMB-C2B-C1B	-4.93	120.20	128.36
26	A	409	DGD	O3G-C3G-C2G	-4.70	99.80	110.99
26	a	408	DGD	O3G-C3G-C2G	-4.55	100.16	110.99
26	C	516	DGD	O3G-C3G-C2G	-4.43	100.45	110.99
31	d	409	LMG	C1-C2-C3	-4.32	101.46	109.97
31	D	406	LMG	C1-C2-C3	-4.28	101.54	109.97
26	c	517	DGD	O3G-C3G-C2G	-4.13	101.16	110.99
22	c	507	CLA	CMB-C2B-C1B	-3.82	122.04	128.36
22	B	612	CLA	CMB-C2B-C1B	-3.78	122.11	128.36
22	C	507	CLA	CMB-C2B-C1B	-3.74	122.17	128.36
22	b	617	CLA	CMB-C2B-C1B	-3.74	122.17	128.36
26	c	516	DGD	O5D-C6D-C5D	-3.73	102.32	109.08
26	c	516	DGD	O3G-C3G-C2G	-3.72	102.14	110.99
26	C	515	DGD	O3G-C3G-C2G	-3.72	102.15	110.99
25	J	102	BCR	C11-C10-C9	-3.69	121.86	127.20
26	C	515	DGD	O5D-C6D-C5D	-3.65	102.47	109.08
26	d	410	DGD	O6D-C1D-O3G	-3.63	101.32	110.05
26	b	625	DGD	O3G-C3G-C2G	-3.61	102.40	110.99
25	B	617	BCR	C33-C5-C6	-3.61	121.06	124.61
25	b	622	BCR	C33-C5-C6	-3.58	121.09	124.61
22	B	607	CLA	CMB-C2B-C1B	-3.58	122.44	128.36
30	f	103	SQD	O9-S-O7	-3.57	100.46	113.48
25	x	101	BCR	C33-C5-C6	-3.56	121.11	124.61
30	d	403	SQD	O9-S-O7	-3.56	100.50	113.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	612	CLA	CMB-C2B-C1B	-3.55	122.49	128.36
26	D	407	DGD	O6D-C1D-O3G	-3.55	101.52	110.05
26	c	515	DGD	O3G-C3G-C2G	-3.54	102.58	110.99
30	F	103	SQD	O9-S-O7	-3.53	100.61	113.48
26	B	620	DGD	O3G-C3G-C2G	-3.52	102.61	110.99
25	F	102	BCR	C33-C5-C6	-3.51	121.16	124.61
22	B	609	CLA	CMB-C2B-C1B	-3.51	122.56	128.36
25	H	102	BCR	C33-C5-C6	-3.51	121.16	124.61
30	B	622	SQD	O9-S-O7	-3.50	100.72	113.48
22	b	614	CLA	CMB-C2B-C1B	-3.50	122.57	128.36
30	a	412	SQD	O9-S-O7	-3.48	100.80	113.48
25	f	102	BCR	C33-C5-C6	-3.47	121.20	124.61
25	g	101	BCR	C38-C26-C25	-3.46	121.21	124.61
30	A	413	SQD	O9-S-O7	-3.45	100.90	113.48
30	a	401	SQD	O9-S-O7	-3.44	100.95	113.48
25	j	102	BCR	C11-C10-C9	-3.42	122.26	127.20
30	b	602	SQD	O9-S-O7	-3.41	101.04	113.48
22	B	613	CLA	CMB-C2B-C1B	-3.41	122.72	128.36
26	C	514	DGD	O3G-C3G-C2G	-3.40	102.89	110.99
22	B	611	CLA	CMB-C2B-C1B	-3.40	122.74	128.36
22	c	505	CLA	CMB-C2B-C1B	-3.40	122.74	128.36
30	B	627	SQD	O9-S-O7	-3.38	101.15	113.48
30	A	414	SQD	O9-S-O7	-3.38	101.17	113.48
22	c	506	CLA	CMB-C2B-C1B	-3.36	122.80	128.36
22	B	601	CLA	CMB-C2B-C1B	-3.35	122.82	128.36
22	b	618	CLA	CMB-C2B-C1B	-3.34	122.85	128.36
22	B	602	CLA	CMB-C2B-C1B	-3.33	122.86	128.36
22	C	505	CLA	CMB-C2B-C1B	-3.32	122.86	128.36
26	b	625	DGD	O6D-C1D-O3G	-3.32	102.06	110.05
22	c	508	CLA	CMB-C2B-C1B	-3.32	122.87	128.36
22	b	605	CLA	CMB-C2B-C1B	-3.32	122.88	128.36
22	c	512	CLA	CMB-C2B-C1B	-3.32	122.88	128.36
25	y	101	BCR	C38-C26-C25	-3.31	121.36	124.61
22	c	510	CLA	CMB-C2B-C1B	-3.30	122.90	128.36
22	A	406	CLA	CMB-C2B-C1B	-3.30	122.90	128.36
22	b	616	CLA	CMB-C2B-C1B	-3.30	122.90	128.36
22	C	510	CLA	CMB-C2B-C1B	-3.29	122.92	128.36
22	C	508	CLA	CMB-C2B-C1B	-3.29	122.93	128.36
25	b	621	BCR	C33-C5-C6	-3.27	121.40	124.61
22	C	512	CLA	CMB-C2B-C1B	-3.26	122.96	128.36
22	c	502	CLA	CMB-C2B-C1B	-3.26	122.97	128.36
22	b	607	CLA	CMB-C2B-C1B	-3.25	122.98	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	DGD	O6D-C1D-O3G	-3.24	102.26	110.05
22	c	503	CLA	CMB-C2B-C1B	-3.24	123.01	128.36
25	j	102	BCR	C7-C8-C9	-3.24	121.28	126.22
22	C	502	CLA	CMB-C2B-C1B	-3.23	123.02	128.36
22	c	509	CLA	CMB-C2B-C1B	-3.23	123.02	128.36
25	B	616	BCR	C33-C5-C6	-3.22	121.44	124.61
22	C	503	CLA	CMB-C2B-C1B	-3.22	123.04	128.36
22	B	605	CLA	CMB-C2B-C1B	-3.21	123.05	128.36
22	C	509	CLA	CMB-C2B-C1B	-3.21	123.05	128.36
22	c	520	CLA	CMB-C2B-C1B	-3.21	123.05	128.36
22	c	503	CLA	O2D-CGD-O1D	-3.20	117.17	123.79
22	a	404	CLA	CMB-C2B-C1B	-3.20	123.07	128.36
22	C	519	CLA	CMB-C2B-C1B	-3.20	123.08	128.36
22	C	506	CLA	CMB-C2B-C1B	-3.19	123.08	128.36
32	b	604	LMT	C1'-O5'-C5'	-3.19	107.55	113.75
22	D	404	CLA	CMB-C2B-C1B	-3.19	123.09	128.36
22	b	618	CLA	O2D-CGD-O1D	-3.18	117.22	123.79
22	b	606	CLA	CMB-C2B-C1B	-3.17	123.11	128.36
26	c	516	DGD	O6D-C1D-O3G	-3.17	102.42	110.05
22	b	609	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
22	a	406	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
24	J	101	PL9	C7-C8-C9	-3.17	121.33	126.70
32	B	629	LMT	C1'-O5'-C5'	-3.17	107.60	113.75
22	C	511	CLA	CMB-C2B-C1B	-3.15	123.15	128.36
22	A	402	CLA	CMB-C2B-C1B	-3.14	123.16	128.36
22	a	403	CLA	CMB-C2B-C1B	-3.14	123.17	128.36
26	c	517	DGD	O5D-C6D-C5D	-3.14	103.40	109.08
22	c	511	CLA	CMB-C2B-C1B	-3.13	123.19	128.36
25	J	102	BCR	C7-C8-C9	-3.12	121.45	126.22
26	d	410	DGD	O3G-C3G-C2G	-3.12	103.56	110.99
22	B	604	CLA	CMB-C2B-C1B	-3.12	123.20	128.36
25	J	102	BCR	C24-C23-C22	-3.12	121.46	126.22
24	j	101	PL9	C7-C8-C9	-3.10	121.45	126.70
22	B	614	CLA	CMB-C2B-C1B	-3.09	123.25	128.36
22	D	403	CLA	CMB-C2B-C1B	-3.08	123.28	128.36
24	A	407	PL9	C22-C23-C24	-3.07	121.09	127.76
22	C	503	CLA	O2D-CGD-O1D	-3.07	117.45	123.79
25	B	617	BCR	C15-C16-C17	-3.07	116.61	123.39
25	b	624	BCR	C3-C4-C5	-3.07	109.00	113.87
22	d	406	CLA	CMB-C2B-C1B	-3.06	123.29	128.36
25	b	623	BCR	C24-C23-C22	-3.06	121.55	126.22
22	b	619	CLA	CMB-C2B-C1B	-3.06	123.30	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	409	DGD	O6D-C1D-O3G	-3.06	102.69	110.05
22	B	603	CLA	O2D-CGD-O1D	-3.06	117.48	123.79
22	B	606	CLA	CMB-C2B-C1B	-3.06	123.31	128.36
26	C	516	DGD	O5D-C6D-C5D	-3.05	103.55	109.08
22	B	613	CLA	O2D-CGD-O1D	-3.05	117.49	123.79
26	D	407	DGD	O3G-C3G-C2G	-3.04	103.75	110.99
25	J	102	BCR	C38-C26-C25	-3.04	121.62	124.61
22	A	403	CLA	CMB-C2B-C1B	-3.04	123.34	128.36
22	B	603	CLA	CMB-C2B-C1B	-3.04	123.34	128.36
31	B	625	LMG	O6-C1-O1	-3.04	102.75	110.05
26	b	601	DGD	O3G-C3G-C2G	-3.04	103.77	110.99
24	a	407	PL9	C22-C23-C24	-3.03	121.17	127.76
22	c	504	CLA	O2D-CGD-O1D	-3.03	117.53	123.79
22	b	608	CLA	CMB-C2B-C1B	-3.02	123.36	128.36
25	j	102	BCR	C38-C26-C25	-3.02	121.64	124.61
22	a	405	CLA	CMB-C2B-C1B	-3.02	123.37	128.36
22	A	404	CLA	CMB-C2B-C1B	-3.01	123.38	128.36
22	d	405	CLA	CMB-C2B-C1B	-3.00	123.40	128.36
22	B	615	CLA	CMB-C2B-C1B	-3.00	123.40	128.36
25	B	617	BCR	C28-C27-C26	-3.00	109.11	113.87
22	b	611	CLA	CMB-C2B-C1B	-3.00	123.41	128.36
26	C	515	DGD	O6D-C1D-O3G	-3.00	102.84	110.05
26	c	515	DGD	O6D-C1D-O3G	-2.99	102.86	110.05
32	M	102	LMT	C1'-O5'-C5'	-2.99	107.95	113.75
22	b	610	CLA	CMB-C2B-C1B	-2.98	123.43	128.36
25	B	619	BCR	C3-C4-C5	-2.98	109.14	113.87
26	A	409	DGD	O5D-C6D-C5D	-2.97	103.69	109.08
26	C	516	DGD	C1D-C2D-C3D	-2.97	104.12	109.97
25	b	622	BCR	C28-C27-C26	-2.97	109.16	113.87
22	C	502	CLA	O2D-CGD-O1D	-2.96	117.67	123.79
26	d	410	DGD	C3D-C4D-C5D	-2.96	105.03	110.20
25	c	514	BCR	C33-C5-C6	-2.96	121.70	124.61
26	B	626	DGD	O3G-C3G-C2G	-2.96	103.95	110.99
26	C	516	DGD	CDB-CCB-CBB	-2.96	99.27	114.53
25	b	622	BCR	C15-C16-C17	-2.95	116.87	123.39
25	j	102	BCR	C24-C23-C22	-2.94	121.74	126.22
22	C	507	CLA	O2D-CGD-O1D	-2.94	117.73	123.79
22	H	101	CLA	CMB-C2B-C1B	-2.93	123.51	128.36
25	C	513	BCR	C33-C5-C6	-2.93	121.73	124.61
31	d	408	LMG	O6-C1-O1	-2.93	103.00	110.05
26	c	517	DGD	CDB-CCB-CBB	-2.93	99.40	114.53
22	B	608	CLA	CMB-C2B-C1B	-2.92	123.54	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	O2D-CGD-O1D	-2.91	117.77	123.79
22	b	620	CLA	CMB-C2B-C1B	-2.91	123.55	128.36
22	C	504	CLA	O2D-CGD-O1D	-2.91	117.78	123.79
22	a	403	CLA	O2D-CGD-O1D	-2.90	117.80	123.79
22	B	605	CLA	O2D-CGD-O1D	-2.90	117.80	123.79
24	d	407	PL9	C22-C23-C24	-2.90	121.45	127.76
25	B	618	BCR	C24-C23-C22	-2.90	121.79	126.22
25	J	102	BCR	C3-C4-C5	-2.90	109.27	113.87
24	D	405	PL9	C22-C23-C24	-2.89	121.47	127.76
22	b	613	CLA	CMB-C2B-C1B	-2.88	123.59	128.36
24	d	407	PL9	C7-C8-C9	-2.88	121.81	126.70
32	b	629	LMT	C3'-C4'-C5'	-2.88	104.32	110.84
26	a	408	DGD	O6D-C1D-O3G	-2.88	103.12	110.05
32	B	624	LMT	C3'-C4'-C5'	-2.88	104.33	110.84
22	B	608	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
25	b	624	BCR	C7-C8-C9	-2.88	121.83	126.22
22	B	606	CLA	O2D-CGD-O1D	-2.87	117.86	123.79
26	C	514	DGD	O6D-C1D-O3G	-2.87	103.14	110.05
26	c	517	DGD	C1D-O6D-C5D	-2.87	108.18	113.75
25	J	102	BCR	C35-C13-C14	-2.86	118.67	122.90
22	c	507	CLA	O2D-CGD-O1D	-2.86	117.89	123.79
32	B	628	LMT	C1'-O5'-C5'	-2.86	108.20	113.75
24	J	101	PL9	C22-C23-C24	-2.86	121.55	127.76
22	a	405	CLA	O2D-CGD-O1D	-2.85	117.90	123.79
24	j	101	PL9	C22-C23-C24	-2.85	121.57	127.76
22	b	607	CLA	O2D-CGD-O1D	-2.85	117.91	123.79
22	c	510	CLA	O2D-CGD-O1D	-2.84	117.92	123.79
26	c	516	DGD	CDB-CCB-CBB	-2.82	99.94	114.53
22	b	614	CLA	O2D-CGD-O1D	-2.82	117.96	123.79
26	B	626	DGD	C3G-C2G-C1G	-2.82	105.47	112.07
26	b	601	DGD	C3G-C2G-C1G	-2.82	105.48	112.07
22	b	613	CLA	O2D-CGD-O1D	-2.81	117.98	123.79
26	d	410	DGD	CDB-CCB-CBB	-2.81	100.02	114.53
25	i	101	BCR	C33-C5-C6	-2.81	121.84	124.61
26	b	601	DGD	C1D-C2D-C3D	-2.81	104.44	109.97
22	b	612	CLA	O2D-CGD-O1D	-2.81	117.99	123.79
22	B	602	CLA	O2D-CGD-O1D	-2.81	117.99	123.79
22	A	403	CLA	O2D-CGD-O1D	-2.81	118.00	123.79
22	C	505	CLA	O2D-CGD-O1D	-2.81	118.00	123.79
22	C	501	CLA	O2D-CGD-O1D	-2.80	118.00	123.79
24	d	407	PL9	C37-C38-C39	-2.80	121.67	127.76
22	b	605	CLA	O2D-CGD-O1D	-2.80	118.01	123.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	BCR	C33-C5-C6	-2.80	121.86	124.61
22	c	520	CLA	O2D-CGD-O1D	-2.79	118.02	123.79
26	c	517	DGD	C1D-C2D-C3D	-2.79	104.48	109.97
22	A	402	CLA	O2D-CGD-O1D	-2.79	118.03	123.79
22	c	505	CLA	O2D-CGD-O1D	-2.79	118.03	123.79
26	D	407	DGD	CDB-CCB-CBB	-2.79	100.14	114.53
26	C	515	DGD	CDB-CCB-CBB	-2.79	100.14	114.53
25	B	619	BCR	C7-C8-C9	-2.79	121.97	126.22
32	b	628	LMT	C1'-O5'-C5'	-2.79	108.34	113.75
25	c	514	BCR	C28-C27-C26	-2.78	109.45	113.87
31	i	102	LMG	O6-C1-O1	-2.78	103.36	110.05
22	b	608	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
22	b	610	CLA	O2D-CGD-O1D	-2.78	118.05	123.79
24	D	405	PL9	C7-C8-C9	-2.77	122.00	126.70
22	c	502	CLA	O2D-CGD-O1D	-2.77	118.07	123.79
22	c	504	CLA	CMB-C2B-C1B	-2.77	123.78	128.36
25	J	102	BCR	C15-C14-C13	-2.77	123.20	127.20
25	c	521	BCR	C15-C16-C17	-2.77	117.27	123.39
22	B	601	CLA	O2D-CGD-O1D	-2.76	118.08	123.79
25	b	624	BCR	C38-C26-C25	-2.76	121.89	124.61
22	c	512	CLA	O2D-CGD-O1D	-2.76	118.09	123.79
25	C	513	BCR	C28-C27-C26	-2.76	109.49	113.87
22	A	404	CLA	O2D-CGD-O1D	-2.75	118.11	123.79
31	C	517	LMG	O6-C1-O1	-2.74	103.45	110.05
25	B	619	BCR	C38-C26-C25	-2.74	121.92	124.61
25	C	513	BCR	C15-C16-C17	-2.74	117.34	123.39
25	g	101	BCR	C7-C8-C9	-2.73	122.05	126.22
25	K	101	BCR	C24-C23-C22	-2.73	122.05	126.22
32	B	623	LMT	C1'-O5'-C5'	-2.73	108.45	113.75
31	c	518	LMG	O6-C1-O1	-2.73	103.49	110.05
22	B	609	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
22	c	501	CLA	O2D-CGD-O1D	-2.72	118.17	123.79
25	j	102	BCR	C3-C4-C5	-2.71	109.56	113.87
22	B	610	CLA	O2D-CGD-O1D	-2.71	118.20	123.79
22	C	510	CLA	O2D-CGD-O1D	-2.70	118.21	123.79
22	b	609	CLA	O2D-CGD-O1D	-2.70	118.21	123.79
25	B	618	BCR	C11-C10-C9	-2.70	123.30	127.20
22	c	511	CLA	O2D-CGD-O1D	-2.70	118.22	123.79
22	C	506	CLA	O2D-CGD-O1D	-2.69	118.23	123.79
26	B	626	DGD	C1D-C2D-C3D	-2.69	104.66	109.97
24	D	405	PL9	C37-C38-C39	-2.69	121.92	127.76
22	b	611	CLA	O2D-CGD-O1D	-2.69	118.24	123.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	506	CLA	O2D-CGD-O1D	-2.68	118.25	123.79
25	C	513	BCR	C38-C26-C25	-2.68	121.97	124.61
25	y	101	BCR	C33-C5-C6	-2.68	121.97	124.61
31	I	101	LMG	O6-C1-O1	-2.68	103.61	110.05
25	c	514	BCR	C38-C26-C25	-2.68	121.98	124.61
22	B	607	CLA	O2D-CGD-O1D	-2.67	118.27	123.79
26	c	516	DGD	C3G-C2G-C1G	-2.66	105.84	112.07
24	d	407	PL9	C32-C33-C34	-2.66	121.98	127.76
22	d	406	CLA	O2D-CGD-O1D	-2.66	118.31	123.79
25	y	101	BCR	C7-C8-C9	-2.66	122.17	126.22
22	b	619	CLA	O2D-CGD-O1D	-2.65	118.31	123.79
25	B	617	BCR	C15-C14-C13	-2.65	123.37	127.20
24	a	407	PL9	C27-C28-C29	-2.65	122.00	127.76
25	c	521	BCR	C33-C5-C6	-2.64	122.01	124.61
25	C	520	BCR	C33-C5-C6	-2.64	122.02	124.61
22	C	504	CLA	CMB-C2B-C1B	-2.64	124.00	128.36
25	A	408	BCR	C38-C26-C25	-2.64	122.02	124.61
24	D	405	PL9	C32-C33-C34	-2.63	122.04	127.76
22	C	519	CLA	O2D-CGD-O1D	-2.63	118.35	123.79
26	C	516	DGD	C1D-O6D-C5D	-2.63	108.64	113.75
24	D	405	PL9	C27-C28-C29	-2.62	122.06	127.76
22	C	511	CLA	O2D-CGD-O1D	-2.62	118.37	123.79
22	b	617	CLA	O2D-CGD-O1D	-2.62	118.37	123.79
22	B	614	CLA	O2D-CGD-O1D	-2.62	118.38	123.79
31	E	101	LMG	C1-C2-C3	-2.62	104.81	109.97
26	C	515	DGD	C3G-C2G-C1G	-2.62	105.95	112.07
32	d	411	LMT	C3'-C4'-C5'	-2.62	104.92	110.84
23	d	401	PHO	CBD-CHA-C4D	-2.61	105.53	108.46
23	D	401	PHO	O2D-CGD-O1D	-2.61	118.41	123.79
25	j	102	BCR	C35-C13-C14	-2.61	119.05	122.90
26	d	410	DGD	CFB-CEB-CDB	-2.60	101.08	114.53
32	D	408	LMT	C3'-C4'-C5'	-2.60	104.95	110.84
25	i	101	BCR	C38-C26-C25	-2.60	122.05	124.61
22	C	512	CLA	O2D-CGD-O1D	-2.60	118.43	123.79
22	B	612	CLA	O2D-CGD-O1D	-2.60	118.43	123.79
26	D	407	DGD	CFB-CEB-CDB	-2.60	101.13	114.53
23	d	401	PHO	O2D-CGD-O1D	-2.59	118.44	123.79
31	D	409	LMG	C38-C37-C36	-2.58	101.18	114.53
24	d	407	PL9	C27-C28-C29	-2.58	122.14	127.76
25	g	101	BCR	C33-C5-C6	-2.58	122.07	124.61
22	b	615	CLA	O2D-CGD-O1D	-2.58	118.46	123.79
26	A	409	DGD	CBB-CAB-C9B	-2.58	101.20	114.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	404	CLA	O2D-CGD-O1D	-2.58	118.47	123.79
25	b	623	BCR	C15-C16-C17	-2.58	117.70	123.39
23	d	402	PHO	CBD-CHA-C4D	-2.57	105.58	108.46
22	H	101	CLA	O2D-CGD-O1D	-2.57	118.49	123.79
25	c	514	BCR	C11-C10-C9	-2.57	123.49	127.20
25	b	623	BCR	C11-C10-C9	-2.56	123.50	127.20
25	b	622	BCR	C15-C14-C13	-2.55	123.51	127.20
23	A	405	PHO	O2D-CGD-O1D	-2.55	118.52	123.79
25	b	623	BCR	C33-C5-C6	-2.55	122.10	124.61
26	c	515	DGD	C3G-C2G-C1G	-2.55	106.11	112.07
32	M	103	LMT	C1'-O5'-C5'	-2.55	108.81	113.75
25	B	616	BCR	C38-C26-C25	-2.54	122.11	124.61
31	d	412	LMG	C38-C37-C36	-2.54	101.42	114.53
22	D	404	CLA	O2D-CGD-O1D	-2.54	118.55	123.79
32	b	603	LMT	C1'-O5'-C5'	-2.54	108.82	113.75
32	i	103	LMT	C1'-O5'-C5'	-2.53	108.83	113.75
26	d	410	DGD	C3G-C2G-C1G	-2.53	106.14	112.07
31	d	408	LMG	O2-C2-C1	-2.53	104.48	110.02
23	D	401	PHO	CBD-CHA-C4D	-2.53	105.63	108.46
22	c	509	CLA	O2D-CGD-O1D	-2.53	118.57	123.79
26	b	625	DGD	CBB-CAB-C9B	-2.53	101.49	114.53
25	c	513	BCR	C24-C23-C22	-2.52	122.37	126.22
31	d	408	LMG	C38-C37-C36	-2.52	101.52	114.53
26	C	516	DGD	CFB-CEB-CDB	-2.52	101.53	114.53
26	B	620	DGD	C3G-C2G-C1G	-2.51	106.20	112.07
26	b	625	DGD	C3G-C2G-C1G	-2.51	106.20	112.07
25	J	102	BCR	C33-C5-C6	-2.51	122.14	124.61
25	B	618	BCR	C15-C14-C13	-2.51	123.57	127.20
26	C	515	DGD	O6E-C1E-O5D	-2.51	104.02	110.05
26	a	408	DGD	CBB-CAB-C9B	-2.50	101.60	114.53
25	c	513	BCR	C7-C8-C9	-2.50	122.40	126.22
31	d	409	LMG	C38-C37-C36	-2.50	101.62	114.53
32	b	629	LMT	C1'-O5'-C5'	-2.50	108.90	113.75
25	C	520	BCR	C38-C26-C25	-2.50	122.16	124.61
22	b	606	CLA	O2D-CGD-O1D	-2.49	118.64	123.79
31	B	625	LMG	O2-C2-C1	-2.49	104.56	110.02
25	c	514	BCR	C15-C16-C17	-2.49	117.89	123.39
22	D	403	CLA	O2D-CGD-O1D	-2.49	118.65	123.79
25	B	619	BCR	C33-C5-C6	-2.49	122.16	124.61
22	c	501	CLA	CMB-C2B-C1B	-2.49	124.25	128.36
31	b	627	LMG	O6-C1-O1	-2.49	104.07	110.05
31	a	402	LMG	O6-C1-O1	-2.48	104.07	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	616	BCR	C7-C8-C9	-2.48	122.43	126.22
27	C	518	LHG	C11-C10-C9	-2.48	101.73	114.53
25	c	521	BCR	C15-C14-C13	-2.48	123.62	127.20
26	c	517	DGD	CFB-CEB-CDB	-2.47	101.76	114.53
31	B	625	LMG	C38-C37-C36	-2.47	101.77	114.53
31	L	101	LMG	C1-C2-C3	-2.46	105.12	109.97
26	c	516	DGD	O6E-C1E-O5D	-2.46	104.13	110.05
31	L	101	LMG	C40-C39-C38	-2.46	101.83	114.53
31	m	101	LMG	O2-C2-C1	-2.45	104.64	110.02
31	b	626	LMG	O2-C2-C1	-2.45	104.65	110.02
25	B	618	BCR	C15-C16-C17	-2.45	117.97	123.39
25	b	624	BCR	C33-C5-C6	-2.45	122.20	124.61
31	D	406	LMG	C38-C37-C36	-2.45	101.88	114.53
23	A	405	PHO	CBD-CHA-C4D	-2.45	105.72	108.46
26	a	408	DGD	C3G-C2G-C1G	-2.45	106.35	112.07
25	B	616	BCR	C11-C10-C9	-2.45	123.66	127.20
25	B	618	BCR	C33-C5-C6	-2.44	122.21	124.61
22	a	406	CLA	O2D-CGD-O1D	-2.44	118.75	123.79
25	C	520	BCR	C15-C16-C17	-2.44	117.99	123.39
31	D	409	LMG	C1-C2-C3	-2.44	105.16	109.97
26	B	620	DGD	CBB-CAB-C9B	-2.44	101.94	114.53
25	c	514	BCR	C15-C14-C13	-2.44	123.68	127.20
24	D	405	PL9	C31-C32-C33	-2.43	105.32	111.69
24	d	407	PL9	C31-C32-C33	-2.43	105.32	111.69
24	A	407	PL9	C27-C28-C29	-2.43	122.48	127.76
31	c	522	LMG	C40-C39-C38	-2.43	101.98	114.53
24	a	407	PL9	C31-C32-C33	-2.43	105.33	111.69
22	A	406	CLA	O2D-CGD-O1D	-2.42	118.79	123.79
31	B	625	LMG	O3-C3-C2	-2.42	104.89	110.34
31	b	626	LMG	C40-C39-C38	-2.42	102.05	114.53
25	b	622	BCR	C35-C13-C14	-2.42	119.33	122.90
22	C	501	CLA	CMB-C2B-C1B	-2.41	124.37	128.36
31	B	621	LMG	C1-C2-C3	-2.41	105.23	109.97
23	d	402	PHO	O2D-CGD-O1D	-2.41	118.82	123.79
31	C	521	LMG	O2-C2-C1	-2.40	104.75	110.02
25	f	102	BCR	C38-C26-C25	-2.40	122.25	124.61
31	l	101	LMG	C40-C39-C38	-2.40	102.14	114.53
27	c	519	LHG	C11-C10-C9	-2.40	102.14	114.53
31	c	518	LMG	O2-C2-C1	-2.40	104.76	110.02
25	J	102	BCR	C15-C16-C17	-2.40	118.09	123.39
31	I	101	LMG	O2-C2-C1	-2.40	104.77	110.02
25	c	521	BCR	C38-C26-C25	-2.40	122.25	124.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	101	BCR	C11-C10-C9	-2.39	123.74	127.20
25	C	513	BCR	C15-C14-C13	-2.39	123.74	127.20
24	a	407	PL9	C7-C8-C9	-2.39	122.65	126.70
31	b	626	LMG	C1-C2-C3	-2.39	105.27	109.97
22	d	405	CLA	O2D-CGD-O1D	-2.39	118.86	123.79
32	I	102	LMT	C1'-O5'-C5'	-2.39	109.11	113.75
25	H	102	BCR	C38-C26-C25	-2.38	122.27	124.61
31	c	522	LMG	O2-C2-C1	-2.38	104.80	110.02
25	j	102	BCR	C33-C5-C6	-2.38	122.27	124.61
25	b	622	BCR	C38-C26-C25	-2.38	122.27	124.61
25	F	102	BCR	C38-C26-C25	-2.38	122.27	124.61
24	A	407	PL9	C7-C8-C9	-2.38	122.67	126.70
25	b	621	BCR	C38-C26-C25	-2.38	122.27	124.61
31	C	521	LMG	C40-C39-C38	-2.38	102.26	114.53
26	a	408	DGD	O5D-C6D-C5D	-2.37	104.78	109.08
31	d	408	LMG	O1-C1-C2	-2.37	105.05	108.04
32	M	103	LMT	C3'-C4'-C5'	-2.37	105.48	110.84
22	C	509	CLA	O2D-CGD-O1D	-2.37	118.90	123.79
22	B	610	CLA	C4B-CHC-C1C	-2.37	124.18	129.26
26	A	409	DGD	C3G-C2G-C1G	-2.37	106.54	112.07
22	b	620	CLA	O2D-CGD-O1D	-2.36	118.92	123.79
25	K	101	BCR	C7-C8-C9	-2.36	122.62	126.22
25	c	513	BCR	C33-C5-C6	-2.36	122.29	124.61
22	c	508	CLA	O2D-CGD-O1D	-2.36	118.92	123.79
31	D	409	LMG	O3-C3-C2	-2.36	105.03	110.34
26	c	516	DGD	CFB-CEB-CDB	-2.36	102.36	114.53
22	C	511	CLA	O2A-CGA-O1A	-2.35	117.42	123.49
31	L	101	LMG	C38-C37-C36	-2.35	102.38	114.53
31	M	101	LMG	O2-C2-C1	-2.35	104.86	110.02
31	m	101	LMG	C1-O6-C5	-2.35	109.18	113.75
31	l	101	LMG	C1-C2-C3	-2.35	105.34	109.97
31	C	517	LMG	C38-C37-C36	-2.35	102.40	114.53
25	b	623	BCR	C15-C14-C13	-2.35	123.81	127.20
25	b	624	BCR	C11-C10-C9	-2.35	123.81	127.20
31	m	101	LMG	C1-C2-C3	-2.35	105.35	109.97
31	i	102	LMG	O2-C2-C1	-2.34	104.88	110.02
31	d	408	LMG	O3-C3-C2	-2.34	105.06	110.34
31	D	406	LMG	O6-C1-C2	-2.34	105.47	110.28
25	C	513	BCR	C11-C10-C9	-2.34	123.82	127.20
31	b	626	LMG	O6-C1-O1	-2.34	104.42	110.05
31	B	621	LMG	O2-C2-C1	-2.34	104.90	110.02
25	B	618	BCR	C7-C8-C9	-2.34	122.66	126.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	101	LMG	C1-O6-C5	-2.34	109.21	113.75
31	d	412	LMG	O6-C1-O1	-2.33	104.44	110.05
25	K	101	BCR	C38-C26-C25	-2.33	122.32	124.61
25	b	621	BCR	C15-C14-C13	-2.33	123.83	127.20
31	C	517	LMG	O2-C2-C1	-2.33	104.92	110.02
31	d	412	LMG	O3-C3-C2	-2.33	105.10	110.34
25	B	617	BCR	C38-C26-C25	-2.33	122.32	124.61
22	c	511	CLA	O2A-CGA-O1A	-2.32	117.50	123.49
25	b	623	BCR	C7-C8-C9	-2.32	122.68	126.22
32	D	408	LMT	C1'-O5'-C5'	-2.32	109.24	113.75
31	L	101	LMG	O3-C3-C2	-2.32	105.11	110.34
31	B	621	LMG	C40-C39-C38	-2.32	102.56	114.53
24	D	405	PL9	C46-C47-C48	-2.31	105.63	111.69
25	y	101	BCR	C1-C6-C5	-2.31	119.26	122.66
31	l	101	LMG	O3-C3-C2	-2.31	105.13	110.34
31	e	101	LMG	C1-C2-C3	-2.31	105.42	109.97
31	d	409	LMG	O6-C1-C2	-2.31	105.54	110.28
31	e	101	LMG	O6-C1-O1	-2.31	104.50	110.05
31	l	101	LMG	C38-C37-C36	-2.30	102.64	114.53
26	b	601	DGD	O6D-C1D-O3G	-2.30	104.51	110.05
26	c	516	DGD	C3D-C4D-C5D	-2.30	106.19	110.20
25	c	513	BCR	C11-C10-C9	-2.30	123.87	127.20
26	C	515	DGD	CFB-CEB-CDB	-2.30	102.68	114.53
31	c	522	LMG	C38-C37-C36	-2.29	102.69	114.53
31	c	518	LMG	C38-C37-C36	-2.29	102.69	114.53
25	c	513	BCR	C38-C26-C25	-2.29	122.36	124.61
22	C	508	CLA	O2D-CGD-O1D	-2.29	119.06	123.79
31	b	626	LMG	C38-C37-C36	-2.29	102.72	114.53
26	B	626	DGD	O6D-C1D-O3G	-2.29	104.55	110.05
31	c	518	LMG	O1-C7-C8	-2.28	105.56	110.99
25	A	408	BCR	C15-C14-C13	-2.28	123.90	127.20
32	B	624	LMT	C1'-O5'-C5'	-2.28	109.32	113.75
31	M	101	LMG	C1-C2-C3	-2.28	105.48	109.97
25	b	623	BCR	C38-C26-C25	-2.28	122.37	124.61
25	i	101	BCR	C15-C16-C17	-2.27	118.36	123.39
24	A	407	PL9	C11-C12-C13	-2.27	105.75	111.69
26	c	516	DGD	O3D-C3D-C4D	-2.26	105.24	110.34
25	j	102	BCR	C15-C14-C13	-2.26	123.93	127.20
31	e	101	LMG	O3-C3-C2	-2.26	105.25	110.34
24	d	407	PL9	C46-C47-C48	-2.26	105.77	111.69
25	c	513	BCR	C15-C16-C17	-2.26	118.40	123.39
25	g	101	BCR	C1-C6-C5	-2.26	119.35	122.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	x	101	BCR	C38-C26-C25	-2.26	122.39	124.61
31	B	621	LMG	O3-C3-C2	-2.25	105.26	110.34
25	B	617	BCR	C35-C13-C14	-2.25	119.58	122.90
24	a	407	PL9	C11-C12-C13	-2.25	105.79	111.69
24	A	407	PL9	C31-C32-C33	-2.25	105.81	111.69
31	C	521	LMG	C38-C37-C36	-2.25	102.94	114.53
34	F	101	HEM	CAA-CBA-CGA	-2.25	108.63	112.75
34	f	101	HEM	CAA-CBA-CGA	-2.24	108.63	112.75
31	B	621	LMG	O6-C1-O1	-2.24	104.65	110.05
24	j	101	PL9	C12-C13-C14	-2.24	122.88	127.76
26	c	515	DGD	C1D-C2D-C3D	-2.24	105.55	109.97
31	C	521	LMG	O3-C3-C2	-2.24	105.29	110.34
25	K	101	BCR	C3-C4-C5	-2.24	110.31	113.87
31	E	101	LMG	O6-C1-O1	-2.24	104.67	110.05
26	C	514	DGD	C3G-C2G-C1G	-2.24	106.84	112.07
24	a	407	PL9	C32-C33-C34	-2.24	122.90	127.76
24	j	101	PL9	O2-C1-C2	-2.23	116.86	121.89
31	a	402	LMG	O3-C3-C2	-2.23	105.31	110.34
24	J	101	PL9	C12-C13-C14	-2.23	122.91	127.76
31	B	621	LMG	C38-C37-C36	-2.23	103.00	114.53
26	b	625	DGD	C1D-C2D-C3D	-2.23	105.58	109.97
31	B	625	LMG	O1-C1-C2	-2.23	105.22	108.04
25	C	520	BCR	C24-C23-C22	-2.23	122.82	126.22
25	C	513	BCR	C24-C23-C22	-2.23	122.82	126.22
31	D	406	LMG	O6-C1-O1	-2.23	104.69	110.05
25	K	101	BCR	C15-C16-C17	-2.23	118.47	123.39
31	i	102	LMG	O3-C3-C2	-2.23	105.32	110.34
31	a	402	LMG	O1-C7-C8	-2.23	105.69	110.99
31	C	521	LMG	O6-C1-O1	-2.23	104.69	110.05
24	d	407	PL9	O2-C1-C2	-2.23	116.88	121.89
25	C	520	BCR	C11-C10-C9	-2.23	123.98	127.20
26	b	601	DGD	CBB-CAB-C9B	-2.23	103.04	114.53
31	d	412	LMG	C1-C2-C3	-2.22	105.59	109.97
31	c	522	LMG	O6-C1-O1	-2.22	104.70	110.05
22	b	616	CLA	O2D-CGD-O1D	-2.22	119.20	123.79
22	B	615	CLA	O2D-CGD-O1D	-2.22	119.20	123.79
25	j	102	BCR	C15-C16-C17	-2.22	118.48	123.39
25	b	624	BCR	C24-C23-C22	-2.22	122.83	126.22
24	D	405	PL9	C42-C43-C44	-2.22	122.94	127.76
31	b	627	LMG	O1-C7-C8	-2.21	105.72	110.99
24	D	405	PL9	O2-C1-C2	-2.21	116.90	121.89
26	b	601	DGD	CAB-C9B-C8B	-2.21	103.10	114.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	DGD	C4E-C3E-C2E	-2.21	106.66	110.79
31	b	626	LMG	O3-C3-C2	-2.21	105.36	110.34
32	d	411	LMT	C1'-O5'-C5'	-2.21	109.45	113.75
26	a	408	DGD	CAB-C9B-C8B	-2.21	103.12	114.53
22	b	615	CLA	C4B-CHC-C1C	-2.20	124.53	129.26
25	c	513	BCR	C15-C14-C13	-2.20	124.02	127.20
24	a	407	PL9	O2-C1-C2	-2.20	116.94	121.89
31	D	409	LMG	O2-C2-C1	-2.20	105.20	110.02
31	C	517	LMG	O1-C7-C8	-2.20	105.76	110.99
31	C	517	LMG	O3-C3-C2	-2.20	105.39	110.34
31	c	518	LMG	O3-C3-C2	-2.20	105.39	110.34
25	g	101	BCR	C3-C2-C1	-2.19	106.71	114.83
26	c	516	DGD	CBB-CAB-C9B	-2.19	103.22	114.53
24	J	101	PL9	O2-C1-C2	-2.19	116.95	121.89
22	B	611	CLA	O2D-CGD-O1D	-2.19	119.27	123.79
31	c	522	LMG	O3-C3-C2	-2.19	105.41	110.34
31	I	101	LMG	O3-C3-C2	-2.19	105.41	110.34
34	f	101	HEM	C3B-C4B-NB	-2.19	107.45	111.63
26	A	409	DGD	CAB-C9B-C8B	-2.19	103.25	114.53
31	d	409	LMG	O6-C1-O1	-2.18	104.80	110.05
24	A	407	PL9	O2-C1-C2	-2.18	116.97	121.89
25	c	521	BCR	C24-C23-C22	-2.18	122.89	126.22
24	D	405	PL9	C3-C2-C1	-2.18	121.64	122.97
25	K	101	BCR	C33-C5-C6	-2.18	122.47	124.61
24	d	407	PL9	C36-C34-C33	-2.18	116.92	121.05
31	L	101	LMG	O1-C1-C2	-2.18	105.29	108.04
31	l	101	LMG	O2-C2-C1	-2.18	105.25	110.02
25	c	513	BCR	C3-C4-C5	-2.17	110.42	113.87
24	D	405	PL9	C12-C13-C14	-2.17	123.04	127.76
31	E	101	LMG	O2-C2-C1	-2.17	105.26	110.02
26	B	626	DGD	CAB-C9B-C8B	-2.16	103.35	114.53
26	C	515	DGD	CBB-CAB-C9B	-2.16	103.35	114.53
31	E	101	LMG	O3-C3-C2	-2.16	105.47	110.34
22	c	509	CLA	O2A-CGA-O1A	-2.16	117.92	123.49
34	F	101	HEM	C3B-C4B-NB	-2.16	107.50	111.63
24	A	407	PL9	C32-C33-C34	-2.16	123.08	127.76
26	C	516	DGD	CBB-CAB-C9B	-2.15	103.40	114.53
25	F	102	BCR	C15-C16-C17	-2.15	118.63	123.39
24	d	407	PL9	C3-C2-C1	-2.15	121.66	122.97
25	F	102	BCR	C7-C8-C9	-2.15	122.93	126.22
31	b	627	LMG	O3-C3-C2	-2.15	105.49	110.34
26	C	515	DGD	O3D-C3D-C4D	-2.15	105.50	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	520	BCR	C7-C8-C9	-2.15	122.94	126.22
25	B	618	BCR	C38-C26-C25	-2.15	122.49	124.61
32	M	102	LMT	C3'-C4'-C5'	-2.15	105.99	110.84
27	a	409	LHG	C27-C26-C25	-2.14	103.48	114.53
27	A	410	LHG	C27-C26-C25	-2.14	103.48	114.53
22	b	619	CLA	O2A-CGA-O1A	-2.14	117.97	123.49
22	B	611	CLA	O2A-CGA-O1A	-2.14	117.97	123.49
25	F	102	BCR	C11-C10-C9	-2.14	124.11	127.20
25	B	619	BCR	C24-C23-C22	-2.14	122.96	126.22
26	D	407	DGD	C3D-C4D-C5D	-2.14	106.47	110.20
31	e	101	LMG	O2-C2-C1	-2.13	105.34	110.02
26	a	408	DGD	C1D-C2D-C3D	-2.13	105.77	109.97
24	d	407	PL9	C11-C12-C13	-2.13	106.11	111.69
22	b	616	CLA	O2A-CGA-O1A	-2.13	118.01	123.49
26	C	514	DGD	O5D-C6D-C5D	-2.12	105.23	109.08
26	d	410	DGD	CAB-C9B-C8B	-2.12	103.57	114.53
25	B	617	BCR	C24-C23-C22	-2.12	122.98	126.22
26	B	626	DGD	CBB-CAB-C9B	-2.12	103.58	114.53
26	C	514	DGD	C5B-C4B-C3B	-2.12	103.59	114.53
31	M	101	LMG	O3-C3-C2	-2.12	105.57	110.34
24	D	405	PL9	C36-C34-C33	-2.12	117.03	121.05
24	A	407	PL9	C12-C13-C14	-2.12	123.16	127.76
25	g	101	BCR	C15-C16-C17	-2.12	118.71	123.39
24	D	405	PL9	C11-C12-C13	-2.11	106.15	111.69
31	d	412	LMG	O2-C2-C1	-2.11	105.39	110.02
26	c	516	DGD	CAB-C9B-C8B	-2.11	103.62	114.53
26	b	625	DGD	CAB-C9B-C8B	-2.11	103.63	114.53
31	L	101	LMG	O2-C2-C1	-2.11	105.40	110.02
25	J	102	BCR	C20-C21-C22	-2.11	124.15	127.20
31	C	517	LMG	O1-C1-C2	-2.11	105.38	108.04
31	b	626	LMG	O1-C7-C8	-2.10	105.98	110.99
25	b	621	BCR	C15-C16-C17	-2.10	118.75	123.39
22	d	405	CLA	O2A-CGA-O1A	-2.10	118.07	123.49
26	D	407	DGD	C3G-C2G-C1G	-2.10	107.16	112.07
26	c	515	DGD	C5B-C4B-C3B	-2.10	103.71	114.53
26	C	515	DGD	CAB-C9B-C8B	-2.09	103.74	114.53
26	c	517	DGD	CBB-CAB-C9B	-2.09	103.74	114.53
25	b	622	BCR	C24-C23-C22	-2.08	123.04	126.22
31	m	101	LMG	O3-C3-C2	-2.08	105.65	110.34
34	f	101	HEM	CBD-CAD-C3D	-2.08	107.49	113.55
25	f	102	BCR	C11-C10-C9	-2.08	124.19	127.20
25	g	101	BCR	C24-C23-C22	-2.08	123.04	126.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	H	102	BCR	C16-C15-C14	-2.08	118.80	123.39
26	D	407	DGD	CAB-C9B-C8B	-2.08	103.81	114.53
25	f	102	BCR	C15-C16-C17	-2.07	118.81	123.39
26	C	515	DGD	O2D-C2D-C1D	-2.07	105.48	110.02
31	I	101	LMG	O1-C7-C8	-2.07	106.06	110.99
25	y	101	BCR	C3-C2-C1	-2.07	107.16	114.83
25	B	618	BCR	C3-C4-C5	-2.07	110.58	113.87
26	C	516	DGD	C3G-C2G-C1G	-2.07	107.23	112.07
26	C	514	DGD	C1D-C2D-C3D	-2.07	105.90	109.97
26	C	515	DGD	C5B-C4B-C3B	-2.07	103.86	114.53
24	a	407	PL9	C3-C2-C1	-2.07	121.71	122.97
25	A	408	BCR	C24-C23-C22	-2.06	123.07	126.22
25	K	101	BCR	C15-C14-C13	-2.06	124.22	127.20
27	c	519	LHG	C27-C26-C25	-2.06	103.89	114.53
26	c	515	DGD	O5D-C6D-C5D	-2.06	105.35	109.08
26	C	515	DGD	C3D-C4D-C5D	-2.06	106.61	110.20
26	C	516	DGD	CAB-C9B-C8B	-2.06	103.90	114.53
24	a	407	PL9	C36-C34-C33	-2.06	117.15	121.05
26	c	517	DGD	C3G-C2G-C1G	-2.06	107.26	112.07
31	d	408	LMG	O1-C7-C8	-2.06	106.10	110.99
23	d	402	PHO	CMB-C2B-C1B	-2.05	121.71	125.06
24	d	407	PL9	C42-C43-C44	-2.05	123.30	127.76
24	a	407	PL9	C12-C13-C14	-2.05	123.30	127.76
22	B	602	CLA	O2A-CGA-O1A	-2.05	118.19	123.49
26	d	410	DGD	C5B-C4B-C3B	-2.05	103.93	114.53
23	D	401	PHO	CMB-C2B-C1B	-2.05	121.72	125.06
22	D	403	CLA	O2A-CGA-O1A	-2.05	118.20	123.49
27	C	518	LHG	C27-C26-C25	-2.05	103.94	114.53
26	D	407	DGD	C5B-C4B-C3B	-2.05	103.95	114.53
22	b	607	CLA	O2A-CGA-O1A	-2.05	118.21	123.49
26	c	516	DGD	O2D-C2D-C1D	-2.05	105.53	110.02
26	b	601	DGD	O3E-C3E-C2E	-2.04	105.73	110.34
22	c	508	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
25	i	101	BCR	C15-C14-C13	-2.04	124.25	127.20
26	D	407	DGD	CBB-CAB-C9B	-2.04	103.99	114.53
24	a	407	PL9	C36-C37-C38	-2.04	106.35	111.69
26	d	410	DGD	CBB-CAB-C9B	-2.03	104.03	114.53
26	B	626	DGD	O3E-C3E-C2E	-2.03	105.77	110.34
25	b	624	BCR	C15-C16-C17	-2.03	118.91	123.39
24	D	405	PL9	O1-C4-C3	-2.03	118.19	120.71
31	b	627	LMG	O2-C2-C1	-2.03	105.57	110.02
22	b	617	CLA	O2A-CGA-O1A	-2.03	118.26	123.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	513	BCR	C8-C7-C6	-2.03	121.23	127.32
26	c	515	DGD	O3E-C3E-C2E	-2.02	105.79	110.34
31	d	408	LMG	C22-C21-C20	-2.02	104.11	114.53
22	B	603	CLA	O2A-CGA-O1A	-2.02	118.28	123.49
31	D	406	LMG	O3-C3-C2	-2.02	105.79	110.34
26	a	408	DGD	C5B-C4B-C3B	-2.02	104.11	114.53
26	A	409	DGD	C5B-C4B-C3B	-2.02	104.11	114.53
31	e	101	LMG	O1-C7-C8	-2.02	106.19	110.99
31	c	518	LMG	O1-C1-C2	-2.02	105.49	108.04
25	x	101	BCR	C15-C16-C17	-2.02	118.94	123.39
22	C	519	CLA	O2A-CGA-O1A	-2.01	118.29	123.49
26	c	517	DGD	CAB-C9B-C8B	-2.01	104.13	114.53
25	A	408	BCR	C15-C16-C17	-2.01	118.94	123.39
26	C	514	DGD	O3E-C3E-C2E	-2.01	105.80	110.34
25	B	619	BCR	C11-C10-C9	-2.01	124.29	127.20
22	C	512	CLA	O2A-CGA-O1A	-2.01	118.30	123.49
22	C	501	CLA	O2A-CGA-O1A	-2.01	118.30	123.49
31	c	522	LMG	C1-C2-C3	-2.01	106.01	109.97
22	C	508	CLA	O2A-CGA-O1A	-2.01	118.30	123.49
22	B	614	CLA	O2A-CGA-O1A	-2.01	118.30	123.49
26	C	516	DGD	C5B-C4B-C3B	-2.01	104.16	114.53
25	b	623	BCR	C3-C4-C5	-2.01	110.68	113.87
31	a	402	LMG	O2-C2-C1	-2.01	105.62	110.02
31	B	625	LMG	O1-C7-C8	-2.01	106.21	110.99
24	d	407	PL9	C12-C13-C14	-2.01	123.40	127.76
26	B	620	DGD	C1D-C2D-C3D	-2.00	106.02	109.97
22	C	504	CLA	O2A-CGA-O1A	-2.00	118.32	123.49
22	c	506	CLA	O2A-CGA-O1A	-2.00	118.32	123.49
31	l	101	LMG	O6-C1-O1	-2.00	105.23	110.05
25	j	102	BCR	C20-C21-C22	-2.00	124.31	127.20
31	B	625	LMG	C22-C21-C20	-2.00	104.20	114.53
26	A	409	DGD	C1D-C2D-C3D	-2.00	106.03	109.97
31	i	102	LMG	O1-C7-C8	-2.00	106.23	110.99
26	c	517	DGD	O2D-C2D-C1D	-2.00	105.64	110.02
23	A	405	PHO	C1B-NB-C4B	2.00	110.47	106.51
22	B	604	CLA	CMD-C2D-C3D	2.01	129.01	125.09
22	B	615	CLA	O2D-CGD-CBD	2.01	114.05	111.30
22	B	613	CLA	O1D-CGD-CBD	2.01	127.50	124.62
22	C	506	CLA	O2D-CGD-CBD	2.01	114.05	111.30
22	c	512	CLA	CMD-C2D-C3D	2.01	129.02	125.09
22	B	602	CLA	O1D-CGD-CBD	2.01	127.50	124.62
22	B	609	CLA	C1D-CHD-C4C	2.01	125.65	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	501	CLA	CMB-C2B-C3B	2.02	129.04	125.09
22	c	510	CLA	CMD-C2D-C3D	2.02	129.04	125.09
22	H	101	CLA	CMD-C2D-C3D	2.02	129.04	125.09
22	B	614	CLA	O2D-CGD-CBD	2.03	114.08	111.30
22	A	404	CLA	CMD-C2D-C3D	2.03	129.06	125.09
22	C	511	CLA	O1D-CGD-CBD	2.03	127.53	124.62
23	d	402	PHO	C1B-NB-C4B	2.03	110.53	106.51
22	B	614	CLA	O1D-CGD-CBD	2.04	127.54	124.62
22	C	511	CLA	O2D-CGD-CBD	2.04	114.09	111.30
26	D	407	DGD	O5D-C1E-C2E	2.04	110.62	108.04
26	A	409	DGD	O5D-C1E-C2E	2.04	110.62	108.04
23	D	401	PHO	C1B-NB-C4B	2.04	110.56	106.51
23	d	401	PHO	CHB-C1B-NB	2.05	128.49	124.66
22	C	507	CLA	CMD-C2D-C3D	2.05	129.10	125.09
22	b	619	CLA	O1D-CGD-CBD	2.05	127.56	124.62
22	B	606	CLA	O1D-CGD-CBD	2.06	127.57	124.62
22	b	615	CLA	CHB-C4A-NA	2.06	127.36	124.51
26	a	408	DGD	O5D-C1E-C2E	2.06	110.64	108.04
22	b	619	CLA	O2D-CGD-CBD	2.06	114.13	111.30
22	b	609	CLA	O2D-CGD-CBD	2.07	114.13	111.30
26	b	625	DGD	O5D-C1E-C2E	2.07	110.65	108.04
22	B	604	CLA	O1D-CGD-CBD	2.07	127.59	124.62
22	C	504	CLA	CBA-CAA-C2A	2.08	119.59	113.73
22	b	619	CLA	CMD-C2D-C3D	2.08	129.16	125.09
30	a	401	SQD	O6-C1-C2	2.08	110.67	108.04
22	a	405	CLA	O1D-CGD-CBD	2.08	127.61	124.62
22	b	620	CLA	O2D-CGD-CBD	2.08	114.16	111.30
22	B	606	CLA	CMD-C2D-C3D	2.09	129.17	125.09
22	C	506	CLA	CMD-C2D-C3D	2.09	129.17	125.09
26	C	516	DGD	O5D-C1E-C2E	2.09	110.68	108.04
22	B	608	CLA	O1D-CGD-CBD	2.09	127.62	124.62
25	J	102	BCR	C29-C30-C25	2.09	113.67	110.36
22	c	520	CLA	O1D-CGD-CBD	2.09	127.62	124.62
22	C	512	CLA	CMD-C2D-C3D	2.09	129.18	125.09
25	j	102	BCR	C29-C30-C25	2.09	113.68	110.36
22	B	610	CLA	CHB-C4A-NA	2.10	127.41	124.51
22	B	603	CLA	CMD-C2D-C3D	2.10	129.19	125.09
34	V	201	HEM	C2D-C3D-C4D	2.10	105.06	101.50
22	c	501	CLA	CMD-C2D-C3D	2.10	129.19	125.09
22	b	607	CLA	CMD-C2D-C3D	2.10	129.20	125.09
22	c	502	CLA	O2D-CGD-CBD	2.11	114.19	111.30
22	c	520	CLA	CMD-C2D-C3D	2.11	129.21	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	b	608	CLA	CMD-C2D-C3D	2.11	129.22	125.09
22	B	602	CLA	CMD-C2D-C3D	2.11	129.22	125.09
22	c	506	CLA	CMD-C2D-C3D	2.11	129.22	125.09
22	b	609	CLA	O1D-CGD-CBD	2.11	127.65	124.62
32	M	103	LMT	O1'-C1'-C2'	2.12	110.72	108.04
22	b	614	CLA	CMD-C2D-C3D	2.12	129.23	125.09
22	b	614	CLA	O1D-CGD-CBD	2.12	127.66	124.62
22	B	613	CLA	CMD-C2D-C3D	2.12	129.24	125.09
30	A	414	SQD	O6-C1-C2	2.12	110.72	108.04
22	C	519	CLA	O2D-CGD-CBD	2.12	114.21	111.30
22	a	404	CLA	O2D-CGD-CBD	2.13	114.22	111.30
22	d	406	CLA	CMD-C2D-C3D	2.13	129.25	125.09
22	c	505	CLA	CMD-C2D-C3D	2.13	129.25	125.09
22	d	405	CLA	CHB-C4A-NA	2.13	127.46	124.51
22	A	406	CLA	CMD-C2D-C3D	2.15	129.29	125.09
30	d	403	SQD	C4-C3-C2	2.15	114.81	110.79
30	F	103	SQD	O48-C23-C24	2.15	118.46	111.90
30	f	103	SQD	O48-C23-C24	2.15	118.46	111.90
25	x	101	BCR	C27-C26-C25	2.15	125.52	122.78
22	c	503	CLA	CMD-C2D-C3D	2.15	129.30	125.09
22	b	618	CLA	CMD-C2D-C3D	2.15	129.30	125.09
22	b	605	CLA	O1D-CGD-CBD	2.16	127.72	124.62
22	B	610	CLA	C4A-NA-C1A	2.16	109.15	106.36
22	C	501	CLA	CMD-C2D-C3D	2.16	129.31	125.09
22	C	506	CLA	O1D-CGD-CBD	2.16	127.72	124.62
22	b	612	CLA	CMD-C2D-C3D	2.16	129.32	125.09
22	c	502	CLA	O1D-CGD-CBD	2.17	127.73	124.62
22	b	605	CLA	O2D-CGD-CBD	2.17	114.28	111.30
22	c	507	CLA	CMD-C2D-C3D	2.17	129.34	125.09
22	C	503	CLA	CMD-C2D-C3D	2.18	129.34	125.09
32	B	623	LMT	O1'-C1'-C2'	2.18	110.79	108.04
22	C	505	CLA	CMD-C2D-C3D	2.18	129.35	125.09
22	C	519	CLA	CMD-C2D-C3D	2.19	129.38	125.09
22	b	605	CLA	CHB-C4A-NA	2.19	127.55	124.51
22	B	610	CLA	C1D-CHD-C4C	2.20	125.93	122.60
30	B	622	SQD	C4-C3-C2	2.20	114.90	110.79
22	B	610	CLA	CMD-C2D-C3D	2.20	129.39	125.09
22	B	612	CLA	CMD-C2D-C3D	2.21	129.41	125.09
26	c	515	DGD	O5D-C1E-C2E	2.21	110.83	108.04
22	b	605	CLA	CMD-C2D-C3D	2.21	129.41	125.09
34	F	101	HEM	C2D-C3D-C4D	2.22	105.26	101.50
25	H	102	BCR	C29-C30-C25	2.22	113.87	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	a	406	CLA	CMD-C2D-C3D	2.22	129.44	125.09
22	B	601	CLA	CMD-C2D-C3D	2.22	129.44	125.09
22	c	520	CLA	O2D-CGD-CBD	2.23	114.36	111.30
22	c	506	CLA	O1D-CGD-CBD	2.24	127.83	124.62
30	b	602	SQD	O48-C23-C24	2.24	118.72	111.90
22	b	617	CLA	O1D-CGD-CBD	2.24	127.83	124.62
22	B	601	CLA	CHB-C4A-NA	2.24	127.61	124.51
22	b	615	CLA	C4A-NA-C1A	2.24	109.26	106.36
22	b	614	CLA	O2D-CGD-CBD	2.25	114.38	111.30
22	C	504	CLA	CMB-C2B-C3B	2.25	129.48	125.09
30	a	412	SQD	C44-O6-C1	2.25	118.54	113.82
22	c	511	CLA	O1D-CGD-CBD	2.25	127.85	124.62
30	f	103	SQD	C1-O5-C5	2.25	118.11	113.75
32	b	629	LMT	O1'-C1'-C2'	2.25	110.89	108.04
22	c	504	CLA	CBA-CAA-C2A	2.26	120.10	113.73
22	a	403	CLA	CMB-C2B-C3B	2.26	129.50	125.09
22	C	509	CLA	O1D-CGD-CBD	2.26	127.86	124.62
22	B	608	CLA	CMD-C2D-C3D	2.26	129.51	125.09
22	D	403	CLA	CMD-C2D-C3D	2.27	129.52	125.09
22	C	502	CLA	CMD-C2D-C3D	2.27	129.53	125.09
22	b	616	CLA	CMD-C2D-C3D	2.27	129.53	125.09
22	B	607	CLA	CMD-C2D-C3D	2.27	129.53	125.09
22	D	403	CLA	CHB-C4A-NA	2.27	127.65	124.51
22	c	504	CLA	CMB-C2B-C3B	2.27	129.54	125.09
22	c	508	CLA	O1D-CGD-CBD	2.28	127.89	124.62
32	b	628	LMT	O1'-C1'-C2'	2.29	110.93	108.04
22	b	614	CLA	C4A-NA-C1A	2.29	109.32	106.36
25	x	101	BCR	C29-C30-C25	2.29	113.99	110.36
22	A	402	CLA	CMB-C2B-C3B	2.29	129.57	125.09
22	D	404	CLA	CMD-C2D-C3D	2.29	129.57	125.09
25	B	618	BCR	C27-C26-C25	2.29	125.70	122.78
24	a	407	PL9	C41-C39-C40	2.29	120.28	114.64
34	f	101	HEM	C2D-C3D-C4D	2.30	105.39	101.50
30	A	414	SQD	C1-O5-C5	2.30	118.21	113.75
22	b	620	CLA	CMB-C2B-C3B	2.30	129.59	125.09
22	A	406	CLA	O1D-CGD-CBD	2.30	127.92	124.62
22	b	607	CLA	C4A-NA-C1A	2.32	109.36	106.36
22	A	404	CLA	O2D-CGD-CBD	2.32	114.48	111.30
25	f	102	BCR	C27-C26-C25	2.32	125.74	122.78
22	c	509	CLA	O1D-CGD-CBD	2.32	127.95	124.62
22	d	405	CLA	CMD-C2D-C3D	2.32	129.63	125.09
22	b	613	CLA	CMD-C2D-C3D	2.32	129.63	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	v	201	HEM	C2D-C3D-C4D	2.33	105.44	101.50
25	H	102	BCR	C27-C26-C25	2.33	125.74	122.78
22	a	405	CLA	O2D-CGD-CBD	2.33	114.49	111.30
22	B	602	CLA	O2D-CGD-CBD	2.33	114.50	111.30
22	B	615	CLA	CMB-C2B-C3B	2.34	129.66	125.09
22	b	614	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	j	101	PL9	C20-C19-C21	2.34	118.98	115.41
32	B	628	LMT	O1'-C1'-C2'	2.35	111.00	108.04
30	a	401	SQD	O48-C23-C24	2.35	119.05	111.90
22	B	611	CLA	CMD-C2D-C3D	2.35	129.69	125.09
30	f	103	SQD	C3-C4-C5	2.36	114.30	110.20
26	d	410	DGD	O5D-C1E-C2E	2.36	111.02	108.04
22	b	613	CLA	C4A-NA-C1A	2.36	109.41	106.36
22	B	608	CLA	O2D-CGD-CBD	2.36	114.53	111.30
22	C	511	CLA	CMD-C2D-C3D	2.36	129.70	125.09
22	H	101	CLA	CMB-C2B-C3B	2.36	129.71	125.09
22	C	502	CLA	CHB-C4A-NA	2.36	127.78	124.51
22	b	611	CLA	O2D-CGD-CBD	2.36	114.54	111.30
25	b	622	BCR	C29-C30-C25	2.36	114.11	110.36
22	b	606	CLA	CMD-C2D-C3D	2.37	129.71	125.09
22	b	607	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	B	601	CLA	C4A-NA-C1A	2.37	109.42	106.36
30	A	414	SQD	O48-C23-C24	2.37	119.11	111.90
22	B	601	CLA	O1D-CGD-CBD	2.37	128.02	124.62
22	B	612	CLA	O1D-CGD-CBD	2.38	128.03	124.62
22	C	509	CLA	CHB-C4A-NA	2.38	127.80	124.51
22	A	403	CLA	CMB-C2B-C3B	2.38	129.74	125.09
22	C	508	CLA	O1D-CGD-CBD	2.38	128.03	124.62
22	B	603	CLA	CMB-C2B-C3B	2.38	129.74	125.09
22	b	605	CLA	C4A-NA-C1A	2.38	109.44	106.36
22	d	406	CLA	O1D-CGD-CBD	2.38	128.04	124.62
22	c	504	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	A	406	CLA	CHB-C4A-NA	2.39	127.81	124.51
22	B	606	CLA	O2D-CGD-CBD	2.39	114.58	111.30
30	F	103	SQD	C3-C4-C5	2.39	114.37	110.20
22	c	501	CLA	O1D-CGD-CBD	2.39	128.05	124.62
22	b	617	CLA	CHB-C4A-NA	2.40	127.83	124.51
30	B	622	SQD	O48-C23-C24	2.40	119.20	111.90
22	C	502	CLA	C4A-NA-C1A	2.40	109.46	106.36
25	B	616	BCR	C2-C1-C6	2.40	114.16	110.36
22	A	402	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	F	102	BCR	C27-C26-C25	2.40	125.84	122.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	511	CLA	CMD-C2D-C3D	2.40	129.79	125.09
22	b	615	CLA	CMD-C2D-C3D	2.41	129.79	125.09
25	K	101	BCR	C27-C26-C25	2.41	125.85	122.78
22	c	505	CLA	O2D-CGD-CBD	2.41	114.60	111.30
22	A	403	CLA	O2D-CGD-CBD	2.41	114.60	111.30
25	B	617	BCR	C29-C30-C25	2.41	114.18	110.36
22	B	610	CLA	O1D-CGD-CBD	2.41	128.08	124.62
22	b	611	CLA	CHB-C4A-NA	2.41	127.85	124.51
22	B	614	CLA	CMB-C2B-C3B	2.42	129.81	125.09
22	b	616	CLA	O1D-CGD-CBD	2.42	128.09	124.62
24	A	407	PL9	C41-C39-C40	2.42	120.58	114.64
25	b	623	BCR	C27-C26-C25	2.42	125.86	122.78
25	b	621	BCR	C2-C1-C6	2.42	114.20	110.36
30	F	103	SQD	C1-O5-C5	2.42	118.45	113.75
22	B	608	CLA	CMB-C2B-C3B	2.42	129.83	125.09
22	a	405	CLA	CHB-C4A-NA	2.42	127.86	124.51
22	a	405	CLA	CMB-C2B-C3B	2.43	129.83	125.09
30	a	401	SQD	C1-O5-C5	2.43	118.45	113.75
22	b	613	CLA	O2D-CGD-CBD	2.43	114.63	111.30
22	b	620	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	c	510	CLA	CHB-C4A-NA	2.43	127.87	124.51
22	D	404	CLA	C4A-NA-C1A	2.43	109.50	106.36
22	B	604	CLA	O2D-CGD-CBD	2.43	114.64	111.30
22	C	505	CLA	C4A-NA-C1A	2.43	109.50	106.36
22	B	609	CLA	O1D-CGD-CBD	2.44	128.11	124.62
22	b	610	CLA	CMB-C2B-C3B	2.44	129.85	125.09
22	b	611	CLA	C4A-NA-C1A	2.45	109.52	106.36
24	A	407	PL9	C20-C19-C21	2.45	119.15	115.41
22	B	615	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	B	609	CLA	C4A-NA-C1A	2.45	109.53	106.36
22	b	611	CLA	CMB-C2B-C3B	2.45	129.89	125.09
22	c	520	CLA	CMB-C2B-C3B	2.45	129.89	125.09
25	c	513	BCR	C27-C26-C25	2.46	125.91	122.78
22	b	613	CLA	CMB-C2B-C3B	2.46	129.90	125.09
22	a	405	CLA	C4A-NA-C1A	2.46	109.54	106.36
22	C	505	CLA	O2D-CGD-CBD	2.46	114.68	111.30
22	C	510	CLA	O1D-CGD-CBD	2.47	128.16	124.62
30	B	627	SQD	O48-C23-C24	2.47	119.42	111.90
22	A	404	CLA	CMB-C2B-C3B	2.47	129.91	125.09
22	B	602	CLA	C4A-NA-C1A	2.47	109.55	106.36
22	a	406	CLA	O1D-CGD-CBD	2.47	128.16	124.62
22	B	611	CLA	O1D-CGD-CBD	2.47	128.16	124.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	402	CLA	C4A-NA-C1A	2.47	109.55	106.36
22	b	608	CLA	CMB-C2B-C3B	2.47	129.93	125.09
22	c	506	CLA	C4A-NA-C1A	2.47	109.56	106.36
22	C	509	CLA	C4A-NA-C1A	2.47	109.56	106.36
22	B	602	CLA	CHB-C4A-NA	2.48	127.94	124.51
22	D	404	CLA	O1D-CGD-CBD	2.48	128.17	124.62
22	B	607	CLA	C4A-NA-C1A	2.48	109.56	106.36
22	d	405	CLA	CMB-C2B-C3B	2.48	129.94	125.09
22	H	101	CLA	CHB-C4A-NA	2.48	127.94	124.51
24	J	101	PL9	C20-C19-C21	2.48	119.20	115.41
22	b	606	CLA	O1D-CGD-CBD	2.48	128.18	124.62
22	B	614	CLA	CHB-C4A-NA	2.48	127.94	124.51
30	A	413	SQD	O48-C23-C24	2.48	119.47	111.90
22	B	608	CLA	C4A-NA-C1A	2.49	109.57	106.36
22	B	606	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	C	505	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	b	612	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	a	403	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	b	613	CLA	CHB-C4A-NA	2.49	127.95	124.51
22	c	502	CLA	CMD-C2D-C3D	2.49	129.96	125.09
22	c	510	CLA	C4A-NA-C1A	2.49	109.58	106.36
22	a	403	CLA	C4A-NA-C1A	2.49	109.58	106.36
22	b	606	CLA	C4A-NA-C1A	2.49	109.58	106.36
22	b	612	CLA	C4A-NA-C1A	2.50	109.59	106.36
22	D	403	CLA	C4A-NA-C1A	2.50	109.59	106.36
24	a	407	PL9	C20-C19-C21	2.50	119.22	115.41
30	d	403	SQD	O48-C23-C24	2.50	119.52	111.90
30	A	413	SQD	C44-O6-C1	2.50	119.07	113.82
22	c	504	CLA	CMD-C2D-C3D	2.50	129.98	125.09
22	C	508	CLA	C4A-NA-C1A	2.50	109.59	106.36
22	A	404	CLA	C4A-NA-C1A	2.50	109.59	106.36
22	c	502	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	b	605	CLA	CMB-C2B-C3B	2.50	129.98	125.09
22	d	406	CLA	CMB-C2B-C3B	2.51	130.00	125.09
22	b	618	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	C	509	CLA	CMB-C2B-C3B	2.51	130.00	125.09
22	b	616	CLA	CHB-C4A-NA	2.51	127.98	124.51
22	C	508	CLA	CMB-C2B-C3B	2.51	130.00	125.09
22	C	507	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	B	611	CLA	CHB-C4A-NA	2.51	127.99	124.51
22	D	403	CLA	O1D-CGD-CBD	2.52	128.23	124.62
22	B	606	CLA	C4A-NA-C1A	2.52	109.62	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	c	512	CLA	O1D-CGD-CBD	2.52	128.23	124.62
22	c	509	CLA	CHB-C4A-NA	2.52	128.00	124.51
22	b	619	CLA	CMB-C2B-C3B	2.52	130.02	125.09
22	c	511	CLA	CMB-C2B-C3B	2.53	130.03	125.09
22	B	607	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	c	509	CLA	CMB-C2B-C3B	2.53	130.03	125.09
25	B	618	BCR	C29-C30-C25	2.53	114.37	110.36
22	D	404	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	b	607	CLA	O2D-CGD-CBD	2.53	114.77	111.30
22	c	503	CLA	CHB-C4A-NA	2.53	128.01	124.51
22	C	512	CLA	CHB-C4A-NA	2.53	128.02	124.51
22	H	101	CLA	O1D-CGD-CBD	2.53	128.25	124.62
22	c	502	CLA	C4A-NA-C1A	2.54	109.64	106.36
22	B	609	CLA	CHB-C4A-NA	2.54	128.02	124.51
22	C	501	CLA	O1D-CGD-CBD	2.54	128.26	124.62
22	b	618	CLA	C4A-NA-C1A	2.54	109.64	106.36
22	c	509	CLA	C4A-NA-C1A	2.54	109.64	106.36
25	c	514	BCR	C29-C30-C25	2.54	114.38	110.36
22	a	404	CLA	CMB-C2B-C3B	2.54	130.06	125.09
24	d	407	PL9	C20-C19-C21	2.54	119.29	115.41
22	C	508	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	a	404	CLA	C4A-NA-C1A	2.55	109.66	106.36
22	C	519	CLA	C4A-NA-C1A	2.55	109.66	106.36
22	B	606	CLA	CMB-C2B-C3B	2.55	130.08	125.09
22	c	507	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	c	520	CLA	CHB-C4A-NA	2.56	128.05	124.51
22	B	604	CLA	CMB-C2B-C3B	2.56	130.10	125.09
22	c	508	CLA	C4A-NA-C1A	2.56	109.67	106.36
22	B	601	CLA	CMB-C2B-C3B	2.56	130.10	125.09
22	C	504	CLA	CMD-C2D-C3D	2.57	130.11	125.09
25	b	621	BCR	C27-C26-C25	2.57	126.05	122.78
22	a	404	CLA	CHB-C4A-NA	2.57	128.06	124.51
22	b	612	CLA	O1D-CGD-CBD	2.57	128.30	124.62
22	B	612	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	c	505	CLA	C4A-NA-C1A	2.57	109.68	106.36
22	A	404	CLA	CHB-C4A-NA	2.57	128.07	124.51
30	a	412	SQD	O48-C23-C24	2.57	119.74	111.90
22	B	608	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	C	519	CLA	CMB-C2B-C3B	2.58	130.13	125.09
22	c	508	CLA	CMB-C2B-C3B	2.58	130.13	125.09
22	b	609	CLA	CMB-C2B-C3B	2.58	130.13	125.09
25	B	616	BCR	C27-C26-C25	2.58	126.07	122.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	503	CLA	CMB-C2B-C3B	2.58	130.14	125.09
22	C	511	CLA	CMB-C2B-C3B	2.58	130.14	125.09
22	c	503	CLA	CMB-C2B-C3B	2.59	130.15	125.09
22	c	505	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	d	406	CLA	CHB-C4A-NA	2.59	128.09	124.51
22	H	101	CLA	C4A-NA-C1A	2.59	109.71	106.36
22	A	406	CLA	C4A-NA-C1A	2.59	109.71	106.36
22	c	512	CLA	C4A-NA-C1A	2.59	109.71	106.36
22	C	519	CLA	CHB-C4A-NA	2.59	128.10	124.51
22	d	405	CLA	O1D-CGD-CBD	2.59	128.34	124.62
22	C	503	CLA	CHB-C4A-NA	2.60	128.10	124.51
22	B	613	CLA	C4A-NA-C1A	2.60	109.72	106.36
25	C	513	BCR	C29-C30-C25	2.60	114.48	110.36
22	C	502	CLA	CMB-C2B-C3B	2.60	130.17	125.09
22	D	403	CLA	CMB-C2B-C3B	2.60	130.18	125.09
22	b	615	CLA	O1D-CGD-CBD	2.60	128.35	124.62
22	b	606	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	b	617	CLA	C4A-NA-C1A	2.61	109.73	106.36
22	C	504	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	c	512	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	a	406	CLA	CHB-C4A-NA	2.61	128.12	124.51
22	C	512	CLA	CMB-C2B-C3B	2.61	130.20	125.09
22	B	612	CLA	CHB-C4A-NA	2.61	128.13	124.51
22	C	502	CLA	O2D-CGD-CBD	2.62	114.89	111.30
22	d	406	CLA	C4A-NA-C1A	2.62	109.74	106.36
22	b	619	CLA	CHB-C4A-NA	2.62	128.13	124.51
22	c	502	CLA	CMB-C2B-C3B	2.63	130.23	125.09
22	B	605	CLA	CMB-C2B-C3B	2.63	130.23	125.09
22	D	404	CLA	CMB-C2B-C3B	2.63	130.23	125.09
22	B	613	CLA	CHB-C4A-NA	2.64	128.16	124.51
22	b	620	CLA	C4A-NA-C1A	2.64	109.77	106.36
22	b	616	CLA	CMB-C2B-C3B	2.64	130.25	125.09
22	C	507	CLA	O2D-CGD-CBD	2.64	114.92	111.30
22	b	619	CLA	C4A-NA-C1A	2.64	109.78	106.36
22	c	507	CLA	C4A-NA-C1A	2.65	109.78	106.36
22	c	511	CLA	CHB-C4A-NA	2.65	128.17	124.51
22	c	510	CLA	CMB-C2B-C3B	2.65	130.27	125.09
22	c	512	CLA	CMB-C2B-C3B	2.65	130.27	125.09
22	c	506	CLA	CHB-C4A-NA	2.65	128.18	124.51
27	C	518	LHG	O8-C23-C24	2.65	119.97	111.90
22	A	406	CLA	CMB-C2B-C3B	2.65	130.28	125.09
22	c	501	CLA	CHB-C4A-NA	2.65	128.18	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	d	405	CLA	C4A-NA-C1A	2.66	109.79	106.36
22	a	406	CLA	C4A-NA-C1A	2.66	109.80	106.36
22	c	511	CLA	C4A-NA-C1A	2.66	109.80	106.36
22	a	406	CLA	CMB-C2B-C3B	2.66	130.29	125.09
30	B	627	SQD	C4-C3-C2	2.66	115.76	110.79
22	c	520	CLA	C4A-NA-C1A	2.67	109.81	106.36
24	D	405	PL9	C20-C19-C21	2.67	119.49	115.41
22	b	610	CLA	CHB-C4A-NA	2.67	128.21	124.51
22	B	603	CLA	CHB-C4A-NA	2.67	128.21	124.51
27	c	519	LHG	O8-C23-C24	2.68	120.05	111.90
22	b	609	CLA	C4A-NA-C1A	2.68	109.82	106.36
25	C	520	BCR	C2-C1-C6	2.68	114.61	110.36
22	B	614	CLA	C4A-NA-C1A	2.68	109.82	106.36
22	C	506	CLA	C4A-NA-C1A	2.68	109.83	106.36
22	C	506	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	b	623	BCR	C29-C30-C25	2.68	114.61	110.36
22	C	511	CLA	CHB-C4A-NA	2.69	128.22	124.51
22	C	501	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	c	508	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	c	510	CLA	O1D-CGD-CBD	2.69	128.47	124.62
22	A	403	CLA	C4A-NA-C1A	2.69	109.84	106.36
30	d	403	SQD	C44-O6-C1	2.70	119.49	113.82
22	b	606	CLA	CMB-C2B-C3B	2.70	130.37	125.09
22	A	403	CLA	CHB-C4A-NA	2.70	128.25	124.51
22	C	512	CLA	C4A-NA-C1A	2.70	109.85	106.36
22	C	510	CLA	CMB-C2B-C3B	2.70	130.38	125.09
25	A	408	BCR	C27-C26-C25	2.71	126.23	122.78
22	B	613	CLA	O2D-CGD-CBD	2.71	115.01	111.30
22	b	618	CLA	CMB-C2B-C3B	2.71	130.38	125.09
22	B	611	CLA	CMB-C2B-C3B	2.71	130.39	125.09
22	C	506	CLA	CMB-C2B-C3B	2.71	130.39	125.09
22	c	504	CLA	C4A-NA-C1A	2.71	109.87	106.36
22	B	604	CLA	C4A-NA-C1A	2.72	109.87	106.36
25	i	101	BCR	C27-C26-C25	2.72	126.25	122.78
22	C	507	CLA	C4A-NA-C1A	2.72	109.88	106.36
22	B	605	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	b	624	BCR	C27-C26-C25	2.73	126.26	122.78
22	B	604	CLA	CHB-C4A-NA	2.74	128.29	124.51
25	B	619	BCR	C27-C26-C25	2.74	126.27	122.78
22	B	615	CLA	C4A-NA-C1A	2.75	109.91	106.36
22	B	607	CLA	O1D-CGD-CBD	2.75	128.56	124.62
22	c	501	CLA	C4A-NA-C1A	2.75	109.91	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	521	BCR	C2-C1-C6	2.75	114.72	110.36
22	C	510	CLA	C4A-NA-C1A	2.75	109.92	106.36
22	C	510	CLA	CHB-C4A-NA	2.76	128.34	124.51
22	C	505	CLA	CMB-C2B-C3B	2.77	130.50	125.09
25	c	521	BCR	C27-C26-C25	2.77	126.31	122.78
22	c	503	CLA	C4A-NA-C1A	2.77	109.94	106.36
22	B	603	CLA	C4A-NA-C1A	2.77	109.94	106.36
22	C	511	CLA	C4A-NA-C1A	2.77	109.94	106.36
22	b	608	CLA	CHB-C4A-NA	2.77	128.34	124.51
22	b	616	CLA	C4A-NA-C1A	2.77	109.94	106.36
22	C	503	CLA	C4A-NA-C1A	2.78	109.95	106.36
22	b	610	CLA	C4A-NA-C1A	2.78	109.95	106.36
30	b	602	SQD	C4-C3-C2	2.78	115.98	110.79
22	C	501	CLA	C4A-NA-C1A	2.78	109.96	106.36
22	a	403	CLA	O1D-CGD-CBD	2.79	128.62	124.62
22	b	614	CLA	CMB-C2B-C3B	2.79	130.54	125.09
22	c	505	CLA	CMB-C2B-C3B	2.79	130.55	125.09
22	b	607	CLA	CMB-C2B-C3B	2.80	130.56	125.09
22	c	507	CLA	O2D-CGD-CBD	2.80	115.14	111.30
25	f	102	BCR	C29-C30-C25	2.81	114.81	110.36
22	C	507	CLA	CMB-C2B-C3B	2.81	130.59	125.09
22	C	512	CLA	O1D-CGD-CBD	2.82	128.66	124.62
22	b	608	CLA	C4A-NA-C1A	2.82	110.01	106.36
22	b	609	CLA	CHB-C4A-NA	2.83	128.42	124.51
25	F	102	BCR	C29-C30-C25	2.83	114.85	110.36
25	B	619	BCR	C2-C1-C6	2.83	114.85	110.36
22	B	602	CLA	CMB-C2B-C3B	2.83	130.63	125.09
22	B	605	CLA	C4A-NA-C1A	2.84	110.03	106.36
25	b	624	BCR	C2-C1-C6	2.84	114.86	110.36
22	A	402	CLA	O1D-CGD-CBD	2.85	128.71	124.62
30	A	413	SQD	C3-C4-C5	2.85	115.17	110.20
22	B	609	CLA	CMB-C2B-C3B	2.86	130.69	125.09
30	F	103	SQD	C44-O6-C1	2.87	119.84	113.82
25	C	520	BCR	C27-C26-C25	2.87	126.43	122.78
22	b	612	CLA	CMB-C2B-C3B	2.87	130.70	125.09
30	f	103	SQD	C44-O6-C1	2.87	119.85	113.82
34	f	101	HEM	CMD-C2D-C3D	2.87	127.05	114.35
30	B	622	SQD	C44-O6-C1	2.87	119.85	113.82
22	c	506	CLA	CMB-C2B-C3B	2.87	130.71	125.09
27	A	410	LHG	O8-C23-C24	2.89	120.71	111.90
22	B	611	CLA	C4A-NA-C1A	2.89	110.10	106.36
24	D	405	PL9	C40-C39-C41	2.90	119.83	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	503	CLA	O2D-CGD-CBD	2.91	115.29	111.30
22	C	504	CLA	C4A-NA-C1A	2.91	110.12	106.36
27	a	409	LHG	O8-C23-C24	2.92	120.81	111.90
34	F	101	HEM	CMD-C2D-C3D	2.93	127.31	114.35
22	B	607	CLA	CMB-C2B-C3B	2.94	130.83	125.09
30	b	602	SQD	C3-C4-C5	2.94	115.32	110.20
22	B	613	CLA	CMB-C2B-C3B	2.95	130.86	125.09
22	b	618	CLA	O2D-CGD-CBD	2.96	115.36	111.30
22	c	507	CLA	CMB-C2B-C3B	2.97	130.90	125.09
22	b	610	CLA	O1D-CGD-CBD	2.99	128.91	124.62
22	b	615	CLA	CMB-C2B-C3B	3.00	130.95	125.09
25	b	623	BCR	C2-C1-C6	3.01	115.14	110.36
22	b	617	CLA	CMB-C2B-C3B	3.02	130.99	125.09
22	c	503	CLA	O2D-CGD-CBD	3.04	115.47	111.30
22	C	504	CLA	O1D-CGD-CBD	3.04	128.98	124.62
30	a	412	SQD	C3-C4-C5	3.06	115.53	110.20
25	i	101	BCR	C2-C1-C6	3.07	115.22	110.36
22	c	504	CLA	O1D-CGD-CBD	3.08	129.04	124.62
34	v	201	HEM	CMD-C2D-C3D	3.09	128.04	114.35
34	F	101	HEM	C3B-C4B-CHC	3.11	127.54	123.16
22	B	610	CLA	CMB-C2B-C3B	3.11	131.17	125.09
24	d	407	PL9	C40-C39-C41	3.12	120.17	115.41
25	y	101	BCR	C27-C26-C25	3.12	126.76	122.78
22	B	605	CLA	O1D-CGD-CBD	3.13	129.10	124.62
30	A	414	SQD	C44-O6-C1	3.13	120.39	113.82
30	B	622	SQD	C3-C4-C5	3.13	115.66	110.20
25	B	618	BCR	C2-C1-C6	3.14	115.33	110.36
25	g	101	BCR	C27-C26-C25	3.15	126.79	122.78
22	b	608	CLA	O1D-CGD-CBD	3.15	129.13	124.62
30	f	103	SQD	O47-C7-C8	3.15	118.37	111.53
30	a	401	SQD	O47-C7-C8	3.15	118.38	111.53
22	B	612	CLA	CMB-C2B-C3B	3.16	131.28	125.09
34	f	101	HEM	C3B-C4B-CHC	3.18	127.64	123.16
30	d	403	SQD	C3-C4-C5	3.18	115.73	110.20
25	j	102	BCR	C27-C26-C25	3.19	126.85	122.78
23	A	405	PHO	O1D-CGD-CBD	3.21	129.22	124.62
25	J	102	BCR	C27-C26-C25	3.22	126.88	122.78
34	V	201	HEM	CMD-C2D-C3D	3.25	128.70	114.35
23	d	401	PHO	O1D-CGD-CBD	3.28	129.32	124.62
22	B	603	CLA	O1D-CGD-CBD	3.30	129.36	124.62
23	D	401	PHO	O1D-CGD-CBD	3.31	129.37	124.62
30	A	414	SQD	O47-C7-C8	3.31	118.72	111.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	408	BCR	C2-C1-C6	3.31	115.61	110.36
30	B	627	SQD	C3-C4-C5	3.33	116.00	110.20
30	F	103	SQD	O47-C7-C8	3.37	118.85	111.53
30	a	401	SQD	C44-O6-C1	3.38	120.92	113.82
23	d	402	PHO	O1D-CGD-CBD	3.39	129.48	124.62
30	d	403	SQD	O47-C7-C8	3.39	118.90	111.53
30	B	622	SQD	O47-C7-C8	3.46	119.04	111.53
34	v	201	HEM	CMC-C2C-C3C	3.50	125.27	116.53
30	A	413	SQD	O5-C5-C4	3.55	116.35	109.68
30	a	412	SQD	O5-C5-C4	3.59	116.41	109.68
30	a	401	SQD	O5-C5-C4	3.60	116.44	109.68
30	b	602	SQD	O5-C5-C4	3.62	116.48	109.68
34	f	101	HEM	CMB-C2B-C3B	3.62	125.57	116.53
30	B	627	SQD	O5-C5-C4	3.66	116.55	109.68
30	f	103	SQD	O5-C5-C4	3.67	116.56	109.68
25	J	102	BCR	C2-C1-C6	3.68	116.18	110.36
30	B	627	SQD	O47-C7-C8	3.68	119.53	111.53
30	F	103	SQD	O5-C5-C4	3.70	116.62	109.68
30	a	412	SQD	O47-C7-C8	3.70	119.57	111.53
30	A	414	SQD	O5-C5-C4	3.75	116.72	109.68
25	K	101	BCR	C2-C1-C6	3.76	116.31	110.36
26	b	601	DGD	O5D-C1E-C2E	3.76	112.79	108.04
34	V	201	HEM	CMC-C2C-C3C	3.76	125.91	116.53
25	c	513	BCR	C2-C1-C6	3.76	116.32	110.36
25	j	102	BCR	C2-C1-C6	3.77	116.33	110.36
34	V	201	HEM	CAD-C3D-C4D	3.77	125.76	112.47
32	I	102	LMT	O1'-C1'-C2'	3.77	112.80	108.04
30	b	602	SQD	O47-C7-C8	3.78	119.75	111.53
27	A	410	LHG	O4-P-O5	3.79	133.06	112.53
34	F	101	HEM	CMB-C2B-C3B	3.79	125.99	116.53
27	c	519	LHG	O4-P-O5	3.80	133.13	112.53
27	a	409	LHG	O4-P-O5	3.81	133.17	112.53
30	A	413	SQD	O47-C7-C8	3.82	119.83	111.53
27	C	518	LHG	O4-P-O5	3.82	133.25	112.53
26	B	626	DGD	O5D-C1E-C2E	3.83	112.88	108.04
34	v	201	HEM	CAD-C3D-C4D	3.88	126.14	112.47
32	i	103	LMT	O1'-C1'-C2'	3.91	112.97	108.04
34	F	101	HEM	CAD-C3D-C4D	3.92	126.30	112.47
34	f	101	HEM	CAD-C3D-C4D	4.05	126.75	112.47
30	B	622	SQD	O5-C5-C4	4.14	117.45	109.68
30	d	403	SQD	O5-C5-C4	4.16	117.49	109.68
30	f	103	SQD	O6-C1-C2	4.32	113.50	108.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	F	103	SQD	O6-C1-C2	4.50	113.72	108.04
30	B	622	SQD	O9-S-C6	4.55	110.78	106.94
30	f	103	SQD	O9-S-C6	4.71	110.91	106.94
34	F	101	HEM	CMC-C2C-C3C	4.81	128.54	116.53
34	V	201	HEM	CMB-C2B-C3B	4.83	128.59	116.53
34	f	101	HEM	CMC-C2C-C3C	4.84	128.62	116.53
30	a	401	SQD	O9-S-C6	4.85	111.03	106.94
30	d	403	SQD	O6-C1-C2	4.88	114.20	108.04
34	v	201	HEM	CMB-C2B-C3B	4.92	128.82	116.53
30	A	414	SQD	O9-S-C6	4.93	111.10	106.94
30	F	103	SQD	O9-S-C6	5.03	111.18	106.94
34	f	101	HEM	CAD-C3D-C2D	5.09	127.86	113.22
30	A	413	SQD	O7-S-C6	5.11	111.25	106.94
30	d	403	SQD	O9-S-C6	5.11	111.25	106.94
30	a	412	SQD	O7-S-C6	5.24	111.36	106.94
30	B	622	SQD	O6-C1-C2	5.25	114.67	108.04
34	v	201	HEM	CAD-C3D-C2D	5.29	128.42	113.22
34	F	101	HEM	CAD-C3D-C2D	5.30	128.44	113.22
30	B	627	SQD	O7-S-C6	5.36	111.46	106.94
34	V	201	HEM	CAD-C3D-C2D	5.55	129.19	113.22
30	b	602	SQD	O9-S-C6	5.68	111.73	106.94
30	d	403	SQD	O7-S-C6	5.69	111.74	106.94
30	b	602	SQD	O7-S-C6	5.74	111.78	106.94
30	B	627	SQD	O9-S-C6	5.85	111.87	106.94
30	A	414	SQD	O7-S-C6	5.89	111.91	106.94
30	F	103	SQD	O7-S-C6	6.00	112.00	106.94
30	a	401	SQD	O7-S-C6	6.19	112.16	106.94
30	f	103	SQD	O7-S-C6	6.44	112.37	106.94
30	B	622	SQD	O7-S-C6	6.67	112.56	106.94
30	a	412	SQD	O9-S-C6	6.73	112.61	106.94
30	a	412	SQD	O6-C1-C2	6.98	116.86	108.04
30	A	413	SQD	O6-C1-C2	6.99	116.86	108.04
30	A	413	SQD	O9-S-C6	7.36	113.14	106.94
30	B	627	SQD	O6-C1-C2	7.45	117.45	108.04
30	b	602	SQD	O6-C1-C2	7.78	117.87	108.04

All (208) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
22	C	501	CLA	NC
22	C	501	CLA	ND
22	C	501	CLA	NA
22	c	502	CLA	NC
22	c	502	CLA	ND
22	c	502	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	C	519	CLA	NC
22	C	519	CLA	ND
22	C	519	CLA	NA
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	A	403	CLA	NC
22	A	403	CLA	ND
22	A	403	CLA	NA
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	511	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	ND
22	b	609	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	ND
22	b	612	CLA	NA
22	a	406	CLA	NC
22	a	406	CLA	ND
22	a	406	CLA	NA
22	c	510	CLA	NC
22	c	510	CLA	ND
22	c	510	CLA	NA
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
22	B	613	CLA	NC
22	B	613	CLA	ND
22	B	613	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA
22	C	504	CLA	NC
22	C	504	CLA	ND
22	C	504	CLA	NA
22	c	506	CLA	NC
22	c	506	CLA	ND
22	c	506	CLA	NA
22	c	504	CLA	NC
22	c	504	CLA	ND
22	c	504	CLA	NA
22	c	508	CLA	NC
22	c	508	CLA	ND
22	c	508	CLA	NA
22	c	512	CLA	NC
22	c	512	CLA	ND
22	c	512	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	c	503	CLA	NC
22	c	503	CLA	ND
22	c	503	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	b	613	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	ND
22	B	606	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	A	404	CLA	NC
22	A	404	CLA	ND
22	A	404	CLA	NA
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	B	601	CLA	NC
22	B	601	CLA	ND
22	B	601	CLA	NA
22	c	511	CLA	NC
22	c	511	CLA	ND
22	c	511	CLA	NA
22	b	610	CLA	NC
22	b	610	CLA	ND
22	b	610	CLA	NA
22	a	404	CLA	NC
22	a	404	CLA	ND
22	a	404	CLA	NA
22	D	404	CLA	NC
22	D	404	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	ND
22	b	617	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	d	406	CLA	NC
22	d	406	CLA	NA
22	A	402	CLA	NC
22	A	402	CLA	ND
22	A	402	CLA	NA
22	a	403	CLA	NC
22	a	403	CLA	ND
22	a	403	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
22	C	512	CLA	NA
22	c	507	CLA	NC
22	c	507	CLA	ND
22	c	507	CLA	NA
22	b	620	CLA	NC
22	b	620	CLA	ND
22	b	620	CLA	NA
22	A	406	CLA	NC
22	A	406	CLA	ND
22	A	406	CLA	NA
22	b	618	CLA	NC
22	b	618	CLA	ND
22	b	618	CLA	NA
22	d	405	CLA	NC
22	d	405	CLA	ND
22	d	405	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	ND
22	C	510	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	ND
22	C	505	CLA	NA
22	B	609	CLA	NC
22	B	609	CLA	ND
22	B	609	CLA	NA
22	b	619	CLA	NC
22	b	619	CLA	ND
22	b	619	CLA	NA
22	c	505	CLA	NC
22	c	505	CLA	ND
22	c	505	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	B	607	CLA	NC
22	B	607	CLA	ND
22	B	607	CLA	NA
22	C	503	CLA	NC
22	C	503	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
22	C	503	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	c	501	CLA	NC
22	c	501	CLA	ND
22	c	501	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	H	101	CLA	NC
22	H	101	CLA	ND
22	H	101	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA
22	c	520	CLA	NC
22	c	520	CLA	ND
22	c	520	CLA	NA
22	D	403	CLA	NC
22	D	403	CLA	ND
22	D	403	CLA	NA
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	a	405	CLA	NC
22	a	405	CLA	ND
22	a	405	CLA	NA
22	c	509	CLA	NC
22	c	509	CLA	ND
22	c	509	CLA	NA
22	C	506	CLA	NC
22	C	506	CLA	ND
22	C	506	CLA	NA

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	c	516	DGD	C2G-O2G-C1B-C2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	515	DGD	C2G-O2G-C1B-C2B
30	B	622	SQD	C45-O47-C7-C8
30	d	403	SQD	C45-O47-C7-C8

There are no ring outliers.

81 monomers are involved in 329 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	402	CLA	10	0
22	A	403	CLA	19	0
22	A	404	CLA	12	0
23	A	405	PHO	6	0
22	A	406	CLA	3	0
24	A	407	PL9	6	0
25	A	408	BCR	3	0
26	A	409	DGD	1	0
27	A	410	LHG	2	0
30	A	413	SQD	3	0
30	A	414	SQD	3	0
22	B	601	CLA	1	0
22	B	602	CLA	11	0
22	B	603	CLA	6	0
22	B	604	CLA	10	0
22	B	605	CLA	7	0
22	B	606	CLA	12	0
22	B	607	CLA	18	0
22	B	608	CLA	9	0
22	B	609	CLA	9	0
22	B	610	CLA	6	0
22	B	611	CLA	6	0
22	B	612	CLA	10	0
22	B	613	CLA	10	0
22	B	614	CLA	4	0
22	B	615	CLA	5	0
25	B	616	BCR	6	0
25	B	617	BCR	2	0
25	B	618	BCR	4	0
25	B	619	BCR	2	0
26	B	620	DGD	3	0
31	B	621	LMG	3	0
30	B	622	SQD	2	0
32	B	623	LMT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	B	624	LMT	1	0
31	B	625	LMG	3	0
26	B	626	DGD	1	0
30	B	627	SQD	1	0
32	B	628	LMT	2	0
32	B	629	LMT	1	0
22	C	501	CLA	6	0
22	C	502	CLA	1	0
22	C	503	CLA	2	0
22	C	504	CLA	2	0
22	C	505	CLA	3	0
22	C	506	CLA	6	0
22	C	507	CLA	5	0
22	C	508	CLA	3	0
22	C	509	CLA	7	0
22	C	510	CLA	9	0
22	C	511	CLA	1	0
22	C	512	CLA	3	0
25	C	513	BCR	10	0
26	C	514	DGD	3	0
26	C	515	DGD	6	0
26	C	516	DGD	9	0
31	C	517	LMG	2	0
27	C	518	LHG	3	0
22	C	519	CLA	3	0
25	C	520	BCR	5	0
31	C	521	LMG	1	0
23	D	401	PHO	12	0
22	D	403	CLA	11	0
22	D	404	CLA	2	0
24	D	405	PL9	10	0
31	D	406	LMG	7	0
26	D	407	DGD	2	0
31	D	409	LMG	8	0
31	E	101	LMG	2	0
34	F	101	HEM	5	0
25	F	102	BCR	3	0
30	F	103	SQD	3	0
22	H	101	CLA	11	0
25	H	102	BCR	2	0
31	I	101	LMG	1	0
32	I	102	LMT	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	J	102	BCR	3	0
25	K	101	BCR	3	0
31	L	101	LMG	2	0
31	M	101	LMG	3	0
34	V	201	HEM	3	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	335/344 (97%)	0.76	46 (13%) 4 6	206, 208, 208, 209	0
1	a	335/344 (97%)	0.93	69 (20%) 1 3	206, 208, 209, 209	0
2	B	490/510 (96%)	0.50	50 (10%) 9 10	206, 207, 209, 210	0
2	b	490/510 (96%)	0.75	89 (18%) 2 4	206, 208, 209, 210	0
3	C	447/461 (96%)	0.62	57 (12%) 5 7	206, 208, 209, 209	0
3	c	447/461 (96%)	0.47	41 (9%) 11 11	205, 208, 209, 210	0
4	D	340/352 (96%)	0.40	26 (7%) 17 15	205, 207, 208, 210	0
4	d	340/352 (96%)	0.63	40 (11%) 6 8	206, 208, 209, 209	0
5	E	82/84 (97%)	0.72	9 (10%) 7 8	206, 208, 209, 209	0
5	e	82/84 (97%)	0.44	5 (6%) 25 20	207, 208, 209, 209	0
6	F	35/45 (77%)	0.12	2 (5%) 27 23	207, 207, 208, 209	0
6	f	35/45 (77%)	0.17	5 (14%) 4 6	207, 208, 209, 209	0
7	H	65/66 (98%)	0.83	15 (23%) 1 3	206, 208, 209, 209	0
7	h	65/66 (98%)	1.28	24 (36%) 0 2	207, 208, 209, 209	0
8	I	35/38 (92%)	1.16	10 (28%) 1 3	207, 208, 209, 209	0
8	i	35/38 (92%)	0.39	2 (5%) 27 23	206, 207, 209, 210	0
9	J	34/40 (85%)	0.54	4 (11%) 6 8	207, 208, 208, 209	0
9	j	34/40 (85%)	-0.32	0 100 100	206, 208, 209, 209	0
10	K	37/46 (80%)	0.18	2 (5%) 29 25	207, 208, 209, 209	0
10	k	37/46 (80%)	0.24	4 (10%) 8 9	207, 208, 209, 209	0
11	L	37/37 (100%)	0.76	5 (13%) 4 6	207, 208, 209, 209	0
11	l	37/37 (100%)	0.60	5 (13%) 4 6	206, 208, 209, 210	0
12	M	34/36 (94%)	0.63	4 (11%) 6 8	206, 207, 208, 209	0
12	m	34/36 (94%)	0.36	2 (5%) 26 21	207, 207, 208, 209	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/272 (89%)	1.05	48 (19%) 1 4	205, 208, 209, 210	0
13	o	243/272 (89%)	1.00	39 (16%) 3 5	206, 208, 209, 210	0
14	T	32/32 (100%)	0.47	2 (6%) 23 19	206, 208, 208, 209	0
14	t	32/32 (100%)	0.74	3 (9%) 11 11	206, 207, 209, 209	0
15	U	97/134 (72%)	1.06	12 (12%) 5 7	206, 207, 208, 209	0
15	u	97/134 (72%)	1.25	22 (22%) 1 3	206, 207, 208, 209	0
16	V	137/163 (84%)	0.46	11 (8%) 15 14	206, 207, 208, 209	0
16	v	137/163 (84%)	0.85	20 (14%) 3 5	206, 208, 209, 209	0
17	g	28/46 (60%)	0.24	2 (7%) 19 16	207, 208, 209, 209	0
17	y	28/46 (60%)	0.47	2 (7%) 19 16	206, 208, 209, 209	0
18	X	37/41 (90%)	0.75	7 (18%) 2 4	206, 208, 209, 210	0
18	x	37/41 (90%)	0.96	7 (18%) 2 4	207, 208, 208, 209	0
19	G	0/28	-	-	-	-
19	Y	0/28	-	-	-	-
20	Z	62/62 (100%)	0.30	1 (1%) 74 67	206, 207, 208, 209	0
20	z	62/62 (100%)	0.65	4 (6%) 22 18	207, 208, 209, 210	0
All	All	5214/5674 (91%)	0.67	696 (13%) 4 6	205, 208, 209, 210	0

All (696) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	84	LYS	9.4
1	A	190	HIS	7.2
2	B	84	THR	7.0
3	c	202	PRO	6.9
1	a	299	GLY	6.8
1	A	299	GLY	6.6
7	H	4	ARG	6.0
1	A	11	ALA	6.0
1	a	190	HIS	5.9
4	d	295	SER	5.9
14	t	31	LYS	5.9
13	O	90	GLU	5.9
13	o	55	ALA	5.8
2	b	431	GLU	5.8
13	o	54	GLY	5.8
1	A	10	SER	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	o	51	THR	5.5
1	A	175	GLY	5.3
3	c	201	ASN	5.3
16	v	111	GLU	5.3
3	C	212	TYR	5.3
3	C	147	PHE	5.3
3	C	149	TYR	5.3
2	B	85	GLY	5.1
1	A	298	ASN	5.1
7	h	56	ASP	5.0
2	b	133	LEU	5.0
7	h	66	GLY	4.9
13	O	220	LYS	4.8
1	a	236	GLY	4.8
14	t	32	LYS	4.8
1	A	179	THR	4.7
13	O	91	PHE	4.7
1	a	179	THR	4.7
2	b	490	GLN	4.7
3	C	148	GLY	4.6
3	c	203	THR	4.6
7	h	3	ARG	4.6
18	X	47	GLN	4.6
3	C	266	TRP	4.6
6	f	13	TYR	4.6
13	O	175	PRO	4.6
2	B	83	GLU	4.5
6	f	11	VAL	4.5
4	d	197	HIS	4.5
2	B	378	LYS	4.5
16	v	35	THR	4.5
3	c	372	PRO	4.4
3	C	209	ILE	4.4
7	h	26	GLY	4.4
13	o	84	ASN	4.4
4	D	192	THR	4.4
1	A	195	HIS	4.4
2	b	482	ILE	4.4
1	A	165	GLN	4.3
5	e	82	GLN	4.3
3	c	199	ILE	4.3
3	c	200	THR	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	c	209	ILE	4.3
1	a	175	GLY	4.3
18	X	46	VAL	4.2
13	o	53	ARG	4.2
14	t	30	THR	4.2
1	a	198	HIS	4.2
3	c	260	ALA	4.2
2	b	127	ARG	4.2
16	v	34	LEU	4.2
2	b	126	PRO	4.1
3	c	178	LYS	4.1
4	d	241	GLU	4.1
15	u	107	GLU	4.1
1	A	177	SER	4.1
2	B	411	PHE	4.1
3	c	373	ASN	4.1
2	b	120	LEU	4.1
13	O	170	GLY	4.1
18	x	13	THR	4.1
3	c	184	GLY	4.0
3	C	325	GLY	4.0
13	O	89	ALA	4.0
13	O	244	GLU	4.0
2	B	164	PRO	4.0
1	a	298	ASN	4.0
2	b	402	TYR	4.0
3	C	210	PHE	4.0
4	D	295	SER	4.0
4	d	294	ARG	4.0
1	a	171	GLY	4.0
2	b	70	GLY	4.0
2	b	483	ASP	4.0
7	h	2	ALA	4.0
2	b	302	TRP	3.9
3	C	402	GLY	3.9
4	d	206	GLY	3.9
7	h	4	ARG	3.9
13	O	46	PRO	3.9
13	o	215	ARG	3.9
5	e	84	LYS	3.9
2	b	491	VAL	3.9
2	b	296	ALA	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	d	139	ARG	3.9
1	A	294	ALA	3.9
13	o	52	ALA	3.9
2	B	69	LEU	3.8
15	U	39	LEU	3.8
8	I	1	MET	3.8
13	O	50	ASP	3.8
9	J	7	ARG	3.8
15	u	74	THR	3.8
4	d	194	ASN	3.8
16	v	36	VAL	3.8
4	d	191	TRP	3.8
9	J	8	ILE	3.8
5	e	3	GLY	3.8
13	O	224	SER	3.8
2	b	304	ALA	3.8
13	o	213	VAL	3.8
11	L	33	SER	3.7
15	u	65	PHE	3.7
2	B	306	PRO	3.7
7	h	27	THR	3.7
6	f	12	SER	3.7
20	z	1	MET	3.7
3	c	204	LEU	3.7
13	o	220	LYS	3.7
4	D	197	HIS	3.7
4	d	201	VAL	3.7
3	C	155	ASN	3.7
13	O	79	LYS	3.7
18	X	45	LYS	3.7
3	c	256	PRO	3.7
4	D	198	MET	3.7
2	b	305	ILE	3.6
7	H	64	ALA	3.7
2	b	485	GLU	3.6
3	C	150	ASP	3.6
3	c	180	MET	3.6
3	c	264	PHE	3.6
2	b	119	ASP	3.6
2	b	298	LEU	3.6
13	O	258	GLU	3.6
18	x	42	GLN	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	265	ILE	3.6
16	v	47	LEU	3.6
1	a	199	GLN	3.5
13	O	242	GLU	3.5
1	A	178	GLY	3.5
18	X	12	ILE	3.5
1	A	80	GLY	3.5
15	U	38	GLU	3.5
15	U	40	VAL	3.5
1	a	178	GLY	3.5
4	d	239	GLN	3.5
13	O	76	PHE	3.5
16	v	46	THR	3.5
1	A	266	ASN	3.5
1	a	293	MET	3.5
3	C	201	ASN	3.5
3	c	179	ALA	3.5
15	u	70	GLY	3.5
7	H	6	TRP	3.5
2	b	397	VAL	3.5
5	E	17	VAL	3.5
16	v	44	THR	3.5
18	x	11	THR	3.5
2	b	178	VAL	3.5
13	o	190	LEU	3.5
7	H	63	LYS	3.5
1	a	246	TYR	3.4
3	c	259	TRP	3.4
4	d	199	MET	3.4
2	b	122	LEU	3.4
7	h	14	LEU	3.4
13	o	171	GLU	3.4
1	a	80	GLY	3.4
18	X	13	THR	3.4
4	d	177	ALA	3.4
5	E	56	TYR	3.4
7	h	23	PRO	3.4
1	A	137	LEU	3.4
5	E	60	GLN	3.4
20	Z	1	MET	3.4
10	K	42	ALA	3.4
1	A	198	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	293	MET	3.4
4	d	172	SER	3.4
16	V	28	GLU	3.4
3	C	154	LYS	3.4
13	O	219	THR	3.4
1	A	192	ILE	3.3
7	H	3	ARG	3.3
13	o	238	ALA	3.3
1	A	191	ASN	3.3
2	b	303	SER	3.3
3	C	203	THR	3.3
3	c	261	ARG	3.3
8	I	32	PRO	3.3
4	d	240	ALA	3.3
13	O	49	ASP	3.3
2	b	411	PHE	3.3
3	c	149	TYR	3.3
13	O	222	GLN	3.3
1	a	245	THR	3.3
13	O	54	GLY	3.3
13	o	189	GLY	3.3
1	a	165	GLN	3.3
13	O	171	GLU	3.3
3	c	210	PHE	3.3
2	b	166	MET	3.3
16	V	30	THR	3.3
1	a	286	THR	3.3
7	H	62	TRP	3.3
4	D	174	GLY	3.3
13	O	223	ILE	3.3
7	h	5	THR	3.3
3	C	204	LEU	3.2
1	A	181	ASN	3.2
13	O	84	ASN	3.2
1	a	244	GLU	3.2
3	c	365	TRP	3.2
1	A	138	GLY	3.2
3	C	142	GLU	3.2
3	C	263	ALA	3.2
13	O	53	ARG	3.2
15	u	50	ALA	3.2
2	b	398	THR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	173	ASN	3.2
7	H	5	THR	3.2
1	a	282	GLY	3.2
3	C	143	TYR	3.2
15	u	39	LEU	3.2
1	a	220	THR	3.2
10	k	11	LEU	3.2
13	o	173	ASN	3.2
7	H	55	LEU	3.2
1	A	15	GLU	3.2
1	a	303	ASN	3.2
4	D	199	MET	3.2
1	A	286	THR	3.2
2	b	395	GLN	3.2
16	v	146	LEU	3.2
7	h	6	TRP	3.2
15	u	69	ARG	3.2
2	B	78	TRP	3.2
13	O	169	LYS	3.2
17	y	42	ARG	3.1
15	u	57	LEU	3.1
2	b	299	GLU	3.1
1	a	176	ILE	3.1
2	B	179	GLN	3.1
2	b	167	TRP	3.1
12	M	1	MET	3.1
4	d	176	ALA	3.1
1	a	170	ASP	3.1
17	y	46	LEU	3.1
3	C	403	SER	3.1
13	o	214	LYS	3.1
16	V	39	ASN	3.1
3	C	264	PHE	3.1
7	h	11	LEU	3.1
2	b	378	LYS	3.1
7	h	15	ASN	3.1
4	d	174	GLY	3.1
16	V	47	LEU	3.1
2	B	165	GLY	3.1
18	X	11	THR	3.1
1	A	301	ASN	3.1
16	V	43	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	U	53	GLU	3.1
5	e	4	THR	3.1
4	d	202	ALA	3.0
4	d	265	ARG	3.0
7	h	25	TRP	3.0
13	o	88	GLU	3.0
16	V	44	THR	3.0
3	c	257	PHE	3.0
1	a	319	ASP	3.0
1	a	16	ARG	3.0
13	O	48	LEU	3.0
4	D	25	ASP	3.0
2	b	339	ALA	3.0
3	C	144	SER	3.0
3	C	256	PRO	3.0
4	d	195	PRO	3.0
2	B	70	GLY	3.0
4	d	192	THR	3.0
7	h	16	SER	3.0
13	o	240	THR	3.0
1	a	186	PHE	3.0
2	b	289	GLN	3.0
2	b	219	VAL	3.0
2	b	179	GLN	3.0
2	B	180	PRO	3.0
3	c	258	GLY	3.0
2	b	338	GLN	3.0
4	d	227	GLU	3.0
2	b	117	TYR	3.0
2	b	69	LEU	3.0
3	C	409	GLY	3.0
1	a	240	GLY	2.9
2	B	86	ILE	2.9
2	b	288	VAL	2.9
4	D	190	ASN	2.9
7	h	9	ASP	2.9
3	C	411	ALA	2.9
3	c	197	ARG	2.9
16	V	29	LEU	2.9
1	a	224	ILE	2.9
4	d	203	GLY	2.9
13	O	174	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	18	ARG	2.9
2	B	121	GLU	2.9
2	b	347	ARG	2.9
1	a	301	ASN	2.9
15	U	70	GLY	2.9
3	C	453	ALA	2.9
1	a	247	ASN	2.9
15	u	45	GLU	2.9
2	b	350	GLU	2.9
3	c	147	PHE	2.9
14	T	27	PRO	2.9
3	C	255	THR	2.8
1	a	287	ALA	2.8
2	B	347	ARG	2.8
1	a	139	MET	2.8
7	H	54	ILE	2.8
16	v	45	ILE	2.8
8	I	25	SER	2.8
2	b	349	LYS	2.8
1	A	199	GLN	2.8
13	O	225	LEU	2.8
1	A	12	ASN	2.8
2	B	127	ARG	2.8
13	O	261	ILE	2.8
2	b	132	ALA	2.8
13	O	168	PHE	2.8
4	D	26	ARG	2.8
4	D	227	GLU	2.8
8	i	25	SER	2.8
6	f	15	ILE	2.8
4	D	77	ALA	2.8
1	a	195	HIS	2.8
2	B	490	GLN	2.8
1	a	328	MET	2.8
2	B	166	MET	2.8
6	f	14	PRO	2.8
1	a	325	ASN	2.8
12	M	4	ASN	2.8
3	C	200	THR	2.8
8	I	35	LYS	2.8
13	o	239	GLY	2.8
16	v	29	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	50	PRO	2.8
8	I	3	THR	2.8
3	C	152	LYS	2.8
15	u	71	LEU	2.8
1	A	14	TRP	2.8
1	A	78	ILE	2.8
2	b	125	ASP	2.8
2	b	121	GLU	2.7
4	D	296	TYR	2.7
5	E	57	ALA	2.7
8	I	34	ARG	2.7
18	x	12	ILE	2.7
7	h	55	LEU	2.7
2	B	379	ALA	2.7
15	u	40	VAL	2.7
17	g	27	MET	2.7
2	b	123	PHE	2.7
2	b	297	THR	2.7
3	C	326	ALA	2.7
2	B	185	TRP	2.7
3	C	191	PRO	2.7
1	A	289	GLY	2.7
3	C	141	GLU	2.7
11	l	33	SER	2.7
13	O	243	SER	2.7
3	C	202	PRO	2.7
2	B	356	VAL	2.7
4	d	200	GLY	2.7
1	a	225	ARG	2.7
2	b	341	LYS	2.7
4	d	190	ASN	2.7
1	a	172	MET	2.7
2	B	305	ILE	2.7
4	D	194	ASN	2.7
15	u	44	ASP	2.7
2	b	368	VAL	2.7
3	C	261	ARG	2.7
6	F	15	ILE	2.7
3	c	263	ALA	2.7
7	h	7	LEU	2.7
13	o	124	GLU	2.7
3	c	198	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	388	SER	2.7
15	U	69	ARG	2.7
2	b	185	TRP	2.7
4	d	155	SER	2.7
11	l	8	GLN	2.7
3	C	332	GLN	2.6
4	d	198	MET	2.6
13	o	221	GLY	2.6
2	b	194	ASN	2.6
16	V	38	LEU	2.6
16	v	31	PRO	2.6
3	C	213	LEU	2.6
18	x	16	LEU	2.6
2	B	73	GLY	2.6
16	v	142	ALA	2.6
2	b	295	GLY	2.6
3	C	140	LEU	2.6
1	a	166	GLY	2.6
2	B	370	LEU	2.6
3	c	405	ASN	2.6
15	u	75	LEU	2.6
9	J	11	TRP	2.6
13	o	258	GLU	2.6
3	c	191	PRO	2.6
2	b	177	SER	2.6
1	A	201	GLY	2.6
3	C	151	TRP	2.6
1	A	81	ALA	2.6
3	c	146	PHE	2.6
1	a	153	SER	2.6
13	O	47	THR	2.6
2	B	219	VAL	2.6
13	O	260	LYS	2.6
7	h	18	TYR	2.6
16	v	49	GLU	2.6
15	u	58	ASN	2.6
16	v	132	ASN	2.6
13	o	228	ALA	2.5
7	H	53	LEU	2.5
3	C	157	MET	2.5
2	b	301	ALA	2.5
17	g	23	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	379	ALA	2.5
15	u	42	VAL	2.5
3	C	46	SER	2.5
3	C	181	PHE	2.5
13	O	234	THR	2.5
1	a	192	ILE	2.5
2	b	373	LYS	2.5
1	a	201	GLY	2.5
2	b	403	GLY	2.5
3	c	403	SER	2.5
1	a	223	LEU	2.5
11	l	1	MET	2.5
13	o	89	ALA	2.5
15	U	75	LEU	2.5
2	B	420	TYR	2.5
4	d	95	PRO	2.5
20	z	4	LEU	2.5
1	A	196	PRO	2.5
1	A	161	TYR	2.5
4	d	278	GLY	2.5
13	o	237	ILE	2.5
13	o	210	ARG	2.5
2	b	396	GLY	2.5
13	o	168	PHE	2.5
1	a	221	SER	2.5
13	O	259	VAL	2.5
3	C	340	TYR	2.4
2	b	300	GLU	2.4
4	D	177	ALA	2.4
13	O	218	LEU	2.4
16	v	78	LEU	2.4
2	b	137	LYS	2.4
1	A	16	ARG	2.4
3	c	183	GLY	2.4
2	b	195	PRO	2.4
4	d	138	VAL	2.4
12	M	2	GLU	2.4
15	u	115	THR	2.4
13	o	169	LYS	2.4
2	B	120	LEU	2.4
1	a	169	SER	2.4
16	V	130	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	137	LEU	2.4
2	b	72	THR	2.4
16	v	48	THR	2.4
5	e	60	GLN	2.4
4	D	282	SER	2.4
4	d	187	GLY	2.4
7	h	13	PRO	2.4
13	O	202	GLN	2.4
1	a	289	GLY	2.4
2	b	489	GLU	2.4
2	B	309	LEU	2.4
2	B	181	VAL	2.4
4	D	195	PRO	2.4
13	O	262	GLN	2.4
13	o	230	VAL	2.4
1	a	191	ASN	2.4
2	b	340	TRP	2.4
2	b	408	GLY	2.4
13	O	206	GLU	2.4
13	O	94	THR	2.4
1	a	239	PHE	2.4
6	F	11	VAL	2.4
1	a	149	ALA	2.4
1	a	167	SER	2.4
1	a	181	ASN	2.4
13	o	50	ASP	2.4
2	B	131	PRO	2.3
2	B	293	ALA	2.3
7	h	22	ALA	2.3
13	O	55	ALA	2.3
2	b	364	GLU	2.3
2	b	405	GLU	2.3
11	L	30	LEU	2.3
1	A	290	ILE	2.3
2	b	218	LEU	2.3
2	b	220	ARG	2.3
2	b	385	ARG	2.3
7	h	8	GLY	2.3
2	b	484	PRO	2.3
1	a	19	ASN	2.3
3	C	145	SER	2.3
3	C	199	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	171	PRO	2.3
4	d	179	PHE	2.3
16	V	37	PRO	2.3
1	a	226	GLU	2.3
2	b	322	GLY	2.3
11	l	34	TYR	2.3
3	c	364	PRO	2.3
2	b	351	GLY	2.3
13	o	229	LYS	2.3
3	c	196	VAL	2.3
1	A	180	PHE	2.3
2	B	124	ARG	2.3
13	O	44	LYS	2.3
7	H	27	THR	2.3
7	h	12	ARG	2.3
1	a	187	GLN	2.3
12	m	4	ASN	2.3
2	B	218	LEU	2.3
15	U	65	PHE	2.3
2	B	81	THR	2.3
1	a	327	GLY	2.3
2	b	352	GLU	2.3
4	D	200	GLY	2.3
2	b	134	ASP	2.3
10	k	15	TYR	2.3
13	O	88	GLU	2.3
1	A	76	ASN	2.3
3	C	182	PHE	2.3
1	a	310	LYS	2.3
1	A	291	SER	2.2
3	C	146	PHE	2.2
4	d	242	GLU	2.2
10	K	46	ARG	2.2
13	O	215	ARG	2.2
1	A	268	SER	2.2
13	O	58	ILE	2.2
3	C	211	GLY	2.2
13	o	91	PHE	2.2
13	O	245	GLN	2.2
1	a	202	VAL	2.2
15	u	106	ARG	2.2
16	v	133	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	v	130	MET	2.2
8	I	2	GLU	2.2
2	b	346	PHE	2.2
18	x	15	SER	2.2
3	c	192	GLY	2.2
2	b	430	PHE	2.2
16	v	113	GLU	2.2
8	I	26	GLY	2.2
11	l	2	GLU	2.2
2	b	234	ILE	2.2
4	d	288	GLY	2.2
13	O	51	THR	2.2
20	z	2	THR	2.2
1	A	170	ASP	2.2
1	a	76	ASN	2.2
1	a	81	ALA	2.2
4	D	297	ASP	2.2
2	B	259	GLY	2.2
4	D	278	GLY	2.2
18	x	40	ILE	2.2
3	c	262	ARG	2.2
2	b	78	TRP	2.2
3	C	137	PRO	2.2
3	C	184	GLY	2.2
13	o	151	LEU	2.2
1	a	296	ASN	2.2
4	d	83	ASN	2.2
13	o	269	ILE	2.2
4	d	136	VAL	2.2
8	I	30	ARG	2.2
13	o	172	PHE	2.2
11	L	28	ALA	2.2
1	a	18	CYS	2.2
1	a	285	PHE	2.2
7	H	7	LEU	2.2
1	a	11	ALA	2.1
2	B	171	PRO	2.1
2	B	410	THR	2.1
10	k	12	PRO	2.1
3	c	329	GLY	2.1
15	u	110	GLU	2.1
1	a	10	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	71	VAL	2.1
5	E	21	VAL	2.1
12	m	33	GLN	2.1
4	d	137	GLY	2.1
2	B	72	THR	2.1
4	D	155	SER	2.1
13	o	164	THR	2.1
1	a	162	PRO	2.1
2	B	80	ILE	2.1
13	o	170	GLY	2.1
3	C	465	PRO	2.1
2	b	370	LEU	2.1
1	A	296	ASN	2.1
2	B	183	PRO	2.1
4	D	202	ALA	2.1
3	C	260	ALA	2.1
3	c	266	TRP	2.1
2	b	345	VAL	2.1
15	u	41	ASN	2.1
18	X	42	GLN	2.1
15	u	38	GLU	2.1
2	b	67	ALA	2.1
16	v	51	GLN	2.1
4	d	165	SER	2.1
11	L	37	ASN	2.1
13	o	158	ASN	2.1
13	O	93	PRO	2.1
15	U	55	ILE	2.1
4	d	182	LEU	2.1
10	k	13	GLU	2.1
1	a	322	ASN	2.1
1	A	203	ALA	2.1
2	B	122	LEU	2.1
4	D	176	ALA	2.1
2	B	294	SER	2.1
16	V	36	VAL	2.1
12	M	5	GLN	2.1
2	b	124	ARG	2.1
2	b	481	GLY	2.1
3	C	183	GLY	2.1
5	E	82	GLN	2.1
9	J	9	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	i	24	LEU	2.1
15	U	128	TYR	2.1
7	H	9	ASP	2.1
7	H	56	ASP	2.1
2	B	82	GLY	2.1
13	O	152	VAL	2.1
4	D	24	ARG	2.1
1	a	138	GLY	2.1
1	a	15	GLU	2.1
13	o	152	VAL	2.1
1	a	156	ALA	2.1
2	b	294	SER	2.1
8	I	6	ILE	2.1
2	b	285	ASN	2.1
3	c	430	HIS	2.1
1	A	186	PHE	2.1
13	o	62	GLN	2.1
15	u	55	ILE	2.1
14	T	26	PRO	2.0
7	H	10	ILE	2.0
2	B	128	THR	2.0
5	E	5	THR	2.0
3	C	405	ASN	2.0
4	D	239	GLN	2.0
7	h	10	ILE	2.0
20	z	3	ILE	2.0
2	b	135	LEU	2.0
2	b	421	ALA	2.0
3	c	411	ALA	2.0
4	D	283	ALA	2.0
4	d	148	ALA	2.0
3	C	134	ILE	2.0
15	u	43	VAL	2.0
2	B	172	TYR	2.0
2	b	229	LEU	2.0
1	a	344	ALA	2.0
2	b	348	ASN	2.0
1	A	282	GLY	2.0
3	C	254	THR	2.0
3	C	324	LEU	2.0
15	U	54	LYS	2.0
15	U	106	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	402	TYR	2.0
1	A	169	SER	2.0
1	A	176	ILE	2.0
3	C	257	PHE	2.0
2	B	68	ARG	2.0
3	c	427	ALA	2.0
4	d	283	ALA	2.0
11	L	32	SER	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
32	LMT	i	103	35/35	0.29	1.35	9.05	206,209,210,210	0
25	BCR	B	619	40/40	0.73	1.17	6.96	205,207,208,208	0
22	CLA	a	406	65/65	0.72	0.81	6.22	206,208,208,209	0
25	BCR	c	521	40/40	0.80	1.52	5.98	206,208,209,209	0
25	BCR	K	101	40/40	0.90	0.83	5.14	206,207,208,209	0
31	LMG	C	517	45/55	0.50	1.11	5.09	206,207,209,210	0
24	PL9	j	101	35/55	0.31	0.49	5.03	205,208,209,210	0
24	PL9	J	101	35/55	0.19	0.59	4.71	206,207,210,210	0
22	CLA	b	605	65/65	0.56	1.38	4.63	206,208,210,210	0
26	DGD	D	407	63/66	0.70	0.72	4.29	206,208,209,210	0
25	BCR	g	101	40/40	0.73	0.82	3.56	205,207,208,209	0
32	LMT	I	102	35/35	0.26	1.23	3.51	206,208,210,210	0
25	BCR	c	513	40/40	0.72	0.92	3.43	206,207,208,209	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	D	404	65/65	0.86	0.71	3.40	205,207,208,208	0
25	BCR	b	624	40/40	0.57	1.01	3.25	205,206,207,208	0
32	LMT	D	408	31/35	0.65	0.74	3.21	207,208,210,210	0
25	BCR	i	101	40/40	0.77	0.70	3.13	206,207,208,208	0
25	BCR	y	101	40/40	0.82	0.80	3.12	206,207,208,208	0
31	LMG	c	518	45/55	0.73	0.88	3.10	206,208,209,210	0
26	DGD	d	410	63/66	0.63	0.79	3.08	206,208,210,211	0
32	LMT	d	411	31/35	0.57	0.80	2.99	206,209,210,211	0
25	BCR	F	102	40/40	0.54	0.56	2.87	205,207,208,208	0
30	SQD	a	401	54/54	0.80	0.60	2.82	205,208,210,213	0
22	CLA	A	406	65/65	0.78	0.78	2.81	206,208,209,209	0
22	CLA	B	608	65/65	0.86	0.85	2.77	205,207,209,210	0
22	CLA	d	406	65/65	0.83	0.66	2.72	206,207,209,209	0
25	BCR	H	102	40/40	0.61	1.22	2.70	206,207,209,210	0
30	SQD	B	627	47/54	0.67	0.68	2.62	206,208,210,212	0
22	CLA	c	512	65/65	0.71	0.82	2.59	206,207,209,210	0
25	BCR	C	520	40/40	0.76	1.09	2.47	206,207,209,210	0
22	CLA	B	609	65/65	0.87	0.73	2.35	206,207,209,210	0
22	CLA	B	603	65/65	0.80	0.60	2.32	205,207,208,208	0
32	LMT	b	629	35/35	0.64	0.93	2.31	206,208,209,210	0
26	DGD	B	626	52/66	0.75	0.55	2.29	206,208,210,211	0
25	BCR	c	514	40/40	0.65	1.27	2.23	206,208,208,209	0
22	CLA	c	501	65/65	0.84	0.75	2.03	206,207,209,209	0
22	CLA	c	511	65/65	0.83	0.97	2.02	206,208,209,209	0
22	CLA	B	614	65/65	0.83	0.91	2.02	205,207,208,209	0
30	SQD	d	403	43/54	0.71	0.80	1.91	205,208,209,209	0
28	CL	A	411	1/1	0.59	0.81	1.87	204,204,204,204	0
31	LMG	b	627	42/55	0.49	0.56	1.77	204,207,211,211	0
22	CLA	C	511	65/65	0.77	1.22	1.76	206,207,208,209	0
22	CLA	C	501	65/65	0.83	0.59	1.75	206,208,209,209	0
22	CLA	B	604	65/65	0.87	0.72	1.68	206,207,208,209	0
22	CLA	B	611	65/65	0.93	0.46	1.68	205,207,208,208	0
25	BCR	A	408	40/40	0.75	0.55	1.67	206,207,208,208	0
22	CLA	B	615	65/65	0.82	0.99	1.65	206,207,209,209	0
22	CLA	C	508	65/65	0.74	0.87	1.57	205,207,208,209	0
22	CLA	c	506	65/65	0.82	0.92	1.54	206,208,209,209	0
22	CLA	b	620	65/65	0.66	1.17	1.53	206,208,209,210	0
32	LMT	B	624	35/35	0.74	0.53	1.52	206,207,211,212	0
25	BCR	x	101	40/40	0.71	0.92	1.45	206,207,209,209	0
22	CLA	b	609	65/65	0.87	0.60	1.43	206,207,208,209	0
22	CLA	C	506	65/65	0.77	0.94	1.43	206,207,208,209	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	CLA	b	612	65/65	0.80	0.49	1.42	205,207,209,209	0
34	HEM	v	201	43/43	0.83	0.73	1.39	206,207,208,209	0
25	BCR	f	102	40/40	0.67	0.39	1.39	206,207,208,209	0
26	DGD	b	601	52/66	0.80	0.47	1.37	204,208,209,210	0
26	DGD	a	408	56/66	0.56	0.50	1.36	206,208,210,211	0
31	LMG	e	101	44/55	0.56	0.55	1.35	205,208,209,211	0
33	BCT	d	404	4/4	0.82	0.86	1.32	206,207,208,208	0
30	SQD	f	103	45/54	0.81	0.71	1.30	205,208,210,210	0
22	CLA	b	614	65/65	0.84	0.71	1.29	206,207,209,210	0
22	CLA	c	508	65/65	0.81	0.56	1.28	205,208,209,209	0
34	HEM	F	101	43/43	0.89	0.72	1.28	206,207,208,210	0
22	CLA	B	605	65/65	0.85	0.84	1.28	206,207,208,209	0
22	CLA	b	607	65/65	0.85	0.65	1.27	205,207,208,208	0
22	CLA	c	510	65/65	0.76	0.47	1.25	206,208,209,211	0
25	BCR	C	513	40/40	0.61	1.11	1.23	205,207,208,208	0
30	SQD	b	602	47/54	0.73	0.45	1.14	205,208,209,212	0
22	CLA	B	601	65/65	0.62	0.70	1.13	205,208,209,209	0
22	CLA	c	503	65/65	0.87	0.56	1.13	206,207,208,209	0
22	CLA	C	512	65/65	0.69	0.92	1.10	205,207,209,211	0
22	CLA	b	608	65/65	0.81	0.45	1.04	205,207,208,209	0
30	SQD	B	622	43/54	0.74	0.60	1.03	205,208,209,212	0
22	CLA	C	502	65/65	0.64	0.58	1.03	206,207,208,208	0
22	CLA	B	607	65/65	0.86	0.47	1.02	206,207,208,209	0
26	DGD	A	409	56/66	0.56	0.58	0.93	206,208,210,211	0
22	CLA	b	617	65/65	0.93	0.36	0.91	206,207,208,209	0
22	CLA	b	606	65/65	0.81	0.51	0.90	205,207,209,210	0
22	CLA	B	602	65/65	0.92	0.61	0.87	205,207,208,209	0
22	CLA	b	613	65/65	0.81	0.66	0.86	205,207,208,209	0
22	CLA	c	502	65/65	0.50	0.70	0.86	206,207,208,209	0
22	CLA	b	619	65/65	0.75	0.96	0.81	206,208,209,209	0
22	CLA	b	610	65/65	0.86	0.62	0.80	206,207,209,209	0
25	BCR	B	616	40/40	0.70	0.41	0.78	205,207,208,209	0
22	CLA	c	505	65/65	0.79	0.81	0.77	205,207,208,209	0
22	CLA	b	616	65/65	0.79	0.45	0.74	206,207,208,209	0
32	LMT	B	628	35/35	0.73	0.60	0.73	206,208,210,211	0
31	LMG	m	101	42/55	0.68	0.51	0.71	205,207,209,210	0
32	LMT	b	603	35/35	0.71	0.66	0.68	206,208,210,210	0
25	BCR	b	623	40/40	0.76	0.31	0.67	205,206,207,207	0
22	CLA	C	510	65/65	0.88	0.56	0.67	206,207,209,209	0
30	SQD	F	103	45/54	0.81	0.63	0.67	205,208,209,210	0
22	CLA	C	505	65/65	0.71	0.67	0.58	206,207,209,210	0
22	CLA	H	101	65/65	0.90	0.40	0.57	206,207,208,209	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
25	BCR	B	618	40/40	0.85	0.29	0.53	205,206,208,208	0
22	CLA	a	404	65/65	0.78	0.80	0.50	204,207,208,208	0
24	PL9	a	407	45/55	0.65	0.43	0.49	205,207,208,209	0
31	LMG	a	402	42/55	0.68	0.42	0.47	204,207,209,210	0
34	HEM	f	101	43/43	0.92	0.43	0.46	206,207,209,209	0
24	PL9	A	407	45/55	0.62	0.46	0.46	206,207,208,210	0
22	CLA	C	503	65/65	0.86	0.41	0.45	206,207,208,209	0
34	HEM	V	201	43/43	0.90	0.44	0.43	201,207,208,209	0
22	CLA	C	507	65/65	0.82	0.36	0.39	206,207,208,208	0
31	LMG	M	101	42/55	0.81	0.36	0.38	205,208,209,210	0
31	LMG	E	101	44/55	0.71	0.46	0.35	204,208,209,210	0
31	LMG	C	521	48/55	0.69	0.34	0.33	206,207,208,209	0
24	PL9	d	407	55/55	0.48	0.54	0.30	205,207,208,208	0
31	LMG	c	522	48/55	0.75	0.33	0.29	205,207,209,210	0
22	CLA	B	613	65/65	0.75	0.46	0.26	206,207,208,209	0
30	SQD	A	414	54/54	0.81	0.45	0.26	205,207,209,210	0
22	CLA	c	504	65/65	0.84	0.44	0.26	205,207,208,209	0
22	CLA	c	507	65/65	0.90	0.31	0.23	206,207,209,209	0
26	DGD	B	620	58/66	0.83	0.38	0.20	205,207,209,209	0
33	BCT	D	402	4/4	0.92	0.40	0.20	208,208,208,208	0
32	LMT	B	629	35/35	0.72	0.39	0.15	206,208,209,210	0
31	LMG	D	409	46/55	0.82	0.35	0.12	205,207,208,209	0
25	BCR	B	617	40/40	0.74	0.34	0.11	205,207,208,209	0
23	PHO	d	401	64/64	0.62	0.51	0.10	206,207,208,208	0
22	CLA	C	504	65/65	0.82	0.42	0.10	205,207,208,209	0
26	DGD	b	625	58/66	0.77	0.37	0.04	206,207,208,209	0
31	LMG	d	409	48/55	0.80	0.34	0.03	206,207,209,210	0
22	CLA	C	509	65/65	0.83	0.37	0.02	205,207,208,208	0
22	CLA	A	403	65/65	0.89	0.62	-0.04	205,207,208,208	0
24	PL9	D	405	55/55	0.63	0.43	-0.08	205,207,208,208	0
22	CLA	c	509	65/65	0.90	0.31	-0.08	206,207,209,209	0
22	CLA	b	615	65/65	0.86	0.31	-0.10	205,207,208,209	0
25	BCR	J	102	40/40	0.60	0.36	-0.11	205,207,209,209	0
22	CLA	b	618	65/65	0.78	0.38	-0.14	206,207,209,210	0
25	BCR	j	102	40/40	0.73	0.26	-0.19	206,208,209,210	0
23	PHO	D	401	64/64	0.83	0.36	-0.19	205,207,208,209	0
22	CLA	B	610	65/65	0.90	0.32	-0.20	205,207,208,208	0
32	LMT	b	604	35/35	0.70	0.35	-0.23	207,208,210,210	0
22	CLA	A	404	65/65	0.81	0.44	-0.26	204,207,208,209	0
25	BCR	b	621	40/40	0.86	0.28	-0.27	206,207,208,208	0
23	PHO	A	405	64/64	0.80	0.40	-0.29	205,207,208,209	0
22	CLA	c	520	65/65	0.88	0.33	-0.32	206,207,208,209	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	LMG	D	406	48/55	0.85	0.28	-0.33	204,207,208,209	0
31	LMG	l	101	51/55	0.83	0.29	-0.33	206,207,209,209	0
30	SQD	A	413	51/54	0.84	0.26	-0.35	204,207,209,209	0
26	DGD	C	516	66/66	0.64	0.43	-0.35	205,207,208,208	0
25	BCR	b	622	40/40	0.75	0.32	-0.38	205,207,208,208	0
26	DGD	c	515	53/66	0.87	0.34	-0.39	205,207,209,210	0
22	CLA	B	612	65/65	0.92	0.26	-0.42	203,207,208,209	0
31	LMG	d	412	46/55	0.90	0.21	-0.45	205,207,208,209	0
22	CLA	a	403	65/65	0.80	0.58	-0.45	205,207,208,210	0
22	CLA	A	402	65/65	0.89	0.46	-0.45	206,207,208,209	0
29	OEX	a	411	10/10	0.97	0.54	-0.48	200,204,205,206	0
26	DGD	C	514	53/66	0.89	0.30	-0.49	205,206,208,209	0
30	SQD	a	412	51/54	0.89	0.23	-0.50	205,207,208,209	0
31	LMG	L	101	51/55	0.85	0.31	-0.51	205,207,208,209	0
22	CLA	a	405	65/65	0.75	0.42	-0.54	205,207,209,209	0
32	LMT	M	102	35/35	0.69	0.42	-0.55	205,208,209,209	0
29	OEX	A	412	10/10	0.94	0.49	-0.55	197,202,205,206	0
22	CLA	d	405	65/65	0.77	0.46	-0.57	205,207,208,208	0
27	LHG	a	409	39/49	0.81	0.32	-0.60	206,207,209,209	0
22	CLA	C	519	65/65	0.84	0.31	-0.69	205,207,209,209	0
23	PHO	d	402	64/64	0.82	0.27	-0.75	206,207,209,209	0
27	LHG	A	410	39/49	0.86	0.25	-0.75	206,207,209,210	0
26	DGD	C	515	62/66	0.85	0.34	-0.76	205,207,209,210	0
27	LHG	C	518	37/49	0.81	0.30	-0.83	205,208,210,211	0
22	CLA	D	403	65/65	0.88	0.36	-0.88	205,207,208,208	0
22	CLA	B	606	65/65	0.91	0.27	-0.89	205,207,208,209	0
31	LMG	d	408	49/55	0.86	0.24	-0.90	205,207,208,209	0
27	LHG	c	519	37/49	0.79	0.28	-0.92	204,207,210,213	0
22	CLA	b	611	65/65	0.90	0.27	-0.96	206,207,208,209	0
26	DGD	c	517	66/66	0.84	0.25	-0.96	206,207,209,209	0
32	LMT	M	103	35/35	0.77	0.35	-0.99	206,208,209,209	0
31	LMG	B	621	49/55	0.85	0.23	-1.15	206,207,208,209	0
31	LMG	B	625	49/55	0.86	0.23	-1.30	205,207,208,208	0
21	FE2	a	413	1/1	0.57	0.24	-1.42	206,206,206,206	0
26	DGD	c	516	62/66	0.90	0.21	-1.44	206,208,208,209	0
31	LMG	b	626	49/55	0.87	0.23	-1.87	205,207,209,209	0
28	CL	a	410	1/1	0.94	0.40	-1.96	205,205,205,205	0
21	FE2	A	401	1/1	0.64	0.17	-2.83	209,209,209,209	0
31	LMG	i	102	43/55	0.64	0.83	-	205,207,209,210	0
35	CA	K	102	1/1	0.43	0.74	-	210,210,210,210	0
35	CA	o	301	1/1	0.62	0.63	-	209,209,209,209	0
32	LMT	B	623	35/35	0.69	0.81	-	206,208,210,210	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
35	CA	O	301	1/1	0.34	0.45	-	208,208,208,208	0
35	CA	k	101	1/1	0.83	0.29	-	208,208,208,208	0
32	LMT	b	628	35/35	0.65	0.54	-	206,208,210,210	0
31	LMG	I	101	43/55	0.49	1.17	-	205,208,210,211	0

6.5 Other polymers

There are no such residues in this entry.