



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 07:44 am GMT

PDB ID : 4IXR
Title : RT fs X-ray diffraction of Photosystem II, first illuminated state
Authors : Kern, J.; Alonso-Mori, R.; Tran, R.; Hattne, J.; Gildea, R.J.; Echols, N.; Gloeckner, C.; Hellmich, J.; Laksmono, H.; Sierra, R.G.; Lassalle-Kaiser, B.; Koroidov, S.; Lampe, A.; Han, G.; Gul, S.; DiFiore, D.; Milathianaki, D.; Fry, A.R.; Miahnahri, A.; Schafer, D.W.; Messerschmidt, M.; Seibert, M.M.; Koglin, J.E.; Sokaras, D.; Weng, T.-C.; Sellberg, J.; Latimer, M.J.; Grosse-Kunstleve, R.W.; Zwart, P.H.; White, W.E.; Glatzel, P.; Adams, P.D.; Bogan, M.J.; Williams, G.J.; Boutet, S.; Messinger, J.; Zouni, A.; Sauter, N.K.; Yachandra, V.K.; Bergmann, U.; Yano, J.
Deposited on : 2013-01-27
Resolution : 5.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

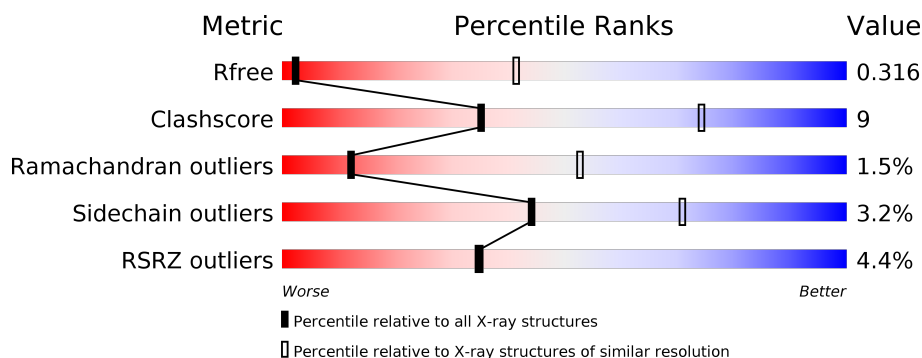
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1083 (8.00-3.70)
Clashscore	112137	1016 (8.00-3.80)
Ramachandran outliers	110173	1000 (8.00-3.72)
Sidechain outliers	110143	1083 (8.00-3.70)
RSRZ outliers	101464	1092 (8.00-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	<div> <div>3%</div> <div> <div></div> <div>61%</div> <div>31%</div> <div>7%</div> </div> </div>
1	a	360	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> </div>
2	B	510	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>27%</div> <div>•</div> </div> </div>
2	b	510	<div> <div>5%</div> <div> <div></div> <div>93%</div> <div>•</div> </div> </div>

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	V	163	
16	v	163	
17	g	46	
17	y	46	
18	X	41	
18	x	41	
19	Z	62	
19	z	62	
20	G	28	
20	Y	28	

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	BCT	d	401	-	-	-	X
23	CLA	A	403	X	-	-	-
23	CLA	A	404	X	-	X	-
23	CLA	A	405	X	-	-	-
23	CLA	A	407	X	-	-	X
23	CLA	B	601	X	-	-	X
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	X
23	CLA	B	604	X	-	-	X
23	CLA	B	605	X	-	-	X
23	CLA	B	606	X	-	-	X
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	X
23	CLA	B	609	X	-	-	X
23	CLA	B	610	X	-	-	X
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	X
23	CLA	B	613	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	B	614	X	-	-	X
23	CLA	B	615	X	-	-	X
23	CLA	B	616	X	-	-	X
23	CLA	C	501	X	-	-	X
23	CLA	C	502	X	-	-	X
23	CLA	C	503	X	-	-	X
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	X
23	CLA	C	506	X	-	-	X
23	CLA	C	507	X	-	-	X
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	X
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	X
23	CLA	C	512	X	-	-	X
23	CLA	C	513	X	-	-	X
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	X
23	CLA	a	404	X	-	-	-
23	CLA	a	405	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	409	X	-	-	X
23	CLA	b	605	X	-	-	X
23	CLA	b	606	X	-	-	X
23	CLA	b	607	X	-	-	X
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	X
23	CLA	b	610	X	-	-	X
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	X
23	CLA	b	613	X	-	-	X
23	CLA	b	614	X	-	-	X
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	b	618	X	-	-	-
23	CLA	b	619	X	-	-	X
23	CLA	b	620	X	-	-	X
23	CLA	c	501	X	-	-	X
23	CLA	c	502	X	-	-	X
23	CLA	c	503	X	-	-	X
23	CLA	c	504	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	X
23	CLA	c	507	X	-	-	X
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	X
23	CLA	c	510	X	-	-	X
23	CLA	c	511	X	-	-	X
23	CLA	c	512	X	-	-	X
23	CLA	c	513	X	-	-	X
23	CLA	d	402	X	-	-	-
23	CLA	d	403	X	-	-	X
25	PL9	A	408	-	-	-	X
25	PL9	J	101	-	-	-	X
25	PL9	a	410	-	-	-	X
25	PL9	j	101	-	-	-	X
26	OEC	A	409	-	-	-	X
27	BCR	A	410	-	-	-	X
27	BCR	B	620	-	-	-	X
27	BCR	C	514	-	-	-	X
27	BCR	C	515	-	-	-	X
27	BCR	C	516	-	-	-	X
27	BCR	D	405	-	-	-	X
27	BCR	H	101	-	-	-	X
27	BCR	J	102	-	-	-	X
27	BCR	a	412	-	-	-	X
27	BCR	b	622	-	-	-	X
27	BCR	c	514	-	-	-	X
27	BCR	c	515	-	-	-	X
27	BCR	h	101	-	-	-	X
27	BCR	j	102	-	-	-	X
27	BCR	k	102	-	-	-	X
27	BCR	y	101	-	-	-	X
27	BCR	z	101	-	-	-	X
28	DGD	B	627	-	-	-	X
28	DGD	C	519	-	-	-	X
28	DGD	D	409	-	-	-	X
28	DGD	b	602	-	-	-	X
28	DGD	d	409	-	-	-	X
29	LHG	A	415	-	-	-	X
29	LHG	a	414	-	-	-	X
30	SQD	B	626	-	-	-	X
30	SQD	D	408	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	SQD	F	102	-	-	-	X
30	SQD	a	401	-	-	-	X
30	SQD	b	601	-	-	-	X
30	SQD	d	408	-	-	-	X
30	SQD	f	102	-	-	-	X
31	LMG	A	418	-	-	-	X
31	LMG	C	521	-	-	-	X
31	LMG	E	101	-	-	-	X
31	LMG	I	101	-	-	-	X
31	LMG	a	402	-	-	-	X
31	LMG	c	519	-	-	-	X
31	LMG	e	101	-	-	-	X
31	LMG	i	101	-	-	-	X
31	LMG	k	103	-	-	-	X
32	CL	A	416	-	-	-	X
32	CL	a	418	-	-	-	X
33	LMT	B	625	-	-	-	X
33	LMT	B	628	-	-	-	X
33	LMT	B	629	-	-	-	X
33	LMT	D	410	-	-	-	X
33	LMT	I	102	-	-	-	X
33	LMT	M	102	-	-	-	X
33	LMT	b	603	-	-	-	X
33	LMT	b	604	-	-	-	X
33	LMT	b	627	-	-	-	X
33	LMT	d	410	-	-	-	X
33	LMT	i	102	-	-	-	X
33	LMT	m	101	-	-	-	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 50232 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
			2627	1720	432	460	15			
1	a	335	Total	C	N	O	S	0	0	0
			2627	1720	432	460	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 Z.

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

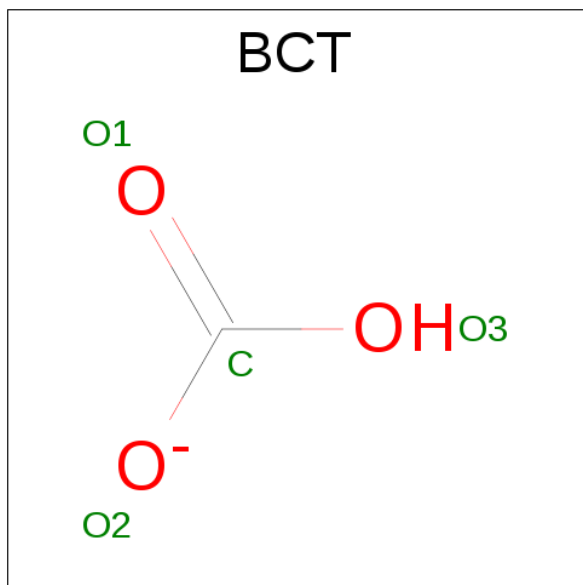
- Molecule 20 is a protein called Photosystem II reaction center protein Y.

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

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

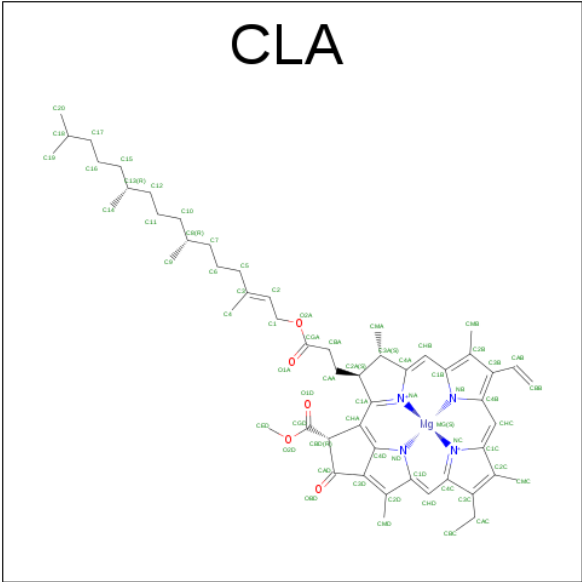
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			4	1	3		
22	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

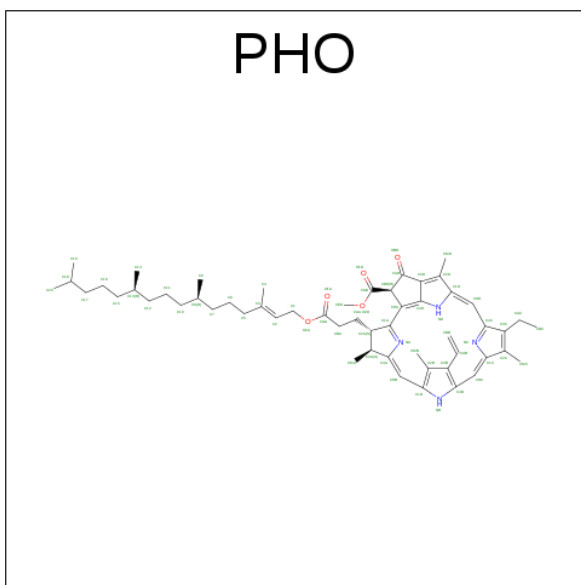
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

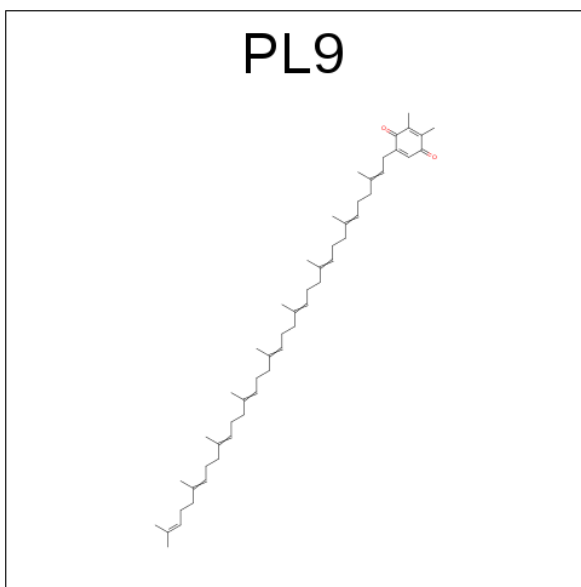
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



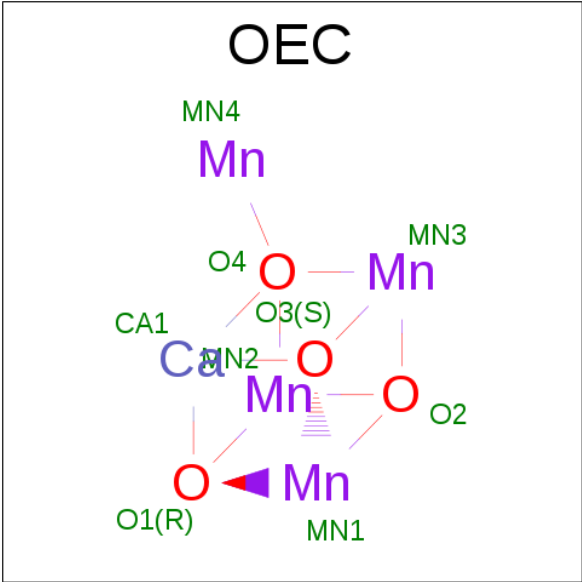
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is 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: C₅₃H₈₀O₂).



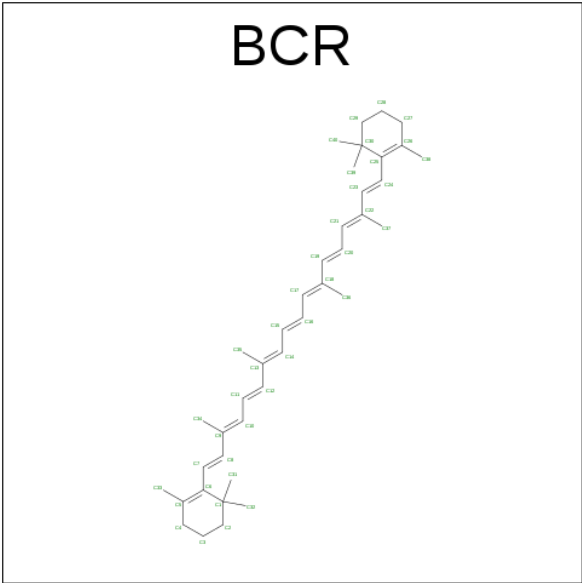
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	A	1	Total	C	O	0	0
			45	43	2		
25	D	1	Total	C	O	0	0
			55	53	2		
25	J	1	Total	C	O	0	0
			35	33	2		
25	a	1	Total	C	O	0	0
			45	43	2		
25	d	1	Total	C	O	0	0
			55	53	2		
25	j	1	Total	C	O	0	0
			35	33	2		

- Molecule 26 is OXYGEN EVOLVING SYSTEM (three-letter code: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	Ca	Mn	0	0
			5	1	4		
26	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	1	Total	C	0	0
			40	40		
27	B	1	Total	C	0	0
			40	40		

Continued on next page...

Continued from previous page...

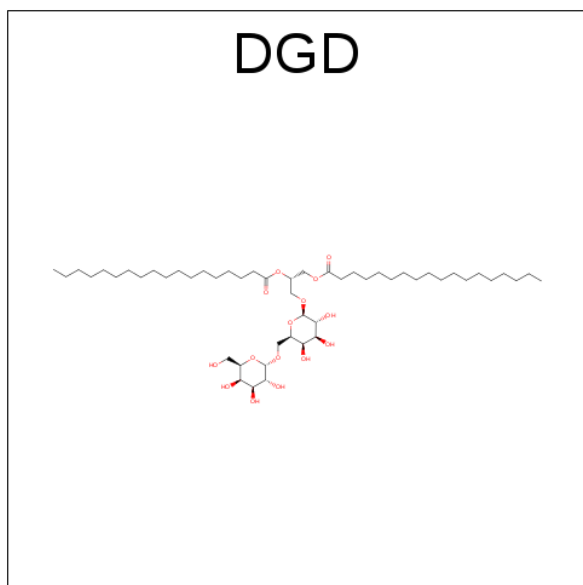
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	B	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	C	1	Total C 40 40	0	0
27	D	1	Total C 40 40	0	0
27	H	1	Total C 40 40	0	0
27	J	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	T	1	Total C 40 40	0	0
27	y	1	Total C 40 40	0	0
27	a	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	b	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	c	1	Total C 40 40	0	0
27	d	1	Total C 40 40	0	0
27	h	1	Total C 40 40	0	0
27	j	1	Total C 40 40	0	0
27	k	1	Total C 40 40	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	z	1	Total C 40 40	0	0

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



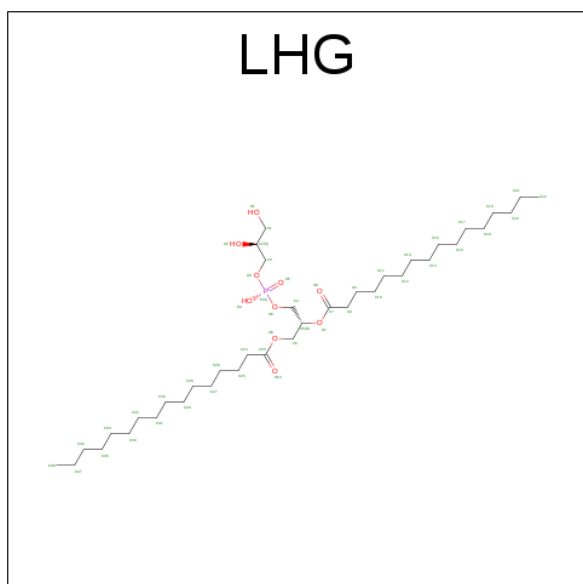
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 56 41 15	0	0
28	B	1	Total C O 58 43 15	0	0
28	B	1	Total C O 52 37 15	0	0
28	C	1	Total C O 53 38 15	0	0
28	C	1	Total C O 62 47 15	0	0
28	C	1	Total C O 66 51 15	0	0
28	D	1	Total C O 63 48 15	0	0
28	a	1	Total C O 56 41 15	0	0
28	b	1	Total C O 52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

Continued on next page...

Continued from previous page...

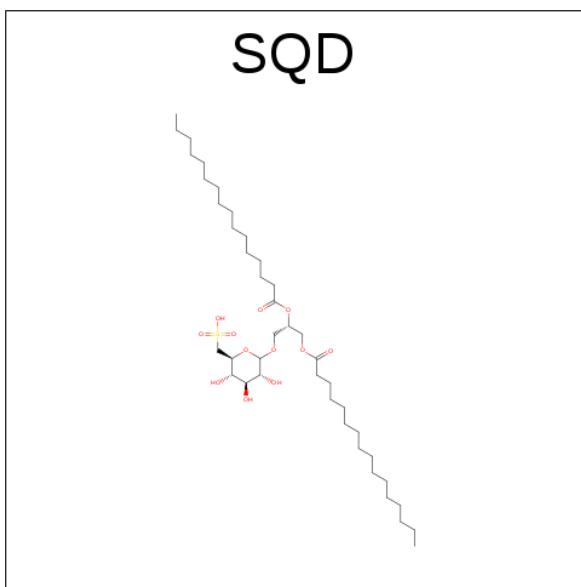
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	c	1	Total	C	O	0	0
			53	38	15		
28	c	1	Total	C	O	0	0
			62	47	15		
28	c	1	Total	C	O	0	0
			66	51	15		
28	d	1	Total	C	O	0	0
			63	48	15		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



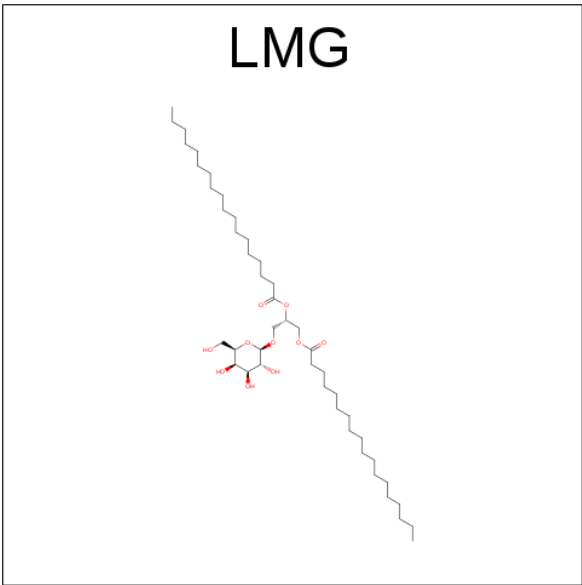
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	O	P	0	0
			39	28	10	1		
29	A	1	Total	C	O	P	0	0
			37	26	10	1		
29	a	1	Total	C	O	P	0	0
			39	28	10	1		
29	a	1	Total	C	O	P	0	0
			37	26	10	1		

- 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		
30	A	1	Total	C	O	S	0	0
			54	41	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		
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: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			51	41	10		
31	A	1	Total	C	O	0	0
			42	32	10		
31	B	1	Total	C	O	0	0
			49	39	10		
31	B	1	Total	C	O	0	0
			49	39	10		
31	C	1	Total	C	O	0	0
			48	38	10		
31	C	1	Total	C	O	0	0
			45	35	10		
31	D	1	Total	C	O	0	0
			46	36	10		
31	D	1	Total	C	O	0	0
			48	38	10		
31	E	1	Total	C	O	0	0
			44	34	10		
31	I	1	Total	C	O	0	0
			43	33	10		
31	M	1	Total	C	O	0	0
			42	32	10		
31	a	1	Total	C	O	0	0
			42	32	10		
31	a	1	Total	C	O	0	0
			51	41	10		
31	b	1	Total	C	O	0	0
			49	39	10		

Continued on next page...

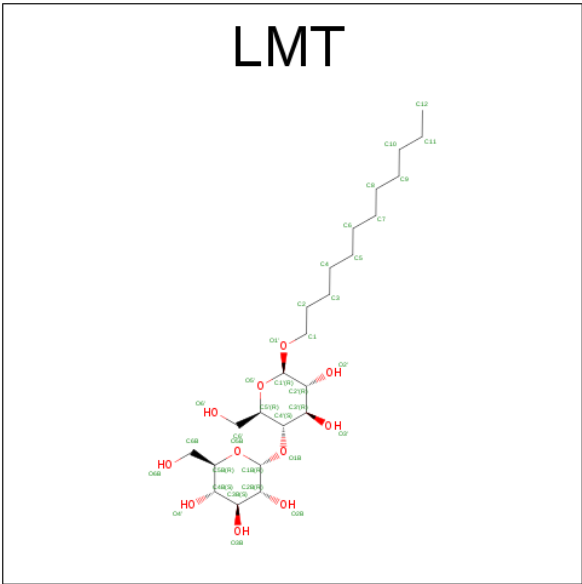
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	b	1	Total	C	O	0	0
			49	39	10		
31	c	1	Total	C	O	0	0
			45	35	10		
31	d	1	Total	C	O	0	0
			46	36	10		
31	d	1	Total	C	O	0	0
			48	38	10		
31	e	1	Total	C	O	0	0
			44	34	10		
31	i	1	Total	C	O	0	0
			43	33	10		
31	k	1	Total	C	O	0	0
			48	38	10		
31	m	1	Total	C	O	0	0
			42	32	10		

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

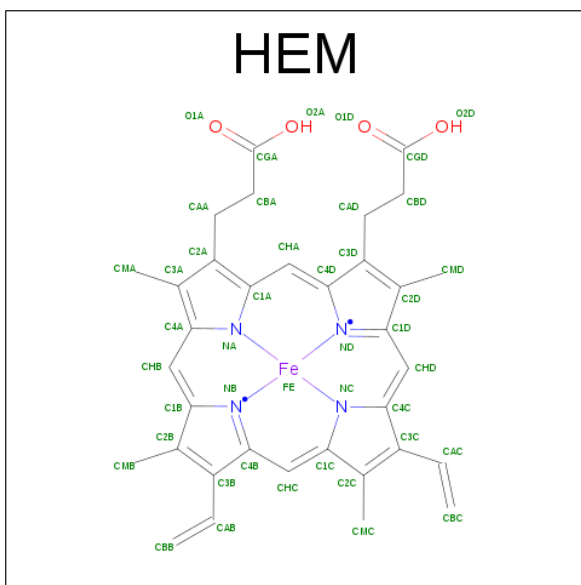
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Cl	0	0
			1	1		
32	a	1	Total	Cl	0	0
			1	1		

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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

- 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	
			43	34	1	4	4	
34	V	1	Total	C	Fe	N	O	
			43	34	1	4	4	
34	f	1	Total	C	Fe	N	O	
			43	34	1	4	4	
34	v	1	Total	C	Fe	N	O	
			43	34	1	4	4	

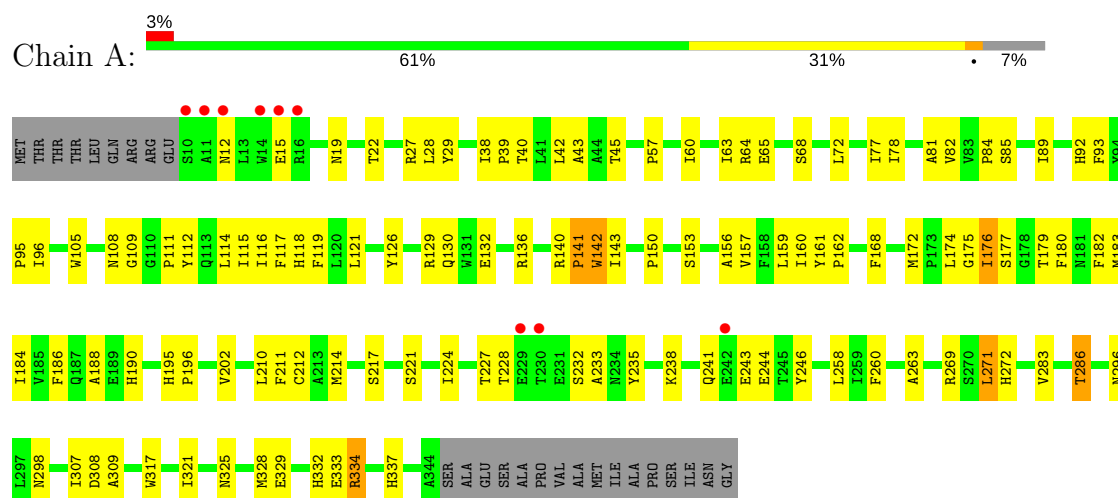
- Molecule 35 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

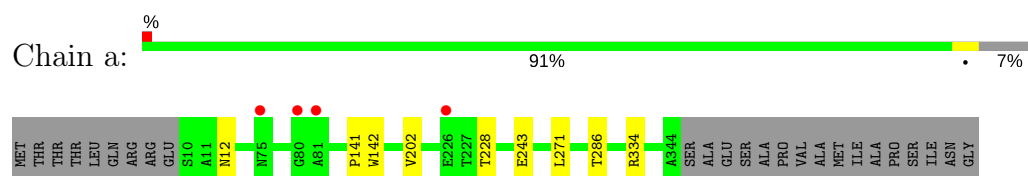
3 Residue-property plots

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

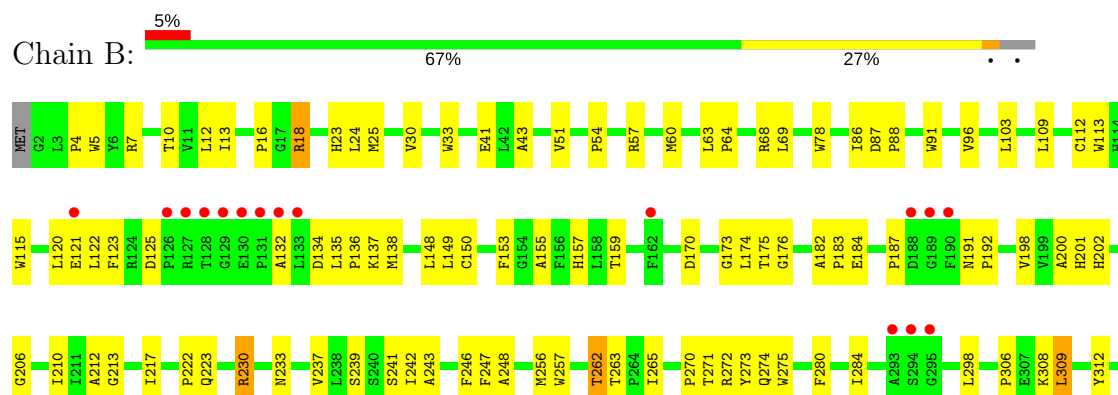
• Molecule 1: Photosystem Q(B) protein 1

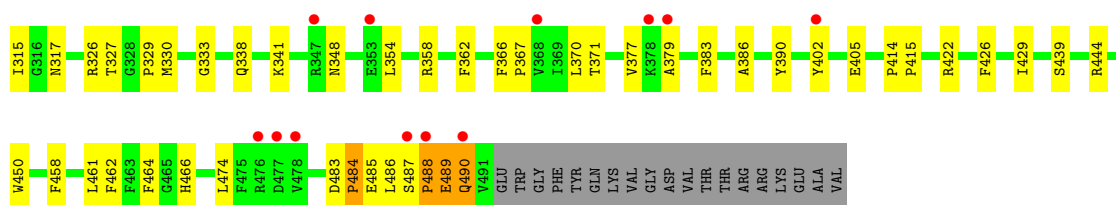


• Molecule 1: Photosystem Q(B) protein 1

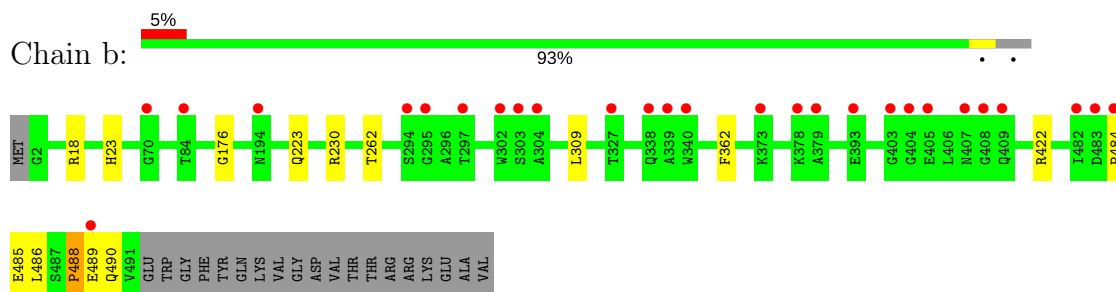


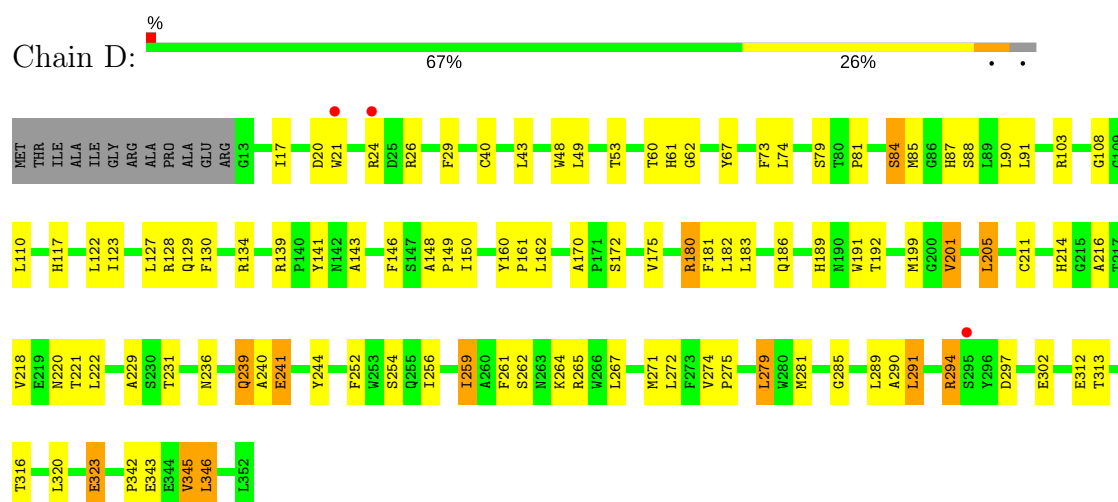
• Molecule 2: Photosystem II core light harvesting protein



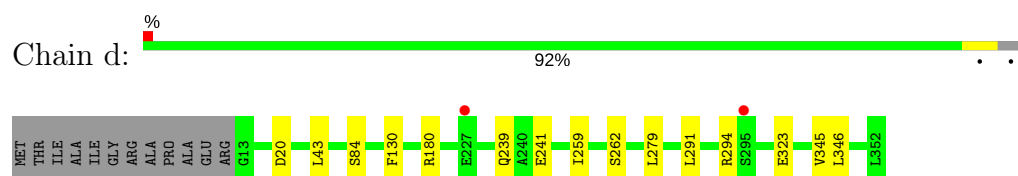


• Molecule 2: Photosystem II core light harvesting protein

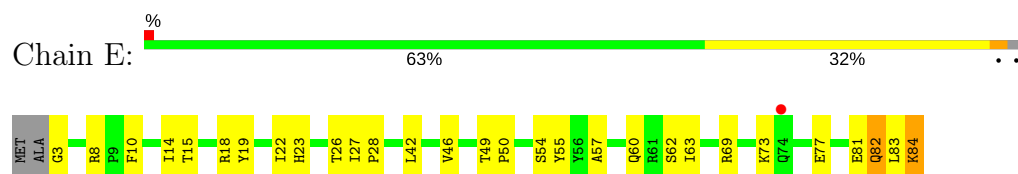




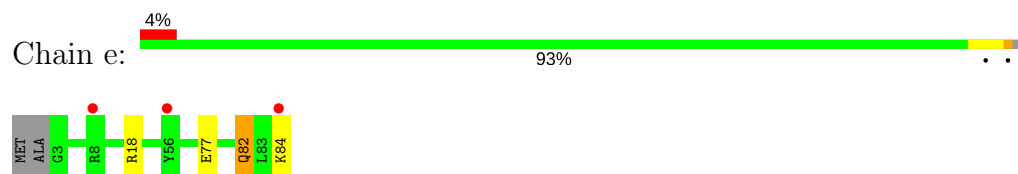
- Molecule 4: Photosystem II D2 protein



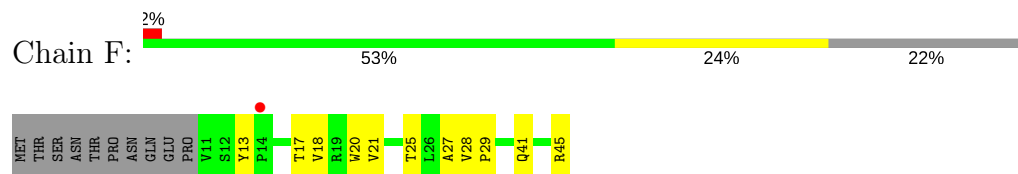
- Molecule 5: Cytochrome b559 subunit alpha



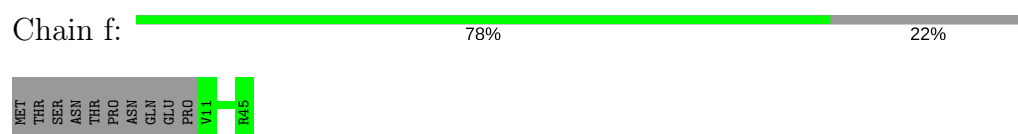
- Molecule 5: Cytochrome b559 subunit alpha



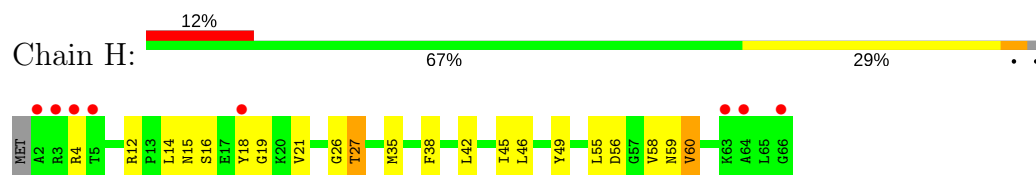
- Molecule 6: Cytochrome b559 subunit beta



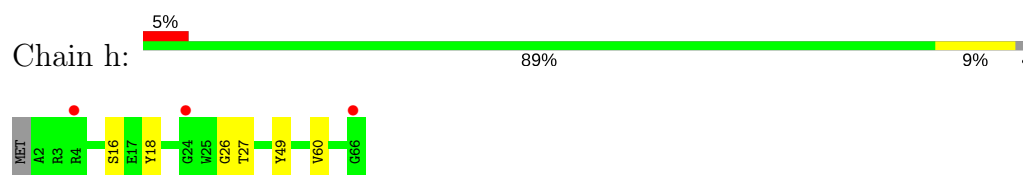
- Molecule 6: Cytochrome b559 subunit beta



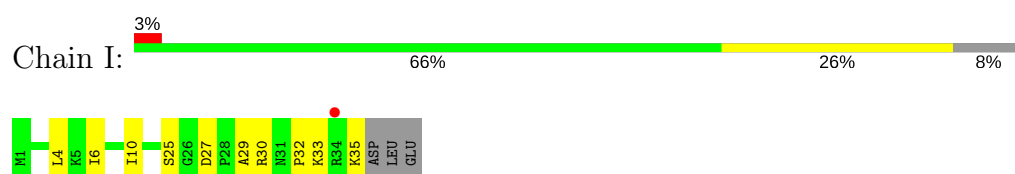
- Molecule 7: Photosystem II reaction center protein H



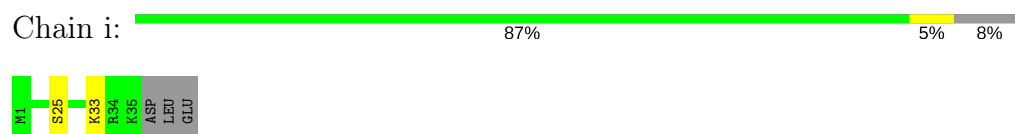
- Molecule 7: Photosystem II reaction center protein H



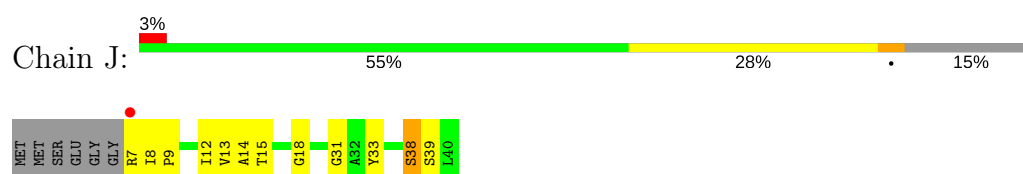
- Molecule 8: Photosystem II reaction center protein I



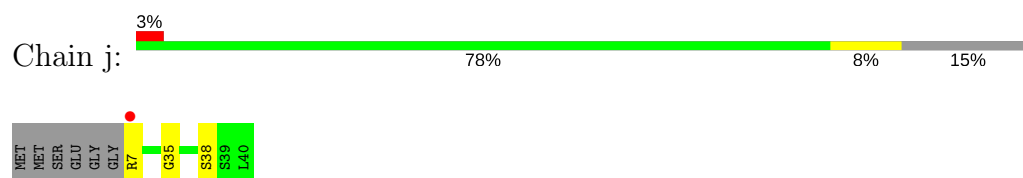
- Molecule 8: Photosystem II reaction center protein I



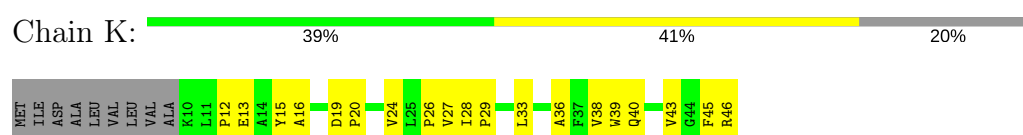
- Molecule 9: Photosystem II reaction center protein J



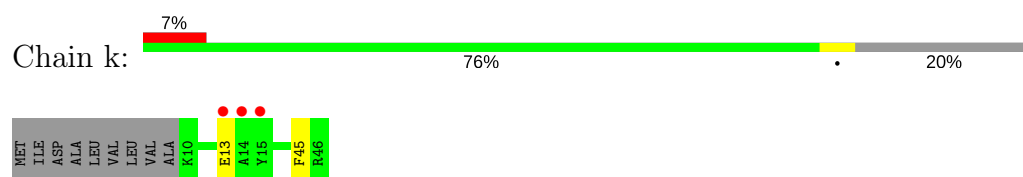
- Molecule 9: Photosystem II reaction center protein J



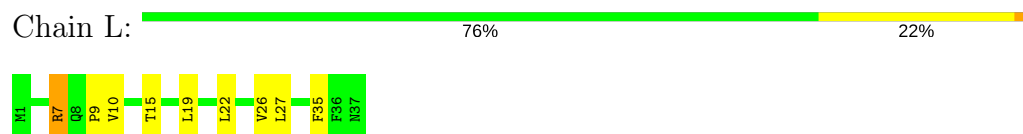
- Molecule 10: Photosystem II reaction center protein K



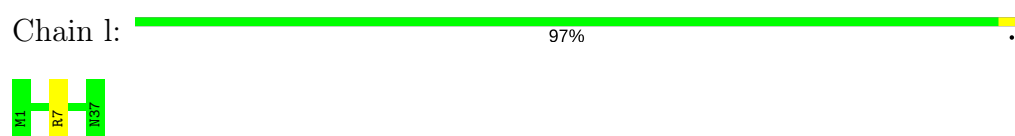
- Molecule 10: Photosystem II reaction center protein K



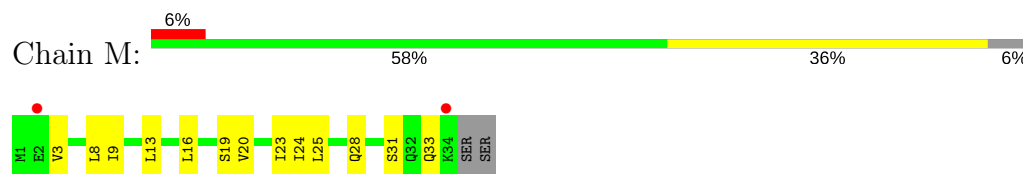
- Molecule 11: Photosystem II reaction center protein L



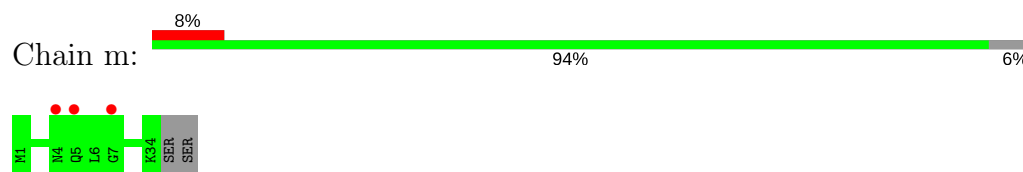
- Molecule 11: Photosystem II reaction center protein L



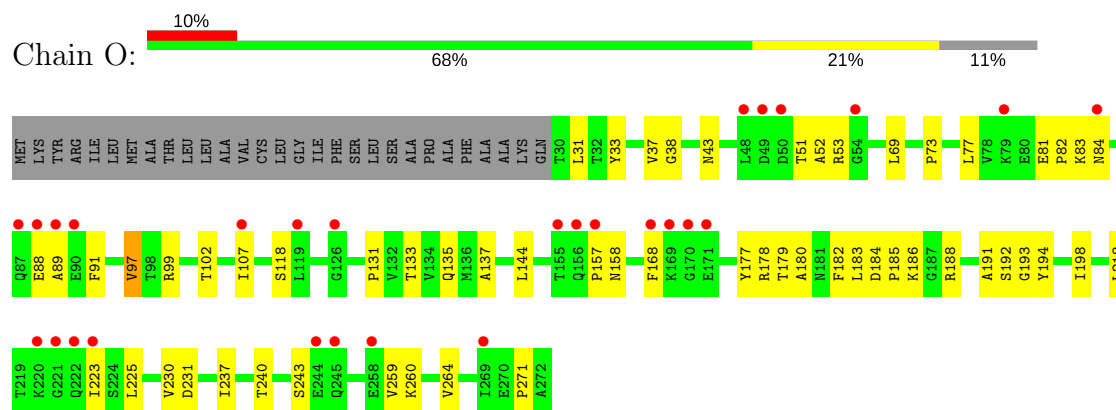
- Molecule 12: Photosystem II reaction center protein M



- Molecule 12: Photosystem II reaction center protein M

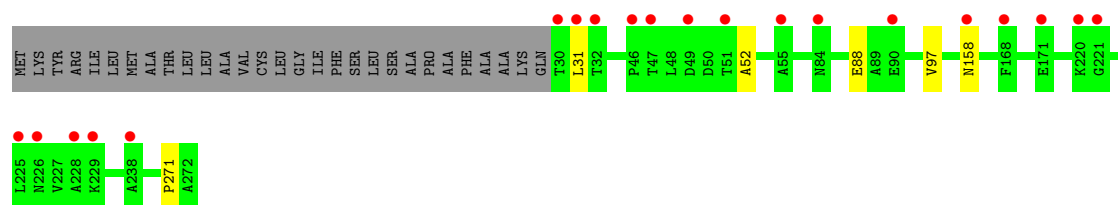


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





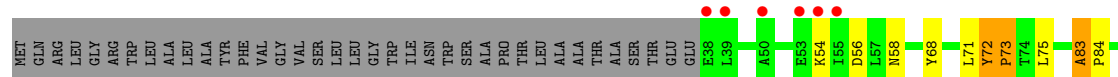
- Molecule 14: Photosystem II reaction center protein T



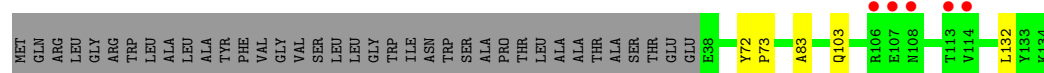
- Molecule 14: Photosystem II reaction center protein T



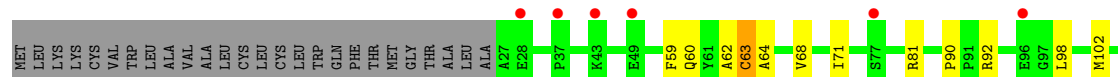
- Molecule 15: Photosystem II 12 kDa extrinsic protein



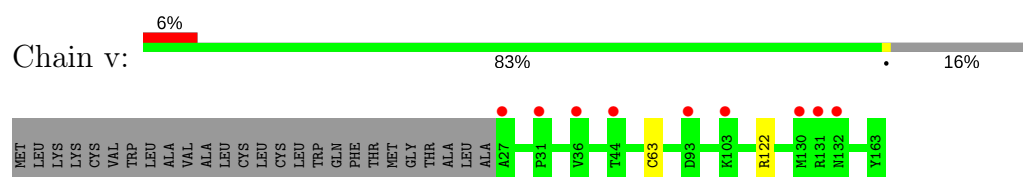
- Molecule 15: Photosystem II 12 kDa extrinsic protein



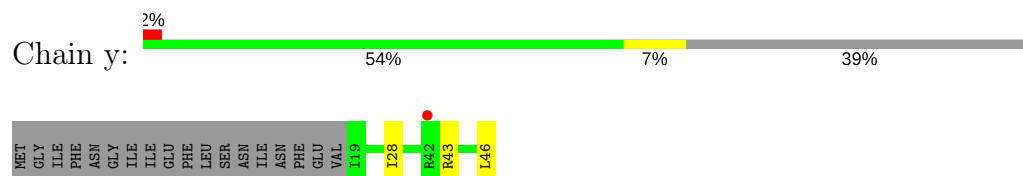
- Molecule 16: Cytochrome c-550



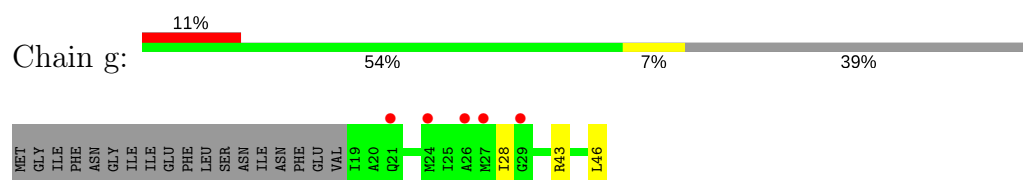
- Molecule 16: Cytochrome c-550



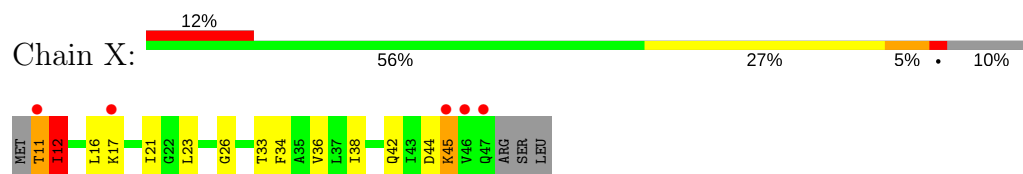
- Molecule 17: Photosystem II reaction center protein ycf12



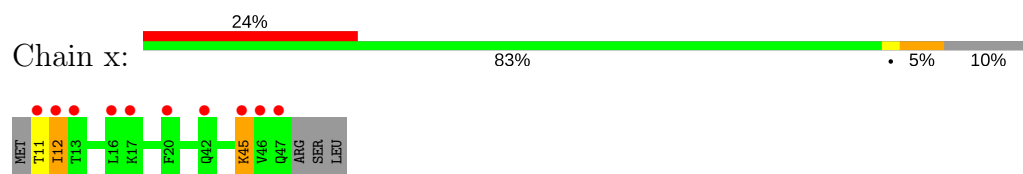
- Molecule 17: Photosystem II reaction center protein ycf12



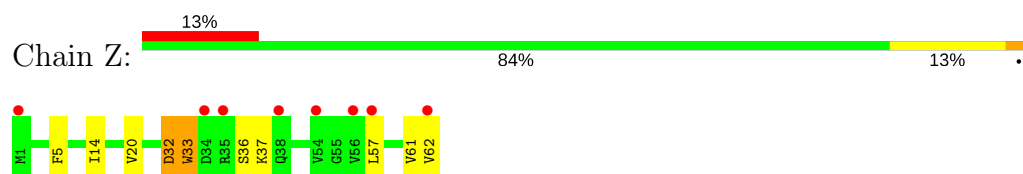
- Molecule 18: Photosystem II reaction center X protein



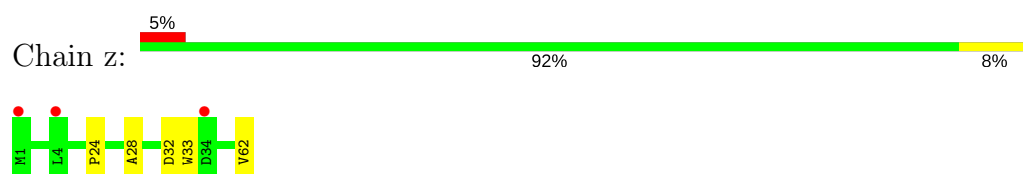
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



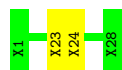
- Molecule 20: Photosystem II reaction center protein Y

Chain G:  93% 7%



- Molecule 20: Photosystem II reaction center protein Y

Chain Y:  93% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.98Å 227.57Å 306.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.97 – 5.90 82.97 – 5.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (82.97-5.90) 98.5 (82.97-5.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 5.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1265)	Depositor
R, R_{free}	0.285 , 0.313 0.308 , 0.316	Depositor DCC
R_{free} test set	1200 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	1.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	50232	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, PHO, DGD, CL, CA, LMT, CLA, PL9, BCT, FE2, OEC, 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	0.31	0/2712	0.48	0/3700
1	a	0.30	0/2712	0.48	0/3700
2	B	0.29	0/3986	0.46	0/5433
2	b	0.28	0/3986	0.46	0/5433
3	C	0.28	0/3556	0.46	0/4842
3	c	0.27	0/3556	0.46	0/4842
4	D	0.28	0/2801	0.46	0/3818
4	d	0.30	0/2801	0.46	0/3818
5	E	0.29	0/685	0.48	0/933
5	e	0.28	0/685	0.48	0/933
6	F	0.28	0/291	0.45	0/397
6	f	0.26	0/291	0.45	0/397
7	H	0.26	0/520	0.49	0/709
7	h	0.27	0/520	0.50	0/709
8	I	0.28	0/293	0.48	0/395
8	i	0.32	0/293	0.49	0/395
9	J	0.29	0/255	0.46	0/346
9	j	0.28	0/255	0.44	0/346
10	K	0.29	0/303	0.52	0/416
10	k	0.28	0/303	0.53	0/416
11	L	0.25	0/311	0.43	0/422
11	l	0.24	0/311	0.45	0/422
12	M	0.41	0/270	0.65	0/367
12	m	0.41	0/270	0.65	0/367
13	O	0.27	0/1876	0.48	0/2548
13	o	0.28	0/1876	0.49	0/2548
14	T	0.36	0/284	0.49	0/381
14	t	0.35	0/284	0.47	0/381
15	U	0.27	0/785	0.49	0/1064
15	u	0.32	0/785	0.55	0/1064
16	V	0.30	0/1081	0.52	0/1468
16	v	0.26	0/1081	0.46	0/1468

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	g	0.24	0/202	0.51	0/272
17	y	0.25	0/202	0.52	0/272
18	X	0.30	0/273	0.52	0/370
18	x	0.32	0/273	0.50	0/370
19	Z	0.30	0/490	0.50	0/669
19	z	0.28	0/490	0.48	0/669
All	All	0.29	0/41948	0.48	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	2627	0	2524	105	0
1	a	2627	0	2524	0	0
2	B	3850	0	3718	137	0
2	b	3850	0	3718	0	0
3	C	3444	0	3365	116	0
3	c	3444	0	3365	0	0
4	D	2706	0	2608	95	0
4	d	2706	0	2608	0	0
5	E	666	0	651	24	0
5	e	666	0	651	0	0
6	F	282	0	291	11	0
6	f	282	0	291	0	0
7	H	507	0	521	20	0
7	h	507	0	521	0	0
8	I	286	0	308	5	0
8	i	286	0	308	0	0
9	J	249	0	262	8	0
9	j	249	0	262	0	0
10	K	293	0	305	16	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	10	0
11	l	304	0	316	0	0
12	M	267	0	289	13	0
12	m	267	0	289	0	0
13	O	1845	0	1801	39	0
13	o	1845	0	1801	0	0
14	T	275	0	288	17	0
14	t	275	0	288	0	0
15	U	774	0	773	13	0
15	u	774	0	773	0	0
16	V	1060	0	1068	13	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	12	0
18	x	270	0	299	0	0
19	Z	479	0	516	9	0
19	z	479	0	516	0	0
20	G	140	0	32	1	0
20	Y	140	0	32	1	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	1	0	0
22	d	4	0	1	0	0
23	A	260	0	288	48	0
23	B	1040	0	1152	131	0
23	C	845	0	936	66	0
23	D	130	0	144	10	0
23	a	260	0	288	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	130	0	144	0	0
24	A	64	0	74	5	0
24	D	64	0	74	6	0
24	a	128	0	148	0	0
25	A	45	0	61	2	0
25	D	55	0	80	12	0
25	J	35	0	45	1	0
25	a	45	0	61	0	0
25	d	55	0	80	0	0
25	j	35	0	45	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	5	0	0	0	0
26	a	5	0	0	0	0
27	A	40	0	56	7	0
27	B	160	0	224	21	0
27	C	120	0	168	22	0
27	D	40	0	56	3	0
27	H	40	0	56	7	0
27	J	40	0	56	4	0
27	T	80	0	112	11	0
27	a	40	0	56	0	0
27	b	80	0	112	0	0
27	c	80	0	112	0	0
27	d	40	0	56	0	0
27	h	40	0	56	0	0
27	j	40	0	56	0	0
27	k	40	0	56	0	0
27	y	40	0	56	0	0
27	z	40	0	56	0	0
28	A	56	0	70	1	0
28	B	110	0	136	2	0
28	C	181	0	245	21	0
28	D	63	0	87	2	0
28	a	56	0	70	0	0
28	b	110	0	136	0	0
28	c	181	0	244	0	0
28	d	63	0	87	0	0
29	A	76	0	95	7	0
29	a	76	0	95	0	0
30	A	105	0	147	12	0
30	B	47	0	61	2	0
30	D	43	0	50	5	0
30	F	45	0	54	2	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	A	93	0	125	5	0
31	B	98	0	135	8	0
31	C	93	0	126	5	0
31	D	94	0	126	8	0
31	E	44	0	58	1	0
31	I	43	0	55	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	M	42	0	53	2	0
31	a	93	0	124	0	0
31	b	98	0	135	0	0
31	c	45	0	59	0	0
31	d	94	0	126	0	0
31	e	44	0	58	0	0
31	i	43	0	55	0	0
31	k	48	0	66	0	0
31	m	42	0	53	0	0
32	A	1	0	0	0	0
32	a	1	0	0	0	0
33	B	140	0	184	5	0
33	D	31	0	35	1	0
33	I	35	0	46	2	0
33	M	35	0	46	1	0
33	b	140	0	184	0	0
33	d	31	0	35	0	0
33	i	35	0	46	0	0
33	m	35	0	46	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	50232	0	51361	801	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 9.

All (801) 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)
4:D:26:ARG:HD3	6:F:18:VAL:HG11	1.58	0.88
3:C:39:ASN:HB2	23:C:508:CLA:HBA1	1.57	0.86
12:M:33:GLN:HB3	12:M:33:GLN:HB3	0.00	0.86
13:O:82:PRO:HG3	13:O:89:ALA:HB2	1.59	0.83
27:B:617:BCR:H383	30:B:626:SQD:H92	1.62	0.82
2:B:187:PRO:HB3	23:B:601:CLA:HMB2	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:D:408:SQD:H301	30:D:408:SQD:H171	1.66	0.77
13:O:69:LEU:HB3	13:O:107:ILE:HB	1.66	0.77
23:C:507:CLA:H112	27:C:516:BCR:H362	1.66	0.77
12:M:28:GLN:HA	12:M:28:GLN:HA	0.00	0.77
3:C:297:TYR:O	3:C:423:ARG:NH2	2.31	0.77
3:C:250:TRP:O	3:C:254:THR:OG1	2.03	0.76
3:C:362:ARG:H	28:C:517:DGD:HE4	1.52	0.75
4:D:199:MET:HG2	25:D:404:PL9:H322	1.68	0.75
4:D:29:PHE:O	4:D:128:ARG:NH2	2.23	0.74
23:B:608:CLA:HBA2	30:D:408:SQD:H101	1.70	0.74
24:A:406:PHO:HBC3	4:D:279:LEU:HG	1.70	0.74
23:A:404:CLA:HED1	25:D:404:PL9:H372	1.69	0.73
3:C:291:TRP:O	3:C:305:THR:OG1	2.05	0.73
2:B:121:GLU:HG2	7:H:4:ARG:HG2	1.73	0.73
34:V:201:HEM:HBC2	34:V:201:HEM:HHD	1.70	0.73
23:C:508:CLA:HBC3	23:C:510:CLA:H92	1.69	0.73
12:M:25:LEU:O	12:M:28:GLN:HG3	1.93	0.73
23:B:612:CLA:H42	4:D:127:LEU:HD11	30.04	0.73
27:B:618:BCR:H10C	14:T:18:PHE:HB2	43.71	0.73
1:A:183:MET:HB3	23:A:404:CLA:HBC2	5.97	0.72
4:D:259:ILE:HG12	31:D:407:LMG:H292	1.87	0.72
2:B:262:THR:HG22	2:B:263:THR:HG23	1.77	0.71
23:B:608:CLA:H42	4:D:127:LEU:HD11	1.72	0.71
1:A:63:ILE:HB	3:C:335:THR:HG21	1.70	0.71
23:B:609:CLA:HBB1	23:B:610:CLA:H51	9.02	0.71
1:A:129:ARG:HH21	4:D:256:ILE:HD12	1.60	0.71
14:T:18:PHE:HB2	27:T:102:BCR:H10C	1.72	0.71
5:E:60:GLN:OE1	5:E:84:LYS:NZ	2.24	0.71
34:F:101:HEM:HHC	34:F:101:HEM:HBB2	1.77	0.71
23:A:405:CLA:HED1	25:D:404:PL9:H372	28.53	0.70
2:B:187:PRO:HB3	23:B:605:CLA:HMB2	31.39	0.70
23:A:403:CLA:H71	23:A:404:CLA:HAB	1.75	0.69
7:H:38:PHE:HB2	27:H:101:BCR:H10C	1.73	0.69
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.96	0.69
11:L:9:PRO:HB3	31:M:101:LMG:HC61	14.40	0.69
23:B:606:CLA:H72	27:B:620:BCR:H311	1.74	0.69
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.74	0.69
4:D:236:ASN:ND2	4:D:239:GLN:O	2.25	0.69
3:C:48:LYS:NZ	3:C:133:ALA:O	2.25	0.69
23:D:403:CLA:H42	18:X:26:GLY:HA3	1.76	0.68
1:A:15:GLU:O	1:A:19:ASN:ND2	2.25	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:415:LHG:H271	29:A:415:LHG:H101	1.76	0.67
12:M:20:VAL:O	12:M:24:ILE:HG13	1.94	0.67
1:A:29:TYR:O	1:A:129:ARG:NH1	2.29	0.67
2:B:12:LEU:HB2	23:B:612:CLA:HMC2	1.77	0.67
3:C:449:ARG:HE	23:C:505:CLA:HED1	1.59	0.67
1:A:183:MET:HA	23:A:403:CLA:HMD2	1.77	0.67
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.83	0.67
4:D:21:TRP:O	4:D:26:ARG:NH2	2.25	0.67
2:B:149:LEU:HG	23:B:607:CLA:HBC1	27.84	0.66
1:A:221:SER:HB3	4:D:141:TYR:HB2	1.77	0.66
3:C:405:ASN:HB2	28:C:518:DGD:HG31	10.27	0.66
3:C:216:SER:HB3	3:C:221:GLU:HB2	1.85	0.66
2:B:271:THR:HG22	2:B:273:TYR:H	1.63	0.66
27:B:618:BCR:H19C	27:B:619:BCR:H363	1.75	0.66
2:B:149:LEU:HG	23:B:603:CLA:HBC1	1.76	0.65
23:B:607:CLA:H193	7:H:42:LEU:HD12	33.83	0.65
23:B:605:CLA:HBB1	23:B:606:CLA:H51	1.77	0.65
4:D:186:GLN:HB2	23:D:401:CLA:HBC1	1.76	0.65
1:A:329:GLU:O	1:A:332:HIS:ND1	2.43	0.65
4:D:24:ARG:NH2	18:X:44:ASP:O	2.29	0.65
23:C:511:CLA:H171	19:Z:20:VAL:HA	1.78	0.65
2:B:103:LEU:HD21	23:B:609:CLA:HMC3	26.64	0.65
31:A:418:LMG:H112	2:B:43:ALA:HA	42.32	0.64
2:B:150:CYS:HB2	23:B:603:CLA:HMC3	1.80	0.64
1:A:317:TRP:CZ3	4:D:180:ARG:HD3	2.32	0.64
2:B:103:LEU:HD21	23:B:605:CLA:HMC3	1.79	0.64
3:C:118:HIS:CE1	31:C:521:LMG:H192	2.33	0.64
16:V:62:ALA:O	34:V:201:HEM:HAB	1.98	0.64
6:F:17:THR:HG23	6:F:20:TRP:H	1.63	0.63
23:B:603:CLA:H193	7:H:42:LEU:HD12	1.80	0.63
7:H:55:LEU:HB2	7:H:58:VAL:HG12	1.83	0.63
15:U:56:ASP:OD2	15:U:115:THR:OG1	2.26	0.63
23:C:503:CLA:H172	23:C:510:CLA:HBB2	1.80	0.63
23:C:507:CLA:H112	27:C:515:BCR:H362	29.07	0.63
3:C:405:ASN:HB2	28:C:519:DGD:HG31	1.80	0.63
31:A:414:LMG:H231	25:D:404:PL9:H352	1.81	0.63
2:B:24:LEU:HD21	23:B:616:CLA:HAB	1.81	0.63
3:C:42:LEU:HD21	23:C:511:CLA:H2A	1.83	0.63
1:A:140:ARG:HH22	29:A:412:LHG:P	2.22	0.63
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.63
31:D:407:LMG:HO4	31:D:407:LMG:HO5	2.22	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:MET:HB3	23:A:403:CLA:HBC2	1.80	0.62
30:A:413:SQD:H241	29:A:415:LHG:HC81	1.82	0.62
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.81	0.62
31:D:407:LMG:H111	11:L:19:LEU:HD21	1.81	0.62
2:B:5:TRP:HZ3	23:B:611:CLA:H51	1.64	0.61
23:D:403:CLA:H43	18:X:23:LEU:HA	1.83	0.61
3:C:406:SER:O	3:C:418:ASN:ND2	2.39	0.61
23:C:509:CLA:HBD	23:C:509:CLA:H121	1.84	0.61
4:D:192:THR:HG23	23:D:401:CLA:HBC2	1.82	0.61
1:A:183:MET:HA	23:A:404:CLA:HMD2	8.46	0.60
4:D:302:GLU:OE1	13:O:186:LYS:NZ	2.30	0.60
23:A:405:CLA:H42	25:D:404:PL9:H162	18.91	0.60
2:B:458:PHE:HB3	23:B:608:CLA:HBC2	12.78	0.60
13:O:178:ARG:HG3	13:O:178:ARG:HH11	1.69	0.60
1:A:72:LEU:HD13	31:A:418:LMG:H111	1.84	0.60
2:B:327:THR:HG21	31:B:623:LMG:H111	1.85	0.59
1:A:28:LEU:HB2	30:A:417:SQD:H91	1.83	0.59
3:C:164:HIS:ND1	23:C:507:CLA:OBD	2.42	0.59
23:B:612:CLA:H151	23:B:613:CLA:H203	19.91	0.59
1:A:64:ARG:O	13:O:178:ARG:NH2	2.36	0.59
2:B:270:PRO:HG3	2:B:312:TYR:HD2	1.87	0.59
3:C:49:LEU:O	3:C:53:HIS:ND1	2.34	0.59
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.68	0.58
1:A:217:SER:HA	4:D:272:LEU:HD12	1.94	0.58
2:B:383:PHE:CZ	13:O:193:GLY:HA2	2.47	0.58
16:V:59:PHE:HA	16:V:63:CYS:SG	2.48	0.58
23:C:501:CLA:HMB3	27:C:516:BCR:H403	1.86	0.58
13:O:180:ALA:HB1	13:O:191:ALA:HB2	1.88	0.58
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.84	0.58
23:B:606:CLA:HBD	23:B:606:CLA:H2	8.35	0.58
3:C:165:LEU:HD21	23:C:506:CLA:HAB	1.85	0.58
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.58
23:A:405:CLA:H142	23:D:401:CLA:H151	1.85	0.58
14:T:21:ILE:HD12	27:T:102:BCR:H332	1.85	0.58
30:A:413:SQD:H223	28:C:519:DGD:HAE1	1.86	0.57
3:C:178:LYS:HA	3:C:182:PHE:HB2	1.85	0.57
3:C:437:PHE:CZ	23:C:510:CLA:HMB3	2.39	0.57
23:B:613:CLA:HMC2	27:H:101:BCR:H343	25.62	0.57
1:A:334:ARG:NH1	13:O:183:LEU:O	2.46	0.57
3:C:215:LYS:HB3	3:C:223:TRP:HA	1.93	0.57
1:A:317:TRP:HZ3	4:D:180:ARG:HD3	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:601:CLA:HMB3	27:H:101:BCR:H281	1.86	0.57
34:F:101:HEM:HMC2	34:F:101:HEM:HBC2	1.87	0.57
13:O:73:PRO:HG2	13:O:102:THR:HB	1.89	0.57
1:A:65:GLU:OE2	1:A:334:ARG:NH2	2.43	0.56
3:C:229:ASN:ND2	3:C:232:ASP:OD1	2.43	0.56
23:B:603:CLA:C2D	23:B:605:CLA:H2	2.35	0.56
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.76	0.56
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.45	0.56
3:C:305:THR:HG23	3:C:307:PRO:HD2	1.88	0.56
30:D:408:SQD:H241	30:D:408:SQD:H111	1.85	0.56
19:Z:33:TRP:O	19:Z:37:LYS:HB2	2.05	0.56
1:A:89:ILE:HD11	1:A:108:ASN:HB3	1.86	0.56
1:A:153:SER:HB3	23:A:404:CLA:HED1	17.23	0.56
2:B:150:CYS:HA	23:B:607:CLA:HBC2	29.73	0.56
3:C:131:TYR:HE1	3:C:135:ARG:HD2	1.80	0.56
15:U:54:LYS:HD2	15:U:113:THR:HG23	2.01	0.56
2:B:212:ALA:HB2	23:B:609:CLA:HMC3	1.87	0.56
23:C:505:CLA:H11	27:C:515:BCR:H312	50.03	0.56
4:D:222:LEU:HD23	4:D:244:TYR:HB3	1.86	0.56
2:B:150:CYS:HA	23:B:603:CLA:HBC2	1.87	0.56
23:C:511:CLA:HMB2	27:C:514:BCR:H382	1.88	0.56
1:A:190:HIS:O	1:A:298:ASN:HB3	2.12	0.55
2:B:150:CYS:HB2	23:B:607:CLA:HMC3	24.82	0.55
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.40	0.55
23:B:609:CLA:H202	23:B:613:CLA:HBB2	21.83	0.55
2:B:121:GLU:O	7:H:12:ARG:NH2	2.41	0.55
23:B:612:CLA:HBA2	30:D:408:SQD:H101	22.81	0.55
1:A:227:THR:HG21	1:A:233:ALA:HA	1.89	0.55
30:A:413:SQD:H311	23:C:508:CLA:H71	1.89	0.55
23:C:513:CLA:HAB	27:C:515:BCR:H24C	1.89	0.55
2:B:239:SER:O	2:B:466:HIS:ND1	2.39	0.55
23:B:608:CLA:H151	23:B:609:CLA:H203	1.89	0.55
2:B:212:ALA:HB2	23:B:613:CLA:HMC3	27.33	0.55
3:C:284:PHE:HB3	28:C:517:DGD:HA51	1.89	0.55
24:A:406:PHO:H151	23:D:401:CLA:H172	1.88	0.55
23:C:501:CLA:C2D	23:C:503:CLA:H2	2.37	0.55
27:C:514:BCR:H391	10:K:36:ALA:HB2	2.00	0.55
2:B:78:TRP:HB3	13:O:137:ALA:HB1	59.82	0.54
13:O:83:LYS:HG2	13:O:84:ASN:H	1.75	0.54
1:A:84:PRO:HA	1:A:112:TYR:CG	2.42	0.54
13:O:240:THR:HG22	13:O:264:VAL:HG12	1.99	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:473:ASP:HB2	14:T:26:PRO:HB3	1.90	0.54
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.88	0.54
23:A:405:CLA:HAA1	25:D:404:PL9:H362	24.29	0.54
4:D:129:GLN:OE1	4:D:143:ALA:HA	2.07	0.54
23:C:505:CLA:HBA1	23:C:505:CLA:HBD	2.00	0.54
2:B:201:HIS:HD2	2:B:202:HIS:CE1	2.50	0.54
2:B:371:THR:HG22	2:B:377:VAL:HA	1.93	0.54
23:B:608:CLA:HBD	23:B:609:CLA:H43	4.18	0.54
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.43	0.54
23:B:615:CLA:H172	23:B:615:CLA:H111	1.90	0.54
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.89	0.54
28:C:518:DGD:HA41	31:C:520:LMG:H391	1.89	0.54
31:C:520:LMG:HC62	27:J:102:BCR:H271	1.90	0.54
12:M:31:SER:HA	31:M:101:LMG:HC1	1.90	0.54
1:A:111:PRO:O	1:A:115:ILE:HG13	2.08	0.53
2:B:41:GLU:HB3	2:B:60:MET:SD	2.48	0.53
2:B:96:VAL:HG22	23:B:610:CLA:HBA1	23.24	0.53
3:C:461:ARG:NH1	4:D:241:GLU:OE1	2.57	0.53
15:U:98:THR:O	15:U:102:LYS:HG3	2.88	0.53
1:A:211:PHE:HA	1:A:214:MET:HB2	1.89	0.53
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.94	0.53
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.00	0.53
2:B:341:LYS:HA	2:B:405:GLU:HB2	1.89	0.53
33:B:628:LMT:H122	14:T:7:VAL:HG12	34.77	0.53
23:A:404:CLA:HHC	23:A:404:CLA:HBB1	2.46	0.53
2:B:271:THR:HB	2:B:274:GLN:HG3	1.90	0.53
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.46	0.53
5:E:15:THR:HG23	9:J:8:ILE:O	2.10	0.53
23:B:603:CLA:C3D	23:B:605:CLA:H2	2.39	0.53
23:B:604:CLA:HBB1	23:B:607:CLA:CBB	2.38	0.53
4:D:214:HIS:ND1	25:D:404:PL9:O2	2.27	0.53
15:U:68:TYR:HB2	15:U:71:LEU:HD12	1.90	0.53
1:A:210:LEU:HG	24:A:406:PHO:NC	2.24	0.53
2:B:198:VAL:O	2:B:202:HIS:ND1	2.35	0.53
4:D:49:LEU:O	4:D:53:THR:HG23	2.09	0.53
13:O:230:VAL:HG13	13:O:237:ILE:HG22	1.91	0.53
1:A:244:GLU:HG3	1:A:246:TYR:H	1.73	0.53
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.98	0.53
2:B:125:ASP:HB2	2:B:132:ALA:HB3	1.91	0.53
28:B:627:DGD:HB22	33:B:629:LMT:H72	1.91	0.53
1:A:141:PRO:O	1:A:143:ILE:N	2.47	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:O	1:A:176:ILE:HB	2.09	0.52
1:A:140:ARG:NH2	29:A:412:LHG:O5	2.36	0.52
23:B:602:CLA:H42	7:H:45:ILE:HD11	1.90	0.52
3:C:437:PHE:HZ	23:C:510:CLA:HMB3	1.75	0.52
23:A:403:CLA:H122	24:D:402:PHO:H3A	1.91	0.52
23:A:404:CLA:H203	24:D:402:PHO:H71	1.92	0.52
23:B:605:CLA:HMB3	27:H:101:BCR:H281	36.59	0.52
23:C:501:CLA:H171	23:C:507:CLA:HMB3	1.91	0.52
1:A:153:SER:HB2	23:A:404:CLA:H43	14.47	0.52
27:A:410:BCR:H311	30:A:417:SQD:H351	1.92	0.52
2:B:241:SER:HB3	23:B:612:CLA:HED3	1.91	0.52
3:C:305:THR:HG22	3:C:308:GLU:HB2	1.94	0.52
23:A:405:CLA:H93	23:D:401:CLA:H152	1.92	0.52
3:C:29:GLU:HB3	10:K:46:ARG:HH11	1.80	0.52
31:D:407:LMG:O6	11:L:15:THR:HG21	2.10	0.52
3:C:334:PRO:HA	13:O:179:THR:OG1	2.22	0.52
19:Z:33:TRP:HA	19:Z:36:SER:HB3	1.95	0.52
19:Z:32:ASP:CG	19:Z:33:TRP:H	2.18	0.52
2:B:112:CYS:HG	14:T:18:PHE:HZ	45.61	0.51
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.44	0.51
27:A:410:BCR:H342	30:A:417:SQD:H342	1.92	0.51
2:B:222:PRO:HG3	7:H:27:THR:H	1.75	0.51
3:C:393:ALA:HB1	34:V:201:HEM:HBC1	1.99	0.51
1:A:332:HIS:CD2	1:A:333:GLU:HG3	2.46	0.51
3:C:158:THR:O	3:C:251:HIS:HB3	2.09	0.51
23:C:512:CLA:H143	23:C:513:CLA:H162	2.03	0.51
3:C:75:PHE:HD1	3:C:86:LEU:HD21	1.75	0.51
2:B:122:LEU:O	7:H:15:ASN:ND2	2.40	0.51
10:K:40:GLN:HA	10:K:43:VAL:HG12	2.06	0.51
23:A:404:CLA:H71	23:A:405:CLA:HAB	27.58	0.51
30:A:417:SQD:H332	23:B:610:CLA:H203	66.31	0.51
23:B:603:CLA:CBB	23:B:605:CLA:H152	2.41	0.51
2:B:462:PHE:CZ	23:B:613:CLA:HMB3	2.46	0.51
3:C:380:ILE:HA	3:C:384:ILE:HD11	2.03	0.51
2:B:474:LEU:O	4:D:134:ARG:NH1	2.47	0.51
23:A:404:CLA:HAA1	25:D:404:PL9:H362	1.91	0.51
13:O:230:VAL:HG12	13:O:231:ASP:H	1.74	0.51
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.48	0.51
23:B:609:CLA:HMD1	7:H:27:THR:HB	1.92	0.51
2:B:213:GLY:O	2:B:217:ILE:HG13	2.10	0.51
23:B:606:CLA:H42	7:H:45:ILE:HD11	29.61	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:225:VAL:HG13	3:C:289:PHE:HA	2.01	0.51
3:C:85:GLY:N	28:C:518:DGD:HE4	2.25	0.51
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.93	0.51
1:A:238:LYS:HD2	14:T:32:LYS:HB3	1.93	0.51
3:C:130:VAL:O	3:C:134:ILE:HG12	2.14	0.51
33:D:410:LMT:H72	18:X:26:GLY:HA2	1.92	0.51
4:D:189:HIS:HA	4:D:294:ARG:HD2	1.93	0.50
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.92	0.50
2:B:241:SER:HB3	23:B:616:CLA:HED3	28.40	0.50
23:B:602:CLA:HBD	23:B:602:CLA:H2	1.92	0.50
3:C:425:TRP:CE2	23:C:504:CLA:HBA1	2.57	0.50
10:K:12:PRO:HB2	10:K:15:TYR:HD2	1.76	0.50
30:F:102:SQD:H131	18:X:36:VAL:HG11	1.93	0.50
23:B:611:CLA:H171	23:B:613:CLA:ND	2.26	0.50
3:C:60:ILE:HG23	23:C:510:CLA:HMC2	2.02	0.50
4:D:49:LEU:HD13	27:D:405:BCR:C15	2.45	0.50
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.94	0.50
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.50
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.41	0.50
2:B:25:MET:HG2	27:T:101:BCR:H23C	37.32	0.50
27:B:618:BCR:H332	14:T:21:ILE:HD12	49.29	0.50
27:C:514:BCR:H311	27:C:514:BCR:H343	1.98	0.50
11:L:10:VAL:O	12:M:28:GLN:NE2	2.34	0.50
2:B:184:GLU:H	2:B:200:ALA:HB2	1.77	0.50
4:D:221:THR:HG23	4:D:244:TYR:HB2	2.01	0.50
1:A:119:PHE:HZ	23:A:403:CLA:H8	1.76	0.50
2:B:155:ALA:O	2:B:159:THR:OG1	2.26	0.50
4:D:87:HIS:CD2	4:D:162:LEU:HA	2.46	0.50
23:B:607:CLA:C3D	23:B:609:CLA:H2	40.36	0.50
27:B:617:BCR:H341	27:B:618:BCR:H24C	1.93	0.50
5:E:55:TYR:O	5:E:84:LYS:HE3	2.29	0.50
9:J:14:ALA:O	9:J:18:GLY:N	2.42	0.50
2:B:12:LEU:HB2	23:B:616:CLA:HMC2	13.50	0.50
3:C:186:TYR:HE2	3:C:188:THR:HG22	1.82	0.50
3:C:429:SER:HB3	28:C:517:DGD:HA81	17.09	0.50
3:C:361:PHE:HA	28:C:517:DGD:HE62	1.92	0.49
30:F:102:SQD:H162	18:X:33:THR:HA	1.93	0.49
13:O:118:SER:HB3	13:O:157:PRO:HA	1.95	0.49
2:B:329:PRO:HB3	23:B:607:CLA:HED1	1.94	0.49
23:B:604:CLA:HBB1	23:B:607:CLA:HBB2	1.93	0.49
23:B:612:CLA:H51	23:B:613:CLA:H101	18.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:ARG:HH21	31:B:622:LMG:HC3	1.76	0.49
23:C:501:CLA:HMB3	27:C:515:BCR:H403	24.91	0.49
2:B:135:LEU:HB2	2:B:136:PRO:HD3	1.93	0.49
29:A:412:LHG:HC32	4:D:229:ALA:O	2.12	0.49
18:X:34:PHE:O	18:X:38:ILE:HG12	2.12	0.49
23:B:613:CLA:HMB1	23:B:613:CLA:HBB1	1.95	0.49
23:A:404:CLA:CHA	23:A:404:CLA:HBA1	2.42	0.49
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.94	0.49
3:C:56:HIS:HE1	3:C:60:ILE:HD11	1.78	0.49
23:B:607:CLA:C2D	23:B:609:CLA:H2	40.11	0.49
3:C:248:GLY:O	3:C:252:ILE:HG12	2.24	0.49
3:C:319:ILE:HG21	3:C:389:GLU:HG3	1.98	0.49
13:O:77:LEU:HB2	13:O:260:LYS:HB3	1.95	0.49
1:A:283:VAL:O	1:A:286:THR:HG22	2.14	0.49
4:D:60:THR:HG23	4:D:61:HIS:CD2	2.49	0.49
1:A:116:ILE:HG13	1:A:117:PHE:N	2.27	0.49
1:A:85:SER:HA	1:A:109:GLY:HA3	2.09	0.49
3:C:405:ASN:CB	28:C:518:DGD:HG31	10.72	0.49
12:M:28:GLN:O	12:M:31:SER:OG	3.44	0.49
2:B:25:MET:HG2	27:T:101:BCR:C23	36.57	0.49
3:C:405:ASN:CB	28:C:519:DGD:HG31	2.43	0.49
3:C:62:PHE:HZ	10:K:28:ILE:HD12	1.77	0.49
3:C:131:TYR:CE1	3:C:135:ARG:HD2	2.58	0.48
23:C:508:CLA:H172	28:C:518:DGD:HBW2	1.95	0.48
23:B:611:CLA:H41	23:B:614:CLA:HBC3	1.95	0.48
27:B:618:BCR:H352	27:B:619:BCR:H382	1.95	0.48
3:C:90:PRO:O	3:C:94:THR:HG23	2.12	0.48
4:D:244:TYR:OH	4:D:264:LYS:HE3	2.13	0.48
1:A:232:SER:OG	31:A:414:LMG:O3	2.21	0.48
23:B:606:CLA:HAA2	7:H:45:ILE:HD12	27.42	0.48
12:M:19:SER:O	12:M:23:ILE:HG13	2.14	0.48
2:B:458:PHE:HB3	23:B:604:CLA:HBC2	1.95	0.48
23:B:607:CLA:H2	23:B:609:CLA:H93	34.05	0.48
3:C:343:ARG:NH1	3:C:347:GLY:O	2.46	0.48
3:C:53:HIS:HB3	23:C:512:CLA:OBD	2.29	0.48
2:B:327:THR:HG22	23:B:607:CLA:H12	1.94	0.48
3:C:429:SER:HB3	28:C:518:DGD:HA81	1.95	0.48
23:A:405:CLA:HAB	23:D:401:CLA:H72	1.96	0.48
23:A:403:CLA:H51	24:D:402:PHO:C3B	2.43	0.48
23:A:405:CLA:HBA1	23:A:405:CLA:CHA	3.90	0.48
4:D:73:PHE:CZ	31:D:406:LMG:H172	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:403:CLA:HBB1	23:A:403:CLA:HHC	1.95	0.48
23:B:616:CLA:H72	23:B:616:CLA:H12	1.96	0.48
1:A:232:SER:HB3	1:A:235:TYR:HD1	1.95	0.48
2:B:488:PRO:O	2:B:490:GLN:N	2.47	0.48
3:C:42:LEU:HD13	23:C:511:CLA:HMA3	1.95	0.48
9:J:9:PRO:HB2	9:J:12:ILE:HG13	2.00	0.48
14:T:4:ILE:HD13	27:T:102:BCR:H381	1.94	0.48
23:A:404:CLA:H122	23:A:404:CLA:HMA1	1.95	0.48
3:C:91:HIS:O	3:C:94:THR:OG1	2.42	0.48
9:J:38:SER:OG	9:J:39:SER:N	2.49	0.48
27:A:410:BCR:H342	30:A:417:SQD:H311	1.95	0.48
1:A:57:PRO:HG3	1:A:68:SER:CB	2.51	0.48
4:D:146:PHE:O	4:D:149:PRO:HD2	2.13	0.48
15:U:117:VAL:HG13	15:U:122:VAL:HG21	2.08	0.48
23:B:606:CLA:H162	23:B:606:CLA:H122	4.25	0.47
23:B:607:CLA:H41	23:B:607:CLA:H61	3.01	0.47
3:C:337:LEU:HA	13:O:131:PRO:HG3	2.04	0.47
3:C:363:GLY:O	3:C:367:GLU:HG2	2.13	0.47
23:A:404:CLA:H42	25:D:404:PL9:H162	1.96	0.47
1:A:157:VAL:HG13	1:A:172:MET:HB3	1.95	0.47
1:A:328:MET:HE1	4:D:183:LEU:HD22	1.96	0.47
27:B:620:BCR:H351	27:B:620:BCR:H15C	1.75	0.47
23:A:405:CLA:H122	23:A:405:CLA:HMA1	8.91	0.47
1:A:43:ALA:HB1	27:A:410:BCR:H362	1.96	0.47
2:B:257:TRP:CE2	4:D:291:LEU:HD12	2.54	0.47
23:B:602:CLA:H162	23:B:602:CLA:H122	1.54	0.47
23:B:611:CLA:H193	11:L:27:LEU:HD11	15.90	0.47
2:B:25:MET:HG2	27:B:617:BCR:C23	2.45	0.47
1:A:269:ARG:NH1	4:D:231:THR:HB	2.36	0.47
23:C:501:CLA:H193	23:C:507:CLA:H111	2.03	0.47
27:B:618:BCR:HC32	31:D:407:LMG:H392	57.86	0.47
1:A:174:LEU:HD22	24:D:402:PHO:H151	1.97	0.47
27:A:410:BCR:H341	27:A:410:BCR:H11C	1.79	0.47
23:B:609:CLA:HMA1	23:B:610:CLA:HBA2	10.53	0.47
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.50	0.47
2:B:487:SER:N	2:B:488:PRO:HD2	2.30	0.47
3:C:425:TRP:CZ2	23:C:504:CLA:HBA1	2.61	0.47
1:A:114:LEU:O	1:A:118:HIS:ND1	2.53	0.47
2:B:33:TRP:CD1	27:B:618:BCR:H391	2.50	0.47
3:C:240:ILE:O	3:C:244:CYS:HB2	2.22	0.47
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:343:GLU:HG2	16:V:161:VAL:HG11	2.04	0.47
1:A:89:ILE:HG12	13:O:99:ARG:NH2	2.30	0.47
16:V:90:PRO:O	16:V:92:ARG:HD3	2.15	0.47
1:A:221:SER:HB2	4:D:139:ARG:O	2.15	0.47
23:A:404:CLA:H3A	23:A:404:CLA:HBA1	3.88	0.47
3:C:386:PRO:HB3	16:V:116:GLU:HG2	2.01	0.47
10:K:16:ALA:O	10:K:19:ASP:HB2	2.15	0.47
13:O:223:ILE:HG13	13:O:243:SER:HB3	1.96	0.47
2:B:135:LEU:HA	2:B:138:MET:HE3	2.03	0.47
23:B:602:CLA:H62	23:B:602:CLA:H41	1.50	0.47
23:B:608:CLA:HBA1	23:B:608:CLA:CHA	2.45	0.47
27:C:514:BCR:HC7	27:C:514:BCR:H331	1.60	0.47
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.97	0.47
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.46
2:B:317:ASN:HA	2:B:330:MET:HE1	2.06	0.46
2:B:326:ARG:HB3	2:B:444:ARG:HG2	2.15	0.46
23:B:612:CLA:HBA1	23:B:612:CLA:CHA	3.80	0.46
2:B:120:LEU:HD13	23:B:616:CLA:HMD2	1.97	0.46
2:B:348:ASN:HB3	2:B:354:LEU:HD21	2.04	0.46
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.97	0.46
4:D:312:GLU:HB2	13:O:185:PRO:CG	2.45	0.46
16:V:98:LEU:O	16:V:102:MET:HG3	2.15	0.46
23:A:404:CLA:HBD	23:A:405:CLA:HAC2	15.21	0.46
2:B:25:MET:HG2	27:B:617:BCR:H23C	1.97	0.46
23:C:502:CLA:HBB2	23:C:510:CLA:H152	1.97	0.46
23:C:505:CLA:H11	27:C:516:BCR:H312	1.96	0.46
27:C:516:BCR:H351	27:C:516:BCR:H15C	1.78	0.46
8:I:29:ALA:HA	8:I:35:LYS:HB2	1.97	0.46
23:C:511:CLA:H151	19:Z:20:VAL:O	2.15	0.46
1:A:156:ALA:HA	1:A:160:ILE:HB	1.98	0.46
2:B:256:MET:HA	2:B:263:THR:HG21	1.97	0.46
33:B:629:LMT:H62	8:I:4:LEU:HD22	81.59	0.46
23:C:509:CLA:H11	23:C:509:CLA:H51	1.71	0.46
15:U:75:LEU:HD21	15:U:101:GLN:HB3	2.05	0.46
1:A:129:ARG:NH2	4:D:256:ILE:HD12	2.34	0.46
1:A:93:PHE:CD2	1:A:95:PRO:HD3	2.51	0.46
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.51	0.46
2:B:18:ARG:NH2	30:B:626:SQD:O9	2.49	0.46
23:B:608:CLA:HBB1	23:B:611:CLA:CBB	17.30	0.46
27:B:620:BCR:H11C	27:B:620:BCR:H341	1.82	0.46
23:C:506:CLA:H202	23:C:506:CLA:H161	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:404:CLA:H191	31:D:407:LMG:H352	7.96	0.46
5:E:81:GLU:C	5:E:83:LEU:H	2.19	0.46
3:C:85:GLY:N	28:C:517:DGD:HE4	23.32	0.46
5:E:19:TYR:O	5:E:23:HIS:ND1	2.40	0.46
1:A:180:PHE:HA	1:A:183:MET:HE2	2.11	0.46
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.98	0.46
23:B:612:CLA:H171	23:B:613:CLA:HBB2	1.98	0.46
2:B:464:PHE:HD2	23:B:615:CLA:HAC2	28.72	0.46
3:C:245:ILE:O	3:C:249:ILE:HG12	2.15	0.46
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.98	0.46
18:X:12:ILE:HA	18:X:16:LEU:HD12	2.12	0.46
2:B:137:LYS:HD2	7:H:14:LEU:O	2.16	0.46
23:B:613:CLA:H191	27:B:619:BCR:H333	1.98	0.46
23:C:511:CLA:H93	27:C:514:BCR:H272	1.99	0.46
4:D:17:ILE:HG21	18:X:42:GLN:HG3	1.98	0.46
24:D:402:PHO:H62	24:D:402:PHO:H41	1.38	0.46
31:I:101:LMG:H221	33:I:102:LMT:H81	2.01	0.46
24:A:406:PHO:HMA2	25:A:408:PL9:H222	1.98	0.45
2:B:201:HIS:HD2	2:B:202:HIS:ND1	2.35	0.45
3:C:56:HIS:CE1	3:C:60:ILE:HD11	2.51	0.45
4:D:252:PHE:O	4:D:256:ILE:HG22	2.19	0.45
1:A:153:SER:HB3	23:A:403:CLA:HED1	1.98	0.45
2:B:247:PHE:HB2	23:B:608:CLA:HBC1	1.98	0.45
3:C:137:PRO:HB2	3:C:139:THR:O	2.16	0.45
3:C:224:ILE:O	3:C:227:VAL:HG23	2.16	0.45
27:C:514:BCR:H351	27:C:514:BCR:H15C	1.74	0.45
23:C:504:CLA:H2	28:C:517:DGD:HA22	25.68	0.45
5:E:26:THR:HB	34:F:101:HEM:CAB	2.51	0.45
12:M:8:LEU:HG	12:M:9:ILE:HD12	7.09	0.45
13:O:240:THR:HA	13:O:264:VAL:HA	1.98	0.45
23:C:507:CLA:H62	23:C:507:CLA:H92	1.72	0.45
4:D:146:PHE:C	4:D:149:PRO:HD2	2.36	0.45
23:A:407:CLA:H162	23:A:407:CLA:H141	1.63	0.45
23:B:603:CLA:H192	23:B:603:CLA:H162	1.78	0.45
2:B:464:PHE:HD2	23:B:611:CLA:HAC2	1.80	0.45
5:E:50:PRO:HB3	5:E:54:SER:O	2.16	0.45
23:B:613:CLA:HMD1	7:H:27:THR:HB	39.53	0.45
1:A:161:TYR:HB3	1:A:162:PRO:HD3	2.00	0.45
1:A:244:GLU:CD	4:D:264:LYS:HZ3	2.20	0.45
23:A:403:CLA:H172	24:D:402:PHO:H43	1.97	0.45
2:B:329:PRO:HB3	23:B:611:CLA:HED1	41.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:603:CLA:H2	23:B:605:CLA:H93	1.97	0.45
3:C:166:ILE:O	3:C:170:ILE:HG13	2.20	0.45
3:C:229:ASN:ND2	3:C:231:GLU:HB2	2.39	0.45
23:C:506:CLA:HMC2	23:C:507:CLA:H102	1.98	0.45
4:D:274:VAL:HG13	25:D:404:PL9:C23	2.57	0.45
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.32	0.45
5:E:57:ALA:HB3	5:E:60:GLN:HB3	1.99	0.45
13:O:177:TYR:HD2	13:O:178:ARG:HG2	1.81	0.45
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.73	0.45
13:O:192:SER:OG	13:O:193:GLY:N	2.55	0.45
2:B:270:PRO:HG3	2:B:312:TYR:CD2	2.72	0.45
23:A:403:CLA:HBA1	23:A:403:CLA:H3A	1.61	0.45
5:E:10:PHE:N	31:E:101:LMG:O3	2.52	0.45
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.45
23:B:612:CLA:HMA1	4:D:130:PHE:CE1	22.72	0.45
4:D:85:MET:HA	5:E:69:ARG:HB3	2.15	0.45
6:F:27:ALA:HB1	34:F:101:HEM:CAC	2.47	0.45
15:U:106:ARG:HA	15:U:109:LEU:HG	1.98	0.45
33:B:628:LMT:H1B	33:B:628:LMT:H3'	1.56	0.45
28:A:411:DGD:HAT2	3:C:281:MET:HG3	1.98	0.45
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.57	0.45
3:C:29:GLU:HB2	3:C:30:SER:H	1.66	0.45
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.99	0.45
5:E:60:GLN:HG2	5:E:62:SER:H	1.88	0.45
30:A:413:SQD:H162	25:J:101:PL9:H533	1.99	0.45
27:T:101:BCR:H341	27:T:102:BCR:H24C	1.98	0.45
23:A:404:CLA:H202	23:A:404:CLA:H162	1.75	0.45
23:A:405:CLA:H162	23:A:405:CLA:H202	4.13	0.45
23:B:603:CLA:H41	23:B:603:CLA:H61	1.80	0.45
31:C:521:LMG:H292	31:C:521:LMG:H111	1.99	0.45
27:H:101:BCR:H15C	27:H:101:BCR:H351	1.85	0.45
31:I:101:LMG:H181	33:I:102:LMT:H42	2.01	0.45
1:A:333:GLU:HB2	1:A:337:HIS:HE1	1.89	0.44
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.05	0.44
23:D:401:CLA:H61	23:D:401:CLA:H41	1.65	0.44
30:D:408:SQD:H3	30:D:408:SQD:H441	2.01	0.44
23:C:511:CLA:H141	19:Z:20:VAL:HG13	2.02	0.44
2:B:96:VAL:HG22	23:B:606:CLA:HBA1	1.98	0.44
23:B:614:CLA:H112	23:B:614:CLA:H91	1.76	0.44
4:D:216:ALA:O	4:D:220:ASN:ND2	2.52	0.44
4:D:261:PHE:HB2	25:D:404:PL9:H522	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:294:ARG:HG2	4:D:294:ARG:H	1.65	0.44
27:D:405:BCR:H351	27:D:405:BCR:H15C	1.82	0.44
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.99	0.44
1:A:232:SER:HB3	1:A:235:TYR:CD1	2.68	0.44
2:B:247:PHE:HE1	23:B:602:CLA:H101	1.82	0.44
27:C:515:BCR:H15C	27:C:515:BCR:H351	1.76	0.44
4:D:40:CYS:HB3	4:D:117:HIS:O	2.18	0.44
23:C:511:CLA:H93	23:C:511:CLA:H61	1.81	0.44
1:A:298:ASN:ND2	3:C:402:GLY:O	2.50	0.44
2:B:327:THR:HG22	23:B:611:CLA:H12	26.94	0.44
3:C:240:ILE:HD11	27:C:516:BCR:H372	1.99	0.44
3:C:456:GLU:HG2	3:C:457:LYS:HG3	1.99	0.44
23:C:501:CLA:C1D	23:C:503:CLA:H2	2.47	0.44
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.08	0.44
2:B:68:ARG:HH22	23:B:604:CLA:HED1	1.82	0.44
23:B:608:CLA:H161	23:B:608:CLA:H202	4.72	0.44
3:C:361:PHE:HD1	28:C:517:DGD:HE61	1.83	0.44
23:C:504:CLA:H121	28:C:518:DGD:HBE2	1.99	0.44
1:A:29:TYR:O	1:A:129:ARG:HD2	2.18	0.44
23:A:403:CLA:H202	23:A:404:CLA:H93	2.00	0.44
1:A:57:PRO:HA	1:A:68:SER:HA	2.00	0.44
2:B:148:LEU:HA	2:B:210:ILE:HD11	2.00	0.44
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.00	0.44
27:B:619:BCR:H341	27:B:619:BCR:H11C	1.84	0.44
23:C:510:CLA:H2	23:C:510:CLA:H61	1.73	0.44
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.18	0.44
13:O:81:GLU:HA	13:O:82:PRO:HD3	1.81	0.44
2:B:338:GLN:HB3	13:O:84:ASN:HB3	38.65	0.44
1:A:141:PRO:HB2	1:A:142:TRP:H	1.62	0.44
27:A:410:BCR:H15C	27:A:410:BCR:H351	1.80	0.44
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.99	0.44
23:B:606:CLA:H3A	23:B:606:CLA:HBA2	1.30	0.44
23:B:610:CLA:H3A	23:B:610:CLA:HBA2	2.62	0.44
2:B:462:PHE:CE1	23:B:613:CLA:HMB3	2.53	0.44
3:C:163:PHE:CG	23:C:512:CLA:HAB	2.54	0.44
23:D:403:CLA:H61	23:D:403:CLA:H41	1.89	0.44
6:F:17:THR:OG1	6:F:18:VAL:N	2.52	0.44
15:U:58:ASN:ND2	15:U:114:VAL:HG13	2.46	0.44
16:V:160:LYS:HA	16:V:163:TYR:CD2	2.53	0.44
2:B:333:GLY:O	2:B:439:SER:HB3	2.23	0.44
3:C:52:ALA:HA	23:C:511:CLA:HMB3	2.03	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:320:LEU:HD23	4:D:323:GLU:OE1	2.18	0.44
27:H:101:BCR:H371	27:H:101:BCR:H24C	1.81	0.44
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.51	0.43
2:B:134:ASP:OD2	2:B:137:LYS:HE3	2.18	0.43
2:B:174:LEU:HD23	2:B:308:LYS:HG2	1.99	0.43
2:B:135:LEU:HD22	2:B:237:VAL:HG21	2.09	0.43
8:I:6:ILE:O	8:I:10:ILE:HG12	2.30	0.43
1:A:150:PRO:HB2	23:A:404:CLA:H61	9.28	0.43
23:B:604:CLA:HBD	23:B:605:CLA:H43	2.00	0.43
3:C:265:ILE:HG12	23:C:505:CLA:HED1	2.00	0.43
3:C:386:PRO:O	3:C:390:ARG:HG2	2.26	0.43
27:C:514:BCR:H11C	27:C:514:BCR:H341	1.79	0.43
4:D:110:LEU:HA	4:D:110:LEU:HD23	1.90	0.43
4:D:285:GLY:O	4:D:289:LEU:HG	2.18	0.43
24:A:406:PHO:H161	4:D:48:TRP:CE2	2.53	0.43
9:J:33:TYR:HB3	27:J:102:BCR:H383	2.05	0.43
27:T:102:BCR:H341	27:T:102:BCR:H11C	1.79	0.43
1:A:238:LYS:O	1:A:241:GLN:HG3	2.18	0.43
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.07	0.43
3:C:318:LEU:HD13	3:C:351:PHE:HE1	1.87	0.43
3:C:38:GLY:HA3	23:C:511:CLA:HMD3	2.02	0.43
23:B:607:CLA:H202	4:D:281:MET:SD	2.57	0.43
5:E:81:GLU:O	5:E:83:LEU:N	2.46	0.43
10:K:12:PRO:HB2	10:K:15:TYR:CD2	2.52	0.43
10:K:43:VAL:CG2	10:K:46:ARG:HE	2.32	0.43
19:Z:5:PHE:CG	19:Z:61:VAL:HG21	2.53	0.43
31:A:414:LMG:H211	11:L:26:VAL:HG21	2.00	0.43
2:B:458:PHE:CG	23:B:604:CLA:HMC3	2.54	0.43
23:B:606:CLA:H41	23:B:606:CLA:H62	1.80	0.43
23:B:614:CLA:OBD	11:L:10:VAL:HG21	2.18	0.43
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.53	0.43
23:B:608:CLA:HAB	4:D:123:ILE:HG23	2.01	0.43
4:D:148:ALA:HB1	4:D:279:LEU:HB2	2.00	0.43
27:B:618:BCR:H381	14:T:4:ILE:HD13	25.19	0.43
23:B:602:CLA:H72	7:H:46:LEU:HD13	2.01	0.43
1:A:92:HIS:CD2	3:C:219:GLY:HA3	2.53	0.43
4:D:275:PRO:O	4:D:279:LEU:HD23	2.17	0.43
7:H:12:ARG:HD3	7:H:12:ARG:O	2.21	0.43
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.27	0.43
13:O:218:LEU:HD22	15:U:119:THR:HG21	2.01	0.43
23:A:405:CLA:H11	23:A:405:CLA:H51	4.37	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:A:417:SQD:HO8	2:B:113:TRP:HE1	62.90	0.43
2:B:247:PHE:HB2	23:B:612:CLA:HBC1	19.75	0.43
4:D:313:THR:OG1	4:D:316:THR:HG23	2.18	0.43
1:A:308:ASP:O	6:F:45:ARG:NE	2.66	0.43
23:A:403:CLA:H62	23:A:403:CLA:H102	1.80	0.43
23:A:407:CLA:HMC3	27:A:410:BCR:H12C	1.99	0.43
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.01	0.43
2:B:275:TRP:CH2	2:B:358:ARG:HD3	2.54	0.43
23:B:607:CLA:HBA2	23:B:607:CLA:C4A	2.48	0.43
2:B:326:ARG:NH2	4:D:297:ASP:OD2	2.52	0.43
7:H:19:GLY:O	7:H:21:VAL:HG13	2.20	0.43
27:J:102:BCR:H351	27:J:102:BCR:H15C	1.60	0.43
1:A:153:SER:CB	23:A:404:CLA:H11	11.39	0.43
23:B:607:CLA:H192	31:B:622:LMG:H342	2.01	0.43
3:C:137:PRO:HG3	23:C:513:CLA:HED2	2.00	0.43
3:C:277:GLY:C	23:C:505:CLA:HBC2	2.53	0.43
23:B:612:CLA:HAB	4:D:123:ILE:HG23	27.95	0.43
2:B:191:ASN:HD21	7:H:59:ASN:C	2.36	0.43
27:J:102:BCR:H24C	27:J:102:BCR:H371	1.87	0.43
27:B:618:BCR:C10	14:T:18:PHE:HB2	44.35	0.43
2:B:69:LEU:HD21	23:B:603:CLA:HED3	2.01	0.43
13:O:135:GLN:HB3	13:O:135:GLN:HE21	1.71	0.43
2:B:354:LEU:HB3	2:B:370:LEU:HB3	2.00	0.43
23:B:604:CLA:H11	23:B:605:CLA:H11	2.00	0.43
2:B:248:ALA:HA	23:B:607:CLA:H42	25.07	0.43
23:B:609:CLA:HMC2	27:H:101:BCR:H343	2.00	0.43
23:B:612:CLA:H18	23:B:613:CLA:H192	22.11	0.43
23:C:504:CLA:H202	28:C:519:DGD:HAF2	2.01	0.43
4:D:79:SER:HA	4:D:172:SER:HB3	2.01	0.43
4:D:53:THR:HG22	4:D:67:TYR:CD2	2.55	0.43
2:B:461:LEU:HA	2:B:461:LEU:HD23	1.90	0.42
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.88	0.42
1:A:309:ALA:HA	6:F:45:ARG:HB2	2.01	0.42
2:B:170:ASP:OD1	2:B:175:THR:N	2.53	0.42
2:B:206:GLY:O	2:B:210:ILE:HG13	2.19	0.42
2:B:483:ASP:CB	2:B:484:PRO:HD2	2.49	0.42
23:C:509:CLA:H112	23:C:509:CLA:H142	1.88	0.42
1:A:27:ARG:NH1	4:D:254:SER:O	2.53	0.42
5:E:22:ILE:O	5:E:26:THR:HG23	2.19	0.42
2:B:230:ARG:O	2:B:233:ASN:HB3	2.19	0.42
23:B:608:CLA:H51	23:B:609:CLA:H101	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:627:DGD:O1B	28:B:627:DGD:O2D	2.37	0.42
12:M:16:LEU:O	12:M:20:VAL:HG23	2.20	0.42
13:O:144:LEU:HD13	13:O:259:VAL:HG11	2.01	0.42
13:O:51:THR:O	13:O:53:ARG:N	2.53	0.42
27:T:101:BCR:H351	27:T:101:BCR:H15C	1.80	0.42
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.71	0.42
2:B:450:TRP:NE1	23:B:611:CLA:HBA1	29.68	0.42
23:B:612:CLA:H8	23:B:612:CLA:H122	1.87	0.42
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.04	0.42
13:O:168:PHE:HB2	13:O:225:LEU:HB2	2.02	0.42
1:A:224:ILE:O	4:D:265:ARG:NH2	2.54	0.42
1:A:119:PHE:HZ	23:A:404:CLA:H8	8.98	0.42
3:C:80:PRO:HB3	3:C:82:TYR:CE1	2.55	0.42
4:D:239:GLN:HB3	4:D:240:ALA:H	1.57	0.42
4:D:342:PRO:O	4:D:345:VAL:HG12	2.30	0.42
1:A:81:ALA:HB2	1:A:175:GLY:HA3	2.07	0.42
2:B:386:ALA:HB3	15:U:132:LEU:HD11	2.01	0.42
27:B:618:BCR:H11C	27:B:618:BCR:H341	1.69	0.42
31:C:520:LMG:H322	10:K:27:VAL:HG23	2.02	0.42
4:D:274:VAL:HA	25:D:404:PL9:H253	2.17	0.42
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.05	0.42
19:Z:33:TRP:O	19:Z:33:TRP:CD1	2.73	0.42
1:A:40:THR:HG21	1:A:121:LEU:HD23	2.01	0.42
2:B:18:ARG:NH1	2:B:115:TRP:O	2.43	0.42
2:B:280:PHE:O	2:B:284:ILE:HG13	2.19	0.42
2:B:483:ASP:OD2	2:B:484:PRO:HD2	2.20	0.42
23:B:605:CLA:H41	23:B:605:CLA:H62	1.75	0.42
3:C:72:LEU:HD11	3:C:108:THR:HB	2.10	0.42
3:C:174:LEU:HG	23:C:512:CLA:H92	2.02	0.42
27:C:514:BCR:H24C	27:C:514:BCR:H371	1.88	0.42
18:X:17:LYS:O	18:X:21:ILE:HG13	2.20	0.42
1:A:176:ILE:HD12	23:A:405:CLA:HED3	27.29	0.42
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.64	0.42
2:B:489:GLU:HB2	5:E:3:GLY:N	2.35	0.42
23:C:503:CLA:H161	23:C:503:CLA:H193	1.80	0.42
23:C:503:CLA:HMD2	23:C:503:CLA:H201	2.09	0.42
23:C:512:CLA:H61	23:C:512:CLA:H13	2.02	0.42
27:C:515:BCR:H20C	27:C:515:BCR:H361	1.93	0.42
3:C:418:ASN:HB2	28:C:519:DGD:O4E	2.20	0.42
4:D:180:ARG:HG3	4:D:181:PHE:N	2.34	0.42
4:D:201:VAL:O	4:D:205:LEU:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:MET:SD	1:A:179:THR:HG23	2.81	0.42
1:A:60:ILE:HD12	1:A:84:PRO:HD2	2.01	0.42
23:C:504:CLA:H2	28:C:518:DGD:HA22	2.01	0.42
4:D:62:GLY:HA3	5:E:63:ILE:HD13	2.05	0.42
10:K:24:VAL:O	10:K:27:VAL:HG12	2.20	0.42
18:X:11:THR:HG23	18:X:12:ILE:HG22	2.01	0.42
23:A:404:CLA:HHC	23:A:404:CLA:CBB	2.73	0.42
23:B:614:CLA:H51	23:B:614:CLA:H12	4.49	0.42
4:D:81:PRO:HG3	4:D:108:GLY:O	2.19	0.42
4:D:346:LEU:HD12	4:D:346:LEU:HA	1.85	0.42
4:D:67:TYR:CD1	31:D:406:LMG:HC72	2.67	0.42
28:D:409:DGD:O5E	28:D:409:DGD:O4E	2.31	0.42
2:B:7:ARG:NH2	31:B:622:LMG:HC3	2.35	0.41
3:C:457:LYS:HG2	4:D:229:ALA:HA	2.05	0.41
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.63	0.41
1:A:321:ILE:HG22	1:A:325:ASN:ND2	2.35	0.41
1:A:176:ILE:HD12	23:A:404:CLA:HED3	2.02	0.41
23:B:603:CLA:HBB2	23:B:603:CLA:H92	2.02	0.41
23:B:610:CLA:H12	23:B:610:CLA:H51	1.78	0.41
27:B:619:BCR:H351	27:B:619:BCR:H15C	1.81	0.41
23:C:504:CLA:H141	23:C:504:CLA:H161	1.90	0.41
3:C:86:LEU:HB3	3:C:90:PRO:HD3	2.10	0.41
4:D:122:LEU:HB3	4:D:150:ILE:CD1	2.50	0.41
13:O:33:TYR:O	13:O:37:VAL:HG23	2.26	0.41
3:C:215:LYS:HG2	3:C:221:GLU:HB3	2.12	0.41
3:C:264:PHE:HE1	23:C:507:CLA:HAB	1.86	0.41
23:C:506:CLA:HBB2	23:C:507:CLA:H52	2.08	0.41
23:C:513:CLA:HBA2	23:C:513:CLA:H3A	1.80	0.41
28:D:409:DGD:O2D	28:D:409:DGD:HG32	2.23	0.41
3:C:347:GLY:HA3	13:O:43:ASN:HB2	2.02	0.41
14:T:8:PHE:CD1	27:T:102:BCR:H373	2.55	0.41
14:T:3:THR:O	14:T:7:VAL:HG23	2.21	0.41
23:B:606:CLA:C3D	33:B:624:LMT:H11	2.50	0.41
23:B:614:CLA:H41	23:B:614:CLA:H62	3.58	0.41
23:B:616:CLA:H143	23:B:616:CLA:H111	1.83	0.41
31:B:623:LMG:H142	11:L:35:PHE:CE1	2.56	0.41
2:B:86:ILE:HG13	2:B:86:ILE:H	1.81	0.41
5:E:14:ILE:HG22	9:J:13:VAL:HG11	2.06	0.41
12:M:13:LEU:HD12	27:T:101:BCR:H333	12.28	0.41
16:V:147:VAL:O	16:V:150:LYS:HB2	2.22	0.41
2:B:247:PHE:HE1	23:B:606:CLA:H101	33.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:451:ALA:HA	3:C:456:GLU:CD	2.40	0.41
5:E:49:THR:HA	5:E:50:PRO:HD3	1.93	0.41
6:F:21:VAL:O	6:F:25:THR:HG23	2.20	0.41
7:H:35:MET:HB2	7:H:35:MET:HE3	1.89	0.41
27:T:101:BCR:H11C	27:T:101:BCR:H341	1.86	0.41
1:A:195:HIS:HA	1:A:196:PRO:HD3	1.94	0.41
2:B:272:ARG:HG3	2:B:273:TYR:N	2.41	0.41
2:B:298:LEU:HA	2:B:298:LEU:HD12	1.90	0.41
2:B:242:ILE:HG22	2:B:466:HIS:HB2	2.04	0.41
29:A:412:LHG:H382	23:C:510:CLA:H93	2.02	0.41
23:A:405:CLA:HMD3	4:D:182:LEU:HD11	2.02	0.41
5:E:10:PHE:CE1	34:F:101:HEM:HBD2	2.64	0.41
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.50	0.41
11:L:22:LEU:O	11:L:26:VAL:HG22	2.20	0.41
12:M:20:VAL:HG13	12:M:20:VAL:HG13	0.00	0.41
16:V:81:ARG:NE	16:V:157:GLY:HA3	2.47	0.41
1:A:307:ILE:HD11	6:F:45:ARG:NH2	2.51	0.41
30:A:413:SQD:H172	29:A:415:LHG:H172	2.03	0.41
2:B:153:PHE:O	2:B:157:HIS:HB3	2.20	0.41
2:B:63:LEU:N	2:B:64:PRO:HD2	2.35	0.41
3:C:186:TYR:CE2	3:C:188:THR:HG22	2.59	0.41
3:C:290:VAL:O	3:C:423:ARG:NH1	2.53	0.41
4:D:267:LEU:O	4:D:271:MET:HG3	2.20	0.41
1:A:22:THR:HG21	8:I:30:ARG:HD3	2.11	0.41
13:O:194:TYR:CE1	13:O:198:ILE:HD13	2.56	0.41
1:A:126:TYR:O	1:A:130:GLN:HG3	2.20	0.41
30:A:417:SQD:H311	30:A:417:SQD:H342	1.86	0.41
2:B:182:ALA:HA	2:B:183:PRO:HD3	1.93	0.41
2:B:30:VAL:HG12	23:B:609:CLA:HHD	31.13	0.41
23:B:603:CLA:HBB2	23:B:605:CLA:H152	2.03	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.52	0.41
3:C:318:LEU:HG	3:C:328:VAL:HG11	2.03	0.41
19:Z:5:PHE:HB2	19:Z:57:LEU:HG	2.12	0.41
23:B:604:CLA:H41	23:B:604:CLA:H61	1.91	0.41
14:T:29:ILE:O	14:T:31:LYS:N	2.54	0.41
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.36	0.41
1:A:180:PHE:O	1:A:184:ILE:HG13	2.23	0.41
2:B:10:THR:O	2:B:13:ILE:HG13	2.29	0.41
2:B:257:TRP:CD2	4:D:291:LEU:HD12	2.60	0.41
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.67	0.41
23:B:616:CLA:H8	23:B:616:CLA:H122	3.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:619:BCR:H24C	27:B:619:BCR:H371	1.89	0.41
31:B:623:LMG:HC3	33:M:102:LMT:O2'	2.21	0.41
2:B:87:ASP:HA	2:B:88:PRO:HD2	1.97	0.41
3:C:447:ARG:HH11	3:C:447:ARG:HG2	1.88	0.41
3:C:120:ILE:HD11	27:C:514:BCR:HC8	2.08	0.41
4:D:74:LEU:O	4:D:175:VAL:HB	2.20	0.41
5:E:42:LEU:O	5:E:46:VAL:HG23	2.28	0.41
5:E:8:ARG:HB2	6:F:13:TYR:HB3	2.02	0.41
20:Y:23:UNK:O	20:Y:24:UNK:C	2.68	0.41
2:B:192:PRO:HD2	7:H:60:VAL:HG12	2.09	0.41
2:B:91:TRP:CH2	23:B:606:CLA:H12	2.56	0.41
3:C:101:PRO:O	3:C:104:GLU:HB2	2.33	0.41
3:C:174:LEU:HD13	23:C:502:CLA:H111	2.07	0.41
1:A:296:ASN:HB3	3:C:401:LEU:HD13	2.03	0.41
27:C:515:BCR:H341	27:C:515:BCR:H11C	1.87	0.41
27:D:405:BCR:H11C	27:D:405:BCR:H341	1.75	0.41
4:D:84:SER:HB2	4:D:85:MET:HE2	2.04	0.41
18:X:12:ILE:O	18:X:12:ILE:HG23	2.23	0.41
1:A:271:LEU:HD11	25:A:408:PL9:C4	2.51	0.40
23:A:405:CLA:H62	23:A:405:CLA:H41	3.14	0.40
2:B:109:LEU:O	27:B:620:BCR:H21C	2.21	0.40
23:B:603:CLA:H3A	23:B:603:CLA:CGA	2.51	0.40
3:C:149:TYR:HA	3:C:156:LYS:HD3	2.02	0.40
3:C:406:SER:HA	3:C:420:VAL:HG23	2.02	0.40
23:C:510:CLA:OBD	10:K:33:LEU:HD23	2.39	0.40
1:A:258:LEU:O	4:D:128:ARG:NH1	2.55	0.40
20:G:23:UNK:O	20:G:24:UNK:C	2.68	0.40
23:B:604:CLA:H161	23:B:604:CLA:H202	1.79	0.40
23:B:605:CLA:H202	23:B:605:CLA:H162	1.96	0.40
3:C:107:ASP:O	3:C:110:PRO:HD2	2.27	0.40
23:C:501:CLA:H52	23:C:503:CLA:H92	2.05	0.40
27:C:515:BCR:H24C	27:C:515:BCR:H371	1.79	0.40
3:C:77:PRO:HG2	3:C:78:GLU:OE2	2.27	0.40
10:K:19:ASP:N	10:K:20:PRO:HD2	2.36	0.40
13:O:97:VAL:HG12	13:O:133:THR:O	2.21	0.40
1:A:177:SER:HA	1:A:180:PHE:CD2	2.56	0.40
23:B:607:CLA:H122	31:B:623:LMG:H412	2.03	0.40
23:B:608:CLA:H18	23:B:609:CLA:H192	2.03	0.40
3:C:307:PRO:HB3	3:C:358:PHE:HB3	2.04	0.40
28:C:517:DGD:HAW2	28:C:517:DGD:HA91	4.31	0.40
10:K:43:VAL:HG22	10:K:46:ARG:HE	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:9:ILE:O	14:T:13:ILE:HG13	2.27	0.40
16:V:68:VAL:O	16:V:71:ILE:HG12	2.20	0.40
1:A:182:PHE:O	1:A:186:PHE:HB2	2.22	0.40
2:B:16:PRO:HB2	2:B:123:PHE:CG	2.56	0.40
23:B:607:CLA:HBB1	31:B:623:LMG:H341	2.03	0.40
3:C:416:SER:OG	3:C:417:VAL:N	2.54	0.40
16:V:60:GLN:HA	16:V:64:ALA:HB2	2.02	0.40
1:A:238:LYS:HA	1:A:238:LYS:HD3	1.88	0.40
1:A:42:LEU:HA	1:A:45:THR:HG22	2.03	0.40
2:B:16:PRO:HG2	2:B:123:PHE:HB3	2.04	0.40
23:B:607:CLA:H92	23:B:607:CLA:HBB2	11.47	0.40
23:B:609:CLA:H161	23:B:609:CLA:H141	4.20	0.40
23:C:511:CLA:H42	10:K:39:TRP:CD1	2.56	0.40
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.04	0.40
11:L:7:ARG:HG3	11:L:7:ARG:H	1.73	0.40
15:U:73:PRO:HG2	16:V:107:THR:HB	2.07	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	333/360 (92%)	311 (93%)	17 (5%)	5 (2%)	12	53
1	a	333/360 (92%)	312 (94%)	17 (5%)	4 (1%)	15	57
2	B	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	18	61
2	b	488/510 (96%)	447 (92%)	36 (7%)	5 (1%)	18	61
3	C	445/461 (96%)	406 (91%)	33 (7%)	6 (1%)	14	56
3	c	445/461 (96%)	407 (92%)	32 (7%)	6 (1%)	14	56
4	D	338/352 (96%)	316 (94%)	20 (6%)	2 (1%)	28	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	338/352 (96%)	315 (93%)	21 (6%)	2 (1%)	28	71
5	E	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	14	56
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	14	56
6	F	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
6	f	33/45 (73%)	30 (91%)	3 (9%)	0	100	100
7	H	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	27
7	h	63/66 (96%)	54 (86%)	6 (10%)	3 (5%)	2	27
8	I	33/38 (87%)	27 (82%)	4 (12%)	2 (6%)	2	22
8	i	33/38 (87%)	28 (85%)	4 (12%)	1 (3%)	5	37
9	J	32/40 (80%)	28 (88%)	3 (9%)	1 (3%)	5	36
9	j	32/40 (80%)	28 (88%)	2 (6%)	2 (6%)	1	22
10	K	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	24
10	k	35/46 (76%)	32 (91%)	1 (3%)	2 (6%)	2	24
11	L	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	l	35/37 (95%)	34 (97%)	1 (3%)	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%)	206 (86%)	31 (13%)	4 (2%)	11	50
13	o	241/272 (89%)	208 (86%)	29 (12%)	4 (2%)	11	50
14	T	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	35
14	t	30/32 (94%)	27 (90%)	2 (7%)	1 (3%)	4	35
15	U	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	36
15	u	95/134 (71%)	87 (92%)	5 (5%)	3 (3%)	5	36
16	V	135/163 (83%)	124 (92%)	11 (8%)	0	100	100
16	v	135/163 (83%)	125 (93%)	10 (7%)	0	100	100
17	g	26/46 (56%)	20 (77%)	5 (19%)	1 (4%)	4	32
17	y	26/46 (56%)	19 (73%)	6 (23%)	1 (4%)	4	32
18	X	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	24
18	x	35/41 (85%)	30 (86%)	3 (9%)	2 (6%)	2	24
19	Z	60/62 (97%)	54 (90%)	5 (8%)	1 (2%)	11	50
19	z	60/62 (97%)	54 (90%)	3 (5%)	3 (5%)	2	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5138/5650 (91%)	4681 (91%)	378 (7%)	79 (2%)	12	53

All (79) 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
14	T	30	THR
18	X	45	LYS
1	a	12	ASN
1	a	142	TRP
2	b	484	PRO
2	b	488	PRO
7	h	18	TYR
13	o	52	ALA
14	t	30	THR
18	x	45	LYS
1	A	141	PRO
2	B	489	GLU
3	C	32	GLY
3	C	144	SER
3	C	257	PHE
3	C	416	SER
4	D	239	GLN
7	H	26	GLY
17	y	43	ARG
19	Z	32	ASP
1	a	141	PRO
2	b	489	GLU
3	c	32	GLY
3	c	144	SER
3	c	257	PHE
3	c	416	SER
4	d	239	GLN
5	e	82	GLN
7	h	26	GLY
9	j	38	SER
17	g	43	ARG
19	z	32	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	TRP
3	C	194	GLY
5	E	82	GLN
9	J	38	SER
13	O	88	GLU
15	U	83	ALA
1	a	334	ARG
3	c	194	GLY
13	o	88	GLU
13	o	271	PRO
15	u	72	TYR
1	A	334	ARG
4	D	262	SER
13	O	271	PRO
15	U	72	TYR
4	d	262	SER
7	h	16	SER
8	i	25	SER
10	k	45	PHE
13	o	158	ASN
15	u	83	ALA
2	B	176	GLY
2	B	230	ARG
7	H	16	SER
10	K	13	GLU
10	K	45	PHE
15	U	73	PRO
2	b	176	GLY
10	k	13	GLU
18	x	12	ILE
8	I	25	SER
13	O	158	ASN
18	X	12	ILE
2	b	230	ARG
19	z	28	ALA
15	u	73	PRO
8	I	32	PRO
3	C	209	ILE
1	A	176	ILE
3	c	209	ILE
19	z	24	PRO
9	j	35	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	271/291 (93%)	266 (98%)	5 (2%)	64	84
1	a	271/291 (93%)	266 (98%)	5 (2%)	64	84
2	B	390/407 (96%)	380 (97%)	10 (3%)	51	75
2	b	390/407 (96%)	379 (97%)	11 (3%)	49	74
3	C	347/362 (96%)	333 (96%)	14 (4%)	36	65
3	c	347/362 (96%)	332 (96%)	15 (4%)	33	64
4	D	275/283 (97%)	260 (94%)	15 (6%)	25	58
4	d	275/283 (97%)	262 (95%)	13 (5%)	30	62
5	E	72/73 (99%)	68 (94%)	4 (6%)	25	57
5	e	72/73 (99%)	68 (94%)	4 (6%)	25	57
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%)	16	48
7	h	53/55 (96%)	50 (94%)	3 (6%)	24	57
8	I	32/35 (91%)	31 (97%)	1 (3%)	45	71
8	i	32/35 (91%)	31 (97%)	1 (3%)	45	71
9	J	24/28 (86%)	23 (96%)	1 (4%)	34	64
9	j	24/28 (86%)	23 (96%)	1 (4%)	34	64
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%)	48	73
11	l	35/35 (100%)	34 (97%)	1 (3%)	48	73
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%)	80	90
13	o	202/228 (89%)	200 (99%)	2 (1%)	80	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	T	29/29 (100%)	28 (97%)	1 (3%)	42	70
14	t	29/29 (100%)	28 (97%)	1 (3%)	42	70
15	U	84/112 (75%)	83 (99%)	1 (1%)	75	88
15	u	84/112 (75%)	82 (98%)	2 (2%)	54	78
16	V	116/138 (84%)	114 (98%)	2 (2%)	66	84
16	v	116/138 (84%)	114 (98%)	2 (2%)	66	84
17	g	20/37 (54%)	18 (90%)	2 (10%)	9	34
17	y	20/37 (54%)	18 (90%)	2 (10%)	9	34
18	X	30/34 (88%)	27 (90%)	3 (10%)	9	34
18	x	30/34 (88%)	27 (90%)	3 (10%)	9	34
19	Z	52/52 (100%)	49 (94%)	3 (6%)	23	56
19	z	52/52 (100%)	50 (96%)	2 (4%)	38	67
All	All	4244/4616 (92%)	4107 (97%)	137 (3%)	44	71

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	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	223	GLN
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	232	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	244	CYS
3	C	254	THR
3	C	289	PHE
3	C	305	THR
3	C	355	THR
3	C	382	ASN
3	C	391	ARG
3	C	472	LEU
4	D	20	ASP
4	D	43	LEU
4	D	84	SER
4	D	91	LEU
4	D	180	ARG
4	D	201	VAL
4	D	205	LEU
4	D	241	GLU
4	D	259	ILE
4	D	279	LEU
4	D	291	LEU
4	D	294	ARG
4	D	323	GLU
4	D	345	VAL
4	D	346	LEU
5	E	18	ARG
5	E	77	GLU
5	E	82	GLN
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
16	V	63	CYS
16	V	122	ARG
17	y	28	ILE
17	y	46	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	X	11	THR
18	X	12	ILE
18	X	45	LYS
19	Z	14	ILE
19	Z	33	TRP
19	Z	62	VAL
1	a	202	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	223	GLN
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	488	PRO
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	232	ASP
3	c	244	CYS
3	c	254	THR
3	c	289	PHE
3	c	305	THR
3	c	355	THR
3	c	382	ASN
3	c	391	ARG
3	c	469	MET
3	c	472	LEU
4	d	20	ASP
4	d	43	LEU
4	d	84	SER
4	d	130	PHE
4	d	180	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	d	241	GLU
4	d	259	ILE
4	d	279	LEU
4	d	291	LEU
4	d	294	ARG
4	d	323	GLU
4	d	345	VAL
4	d	346	LEU
5	e	18	ARG
5	e	77	GLU
5	e	82	GLN
5	e	84	LYS
7	h	27	THR
7	h	49	TYR
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	103	GLN
15	u	132	LEU
16	v	63	CYS
16	v	122	ARG
17	g	28	ILE
17	g	46	LEU
18	x	11	THR
18	x	12	ILE
18	x	45	LYS
19	z	33	TRP
19	z	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	303	ASN
4	D	117	HIS
17	y	45	ASN
1	a	241	GLN
2	b	201	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	u	93	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	BCT	A	402	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	A	403	-	56,73,73	1.13	4 (7%)	65,113,113	1.24	9 (13%)
23	CLA	A	404	-	56,73,73	1.09	4 (7%)	65,113,113	1.33	9 (13%)
23	CLA	A	405	-	56,73,73	1.07	4 (7%)	65,113,113	1.31	10 (15%)
24	PHO	A	406	-	67,69,69	1.26	9 (13%)	87,99,99	1.10	8 (9%)
23	CLA	A	407	-	56,73,73	1.09	4 (7%)	65,113,113	1.23	8 (12%)
25	PL9	A	408	-	45,45,55	1.24	7 (15%)	57,57,69	1.53	14 (24%)
26	OEC	A	409	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	A	410	-	41,41,41	0.72	0	56,56,56	1.88	11 (19%)
28	DGD	A	411	-	57,57,67	1.23	7 (12%)	71,71,81	1.60	12 (16%)
29	LHG	A	412	-	38,38,48	1.03	2 (5%)	39,44,54	1.02	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	SQD	A	413	-	50,51,54	0.98	5 (10%)	60,62,65	1.75	10 (16%)
31	LMG	A	414	-	51,51,55	1.15	6 (11%)	59,59,63	1.37	5 (8%)
29	LHG	A	415	-	36,36,48	1.06	2 (5%)	37,42,54	1.14	3 (8%)
30	SQD	A	417	-	53,54,54	1.00	5 (9%)	63,65,65	1.92	13 (20%)
31	LMG	A	418	-	42,42,55	1.22	6 (14%)	50,50,63	1.53	9 (18%)
23	CLA	B	601	-	56,73,73	1.13	5 (8%)	65,113,113	1.25	8 (12%)
23	CLA	B	602	-	56,73,73	1.10	4 (7%)	65,113,113	1.21	7 (10%)
23	CLA	B	603	-	56,73,73	1.12	4 (7%)	65,113,113	1.26	8 (12%)
23	CLA	B	604	-	56,73,73	1.14	4 (7%)	65,113,113	1.22	10 (15%)
23	CLA	B	605	-	56,73,73	1.11	4 (7%)	65,113,113	1.27	9 (13%)
23	CLA	B	606	-	56,73,73	1.09	4 (7%)	65,113,113	1.24	8 (12%)
23	CLA	B	607	-	56,73,73	1.08	4 (7%)	65,113,113	1.33	9 (13%)
23	CLA	B	608	-	56,73,73	1.11	4 (7%)	65,113,113	1.23	8 (12%)
23	CLA	B	609	-	56,73,73	1.10	4 (7%)	65,113,113	1.26	7 (10%)
23	CLA	B	610	-	56,73,73	1.11	5 (8%)	65,113,113	1.28	9 (13%)
23	CLA	B	611	-	56,73,73	1.10	4 (7%)	65,113,113	1.28	9 (13%)
23	CLA	B	612	-	56,73,73	1.11	4 (7%)	65,113,113	1.26	8 (12%)
23	CLA	B	613	-	56,73,73	1.08	4 (7%)	65,113,113	1.18	8 (12%)
23	CLA	B	614	-	56,73,73	1.12	4 (7%)	65,113,113	1.18	6 (9%)
23	CLA	B	615	-	56,73,73	1.12	4 (7%)	65,113,113	1.21	8 (12%)
23	CLA	B	616	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	8 (12%)
27	BCR	B	617	-	41,41,41	0.69	0	56,56,56	1.85	14 (25%)
27	BCR	B	618	-	41,41,41	0.66	0	56,56,56	2.27	20 (35%)
27	BCR	B	619	-	41,41,41	0.66	0	56,56,56	1.86	16 (28%)
27	BCR	B	620	-	41,41,41	0.72	0	56,56,56	2.14	15 (26%)
28	DGD	B	621	-	59,59,67	1.22	9 (15%)	73,73,81	1.14	5 (6%)
31	LMG	B	622	-	49,49,55	1.14	7 (14%)	57,57,63	1.31	6 (10%)
31	LMG	B	623	-	49,49,55	1.19	8 (16%)	57,57,63	1.40	9 (15%)
33	LMT	B	624	-	36,36,36	0.42	0	47,47,47	0.71	0
33	LMT	B	625	-	36,36,36	0.40	0	47,47,47	0.74	1 (2%)
30	SQD	B	626	-	46,47,54	1.03	5 (10%)	56,58,65	1.77	10 (17%)
28	DGD	B	627	-	53,53,67	1.22	6 (11%)	67,67,81	1.45	10 (14%)
33	LMT	B	628	-	36,36,36	0.45	0	47,47,47	0.82	1 (2%)
33	LMT	B	629	-	36,36,36	0.46	0	47,47,47	0.68	1 (2%)
23	CLA	C	501	-	56,73,73	1.12	4 (7%)	65,113,113	1.21	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	502	-	56,73,73	1.13	4 (7%)	65,113,113	1.24	8 (12%)
23	CLA	C	503	-	56,73,73	1.08	4 (7%)	65,113,113	1.26	8 (12%)
23	CLA	C	504	-	56,73,73	1.10	5 (8%)	65,113,113	1.25	9 (13%)
23	CLA	C	505	-	56,73,73	1.13	5 (8%)	65,113,113	1.23	9 (13%)
23	CLA	C	506	-	56,73,73	1.10	4 (7%)	65,113,113	1.31	8 (12%)
23	CLA	C	507	-	56,73,73	1.08	4 (7%)	65,113,113	1.30	8 (12%)
23	CLA	C	508	-	56,73,73	1.11	4 (7%)	65,113,113	1.26	9 (13%)
23	CLA	C	509	-	56,73,73	1.10	5 (8%)	65,113,113	1.21	10 (15%)
23	CLA	C	510	-	56,73,73	1.14	4 (7%)	65,113,113	1.24	8 (12%)
23	CLA	C	511	3	56,73,73	1.15	5 (8%)	65,113,113	1.28	9 (13%)
23	CLA	C	512	-	56,73,73	1.11	4 (7%)	65,113,113	1.29	8 (12%)
23	CLA	C	513	-	56,73,73	1.12	4 (7%)	65,113,113	1.25	10 (15%)
27	BCR	C	514	-	41,41,41	0.72	0	56,56,56	2.34	20 (35%)
27	BCR	C	515	-	41,41,41	0.66	0	56,56,56	1.90	16 (28%)
27	BCR	C	516	-	41,41,41	0.68	0	56,56,56	1.95	16 (28%)
28	DGD	C	517	-	54,54,67	1.21	6 (11%)	68,68,81	1.28	7 (10%)
28	DGD	C	518	-	63,63,67	1.22	10 (15%)	77,77,81	1.32	7 (9%)
28	DGD	C	519	-	67,67,67	1.12	6 (8%)	81,81,81	1.44	10 (12%)
31	LMG	C	520	-	48,48,55	1.13	6 (12%)	56,56,63	1.33	6 (10%)
31	LMG	C	521	-	45,45,55	1.19	8 (17%)	53,53,63	1.39	9 (16%)
23	CLA	D	401	-	56,73,73	1.09	4 (7%)	65,113,113	1.28	9 (13%)
24	PHO	D	402	-	67,69,69	1.21	9 (13%)	87,99,99	1.06	8 (9%)
23	CLA	D	403	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	8 (12%)
25	PL9	D	404	-	55,55,55	1.20	8 (14%)	69,69,69	1.58	16 (23%)
27	BCR	D	405	-	41,41,41	0.66	0	56,56,56	2.19	17 (30%)
31	LMG	D	406	-	46,46,55	1.17	7 (15%)	54,54,63	1.41	6 (11%)
31	LMG	D	407	-	48,48,55	1.18	8 (16%)	56,56,63	1.44	8 (14%)
30	SQD	D	408	-	42,43,54	1.11	5 (11%)	52,54,65	2.15	10 (19%)
28	DGD	D	409	-	64,64,67	1.14	6 (9%)	78,78,81	1.44	11 (14%)
33	LMT	D	410	-	32,32,36	0.50	1 (3%)	43,43,47	0.72	1 (2%)
31	LMG	E	101	-	44,44,55	1.19	7 (15%)	52,52,63	1.34	8 (15%)
34	HEM	F	101	5,6	28,50,50	2.25	6 (21%)	17,82,82	1.44	2 (11%)
30	SQD	F	102	-	44,45,54	1.04	5 (11%)	54,56,65	1.89	10 (18%)
27	BCR	H	101	-	41,41,41	0.70	0	56,56,56	1.74	16 (28%)
31	LMG	I	101	-	43,43,55	1.25	8 (18%)	51,51,63	1.33	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LMT	I	102	-	36,36,36	0.42	0	47,47,47	0.69	1 (2%)
25	PL9	J	101	-	35,35,55	1.16	5 (14%)	45,45,69	1.51	7 (15%)
27	BCR	J	102	-	41,41,41	0.72	0	56,56,56	3.37	26 (46%)
31	LMG	M	101	-	42,42,55	1.28	7 (16%)	50,50,63	1.55	8 (16%)
33	LMT	M	102	-	36,36,36	0.44	0	47,47,47	0.71	1 (2%)
27	BCR	T	101	-	41,41,41	0.68	0	56,56,56	1.78	13 (23%)
27	BCR	T	102	-	41,41,41	0.69	0	56,56,56	2.25	16 (28%)
34	HEM	V	201	16	28,50,50	2.30	7 (25%)	17,82,82	1.30	1 (5%)
30	SQD	a	401	-	53,54,54	0.99	5 (9%)	63,65,65	1.89	13 (20%)
31	LMG	a	402	-	42,42,55	1.23	6 (14%)	50,50,63	1.54	7 (14%)
23	CLA	a	404	-	56,73,73	1.12	4 (7%)	65,113,113	1.28	9 (13%)
23	CLA	a	405	-	56,73,73	1.07	4 (7%)	65,113,113	1.37	10 (15%)
23	CLA	a	406	-	56,73,73	1.10	4 (7%)	65,113,113	1.34	9 (13%)
24	PHO	a	407	-	67,69,69	1.22	9 (13%)	87,99,99	1.06	8 (9%)
24	PHO	a	408	-	67,69,69	1.24	8 (11%)	87,99,99	1.06	4 (4%)
23	CLA	a	409	-	56,73,73	1.10	4 (7%)	65,113,113	1.25	8 (12%)
25	PL9	a	410	-	45,45,55	1.20	7 (15%)	57,57,69	1.59	12 (21%)
26	OEC	a	411	1,3	0,0,13	0.00	-	0,0,27	0.00	-
27	BCR	a	412	-	41,41,41	0.72	0	56,56,56	1.90	12 (21%)
28	DGD	a	413	-	57,57,67	1.19	7 (12%)	71,71,81	1.53	12 (16%)
29	LHG	a	414	-	38,38,48	1.05	2 (5%)	39,44,54	1.05	4 (10%)
30	SQD	a	415	-	50,51,54	0.97	4 (8%)	60,62,65	1.78	12 (20%)
31	LMG	a	416	-	51,51,55	1.11	6 (11%)	59,59,63	1.41	6 (10%)
29	LHG	a	417	-	36,36,48	1.07	2 (5%)	37,42,54	1.07	2 (5%)
30	SQD	b	601	-	46,47,54	1.02	5 (10%)	56,58,65	1.84	10 (17%)
28	DGD	b	602	-	53,53,67	1.23	6 (11%)	67,67,81	1.39	10 (14%)
33	LMT	b	603	-	36,36,36	0.44	0	47,47,47	0.79	1 (2%)
33	LMT	b	604	-	36,36,36	0.40	0	47,47,47	0.66	1 (2%)
23	CLA	b	605	-	56,73,73	1.12	4 (7%)	65,113,113	1.30	10 (15%)
23	CLA	b	606	-	56,73,73	1.09	4 (7%)	65,113,113	1.30	8 (12%)
23	CLA	b	607	-	56,73,73	1.08	4 (7%)	65,113,113	1.29	9 (13%)
23	CLA	b	608	-	56,73,73	1.13	4 (7%)	65,113,113	1.22	10 (15%)
23	CLA	b	609	-	56,73,73	1.11	4 (7%)	65,113,113	1.20	8 (12%)
23	CLA	b	610	-	56,73,73	1.13	4 (7%)	65,113,113	1.24	9 (13%)
23	CLA	b	611	-	56,73,73	1.11	4 (7%)	65,113,113	1.18	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	612	-	56,73,73	1.10	4 (7%)	65,113,113	1.30	10 (15%)
23	CLA	b	613	-	56,73,73	1.10	4 (7%)	65,113,113	1.22	9 (13%)
23	CLA	b	614	-	56,73,73	1.07	4 (7%)	65,113,113	1.29	7 (10%)
23	CLA	b	615	-	56,73,73	1.14	4 (7%)	65,113,113	1.27	9 (13%)
23	CLA	b	616	-	56,73,73	1.08	4 (7%)	65,113,113	1.29	8 (12%)
23	CLA	b	617	-	56,73,73	1.10	4 (7%)	65,113,113	1.33	9 (13%)
23	CLA	b	618	-	56,73,73	1.15	4 (7%)	65,113,113	1.19	6 (9%)
23	CLA	b	619	-	56,73,73	1.09	4 (7%)	65,113,113	1.27	8 (12%)
23	CLA	b	620	-	56,73,73	1.17	6 (10%)	65,113,113	1.16	9 (13%)
27	BCR	b	621	-	41,41,41	0.64	0	56,56,56	1.96	19 (33%)
27	BCR	b	622	-	41,41,41	0.71	0	56,56,56	2.21	17 (30%)
28	DGD	b	623	-	59,59,67	1.20	9 (15%)	73,73,81	1.17	5 (6%)
31	LMG	b	624	-	49,49,55	1.17	7 (14%)	57,57,63	1.32	7 (12%)
31	LMG	b	625	-	49,49,55	1.18	8 (16%)	57,57,63	1.43	10 (17%)
33	LMT	b	626	-	36,36,36	0.39	0	47,47,47	0.76	1 (2%)
33	LMT	b	627	-	36,36,36	0.43	0	47,47,47	0.69	0
23	CLA	c	501	-	56,73,73	1.11	4 (7%)	65,113,113	1.28	10 (15%)
23	CLA	c	502	-	56,73,73	1.12	4 (7%)	65,113,113	1.27	9 (13%)
23	CLA	c	503	-	56,73,73	1.10	4 (7%)	65,113,113	1.20	8 (12%)
23	CLA	c	504	-	56,73,73	1.08	4 (7%)	65,113,113	1.30	8 (12%)
23	CLA	c	505	-	56,73,73	1.12	4 (7%)	65,113,113	1.26	9 (13%)
23	CLA	c	506	-	56,73,73	1.09	4 (7%)	65,113,113	1.36	9 (13%)
23	CLA	c	507	-	56,73,73	1.11	4 (7%)	65,113,113	1.27	10 (15%)
23	CLA	c	508	-	56,73,73	1.10	4 (7%)	65,113,113	1.33	9 (13%)
23	CLA	c	509	-	56,73,73	1.14	4 (7%)	65,113,113	1.19	8 (12%)
23	CLA	c	510	-	56,73,73	1.09	4 (7%)	65,113,113	1.22	7 (10%)
23	CLA	c	511	-	56,73,73	1.17	4 (7%)	65,113,113	1.21	8 (12%)
23	CLA	c	512	-	56,73,73	1.09	4 (7%)	65,113,113	1.29	9 (13%)
23	CLA	c	513	-	56,73,73	1.11	4 (7%)	65,113,113	1.25	9 (13%)
27	BCR	c	514	-	41,41,41	0.69	0	56,56,56	2.38	19 (33%)
27	BCR	c	515	-	41,41,41	0.68	0	56,56,56	1.99	16 (28%)
28	DGD	c	516	-	54,54,67	1.23	6 (11%)	68,68,81	1.29	7 (10%)
28	DGD	c	517	-	63,63,67	1.21	10 (15%)	77,77,81	1.35	7 (9%)
28	DGD	c	518	-	67,67,67	1.11	6 (8%)	81,81,81	1.48	13 (16%)
31	LMG	c	519	-	45,45,55	1.21	8 (17%)	53,53,63	1.35	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCT	d	401	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	d	402	-	56,73,73	1.12	4 (7%)	65,113,113	1.29	9 (13%)
23	CLA	d	403	-	56,73,73	1.14	4 (7%)	65,113,113	1.21	9 (13%)
25	PL9	d	404	-	55,55,55	1.19	8 (14%)	69,69,69	1.66	17 (24%)
27	BCR	d	405	-	41,41,41	0.66	0	56,56,56	2.16	16 (28%)
31	LMG	d	406	-	46,46,55	1.18	7 (15%)	54,54,63	1.35	6 (11%)
31	LMG	d	407	-	48,48,55	1.17	8 (16%)	56,56,63	1.50	8 (14%)
30	SQD	d	408	-	42,43,54	1.12	5 (11%)	52,54,65	2.14	10 (19%)
28	DGD	d	409	-	64,64,67	1.14	5 (7%)	78,78,81	1.45	11 (14%)
33	LMT	d	410	-	32,32,36	0.49	0	43,43,47	0.72	1 (2%)
31	LMG	e	101	-	44,44,55	1.21	8 (18%)	52,52,63	1.36	9 (17%)
34	HEM	f	101	5,6	28,50,50	2.24	6 (21%)	17,82,82	1.50	3 (17%)
30	SQD	f	102	-	44,45,54	1.02	5 (11%)	54,56,65	1.88	10 (18%)
27	BCR	h	101	-	41,41,41	0.72	0	56,56,56	1.75	14 (25%)
31	LMG	i	101	-	43,43,55	1.26	7 (16%)	51,51,63	1.32	6 (11%)
33	LMT	i	102	-	36,36,36	0.48	1 (2%)	47,47,47	0.69	1 (2%)
25	PL9	j	101	-	35,35,55	1.15	5 (14%)	45,45,69	1.50	8 (17%)
27	BCR	j	102	-	41,41,41	0.70	0	56,56,56	3.35	25 (44%)
27	BCR	k	102	-	41,41,41	0.72	0	56,56,56	1.96	15 (26%)
31	LMG	k	103	-	48,48,55	1.13	6 (12%)	56,56,63	1.29	7 (12%)
33	LMT	m	101	-	36,36,36	0.42	0	47,47,47	0.69	0
31	LMG	m	102	-	42,42,55	1.33	7 (16%)	50,50,63	1.62	8 (16%)
34	HEM	v	201	16	28,50,50	2.31	7 (25%)	17,82,82	1.27	1 (5%)
27	BCR	y	101	-	41,41,41	0.71	0	56,56,56	1.94	15 (26%)
27	BCR	z	101	-	41,41,41	0.64	0	56,56,56	1.83	15 (26%)

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	BCT	A	402	21	-	0/0/0/0	0/0/0/0
23	CLA	A	403	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	A	405	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	A	406	-	-	0/53/103/103	0/1/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	407	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	A	408	-	-	0/41/61/73	0/1/1/1
26	OEC	A	409	1,3	-	0/0/0/54	0/0/0/5
27	BCR	A	410	-	-	0/29/63/63	0/2/2/2
28	DGD	A	411	-	-	0/45/85/95	0/2/2/2
29	LHG	A	412	-	-	0/43/43/53	0/0/0/0
30	SQD	A	413	-	-	0/46/66/69	0/1/1/1
31	LMG	A	414	-	-	0/46/66/70	0/1/1/1
29	LHG	A	415	-	-	0/41/41/53	0/0/0/0
30	SQD	A	417	-	-	0/49/69/69	0/1/1/1
31	LMG	A	418	-	-	0/37/57/70	0/1/1/1
23	CLA	B	601	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	602	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	B	617	-	-	0/29/63/63	0/2/2/2
27	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	BCR	B	620	-	-	0/29/63/63	0/2/2/2
28	DGD	B	621	-	-	0/47/87/95	0/2/2/2
31	LMG	B	622	-	-	0/44/64/70	0/1/1/1
31	LMG	B	623	-	-	0/44/64/70	0/1/1/1
33	LMT	B	624	-	-	0/21/61/61	0/2/2/2
33	LMT	B	625	-	-	0/21/61/61	0/2/2/2
30	SQD	B	626	-	-	0/42/62/69	0/1/1/1
28	DGD	B	627	-	-	0/41/81/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	B	628	-	-	0/21/61/61	0/2/2/2
33	LMT	B	629	-	-	0/21/61/61	0/2/2/2
23	CLA	C	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	C	514	-	-	0/29/63/63	0/2/2/2
27	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	BCR	C	516	-	-	0/29/63/63	0/2/2/2
28	DGD	C	517	-	-	0/42/82/95	0/2/2/2
28	DGD	C	518	-	-	2/51/91/95	0/2/2/2
28	DGD	C	519	-	-	0/55/95/95	0/2/2/2
31	LMG	C	520	-	-	0/43/63/70	0/1/1/1
31	LMG	C	521	-	-	0/40/60/70	0/1/1/1
23	CLA	D	401	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
23	CLA	D	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	D	404	-	-	0/53/73/73	0/1/1/1
27	BCR	D	405	-	-	0/29/63/63	0/2/2/2
31	LMG	D	406	-	-	0/41/61/70	0/1/1/1
31	LMG	D	407	-	-	0/43/63/70	0/1/1/1
30	SQD	D	408	-	-	2/38/58/69	0/1/1/1
28	DGD	D	409	-	-	1/52/92/95	0/2/2/2
33	LMT	D	410	-	-	0/17/57/61	0/2/2/2
31	LMG	E	101	-	-	0/39/59/70	0/1/1/1
34	HEM	F	101	5,6	-	0/6/54/54	0/0/8/8
30	SQD	F	102	-	-	0/40/60/69	0/1/1/1
27	BCR	H	101	-	-	0/29/63/63	0/2/2/2
31	LMG	I	101	-	-	0/38/58/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMT	I	102	-	-	0/21/61/61	0/2/2/2
25	PL9	J	101	-	-	0/29/49/73	0/1/1/1
27	BCR	J	102	-	-	0/29/63/63	0/2/2/2
31	LMG	M	101	-	-	1/37/57/70	0/1/1/1
33	LMT	M	102	-	-	0/21/61/61	0/2/2/2
27	BCR	T	101	-	-	0/29/63/63	0/2/2/2
27	BCR	T	102	-	-	0/29/63/63	0/2/2/2
34	HEM	V	201	16	-	0/6/54/54	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
23	CLA	a	404	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	405	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
24	PHO	a	407	-	-	0/53/103/103	0/1/6/6
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6
23	CLA	a	409	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	a	410	-	-	0/41/61/73	0/1/1/1
26	OEC	a	411	1,3	-	0/0/0/54	0/0/0/5
27	BCR	a	412	-	-	0/29/63/63	0/2/2/2
28	DGD	a	413	-	-	0/45/85/95	0/2/2/2
29	LHG	a	414	-	-	0/43/43/53	0/0/0/0
30	SQD	a	415	-	-	0/46/66/69	0/1/1/1
31	LMG	a	416	-	-	0/46/66/70	0/1/1/1
29	LHG	a	417	-	-	0/41/41/53	0/0/0/0
30	SQD	b	601	-	-	0/42/62/69	0/1/1/1
28	DGD	b	602	-	-	0/41/81/95	0/2/2/2
33	LMT	b	603	-	-	0/21/61/61	0/2/2/2
33	LMT	b	604	-	-	0/21/61/61	0/2/2/2
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	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
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	618	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	619	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	620	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	b	621	-	-	0/29/63/63	0/2/2/2
27	BCR	b	622	-	-	0/29/63/63	0/2/2/2
28	DGD	b	623	-	-	0/47/87/95	0/2/2/2
31	LMG	b	624	-	-	0/44/64/70	0/1/1/1
31	LMG	b	625	-	-	0/44/64/70	0/1/1/1
33	LMT	b	626	-	-	0/21/61/61	0/2/2/2
33	LMT	b	627	-	-	0/21/61/61	0/2/2/2
23	CLA	c	501	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	503	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	504	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	505	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	506	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	508	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	511	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	512	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	513	-	3/3/20/25	0/37/135/135	0/0/9/9
27	BCR	c	514	-	-	0/29/63/63	0/2/2/2
27	BCR	c	515	-	-	0/29/63/63	0/2/2/2
28	DGD	c	516	-	-	0/42/82/95	0/2/2/2
28	DGD	c	517	-	-	2/51/91/95	0/2/2/2
28	DGD	c	518	-	-	0/55/95/95	0/2/2/2
31	LMG	c	519	-	-	0/40/60/70	0/1/1/1
22	BCT	d	401	21	-	0/0/0/0	0/0/0/0
23	CLA	d	402	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	d	403	-	3/3/20/25	0/37/135/135	0/0/9/9
25	PL9	d	404	-	-	0/53/73/73	0/1/1/1
27	BCR	d	405	-	-	0/29/63/63	0/2/2/2
31	LMG	d	406	-	-	0/41/61/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMG	d	407	-	-	0/43/63/70	0/1/1/1
30	SQD	d	408	-	-	2/38/58/69	0/1/1/1
28	DGD	d	409	-	-	1/52/92/95	0/2/2/2
33	LMT	d	410	-	-	0/17/57/61	0/2/2/2
31	LMG	e	101	-	-	0/39/59/70	0/1/1/1
34	HEM	f	101	5,6	-	0/6/54/54	0/0/8/8
30	SQD	f	102	-	-	0/40/60/69	0/1/1/1
27	BCR	h	101	-	-	0/29/63/63	0/2/2/2
31	LMG	i	101	-	-	0/38/58/70	0/1/1/1
33	LMT	i	102	-	-	0/21/61/61	0/2/2/2
25	PL9	j	101	-	-	0/29/49/73	0/1/1/1
27	BCR	j	102	-	-	0/29/63/63	0/2/2/2
27	BCR	k	102	-	-	0/29/63/63	0/2/2/2
31	LMG	k	103	-	-	0/43/63/70	0/1/1/1
33	LMT	m	101	-	-	0/21/61/61	0/2/2/2
31	LMG	m	102	-	-	1/37/57/70	0/1/1/1
34	HEM	v	201	16	-	0/6/54/54	0/0/8/8
27	BCR	y	101	-	-	0/29/63/63	0/2/2/2
27	BCR	z	101	-	-	0/29/63/63	0/2/2/2

All (703) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	F	101	HEM	C3B-C2B	-5.17	1.33	1.40
34	V	201	HEM	C3C-C2C	-5.16	1.33	1.40
34	f	101	HEM	C3B-C2B	-5.04	1.33	1.40
34	v	201	HEM	C3C-C2C	-4.95	1.33	1.40
34	V	201	HEM	C3B-C2B	-4.48	1.34	1.40
34	v	201	HEM	C3B-C2B	-4.19	1.34	1.40
34	F	101	HEM	C3C-C2C	-4.01	1.35	1.40
34	f	101	HEM	C3C-C2C	-3.78	1.35	1.40
31	m	102	LMG	O1-C7	-3.12	1.38	1.43
31	D	406	LMG	O7-C8	-3.06	1.38	1.46
28	C	517	DGD	O2G-C2G	-3.06	1.38	1.46
28	B	621	DGD	O2G-C2G	-3.03	1.38	1.46
31	D	407	LMG	O3-C3	-3.02	1.36	1.43
31	i	101	LMG	O7-C8	-2.99	1.38	1.46
31	d	406	LMG	O7-C8	-2.98	1.38	1.46
31	D	407	LMG	O7-C8	-2.98	1.38	1.46
31	B	622	LMG	O7-C8	-2.95	1.38	1.46
28	b	623	DGD	O2G-C2G	-2.90	1.39	1.46
31	C	520	LMG	O7-C8	-2.89	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	414	LMG	O3-C3	-2.89	1.36	1.43
31	b	625	LMG	O3-C3	-2.88	1.36	1.43
31	I	101	LMG	O7-C8	-2.87	1.39	1.46
23	b	615	CLA	CMB-C2B	-2.87	1.45	1.51
31	M	101	LMG	O1-C7	-2.86	1.38	1.43
28	c	516	DGD	O2G-C2G	-2.85	1.39	1.46
31	B	623	LMG	O3-C3	-2.85	1.36	1.43
31	k	103	LMG	O7-C8	-2.85	1.39	1.46
31	m	102	LMG	O7-C8	-2.82	1.39	1.46
31	d	407	LMG	O3-C3	-2.82	1.36	1.43
31	A	418	LMG	O7-C8	-2.82	1.39	1.46
31	b	625	LMG	O7-C8	-2.81	1.39	1.46
31	a	416	LMG	O3-C3	-2.80	1.36	1.43
31	b	624	LMG	O7-C8	-2.79	1.39	1.46
28	a	413	DGD	O2G-C2G	-2.78	1.39	1.46
31	d	407	LMG	O7-C8	-2.78	1.39	1.46
31	a	416	LMG	O7-C8	-2.77	1.39	1.46
31	a	402	LMG	O7-C8	-2.76	1.39	1.46
23	B	611	CLA	CMB-C2B	-2.75	1.46	1.51
28	c	517	DGD	O2G-C2G	-2.75	1.39	1.46
28	B	621	DGD	O3G-C3G	-2.73	1.38	1.43
28	C	518	DGD	O2G-C2G	-2.73	1.39	1.46
31	B	623	LMG	O7-C8	-2.73	1.39	1.46
31	m	102	LMG	O3-C3	-2.72	1.36	1.43
28	D	409	DGD	O2G-C2G	-2.72	1.39	1.46
31	A	418	LMG	O8-C9	-2.72	1.39	1.45
31	D	406	LMG	O3-C3	-2.71	1.36	1.43
31	m	102	LMG	O8-C9	-2.70	1.39	1.45
31	i	101	LMG	O3-C3	-2.70	1.36	1.43
31	c	519	LMG	O3-C3	-2.70	1.36	1.43
31	d	406	LMG	O3-C3	-2.69	1.36	1.43
23	C	510	CLA	CMB-C2B	-2.69	1.46	1.51
31	M	101	LMG	O3-C3	-2.68	1.36	1.43
31	M	101	LMG	O7-C8	-2.68	1.39	1.46
31	a	402	LMG	O3-C3	-2.68	1.36	1.43
31	I	101	LMG	O3-C3	-2.68	1.36	1.43
31	A	414	LMG	O7-C8	-2.67	1.39	1.46
31	i	101	LMG	O8-C9	-2.66	1.39	1.45
31	e	101	LMG	O7-C8	-2.66	1.39	1.46
28	c	518	DGD	O4D-C4D	-2.66	1.36	1.43
23	c	510	CLA	CMD-C2D	-2.63	1.46	1.51
28	C	519	DGD	O4D-C4D	-2.63	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	101	LMG	O8-C9	-2.63	1.39	1.45
23	b	612	CLA	CMB-C2B	-2.63	1.46	1.51
28	d	409	DGD	O2G-C2G	-2.63	1.39	1.46
23	b	605	CLA	CMB-C2B	-2.62	1.46	1.51
31	C	520	LMG	O3-C3	-2.62	1.36	1.43
31	b	624	LMG	O3-C3	-2.61	1.36	1.43
28	B	627	DGD	O2G-C2G	-2.61	1.39	1.46
31	e	101	LMG	O3-C3	-2.61	1.36	1.43
28	A	411	DGD	O4D-C4D	-2.61	1.36	1.43
31	e	101	LMG	O8-C9	-2.61	1.39	1.45
28	B	627	DGD	O6E-C5E	-2.60	1.38	1.44
23	b	610	CLA	CMB-C2B	-2.60	1.46	1.51
31	c	519	LMG	O7-C8	-2.60	1.39	1.46
31	C	521	LMG	O3-C3	-2.60	1.37	1.43
23	B	601	CLA	CMB-C2B	-2.59	1.46	1.51
31	A	418	LMG	O3-C3	-2.58	1.37	1.43
23	b	620	CLA	CMB-C2B	-2.58	1.46	1.51
31	k	103	LMG	O3-C3	-2.58	1.37	1.43
23	B	604	CLA	CMB-C2B	-2.57	1.46	1.51
23	c	508	CLA	CMB-C2B	-2.57	1.46	1.51
31	E	101	LMG	O8-C9	-2.57	1.39	1.45
31	E	101	LMG	O3-C3	-2.56	1.37	1.43
23	C	508	CLA	CMB-C2B	-2.56	1.46	1.51
23	B	610	CLA	CMB-C2B	-2.56	1.46	1.51
31	B	622	LMG	O3-C3	-2.56	1.37	1.43
23	b	617	CLA	CMB-C2B	-2.56	1.46	1.51
23	B	612	CLA	CMD-C2D	-2.55	1.46	1.51
23	B	616	CLA	CMB-C2B	-2.55	1.46	1.51
23	B	603	CLA	CMB-C2B	-2.55	1.46	1.51
31	c	519	LMG	O8-C9	-2.55	1.39	1.45
28	b	623	DGD	O3G-C3G	-2.55	1.39	1.43
23	c	507	CLA	CMB-C2B	-2.55	1.46	1.51
23	B	606	CLA	CMB-C2B	-2.55	1.46	1.51
28	c	517	DGD	O5D-C6D	-2.54	1.39	1.43
28	C	519	DGD	O3G-C3G	-2.54	1.39	1.43
31	B	623	LMG	O8-C9	-2.54	1.39	1.45
28	b	602	DGD	O2G-C2G	-2.54	1.40	1.46
23	C	507	CLA	CMB-C2B	-2.54	1.46	1.51
31	I	101	LMG	O8-C9	-2.54	1.39	1.45
23	A	404	CLA	CMB-C2B	-2.53	1.46	1.51
23	b	618	CLA	CMB-C2B	-2.53	1.46	1.51
31	b	625	LMG	O8-C9	-2.53	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	602	DGD	O6E-C5E	-2.53	1.38	1.44
31	a	416	LMG	O8-C9	-2.53	1.39	1.45
31	b	624	LMG	O6-C5	-2.53	1.38	1.44
28	C	518	DGD	O4D-C4D	-2.53	1.37	1.43
23	c	502	CLA	CMB-C2B	-2.52	1.46	1.51
23	B	608	CLA	CMB-C2B	-2.52	1.46	1.51
23	A	403	CLA	CMD-C2D	-2.52	1.46	1.51
28	C	519	DGD	O2G-C2G	-2.52	1.40	1.46
23	b	606	CLA	CMB-C2B	-2.52	1.46	1.51
28	c	517	DGD	O4D-C4D	-2.51	1.37	1.43
28	A	411	DGD	O2G-C2G	-2.51	1.40	1.46
23	C	504	CLA	CMB-C2B	-2.51	1.46	1.51
31	d	406	LMG	O8-C9	-2.51	1.39	1.45
23	a	405	CLA	CMB-C2B	-2.51	1.46	1.51
23	a	404	CLA	CMD-C2D	-2.50	1.46	1.51
23	c	505	CLA	CMB-C2B	-2.50	1.46	1.51
23	C	505	CLA	CMB-C2B	-2.50	1.46	1.51
31	A	418	LMG	O1-C7	-2.50	1.39	1.43
23	C	505	CLA	CMD-C2D	-2.49	1.46	1.51
31	C	521	LMG	O7-C8	-2.49	1.40	1.46
23	b	614	CLA	CMB-C2B	-2.49	1.46	1.51
23	d	402	CLA	CMD-C2D	-2.49	1.46	1.51
31	B	622	LMG	O8-C9	-2.49	1.39	1.45
31	E	101	LMG	O7-C8	-2.49	1.40	1.46
23	c	510	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	615	CLA	CMB-C2B	-2.49	1.46	1.51
23	b	608	CLA	CMB-C2B	-2.49	1.46	1.51
23	B	608	CLA	CMD-C2D	-2.48	1.46	1.51
23	b	616	CLA	CMD-C2D	-2.48	1.46	1.51
23	C	513	CLA	CMB-C2B	-2.48	1.46	1.51
23	b	607	CLA	CMB-C2B	-2.48	1.46	1.51
31	i	101	LMG	O1-C7	-2.48	1.39	1.43
23	c	504	CLA	CMB-C2B	-2.48	1.46	1.51
23	B	613	CLA	CMB-C2B	-2.48	1.46	1.51
28	a	413	DGD	O4D-C4D	-2.47	1.37	1.43
23	b	611	CLA	CMB-C2B	-2.47	1.46	1.51
23	C	501	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	405	CLA	CMB-C2B	-2.47	1.46	1.51
23	B	607	CLA	CMB-C2B	-2.47	1.46	1.51
23	B	614	CLA	CMD-C2D	-2.47	1.46	1.51
23	B	605	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	407	CLA	CMB-C2B	-2.47	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	CMB-C2B	-2.47	1.46	1.51
28	A	411	DGD	O3G-C3G	-2.47	1.39	1.43
23	c	513	CLA	CMB-C2B	-2.47	1.46	1.51
23	A	403	CLA	CMB-C2B	-2.47	1.46	1.51
31	A	414	LMG	O8-C9	-2.46	1.39	1.45
23	C	509	CLA	CMB-C2B	-2.46	1.46	1.51
28	c	516	DGD	O4D-C4D	-2.46	1.37	1.43
28	c	518	DGD	O2G-C2G	-2.46	1.40	1.46
23	B	604	CLA	CMD-C2D	-2.46	1.46	1.51
31	D	407	LMG	O8-C9	-2.46	1.39	1.45
23	a	404	CLA	CMB-C2B	-2.46	1.46	1.51
30	A	417	SQD	O2-C2	-2.46	1.37	1.43
23	c	505	CLA	CMD-C2D	-2.45	1.46	1.51
23	C	502	CLA	CMB-C2B	-2.45	1.46	1.51
23	c	506	CLA	CMB-C2B	-2.45	1.46	1.51
23	C	512	CLA	CMB-C2B	-2.45	1.46	1.51
31	b	624	LMG	O8-C9	-2.44	1.39	1.45
23	C	510	CLA	CMD-C2D	-2.44	1.46	1.51
23	c	501	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	618	CLA	CMD-C2D	-2.44	1.46	1.51
23	a	406	CLA	CMD-C2D	-2.44	1.46	1.51
23	C	506	CLA	CMB-C2B	-2.44	1.46	1.51
23	D	403	CLA	CMB-C2B	-2.44	1.46	1.51
28	a	413	DGD	O3G-C3G	-2.44	1.39	1.43
23	c	512	CLA	CMB-C2B	-2.44	1.46	1.51
23	b	608	CLA	CMD-C2D	-2.44	1.46	1.51
31	d	407	LMG	O8-C9	-2.43	1.39	1.45
23	B	614	CLA	CMB-C2B	-2.43	1.46	1.51
23	b	609	CLA	CMB-C2B	-2.43	1.46	1.51
31	A	414	LMG	O1-C7	-2.43	1.39	1.43
23	B	602	CLA	CMB-C2B	-2.43	1.46	1.51
31	D	406	LMG	O8-C9	-2.43	1.39	1.45
28	b	602	DGD	O4D-C4D	-2.43	1.37	1.43
28	C	518	DGD	O5D-C6D	-2.42	1.39	1.43
23	B	603	CLA	CMD-C2D	-2.42	1.46	1.51
23	c	502	CLA	CMD-C2D	-2.42	1.46	1.51
23	C	503	CLA	CMB-C2B	-2.42	1.46	1.51
23	B	609	CLA	CMB-C2B	-2.42	1.46	1.51
28	C	517	DGD	O6E-C5E	-2.41	1.38	1.44
31	C	521	LMG	O8-C9	-2.41	1.39	1.45
31	I	101	LMG	O1-C7	-2.41	1.39	1.43
23	b	612	CLA	CMD-C2D	-2.41	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	CMB-C2B	-2.41	1.46	1.51
23	C	508	CLA	CMD-C2D	-2.41	1.46	1.51
23	b	619	CLA	CMB-C2B	-2.41	1.46	1.51
23	D	401	CLA	CMD-C2D	-2.41	1.46	1.51
31	C	520	LMG	O8-C9	-2.41	1.39	1.45
23	b	609	CLA	CMD-C2D	-2.41	1.46	1.51
31	b	624	LMG	O1-C7	-2.40	1.39	1.43
23	d	403	CLA	CMD-C2D	-2.40	1.46	1.51
28	c	516	DGD	O6E-C5E	-2.40	1.38	1.44
23	b	613	CLA	CMB-C2B	-2.40	1.46	1.51
23	d	403	CLA	CMB-C2B	-2.40	1.46	1.51
23	d	402	CLA	CMB-C2B	-2.40	1.46	1.51
23	c	503	CLA	CMB-C2B	-2.40	1.46	1.51
31	B	623	LMG	O1-C7	-2.40	1.39	1.43
23	a	406	CLA	CMB-C2B	-2.40	1.46	1.51
28	c	517	DGD	O6E-C5E	-2.39	1.38	1.44
23	c	509	CLA	CMB-C2B	-2.39	1.46	1.51
23	B	611	CLA	CMD-C2D	-2.39	1.46	1.51
31	d	406	LMG	O1-C7	-2.39	1.39	1.43
23	C	502	CLA	CMD-C2D	-2.39	1.46	1.51
28	B	621	DGD	O4D-C4D	-2.39	1.37	1.43
23	a	409	CLA	CMB-C2B	-2.38	1.46	1.51
23	b	611	CLA	CMD-C2D	-2.38	1.46	1.51
31	B	622	LMG	O6-C5	-2.37	1.38	1.44
28	B	627	DGD	O4D-C4D	-2.37	1.37	1.43
28	C	518	DGD	O6E-C5E	-2.37	1.38	1.44
23	D	403	CLA	CMD-C2D	-2.37	1.46	1.51
23	b	617	CLA	CMD-C2D	-2.37	1.46	1.51
23	c	507	CLA	CMD-C2D	-2.36	1.46	1.51
23	B	605	CLA	CMD-C2D	-2.36	1.46	1.51
23	b	615	CLA	CMD-C2D	-2.36	1.46	1.51
23	B	612	CLA	CMB-C2B	-2.35	1.46	1.51
23	c	501	CLA	CMD-C2D	-2.35	1.46	1.51
23	D	401	CLA	CMB-C2B	-2.34	1.46	1.51
23	b	616	CLA	CMB-C2B	-2.34	1.46	1.51
23	B	606	CLA	CMD-C2D	-2.34	1.46	1.51
23	b	610	CLA	CMD-C2D	-2.33	1.46	1.51
31	a	402	LMG	O8-C9	-2.33	1.40	1.45
30	a	401	SQD	O2-C2	-2.33	1.37	1.43
23	b	605	CLA	CMD-C2D	-2.33	1.46	1.51
23	A	407	CLA	CMD-C2D	-2.32	1.46	1.51
31	a	402	LMG	O1-C7	-2.32	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	CMD-C2D	-2.32	1.46	1.51
31	k	103	LMG	O1-C7	-2.32	1.39	1.43
28	A	411	DGD	O1G-C1G	-2.32	1.40	1.45
23	a	405	CLA	CMD-C2D	-2.31	1.46	1.51
23	b	620	CLA	CMD-C2D	-2.31	1.46	1.51
23	C	506	CLA	CMD-C2D	-2.31	1.46	1.51
23	C	504	CLA	CMD-C2D	-2.31	1.46	1.51
31	a	416	LMG	O1-C7	-2.31	1.39	1.43
23	B	609	CLA	CMD-C2D	-2.30	1.46	1.51
24	A	406	PHO	C1C-NC	-2.30	1.33	1.38
23	B	602	CLA	CMD-C2D	-2.30	1.46	1.51
24	D	402	PHO	C1C-NC	-2.30	1.33	1.38
23	B	607	CLA	CMD-C2D	-2.30	1.46	1.51
23	c	513	CLA	CMD-C2D	-2.30	1.46	1.51
23	B	615	CLA	CMD-C2D	-2.29	1.46	1.51
23	a	409	CLA	CMD-C2D	-2.28	1.46	1.51
23	B	610	CLA	CMD-C2D	-2.28	1.46	1.51
28	c	518	DGD	O3G-C3G	-2.28	1.39	1.43
30	B	626	SQD	O2-C2	-2.28	1.37	1.43
23	b	606	CLA	CMD-C2D	-2.28	1.46	1.51
23	C	512	CLA	CMD-C2D	-2.28	1.46	1.51
23	c	506	CLA	CMD-C2D	-2.28	1.46	1.51
23	A	404	CLA	CMD-C2D	-2.28	1.46	1.51
30	A	417	SQD	C4-C5	-2.28	1.48	1.53
31	k	103	LMG	O8-C9	-2.28	1.40	1.45
23	A	405	CLA	CMD-C2D	-2.28	1.46	1.51
31	D	407	LMG	O2-C2	-2.28	1.37	1.43
23	c	511	CLA	CMD-C2D	-2.27	1.46	1.51
28	C	517	DGD	O4D-C4D	-2.27	1.37	1.43
28	C	518	DGD	C4D-C5D	-2.27	1.48	1.53
31	i	101	LMG	O6-C5	-2.27	1.38	1.44
23	b	613	CLA	CMD-C2D	-2.26	1.46	1.51
23	c	504	CLA	CMD-C2D	-2.26	1.46	1.51
31	d	407	LMG	O2-C2	-2.26	1.37	1.43
24	a	408	PHO	C1C-NC	-2.25	1.33	1.38
23	c	512	CLA	CMD-C2D	-2.25	1.46	1.51
23	c	503	CLA	CMD-C2D	-2.25	1.46	1.51
23	C	513	CLA	CMD-C2D	-2.25	1.46	1.51
31	I	101	LMG	O6-C5	-2.25	1.38	1.44
23	b	607	CLA	CMD-C2D	-2.24	1.46	1.51
23	C	503	CLA	CMD-C2D	-2.24	1.46	1.51
31	d	407	LMG	O1-C7	-2.24	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	CMD-C2D	-2.24	1.46	1.51
31	m	102	LMG	O6-C5	-2.23	1.38	1.44
23	C	511	CLA	CMD-C2D	-2.23	1.46	1.51
23	b	619	CLA	CMD-C2D	-2.23	1.46	1.51
23	C	501	CLA	CMD-C2D	-2.23	1.46	1.51
28	c	517	DGD	O1G-C1G	-2.23	1.40	1.45
31	D	407	LMG	O6-C5	-2.22	1.38	1.44
23	c	509	CLA	CMD-C2D	-2.22	1.46	1.51
23	c	508	CLA	CMD-C2D	-2.22	1.46	1.51
28	B	621	DGD	O6D-C5D	-2.22	1.38	1.44
28	d	409	DGD	O4D-C4D	-2.21	1.37	1.43
28	b	623	DGD	O6E-C5E	-2.21	1.39	1.44
30	b	601	SQD	O2-C2	-2.21	1.37	1.43
23	C	509	CLA	CMD-C2D	-2.21	1.46	1.51
31	B	623	LMG	O6-C5	-2.21	1.39	1.44
23	C	507	CLA	CMD-C2D	-2.20	1.46	1.51
28	c	517	DGD	O6D-C5D	-2.20	1.39	1.44
28	C	518	DGD	O5D-C1E	-2.20	1.36	1.40
30	A	413	SQD	O2-C2	-2.20	1.37	1.43
31	c	519	LMG	O6-C5	-2.19	1.39	1.44
28	D	409	DGD	O4D-C4D	-2.19	1.37	1.43
28	a	413	DGD	O1G-C1G	-2.18	1.40	1.45
28	b	623	DGD	O4D-C4D	-2.18	1.37	1.43
28	D	409	DGD	O5D-C6D	-2.17	1.39	1.43
31	E	101	LMG	O6-C5	-2.17	1.39	1.44
31	d	407	LMG	O6-C5	-2.16	1.39	1.44
31	C	520	LMG	O1-C7	-2.16	1.39	1.43
31	b	625	LMG	O6-C5	-2.16	1.39	1.44
30	D	408	SQD	O3-C3	-2.16	1.38	1.43
30	d	408	SQD	O3-C3	-2.15	1.38	1.43
31	e	101	LMG	O6-C5	-2.15	1.39	1.44
30	F	102	SQD	O2-C2	-2.15	1.38	1.43
23	B	613	CLA	CMD-C2D	-2.14	1.47	1.51
24	a	407	PHO	C1C-NC	-2.14	1.33	1.38
28	D	409	DGD	O6E-C5E	-2.14	1.39	1.44
31	b	625	LMG	O2-C2	-2.14	1.38	1.43
31	b	625	LMG	O1-C7	-2.14	1.40	1.43
23	b	614	CLA	CMD-C2D	-2.14	1.47	1.51
31	D	407	LMG	O1-C7	-2.13	1.40	1.43
30	D	408	SQD	O4-C4	-2.13	1.38	1.43
30	f	102	SQD	O2-C2	-2.12	1.38	1.43
30	B	626	SQD	O3-C3	-2.12	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	E	101	LMG	O2-C2	-2.12	1.38	1.43
31	C	521	LMG	O6-C5	-2.12	1.39	1.44
28	a	413	DGD	O6E-C5E	-2.12	1.39	1.44
31	B	623	LMG	O2-C2	-2.11	1.38	1.43
28	c	517	DGD	O5D-C1E	-2.11	1.36	1.40
28	B	621	DGD	O6E-C5E	-2.11	1.39	1.44
31	B	622	LMG	O1-C7	-2.10	1.40	1.43
30	d	408	SQD	O4-C4	-2.10	1.38	1.43
30	b	601	SQD	O3-C3	-2.10	1.38	1.43
30	a	401	SQD	C4-C5	-2.10	1.48	1.53
30	F	102	SQD	O3-C3	-2.10	1.38	1.43
28	C	518	DGD	O6D-C5D	-2.10	1.39	1.44
28	C	519	DGD	O1G-C1G	-2.10	1.40	1.45
28	B	621	DGD	O1G-C1G	-2.10	1.40	1.45
31	e	101	LMG	O2-C2	-2.10	1.38	1.43
23	C	511	CLA	C3B-C2B	-2.09	1.37	1.40
31	c	519	LMG	O1-C7	-2.09	1.40	1.43
31	M	101	LMG	O6-C5	-2.09	1.39	1.44
23	C	509	CLA	C3B-C2B	-2.09	1.37	1.40
28	d	409	DGD	O6E-C5E	-2.09	1.39	1.44
23	b	620	CLA	C3B-C2B	-2.09	1.37	1.40
28	b	623	DGD	O6D-C5D	-2.09	1.39	1.44
30	a	415	SQD	O2-C2	-2.08	1.38	1.43
23	C	504	CLA	C3B-CAB	-2.08	1.43	1.47
30	a	415	SQD	O3-C3	-2.08	1.38	1.43
28	c	518	DGD	O6E-C5E	-2.08	1.39	1.44
28	b	602	DGD	O5D-C6D	-2.08	1.40	1.43
28	B	627	DGD	C4E-C5E	-2.08	1.48	1.53
28	C	517	DGD	C4E-C5E	-2.08	1.48	1.53
28	A	411	DGD	O6E-C5E	-2.07	1.39	1.44
30	B	626	SQD	O4-C4	-2.07	1.38	1.43
31	I	101	LMG	C4-C5	-2.07	1.48	1.53
30	D	408	SQD	O2-C2	-2.07	1.38	1.43
28	C	518	DGD	C4E-C5E	-2.07	1.48	1.53
31	d	406	LMG	O6-C5	-2.06	1.39	1.44
28	c	517	DGD	C4D-C5D	-2.06	1.48	1.53
31	e	101	LMG	C4-C5	-2.06	1.48	1.53
23	C	505	CLA	C3B-C2B	-2.06	1.37	1.40
31	D	406	LMG	O6-C5	-2.05	1.39	1.44
30	F	102	SQD	O4-C4	-2.05	1.38	1.43
30	f	102	SQD	O3-C3	-2.04	1.38	1.43
30	b	601	SQD	O4-C4	-2.04	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	401	SQD	O4-C4	-2.04	1.38	1.43
30	f	102	SQD	O4-C4	-2.03	1.38	1.43
30	A	413	SQD	O3-C3	-2.03	1.38	1.43
31	C	521	LMG	O1-C7	-2.03	1.40	1.43
31	C	521	LMG	O2-C2	-2.03	1.38	1.43
28	B	621	DGD	O5D-C6D	-2.02	1.40	1.43
31	D	406	LMG	O1-C7	-2.02	1.40	1.43
28	b	623	DGD	O5D-C6D	-2.02	1.40	1.43
30	A	417	SQD	O4-C4	-2.02	1.38	1.43
23	B	610	CLA	C3B-CAB	-2.01	1.43	1.47
31	c	519	LMG	O2-C2	-2.01	1.38	1.43
28	b	623	DGD	O1G-C1G	-2.01	1.40	1.45
30	d	408	SQD	O2-C2	-2.01	1.38	1.43
23	b	620	CLA	C3B-CAB	-2.01	1.43	1.47
30	A	413	SQD	O4-C4	-2.01	1.38	1.43
28	c	516	DGD	C4E-C5E	-2.00	1.48	1.53
24	a	407	PHO	C4B-NB	2.00	1.41	1.36
34	v	201	HEM	C1B-NB	2.03	1.39	1.36
33	D	410	LMT	O1'-C1'	2.03	1.43	1.40
33	i	102	LMT	O1'-C1'	2.05	1.43	1.40
24	a	407	PHO	CHD-C1D	2.06	1.42	1.38
23	B	601	CLA	C4C-NC	2.07	1.40	1.37
24	a	408	PHO	C4B-NB	2.08	1.41	1.36
24	D	402	PHO	C1B-C2B	2.13	1.50	1.45
24	a	407	PHO	C1B-C2B	2.14	1.50	1.45
24	A	406	PHO	C4B-NB	2.14	1.41	1.36
34	V	201	HEM	CAA-C2A	2.15	1.55	1.52
24	A	406	PHO	C1C-C2C	2.15	1.50	1.45
24	D	402	PHO	C4B-NB	2.15	1.41	1.36
24	a	407	PHO	C4C-C3C	2.18	1.49	1.45
24	D	402	PHO	CHD-C1D	2.21	1.43	1.38
24	A	406	PHO	C4C-C3C	2.22	1.49	1.45
25	D	404	PL9	C28-C29	2.24	1.38	1.33
25	j	101	PL9	C28-C29	2.27	1.38	1.32
25	J	101	PL9	C28-C29	2.28	1.39	1.32
25	a	410	PL9	C28-C29	2.28	1.38	1.33
24	D	402	PHO	C4C-C3C	2.32	1.49	1.45
23	d	402	CLA	CHC-C1C	2.34	1.42	1.35
25	A	408	PL9	C28-C29	2.36	1.38	1.33
28	B	621	DGD	O2G-C1B	2.40	1.41	1.34
25	D	404	PL9	C13-C14	2.40	1.39	1.33
31	A	418	LMG	O8-C28	2.40	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	404	PL9	C28-C29	2.41	1.39	1.33
24	D	402	PHO	C1A-NA	2.42	1.42	1.37
25	D	404	PL9	C8-C9	2.42	1.39	1.33
25	a	410	PL9	C18-C19	2.42	1.39	1.33
23	C	502	CLA	CHC-C1C	2.43	1.42	1.35
24	a	408	PHO	C1A-NA	2.43	1.42	1.37
24	A	406	PHO	C1A-NA	2.43	1.42	1.37
25	a	410	PL9	C8-C9	2.43	1.39	1.33
28	D	409	DGD	O2G-C1B	2.43	1.41	1.34
23	b	605	CLA	CHC-C1C	2.43	1.42	1.35
23	c	507	CLA	CHC-C1C	2.44	1.42	1.35
31	i	101	LMG	O8-C28	2.45	1.40	1.33
23	b	616	CLA	CHC-C1C	2.45	1.42	1.35
23	b	608	CLA	CHC-C1C	2.46	1.42	1.35
24	A	406	PHO	CHD-C1D	2.47	1.43	1.38
28	b	623	DGD	O2G-C1B	2.47	1.41	1.34
34	F	101	HEM	C4D-ND	2.48	1.39	1.36
23	B	606	CLA	CHC-C1C	2.48	1.42	1.35
24	D	402	PHO	C4C-NC	2.49	1.42	1.36
23	b	615	CLA	CHC-C1C	2.49	1.42	1.35
25	d	404	PL9	C8-C9	2.50	1.39	1.33
31	D	406	LMG	O8-C28	2.50	1.40	1.33
34	f	101	HEM	C4D-ND	2.51	1.39	1.36
28	d	409	DGD	O2G-C1B	2.51	1.41	1.34
25	d	404	PL9	C18-C19	2.51	1.39	1.33
31	D	407	LMG	O7-C10	2.51	1.41	1.34
31	D	406	LMG	O7-C10	2.52	1.41	1.34
23	b	620	CLA	CHC-C1C	2.52	1.42	1.35
23	c	513	CLA	CHC-C1C	2.52	1.42	1.35
31	d	406	LMG	O8-C28	2.52	1.40	1.33
31	k	103	LMG	O7-C10	2.53	1.41	1.34
23	B	616	CLA	CHC-C1C	2.53	1.42	1.35
23	b	612	CLA	CHC-C1C	2.53	1.42	1.35
25	d	404	PL9	C13-C14	2.54	1.39	1.33
31	b	625	LMG	O8-C28	2.54	1.40	1.33
23	a	404	CLA	CHC-C1C	2.54	1.42	1.35
24	a	408	PHO	C4C-C3C	2.55	1.49	1.45
23	A	407	CLA	CHC-C1C	2.55	1.42	1.35
25	A	408	PL9	C8-C9	2.55	1.39	1.33
31	C	520	LMG	O7-C10	2.56	1.41	1.34
23	b	617	CLA	CHC-C1C	2.56	1.42	1.35
25	D	404	PL9	C23-C24	2.56	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CHC-C1C	2.56	1.42	1.35
25	a	410	PL9	C23-C24	2.56	1.39	1.33
23	C	510	CLA	CHC-C1C	2.56	1.42	1.35
31	B	623	LMG	O8-C28	2.57	1.40	1.33
25	A	408	PL9	C23-C24	2.58	1.39	1.33
31	d	406	LMG	O7-C10	2.58	1.41	1.34
31	i	101	LMG	O7-C10	2.58	1.41	1.34
23	B	615	CLA	CHC-C1C	2.58	1.42	1.35
28	a	413	DGD	O2G-C1B	2.58	1.41	1.34
25	a	410	PL9	C13-C14	2.59	1.39	1.33
23	A	405	CLA	CHC-C1C	2.59	1.42	1.35
23	C	505	CLA	CHC-C1C	2.59	1.42	1.35
28	C	517	DGD	O2G-C1B	2.59	1.41	1.34
24	D	402	PHO	CHC-C1C	2.60	1.43	1.38
25	A	408	PL9	C13-C14	2.60	1.39	1.33
31	I	101	LMG	O8-C28	2.60	1.41	1.33
23	b	607	CLA	CHC-C1C	2.60	1.42	1.35
24	A	406	PHO	C4C-NC	2.60	1.42	1.36
25	D	404	PL9	C18-C19	2.60	1.39	1.33
31	B	622	LMG	O8-C28	2.61	1.41	1.33
23	c	505	CLA	CHC-C1C	2.61	1.42	1.35
25	J	101	PL9	C18-C19	2.61	1.39	1.33
25	d	404	PL9	C23-C24	2.61	1.39	1.33
31	D	407	LMG	O8-C28	2.61	1.41	1.33
25	J	101	PL9	C13-C14	2.61	1.39	1.33
23	C	501	CLA	CHC-C1C	2.61	1.42	1.35
23	C	503	CLA	CHC-C1C	2.61	1.42	1.35
23	a	405	CLA	CHC-C1C	2.61	1.42	1.35
23	b	611	CLA	CHC-C1C	2.61	1.42	1.35
23	C	507	CLA	CHC-C1C	2.61	1.42	1.35
25	j	101	PL9	C8-C9	2.62	1.39	1.33
23	B	611	CLA	CHC-C1C	2.62	1.42	1.35
24	a	408	PHO	CHD-C1D	2.62	1.43	1.38
31	B	622	LMG	O7-C10	2.62	1.41	1.34
23	D	401	CLA	CHC-C1C	2.62	1.42	1.35
23	c	503	CLA	CHC-C1C	2.62	1.42	1.35
31	A	414	LMG	O8-C28	2.62	1.41	1.33
23	c	512	CLA	CHC-C1C	2.62	1.42	1.35
23	b	610	CLA	CHC-C1C	2.62	1.42	1.35
23	c	501	CLA	CHC-C1C	2.62	1.42	1.35
23	B	613	CLA	CHC-C1C	2.63	1.42	1.35
23	B	604	CLA	CHC-C1C	2.63	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	CHC-C1C	2.63	1.42	1.35
24	a	407	PHO	C4C-NC	2.63	1.42	1.36
24	a	408	PHO	C4C-NC	2.63	1.42	1.36
23	C	511	CLA	CHC-C1C	2.64	1.43	1.35
31	d	407	LMG	O7-C10	2.64	1.41	1.34
34	V	201	HEM	C4D-ND	2.64	1.39	1.36
28	C	518	DGD	O2G-C1B	2.64	1.41	1.34
31	a	416	LMG	O8-C28	2.64	1.41	1.33
31	d	407	LMG	O8-C28	2.64	1.41	1.33
25	A	408	PL9	C18-C19	2.64	1.39	1.33
24	a	407	PHO	C1A-NA	2.65	1.43	1.37
23	d	403	CLA	CHC-C1C	2.65	1.43	1.35
23	A	403	CLA	CHC-C1C	2.65	1.43	1.35
31	e	101	LMG	O8-C28	2.65	1.41	1.33
23	B	601	CLA	CHC-C1C	2.65	1.43	1.35
31	C	520	LMG	O8-C28	2.65	1.41	1.33
25	J	101	PL9	C8-C9	2.65	1.39	1.33
25	j	101	PL9	C23-C24	2.66	1.39	1.33
28	c	517	DGD	O1G-C1A	2.66	1.41	1.33
23	C	512	CLA	CHC-C1C	2.66	1.43	1.35
31	a	402	LMG	O8-C28	2.66	1.41	1.33
30	a	415	SQD	O47-C7	2.66	1.42	1.34
31	E	101	LMG	O8-C28	2.67	1.41	1.33
25	j	101	PL9	C18-C19	2.67	1.39	1.33
23	b	614	CLA	CHC-C1C	2.67	1.43	1.35
28	c	517	DGD	O2G-C1B	2.67	1.42	1.34
23	c	502	CLA	CHC-C1C	2.68	1.43	1.35
31	b	624	LMG	O8-C28	2.68	1.41	1.33
30	B	626	SQD	O47-C7	2.68	1.42	1.34
23	B	612	CLA	CHC-C1C	2.68	1.43	1.35
31	b	624	LMG	O7-C10	2.68	1.42	1.34
23	B	614	CLA	CHC-C1C	2.68	1.43	1.35
31	I	101	LMG	O7-C10	2.69	1.42	1.34
31	e	101	LMG	O7-C10	2.69	1.42	1.34
31	M	101	LMG	O8-C28	2.69	1.41	1.33
31	c	519	LMG	O8-C28	2.69	1.41	1.33
23	C	508	CLA	CHC-C1C	2.70	1.43	1.35
30	A	413	SQD	O47-C7	2.70	1.42	1.34
23	B	605	CLA	CHC-C1C	2.70	1.43	1.35
23	D	403	CLA	CHC-C1C	2.70	1.43	1.35
23	C	506	CLA	CHC-C1C	2.70	1.43	1.35
23	c	508	CLA	CHC-C1C	2.70	1.43	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	413	DGD	O1G-C1A	2.71	1.41	1.33
23	C	509	CLA	CHC-C1C	2.71	1.43	1.35
31	a	402	LMG	O7-C10	2.71	1.42	1.34
31	A	418	LMG	O7-C10	2.71	1.42	1.34
28	B	621	DGD	O1G-C1A	2.72	1.41	1.33
23	C	504	CLA	CHC-C1C	2.72	1.43	1.35
25	j	101	PL9	C13-C14	2.72	1.39	1.33
31	b	625	LMG	O7-C10	2.72	1.42	1.34
30	f	102	SQD	O47-C7	2.72	1.42	1.34
23	b	618	CLA	CHC-C1C	2.72	1.43	1.35
28	A	411	DGD	O1G-C1A	2.72	1.41	1.33
23	c	506	CLA	CHC-C1C	2.73	1.43	1.35
23	C	513	CLA	CHC-C1C	2.73	1.43	1.35
23	B	603	CLA	CHC-C1C	2.73	1.43	1.35
23	B	610	CLA	CHC-C1C	2.73	1.43	1.35
23	a	406	CLA	CHC-C1C	2.73	1.43	1.35
31	m	102	LMG	O8-C28	2.73	1.41	1.33
23	b	609	CLA	CHC-C1C	2.74	1.43	1.35
23	B	607	CLA	CHC-C1C	2.74	1.43	1.35
28	C	519	DGD	O1G-C1A	2.75	1.41	1.33
31	C	521	LMG	O8-C28	2.76	1.41	1.33
30	a	401	SQD	O47-C7	2.76	1.42	1.34
23	B	602	CLA	CHC-C1C	2.76	1.43	1.35
23	c	509	CLA	CHC-C1C	2.76	1.43	1.35
23	c	510	CLA	CHC-C1C	2.77	1.43	1.35
31	k	103	LMG	O8-C28	2.77	1.41	1.33
23	B	608	CLA	CHC-C1C	2.77	1.43	1.35
23	B	609	CLA	CHC-C1C	2.78	1.43	1.35
28	c	516	DGD	O2G-C1B	2.78	1.42	1.34
31	E	101	LMG	O7-C10	2.78	1.42	1.34
31	m	102	LMG	O7-C10	2.78	1.42	1.34
23	b	619	CLA	CHC-C1C	2.79	1.43	1.35
30	b	601	SQD	O47-C7	2.79	1.42	1.34
28	c	518	DGD	O1G-C1A	2.80	1.41	1.33
24	a	407	PHO	CHC-C1C	2.80	1.44	1.38
28	b	623	DGD	O1G-C1A	2.81	1.41	1.33
28	b	602	DGD	O2G-C1B	2.82	1.42	1.34
23	c	511	CLA	CHC-C1C	2.82	1.43	1.35
23	A	404	CLA	CHC-C1C	2.83	1.43	1.35
31	a	416	LMG	O7-C10	2.83	1.42	1.34
23	a	409	CLA	CHC-C1C	2.84	1.43	1.35
25	J	101	PL9	C23-C24	2.84	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	v	201	HEM	C4D-ND	2.84	1.40	1.36
30	A	417	SQD	O47-C7	2.85	1.42	1.34
28	B	627	DGD	O2G-C1B	2.86	1.42	1.34
25	d	404	PL9	C43-C44	2.86	1.40	1.33
31	A	414	LMG	O7-C10	2.87	1.42	1.34
31	c	519	LMG	O7-C10	2.87	1.42	1.34
23	b	606	CLA	CHC-C1C	2.87	1.43	1.35
28	C	518	DGD	O1G-C1A	2.88	1.41	1.33
30	F	102	SQD	O47-C7	2.88	1.42	1.34
28	A	411	DGD	O2G-C1B	2.88	1.42	1.34
31	M	101	LMG	O7-C10	2.89	1.42	1.34
31	B	623	LMG	O7-C10	2.90	1.42	1.34
28	d	409	DGD	O1G-C1A	2.90	1.41	1.33
24	a	407	PHO	C3B-C4B	2.91	1.49	1.43
30	D	408	SQD	O47-C7	2.91	1.42	1.34
28	C	517	DGD	O1G-C1A	2.92	1.41	1.33
31	C	521	LMG	O7-C10	2.92	1.42	1.34
30	d	408	SQD	O47-C7	2.93	1.42	1.34
28	B	627	DGD	O1G-C1A	2.93	1.42	1.33
28	D	409	DGD	O1G-C1A	2.95	1.42	1.33
24	a	408	PHO	CHC-C1C	2.97	1.44	1.38
30	F	102	SQD	O48-C23	3.01	1.42	1.33
24	D	402	PHO	C3B-C4B	3.01	1.49	1.43
28	c	518	DGD	O2G-C1B	3.04	1.43	1.34
30	f	102	SQD	O48-C23	3.04	1.42	1.33
28	C	519	DGD	O2G-C1B	3.06	1.43	1.34
25	D	404	PL9	C43-C44	3.06	1.40	1.33
28	c	516	DGD	O1G-C1A	3.07	1.42	1.33
30	B	626	SQD	O48-C23	3.07	1.42	1.33
30	A	417	SQD	O48-C23	3.08	1.42	1.33
25	A	408	PL9	C38-C39	3.09	1.41	1.32
25	d	404	PL9	C33-C34	3.09	1.40	1.33
25	a	410	PL9	C38-C39	3.12	1.41	1.32
30	b	601	SQD	O48-C23	3.12	1.42	1.33
25	D	404	PL9	C33-C34	3.14	1.40	1.33
28	b	602	DGD	O1G-C1A	3.14	1.42	1.33
25	a	410	PL9	C33-C34	3.15	1.40	1.33
25	d	404	PL9	C38-C39	3.15	1.40	1.33
24	a	408	PHO	C3B-C4B	3.17	1.50	1.43
30	a	415	SQD	O48-C23	3.17	1.42	1.33
30	A	413	SQD	O48-C23	3.18	1.42	1.33
30	D	408	SQD	O48-C23	3.19	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	401	SQD	O48-C23	3.22	1.42	1.33
30	d	408	SQD	O48-C23	3.24	1.42	1.33
25	D	404	PL9	C38-C39	3.24	1.41	1.33
24	A	406	PHO	CHC-C1C	3.31	1.45	1.38
25	A	408	PL9	C33-C34	3.32	1.41	1.33
24	A	406	PHO	C3B-C4B	3.39	1.50	1.43
34	V	201	HEM	C3B-CAB	3.42	1.54	1.47
23	b	606	CLA	CHB-C4A	3.48	1.38	1.33
34	v	201	HEM	C3B-CAB	3.56	1.55	1.47
23	a	405	CLA	CHB-C4A	3.59	1.38	1.33
23	A	404	CLA	CHB-C4A	3.70	1.38	1.33
23	C	509	CLA	CHB-C4A	3.72	1.38	1.33
23	b	614	CLA	CHB-C4A	3.73	1.38	1.33
34	f	101	HEM	C3B-CAB	3.73	1.55	1.47
23	c	510	CLA	CHB-C4A	3.76	1.38	1.33
23	C	504	CLA	CHB-C4A	3.77	1.38	1.33
23	B	609	CLA	CHB-C4A	3.77	1.38	1.33
34	F	101	HEM	C3B-CAB	3.79	1.55	1.47
34	V	201	HEM	C3C-CAC	3.79	1.55	1.47
23	C	507	CLA	CHB-C4A	3.82	1.38	1.33
23	b	612	CLA	CHB-C4A	3.83	1.38	1.33
23	b	619	CLA	CHB-C4A	3.83	1.38	1.33
23	B	610	CLA	CHB-C4A	3.84	1.38	1.33
23	C	506	CLA	CHB-C4A	3.85	1.38	1.33
34	v	201	HEM	C3C-CAC	3.86	1.55	1.47
23	A	405	CLA	CHB-C4A	3.86	1.38	1.33
23	B	611	CLA	CHB-C4A	3.90	1.38	1.33
23	B	613	CLA	CHB-C4A	3.91	1.38	1.33
23	B	606	CLA	CHB-C4A	3.91	1.38	1.33
34	f	101	HEM	C3C-CAC	3.92	1.55	1.47
23	c	506	CLA	CHB-C4A	3.94	1.38	1.33
23	B	601	CLA	CHB-C4A	3.95	1.38	1.33
23	b	607	CLA	CHB-C4A	3.95	1.38	1.33
34	F	101	HEM	C3C-CAC	3.97	1.55	1.47
23	b	617	CLA	CHB-C4A	3.98	1.38	1.33
23	b	616	CLA	CHB-C4A	3.98	1.38	1.33
23	A	407	CLA	CHB-C4A	4.00	1.38	1.33
23	c	502	CLA	CHB-C4A	4.01	1.38	1.33
23	B	607	CLA	CHB-C4A	4.02	1.38	1.33
23	B	602	CLA	CHB-C4A	4.03	1.38	1.33
23	b	609	CLA	CHB-C4A	4.03	1.38	1.33
23	a	409	CLA	CHB-C4A	4.04	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	415	LHG	O7-C7	4.04	1.46	1.34
23	c	508	CLA	CHB-C4A	4.04	1.38	1.33
29	A	412	LHG	O7-C7	4.05	1.46	1.34
29	a	414	LHG	O7-C7	4.06	1.46	1.34
23	b	611	CLA	CHB-C4A	4.06	1.38	1.33
23	D	403	CLA	CHB-C4A	4.06	1.38	1.33
23	C	513	CLA	CHB-C4A	4.07	1.38	1.33
23	B	603	CLA	CHB-C4A	4.08	1.38	1.33
23	B	608	CLA	CHB-C4A	4.09	1.38	1.33
23	B	605	CLA	CHB-C4A	4.09	1.38	1.33
23	B	616	CLA	CHB-C4A	4.10	1.38	1.33
29	a	417	LHG	O7-C7	4.10	1.46	1.34
23	B	612	CLA	CHB-C4A	4.10	1.38	1.33
23	C	503	CLA	CHB-C4A	4.11	1.38	1.33
23	c	504	CLA	CHB-C4A	4.13	1.38	1.33
23	c	512	CLA	CHB-C4A	4.14	1.38	1.33
23	D	401	CLA	CHB-C4A	4.17	1.38	1.33
23	C	505	CLA	CHB-C4A	4.18	1.38	1.33
23	b	613	CLA	CHB-C4A	4.18	1.38	1.33
23	c	507	CLA	CHB-C4A	4.20	1.38	1.33
23	C	512	CLA	CHB-C4A	4.20	1.38	1.33
23	b	605	CLA	CHB-C4A	4.21	1.38	1.33
29	A	412	LHG	O8-C23	4.21	1.45	1.33
23	c	505	CLA	CHB-C4A	4.22	1.38	1.33
23	C	508	CLA	CHB-C4A	4.23	1.38	1.33
23	a	406	CLA	CHB-C4A	4.23	1.38	1.33
29	A	415	LHG	O8-C23	4.24	1.45	1.33
23	b	610	CLA	CHB-C4A	4.25	1.38	1.33
23	C	510	CLA	CHB-C4A	4.26	1.39	1.33
29	a	417	LHG	O8-C23	4.26	1.45	1.33
23	B	614	CLA	CHB-C4A	4.27	1.39	1.33
23	c	501	CLA	CHB-C4A	4.27	1.39	1.33
23	B	615	CLA	CHB-C4A	4.28	1.39	1.33
23	c	513	CLA	CHB-C4A	4.28	1.39	1.33
23	c	503	CLA	CHB-C4A	4.28	1.39	1.33
23	a	404	CLA	CHB-C4A	4.31	1.39	1.33
23	C	501	CLA	CHB-C4A	4.32	1.39	1.33
29	a	414	LHG	O8-C23	4.32	1.46	1.33
23	B	604	CLA	CHB-C4A	4.37	1.39	1.33
23	b	615	CLA	CHB-C4A	4.39	1.39	1.33
23	c	509	CLA	CHB-C4A	4.42	1.39	1.33
23	b	608	CLA	CHB-C4A	4.44	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	618	CLA	CHB-C4A	4.47	1.39	1.33
23	A	403	CLA	CHB-C4A	4.51	1.39	1.33
23	d	403	CLA	CHB-C4A	4.52	1.39	1.33
23	d	402	CLA	CHB-C4A	4.52	1.39	1.33
23	C	511	CLA	CHB-C4A	4.52	1.39	1.33
23	C	502	CLA	CHB-C4A	4.63	1.39	1.33
23	b	620	CLA	CHB-C4A	4.63	1.39	1.33
23	c	511	CLA	CHB-C4A	4.77	1.39	1.33
34	F	101	HEM	C3D-C2D	5.48	1.53	1.37
34	f	101	HEM	C3D-C2D	5.50	1.54	1.37
34	V	201	HEM	C3D-C2D	5.54	1.54	1.37
34	v	201	HEM	C3D-C2D	5.70	1.54	1.37

All (1529) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	j	102	BCR	C32-C1-C6	-13.67	88.14	110.31
27	J	102	BCR	C32-C1-C6	-13.38	88.62	110.31
27	T	102	BCR	C7-C8-C9	-8.82	112.96	126.21
27	B	618	BCR	C7-C8-C9	-8.67	113.18	126.21
27	J	102	BCR	C32-C1-C31	-8.47	82.55	108.50
27	j	102	BCR	C32-C1-C31	-8.45	82.62	108.50
27	d	405	BCR	C7-C8-C9	-6.77	116.04	126.21
30	A	417	SQD	C5-C6-S	-6.50	105.28	114.34
27	D	405	BCR	C7-C8-C9	-6.47	116.49	126.21
27	J	102	BCR	C15-C14-C13	-6.18	118.48	127.31
27	b	622	BCR	C24-C23-C22	-6.06	117.11	126.21
27	B	618	BCR	C11-C10-C9	-5.60	119.32	127.31
30	a	401	SQD	C5-C6-S	-5.58	106.56	114.34
27	J	102	BCR	C28-C27-C26	-5.55	104.23	113.78
27	c	514	BCR	C15-C14-C13	-5.54	119.40	127.31
27	J	102	BCR	C32-C1-C2	-5.47	87.22	108.80
27	j	102	BCR	C15-C14-C13	-5.45	119.54	127.31
27	j	102	BCR	C32-C1-C2	-5.40	87.49	108.80
27	z	101	BCR	C15-C14-C13	-5.39	119.62	127.31
27	B	620	BCR	C24-C23-C22	-5.39	118.12	126.21
27	b	622	BCR	C3-C4-C5	-5.37	104.54	113.78
27	j	102	BCR	C28-C27-C26	-5.27	104.72	113.78
27	D	405	BCR	C28-C27-C26	-5.11	105.00	113.78
27	D	405	BCR	C11-C10-C9	-5.09	120.04	127.31
27	j	102	BCR	C20-C21-C22	-5.07	120.07	127.31
27	a	412	BCR	C33-C5-C6	-5.03	118.88	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	d	405	BCR	C28-C27-C26	-4.97	105.24	113.78
27	j	102	BCR	C11-C10-C9	-4.97	120.22	127.31
27	J	102	BCR	C20-C21-C22	-4.96	120.23	127.31
27	C	516	BCR	C7-C8-C9	-4.96	118.76	126.21
27	j	102	BCR	C24-C23-C22	-4.94	118.79	126.21
27	y	101	BCR	C15-C14-C13	-4.90	120.32	127.31
27	c	514	BCR	C33-C5-C6	-4.86	119.07	124.51
27	B	618	BCR	C3-C4-C5	-4.84	105.46	113.78
28	c	517	DGD	O5D-C6D-C5D	-4.83	100.87	108.94
27	B	620	BCR	C3-C4-C5	-4.81	105.51	113.78
27	C	515	BCR	C15-C14-C13	-4.79	120.47	127.31
27	T	102	BCR	C28-C27-C26	-4.77	105.58	113.78
27	C	514	BCR	C33-C5-C6	-4.73	119.21	124.51
27	B	620	BCR	C16-C17-C18	-4.71	120.59	127.31
27	T	102	BCR	C3-C4-C5	-4.70	105.70	113.78
27	J	102	BCR	C24-C23-C22	-4.65	119.23	126.21
27	T	102	BCR	C11-C10-C9	-4.64	120.68	127.31
27	c	515	BCR	C7-C8-C9	-4.64	119.24	126.21
27	k	102	BCR	C15-C14-C13	-4.63	120.70	127.31
27	A	410	BCR	C33-C5-C6	-4.62	119.33	124.51
27	b	622	BCR	C16-C17-C18	-4.56	120.80	127.31
27	J	102	BCR	C11-C10-C9	-4.55	120.82	127.31
27	C	514	BCR	C15-C14-C13	-4.47	120.93	127.31
28	C	518	DGD	O5D-C6D-C5D	-4.47	101.47	108.94
27	b	621	BCR	C15-C14-C13	-4.45	120.96	127.31
27	k	102	BCR	C24-C23-C22	-4.44	119.54	126.21
27	c	515	BCR	C15-C14-C13	-4.43	120.99	127.31
27	y	101	BCR	C16-C17-C18	-4.41	121.01	127.31
27	y	101	BCR	C7-C8-C9	-4.41	119.59	126.21
27	J	102	BCR	C16-C17-C18	-4.41	121.02	127.31
27	B	619	BCR	C20-C21-C22	-4.40	121.03	127.31
27	B	617	BCR	C16-C17-C18	-4.40	121.03	127.31
27	B	620	BCR	C15-C14-C13	-4.38	121.06	127.31
28	C	519	DGD	C1D-O6D-C5D	-4.37	105.49	113.72
28	c	518	DGD	C1D-O6D-C5D	-4.36	105.50	113.72
27	B	619	BCR	C28-C27-C26	-4.36	106.29	113.78
27	C	516	BCR	C15-C14-C13	-4.29	121.19	127.31
27	b	621	BCR	C28-C27-C26	-4.27	106.44	113.78
27	j	102	BCR	C7-C8-C9	-4.26	119.81	126.21
27	B	618	BCR	C28-C27-C26	-4.24	106.48	113.78
27	k	102	BCR	C38-C26-C25	-4.24	119.77	124.51
27	H	101	BCR	C33-C5-C6	-4.22	119.78	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	621	BCR	C7-C8-C9	-4.22	119.87	126.21
27	a	412	BCR	C16-C17-C18	-4.20	121.31	127.31
27	B	620	BCR	C38-C26-C25	-4.20	119.80	124.51
23	b	614	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
23	B	610	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
27	C	515	BCR	C16-C17-C18	-4.18	121.34	127.31
27	D	405	BCR	C16-C17-C18	-4.18	121.34	127.31
27	b	622	BCR	C7-C8-C9	-4.18	119.94	126.21
27	d	405	BCR	C15-C14-C13	-4.16	121.37	127.31
27	d	405	BCR	C33-C5-C6	-4.16	119.85	124.51
27	d	405	BCR	C11-C10-C9	-4.16	121.37	127.31
27	D	405	BCR	C33-C5-C6	-4.16	119.86	124.51
27	c	515	BCR	C16-C17-C18	-4.13	121.41	127.31
27	A	410	BCR	C15-C14-C13	-4.12	121.42	127.31
27	C	514	BCR	C3-C4-C5	-4.12	106.70	113.78
27	z	101	BCR	C16-C17-C18	-4.09	121.47	127.31
27	b	621	BCR	C20-C21-C22	-4.08	121.48	127.31
27	T	101	BCR	C24-C23-C22	-4.07	120.10	126.21
27	c	515	BCR	C28-C27-C26	-4.06	106.80	113.78
27	a	412	BCR	C24-C23-C22	-4.04	120.14	126.21
27	B	617	BCR	C7-C8-C9	-4.04	120.14	126.21
27	B	617	BCR	C15-C14-C13	-4.04	121.55	127.31
28	A	411	DGD	C1D-O6D-C5D	-4.02	106.15	113.72
27	b	622	BCR	C15-C14-C13	-4.02	121.58	127.31
27	D	405	BCR	C15-C14-C13	-4.01	121.59	127.31
27	a	412	BCR	C38-C26-C25	-4.00	120.03	124.51
27	k	102	BCR	C7-C8-C9	-4.00	120.20	126.21
27	a	412	BCR	C15-C14-C13	-4.00	121.61	127.31
27	b	622	BCR	C38-C26-C25	-3.99	120.04	124.51
27	B	617	BCR	C24-C23-C22	-3.99	120.22	126.21
27	T	101	BCR	C15-C14-C13	-3.98	121.64	127.31
27	c	514	BCR	C11-C10-C9	-3.96	121.66	127.31
23	b	616	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
27	B	620	BCR	C20-C21-C22	-3.95	121.67	127.31
27	y	101	BCR	C3-C4-C5	-3.95	106.99	113.78
27	T	101	BCR	C33-C5-C6	-3.94	120.10	124.51
27	T	101	BCR	C20-C21-C22	-3.94	121.69	127.31
27	k	102	BCR	C16-C17-C18	-3.93	121.70	127.31
27	h	101	BCR	C33-C5-C6	-3.93	120.11	124.51
27	B	619	BCR	C15-C14-C13	-3.93	121.70	127.31
23	b	617	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
27	C	515	BCR	C24-C23-C22	-3.90	120.35	126.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	h	101	BCR	C16-C17-C18	-3.90	121.75	127.31
23	c	504	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
27	b	622	BCR	C11-C10-C9	-3.87	121.79	127.31
27	d	405	BCR	C16-C17-C18	-3.87	121.79	127.31
23	B	613	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
27	J	102	BCR	C7-C8-C9	-3.84	120.44	126.21
27	b	621	BCR	C24-C23-C22	-3.84	120.45	126.21
23	C	507	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
23	B	603	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
23	d	402	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
27	C	516	BCR	C28-C27-C26	-3.82	107.21	113.78
27	j	102	BCR	C16-C17-C18	-3.82	121.86	127.31
30	f	102	SQD	O9-S-O7	-3.81	100.65	113.86
27	D	405	BCR	C24-C23-C22	-3.81	120.49	126.21
31	d	407	LMG	C1-O6-C5	-3.80	106.56	113.72
30	a	415	SQD	O9-S-O7	-3.79	100.72	113.86
27	y	101	BCR	C38-C26-C25	-3.79	120.27	124.51
30	A	413	SQD	O9-S-O7	-3.78	100.74	113.86
30	F	102	SQD	O9-S-O7	-3.78	100.75	113.86
27	B	617	BCR	C33-C5-C6	-3.77	120.28	124.51
27	a	412	BCR	C3-C4-C5	-3.77	107.30	113.78
23	D	401	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
23	B	612	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
23	C	508	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
30	D	408	SQD	O9-S-O7	-3.75	100.87	113.86
23	B	614	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
27	C	515	BCR	C33-C5-C6	-3.73	120.33	124.51
23	A	407	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
23	c	506	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
27	A	410	BCR	C16-C17-C18	-3.71	122.01	127.31
30	d	408	SQD	O9-S-O7	-3.71	100.99	113.86
27	h	101	BCR	C15-C14-C13	-3.71	122.02	127.31
23	c	508	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
27	z	101	BCR	C24-C23-C22	-3.70	120.65	126.21
27	c	515	BCR	C11-C10-C9	-3.70	122.03	127.31
31	m	102	LMG	C1-O6-C5	-3.70	106.75	113.72
23	B	611	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
27	A	410	BCR	C3-C4-C5	-3.69	107.44	113.78
27	c	514	BCR	C3-C4-C5	-3.68	107.44	113.78
23	A	404	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
27	C	516	BCR	C38-C26-C25	-3.67	120.40	124.51
27	H	101	BCR	C24-C23-C22	-3.65	120.72	126.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
27	b	621	BCR	C3-C4-C5	-3.65	107.50	113.78
23	B	606	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
23	B	608	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
23	a	405	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
23	C	503	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
27	d	405	BCR	C24-C23-C22	-3.61	120.79	126.21
23	c	507	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
27	C	516	BCR	C16-C17-C18	-3.60	122.17	127.31
23	B	616	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
23	b	619	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
30	b	601	SQD	O9-S-O7	-3.59	101.43	113.86
27	b	622	BCR	C4-C5-C6	-3.55	117.53	122.74
27	c	514	BCR	C35-C13-C14	-3.55	117.96	122.92
23	a	404	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
27	B	620	BCR	C11-C10-C9	-3.54	122.25	127.31
27	A	410	BCR	C38-C26-C25	-3.54	120.54	124.51
23	b	607	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
23	B	607	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
28	b	623	DGD	C1D-O6D-C5D	-3.54	107.05	113.72
23	C	504	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
23	b	606	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
27	k	102	BCR	C3-C4-C5	-3.52	107.72	113.78
27	z	101	BCR	C3-C4-C5	-3.52	107.73	113.78
30	B	626	SQD	O9-S-O7	-3.50	101.72	113.86
27	C	515	BCR	C3-C4-C5	-3.50	107.76	113.78
27	C	514	BCR	C11-C10-C9	-3.50	122.32	127.31
27	k	102	BCR	C20-C21-C22	-3.49	122.33	127.31
23	C	506	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
23	D	403	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
23	c	510	CLA	CMB-C2B-C1B	-3.47	123.12	128.46
27	c	514	BCR	C16-C17-C18	-3.47	122.35	127.31
27	h	101	BCR	C24-C23-C22	-3.47	121.00	126.21
23	b	615	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	b	618	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
27	C	516	BCR	C33-C5-C6	-3.44	120.65	124.51
28	B	621	DGD	C1D-O6D-C5D	-3.44	107.23	113.72
31	A	414	LMG	C1-O6-C5	-3.43	107.25	113.72
23	A	405	CLA	O2D-CGD-O1D	-3.43	116.91	123.82
23	b	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
27	z	101	BCR	C33-C5-C6	-3.43	120.67	124.51
23	c	513	CLA	CMB-C2B-C1B	-3.42	123.20	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	401	SQD	O9-S-O7	-3.42	102.02	113.86
27	B	617	BCR	C11-C10-C9	-3.41	122.44	127.31
27	H	101	BCR	C16-C17-C18	-3.41	122.44	127.31
27	C	515	BCR	C11-C10-C9	-3.41	122.44	127.31
27	A	410	BCR	C20-C21-C22	-3.41	122.44	127.31
27	c	515	BCR	C33-C5-C6	-3.41	120.69	124.51
31	M	101	LMG	C1-O6-C5	-3.41	107.30	113.72
23	A	403	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
31	m	102	LMG	C6-C5-C4	-3.39	105.07	113.00
28	A	411	DGD	C3G-C2G-C1G	-3.39	104.21	111.86
27	B	618	BCR	C38-C26-C25	-3.38	120.73	124.51
27	b	622	BCR	C20-C21-C22	-3.37	122.50	127.31
27	c	515	BCR	C38-C26-C25	-3.37	120.73	124.51
23	C	502	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
23	C	512	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
23	a	406	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
27	B	620	BCR	C4-C5-C6	-3.36	117.81	122.74
23	C	510	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
23	a	405	CLA	C1-C2-C3	-3.35	119.79	125.96
27	c	514	BCR	C7-C6-C5	-3.34	113.58	121.54
27	b	621	BCR	C16-C17-C18	-3.34	122.55	127.31
23	B	615	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
27	A	410	BCR	C11-C10-C9	-3.32	122.57	127.31
27	T	102	BCR	C38-C26-C25	-3.32	120.79	124.51
23	A	405	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
27	C	514	BCR	C20-C21-C22	-3.32	122.57	127.31
23	B	609	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
31	M	101	LMG	C6-C5-C4	-3.31	105.25	113.00
24	A	406	PHO	O2D-CGD-O1D	-3.30	117.17	123.82
23	B	606	CLA	O2D-CGD-O1D	-3.30	117.17	123.82
30	A	417	SQD	O9-S-O7	-3.29	102.45	113.86
27	T	101	BCR	C7-C8-C9	-3.29	121.27	126.21
27	c	514	BCR	C20-C21-C22	-3.29	122.62	127.31
23	b	611	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
23	c	503	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
27	B	619	BCR	C3-C4-C5	-3.28	108.15	113.78
23	B	605	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
27	k	102	BCR	C33-C5-C6	-3.27	120.84	124.51
23	b	612	CLA	O2D-CGD-O1D	-3.27	117.24	123.82
23	c	502	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
23	b	605	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
23	B	607	CLA	O2D-CGD-O1D	-3.25	117.29	123.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	101	BCR	C11-C10-C9	-3.24	122.69	127.31
23	B	601	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
23	B	602	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
31	c	519	LMG	C1-O6-C5	-3.21	107.66	113.72
27	T	101	BCR	C16-C17-C18	-3.21	122.72	127.31
27	y	101	BCR	C24-C23-C22	-3.21	121.39	126.21
27	c	515	BCR	C3-C4-C5	-3.21	108.26	113.78
27	C	514	BCR	C7-C6-C5	-3.21	113.90	121.54
23	a	409	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
27	A	410	BCR	C24-C23-C22	-3.20	121.41	126.21
27	B	619	BCR	C16-C17-C18	-3.19	122.75	127.31
28	a	413	DGD	C1D-O6D-C5D	-3.19	107.70	113.72
31	d	407	LMG	C1-C2-C3	-3.19	104.05	109.98
23	c	512	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
27	C	516	BCR	C20-C21-C22	-3.18	122.77	127.31
27	H	101	BCR	C15-C14-C13	-3.17	122.78	127.31
27	z	101	BCR	C20-C21-C22	-3.17	122.79	127.31
23	C	513	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
31	D	407	LMG	C1-O6-C5	-3.16	107.77	113.72
27	C	516	BCR	C3-C4-C5	-3.15	108.37	113.78
23	d	403	CLA	O2D-CGD-O1D	-3.14	117.51	123.82
27	C	514	BCR	C28-C27-C26	-3.13	108.40	113.78
23	c	505	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
31	C	520	LMG	C1-O6-C5	-3.12	107.83	113.72
25	d	404	PL9	C7-C8-C9	-3.12	121.49	126.71
23	b	607	CLA	O2D-CGD-O1D	-3.12	117.54	123.82
31	a	402	LMG	C6-C5-C4	-3.11	105.72	113.00
27	j	102	BCR	C27-C26-C25	-3.11	118.17	122.74
23	D	401	CLA	O2D-CGD-O1D	-3.10	117.58	123.82
34	F	101	HEM	CBA-CAA-C2A	-3.09	106.58	112.48
27	y	101	BCR	C33-C5-C6	-3.08	121.06	124.51
23	c	512	CLA	O2D-CGD-O1D	-3.08	117.62	123.82
27	H	101	BCR	C20-C21-C22	-3.08	122.92	127.31
25	D	404	PL9	C22-C23-C24	-3.07	119.96	127.68
23	c	502	CLA	O2D-CGD-O1D	-3.06	117.67	123.82
27	b	621	BCR	C11-C10-C9	-3.05	122.95	127.31
23	A	404	CLA	C1-C2-C3	-3.05	120.34	125.96
23	C	507	CLA	O2D-CGD-O1D	-3.04	117.71	123.82
23	b	608	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
23	C	511	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
27	B	620	BCR	C7-C8-C9	-3.03	121.66	126.21
27	H	101	BCR	C8-C7-C6	-3.03	118.77	127.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	619	BCR	C33-C5-C6	-3.02	121.12	124.51
34	f	101	HEM	CBA-CAA-C2A	-3.02	106.72	112.48
23	C	509	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
23	c	503	CLA	O2D-CGD-O1D	-3.01	117.76	123.82
23	a	406	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
23	C	511	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
27	B	617	BCR	C38-C26-C25	-3.00	121.15	124.51
27	C	514	BCR	C38-C26-C25	-3.00	121.15	124.51
23	c	501	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
27	J	102	BCR	C27-C26-C25	-2.99	118.36	122.74
31	a	416	LMG	C1-O6-C5	-2.98	108.10	113.72
23	C	510	CLA	O2D-CGD-O1D	-2.97	117.84	123.82
23	d	403	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
23	c	504	CLA	O2D-CGD-O1D	-2.97	117.85	123.82
27	B	619	BCR	C11-C10-C9	-2.97	123.07	127.31
23	c	511	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
31	D	407	LMG	C1-C2-C3	-2.96	104.47	109.98
27	C	515	BCR	C20-C21-C22	-2.96	123.08	127.31
27	B	618	BCR	C4-C5-C6	-2.96	118.40	122.74
27	c	514	BCR	C34-C9-C10	-2.96	118.78	122.92
23	c	501	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
23	b	605	CLA	O2D-CGD-O1D	-2.95	117.89	123.82
27	h	101	BCR	C10-C11-C12	-2.94	114.22	123.23
23	b	613	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
23	c	510	CLA	O2D-CGD-O1D	-2.94	117.91	123.82
31	A	418	LMG	C6-C5-C4	-2.93	106.14	113.00
23	b	606	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
25	d	404	PL9	C37-C38-C39	-2.92	120.35	127.68
23	B	604	CLA	O2D-CGD-O1D	-2.92	117.95	123.82
23	c	506	CLA	O2D-CGD-O1D	-2.92	117.95	123.82
23	C	505	CLA	O2D-CGD-O1D	-2.91	117.96	123.82
27	c	514	BCR	C28-C27-C26	-2.91	108.78	113.78
25	D	404	PL9	C12-C13-C14	-2.91	120.38	127.68
27	h	101	BCR	C20-C21-C22	-2.90	123.17	127.31
25	a	410	PL9	C22-C23-C24	-2.89	120.42	127.68
28	A	411	DGD	C4D-C3D-C2D	-2.89	105.74	110.84
23	B	604	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
31	C	521	LMG	C1-O6-C5	-2.87	108.30	113.72
27	b	621	BCR	C33-C5-C6	-2.87	121.29	124.51
25	d	404	PL9	C22-C23-C24	-2.87	120.47	127.68
24	a	407	PHO	O2D-CGD-O1D	-2.87	118.05	123.82
27	c	515	BCR	C20-C21-C22	-2.87	123.22	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	O2D-CGD-O1D	-2.86	118.07	123.82
27	B	619	BCR	C24-C23-C22	-2.86	121.92	126.21
24	D	402	PHO	CBD-CHA-C4D	-2.86	105.32	108.54
27	J	102	BCR	C35-C13-C14	-2.86	118.92	122.92
31	k	103	LMG	C1-O6-C5	-2.86	108.33	113.72
23	b	610	CLA	O2D-CGD-O1D	-2.85	118.08	123.82
27	j	102	BCR	C33-C5-C6	-2.85	121.32	124.51
27	B	617	BCR	C20-C21-C22	-2.84	123.25	127.31
25	D	404	PL9	C37-C38-C39	-2.84	120.55	127.68
27	C	514	BCR	C34-C9-C10	-2.84	118.95	122.92
31	B	623	LMG	C1-O6-C5	-2.83	108.38	113.72
23	b	609	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
24	A	406	PHO	CBD-CHA-C4D	-2.83	105.35	108.54
27	J	102	BCR	C33-C5-C6	-2.82	121.35	124.51
23	C	505	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
23	c	513	CLA	O2D-CGD-O1D	-2.81	118.17	123.82
23	b	613	CLA	O2D-CGD-O1D	-2.80	118.18	123.82
24	a	408	PHO	O2D-CGD-O1D	-2.80	118.18	123.82
33	D	410	LMT	C1B-O1B-C4'	-2.80	111.17	118.00
27	C	515	BCR	C15-C16-C17	-2.80	117.49	123.46
27	D	405	BCR	C3-C4-C5	-2.80	108.97	113.78
23	b	615	CLA	O2D-CGD-O1D	-2.79	118.20	123.82
27	C	515	BCR	C7-C8-C9	-2.79	122.02	126.21
25	d	404	PL9	C7-C3-C2	-2.79	119.26	123.23
23	b	614	CLA	O2D-CGD-O1D	-2.78	118.24	123.82
31	D	406	LMG	O8-C28-O10	-2.77	116.67	123.55
23	B	607	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
23	b	617	CLA	O2D-CGD-O1D	-2.77	118.25	123.82
28	A	411	DGD	O4D-C4D-C5D	-2.77	102.31	109.28
25	A	408	PL9	C22-C23-C24	-2.76	120.74	127.68
23	c	508	CLA	O2D-CGD-O1D	-2.76	118.27	123.82
23	B	614	CLA	O2D-CGD-O1D	-2.75	118.28	123.82
27	H	101	BCR	C10-C11-C12	-2.75	114.80	123.23
23	C	503	CLA	O2D-CGD-O1D	-2.74	118.30	123.82
23	B	609	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
28	a	413	DGD	C3G-C2G-C1G	-2.74	105.67	111.86
31	I	101	LMG	C1-O6-C5	-2.74	108.55	113.72
31	i	101	LMG	C1-O6-C5	-2.74	108.56	113.72
23	C	501	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
27	C	514	BCR	C16-C17-C18	-2.74	123.40	127.31
27	B	618	BCR	C21-C20-C19	-2.74	114.84	123.23
28	c	516	DGD	C1D-O6D-C5D	-2.74	108.56	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
27	a	412	BCR	C34-C9-C10	-2.73	119.10	122.92
31	d	406	LMG	O8-C28-O10	-2.72	116.78	123.55
28	c	518	DGD	C4D-C3D-C2D	-2.72	106.04	110.84
23	C	502	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
23	b	618	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
23	b	620	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
23	C	504	CLA	C1B-CHB-C4A	-2.71	124.76	130.12
23	B	611	CLA	O2D-CGD-O1D	-2.71	118.38	123.82
23	A	403	CLA	O2D-CGD-O1D	-2.69	118.40	123.82
28	b	602	DGD	C6D-C5D-C4D	-2.69	106.28	112.00
23	c	509	CLA	CMB-C2B-C1B	-2.69	124.34	128.46
27	k	102	BCR	C35-C13-C14	-2.68	119.17	122.92
23	C	512	CLA	O2D-CGD-O1D	-2.68	118.42	123.82
23	C	501	CLA	O2D-CGD-O1D	-2.68	118.42	123.82
23	A	404	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
27	T	102	BCR	C4-C5-C6	-2.68	118.81	122.74
23	b	611	CLA	O2D-CGD-O1D	-2.68	118.43	123.82
23	C	506	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
23	C	506	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
27	C	516	BCR	C11-C10-C9	-2.67	123.50	127.31
27	T	102	BCR	C21-C20-C19	-2.67	115.06	123.23
23	b	606	CLA	O2D-CGD-O1D	-2.67	118.46	123.82
27	y	101	BCR	C20-C21-C22	-2.66	123.51	127.31
23	A	405	CLA	C1-C2-C3	-2.66	121.06	125.96
28	C	518	DGD	O4D-C4D-C5D	-2.66	102.58	109.28
27	D	405	BCR	C23-C24-C25	-2.66	119.82	127.25
27	C	515	BCR	C8-C7-C6	-2.65	119.82	127.25
27	d	405	BCR	C38-C26-C25	-2.65	121.54	124.51
23	B	605	CLA	O2D-CGD-O1D	-2.65	118.49	123.82
23	a	404	CLA	O2A-CGA-O1A	-2.65	116.97	123.55
31	a	402	LMG	C1-O6-C5	-2.64	108.75	113.72
23	c	510	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
27	A	410	BCR	C34-C9-C10	-2.64	119.23	122.92
23	C	507	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
27	c	514	BCR	C38-C26-C25	-2.63	121.56	124.51
23	b	620	CLA	O2D-CGD-O1D	-2.62	118.54	123.82
23	a	406	CLA	C1-C2-C3	-2.62	121.12	125.96
27	H	101	BCR	C38-C26-C25	-2.62	121.57	124.51
23	c	506	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
27	h	101	BCR	C38-C26-C25	-2.62	121.58	124.51
23	a	405	CLA	O2D-CGD-O1D	-2.62	118.56	123.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	O2D-CGD-O1D	-2.61	118.56	123.82
23	B	604	CLA	O2A-CGA-O1A	-2.61	117.06	123.55
24	a	407	PHO	CBD-CHA-C4D	-2.61	105.60	108.54
23	B	608	CLA	O2D-CGD-O1D	-2.61	118.57	123.82
27	C	514	BCR	C35-C13-C14	-2.61	119.27	122.92
25	J	101	PL9	C7-C3-C2	-2.61	119.52	123.23
25	D	404	PL9	C7-C8-C9	-2.61	122.35	126.71
23	B	610	CLA	O2D-CGD-O1D	-2.61	118.58	123.82
27	a	412	BCR	C11-C10-C9	-2.60	123.59	127.31
27	T	101	BCR	C38-C26-C25	-2.60	121.60	124.51
23	b	619	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
27	J	102	BCR	C36-C18-C17	-2.60	119.28	122.92
23	B	609	CLA	O2D-CGD-O1D	-2.60	118.59	123.82
23	A	404	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
23	C	504	CLA	O2D-CGD-O1D	-2.59	118.62	123.82
23	a	405	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
33	b	626	LMT	C1B-O1B-C4'	-2.58	111.71	118.00
23	b	608	CLA	O2D-CGD-O1D	-2.58	118.63	123.82
27	z	101	BCR	C8-C7-C6	-2.58	120.04	127.25
27	b	621	BCR	C8-C7-C6	-2.57	120.05	127.25
27	C	515	BCR	C28-C27-C26	-2.57	109.36	113.78
23	b	619	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
27	y	101	BCR	C35-C13-C14	-2.57	119.33	122.92
27	J	102	BCR	C1-C6-C5	-2.57	118.98	122.59
27	T	102	BCR	C23-C24-C25	-2.56	120.08	127.25
27	D	405	BCR	C21-C20-C19	-2.56	115.37	123.23
28	C	519	DGD	C4D-C3D-C2D	-2.56	106.32	110.84
34	f	101	HEM	C1D-C2D-C3D	-2.56	105.22	107.00
23	B	615	CLA	O2D-CGD-O1D	-2.56	118.67	123.82
23	B	601	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
27	d	405	BCR	C23-C24-C25	-2.55	120.10	127.25
27	C	514	BCR	C24-C23-C22	-2.55	122.38	126.21
23	B	601	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
23	b	611	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
23	c	502	CLA	C1B-CHB-C4A	-2.55	125.08	130.12
23	a	409	CLA	O2D-CGD-O1D	-2.55	118.70	123.82
23	b	614	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
27	h	101	BCR	C8-C7-C6	-2.54	120.15	127.25
23	c	505	CLA	O2D-CGD-O1D	-2.53	118.72	123.82
23	D	401	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
27	J	102	BCR	C37-C22-C21	-2.53	119.38	122.92
31	m	102	LMG	O4-C4-C3	-2.53	104.86	110.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	415	SQD	C5-C6-S	-2.52	110.83	114.34
23	B	614	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
23	c	507	CLA	O2D-CGD-O1D	-2.51	118.76	123.82
25	d	404	PL9	C32-C33-C34	-2.51	121.37	127.68
25	j	101	PL9	C7-C3-C2	-2.51	119.66	123.23
23	b	612	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	a	404	CLA	O2D-CGD-O1D	-2.51	118.77	123.82
23	a	409	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
23	B	611	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
31	b	625	LMG	C1-O6-C5	-2.50	109.02	113.72
27	j	102	BCR	C35-C13-C14	-2.49	119.43	122.92
27	T	102	BCR	C15-C14-C13	-2.49	123.75	127.31
23	C	513	CLA	O2D-CGD-O1D	-2.49	118.81	123.82
23	d	402	CLA	O2D-CGD-O1D	-2.48	118.82	123.82
23	C	513	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
33	d	410	LMT	C1B-O1B-C4'	-2.48	111.96	118.00
23	B	602	CLA	O2D-CGD-O1D	-2.48	118.84	123.82
31	m	102	LMG	O8-C9-C8	-2.47	102.44	108.66
23	D	401	CLA	O2A-CGA-O1A	-2.47	117.42	123.55
28	C	518	DGD	C1D-O6D-C5D	-2.46	109.07	113.72
23	A	405	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
27	d	405	BCR	C16-C15-C14	-2.46	118.21	123.46
27	d	405	BCR	C3-C4-C5	-2.46	109.55	113.78
28	c	517	DGD	C1D-O6D-C5D	-2.46	109.08	113.72
31	b	625	LMG	C6-C5-C4	-2.46	107.25	113.00
25	d	404	PL9	C12-C13-C14	-2.46	121.50	127.68
23	C	510	CLA	C1-C2-C3	-2.45	121.44	125.96
23	C	508	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
27	B	617	BCR	C3-C4-C5	-2.45	109.57	113.78
28	b	602	DGD	O4D-C4D-C5D	-2.45	103.11	109.28
23	b	609	CLA	O2D-CGD-O1D	-2.45	118.89	123.82
27	D	405	BCR	C27-C26-C25	-2.45	119.15	122.74
23	c	505	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
27	a	412	BCR	C20-C21-C22	-2.44	123.82	127.31
24	a	407	PHO	C2B-C1B-NB	-2.44	106.20	109.82
28	a	413	DGD	C6E-C5E-C4E	-2.44	107.29	113.00
23	D	403	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
23	B	610	CLA	C1-C2-C3	-2.44	121.46	125.96
23	D	403	CLA	O2D-CGD-O1D	-2.44	118.91	123.82
31	e	101	LMG	C1-O6-C5	-2.44	109.12	113.72
23	C	512	CLA	O2A-CGA-O1A	-2.44	117.50	123.55
23	B	605	CLA	C1B-CHB-C4A	-2.44	125.29	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B	618	BCR	C23-C24-C25	-2.43	120.44	127.25
27	a	412	BCR	C23-C24-C25	-2.43	120.44	127.25
23	B	613	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	B	608	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	c	504	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	A	407	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
27	B	619	BCR	C37-C22-C21	-2.43	119.52	122.92
31	A	418	LMG	C1-O6-C5	-2.42	109.15	113.72
27	h	101	BCR	C15-C16-C17	-2.42	118.29	123.46
27	j	102	BCR	C39-C30-C25	-2.42	106.38	110.31
27	z	101	BCR	C23-C24-C25	-2.42	120.47	127.25
23	b	613	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
31	D	407	LMG	O8-C28-O10	-2.42	117.55	123.55
27	c	514	BCR	C24-C23-C22	-2.41	122.59	126.21
23	a	405	CLA	O2A-CGA-O1A	-2.41	117.57	123.55
23	d	402	CLA	O2A-CGA-O1A	-2.41	117.57	123.55
28	a	413	DGD	O4D-C4D-C5D	-2.41	103.22	109.28
23	B	616	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
27	j	102	BCR	C1-C6-C5	-2.41	119.21	122.59
23	a	409	CLA	O2A-CGA-O1A	-2.41	117.58	123.55
27	d	405	BCR	C21-C20-C19	-2.40	115.86	123.23
27	B	617	BCR	C23-C24-C25	-2.40	120.53	127.25
27	z	101	BCR	C11-C10-C9	-2.40	123.88	127.31
23	a	405	CLA	CAA-C2A-C3A	-2.40	106.23	112.81
25	a	410	PL9	C12-C13-C14	-2.40	121.66	127.68
23	a	406	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
31	a	402	LMG	O3-C3-C4	-2.40	105.14	110.36
23	b	617	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
23	C	513	CLA	O2A-CGA-O1A	-2.39	117.62	123.55
27	B	617	BCR	C36-C18-C17	-2.39	119.58	122.92
23	b	618	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
31	b	624	LMG	C1-O6-C5	-2.38	109.23	113.72
23	b	607	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
27	j	102	BCR	C37-C22-C21	-2.38	119.60	122.92
27	H	101	BCR	C3-C4-C5	-2.37	109.70	113.78
23	b	605	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
24	a	408	PHO	CBD-CHA-C4D	-2.37	105.87	108.54
23	b	617	CLA	O2A-CGA-O1A	-2.37	117.67	123.55
23	b	608	CLA	C1-C2-C3	-2.37	121.60	125.96
31	A	418	LMG	O8-C28-O10	-2.36	117.69	123.55
23	a	404	CLA	C1-C2-C3	-2.36	121.61	125.96
23	c	512	CLA	O2A-CGA-O1A	-2.36	117.69	123.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	405	BCR	C34-C9-C10	-2.36	119.62	122.92
34	F	101	HEM	C1D-C2D-C3D	-2.36	105.36	107.00
27	c	515	BCR	C23-C24-C25	-2.35	120.66	127.25
23	c	509	CLA	O2D-CGD-O1D	-2.35	119.08	123.82
23	B	603	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
27	C	516	BCR	C15-C16-C17	-2.35	118.45	123.46
27	B	618	BCR	C15-C14-C13	-2.35	123.96	127.31
23	C	505	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	B	602	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
31	b	624	LMG	O4-C4-C3	-2.35	105.25	110.36
23	b	616	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
27	T	102	BCR	C15-C16-C17	-2.35	118.46	123.46
27	T	102	BCR	C16-C17-C18	-2.34	123.96	127.31
25	j	101	PL9	C22-C23-C24	-2.34	121.80	127.68
23	c	508	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	C	512	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	c	513	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
23	A	405	CLA	O2A-CGA-O1A	-2.34	117.75	123.55
27	y	101	BCR	C11-C10-C9	-2.33	123.98	127.31
23	c	509	CLA	C1-C2-C3	-2.33	121.67	125.96
28	a	413	DGD	C4D-C3D-C2D	-2.33	106.73	110.84
23	B	610	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
27	J	102	BCR	C11-C12-C13	-2.33	119.87	126.42
31	e	101	LMG	C6-C5-C4	-2.32	107.56	113.00
27	h	101	BCR	C3-C4-C5	-2.32	109.79	113.78
27	j	102	BCR	C34-C9-C10	-2.32	119.67	122.92
27	B	619	BCR	C15-C16-C17	-2.32	118.52	123.46
27	d	405	BCR	C27-C26-C25	-2.31	119.34	122.74
24	D	402	PHO	C2B-C1B-NB	-2.31	106.39	109.82
27	C	515	BCR	C23-C24-C25	-2.31	120.77	127.25
24	D	402	PHO	O2A-CGA-O1A	-2.31	117.81	123.55
31	k	103	LMG	O8-C28-O10	-2.31	117.81	123.55
25	a	410	PL9	C7-C3-C2	-2.31	119.94	123.23
31	b	625	LMG	O3-C3-C4	-2.31	105.33	110.36
27	z	101	BCR	C28-C27-C26	-2.31	109.81	113.78
27	T	101	BCR	C3-C4-C5	-2.31	109.81	113.78
27	T	102	BCR	C24-C23-C22	-2.31	122.75	126.21
27	B	618	BCR	C34-C9-C10	-2.31	119.69	122.92
23	B	605	CLA	O2A-CGA-O1A	-2.30	117.84	123.55
23	B	601	CLA	O2A-CGA-O1A	-2.30	117.85	123.55
27	B	618	BCR	C16-C17-C18	-2.29	124.04	127.31
23	C	510	CLA	C1B-CHB-C4A	-2.29	125.58	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	405	BCR	C38-C26-C25	-2.29	121.94	124.51
31	i	101	LMG	O8-C28-O10	-2.29	117.86	123.55
28	C	519	DGD	O1G-C1A-O1A	-2.29	117.87	123.55
23	C	509	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
25	j	101	PL9	C12-C13-C14	-2.28	121.94	127.68
27	T	101	BCR	C23-C24-C25	-2.28	120.86	127.25
28	c	516	DGD	C6E-C5E-C4E	-2.28	107.66	113.00
23	C	503	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
30	A	417	SQD	O2-C2-C3	-2.28	105.39	110.36
31	c	519	LMG	C6-C5-C4	-2.28	107.67	113.00
23	C	511	CLA	O2A-CGA-O1A	-2.27	117.91	123.55
31	I	101	LMG	C6-C5-C4	-2.27	107.68	113.00
23	B	611	CLA	C1-C2-C3	-2.27	121.77	125.96
24	A	406	PHO	CMB-C2B-C1B	-2.27	121.51	125.04
25	a	410	PL9	C7-C8-C9	-2.27	122.92	126.71
25	d	404	PL9	C36-C34-C33	-2.26	116.47	121.10
25	J	101	PL9	C12-C13-C14	-2.26	122.00	127.68
23	d	402	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	B	606	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
23	A	403	CLA	O2A-CGA-O1A	-2.26	117.94	123.55
23	b	605	CLA	C1-C2-C3	-2.26	121.80	125.96
31	M	101	LMG	O8-C9-C8	-2.26	102.99	108.66
23	A	407	CLA	O2D-CGD-O1D	-2.25	119.29	123.82
27	b	621	BCR	C27-C26-C25	-2.25	119.43	122.74
28	A	411	DGD	C6E-C5E-C4E	-2.25	107.73	113.00
27	C	516	BCR	C21-C20-C19	-2.25	116.33	123.23
23	c	502	CLA	C1-C2-C3	-2.25	121.81	125.96
31	B	622	LMG	O4-C4-C3	-2.25	105.47	110.36
23	b	605	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
25	A	408	PL9	C26-C24-C23	-2.25	116.50	121.10
23	c	508	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
27	C	515	BCR	C10-C11-C12	-2.25	116.34	123.23
23	b	613	CLA	O2A-CGA-O1A	-2.25	117.97	123.55
34	f	101	HEM	CBD-CAD-C3D	-2.24	108.19	112.47
27	C	515	BCR	C38-C26-C25	-2.24	122.00	124.51
30	B	626	SQD	C10-C9-C8	-2.24	105.02	113.24
23	b	610	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
28	c	517	DGD	O4D-C4D-C5D	-2.24	103.64	109.28
23	c	506	CLA	C1-C2-C3	-2.24	121.83	125.96
25	A	408	PL9	C7-C3-C2	-2.24	120.04	123.23
23	c	507	CLA	O2A-CGA-O1A	-2.24	117.99	123.55
31	E	101	LMG	O9-C10-C11	-2.24	114.83	123.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	627	DGD	C4D-C3D-C2D	-2.24	106.89	110.84
23	b	610	CLA	O2A-CGA-O1A	-2.23	118.00	123.55
27	H	101	BCR	C7-C8-C9	-2.23	122.86	126.21
31	C	520	LMG	O8-C28-O10	-2.23	118.01	123.55
30	b	601	SQD	C10-C9-C8	-2.23	105.06	113.24
25	a	410	PL9	C32-C33-C34	-2.23	122.08	127.68
31	B	623	LMG	O8-C28-O10	-2.23	118.02	123.55
31	e	101	LMG	O7-C10-O9	-2.23	118.12	123.68
27	z	101	BCR	C38-C26-C25	-2.23	122.02	124.51
23	b	619	CLA	O2A-CGA-O1A	-2.23	118.02	123.55
27	C	516	BCR	C23-C24-C25	-2.23	121.02	127.25
23	c	501	CLA	O2A-CGA-O1A	-2.23	118.03	123.55
23	C	504	CLA	O2A-CGA-O1A	-2.22	118.03	123.55
25	A	408	PL9	C12-C13-C14	-2.22	122.09	127.68
23	d	403	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
25	a	410	PL9	C17-C18-C19	-2.22	122.10	127.68
23	B	603	CLA	O2D-CGD-O1D	-2.22	119.35	123.82
24	D	402	PHO	O2D-CGD-O1D	-2.22	119.35	123.82
25	D	404	PL9	C32-C33-C34	-2.22	122.11	127.68
31	B	623	LMG	O3-C3-C4	-2.22	105.53	110.36
23	c	513	CLA	O2A-CGA-O1A	-2.21	118.05	123.55
23	C	502	CLA	C1-C2-C3	-2.21	121.88	125.96
23	b	615	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
31	E	101	LMG	C1-O6-C5	-2.21	109.56	113.72
23	c	507	CLA	C1-C2-C3	-2.20	121.90	125.96
31	d	406	LMG	C6-C5-C4	-2.20	107.84	113.00
23	C	508	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
23	b	615	CLA	C1-C2-C3	-2.20	121.91	125.96
23	C	501	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
23	C	513	CLA	C1-C2-C3	-2.19	121.91	125.96
23	c	503	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
23	c	509	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
27	B	618	BCR	C31-C1-C6	-2.19	106.75	110.31
25	A	408	PL9	C11-C9-C8	-2.19	116.62	121.10
23	B	604	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	c	501	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
27	b	621	BCR	C35-C13-C14	-2.18	119.86	122.92
23	b	606	CLA	C1-C2-C3	-2.18	121.94	125.96
28	d	409	DGD	O2G-C1B-O1B	-2.18	118.25	123.68
23	B	612	CLA	O2D-CGD-O1D	-2.17	119.45	123.82
23	b	613	CLA	C1-C2-C3	-2.17	121.95	125.96
27	A	410	BCR	C23-C24-C25	-2.17	121.17	127.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	O2A-CGA-O1A	-2.17	118.16	123.55
31	A	418	LMG	O3-C3-C4	-2.17	105.64	110.36
27	B	619	BCR	C7-C8-C9	-2.17	122.95	126.21
23	B	616	CLA	OBD-CAD-CBD	-2.17	122.67	125.94
27	j	102	BCR	C11-C12-C13	-2.17	120.33	126.42
23	D	403	CLA	O2A-CGA-O1A	-2.16	118.18	123.55
28	D	409	DGD	C1D-O6D-C5D	-2.16	109.64	113.72
28	c	518	DGD	C6E-C5E-C4E	-2.16	107.94	113.00
31	M	101	LMG	O3-C3-C4	-2.16	105.66	110.36
23	c	512	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
27	c	515	BCR	C21-C20-C19	-2.16	116.61	123.23
23	C	509	CLA	C1-C2-C3	-2.16	121.98	125.96
31	b	625	LMG	O8-C28-O10	-2.16	118.19	123.55
28	A	411	DGD	C6D-C5D-C4D	-2.15	107.41	112.00
31	D	406	LMG	C1-O6-C5	-2.15	109.66	113.72
27	k	102	BCR	C23-C24-C25	-2.15	121.23	127.25
28	B	627	DGD	C6D-C5D-C4D	-2.15	107.42	112.00
24	a	408	PHO	CMB-C2B-C1B	-2.15	121.69	125.04
23	c	501	CLA	C1-C2-C3	-2.14	122.01	125.96
27	j	102	BCR	C15-C16-C17	-2.14	118.89	123.46
23	c	511	CLA	O2A-CGA-O1A	-2.14	118.24	123.55
23	A	404	CLA	O2A-CGA-O1A	-2.14	118.24	123.55
31	C	521	LMG	O3-C3-C4	-2.14	105.70	110.36
23	b	609	CLA	O2A-CGA-O1A	-2.14	118.24	123.55
27	y	101	BCR	C32-C1-C6	-2.13	106.85	110.31
23	C	501	CLA	O2A-CGA-O1A	-2.13	118.25	123.55
23	B	612	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
28	c	518	DGD	O1G-C1A-O1A	-2.13	118.26	123.55
23	B	608	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
23	b	620	CLA	OBD-CAD-CBD	-2.13	122.72	125.94
27	b	621	BCR	C37-C22-C21	-2.13	119.94	122.92
31	m	102	LMG	O3-C3-C4	-2.13	105.73	110.36
25	d	404	PL9	C42-C43-C44	-2.12	122.35	127.68
24	a	407	PHO	O2A-CGA-O1A	-2.12	118.28	123.55
23	c	507	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
31	E	101	LMG	O7-C10-O9	-2.12	118.39	123.68
27	c	514	BCR	C23-C24-C25	-2.12	121.32	127.25
23	A	403	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
27	c	515	BCR	C15-C16-C17	-2.12	118.94	123.46
23	B	615	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
23	B	607	CLA	O2A-CGA-O1A	-2.11	118.31	123.55
31	C	521	LMG	C6-C5-C4	-2.11	108.07	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
23	A	403	CLA	OBD-CAD-CBD	-2.10	122.76	125.94
31	e	101	LMG	O9-C10-C11	-2.10	115.37	123.68
23	c	505	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
23	b	608	CLA	O2A-CGA-O1A	-2.10	118.33	123.55
23	a	404	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
23	b	616	CLA	O2D-CGD-O1D	-2.10	119.59	123.82
23	B	605	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
27	B	618	BCR	C15-C16-C17	-2.10	118.98	123.46
29	a	414	LHG	C5-O7-C7	-2.10	112.92	117.88
27	j	102	BCR	C36-C18-C17	-2.10	119.99	122.92
27	B	620	BCR	C35-C13-C14	-2.09	119.99	122.92
23	C	508	CLA	C1-C2-C3	-2.09	122.10	125.96
27	b	622	BCR	C28-C27-C26	-2.09	110.18	113.78
25	A	408	PL9	C32-C33-C34	-2.09	122.43	127.68
23	C	511	CLA	C1B-CHB-C4A	-2.09	125.99	130.12
23	C	509	CLA	O2D-CGD-O1D	-2.08	119.62	123.82
27	B	619	BCR	C27-C26-C25	-2.08	119.68	122.74
23	a	406	CLA	O2A-CGA-O1A	-2.08	118.39	123.55
24	A	406	PHO	C2B-C1B-NB	-2.08	106.74	109.82
23	b	612	CLA	C1-C2-C3	-2.08	122.12	125.96
27	k	102	BCR	C32-C1-C6	-2.08	106.94	110.31
31	M	101	LMG	O4-C4-C3	-2.08	105.84	110.36
27	B	617	BCR	C8-C7-C6	-2.08	121.44	127.25
23	c	502	CLA	O2A-CGA-O1A	-2.08	118.39	123.55
27	J	102	BCR	C34-C9-C10	-2.08	120.01	122.92
23	C	511	CLA	C1-C2-C3	-2.08	122.13	125.96
27	b	622	BCR	C23-C24-C25	-2.08	121.44	127.25
27	H	101	BCR	C16-C15-C14	-2.08	119.03	123.46
27	H	101	BCR	C21-C20-C19	-2.07	116.87	123.23
27	b	622	BCR	C21-C20-C19	-2.07	116.87	123.23
27	B	618	BCR	C24-C23-C22	-2.07	123.10	126.21
25	D	404	PL9	C7-C3-C2	-2.07	120.28	123.23
31	d	407	LMG	O8-C28-O10	-2.07	118.41	123.55
31	A	414	LMG	O8-C28-O10	-2.07	118.42	123.55
27	D	405	BCR	C16-C15-C14	-2.07	119.05	123.46
27	C	514	BCR	C23-C24-C25	-2.07	121.47	127.25
28	B	621	DGD	C4D-C3D-C2D	-2.06	107.19	110.84
27	J	102	BCR	C30-C25-C26	-2.06	119.69	122.59
34	V	201	HEM	C1D-C2D-C3D	-2.06	105.56	107.00
28	D	409	DGD	O2G-C1B-O1B	-2.06	118.54	123.68
23	b	608	CLA	C1B-CHB-C4A	-2.06	126.04	130.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	k	103	LMG	C6-C5-C4	-2.06	108.18	113.00
28	D	409	DGD	C6D-O5D-C1E	-2.06	109.54	113.76
27	B	620	BCR	C32-C1-C6	-2.06	106.97	110.31
34	v	201	HEM	CAA-CBA-CGA	-2.06	109.15	112.66
31	B	623	LMG	O4-C4-C3	-2.06	105.88	110.36
23	B	611	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
23	c	511	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
23	B	612	CLA	OBD-CAD-CBD	-2.05	122.84	125.94
33	B	625	LMT	C1B-O1B-C4'	-2.05	113.00	118.00
27	k	102	BCR	C11-C10-C9	-2.05	124.39	127.31
31	C	521	LMG	O8-C28-O10	-2.05	118.46	123.55
27	c	515	BCR	C35-C13-C14	-2.05	120.06	122.92
27	b	622	BCR	C20-C19-C18	-2.05	120.67	126.42
28	d	409	DGD	O1G-C1A-O1A	-2.04	118.47	123.55
27	T	101	BCR	C8-C7-C6	-2.04	121.53	127.25
31	c	519	LMG	O3-C3-C4	-2.04	105.92	110.36
29	A	415	LHG	C6-C5-C4	-2.04	107.26	111.86
28	C	517	DGD	O2G-C1B-O1B	-2.03	118.60	123.68
27	T	101	BCR	C36-C18-C17	-2.03	120.08	122.92
25	J	101	PL9	C22-C23-C24	-2.03	122.57	127.68
27	y	101	BCR	C36-C18-C17	-2.03	120.08	122.92
27	z	101	BCR	C10-C11-C12	-2.03	117.01	123.23
23	b	620	CLA	O2A-CGA-O1A	-2.03	118.52	123.55
23	c	506	CLA	O2A-CGA-O1A	-2.03	118.52	123.55
27	C	514	BCR	C39-C30-C25	-2.03	107.02	110.31
23	B	604	CLA	C1-C2-C3	-2.03	122.22	125.96
27	J	102	BCR	C39-C30-C25	-2.03	107.02	110.31
31	I	101	LMG	O3-C3-C4	-2.02	105.95	110.36
27	z	101	BCR	C35-C13-C14	-2.02	120.09	122.92
27	b	622	BCR	C31-C1-C6	-2.02	107.03	110.31
27	z	101	BCR	C36-C18-C17	-2.02	120.09	122.92
27	B	618	BCR	C35-C13-C14	-2.02	120.10	122.92
27	H	101	BCR	C15-C16-C17	-2.01	119.16	123.46
23	C	503	CLA	O2A-CGA-O1A	-2.01	118.55	123.55
27	b	621	BCR	C31-C1-C6	-2.01	107.05	110.31
27	b	621	BCR	C15-C16-C17	-2.01	119.17	123.46
23	C	509	CLA	O2A-CGA-O1A	-2.01	118.56	123.55
23	b	611	CLA	O2A-CGA-O1A	-2.01	118.56	123.55
27	B	620	BCR	C21-C20-C19	-2.01	117.07	123.23
23	A	407	CLA	O2A-CGA-O1A	-2.01	118.57	123.55
25	D	404	PL9	C27-C28-C29	-2.01	122.64	127.68
25	D	404	PL9	C36-C34-C33	-2.00	117.00	121.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	I	101	LMG	O8-C28-O10	-2.00	118.58	123.55
31	a	416	LMG	O8-C28-O10	-2.00	118.58	123.55
28	c	518	DGD	O6D-C1D-O3G	2.00	114.77	110.02
23	B	607	CLA	O2D-CGD-CBD	2.00	114.88	111.30
23	c	503	CLA	O2D-CGD-CBD	2.01	114.88	111.30
23	B	613	CLA	C1D-CHD-C4C	2.01	125.23	122.48
23	C	509	CLA	C1D-CHD-C4C	2.01	125.23	122.48
23	c	507	CLA	CMD-C2D-C3D	2.01	128.63	124.89
33	i	102	LMT	O1B-C4'-C3'	2.01	112.04	107.19
25	a	410	PL9	C15-C14-C16	2.01	118.78	115.29
27	C	515	BCR	C36-C18-C19	2.01	121.31	118.10
28	D	409	DGD	O3D-C3D-C4D	2.01	114.74	110.36
27	J	102	BCR	C33-C5-C4	2.01	117.28	113.45
23	c	513	CLA	CMD-C2D-C3D	2.02	128.63	124.89
23	C	504	CLA	C3A-C2A-C1A	2.02	104.36	101.34
24	D	402	PHO	CBD-CHA-C1A	2.02	131.12	126.36
31	d	407	LMG	O2-C2-C1	2.02	114.26	110.03
23	C	506	CLA	C1D-CHD-C4C	2.03	125.26	122.48
23	b	612	CLA	C1D-CHD-C4C	2.03	125.26	122.48
23	C	509	CLA	CMD-C2D-C3D	2.03	128.66	124.89
27	C	516	BCR	C2-C1-C6	2.03	113.65	110.48
23	a	405	CLA	CMD-C2D-C3D	2.03	128.66	124.89
25	D	404	PL9	C20-C19-C21	2.03	118.81	115.29
25	A	408	PL9	C10-C9-C11	2.03	118.81	115.29
25	A	408	PL9	C15-C14-C16	2.03	118.82	115.29
24	A	406	PHO	CHB-C1B-NB	2.03	128.63	124.64
23	D	401	CLA	CHB-C4A-NA	2.04	127.33	124.51
31	C	520	LMG	C3-C4-C5	2.04	113.81	110.22
23	b	605	CLA	C1D-CHD-C4C	2.04	125.27	122.48
23	b	620	CLA	CMB-C2B-C3B	2.04	128.68	124.89
23	B	613	CLA	CMD-C2D-C3D	2.04	128.68	124.89
27	b	621	BCR	C2-C1-C6	2.04	113.67	110.48
27	B	619	BCR	C38-C26-C27	2.05	117.33	113.45
23	C	513	CLA	CMD-C2D-C3D	2.05	128.69	124.89
30	a	415	SQD	O5-C1-C2	2.05	114.24	110.30
27	T	101	BCR	C33-C5-C4	2.05	117.33	113.45
25	d	404	PL9	C10-C9-C11	2.05	118.84	115.29
23	b	608	CLA	O1D-CGD-CBD	2.05	128.28	124.60
23	C	513	CLA	C1D-CHD-C4C	2.05	125.29	122.48
30	a	401	SQD	O9-S-C6	2.05	108.58	106.83
23	C	510	CLA	C4A-NA-C1A	2.05	109.00	106.45
23	a	404	CLA	C1D-CHD-C4C	2.06	125.30	122.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	625	LMG	C3-C4-C5	2.06	113.85	110.22
27	B	617	BCR	C33-C5-C4	2.06	117.36	113.45
27	y	101	BCR	C38-C26-C27	2.06	117.37	113.45
31	B	623	LMG	O6-C5-C4	2.07	113.47	109.66
28	a	413	DGD	O6D-C1D-O3G	2.07	114.93	110.02
27	C	514	BCR	C34-C9-C8	2.07	121.39	118.10
23	B	603	CLA	CMD-C2D-C3D	2.07	128.73	124.89
33	b	604	LMT	O1B-C4'-C3'	2.07	112.17	107.19
23	b	614	CLA	CMD-C2D-C3D	2.07	128.74	124.89
23	C	501	CLA	C1D-CHD-C4C	2.07	125.32	122.48
23	c	508	CLA	C1D-CHD-C4C	2.08	125.33	122.48
23	C	510	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	c	509	CLA	CMB-C2B-C3B	2.09	128.76	124.89
28	C	517	DGD	C3G-O3G-C1D	2.09	118.04	113.76
23	C	505	CLA	O1D-CGD-CBD	2.09	128.35	124.60
27	B	617	BCR	C36-C18-C19	2.09	121.43	118.10
24	a	407	PHO	CBD-CHA-C1A	2.09	131.28	126.36
31	D	407	LMG	O2-C2-C1	2.09	114.40	110.03
31	b	625	LMG	O6-C5-C4	2.09	113.51	109.66
23	C	501	CLA	CMD-C2D-C3D	2.09	128.77	124.89
23	b	608	CLA	C1D-CHD-C4C	2.09	125.34	122.48
23	c	504	CLA	C1D-CHD-C4C	2.09	125.35	122.48
23	B	604	CLA	CMD-C2D-C3D	2.10	128.79	124.89
33	B	629	LMT	O1B-C4'-C3'	2.10	112.25	107.19
28	B	627	DGD	C1G-O1G-C1A	2.10	123.45	117.13
23	C	505	CLA	CBA-CAA-C2A	2.10	120.09	113.80
27	H	101	BCR	C36-C18-C19	2.10	121.45	118.10
23	b	610	CLA	O1D-CGD-CBD	2.10	128.38	124.60
23	d	403	CLA	C1D-CHD-C4C	2.10	125.36	122.48
23	c	505	CLA	CBA-CAA-C2A	2.11	120.10	113.80
23	d	403	CLA	CMD-C2D-C3D	2.11	128.80	124.89
23	b	616	CLA	C1D-CHD-C4C	2.11	125.37	122.48
27	A	410	BCR	C33-C5-C4	2.11	117.46	113.45
23	b	611	CLA	C1D-CHD-C4C	2.12	125.38	122.48
23	B	607	CLA	CMD-C2D-C3D	2.12	128.82	124.89
27	C	514	BCR	C29-C30-C25	2.12	113.79	110.48
25	j	101	PL9	C10-C9-C11	2.12	118.97	115.29
23	B	608	CLA	O1D-CGD-CBD	2.12	128.41	124.60
27	c	514	BCR	C29-C30-C25	2.12	113.80	110.48
24	D	402	PHO	C1B-NB-C4B	2.12	110.72	106.52
23	c	511	CLA	O1D-CGD-CBD	2.12	128.42	124.60
23	d	402	CLA	CHB-C4A-NA	2.12	127.45	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PL9	C53-C6-C1	2.13	119.37	114.84
28	c	518	DGD	O3G-C1D-C2D	2.13	111.71	108.23
23	b	617	CLA	CMD-C2D-C3D	2.13	128.85	124.89
27	B	619	BCR	C33-C5-C4	2.13	117.50	113.45
23	C	508	CLA	O1D-CGD-CBD	2.13	128.44	124.60
23	b	615	CLA	CMD-C2D-C3D	2.14	128.87	124.89
28	C	517	DGD	C1G-O1G-C1A	2.14	123.57	117.13
25	a	410	PL9	C53-C6-C1	2.14	119.39	114.84
23	c	505	CLA	CMD-C2D-C3D	2.14	128.87	124.89
25	D	404	PL9	C51-C49-C50	2.14	119.60	114.60
27	c	515	BCR	C33-C5-C4	2.14	117.52	113.45
23	B	616	CLA	CHB-C4A-NA	2.15	127.48	124.51
28	C	519	DGD	O3D-C3D-C4D	2.15	115.03	110.36
25	D	404	PL9	C53-C6-C1	2.15	119.40	114.84
23	B	604	CLA	O1D-CGD-CBD	2.15	128.46	124.60
31	I	101	LMG	C8-O7-C10	2.15	122.95	117.88
31	k	103	LMG	C3-C4-C5	2.15	114.00	110.22
23	b	612	CLA	O1D-CGD-CBD	2.15	128.47	124.60
23	c	501	CLA	C1D-CHD-C4C	2.15	125.43	122.48
33	M	102	LMT	O1B-C1B-C2B	2.16	112.97	108.11
25	j	101	PL9	C20-C19-C21	2.16	119.03	115.29
28	D	409	DGD	O2G-C1B-C2B	2.16	116.03	111.55
27	a	412	BCR	C38-C26-C27	2.16	117.55	113.45
28	b	602	DGD	C1E-C2E-C3E	2.16	114.00	109.98
30	a	401	SQD	O8-S-C6	2.16	108.65	106.01
23	A	405	CLA	C4A-NA-C1A	2.16	109.14	106.45
27	h	101	BCR	C36-C18-C19	2.16	121.54	118.10
27	y	101	BCR	C35-C13-C12	2.16	121.55	118.10
23	C	501	CLA	CMB-C2B-C3B	2.16	128.91	124.89
23	b	620	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	c	512	CLA	CMD-C2D-C3D	2.17	128.91	124.89
27	k	102	BCR	C35-C13-C12	2.17	121.55	118.10
23	B	615	CLA	CMD-C2D-C3D	2.17	128.91	124.89
30	a	415	SQD	O6-C1-C2	2.17	111.77	108.23
27	z	101	BCR	C33-C5-C4	2.17	117.57	113.45
23	B	615	CLA	C1D-CHD-C4C	2.17	125.45	122.48
27	c	514	BCR	C12-C13-C14	2.17	122.28	118.94
23	B	610	CLA	C1D-CHD-C4C	2.18	125.46	122.48
30	b	601	SQD	C1-O5-C5	2.18	117.82	113.72
25	d	404	PL9	C15-C14-C16	2.18	119.07	115.29
33	I	102	LMT	O1B-C4'-C3'	2.18	112.44	107.19
24	A	406	PHO	C4A-NA-C1A	2.18	109.92	108.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	E	101	LMG	O1-C1-C2	2.18	111.79	108.23
25	A	408	PL9	C30-C29-C31	2.18	119.08	115.29
23	d	402	CLA	CMD-C2D-C3D	2.19	128.95	124.89
23	b	617	CLA	C1D-CHD-C4C	2.19	125.48	122.48
31	b	624	LMG	C3-C4-C5	2.19	114.08	110.22
23	b	613	CLA	CHB-C4A-NA	2.20	127.55	124.51
23	B	614	CLA	CHB-C4A-NA	2.20	127.55	124.51
31	A	418	LMG	O1-C1-C2	2.20	111.83	108.23
23	A	403	CLA	CHB-C4A-NA	2.22	127.58	124.51
24	D	402	PHO	C4A-NA-C1A	2.22	109.95	108.16
29	A	412	LHG	O8-C23-C24	2.22	118.36	111.90
23	b	607	CLA	O2D-CGD-CBD	2.23	115.28	111.30
28	D	409	DGD	O5D-C6D-C5D	2.23	112.68	108.94
30	B	626	SQD	C1-O5-C5	2.23	117.92	113.72
31	I	101	LMG	C3-C4-C5	2.24	114.16	110.22
24	a	407	PHO	C1B-NB-C4B	2.24	110.96	106.52
23	a	405	CLA	C4A-NA-C1A	2.25	109.24	106.45
23	B	615	CLA	CHB-C4A-NA	2.25	127.62	124.51
23	c	501	CLA	CMD-C2D-C3D	2.25	129.06	124.89
25	J	101	PL9	C15-C14-C16	2.25	119.19	115.29
23	b	615	CLA	C1D-CHD-C4C	2.25	125.56	122.48
25	j	101	PL9	C15-C14-C16	2.25	119.19	115.29
23	c	509	CLA	CMD-C2D-C3D	2.25	129.07	124.89
23	c	511	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	a	414	LHG	C6-O8-C23	2.25	123.91	117.13
23	b	612	CLA	CMD-C2D-C3D	2.25	129.08	124.89
23	c	510	CLA	C4A-NA-C1A	2.26	109.25	106.45
23	B	604	CLA	CMB-C2B-C3B	2.26	129.08	124.89
24	A	406	PHO	C1B-NB-C4B	2.26	110.99	106.52
25	d	404	PL9	C51-C49-C50	2.26	119.88	114.60
29	a	414	LHG	O8-C23-C24	2.26	118.49	111.90
23	C	505	CLA	CMB-C2B-C3B	2.26	129.09	124.89
23	C	507	CLA	O2D-CGD-CBD	2.27	115.35	111.30
23	C	502	CLA	CHB-C4A-NA	2.27	127.64	124.51
23	c	507	CLA	CHB-C4A-NA	2.27	127.65	124.51
27	B	618	BCR	C35-C13-C12	2.27	121.71	118.10
25	a	410	PL9	C20-C19-C21	2.27	119.22	115.29
23	B	606	CLA	C4A-NA-C1A	2.27	109.27	106.45
25	d	404	PL9	C53-C6-C1	2.27	119.67	114.84
27	h	101	BCR	C33-C5-C4	2.28	117.77	113.45
27	C	516	BCR	C33-C5-C4	2.28	117.77	113.45
30	A	413	SQD	C44-O6-C1	2.28	118.43	113.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	623	LMG	C3-C4-C5	2.28	114.24	110.22
23	b	620	CLA	C1D-CHD-C4C	2.29	125.61	122.48
31	B	622	LMG	C4-C3-C2	2.29	114.87	110.84
23	C	502	CLA	C1D-CHD-C4C	2.29	125.61	122.48
23	B	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
27	b	621	BCR	C33-C5-C4	2.29	117.80	113.45
23	b	612	CLA	CHB-C4A-NA	2.29	127.68	124.51
23	b	605	CLA	CHB-C4A-NA	2.29	127.68	124.51
31	b	624	LMG	C4-C3-C2	2.30	114.89	110.84
23	A	404	CLA	CMD-C2D-C3D	2.30	129.16	124.89
23	d	403	CLA	CMB-C2B-C3B	2.30	129.16	124.89
27	h	101	BCR	C35-C13-C12	2.30	121.77	118.10
31	C	521	LMG	C3-C4-C5	2.30	114.28	110.22
23	B	611	CLA	CMD-C2D-C3D	2.31	129.18	124.89
23	c	512	CLA	C1D-CHD-C4C	2.31	125.64	122.48
30	A	413	SQD	O5-C1-C2	2.31	114.76	110.30
23	C	511	CLA	CMD-C2D-C3D	2.31	129.19	124.89
23	b	608	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	b	612	CLA	C4A-NA-C1A	2.32	109.33	106.45
31	c	519	LMG	C3-C4-C5	2.32	114.30	110.22
31	k	103	LMG	C7-O1-C1	2.32	118.51	113.76
27	B	619	BCR	C2-C1-C6	2.32	114.11	110.48
23	b	620	CLA	CMD-C2D-C3D	2.32	129.20	124.89
23	b	613	CLA	C4A-NA-C1A	2.32	109.33	106.45
25	D	404	PL9	C15-C14-C16	2.33	119.32	115.29
23	c	511	CLA	CMB-C2B-C3B	2.33	129.21	124.89
23	B	616	CLA	C4A-NA-C1A	2.33	109.34	106.45
27	D	405	BCR	C33-C5-C4	2.33	117.87	113.45
27	b	621	BCR	C38-C26-C27	2.33	117.87	113.45
31	e	101	LMG	O1-C1-C2	2.33	112.04	108.23
23	A	407	CLA	CMD-C2D-C3D	2.33	129.22	124.89
25	d	404	PL9	C20-C19-C21	2.34	119.34	115.29
23	B	606	CLA	O1D-CGD-CBD	2.34	128.80	124.60
28	d	409	DGD	C2G-O2G-C1B	2.34	123.40	117.88
23	c	513	CLA	C1D-CHD-C4C	2.34	125.68	122.48
28	c	516	DGD	O3D-C3D-C4D	2.35	115.46	110.36
23	C	505	CLA	CHB-C4A-NA	2.35	127.76	124.51
25	A	408	PL9	C20-C19-C21	2.35	119.37	115.29
31	e	101	LMG	C8-O7-C10	2.35	123.43	117.88
23	B	610	CLA	C4A-NA-C1A	2.35	109.37	106.45
23	B	604	CLA	CHB-C4A-NA	2.35	127.76	124.51
27	C	515	BCR	C33-C5-C4	2.35	117.92	113.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	c	518	DGD	O2G-C1B-C2B	2.35	116.44	111.55
23	A	405	CLA	CHB-C4A-NA	2.36	127.77	124.51
23	c	507	CLA	C1D-CHD-C4C	2.36	125.71	122.48
25	d	404	PL9	C40-C39-C41	2.36	119.38	115.29
23	D	403	CLA	CHB-C4A-NA	2.36	127.77	124.51
28	b	623	DGD	C3G-O3G-C1D	2.36	118.59	113.76
23	d	403	CLA	O2D-CGD-CBD	2.36	115.52	111.30
23	b	615	CLA	CHB-C4A-NA	2.36	127.78	124.51
27	k	102	BCR	C38-C26-C27	2.36	117.94	113.45
30	F	102	SQD	O48-C23-C24	2.37	118.79	111.90
27	C	514	BCR	C33-C5-C4	2.37	117.95	113.45
31	i	101	LMG	C3-C4-C5	2.37	114.40	110.22
23	C	510	CLA	C1D-CHD-C4C	2.37	125.73	122.48
23	B	606	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	c	503	CLA	CMD-C2D-C3D	2.38	129.31	124.89
31	a	416	LMG	O6-C5-C6	2.38	112.12	106.41
30	b	601	SQD	O8-S-C6	2.39	108.92	106.01
23	b	607	CLA	C1D-CHD-C4C	2.39	125.75	122.48
28	b	602	DGD	C1G-O1G-C1A	2.39	124.32	117.13
23	c	503	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	b	610	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	f	102	SQD	O5-C1-C2	2.39	114.90	110.30
23	b	608	CLA	CMB-C2B-C3B	2.39	129.33	124.89
30	A	417	SQD	O48-C23-C24	2.40	118.87	111.90
23	b	605	CLA	CMD-C2D-C3D	2.40	129.34	124.89
23	B	601	CLA	CMD-C2D-C3D	2.40	129.34	124.89
27	c	514	BCR	C33-C5-C4	2.40	118.00	113.45
23	b	615	CLA	CMB-C2B-C3B	2.40	129.34	124.89
23	b	614	CLA	C4A-NA-C1A	2.40	109.43	106.45
23	d	403	CLA	CHB-C4A-NA	2.40	127.84	124.51
27	H	101	BCR	C35-C13-C12	2.40	121.93	118.10
23	B	603	CLA	C1D-CHD-C4C	2.41	125.77	122.48
23	c	501	CLA	CMB-C2B-C3B	2.41	129.37	124.89
23	D	401	CLA	O1D-CGD-CBD	2.41	128.94	124.60
23	d	402	CLA	O1D-CGD-CBD	2.41	128.94	124.60
23	D	401	CLA	C4A-NA-C1A	2.42	109.45	106.45
27	h	101	BCR	C34-C9-C8	2.42	121.95	118.10
30	f	102	SQD	O48-C23-C24	2.42	118.95	111.90
28	A	411	DGD	O3D-C3D-C4D	2.42	115.63	110.36
31	d	407	LMG	C7-O1-C1	2.42	118.73	113.76
23	C	511	CLA	CMB-C2B-C3B	2.42	129.39	124.89
23	A	404	CLA	C4A-NA-C1A	2.43	109.47	106.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CMD-C2D-C3D	2.43	129.40	124.89
28	d	409	DGD	O2G-C1B-C2B	2.43	116.60	111.55
30	B	626	SQD	O47-C7-C8	2.43	116.60	111.55
28	a	413	DGD	O3D-C3D-C4D	2.43	115.65	110.36
23	A	403	CLA	CMB-C2B-C3B	2.44	129.42	124.89
27	a	412	BCR	C34-C9-C8	2.44	121.99	118.10
23	A	405	CLA	CMD-C2D-C3D	2.44	129.42	124.89
23	D	403	CLA	C4A-NA-C1A	2.44	109.48	106.45
23	c	510	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	C	506	CLA	CMD-C2D-C3D	2.45	129.44	124.89
23	B	611	CLA	C4A-NA-C1A	2.45	109.49	106.45
27	k	102	BCR	C33-C5-C4	2.45	118.10	113.45
31	i	101	LMG	C7-O1-C1	2.45	118.79	113.76
23	c	503	CLA	C4A-NA-C1A	2.45	109.50	106.45
23	B	613	CLA	C4A-NA-C1A	2.45	109.50	106.45
23	C	504	CLA	CMD-C2D-C3D	2.46	129.45	124.89
30	A	413	SQD	O48-C23-C24	2.46	119.05	111.90
28	c	516	DGD	O1G-C1A-C2A	2.46	119.06	111.90
23	B	612	CLA	CHB-C4A-NA	2.46	127.91	124.51
27	B	620	BCR	C38-C26-C27	2.46	118.12	113.45
23	B	606	CLA	CMD-C2D-C3D	2.46	129.46	124.89
23	b	609	CLA	CMB-C2B-C3B	2.46	129.46	124.89
23	a	404	CLA	CHB-C4A-NA	2.46	127.92	124.51
28	b	602	DGD	O6D-C1D-O3G	2.46	115.87	110.02
23	C	510	CLA	CMB-C2B-C3B	2.46	129.47	124.89
23	a	404	CLA	CMB-C2B-C3B	2.47	129.47	124.89
23	C	507	CLA	C4A-NA-C1A	2.47	109.52	106.45
27	D	405	BCR	C29-C30-C25	2.47	114.34	110.48
23	b	605	CLA	C4A-NA-C1A	2.47	109.52	106.45
28	c	518	DGD	O5D-C1E-C2E	2.47	112.27	108.23
23	c	504	CLA	CMD-C2D-C3D	2.48	129.49	124.89
23	C	508	CLA	C1D-CHD-C4C	2.48	125.88	122.48
23	A	407	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	B	605	CLA	CMD-C2D-C3D	2.49	129.51	124.89
27	d	405	BCR	C33-C5-C4	2.49	118.18	113.45
23	a	405	CLA	CHB-C4A-NA	2.49	127.96	124.51
23	A	403	CLA	C4A-NA-C1A	2.49	109.55	106.45
23	B	614	CLA	C4A-NA-C1A	2.50	109.55	106.45
28	b	623	DGD	O1G-C1A-C2A	2.50	119.17	111.90
31	C	520	LMG	C7-O1-C1	2.50	118.89	113.76
23	b	618	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	C	501	CLA	CHB-C4A-NA	2.51	127.98	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	408	SQD	O48-C23-C24	2.51	119.19	111.90
23	B	612	CLA	C4A-NA-C1A	2.51	109.56	106.45
23	B	601	CLA	CMB-C2B-C3B	2.51	129.55	124.89
28	C	519	DGD	O2G-C1B-C2B	2.51	116.76	111.55
23	B	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	B	615	CLA	C4A-NA-C1A	2.51	109.57	106.45
25	D	404	PL9	C40-C39-C41	2.51	119.64	115.29
23	c	501	CLA	CHB-C4A-NA	2.51	127.99	124.51
23	c	510	CLA	CMD-C2D-C3D	2.51	129.56	124.89
23	c	505	CLA	CMB-C2B-C3B	2.51	129.56	124.89
23	b	605	CLA	CMB-C2B-C3B	2.51	129.56	124.89
27	b	622	BCR	C38-C26-C27	2.52	118.22	113.45
23	b	609	CLA	CHB-C4A-NA	2.52	127.99	124.51
28	B	627	DGD	O6D-C1D-O3G	2.52	116.00	110.02
23	A	407	CLA	C4A-NA-C1A	2.52	109.58	106.45
23	C	502	CLA	CMB-C2B-C3B	2.52	129.57	124.89
24	a	407	PHO	C4A-NA-C1A	2.52	110.20	108.16
23	b	615	CLA	C4A-NA-C1A	2.52	109.59	106.45
23	B	611	CLA	CHB-C4A-NA	2.53	128.00	124.51
23	b	607	CLA	CMD-C2D-C3D	2.53	129.59	124.89
23	b	613	CLA	CMB-C2B-C3B	2.53	129.59	124.89
23	B	613	CLA	CHB-C4A-NA	2.53	128.01	124.51
23	c	507	CLA	C4A-NA-C1A	2.53	109.59	106.45
23	C	502	CLA	CMD-C2D-C3D	2.53	129.59	124.89
28	B	627	DGD	C1E-C2E-C3E	2.54	114.69	109.98
23	C	509	CLA	CMB-C2B-C3B	2.54	129.60	124.89
27	c	515	BCR	C38-C26-C27	2.54	118.27	113.45
28	d	409	DGD	O3D-C3D-C4D	2.54	115.88	110.36
28	D	409	DGD	O5D-C1E-C2E	2.55	112.39	108.23
23	b	620	CLA	C4A-NA-C1A	2.55	109.61	106.45
23	c	513	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	A	405	CLA	O2D-CGD-CBD	2.55	115.86	111.30
23	C	503	CLA	CHB-C4A-NA	2.55	128.04	124.51
23	b	607	CLA	C4A-NA-C1A	2.55	109.62	106.45
31	C	521	LMG	C7-O1-C1	2.56	119.00	113.76
28	a	413	DGD	C3D-C4D-C5D	2.56	114.72	110.22
28	B	621	DGD	O2G-C1B-C2B	2.56	116.86	111.55
30	D	408	SQD	O48-C23-C24	2.56	119.35	111.90
23	b	610	CLA	CMD-C2D-C3D	2.56	129.64	124.89
28	A	411	DGD	C3D-C4D-C5D	2.56	114.73	110.22
28	A	411	DGD	O1G-C1A-C2A	2.56	119.36	111.90
27	b	621	BCR	C29-C30-C25	2.56	114.48	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	521	LMG	O1-C1-C2	2.56	112.42	108.23
23	b	609	CLA	C4A-NA-C1A	2.56	109.63	106.45
31	I	101	LMG	C7-O1-C1	2.56	119.02	113.76
23	c	505	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	B	601	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	B	615	CLA	CMB-C2B-C3B	2.58	129.68	124.89
27	B	619	BCR	C29-C30-C25	2.58	114.51	110.48
23	A	404	CLA	CHB-C4A-NA	2.58	128.08	124.51
28	C	517	DGD	O1G-C1A-C2A	2.58	119.41	111.90
23	c	506	CLA	CHB-C4A-NA	2.58	128.09	124.51
23	C	512	CLA	CHB-C4A-NA	2.59	128.09	124.51
27	C	516	BCR	C38-C26-C27	2.59	118.36	113.45
28	c	517	DGD	O6E-C1E-C2E	2.59	115.28	110.30
31	e	101	LMG	O7-C10-C11	2.59	116.92	111.55
23	C	511	CLA	CHB-C4A-NA	2.59	128.09	124.51
30	B	626	SQD	O8-S-C6	2.59	109.17	106.01
23	c	508	CLA	C4A-NA-C1A	2.60	109.68	106.45
23	C	502	CLA	C4A-NA-C1A	2.60	109.68	106.45
23	A	403	CLA	CMD-C2D-C3D	2.60	129.71	124.89
23	C	501	CLA	C4A-NA-C1A	2.60	109.68	106.45
23	C	508	CLA	C4A-NA-C1A	2.60	109.68	106.45
30	A	417	SQD	O8-S-C6	2.60	109.19	106.01
31	c	519	LMG	O1-C1-C2	2.61	112.48	108.23
25	J	101	PL9	C20-C19-C21	2.61	119.81	115.29
29	a	417	LHG	O8-C23-C24	2.61	119.49	111.90
30	a	415	SQD	O48-C23-C24	2.61	119.50	111.90
30	a	401	SQD	O48-C23-C24	2.61	119.50	111.90
23	a	409	CLA	CHB-C4A-NA	2.61	128.12	124.51
23	c	508	CLA	CMD-C2D-C3D	2.61	129.74	124.89
23	b	614	CLA	CHB-C4A-NA	2.61	128.13	124.51
23	d	403	CLA	C4A-NA-C1A	2.62	109.70	106.45
28	C	518	DGD	O3G-C1D-C2D	2.62	112.50	108.23
23	C	505	CLA	CMD-C2D-C3D	2.62	129.75	124.89
23	C	513	CLA	C4A-NA-C1A	2.62	109.70	106.45
23	B	602	CLA	CMB-C2B-C3B	2.62	129.75	124.89
30	b	601	SQD	O47-C7-C8	2.62	117.00	111.55
23	b	606	CLA	C4A-NA-C1A	2.62	109.71	106.45
27	B	618	BCR	C29-C30-C25	2.62	114.58	110.48
23	C	503	CLA	C4A-NA-C1A	2.62	109.71	106.45
23	a	406	CLA	CMB-C2B-C3B	2.62	129.76	124.89
23	B	602	CLA	CMD-C2D-C3D	2.62	129.76	124.89
23	c	501	CLA	C4A-NA-C1A	2.63	109.71	106.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	a	409	CLA	C4A-NA-C1A	2.63	109.71	106.45
28	B	627	DGD	O1G-C1A-C2A	2.63	119.55	111.90
30	F	102	SQD	O5-C1-C2	2.63	115.37	110.30
23	D	401	CLA	CMD-C2D-C3D	2.63	129.78	124.89
23	c	506	CLA	C4A-NA-C1A	2.63	109.72	106.45
23	C	509	CLA	C4A-NA-C1A	2.64	109.72	106.45
31	B	622	LMG	O1-C1-C2	2.64	112.53	108.23
23	C	507	CLA	CHB-C4A-NA	2.64	128.16	124.51
23	c	503	CLA	CMB-C2B-C3B	2.64	129.79	124.89
23	c	513	CLA	C4A-NA-C1A	2.64	109.73	106.45
23	B	609	CLA	C4A-NA-C1A	2.64	109.73	106.45
23	C	506	CLA	C4A-NA-C1A	2.65	109.74	106.45
23	C	504	CLA	C4A-NA-C1A	2.65	109.74	106.45
23	b	608	CLA	C4A-NA-C1A	2.65	109.74	106.45
23	D	403	CLA	CMD-C2D-C3D	2.65	129.81	124.89
23	B	604	CLA	C4A-NA-C1A	2.66	109.75	106.45
23	B	602	CLA	C4A-NA-C1A	2.66	109.76	106.45
23	b	610	CLA	C4A-NA-C1A	2.66	109.76	106.45
23	c	511	CLA	C4A-NA-C1A	2.66	109.76	106.45
28	c	516	DGD	C1G-O1G-C1A	2.66	125.15	117.13
28	C	517	DGD	O3D-C3D-C4D	2.66	116.16	110.36
23	c	502	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	b	607	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	b	616	CLA	C4A-NA-C1A	2.67	109.76	106.45
28	d	409	DGD	O5D-C6D-C5D	2.67	113.40	108.94
23	B	605	CLA	CMB-C2B-C3B	2.67	129.84	124.89
28	c	518	DGD	O3D-C3D-C4D	2.67	116.16	110.36
33	b	603	LMT	O1B-C4'-C3'	2.67	113.62	107.19
30	A	417	SQD	O6-C1-C2	2.67	112.59	108.23
23	b	610	CLA	CMB-C2B-C3B	2.67	129.85	124.89
30	b	601	SQD	O5-C5-C4	2.67	114.58	109.66
23	b	619	CLA	C4A-NA-C1A	2.67	109.77	106.45
23	b	616	CLA	CMD-C2D-C3D	2.67	129.85	124.89
23	B	608	CLA	CHB-C4A-NA	2.67	128.21	124.51
28	B	621	DGD	O1G-C1A-C2A	2.68	119.69	111.90
23	C	513	CLA	CHB-C4A-NA	2.68	128.22	124.51
23	C	507	CLA	CMD-C2D-C3D	2.69	129.88	124.89
30	B	626	SQD	O5-C5-C4	2.69	114.61	109.66
31	E	101	LMG	C8-O7-C10	2.69	124.22	117.88
23	c	502	CLA	C4A-NA-C1A	2.69	109.79	106.45
31	M	101	LMG	O8-C28-C29	2.69	119.73	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	516	BCR	C29-C30-C25	2.69	114.69	110.48
31	E	101	LMG	O7-C10-C11	2.69	117.14	111.55
23	c	512	CLA	CMB-C2B-C3B	2.70	129.89	124.89
31	d	406	LMG	C3-C4-C5	2.70	114.97	110.22
23	B	603	CLA	CHB-C4A-NA	2.70	128.24	124.51
23	b	611	CLA	CHB-C4A-NA	2.70	128.25	124.51
28	a	413	DGD	O1G-C1A-C2A	2.70	119.76	111.90
23	a	406	CLA	CMD-C2D-C3D	2.70	129.91	124.89
23	b	611	CLA	C4A-NA-C1A	2.70	109.81	106.45
23	B	608	CLA	C4A-NA-C1A	2.71	109.81	106.45
31	b	624	LMG	C7-O1-C1	2.71	119.31	113.76
23	C	512	CLA	CMD-C2D-C3D	2.71	129.92	124.89
28	c	516	DGD	O5D-C1E-C2E	2.71	112.66	108.23
23	c	512	CLA	C4A-NA-C1A	2.71	109.82	106.45
24	D	402	PHO	O1D-CGD-CBD	2.71	129.47	124.60
23	b	616	CLA	CHB-C4A-NA	2.71	128.26	124.51
23	c	509	CLA	CHB-C4A-NA	2.71	128.27	124.51
23	C	506	CLA	CHB-C4A-NA	2.72	128.28	124.51
30	f	102	SQD	O5-C5-C4	2.72	114.68	109.66
23	c	513	CLA	CMB-C2B-C3B	2.72	129.94	124.89
30	A	413	SQD	O5-C5-C4	2.72	114.68	109.66
23	C	508	CLA	CHB-C4A-NA	2.72	128.28	124.51
31	D	406	LMG	C3-C4-C5	2.73	115.02	110.22
27	T	102	BCR	C29-C30-C25	2.73	114.74	110.48
28	c	517	DGD	O1G-C1A-C2A	2.73	119.84	111.90
23	B	603	CLA	C4A-NA-C1A	2.73	109.84	106.45
23	a	409	CLA	CMB-C2B-C3B	2.74	129.97	124.89
23	b	619	CLA	CHB-C4A-NA	2.74	128.30	124.51
23	b	613	CLA	CMD-C2D-C3D	2.74	129.97	124.89
27	H	101	BCR	C33-C5-C4	2.74	118.65	113.45
30	B	626	SQD	O48-C23-C24	2.74	119.88	111.90
23	C	503	CLA	CMD-C2D-C3D	2.74	129.98	124.89
23	B	605	CLA	CHB-C4A-NA	2.75	128.31	124.51
23	B	611	CLA	CMB-C2B-C3B	2.75	129.99	124.89
29	A	415	LHG	O8-C23-C24	2.75	119.89	111.90
24	a	407	PHO	O1D-CGD-CBD	2.75	129.54	124.60
23	b	609	CLA	CMD-C2D-C3D	2.75	129.99	124.89
30	b	601	SQD	O48-C23-C24	2.75	119.90	111.90
23	c	508	CLA	CHB-C4A-NA	2.75	128.32	124.51
27	c	515	BCR	C29-C30-C25	2.75	114.78	110.48
28	c	518	DGD	O6D-C5D-C6D	2.75	112.13	106.64
23	C	505	CLA	C4A-NA-C1A	2.75	109.87	106.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405	CLA	CMB-C2B-C3B	2.75	130.00	124.89
23	b	611	CLA	CMB-C2B-C3B	2.76	130.01	124.89
24	a	408	PHO	O1D-CGD-CBD	2.76	129.56	124.60
30	a	415	SQD	O5-C5-C4	2.76	114.74	109.66
23	a	409	CLA	CMD-C2D-C3D	2.76	130.01	124.89
23	B	601	CLA	C4A-NA-C1A	2.76	109.88	106.45
27	d	405	BCR	C29-C30-C25	2.76	114.80	110.48
23	c	504	CLA	CHB-C4A-NA	2.76	128.34	124.51
27	b	622	BCR	C2-C1-C6	2.77	114.80	110.48
23	C	513	CLA	CMB-C2B-C3B	2.77	130.03	124.89
27	T	102	BCR	C33-C5-C4	2.77	118.71	113.45
23	B	609	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	b	619	CLA	CMD-C2D-C3D	2.77	130.04	124.89
23	C	512	CLA	CMB-C2B-C3B	2.77	130.04	124.89
23	c	506	CLA	CMD-C2D-C3D	2.78	130.06	124.89
31	i	101	LMG	O8-C28-C29	2.78	120.00	111.90
30	F	102	SQD	O5-C5-C4	2.78	114.79	109.66
23	a	404	CLA	C4A-NA-C1A	2.79	109.91	106.45
28	b	623	DGD	O2G-C1B-C2B	2.79	117.35	111.55
24	A	406	PHO	O1D-CGD-CBD	2.79	129.62	124.60
27	B	618	BCR	C33-C5-C4	2.79	118.75	113.45
23	B	605	CLA	C4A-NA-C1A	2.79	109.92	106.45
23	c	502	CLA	CMB-C2B-C3B	2.80	130.08	124.89
23	b	606	CLA	CHB-C4A-NA	2.80	128.38	124.51
30	F	102	SQD	C44-O6-C1	2.80	119.50	113.76
28	b	602	DGD	O1G-C1A-C2A	2.80	120.06	111.90
23	c	512	CLA	CHB-C4A-NA	2.81	128.39	124.51
31	b	625	LMG	C7-O1-C1	2.81	119.52	113.76
23	c	504	CLA	C4A-NA-C1A	2.81	109.94	106.45
30	a	415	SQD	C44-O6-C1	2.81	119.52	113.76
23	C	512	CLA	C4A-NA-C1A	2.81	109.94	106.45
23	b	618	CLA	CMB-C2B-C3B	2.82	130.12	124.89
23	a	405	CLA	CMB-C2B-C3B	2.82	130.12	124.89
27	y	101	BCR	C33-C5-C4	2.82	118.80	113.45
23	B	616	CLA	CMB-C2B-C3B	2.83	130.14	124.89
23	a	406	CLA	CHB-C4A-NA	2.83	128.42	124.51
23	c	507	CLA	CMB-C2B-C3B	2.83	130.15	124.89
23	C	509	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	B	612	CLA	CMD-C2D-C3D	2.84	130.17	124.89
23	B	616	CLA	CMD-C2D-C3D	2.85	130.17	124.89
23	D	403	CLA	CMB-C2B-C3B	2.86	130.19	124.89
28	C	518	DGD	O1G-C1A-C2A	2.86	120.22	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	617	CLA	C4A-NA-C1A	2.86	110.00	106.45
31	D	407	LMG	O8-C28-C29	2.86	120.22	111.90
27	D	405	BCR	C38-C26-C27	2.86	118.88	113.45
23	c	510	CLA	CMB-C2B-C3B	2.87	130.22	124.89
23	b	617	CLA	CHB-C4A-NA	2.87	128.48	124.51
27	j	102	BCR	C38-C26-C27	2.87	118.90	113.45
31	m	102	LMG	O8-C28-C29	2.87	120.26	111.90
33	B	628	LMT	O1B-C4'-C3'	2.88	114.12	107.19
31	B	622	LMG	C7-O1-C1	2.88	119.67	113.76
27	T	102	BCR	C2-C1-C6	2.89	115.00	110.48
28	D	409	DGD	O1G-C1A-C2A	2.89	120.32	111.90
23	C	508	CLA	CMB-C2B-C3B	2.89	130.26	124.89
23	c	508	CLA	CMB-C2B-C3B	2.89	130.26	124.89
23	B	609	CLA	CMB-C2B-C3B	2.89	130.26	124.89
27	B	620	BCR	C2-C1-C6	2.90	115.01	110.48
23	a	406	CLA	C4A-NA-C1A	2.90	110.05	106.45
27	B	618	BCR	C2-C1-C6	2.90	115.02	110.48
23	b	618	CLA	C4A-NA-C1A	2.90	110.06	106.45
23	B	608	CLA	CMB-C2B-C3B	2.91	130.29	124.89
28	b	602	DGD	O2G-C1B-C2B	2.91	117.60	111.55
27	J	102	BCR	C38-C26-C27	2.91	118.98	113.45
23	B	606	CLA	CMB-C2B-C3B	2.91	130.30	124.89
23	C	503	CLA	CMB-C2B-C3B	2.91	130.30	124.89
28	b	602	DGD	C3G-O3G-C1D	2.92	119.74	113.76
23	b	606	CLA	CMD-C2D-C3D	2.92	130.31	124.89
28	c	517	DGD	O3G-C1D-C2D	2.92	113.01	108.23
23	c	509	CLA	C4A-NA-C1A	2.93	110.09	106.45
31	a	402	LMG	O8-C28-C29	2.93	120.42	111.90
23	C	506	CLA	CMB-C2B-C3B	2.93	130.33	124.89
27	B	618	BCR	C38-C26-C27	2.93	119.02	113.45
28	b	623	DGD	O3D-C3D-C4D	2.94	116.75	110.36
28	C	519	DGD	O6D-C5D-C6D	2.95	112.53	106.64
28	C	518	DGD	O6E-C1E-C2E	2.97	116.02	110.30
27	d	405	BCR	C38-C26-C27	2.97	119.10	113.45
25	D	404	PL9	C25-C24-C26	2.98	120.45	115.29
31	I	101	LMG	O8-C28-C29	2.98	120.57	111.90
23	d	402	CLA	CMB-C2B-C3B	2.98	130.42	124.89
23	c	504	CLA	CMB-C2B-C3B	2.98	130.42	124.89
23	b	612	CLA	CMB-C2B-C3B	2.99	130.43	124.89
31	B	622	LMG	O8-C28-C29	2.99	120.59	111.90
25	J	101	PL9	C25-C24-C26	2.99	120.48	115.29
31	B	623	LMG	O1-C1-C2	2.99	113.12	108.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	409	DGD	O1G-C1A-C2A	3.00	120.63	111.90
31	E	101	LMG	O8-C28-C29	3.01	120.65	111.90
23	c	505	CLA	C4A-NA-C1A	3.01	110.19	106.45
31	b	624	LMG	O8-C28-C29	3.01	120.66	111.90
23	b	606	CLA	CMB-C2B-C3B	3.01	130.48	124.89
28	C	519	DGD	O5D-C1E-C2E	3.03	113.17	108.23
31	I	101	LMG	O7-C10-C11	3.03	117.84	111.55
31	e	101	LMG	O8-C28-C29	3.03	120.72	111.90
23	B	607	CLA	CMB-C2B-C3B	3.04	130.52	124.89
31	A	418	LMG	O8-C28-C29	3.04	120.74	111.90
31	d	406	LMG	C7-O1-C1	3.04	119.99	113.76
23	c	506	CLA	CMB-C2B-C3B	3.04	130.53	124.89
23	A	407	CLA	CMB-C2B-C3B	3.04	130.53	124.89
23	C	511	CLA	C4A-NA-C1A	3.04	110.23	106.45
23	A	404	CLA	CMB-C2B-C3B	3.05	130.55	124.89
30	f	102	SQD	C44-O6-C1	3.05	120.01	113.76
23	B	612	CLA	CMB-C2B-C3B	3.05	130.56	124.89
23	d	402	CLA	C4A-NA-C1A	3.05	110.24	106.45
31	A	418	LMG	C7-O1-C1	3.05	120.02	113.76
23	c	502	CLA	CMD-C2D-C3D	3.05	130.56	124.89
28	d	409	DGD	O5D-C1E-C2E	3.06	113.22	108.23
28	C	519	DGD	O1G-C1A-C2A	3.06	120.80	111.90
28	A	411	DGD	O6D-C5D-C6D	3.06	112.75	106.64
23	B	607	CLA	C4A-NA-C1A	3.06	110.25	106.45
27	T	102	BCR	C38-C26-C27	3.06	119.26	113.45
30	D	408	SQD	O5-C5-C4	3.07	115.31	109.66
31	A	418	LMG	C3-C4-C5	3.07	115.63	110.22
30	d	408	SQD	O5-C5-C4	3.08	115.33	109.66
23	b	607	CLA	CMB-C2B-C3B	3.08	130.61	124.89
31	d	407	LMG	O8-C28-C29	3.08	120.87	111.90
23	b	619	CLA	CMB-C2B-C3B	3.08	130.62	124.89
23	C	504	CLA	CMB-C2B-C3B	3.09	130.62	124.89
23	B	607	CLA	CHB-C4A-NA	3.09	128.78	124.51
31	a	416	LMG	O8-C28-C29	3.09	120.90	111.90
31	a	402	LMG	C7-O1-C1	3.10	120.11	113.76
28	C	517	DGD	O5D-C1E-C2E	3.10	113.29	108.23
31	D	407	LMG	O7-C10-C11	3.11	118.00	111.55
31	e	101	LMG	C7-O1-C1	3.11	120.13	113.76
31	i	101	LMG	O7-C10-C11	3.11	118.00	111.55
31	b	625	LMG	O1-C1-C2	3.12	113.33	108.23
25	A	408	PL9	C35-C34-C36	3.13	120.71	115.29
25	d	404	PL9	C35-C34-C36	3.13	120.71	115.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	406	LMG	C7-O1-C1	3.13	120.17	113.76
27	B	620	BCR	C33-C5-C4	3.13	119.40	113.45
23	B	614	CLA	CMB-C2B-C3B	3.14	130.72	124.89
28	d	409	DGD	C3G-O3G-C1D	3.14	120.19	113.76
28	c	518	DGD	O1G-C1A-C2A	3.15	121.05	111.90
23	B	603	CLA	CMB-C2B-C3B	3.15	130.73	124.89
27	c	514	BCR	C1-C6-C7	3.15	124.58	115.73
27	J	102	BCR	C29-C30-C25	3.15	115.40	110.48
31	b	625	LMG	O8-C28-C29	3.15	121.07	111.90
23	B	613	CLA	CMB-C2B-C3B	3.15	130.74	124.89
28	b	602	DGD	O5D-C1E-C2E	3.16	113.39	108.23
31	d	406	LMG	O8-C28-C29	3.17	121.12	111.90
31	c	519	LMG	O8-C28-C29	3.19	121.18	111.90
31	E	101	LMG	C7-O1-C1	3.19	120.30	113.76
27	j	102	BCR	C29-C30-C25	3.20	115.47	110.48
31	d	407	LMG	O7-C10-C11	3.20	118.19	111.55
27	C	514	BCR	C1-C6-C7	3.21	124.76	115.73
31	B	623	LMG	O8-C28-C29	3.22	121.26	111.90
25	j	101	PL9	C25-C24-C26	3.23	120.90	115.29
23	D	401	CLA	CMB-C2B-C3B	3.24	130.90	124.89
31	C	520	LMG	O8-C28-C29	3.24	121.33	111.90
23	b	617	CLA	CMB-C2B-C3B	3.24	130.91	124.89
27	b	622	BCR	C33-C5-C4	3.25	119.63	113.45
28	C	517	DGD	O2G-C1B-C2B	3.26	118.31	111.55
25	D	404	PL9	C35-C34-C36	3.26	120.94	115.29
31	A	414	LMG	O8-C28-C29	3.28	121.43	111.90
28	B	621	DGD	O3D-C3D-C4D	3.28	117.50	110.36
31	A	414	LMG	C7-O1-C1	3.29	120.50	113.76
23	C	507	CLA	CMB-C2B-C3B	3.29	131.00	124.89
30	A	417	SQD	C1-C2-C3	3.30	116.12	109.98
30	A	413	SQD	O47-C7-C8	3.31	118.42	111.55
30	b	601	SQD	C44-O6-C1	3.31	120.55	113.76
30	a	401	SQD	O6-C1-C2	3.31	113.64	108.23
28	B	627	DGD	C3G-O3G-C1D	3.33	120.58	113.76
31	a	402	LMG	C3-C4-C5	3.33	116.09	110.22
28	a	413	DGD	O6D-C5D-C6D	3.33	113.29	106.64
28	c	516	DGD	O2G-C1B-C2B	3.34	118.48	111.55
25	A	408	PL9	C25-C24-C26	3.34	121.09	115.29
27	j	102	BCR	C31-C1-C2	3.34	121.99	108.80
31	D	407	LMG	C7-O1-C1	3.35	120.62	113.76
25	D	404	PL9	C7-C3-C4	3.35	119.60	116.88
27	J	102	BCR	C31-C1-C2	3.35	122.03	108.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	521	LMG	O8-C28-C29	3.37	121.71	111.90
30	A	417	SQD	C44-O6-C1	3.38	120.68	113.76
23	B	610	CLA	CMB-C2B-C3B	3.38	131.17	124.89
23	b	616	CLA	CMB-C2B-C3B	3.40	131.20	124.89
31	k	103	LMG	O8-C28-C29	3.41	121.82	111.90
30	D	408	SQD	O8-S-C6	3.41	110.18	106.01
30	F	102	SQD	O8-S-C6	3.42	110.18	106.01
30	B	626	SQD	C44-O6-C1	3.44	120.81	113.76
28	b	602	DGD	C3D-C4D-C5D	3.45	116.30	110.22
31	M	101	LMG	C3-C4-C5	3.45	116.30	110.22
29	A	412	LHG	O7-C7-C8	3.46	118.73	111.55
25	d	404	PL9	C25-C24-C26	3.47	121.31	115.29
31	k	103	LMG	O7-C10-C11	3.48	118.77	111.55
27	j	102	BCR	C2-C1-C6	3.48	115.92	110.48
29	a	414	LHG	O7-C7-C8	3.49	118.79	111.55
25	a	410	PL9	C25-C24-C26	3.49	121.35	115.29
30	a	401	SQD	O5-C1-C2	3.51	117.07	110.30
30	d	408	SQD	O8-S-C6	3.51	110.30	106.01
31	D	406	LMG	O8-C28-C29	3.53	122.16	111.90
30	a	401	SQD	C1-C2-C3	3.53	116.54	109.98
27	J	102	BCR	C2-C1-C6	3.54	116.01	110.48
23	b	614	CLA	CMB-C2B-C3B	3.54	131.46	124.89
30	a	415	SQD	C1-O5-C5	3.54	120.39	113.72
25	a	410	PL9	C35-C34-C36	3.59	121.52	115.29
28	B	627	DGD	C3D-C4D-C5D	3.60	116.57	110.22
28	D	409	DGD	C3G-O3G-C1D	3.62	121.17	113.76
30	a	401	SQD	C44-O6-C1	3.62	121.19	113.76
30	A	417	SQD	O5-C1-C2	3.63	117.29	110.30
31	C	520	LMG	O7-C10-C11	3.66	119.14	111.55
28	C	518	DGD	O2G-C1B-C2B	3.67	119.17	111.55
30	a	401	SQD	O5-C5-C4	3.67	116.43	109.66
30	A	417	SQD	C1-O5-C5	3.68	120.64	113.72
28	c	518	DGD	C2G-O2G-C1B	3.68	126.57	117.88
30	a	415	SQD	O47-C7-C8	3.69	119.22	111.55
30	A	417	SQD	O5-C5-C4	3.70	116.47	109.66
30	f	102	SQD	C1-O5-C5	3.72	120.73	113.72
30	a	415	SQD	O8-S-C6	3.74	110.58	106.01
30	a	401	SQD	C1-O5-C5	3.75	120.79	113.72
31	c	519	LMG	O7-C10-C11	3.75	119.35	111.55
28	c	517	DGD	O2G-C1B-C2B	3.78	119.41	111.55
30	a	401	SQD	O47-C7-C8	3.80	119.44	111.55
31	A	418	LMG	O7-C10-C11	3.80	119.45	111.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	417	LHG	O7-C7-C8	3.81	119.46	111.55
28	C	519	DGD	C2G-O2G-C1B	3.82	126.89	117.88
31	a	402	LMG	O7-C10-C11	3.82	119.49	111.55
28	B	627	DGD	O2G-C1B-C2B	3.82	119.49	111.55
31	b	625	LMG	O7-C10-C11	3.83	119.51	111.55
31	D	407	LMG	O1-C1-C2	3.83	114.49	108.23
31	D	406	LMG	O7-C10-C11	3.85	119.54	111.55
30	D	408	SQD	C1-O5-C5	3.85	120.97	113.72
30	d	408	SQD	C1-O5-C5	3.85	120.97	113.72
30	A	413	SQD	C1-O5-C5	3.85	120.98	113.72
28	B	627	DGD	O5D-C1E-C2E	3.86	114.53	108.23
30	A	417	SQD	O47-C7-C8	3.91	119.67	111.55
25	a	410	PL9	C7-C3-C4	3.92	120.06	116.88
31	C	521	LMG	O7-C10-C11	3.93	119.70	111.55
29	A	415	LHG	O7-C7-C8	3.93	119.72	111.55
31	m	102	LMG	C3-C4-C5	3.94	117.16	110.22
25	A	408	PL9	C7-C3-C4	3.94	120.08	116.88
31	d	406	LMG	O7-C10-C11	3.95	119.74	111.55
30	F	102	SQD	C1-O5-C5	3.95	121.16	113.72
31	a	416	LMG	O7-C10-C11	3.98	119.82	111.55
30	f	102	SQD	O47-C7-C8	3.99	119.85	111.55
31	A	414	LMG	O7-C10-C11	4.00	119.86	111.55
31	B	622	LMG	O7-C10-C11	4.08	120.03	111.55
30	f	102	SQD	O9-S-C6	4.09	110.32	106.83
31	M	101	LMG	O7-C10-C11	4.11	120.09	111.55
31	m	102	LMG	O7-C10-C11	4.12	120.10	111.55
31	b	624	LMG	O7-C10-C11	4.13	120.12	111.55
30	d	408	SQD	O7-S-C6	4.13	110.36	106.83
30	F	102	SQD	O47-C7-C8	4.13	120.12	111.55
28	a	413	DGD	O2G-C1B-C2B	4.13	120.13	111.55
25	d	404	PL9	C7-C3-C4	4.14	120.24	116.88
28	D	409	DGD	O2D-C2D-C1D	4.15	118.71	110.03
30	D	408	SQD	O47-C7-C8	4.15	120.18	111.55
31	d	407	LMG	O1-C1-C2	4.17	115.04	108.23
31	B	623	LMG	O7-C10-C11	4.17	120.22	111.55
30	A	413	SQD	O8-S-C6	4.18	111.11	106.01
30	f	102	SQD	O8-S-C6	4.18	111.11	106.01
28	A	411	DGD	O2G-C1B-C2B	4.21	120.29	111.55
27	c	514	BCR	C8-C7-C6	4.26	139.18	127.25
31	a	416	LMG	C7-O1-C1	4.40	122.77	113.76
28	d	409	DGD	O2D-C2D-C1D	4.43	119.30	110.03
30	d	408	SQD	O47-C7-C8	4.47	120.83	111.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	514	BCR	C8-C7-C6	4.51	139.88	127.25
25	j	101	PL9	C7-C3-C4	4.55	120.58	116.88
25	J	101	PL9	C7-C3-C4	4.82	120.80	116.88
30	B	626	SQD	O9-S-C6	4.86	110.98	106.83
30	D	408	SQD	O7-S-C6	4.90	111.02	106.83
28	d	409	DGD	O3G-C1D-C2D	4.92	116.26	108.23
30	d	408	SQD	C44-O6-C1	5.08	124.17	113.76
28	D	409	DGD	O3G-C1D-C2D	5.11	116.57	108.23
30	A	413	SQD	O7-S-C6	5.15	111.23	106.83
28	C	519	DGD	C3G-O3G-C1D	5.27	124.56	113.76
30	D	408	SQD	C44-O6-C1	5.37	124.76	113.76
30	a	401	SQD	O7-S-C6	5.43	111.47	106.83
30	A	417	SQD	O7-S-C6	5.44	111.47	106.83
28	a	413	DGD	C3G-O3G-C1D	5.52	125.08	113.76
30	a	415	SQD	O9-S-C6	5.59	111.61	106.83
30	b	601	SQD	O9-S-C6	5.61	111.62	106.83
30	d	408	SQD	O6-C1-C2	5.64	117.43	108.23
30	a	415	SQD	O7-S-C6	5.68	111.68	106.83
28	A	411	DGD	C3G-O3G-C1D	5.70	125.44	113.76
30	F	102	SQD	O9-S-C6	5.79	111.77	106.83
28	c	518	DGD	C3G-O3G-C1D	5.81	125.67	113.76
30	A	413	SQD	O9-S-C6	5.85	111.83	106.83
30	F	102	SQD	O7-S-C6	5.85	111.83	106.83
30	D	408	SQD	O6-C1-C2	5.87	117.82	108.23
30	D	408	SQD	O9-S-C6	5.94	111.90	106.83
27	J	102	BCR	C31-C1-C6	6.32	120.55	110.31
27	j	102	BCR	C31-C1-C6	6.38	120.66	110.31
30	d	408	SQD	O9-S-C6	6.63	112.49	106.83
30	B	626	SQD	O7-S-C6	6.64	112.50	106.83
30	f	102	SQD	O7-S-C6	6.88	112.71	106.83
30	b	601	SQD	O7-S-C6	7.16	112.94	106.83
27	c	514	BCR	C7-C8-C9	8.16	138.47	126.21
27	C	514	BCR	C7-C8-C9	8.37	138.79	126.21

All (210) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	b	606	CLA	NC
23	b	606	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	b	606	CLA	NA
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	B	616	CLA	NC
23	B	616	CLA	ND
23	B	616	CLA	NA
23	A	404	CLA	NC
23	A	404	CLA	ND
23	A	404	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	c	511	CLA	NC
23	c	511	CLA	ND
23	c	511	CLA	NA
23	c	502	CLA	NC
23	c	502	CLA	ND
23	c	502	CLA	NA
23	b	618	CLA	NC
23	b	618	CLA	ND
23	b	618	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	ND
23	A	405	CLA	NA
23	c	507	CLA	NC
23	c	507	CLA	ND
23	c	507	CLA	NA
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	c	512	CLA	NC
23	c	512	CLA	ND
23	c	512	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	ND
23	B	610	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	B	607	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	B	602	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	c	508	CLA	NC
23	c	508	CLA	ND
23	c	508	CLA	NA
23	c	506	CLA	NC
23	c	506	CLA	ND
23	c	506	CLA	NA
23	b	620	CLA	NC
23	b	620	CLA	ND
23	b	620	CLA	NA
23	C	503	CLA	NC
23	C	503	CLA	ND
23	C	503	CLA	NA
23	c	504	CLA	NC
23	c	504	CLA	ND
23	c	504	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	a	405	CLA	NC
23	a	405	CLA	ND
23	a	405	CLA	NA
23	B	601	CLA	NC
23	B	601	CLA	ND
23	B	601	CLA	NA
23	d	403	CLA	NC
23	d	403	CLA	ND
23	d	403	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	D	403	CLA	NC
23	D	403	CLA	ND
23	D	403	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	b	617	CLA	NA
23	c	503	CLA	NC
23	c	503	CLA	ND
23	c	503	CLA	NA
23	c	509	CLA	NC
23	c	509	CLA	ND
23	c	509	CLA	NA
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	c	510	CLA	NC
23	c	510	CLA	ND
23	c	510	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	a	404	CLA	NC
23	a	404	CLA	ND
23	a	404	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	C	506	CLA	NC
23	C	506	CLA	ND
23	C	506	CLA	NA
23	b	612	CLA	NC
23	b	612	CLA	ND
23	b	612	CLA	NA
23	b	619	CLA	NC
23	b	619	CLA	ND
23	b	619	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	b	613	CLA	NA
23	c	513	CLA	NC
23	c	513	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	c	513	CLA	NA
23	B	609	CLA	NC
23	B	609	CLA	ND
23	B	609	CLA	NA
23	c	501	CLA	NC
23	c	501	CLA	ND
23	c	501	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	ND
23	a	406	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	C	511	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	ND
23	b	610	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	a	409	CLA	NC
23	a	409	CLA	ND
23	a	409	CLA	NA
23	c	505	CLA	NC
23	c	505	CLA	ND
23	c	505	CLA	NA
23	D	401	CLA	NC
23	D	401	CLA	ND
23	D	401	CLA	NA
23	A	403	CLA	NC
23	A	403	CLA	ND
23	A	403	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	B	613	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	ND
23	C	510	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	ND
23	C	504	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	d	402	CLA	NC
23	d	402	CLA	ND
23	d	402	CLA	NA
23	A	407	CLA	NC
23	A	407	CLA	ND
23	A	407	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	ND
23	C	512	CLA	NA
23	b	609	CLA	NC
23	b	609	CLA	ND
23	b	609	CLA	NA
23	C	501	CLA	NC
23	C	501	CLA	ND
23	C	501	CLA	NA

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	D	409	DGD	C3G-O3G-C1D-O6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	d	409	DGD	C3G-O3G-C1D-O6D
31	m	102	LMG	C8-O7-C10-C11
31	M	101	LMG	C8-O7-C10-C11
28	c	517	DGD	C2G-O2G-C1B-O1B
28	C	518	DGD	C2G-O2G-C1B-O1B
28	c	517	DGD	C2G-O2G-C1B-C2B
28	C	518	DGD	C2G-O2G-C1B-C2B
30	d	408	SQD	C45-O47-C7-O49
30	D	408	SQD	C45-O47-C7-O49
30	D	408	SQD	C45-O47-C7-C8
30	d	408	SQD	C45-O47-C7-C8

There are no ring outliers.

85 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	403	CLA	12	0
23	A	404	CLA	23	0
23	A	405	CLA	15	0
24	A	406	PHO	5	0
23	A	407	CLA	2	0
25	A	408	PL9	2	0
27	A	410	BCR	7	0
28	A	411	DGD	1	0
29	A	412	LHG	4	0
30	A	413	SQD	5	0
31	A	414	LMG	3	0
29	A	415	LHG	3	0
30	A	417	SQD	7	0
31	A	418	LMG	2	0
23	B	601	CLA	2	0
23	B	602	CLA	6	0
23	B	603	CLA	14	0
23	B	604	CLA	9	0
23	B	605	CLA	13	0
23	B	606	CLA	12	0
23	B	607	CLA	19	0
23	B	608	CLA	12	0
23	B	609	CLA	16	0
23	B	610	CLA	6	0
23	B	611	CLA	9	0
23	B	612	CLA	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	613	CLA	13	0
23	B	614	CLA	5	0
23	B	615	CLA	2	0
23	B	616	CLA	7	0
27	B	617	BCR	4	0
27	B	618	BCR	10	0
27	B	619	BCR	6	0
27	B	620	BCR	4	0
31	B	622	LMG	3	0
31	B	623	LMG	5	0
33	B	624	LMT	1	0
30	B	626	SQD	2	0
28	B	627	DGD	2	0
33	B	628	LMT	2	0
33	B	629	LMT	2	0
23	C	501	CLA	7	0
23	C	502	CLA	2	0
23	C	503	CLA	6	0
23	C	504	CLA	7	0
23	C	505	CLA	6	0
23	C	506	CLA	4	0
23	C	507	CLA	9	0
23	C	508	CLA	4	0
23	C	509	CLA	3	0
23	C	510	CLA	9	0
23	C	511	CLA	11	0
23	C	512	CLA	5	0
23	C	513	CLA	4	0
27	C	514	BCR	9	0
27	C	515	BCR	8	0
27	C	516	BCR	5	0
28	C	517	DGD	8	0
28	C	518	DGD	8	0
28	C	519	DGD	5	0
31	C	520	LMG	3	0
31	C	521	LMG	2	0
23	D	401	CLA	7	0
24	D	402	PHO	6	0
23	D	403	CLA	3	0
25	D	404	PL9	12	0
27	D	405	BCR	3	0
31	D	406	LMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	407	LMG	6	0
30	D	408	SQD	5	0
28	D	409	DGD	2	0
33	D	410	LMT	1	0
31	E	101	LMG	1	0
34	F	101	HEM	5	0
30	F	102	SQD	2	0
27	H	101	BCR	7	0
31	I	101	LMG	2	0
33	I	102	LMT	2	0
25	J	101	PL9	1	0
27	J	102	BCR	4	0
31	M	101	LMG	2	0
33	M	102	LMT	1	0
27	T	101	BCR	6	0
27	T	102	BCR	6	0
34	V	201	HEM	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/360 (93%)	0.10	9 (2%) 55 51	43, 64, 104, 149	0
1	a	335/360 (93%)	-0.11	4 (1%) 79 74	44, 65, 106, 149	0
2	B	490/510 (96%)	0.33	28 (5%) 24 27	46, 69, 103, 159	0
2	b	490/510 (96%)	0.30	27 (5%) 26 28	47, 71, 104, 159	0
3	C	447/461 (96%)	0.06	7 (1%) 72 67	54, 79, 106, 132	0
3	c	447/461 (96%)	0.20	10 (2%) 62 59	56, 81, 105, 135	0
4	D	340/352 (96%)	-0.04	3 (0%) 84 80	44, 66, 103, 137	0
4	d	340/352 (96%)	-0.08	2 (0%) 89 86	45, 66, 102, 134	0
5	E	82/84 (97%)	0.07	1 (1%) 79 74	68, 92, 125, 130	0
5	e	82/84 (97%)	0.38	3 (3%) 42 41	70, 92, 125, 129	0
6	F	35/45 (77%)	0.03	1 (2%) 52 49	68, 84, 119, 139	0
6	f	35/45 (77%)	0.33	0 100 100	73, 85, 120, 141	0
7	H	65/66 (98%)	0.78	8 (12%) 5 11	77, 94, 122, 138	0
7	h	65/66 (98%)	0.58	3 (4%) 33 34	73, 93, 120, 144	0
8	I	35/38 (92%)	0.16	1 (2%) 52 49	65, 79, 107, 118	0
8	i	35/38 (92%)	0.04	0 100 100	66, 81, 106, 120	0
9	J	34/40 (85%)	0.01	1 (2%) 52 49	69, 85, 95, 112	0
9	j	34/40 (85%)	-0.25	1 (2%) 52 49	74, 88, 95, 116	0
10	K	37/46 (80%)	0.13	0 100 100	77, 87, 101, 122	0
10	k	37/46 (80%)	0.27	3 (8%) 13 18	73, 88, 108, 123	0
11	L	37/37 (100%)	-0.01	0 100 100	48, 62, 128, 156	0
11	l	37/37 (100%)	-0.12	0 100 100	52, 60, 126, 158	0
12	M	34/36 (94%)	0.09	2 (5%) 23 25	56, 71, 110, 164	0
12	m	34/36 (94%)	0.25	3 (8%) 11 16	55, 69, 108, 165	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%)	0.83	28 (11%) 5 12	50, 78, 122, 169	0
13	o	243/272 (89%)	0.60	20 (8%) 12 18	52, 78, 121, 167	0
14	T	32/32 (100%)	0.27	4 (12%) 4 11	55, 67, 158, 174	0
14	t	32/32 (100%)	-0.08	0 100 100	54, 69, 159, 168	0
15	U	97/134 (72%)	0.92	9 (9%) 9 15	56, 71, 92, 108	0
15	u	97/134 (72%)	0.74	5 (5%) 28 30	55, 71, 91, 111	0
16	V	137/163 (84%)	0.33	7 (5%) 29 31	53, 71, 86, 101	0
16	v	137/163 (84%)	0.72	9 (6%) 19 22	59, 72, 88, 95	0
17	g	28/46 (60%)	0.78	5 (17%) 2 7	95, 108, 126, 132	0
17	y	28/46 (60%)	0.28	1 (3%) 43 41	89, 107, 126, 131	0
18	X	37/41 (90%)	0.95	5 (13%) 3 10	76, 93, 124, 140	0
18	x	37/41 (90%)	0.94	10 (27%) 1 6	75, 90, 126, 141	0
19	Z	62/62 (100%)	1.07	8 (12%) 4 10	87, 104, 168, 185	0
19	z	62/62 (100%)	0.70	3 (4%) 31 33	88, 105, 172, 187	0
20	G	0/28	-	-	-	-
20	Y	0/28	-	-	-	-
All	All	5214/5706 (91%)	0.27	231 (4%) 35 35	43, 75, 115, 187	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	O	170	GLY	5.7
2	B	129	GLY	5.4
13	o	84	ASN	4.2
15	U	54	LYS	4.2
10	k	14	ALA	4.0
2	b	483	ASP	4.0
4	d	295	SER	3.8
15	U	113	THR	3.7
7	H	2	ALA	3.6
7	H	4	ARG	3.6
13	O	90	GLU	3.6
15	u	107	GLU	3.6
2	B	378	LYS	3.6
14	T	28	ARG	3.5
13	o	46	PRO	3.5
2	B	128	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	130	GLU	3.4
14	T	31	LYS	3.4
18	X	47	GLN	3.4
13	o	30	THR	3.3
2	b	482	ILE	3.3
13	O	157	PRO	3.3
2	B	379	ALA	3.2
2	b	302	TRP	3.2
5	e	84	LYS	3.2
16	v	131	ARG	3.2
2	B	294	SER	3.2
19	Z	62	VAL	3.2
19	z	1	MET	3.2
18	x	47	GLN	3.1
2	B	127	ARG	3.1
2	b	405	GLU	3.1
1	A	11	ALA	3.1
2	b	407	ASN	3.1
13	O	169	LYS	3.1
7	H	64	ALA	3.1
2	b	70	GLY	3.1
1	A	16	ARG	3.1
3	C	183	GLY	3.1
13	O	269	ILE	3.0
3	C	184	GLY	3.0
13	o	171	GLU	3.0
3	C	27	ASP	3.0
3	c	372	PRO	3.0
13	O	84	ASN	3.0
13	O	223	ILE	3.0
13	O	79	LYS	3.0
18	X	46	VAL	3.0
10	k	13	GLU	2.9
13	o	221	GLY	2.9
1	A	15	GLU	2.9
2	B	132	ALA	2.9
15	U	53	GLU	2.9
1	A	229	GLU	2.9
9	j	7	ARG	2.9
2	b	484	PRO	2.9
1	A	12	ASN	2.9
2	b	409	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	10	SER	2.8
2	B	133	LEU	2.8
19	Z	34	ASP	2.8
2	B	477	ASP	2.8
2	B	402	TYR	2.8
15	U	38	GLU	2.8
13	O	222	GLN	2.8
18	x	13	THR	2.8
7	H	5	THR	2.8
19	Z	1	MET	2.7
13	O	220	LYS	2.7
2	b	393	GLU	2.7
13	o	47	THR	2.7
15	U	55	ILE	2.7
7	h	24	GLY	2.7
13	O	245	GLN	2.7
2	b	294	SER	2.7
15	u	113	THR	2.7
13	O	119	LEU	2.7
17	y	42	ARG	2.7
2	b	304	ALA	2.6
13	o	158	ASN	2.6
3	C	332	GLN	2.6
13	o	55	ALA	2.6
13	O	155	THR	2.6
18	X	17	LYS	2.6
1	A	230	THR	2.6
1	a	80	GLY	2.6
7	H	18	TYR	2.6
17	g	27	MET	2.6
2	B	476	ARG	2.6
13	O	258	GLU	2.6
4	D	295	SER	2.6
19	Z	54	VAL	2.5
4	d	227	GLU	2.5
18	x	11	THR	2.5
2	B	190	PHE	2.5
2	B	490	GLN	2.5
2	b	194	ASN	2.5
16	v	103	LYS	2.5
13	o	32	THR	2.5
13	O	49	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	126	GLY	2.5
13	O	87	GLN	2.5
13	o	31	LEU	2.4
13	O	168	PHE	2.4
18	x	42	GLN	2.4
16	V	28	GLU	2.4
13	O	107	ILE	2.4
13	O	244	GLU	2.4
2	b	489	GLU	2.4
3	C	145	SER	2.4
2	B	189	GLY	2.4
2	B	293	ALA	2.4
7	H	63	LYS	2.4
12	m	5	GLN	2.4
17	g	21	GLN	2.4
19	z	4	LEU	2.4
2	B	131	PRO	2.4
2	b	339	ALA	2.4
3	c	147	PHE	2.4
7	H	66	GLY	2.4
15	u	114	VAL	2.4
2	B	188	ASP	2.4
4	D	21	TRP	2.4
13	O	171	GLU	2.4
2	b	408	GLY	2.4
17	g	29	GLY	2.4
3	c	142	GLU	2.4
13	O	54	GLY	2.4
5	e	8	ARG	2.3
13	O	50	ASP	2.3
19	Z	56	VAL	2.3
13	o	229	LYS	2.3
2	B	295	GLY	2.3
2	b	403	GLY	2.3
18	x	16	LEU	2.3
13	o	225	LEU	2.3
2	B	347	ARG	2.3
3	C	28	GLN	2.3
19	Z	57	LEU	2.3
16	v	44	THR	2.3
15	U	112	PHE	2.3
18	x	46	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	404	GLY	2.3
3	c	184	GLY	2.3
15	U	123	GLU	2.3
18	x	17	LYS	2.3
3	c	144	SER	2.3
2	b	327	THR	2.3
3	C	258	GLY	2.3
13	O	221	GLY	2.3
16	V	96	GLU	2.3
18	X	45	LYS	2.3
16	v	93	ASP	2.3
6	F	14	PRO	2.3
18	x	20	PHE	2.3
2	b	338	GLN	2.2
2	B	368	VAL	2.2
5	e	56	TYR	2.2
18	x	12	ILE	2.2
7	h	4	ARG	2.2
2	b	379	ALA	2.2
13	O	156	GLN	2.2
3	c	146	PHE	2.2
2	B	162	PHE	2.2
3	c	373	ASN	2.2
16	v	130	MET	2.2
12	M	2	GLU	2.2
13	O	89	ALA	2.2
13	o	51	THR	2.2
2	b	340	TRP	2.2
16	v	27	ALA	2.2
15	U	50	ALA	2.2
17	g	24	MET	2.2
1	A	242	GLU	2.2
2	B	121	GLU	2.2
15	u	106	ARG	2.2
2	B	478	VAL	2.2
13	o	238	ALA	2.2
16	v	132	ASN	2.1
16	V	37	PRO	2.1
13	o	168	PHE	2.1
16	v	36	VAL	2.1
7	H	3	ARG	2.1
7	h	66	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	m	4	ASN	2.1
16	V	49	GLU	2.1
17	g	26	ALA	2.1
1	a	81	ALA	2.1
2	B	353	GLU	2.1
13	O	48	LEU	2.1
16	V	77	SER	2.1
13	o	49	ASP	2.1
3	c	363	GLY	2.1
12	m	7	GLY	2.1
13	o	226	ASN	2.1
15	U	39	LEU	2.1
2	b	303	SER	2.1
12	M	34	LYS	2.1
14	T	27	PRO	2.1
13	o	90	GLU	2.1
15	u	108	ASN	2.1
1	a	226	GLU	2.1
2	b	378	LYS	2.1
16	V	43	LYS	2.1
16	v	31	PRO	2.1
3	c	389	GLU	2.1
2	B	126	PRO	2.1
13	o	228	ALA	2.1
13	O	88	GLU	2.1
5	E	74	GLN	2.1
2	b	84	THR	2.1
2	B	487	SER	2.1
18	x	45	LYS	2.1
14	T	29	ILE	2.1
9	J	7	ARG	2.0
18	X	11	THR	2.0
19	z	34	ASP	2.0
2	b	297	THR	2.0
19	Z	35	ARG	2.0
16	V	111	GLU	2.0
1	A	14	TRP	2.0
2	b	373	LYS	2.0
3	c	145	SER	2.0
19	Z	38	GLN	2.0
8	I	34	ARG	2.0
2	B	488	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	k	15	TYR	2.0
4	D	24	ARG	2.0
13	o	220	LYS	2.0
1	a	75	ASN	2.0
2	b	295	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	LMT	i	102	35/35	0.38	1.07	8.39	99,137,146,152	0
25	PL9	J	101	35/55	0.29	0.53	6.08	119,157,178,182	0
27	BCR	B	620	40/40	0.57	0.94	5.97	75,86,98,103	0
32	CL	A	416	1/1	0.44	1.00	5.64	49,49,49,49	0
27	BCR	C	514	40/40	0.84	1.00	4.73	73,80,87,94	0
27	BCR	c	514	40/40	0.80	1.11	4.57	76,82,88,89	0
27	BCR	z	101	40/40	0.67	1.31	4.55	86,96,112,115	0
31	LMG	C	521	45/55	0.33	1.12	4.28	84,119,143,175	0
33	LMT	B	629	35/35	0.48	0.67	4.21	70,137,165,168	0
28	DGD	D	409	63/66	0.56	0.74	4.05	104,127,181,188	0
23	CLA	b	605	65/65	0.50	0.91	4.01	88,108,124,137	0
31	LMG	c	519	45/55	0.55	0.97	3.91	86,119,142,171	0
33	LMT	b	627	35/35	0.56	0.88	3.74	100,140,152,154	0
23	CLA	C	513	65/65	0.75	0.93	3.68	95,109,142,149	0
27	BCR	C	515	40/40	0.80	1.04	3.66	85,92,115,116	0
28	DGD	d	409	63/66	0.59	0.62	3.56	106,128,181,190	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	c	511	65/65	0.82	0.69	3.55	75,91,102,108	0
22	BCT	d	401	4/4	0.86	0.48	3.48	87,91,92,94	0
27	BCR	j	102	40/40	0.49	0.51	3.47	110,128,180,184	0
33	LMT	I	102	35/35	0.65	0.68	3.46	99,135,144,145	0
23	CLA	B	612	65/65	0.90	0.51	3.44	61,72,82,86	0
23	CLA	c	507	65/65	0.83	0.66	3.41	83,93,105,111	0
23	CLA	c	501	65/65	0.85	0.81	3.38	67,82,92,94	0
27	BCR	b	622	40/40	0.66	0.65	3.38	72,83,94,96	0
23	CLA	b	607	65/65	0.83	0.78	3.36	68,82,92,103	0
23	CLA	c	513	65/65	0.66	1.06	3.31	93,109,142,148	0
23	CLA	D	403	65/65	0.86	0.87	3.30	74,87,123,124	0
31	LMG	E	101	44/55	0.46	0.65	3.30	87,123,132,139	0
27	BCR	y	101	40/40	0.68	0.78	3.26	79,86,106,109	0
33	LMT	D	410	31/35	0.60	0.95	3.26	83,133,154,159	0
33	LMT	B	625	35/35	0.72	0.75	3.22	95,139,149,152	0
23	CLA	c	503	65/65	0.83	0.81	3.16	77,89,97,103	0
23	CLA	B	601	65/65	0.53	1.00	3.09	92,108,131,137	0
28	DGD	B	627	52/66	0.72	0.50	3.07	75,105,178,180	0
23	CLA	B	609	65/65	0.90	0.73	3.06	74,89,104,106	0
23	CLA	B	604	65/65	0.83	0.58	3.05	59,67,104,124	0
23	CLA	c	512	65/65	0.77	1.05	2.97	83,104,146,152	0
23	CLA	C	512	65/65	0.83	0.84	2.96	89,101,144,149	0
27	BCR	c	515	40/40	0.78	0.79	2.95	75,86,95,101	0
27	BCR	H	101	40/40	0.70	1.03	2.90	83,96,130,131	0
23	CLA	B	605	65/65	0.87	0.66	2.88	58,78,86,92	0
31	LMG	i	101	43/55	0.72	0.67	2.77	84,120,162,177	0
30	SQD	d	408	43/54	0.64	0.74	2.73	67,109,152,157	0
33	LMT	B	628	35/35	0.39	0.62	2.70	72,126,141,144	0
33	LMT	d	410	31/35	0.39	0.87	2.69	83,134,157,157	0
23	CLA	b	613	65/65	0.81	0.73	2.68	65,93,104,114	0
23	CLA	C	509	65/65	0.86	0.63	2.59	62,81,95,98	0
31	LMG	a	402	42/55	0.66	0.51	2.57	72,100,119,143	0
23	CLA	B	610	65/65	0.84	0.67	2.44	69,81,88,92	0
23	CLA	A	407	65/65	0.84	0.49	2.30	56,66,127,129	0
23	CLA	B	603	65/65	0.89	0.65	2.27	65,81,94,109	0
33	LMT	b	603	35/35	0.61	0.48	2.27	73,119,136,138	0
31	LMG	I	101	43/55	0.74	0.56	2.25	73,118,166,178	0
33	LMT	b	604	35/35	0.68	0.49	2.25	69,133,158,160	0
32	CL	a	418	1/1	0.78	0.49	2.21	49,49,49,49	0
25	PL9	j	101	35/55	0.32	0.43	2.19	120,160,178,182	0
23	CLA	b	619	65/65	0.81	0.59	2.18	85,97,108,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	CLA	b	612	65/65	0.80	0.51	2.17	63,75,95,98	0
23	CLA	b	609	65/65	0.87	0.51	2.17	61,76,84,88	0
23	CLA	d	403	65/65	0.83	0.67	2.14	72,88,121,128	0
27	BCR	k	102	40/40	0.64	0.78	2.14	72,80,109,111	0
23	CLA	B	608	65/65	0.79	0.64	2.12	64,75,93,97	0
27	BCR	a	412	40/40	0.73	0.42	2.10	54,71,84,87	0
30	SQD	B	626	47/54	0.68	0.42	2.09	75,100,144,148	0
27	BCR	D	405	40/40	0.64	0.53	2.09	68,81,105,110	0
23	CLA	c	509	65/65	0.85	0.52	2.08	67,85,91,97	0
23	CLA	C	501	65/65	0.86	0.47	2.05	69,82,90,95	0
23	CLA	b	608	65/65	0.84	0.40	1.90	61,68,107,117	0
27	BCR	h	101	40/40	0.73	0.94	1.87	85,94,124,127	0
29	LHG	A	415	37/49	0.62	0.59	1.86	104,133,190,202	0
23	CLA	b	614	65/65	0.84	0.60	1.83	66,82,88,91	0
23	CLA	C	507	65/65	0.74	0.66	1.81	79,93,100,104	0
23	CLA	a	409	65/65	0.81	0.46	1.80	55,67,129,133	0
29	LHG	a	417	37/49	0.70	0.38	1.76	110,135,197,206	0
30	SQD	F	102	45/54	0.69	0.77	1.71	87,127,149,152	0
23	CLA	B	606	65/65	0.79	0.72	1.70	67,81,110,121	0
30	SQD	f	102	45/54	0.75	0.59	1.69	88,133,148,152	0
30	SQD	D	408	43/54	0.72	0.66	1.67	71,103,148,152	0
25	PL9	a	410	45/55	0.64	0.46	1.64	82,103,121,125	0
30	SQD	b	601	47/54	0.68	0.41	1.64	81,103,147,151	0
31	LMG	A	418	42/55	0.62	0.44	1.62	81,105,123,147	0
24	PHO	A	406	64/64	0.84	0.37	1.59	50,69,77,81	0
23	CLA	b	620	65/65	0.71	0.59	1.59	75,98,145,147	0
25	PL9	A	408	45/55	0.67	0.47	1.57	89,101,119,127	0
23	CLA	c	502	65/65	0.68	0.61	1.49	63,75,100,106	0
30	SQD	A	413	51/54	0.73	0.40	1.49	81,99,128,131	0
23	CLA	B	615	65/65	0.82	0.82	1.47	83,96,106,116	0
27	BCR	C	516	40/40	0.75	0.57	1.42	74,86,95,100	0
27	BCR	J	102	40/40	0.58	0.45	1.38	108,125,177,180	0
23	CLA	B	602	65/65	0.79	0.63	1.36	68,87,95,96	0
28	DGD	C	519	66/66	0.66	0.44	1.29	55,72,100,114	0
23	CLA	C	502	65/65	0.79	0.50	1.24	59,75,108,111	0
23	CLA	C	503	65/65	0.87	0.50	1.21	71,88,99,105	0
23	CLA	C	506	65/65	0.67	0.60	1.17	79,91,125,133	0
23	CLA	b	616	65/65	0.91	0.34	1.16	61,73,83,86	0
23	CLA	b	606	65/65	0.86	0.47	1.14	70,87,96,97	0
23	CLA	c	506	65/65	0.79	0.49	1.14	78,92,122,128	0
23	CLA	C	510	65/65	0.79	0.38	1.09	67,74,83,93	0
27	BCR	A	410	40/40	0.70	0.47	1.09	52,68,85,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	LMG	M	101	42/55	0.74	0.35	1.07	83,111,135,144	0
31	LMG	d	407	48/55	0.82	0.36	1.00	58,70,85,120	0
27	BCR	d	405	40/40	0.78	0.38	1.00	69,82,102,106	0
27	BCR	B	618	40/40	0.62	0.36	0.98	75,82,94,95	0
28	DGD	a	413	56/66	0.75	0.38	0.96	76,100,145,148	0
28	DGD	A	411	56/66	0.71	0.38	0.95	77,102,146,153	0
30	SQD	A	417	54/54	0.78	0.37	0.94	77,113,147,154	0
23	CLA	C	504	65/65	0.78	0.36	0.91	62,83,138,145	0
23	CLA	c	508	65/65	0.90	0.36	0.88	70,85,118,134	0
23	CLA	c	510	65/65	0.90	0.42	0.88	67,75,84,89	0
23	CLA	C	511	65/65	0.80	0.55	0.87	74,88,102,109	0
23	CLA	d	402	65/65	0.84	0.37	0.85	49,57,81,95	0
28	DGD	B	621	58/66	0.85	0.38	0.81	46,71,101,105	0
23	CLA	B	616	65/65	0.69	0.71	0.80	79,93,147,152	0
27	BCR	B	619	40/40	0.71	0.34	0.80	62,75,83,86	0
23	CLA	c	504	65/65	0.82	0.34	0.80	75,83,133,138	0
29	LHG	a	414	39/49	0.79	0.41	0.80	60,78,94,102	0
23	CLA	b	610	65/65	0.87	0.53	0.79	70,83,112,126	0
34	HEM	V	201	43/43	0.85	0.47	0.76	58,69,74,76	0
30	SQD	a	401	54/54	0.75	0.42	0.75	76,114,149,152	0
34	HEM	F	101	43/43	0.88	0.45	0.74	89,105,127,130	0
23	CLA	c	505	65/65	0.82	0.35	0.72	70,77,83,85	0
27	BCR	B	617	40/40	0.78	0.33	0.64	67,74,81,84	0
31	LMG	m	102	42/55	0.77	0.38	0.60	73,111,128,138	0
33	LMT	M	102	35/35	0.82	0.51	0.60	69,96,112,115	0
28	DGD	c	518	66/66	0.76	0.34	0.60	54,73,105,118	0
28	DGD	b	602	52/66	0.80	0.41	0.58	79,107,180,186	0
26	OEC	A	409	5/9	0.94	0.43	0.55	35,44,57,62	0
28	DGD	b	623	58/66	0.80	0.36	0.53	57,74,99,107	0
24	PHO	a	408	64/64	0.86	0.33	0.52	58,68,79,86	0
23	CLA	C	505	65/65	0.79	0.41	0.52	69,77,86,91	0
23	CLA	B	614	65/65	0.73	0.41	0.50	63,83,125,129	0
23	CLA	a	406	65/65	0.79	0.36	0.47	55,71,140,147	0
34	HEM	f	101	43/43	0.89	0.50	0.44	89,105,124,126	0
23	CLA	a	404	65/65	0.90	0.33	0.44	53,60,67,74	0
23	CLA	b	618	65/65	0.82	0.32	0.43	60,82,123,130	0
31	LMG	k	103	48/55	0.74	0.43	0.43	79,100,112,115	0
28	DGD	c	517	62/66	0.84	0.31	0.40	64,84,132,141	0
27	BCR	T	102	40/40	0.72	0.33	0.39	71,79,86,86	0
29	LHG	A	412	39/49	0.83	0.29	0.38	59,79,89,93	0
34	HEM	v	201	43/43	0.84	0.51	0.34	57,68,75,76	0
31	LMG	e	101	44/55	0.66	0.44	0.32	91,122,132,136	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
30	SQD	a	415	51/54	0.71	0.39	0.31	88,101,128,129	0
23	CLA	B	613	65/65	0.86	0.30	0.31	46,64,88,93	0
31	LMG	D	406	46/55	0.80	0.33	0.31	58,73,116,129	0
25	PL9	d	404	55/55	0.75	0.32	0.29	45,65,78,85	0
31	LMG	a	416	51/55	0.80	0.33	0.27	62,80,93,100	0
28	DGD	C	518	62/66	0.82	0.34	0.26	58,81,134,144	0
23	CLA	b	617	65/65	0.92	0.27	0.23	57,67,91,93	0
23	CLA	A	403	65/65	0.91	0.28	0.19	52,58,66,70	0
25	PL9	D	404	55/55	0.77	0.32	0.15	42,61,71,77	0
31	LMG	B	622	49/55	0.75	0.33	0.15	61,79,105,117	0
28	DGD	C	517	53/66	0.87	0.29	0.14	61,79,96,101	0
28	DGD	c	516	53/66	0.82	0.31	0.14	63,77,96,103	0
31	LMG	C	520	48/55	0.80	0.30	0.10	89,100,109,112	0
23	CLA	B	611	65/65	0.87	0.31	0.09	63,72,80,87	0
23	CLA	b	615	65/65	0.90	0.28	0.05	54,72,80,87	0
23	CLA	C	508	65/65	0.86	0.32	0.05	71,86,117,132	0
27	BCR	b	621	40/40	0.72	0.28	0.03	63,73,84,87	0
23	CLA	A	405	65/65	0.85	0.30	0.03	44,69,140,145	0
24	PHO	D	402	64/64	0.88	0.29	0.01	51,62,72,74	0
23	CLA	a	405	65/65	0.87	0.31	-0.03	44,53,69,73	0
26	OEC	a	411	5/9	0.92	0.35	-0.05	35,44,62,68	0
31	LMG	D	407	48/55	0.86	0.26	-0.08	54,72,81,120	0
27	BCR	T	101	40/40	0.79	0.31	-0.09	68,75,82,83	0
31	LMG	B	623	49/55	0.83	0.31	-0.14	58,76,84,87	0
22	BCT	A	402	4/4	0.87	0.33	-0.16	85,90,90,94	0
24	PHO	a	407	64/64	0.87	0.28	-0.19	53,63,70,73	0
23	CLA	D	401	65/65	0.88	0.27	-0.20	49,59,87,97	0
23	CLA	b	611	65/65	0.87	0.32	-0.22	54,64,89,92	0
31	LMG	b	624	49/55	0.85	0.27	-0.26	59,82,102,113	0
33	LMT	m	101	35/35	0.81	0.41	-0.35	68,93,112,114	0
31	LMG	b	625	49/55	0.81	0.32	-0.39	51,75,86,89	0
23	CLA	A	404	65/65	0.90	0.29	-0.42	44,54,67,74	0
23	CLA	B	607	65/65	0.86	0.28	-0.42	52,66,82,85	0
31	LMG	A	414	51/55	0.84	0.26	-0.45	63,77,92,95	0
31	LMG	d	406	46/55	0.89	0.24	-0.60	63,73,116,130	0
21	FE2	A	401	1/1	0.78	0.17	-1.38	64,64,64,64	0
21	FE2	a	403	1/1	0.87	0.16	-2.83	72,72,72,72	0
33	LMT	B	624	35/35	0.50	0.82	-	80,142,170,171	0
35	CA	K	101	1/1	0.62	0.53	-	86,86,86,86	0
35	CA	o	301	1/1	0.64	0.47	-	98,98,98,98	0
35	CA	O	301	1/1	0.35	0.47	-	112,112,112,112	0
33	LMT	b	626	35/35	0.62	0.67	-	76,139,174,176	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CA	k	101	1/1	0.32	0.53	-	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.