



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2017 – 12:21 AM EST

PDB ID : 5WS6
Title : Native XFEL structure of Photosystem II (preflash two-flash dataset)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2016-12-05
Resolution : 2.35 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 : rb-20029077
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)
Validation Pipeline (wwPDB-VP) : rb-20029077

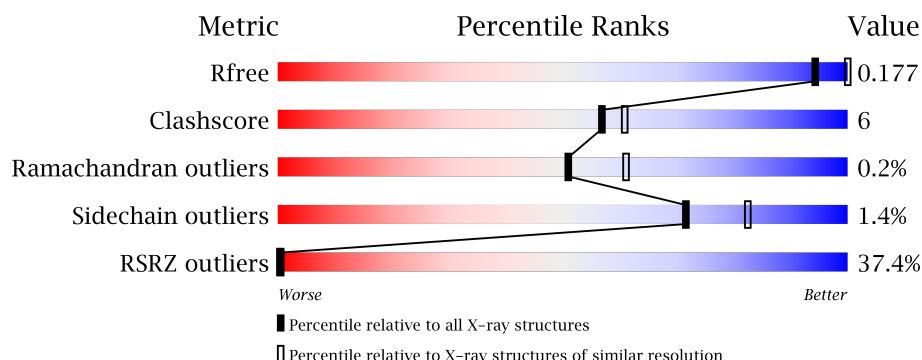
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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	344	<div> <div>24%</div> <div>84%</div> <div>13%</div> <div>.</div> </div>
1	a	344	<div> <div>33%</div> <div>97%</div> <div>..</div> </div>
2	B	505	<div> <div>30%</div> <div>84%</div> <div>16%</div> </div>
2	b	505	<div> <div>34%</div> <div>98%</div> <div>.</div> </div>
3	C	455	<div> <div>38%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

Continued on next page...

Continued from previous page...

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CL	A	402	-	-	-	X
22	CL	a	402	-	-	-	X
24	CLA	A	404	X	-	-	-
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	A	409	X	-	-	-
24	CLA	B	601	X	-	-	X
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	X
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	X
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	X
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	C	514	X	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	350	X	-	-	-
24	CLA	a	403	X	-	-	-
24	CLA	a	404	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	X
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	X
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-
26	BCR	B	617	-	-	-	X
26	BCR	B	618	-	-	-	X
26	BCR	T	101	-	-	-	X
26	BCR	b	618	-	-	-	X
26	BCR	t	102	-	-	-	X
27	SQD	A	411	-	-	-	X
27	SQD	A	413	-	-	-	X
27	SQD	B	620	-	-	-	X
27	SQD	a	411	-	-	-	X
27	SQD	b	620	-	-	-	X
27	SQD	f	101	-	-	-	X
28	GOL	B	626	-	-	-	X
28	GOL	B	627	-	-	-	X
28	GOL	V	202	-	-	-	X
28	GOL	a	410	-	-	-	X
28	GOL	a	416	-	-	-	X
28	GOL	c	502	-	-	-	X
28	GOL	v	202	-	-	-	X
31	PL9	A	416[A]	-	-	-	X
31	PL9	A	416[B]	-	-	-	X
31	PL9	D	405	-	-	-	X
31	PL9	a	414[A]	-	-	-	X
31	PL9	a	414[B]	-	-	-	X
31	PL9	d	405	-	-	-	X
32	UNL	D	408	-	-	-	X
32	UNL	D	409	-	-	-	X
32	UNL	I	102	-	-	-	X
32	UNL	K	101	-	-	-	X
32	UNL	d	409	-	-	-	X
32	UNL	d	410	-	-	-	X
32	UNL	i	101	-	-	-	X
32	UNL	j	102	-	-	-	X
33	LMG	A	418	-	-	-	X
33	LMG	B	621	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	LMG	C	520	-	-	-	X
33	LMG	C	521	-	-	-	X
33	LMG	J	101	-	-	-	X
33	LMG	Z	101	-	-	-	X
33	LMG	a	417	-	-	-	X
33	LMG	c	522	-	-	-	X
33	LMG	z	101	-	-	-	X
34	LMT	A	359	-	-	-	X
34	LMT	B	622	-	-	-	X
34	LMT	B	630	-	-	-	X
34	LMT	E	102	-	-	-	X
34	LMT	I	101	-	-	-	X
34	LMT	M	101	-	-	-	X
34	LMT	M	103	-	-	-	X
34	LMT	a	359	-	-	-	X
34	LMT	a	418	-	-	-	X
34	LMT	b	622	-	-	-	X
34	LMT	b	630	-	-	-	X
34	LMT	e	101	-	-	-	X
34	LMT	m	102	-	-	-	X
34	LMT	t	101	-	-	-	X
35	HTG	B	623	-	-	-	X
35	HTG	B	624	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	410	-	-	-	X
35	HTG	V	204	-	-	-	X
35	HTG	b	623	-	-	-	X
35	HTG	b	624	-	-	-	X
35	HTG	b	625	-	-	-	X
35	HTG	c	526	-	-	-	X
35	HTG	h	101	-	-	-	X
36	DGD	C	518	-	-	-	X
36	DGD	H	102	-	-	-	X
36	DGD	h	103	-	-	-	X
38	LHG	D	357	-	-	-	X
38	LHG	D	406	-	-	-	X
38	LHG	D	407	-	-	-	X
38	LHG	E	101	-	-	-	X
38	LHG	L	101	-	-	-	X
38	LHG	a	419	-	-	-	X
38	LHG	d	406	-	-	-	X
38	LHG	d	407	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
38	LHG	d	408	-	-	-	X
38	LHG	l	101	-	-	-	X
39	HEM	e	102	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 53280 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	29	0
			2850	1865	467	502	16			
1	a	334	Total	C	N	O	S	0	29	0
			2852	1867	466	503	16			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	8	0
			4007	2630	664	700	13			
2	b	504	Total	C	N	O	S	0	4	0
			3986	2618	661	694	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	10	0
			3542	2315	590	624	13			
3	c	455	Total	C	N	O	S	0	10	0
			3577	2340	595	629	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2748	1819	450	467	12			
4	d	341	Total	C	N	O	S	0	3	0
			2739	1814	449	464	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	1	0
			665	434	107	124			
5	e	79	Total	C	N	O	0	0	0
			648	424	105	119			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			514	344	84	84	2			
7	h	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	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	36	Total	C	N	O	0	1	0
			301	202	47	52			
11	l	36	Total	C	N	O	0	1	0
			301	202	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			265	178	38	48	1			
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	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	5	0
			1889	1182	315	387	5			
13	o	243	Total	C	N	O	S	0	2	0
			1873	1171	315	382	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	0	0
			765	486	128	151			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	0	0
			281	188	45	48			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

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

- 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 protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total	C	N	O	0	0	0
			273	186	47	40			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		

Continued on next page...

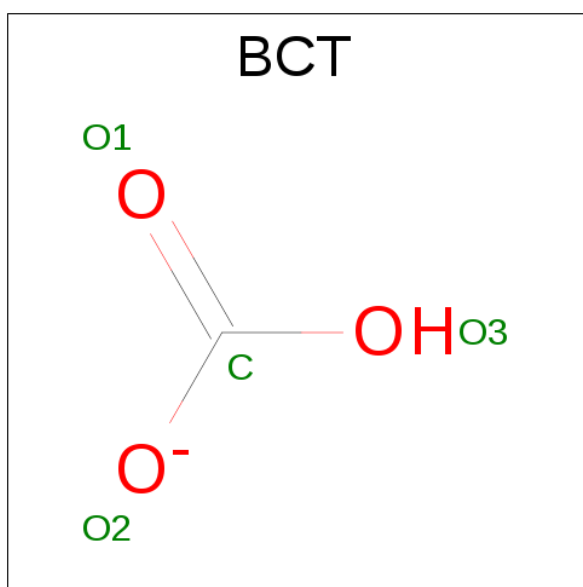
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	a	1	Total	Fe	0	1
			2	2		

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

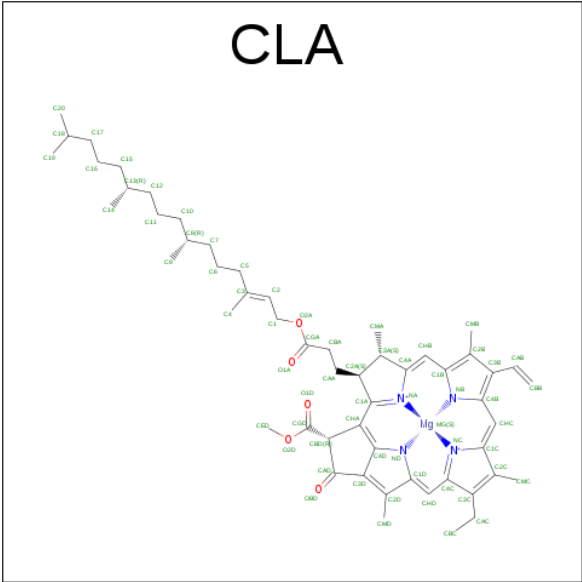
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	1
			8	2	6		
23	a	1	Total	C	O	0	1
			8	2	6		

- Molecule 24 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
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	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
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

Continued on next page...

Continued from previous page...

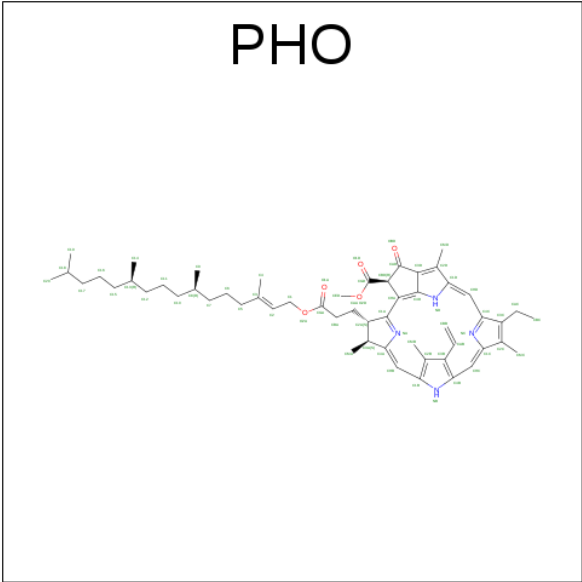
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

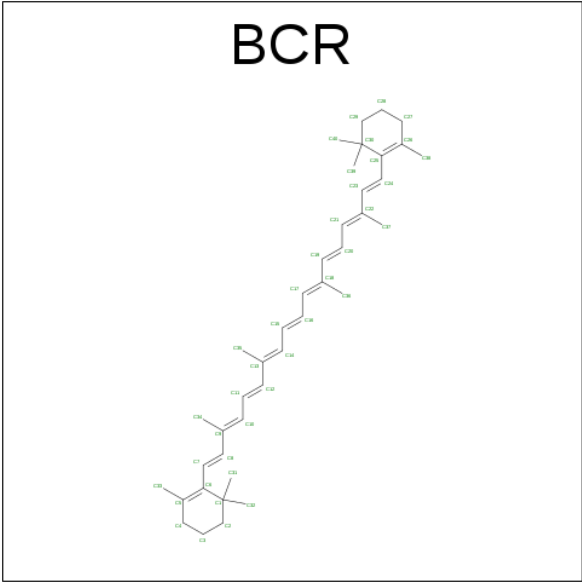
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



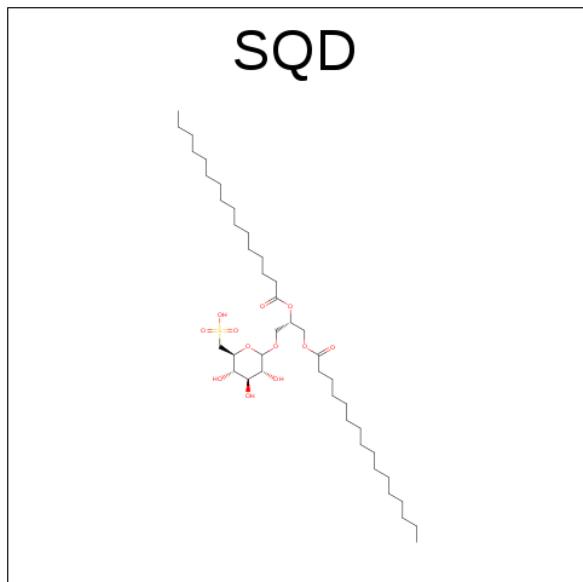
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 26 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



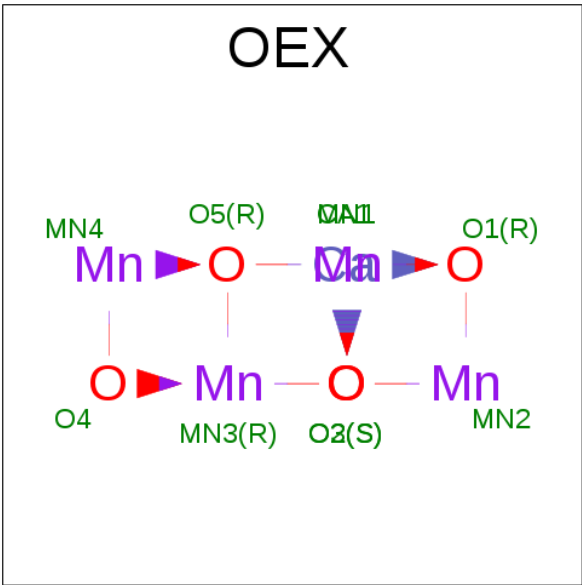
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	b	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



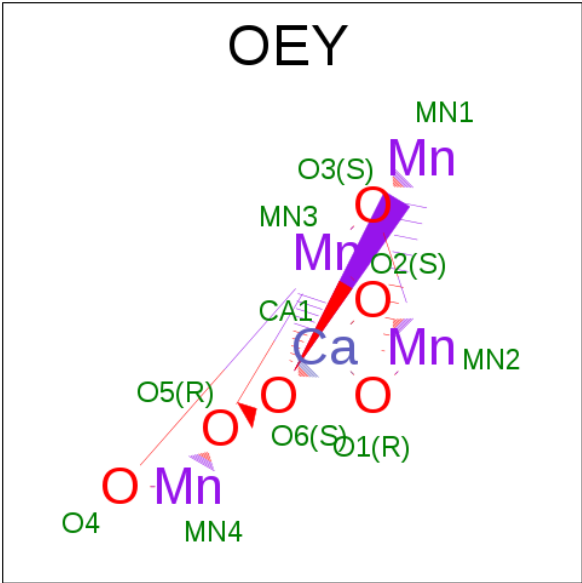
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	C	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

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



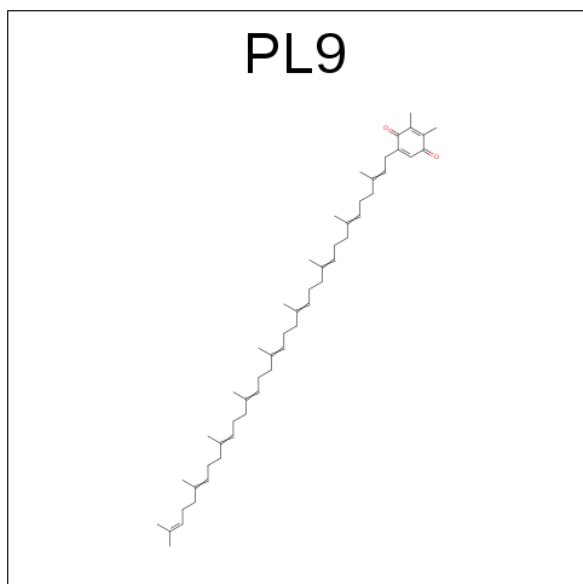
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
29	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 30 is CA-MN4-O6 CLUSTER (three-letter code: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	1
			110	106	4		
31	D	1	Total	C	O	0	0
			55	53	2		
31	a	1	Total	C	O	0	1
			110	106	4		
31	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 32 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

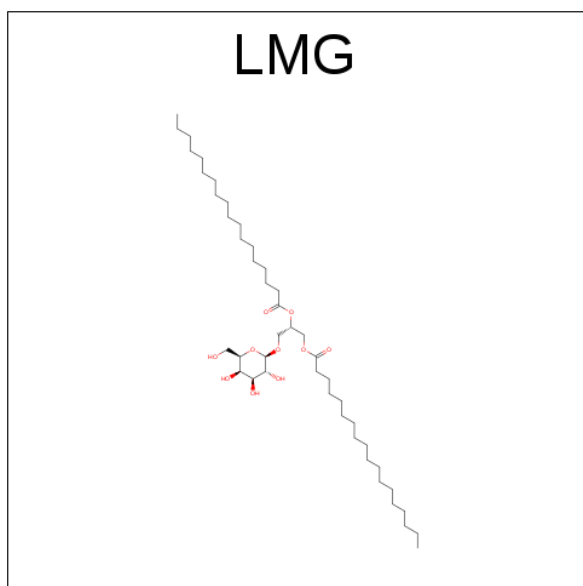
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	J	1	Total	C		0	0
			10	10			
32	i	1	Total	C	O	0	0
			40	35	5		
32	D	2	Total	C	O	0	0
			57	51	6		
32	K	1	Total	C	O	0	0
			34	29	5		
32	B	1	Total	C	O	0	0
			33	28	5		

Continued on next page...

Continued from previous page...

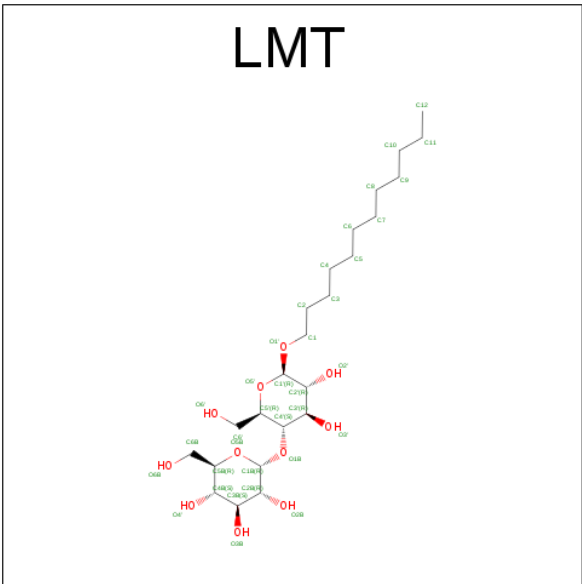
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	I	1	Total	C	O	0	0
			40	35	5		
32	c	1	Total	C	O	0	0
			32	27	5		
32	a	1	Total	C	O	0	0
			30	25	5		
32	x	1	Total	C	O	0	0
			18	16	2		
32	A	1	Total	C	O	0	0
			28	23	5		
32	j	1	Total	C		0	0
			10	10			
32	X	1	Total	C	O	0	0
			18	16	2		
32	d	2	Total	C	O	0	0
			53	47	6		
32	m	1	Total	C		0	0
			10	10			
32	b	1	Total	C	O	0	0
			33	28	5		
32	M	1	Total	C		0	0
			10	10			

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



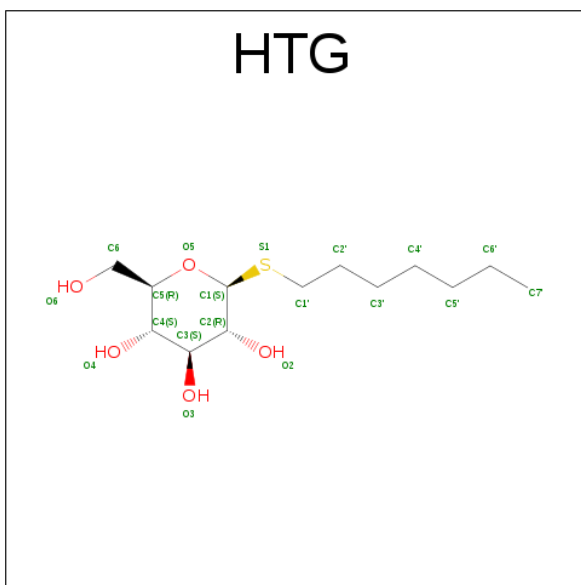
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			51	41	10		
33	B	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	J	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	b	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	j	1	Total	C	O	0	0
			51	41	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	1	Total C O 35 24 11	0	0
34	B	1	Total C O 35 24 11	0	0
34	B	1	Total C O 25 19 6	0	0
34	E	1	Total C O 35 24 11	0	0
34	I	1	Total C O 35 24 11	0	0
34	M	1	Total C O 35 24 11	0	0
34	M	1	Total C O 35 24 11	0	0
34	a	1	Total C O 35 24 11	0	0
34	a	1	Total C O 35 24 11	0	0
34	b	1	Total C O 25 19 6	0	0
34	b	1	Total C O 25 19 6	0	0
34	e	1	Total C O 35 24 11	0	0
34	m	1	Total C O 35 24 11	0	0
34	t	1	Total C O 26 19 7	0	0

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



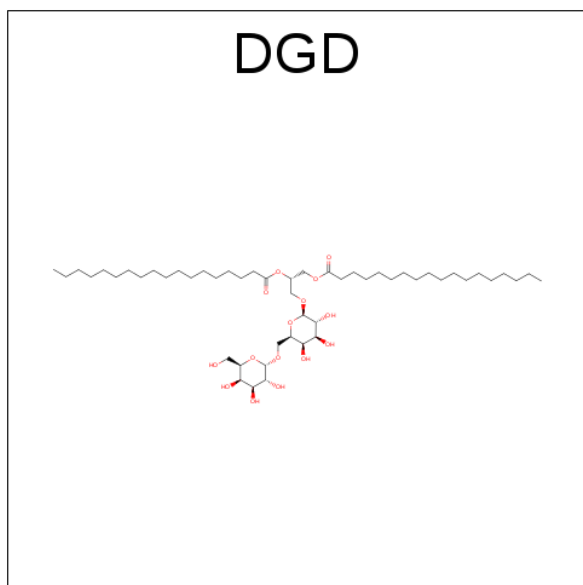
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O		0	0
			11	6	5			
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	h	1	Total	C	O	S	0	0
			16	10	5	1		

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

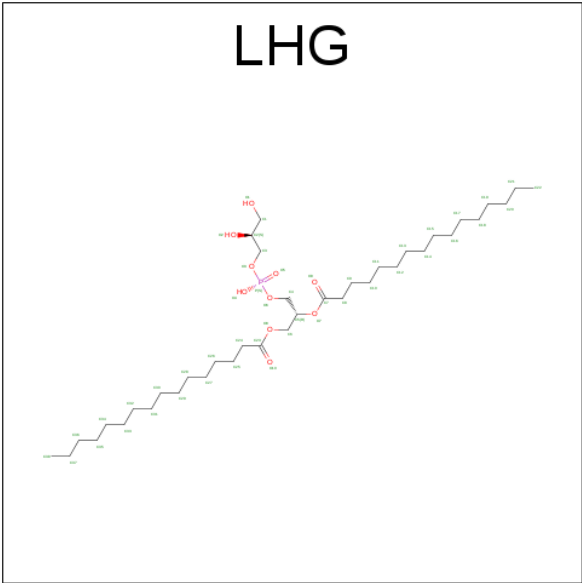


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	C	1	Total	C	O		0	0
			62	47	15			
36	H	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15			
36	c	1	Total	C	O		0	0
			62	47	15	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

- Molecule 37 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	b	1	Total	Ca	0	0
			1	1		
37	C	1	Total	Ca	0	0
			1	1		
37	V	1	Total	Ca	0	0
			1	1		
37	c	2	Total	Ca	0	0
			2	2		
37	v	1	Total	Ca	0	0
			1	1		
37	O	1	Total	Ca	0	0
			1	1		
37	o	1	Total	Ca	0	0
			1	1		

- Molecule 38 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



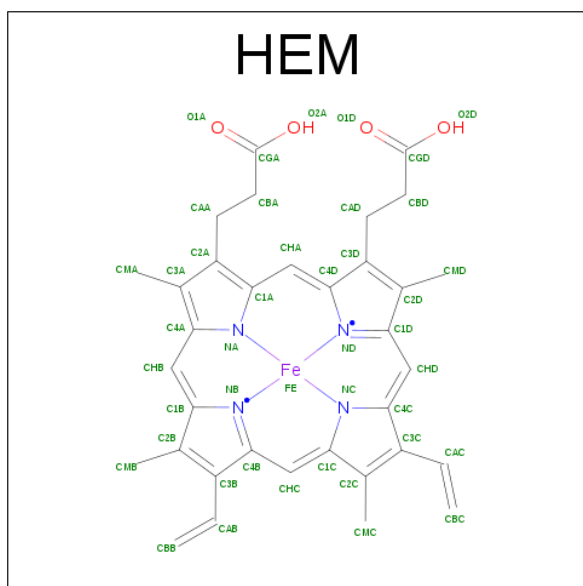
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		

Continued on next page...

Continued from previous page...

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

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 40 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	125	Total O 130 130	0	5
41	B	164	Total O 164 164	0	0
41	C	147	Total O 147 147	0	0
41	D	112	Total O 112 112	0	0
41	E	14	Total O 14 14	0	0
41	F	4	Total O 4 4	0	0
41	H	20	Total O 20 20	0	0
41	I	6	Total O 6 6	0	0
41	J	4	Total O 4 4	0	0
41	K	7	Total O 7 7	0	0
41	L	4	Total O 4 4	0	0
41	M	7	Total O 7 7	0	0
41	O	74	Total O 74 74	0	0
41	T	8	Total O 8 8	0	0
41	U	33	Total O 33 33	0	0
41	V	65	Total O 65 65	0	0
41	X	2	Total O 2 2	0	0
41	Y	1	Total O 1 1	0	0

Continued on next page...

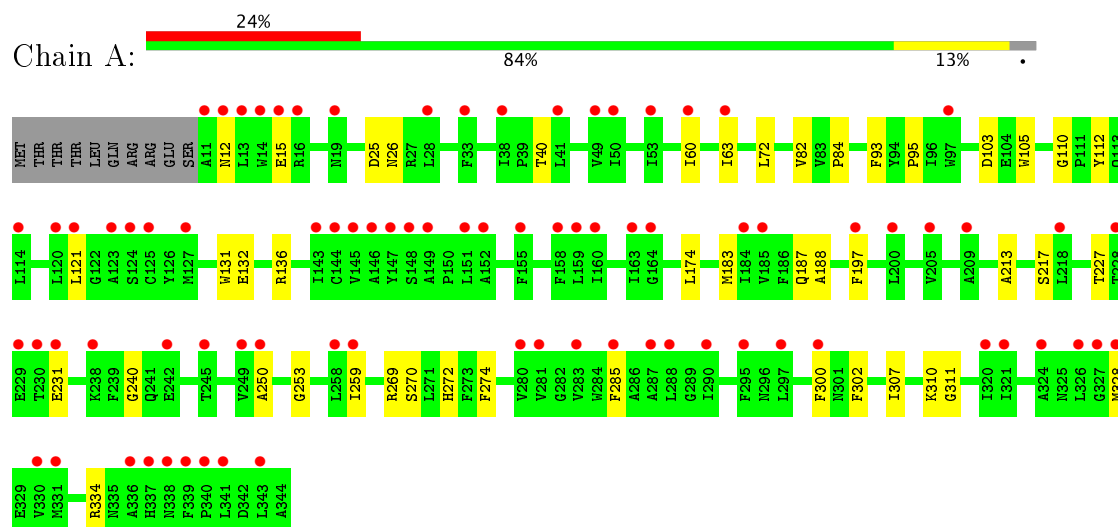
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	a	128	Total 133	O 133	0	5
41	b	185	Total 185	O 185	0	0
41	c	122	Total 122	O 122	0	0
41	d	109	Total 109	O 109	0	0
41	e	7	Total 7	O 7	0	0
41	f	3	Total 3	O 3	0	0
41	h	14	Total 14	O 14	0	0
41	i	3	Total 3	O 3	0	0
41	j	2	Total 2	O 2	0	0
41	k	3	Total 3	O 3	0	0
41	l	6	Total 6	O 6	0	0
41	m	11	Total 11	O 11	0	0
41	o	78	Total 78	O 78	0	0
41	t	5	Total 5	O 5	0	0
41	u	47	Total 47	O 47	0	0
41	v	49	Total 49	O 49	0	0
41	x	4	Total 4	O 4	0	0
41	y	1	Total 1	O 1	0	0

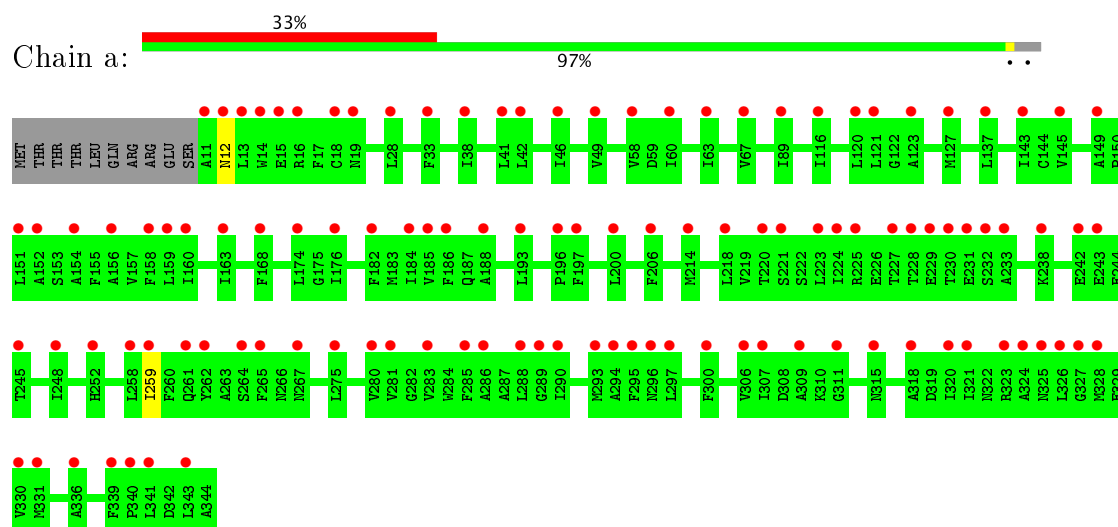
3 Residue-property plots [i](#)

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

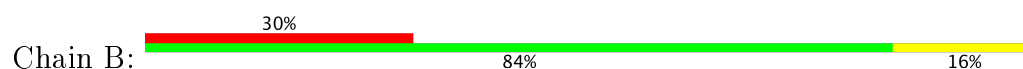
• Molecule 1: Photosystem II D1 protein

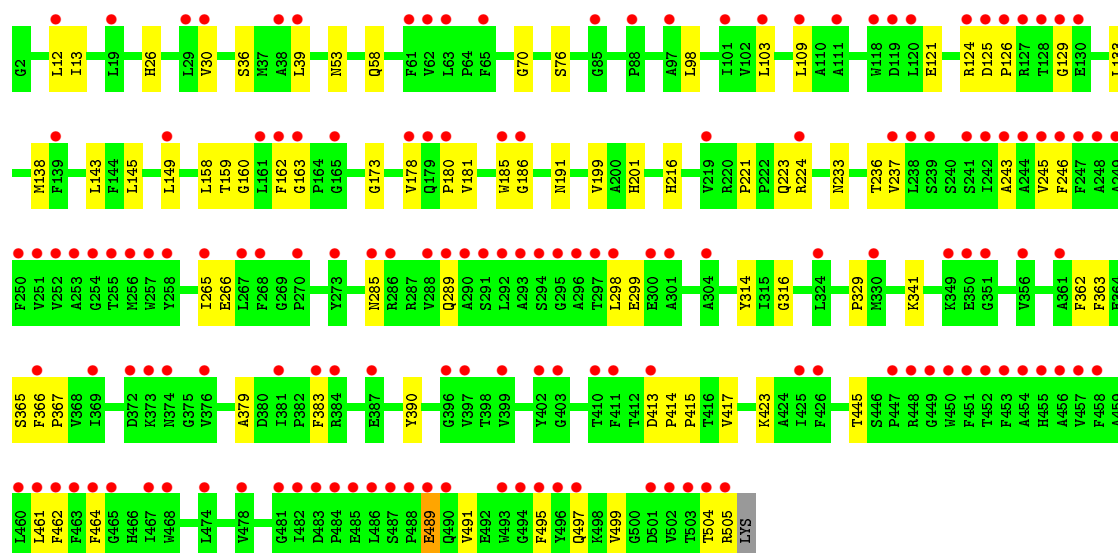


• Molecule 1: Photosystem II D1 protein

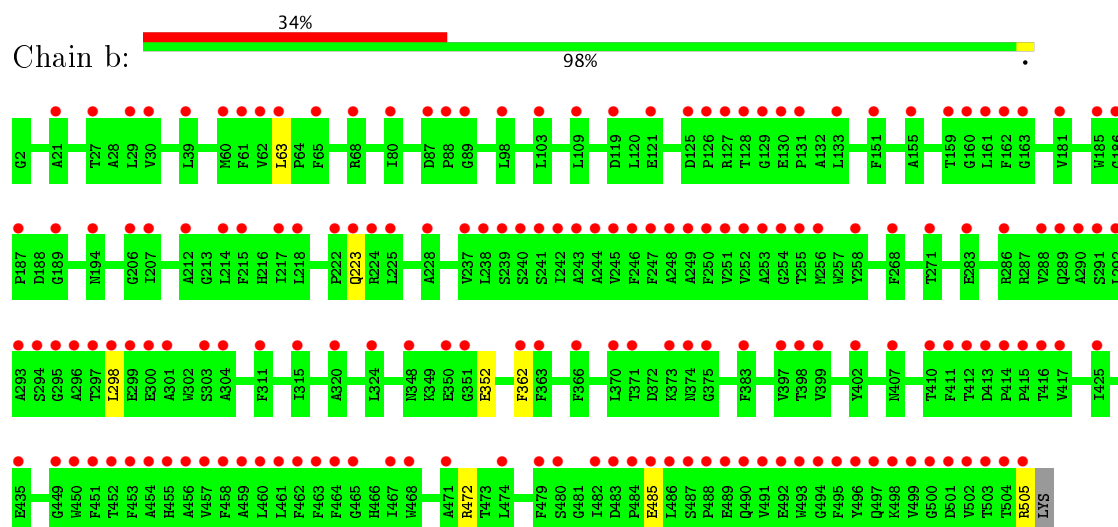


• Molecule 2: Photosystem II CP47 reaction center protein

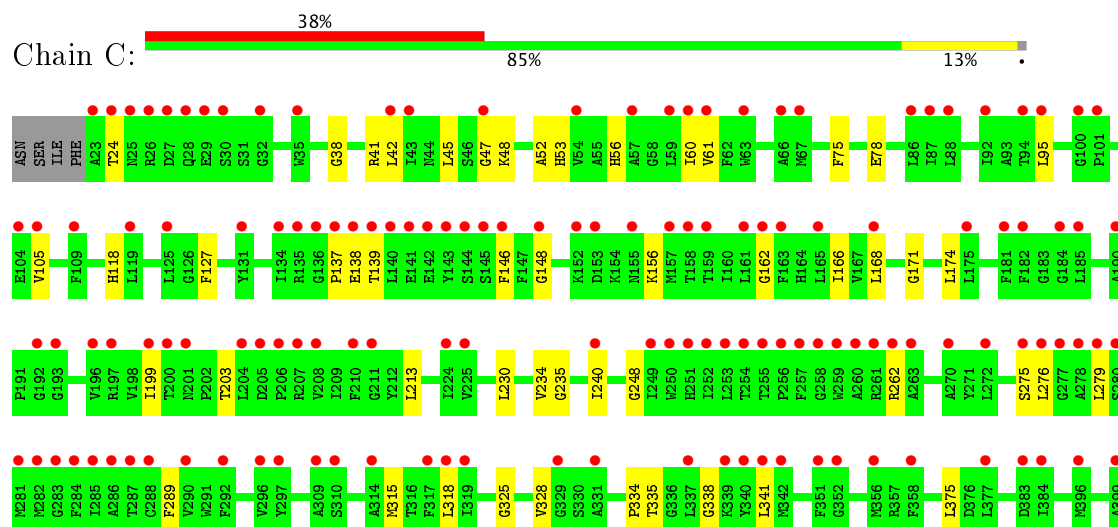


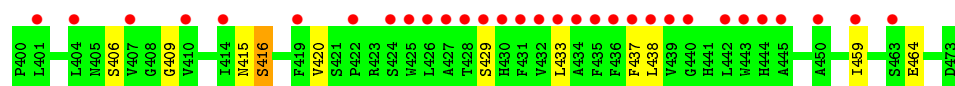


• Molecule 2: Photosystem II CP47 reaction center protein

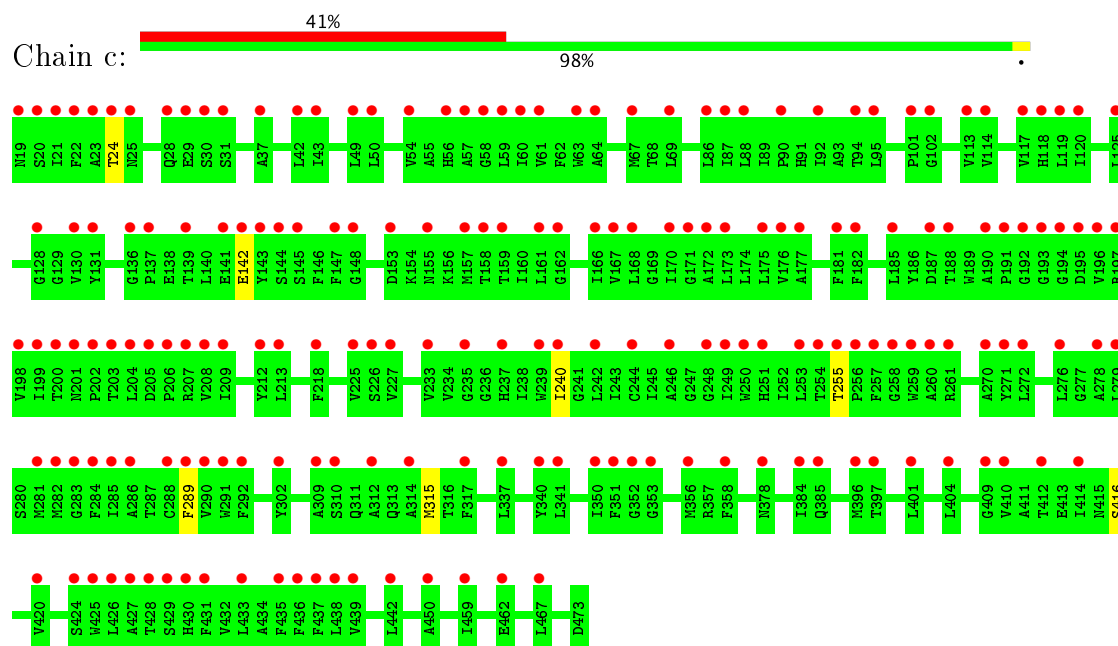


• Molecule 3: Photosystem II CP43 chlorophyll protein

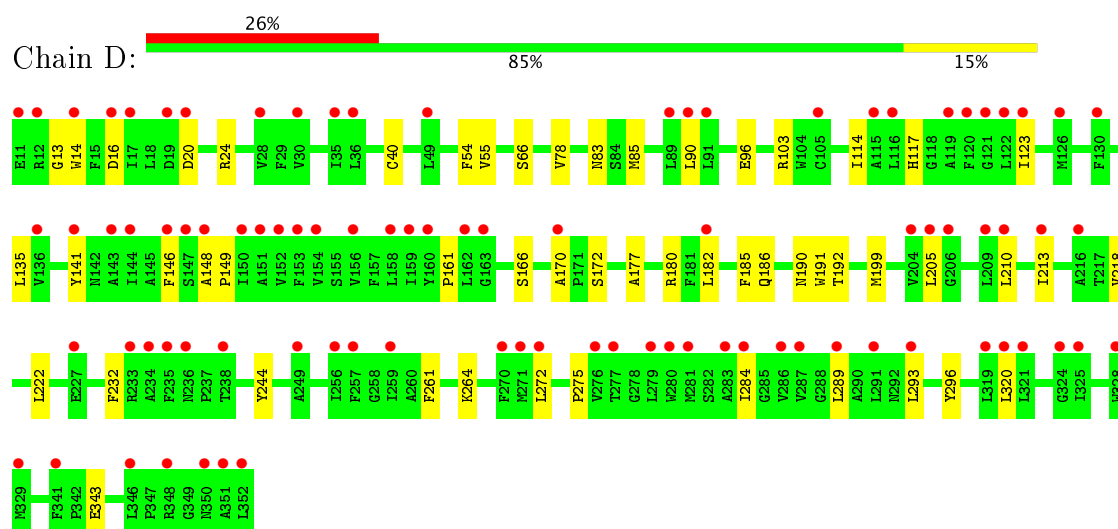




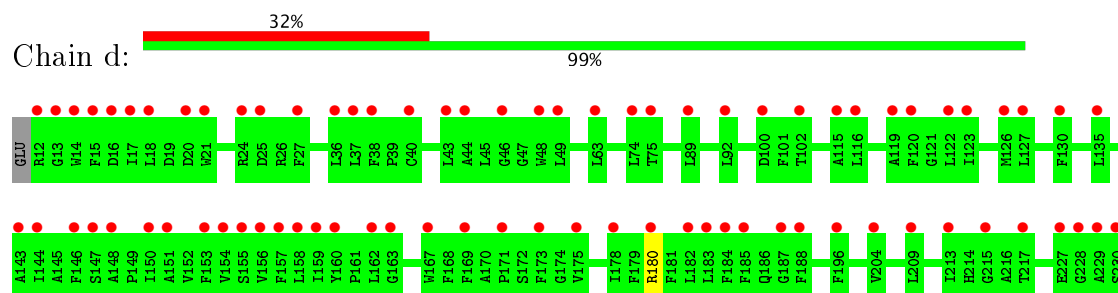
• Molecule 3: Photosystem II CP43 chlorophyll protein

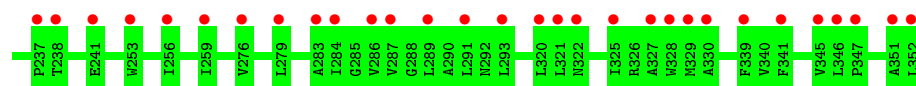


• Molecule 4: Photosystem II D2 protein

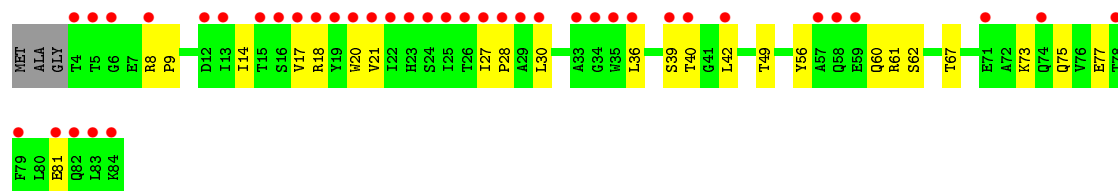


• Molecule 4: Photosystem II D2 protein

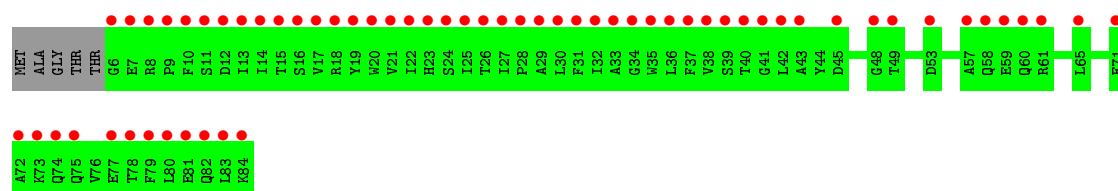
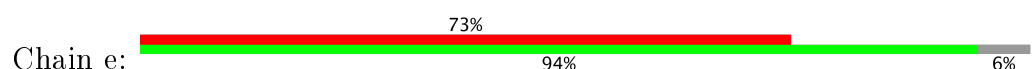




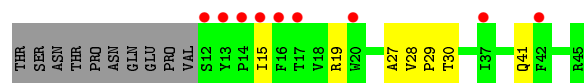
• Molecule 5: Cytochrome b559 subunit alpha



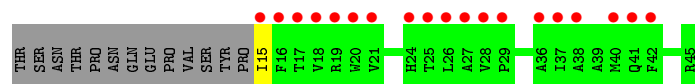
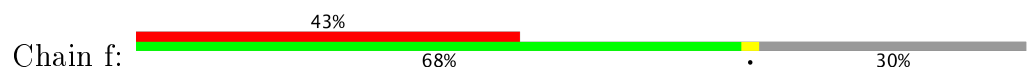
• Molecule 5: Cytochrome b559 subunit alpha



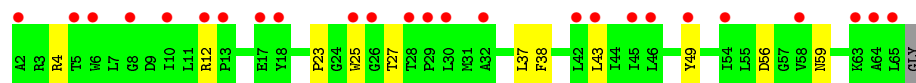
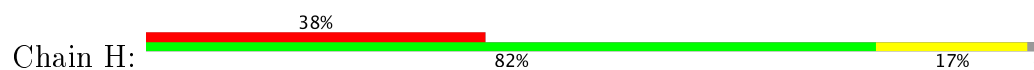
• Molecule 6: Cytochrome b559 subunit beta



• Molecule 6: Cytochrome b559 subunit beta

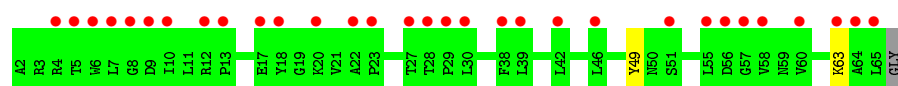


• Molecule 7: Photosystem II reaction center protein H

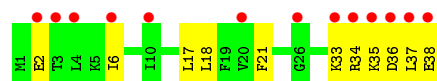


• Molecule 7: Photosystem II reaction center protein H

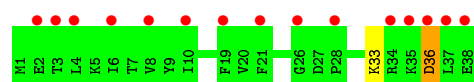




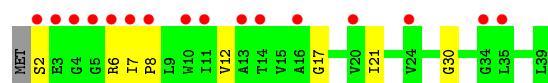
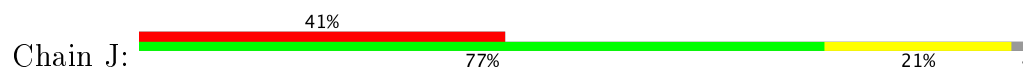
- Molecule 8: Photosystem II reaction center protein I



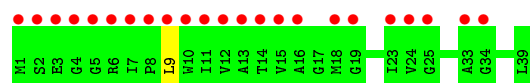
- Molecule 8: Photosystem II reaction center protein I



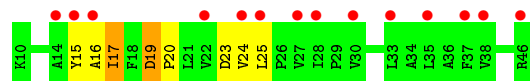
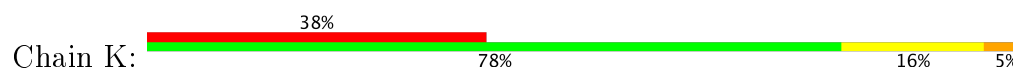
- Molecule 9: Photosystem II reaction center protein J



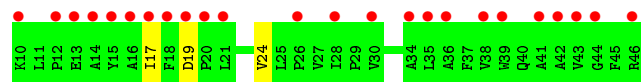
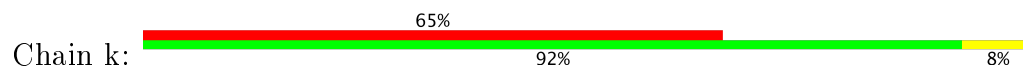
- Molecule 9: Photosystem II reaction center protein J



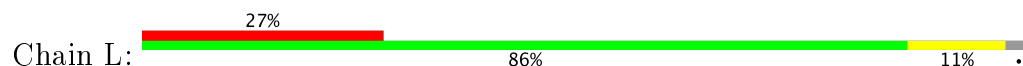
- Molecule 10: Photosystem II reaction center protein K



- Molecule 10: Photosystem II reaction center protein K

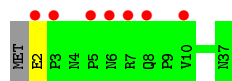


- Molecule 11: Photosystem II reaction center protein L

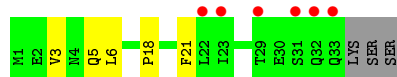
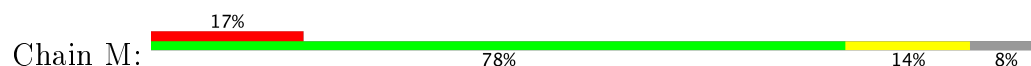




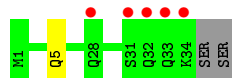
- Molecule 11: Photosystem II reaction center protein L



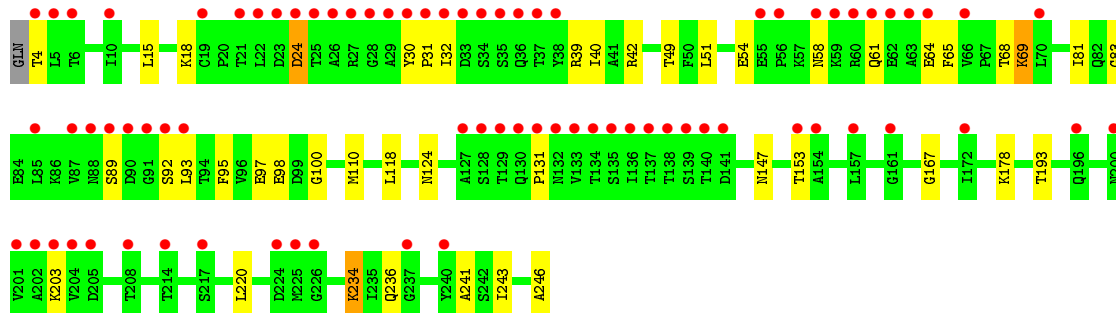
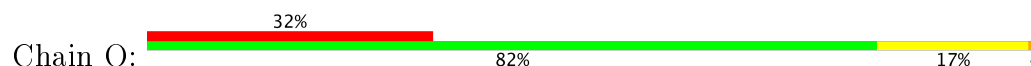
- Molecule 12: Photosystem II reaction center protein M



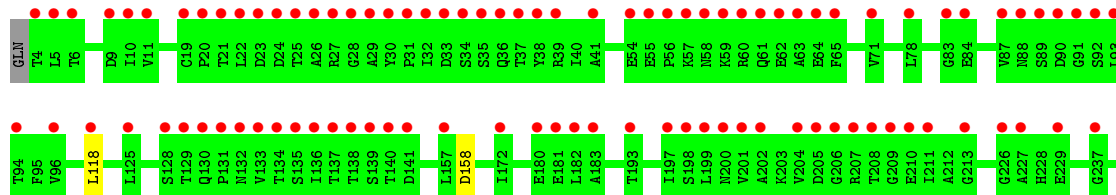
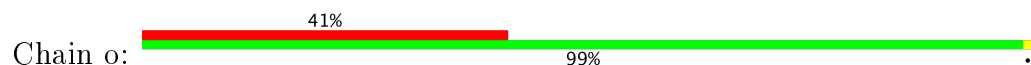
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

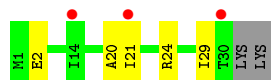
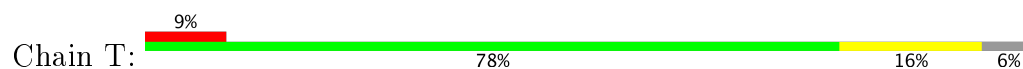


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

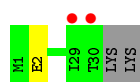




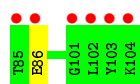
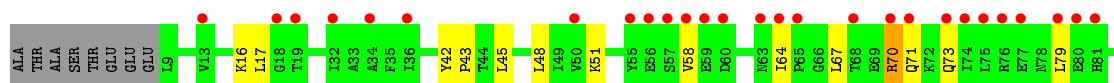
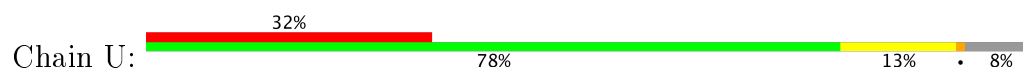
- Molecule 14: Photosystem II reaction center protein T



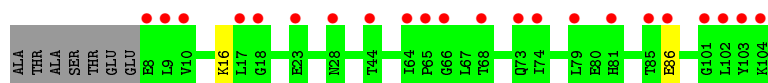
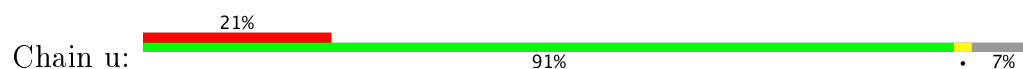
- Molecule 14: Photosystem II reaction center protein T



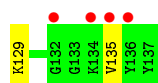
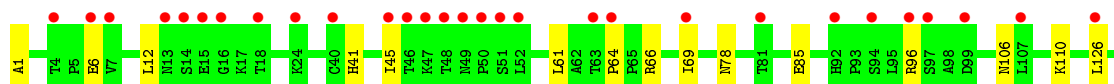
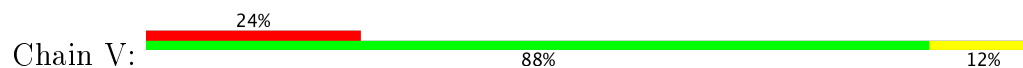
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein

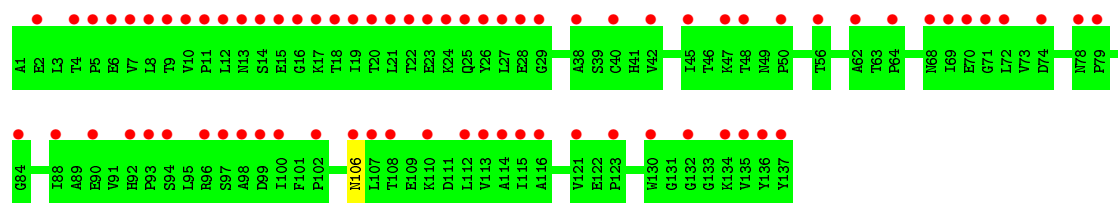


- Molecule 16: Cytochrome c-550

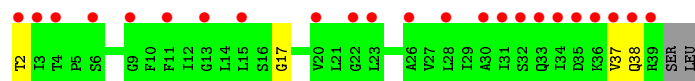
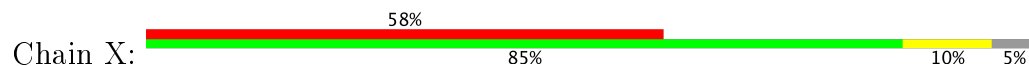


- Molecule 16: Cytochrome c-550

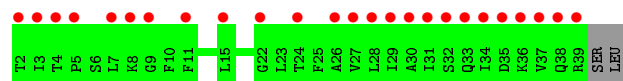




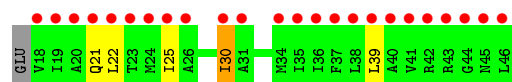
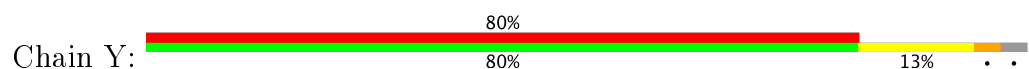
• Molecule 17: Photosystem II reaction center protein X



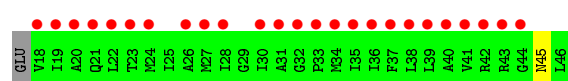
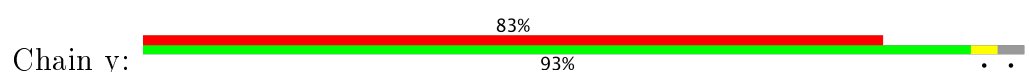
• Molecule 17: Photosystem II reaction center protein X



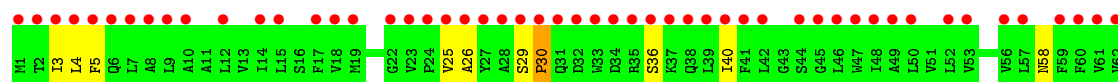
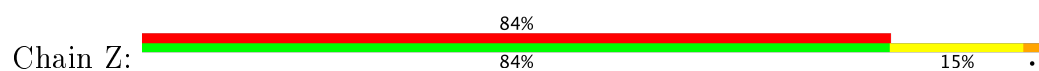
• Molecule 18: Photosystem II reaction center protein Ycf12



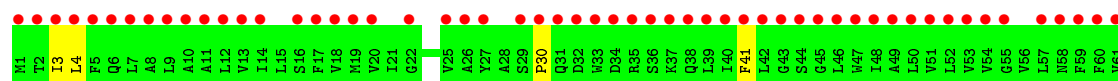
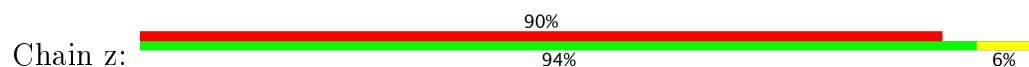
• Molecule 18: Photosystem II reaction center protein Ycf12



• Molecule 19: Photosystem II reaction center protein Z

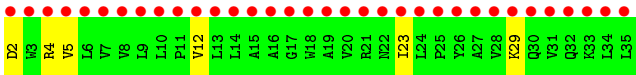
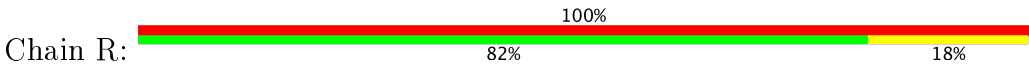


• Molecule 19: Photosystem II reaction center protein Z





● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	124.96Å 230.22Å 286.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 47.05 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.35) 100.0 (47.05-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.129 , 0.175 0.136 , 0.177	Depositor DCC
R_{free} test set	17092 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	53280	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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, GOL, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, OEY, LMG, FE2, BCT, HEM, FME, UNL, HTG, BCR, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.50	0/2952	0.59	0/4019
1	a	0.43	0/2957	0.55	0/4027
2	B	0.43	0/4171	0.54	0/5683
2	b	0.41	0/4138	0.53	0/5640
3	C	0.42	0/3667	0.53	0/4992
3	c	0.38	0/3703	0.50	0/5041
4	D	0.46	0/2847	0.56	0/3878
4	d	0.43	0/2838	0.53	0/3866
5	E	0.36	0/687	0.50	0/936
5	e	0.35	0/667	0.47	0/908
6	F	0.42	0/284	0.50	0/387
6	f	0.38	0/257	0.53	0/349
7	H	0.37	0/530	0.57	0/723
7	h	0.33	0/519	0.50	0/708
8	I	0.37	0/311	0.48	0/419
8	i	0.34	0/311	0.49	0/419
9	J	0.34	0/278	0.46	0/376
9	j	0.32	0/283	0.46	0/383
10	K	0.37	0/303	0.51	0/416
10	k	0.34	0/303	0.49	0/416
11	L	0.43	0/311	0.47	0/423
11	l	0.41	0/311	0.49	0/423
12	M	0.45	0/261	0.61	0/357
12	m	0.42	0/262	0.59	0/357
13	O	0.39	0/1935	0.56	0/2623
13	o	0.39	0/1910	0.57	1/2589 (0.0%)
14	T	0.49	0/257	0.55	0/349
14	t	0.47	0/257	0.51	0/349
15	U	0.38	0/776	0.54	0/1052
15	u	0.37	0/785	0.54	0/1064
16	V	0.38	0/1085	0.49	0/1473

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.34	0/1085	0.48	0/1473
17	X	0.33	0/284	0.46	0/384
17	x	0.31	0/284	0.45	0/384
18	Y	0.29	0/216	0.44	0/289
18	y	0.30	0/216	0.47	0/289
19	Z	0.31	0/490	0.44	0/669
19	z	0.29	0/490	0.39	0/669
20	R	0.28	0/279	0.39	0/383
All	All	0.41	0/43500	0.53	1/59185 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	158	ASP	CB-CG-OD1	5.06	122.86	118.30

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	2850	0	2705	36	0
1	a	2852	0	2708	0	0
2	B	4007	0	3879	71	0
2	b	3986	0	3855	0	0
3	C	3542	0	3462	61	0
3	c	3577	0	3498	0	0
4	D	2748	0	2650	47	0
4	d	2739	0	2644	0	0
5	E	665	0	653	22	0
5	e	648	0	634	0	0
6	F	275	0	282	7	0
6	f	250	0	261	0	0
7	H	514	0	542	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	506	0	529	0	0
8	I	314	0	328	8	0
8	i	314	0	328	0	0
9	J	272	0	279	8	0
9	j	277	0	284	0	0
10	K	293	0	305	8	0
10	k	293	0	305	0	0
11	L	301	0	315	5	0
11	l	301	0	315	0	0
12	M	265	0	286	5	0
12	m	269	0	288	0	0
13	O	1889	0	1871	28	0
13	o	1873	0	1852	0	0
14	T	258	0	261	5	0
14	t	258	0	261	0	0
15	U	765	0	767	9	0
15	u	774	0	773	0	0
16	V	1064	0	1073	12	0
16	v	1064	0	1073	0	0
17	X	281	0	312	6	0
17	x	281	0	312	0	0
18	Y	215	0	246	7	0
18	y	215	0	246	0	0
19	Z	479	0	516	6	0
19	z	479	0	516	0	0
20	R	273	0	305	6	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	19	0
24	B	1040	0	1152	69	0
24	C	845	0	936	92	0
24	D	130	0	144	12	0
24	a	260	0	288	0	0
24	b	1040	0	1152	0	0
24	c	845	0	936	0	0
24	d	130	0	144	0	0
25	A	128	0	148	6	0
25	a	128	0	148	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	40	0	56	2	0
26	B	120	0	168	13	0
26	C	80	0	112	7	0
26	D	40	0	56	5	0
26	H	40	0	56	3	0
26	K	40	0	56	1	0
26	T	40	0	56	6	0
26	Y	40	0	56	4	0
26	a	40	0	56	0	0
26	b	120	0	168	0	0
26	c	80	0	112	0	0
26	d	40	0	56	0	0
26	h	40	0	56	0	0
26	k	40	0	56	0	0
26	t	40	0	56	0	0
26	y	40	0	56	0	0
27	A	108	0	156	8	0
27	B	54	0	78	3	0
27	F	43	0	53	1	0
27	a	108	0	156	0	0
27	b	54	0	78	0	0
27	f	43	0	53	0	0
28	A	6	0	8	0	0
28	B	12	0	16	1	0
28	C	6	0	8	0	0
28	V	6	0	8	0	0
28	a	12	0	16	0	0
28	b	6	0	8	0	0
28	c	6	0	8	0	0
28	v	6	0	8	0	0
29	A	10	0	0	0	0
29	a	10	0	0	0	0
30	A	11	0	0	0	0
30	a	11	0	0	0	0
31	A	110	0	160	9	0
31	D	55	0	80	5	0
31	a	110	0	160	0	0
31	d	55	0	80	0	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	D	57	0	0	1	0
32	I	40	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	J	10	0	0	0	0
32	K	34	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	53	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
32	x	18	0	0	0	0
33	A	51	0	72	1	0
33	B	51	0	72	2	0
33	C	102	0	144	5	0
33	J	51	0	72	6	0
33	Z	37	0	44	6	0
33	a	51	0	72	0	0
33	b	51	0	72	0	0
33	c	102	0	144	0	0
33	j	51	0	72	0	0
33	z	39	0	48	0	0
34	A	35	0	46	4	0
34	B	60	0	81	3	0
34	E	35	0	46	1	0
34	I	35	0	46	1	0
34	M	70	0	92	3	0
34	a	70	0	92	0	0
34	b	50	0	70	0	0
34	e	35	0	46	0	0
34	m	35	0	46	0	0
34	t	26	0	35	0	0
35	B	76	0	104	9	0
35	C	38	0	52	2	0
35	D	16	0	17	2	0
35	V	11	0	10	0	0
35	b	76	0	104	0	0
35	c	38	0	52	0	0
35	h	16	0	17	0	0
36	C	186	0	246	10	0
36	H	62	0	82	2	0
36	c	186	0	246	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	h	62	0	82	0	0
37	C	1	0	0	0	0
37	O	1	0	0	0	0
37	V	1	0	0	0	0
37	b	1	0	0	0	0
37	c	2	0	0	0	0
37	o	1	0	0	0	0
37	v	1	0	0	0	0
38	D	147	0	222	14	0
38	E	42	0	57	6	0
38	L	49	0	74	2	0
38	a	42	0	57	0	0
38	d	147	0	222	0	0
38	l	49	0	74	0	0
39	E	43	0	30	2	0
39	V	43	0	30	0	0
39	e	43	0	30	0	0
39	v	43	0	30	0	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	A	130	0	0	1	0
41	B	164	0	0	4	0
41	C	147	0	0	4	0
41	D	112	0	0	1	0
41	E	14	0	0	1	0
41	F	4	0	0	0	0
41	H	20	0	0	0	0
41	I	6	0	0	1	0
41	J	4	0	0	0	0
41	K	7	0	0	0	0
41	L	4	0	0	0	0
41	M	7	0	0	0	0
41	O	74	0	0	2	0
41	T	8	0	0	0	0
41	U	33	0	0	1	0
41	V	65	0	0	1	0
41	X	2	0	0	0	0
41	Y	1	0	0	0	0
41	a	133	0	0	0	0
41	b	185	0	0	0	0
41	c	122	0	0	0	0
41	d	109	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	e	7	0	0	0	0
41	f	3	0	0	0	0
41	h	14	0	0	0	0
41	i	3	0	0	0	0
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	6	0	0	0	0
41	m	11	0	0	0	0
41	o	78	0	0	0	0
41	t	5	0	0	0	0
41	u	47	0	0	0	0
41	v	49	0	0	0	0
41	x	4	0	0	0	0
41	y	1	0	0	0	0
All	All	53280	0	52671	514	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 6.

All (514) 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)
24:C:514:CLA:HBB1	26:C:515:BCR:H24C	1.35	1.05
24:B:604:CLA:H42	24:B:605:CLA:H2	1.47	0.95
13:O:124:ASN:HD22	13:O:147:ASN:HD22	1.59	0.89
1:A:250:ALA:HA	2:B:491:VAL:HG11	2.54	0.88
5:E:67:THR:H	5:E:75:GLN:HE22	2.55	0.83
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.92	0.79
24:C:506:CLA:CMD	24:C:508:CLA:HAB	2.16	0.76
24:B:601:CLA:H12	24:B:601:CLA:H71	1.70	0.73
1:A:253:GLY:HA3	2:B:491:VAL:HG12	4.24	0.72
3:C:279:LEU:HD22	24:C:511:CLA:HED2	12.68	0.71
24:C:505:CLA:HBB1	24:C:514:CLA:H41	33.05	0.71
31:A:416[A]:PL9:H253	24:D:402:CLA:H141	1.72	0.70
24:A:405:CLA:HBB1	24:A:405:CLA:HHC	1.73	0.70
24:B:606:CLA:HBB1	24:B:606:CLA:HHC	2.64	0.69
24:A:406:CLA:H152	31:A:416[B]:PL9:H252	1.77	0.67
8:I:37:LEU:O	41:I:201:HOH:O	2.12	0.67
1:A:121[B]:LEU:HD11	24:C:506:CLA:H122	1.75	0.67
24:B:614:CLA:H43	27:B:620:SQD:H111	1.76	0.67
24:C:506:CLA:H42	36:C:519:DGD:HB42	34.65	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:6:LEU:HD11	34:M:103:LMT:H11	15.64	0.67
38:D:406:LHG:H212	12:M:18:PRO:HG3	17.78	0.67
2:B:103:LEU:HD21	24:B:605:CLA:HMC3	1.76	0.66
2:B:497:GLN:HB2	2:B:504:THR:HB	2.43	0.66
38:D:407:LHG:H372	38:D:407:LHG:H132	1.77	0.65
33:A:418:LMG:H152	36:C:517:DGD:HA91	1.77	0.65
5:E:40:THR:HB	20:R:4:ARG:HG2	1.79	0.65
24:B:603:CLA:C2D	24:B:605:CLA:H2	4.06	0.65
25:A:408:PHO:H3A	24:D:402:CLA:H142	1.77	0.65
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	1.79	0.64
33:Z:101:LMG:O5	33:Z:101:LMG:O4	2.14	0.64
24:A:404:CLA:HMD3	4:D:182:LEU:HD11	11.66	0.64
24:C:507:CLA:CMD	24:C:509:CLA:HAB	27.45	0.64
2:B:121:GLU:HG2	7:H:4:ARG:HG2	2.40	0.64
1:A:25:ASP:OD1	41:A:501:HOH:O	2.15	0.63
24:C:510:CLA:HBC3	24:C:512:CLA:H71	20.96	0.63
24:B:605:CLA:HHC	24:B:605:CLA:HBB1	2.05	0.63
24:C:504:CLA:HBB1	24:C:504:CLA:HHC	1.81	0.62
33:C:521:LMG:H181	35:C:522:HTG:H6'2	1.80	0.62
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.32	0.62
24:C:503:CLA:C4D	24:C:505:CLA:H2	17.22	0.61
34:A:359:LMT:H71	2:B:39:LEU:HD13	45.37	0.61
3:C:438:LEU:HD11	24:C:507:CLA:HBB1	17.23	0.61
24:C:507:CLA:HMD2	24:C:509:CLA:HAB	27.61	0.61
3:C:279:LEU:HD22	24:C:510:CLA:HED2	1.83	0.60
27:A:411:SQD:H251	38:D:407:LHG:H131	1.84	0.60
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.84	0.60
24:C:504:CLA:H61	24:C:514:CLA:H42	26.26	0.59
3:C:409[B]:GLY:O	41:C:601:HOH:O	23.31	0.59
3:C:406:SER:HA	3:C:420:VAL:HG23	1.85	0.59
2:B:12:LEU:HB2	24:B:612:CLA:HMC2	2.02	0.59
34:A:359:LMT:H6E	35:B:623:HTG:H61	48.71	0.59
31:A:416[B]:PL9:H253	24:D:402:CLA:H141	1.84	0.59
39:E:103:HEM:HAC	6:F:27:ALA:HB1	1.85	0.59
4:D:123:ILE:HD11	36:H:102:DGD:HAH2	1.84	0.59
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.83	0.58
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.38	0.58
2:B:341:LYS:NZ	35:B:624:HTG:S1	3.05	0.58
24:B:616:CLA:HHC	24:B:616:CLA:HBB1	1.85	0.58
3:C:168:LEU:HD21	24:C:511:CLA:H61	22.39	0.58
24:C:506:CLA:H151	24:C:510:CLA:H143	29.83	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:325:GLY:O	15:U:51:LYS:NZ	2.35	0.58
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.57	0.58
24:C:513:CLA:H191	33:Z:101:LMG:H242	28.95	0.58
24:A:409:CLA:H171	24:C:507:CLA:H142	1.86	0.58
24:C:507:CLA:HMC2	24:C:508:CLA:H102	1.86	0.58
7:H:56:ASP:OD1	17:X:2:THR:OG1	3.32	0.58
24:C:514:CLA:H172	33:C:521:LMG:H402	1.86	0.57
24:B:613:CLA:H51	38:D:357:LHG:H361	1.85	0.57
13:O:32:ILE:HG13	13:O:93:LEU:HD11	1.85	0.57
24:C:509:CLA:HBC3	24:C:511:CLA:H71	1.86	0.57
24:B:616:CLA:H43	24:B:616:CLA:HED2	1.87	0.57
38:D:407:LHG:H382	38:D:407:LHG:H112	1.87	0.57
15:U:64:ILE:HB	15:U:67:LEU:HD11	1.87	0.57
13:O:42:ARG:O	13:O:241:ALA:HA	2.06	0.56
2:B:462:PHE:CE1	24:B:613:CLA:HMB3	2.41	0.56
1:A:183:MET:HA	24:A:404:CLA:HMD2	1.88	0.56
24:B:612:CLA:HMB1	24:B:612:CLA:HBB1	1.86	0.56
27:B:620:SQD:H462	27:B:620:SQD:H1	2.03	0.56
24:C:511:CLA:HBB1	24:C:511:CLA:HMB1	1.87	0.56
1:A:227:THR:HB	1:A:231:GLU:HG3	1.87	0.56
13:O:68:THR:HG22	13:O:110[B]:MET:HG2	1.86	0.56
24:C:502:CLA:HBB1	24:C:502:CLA:HHC	1.86	0.56
2:B:145:LEU:HD11	24:B:615:CLA:HMB2	2.06	0.56
3:C:95:LEU:HD13	24:C:503:CLA:H142	1.87	0.56
3:C:334:PRO:HA	13:O:153:THR:OG1	2.06	0.55
13:O:89:SER:N	41:O:402:HOH:O	2.35	0.55
31:D:405:PL9:H33	38:L:101:LHG:H222	1.88	0.55
8:I:35:LYS:O	8:I:37:LEU:N	2.83	0.55
1:A:84:PRO:HA	1:A:112:TYR:CG	2.43	0.55
2:B:186:GLY:O	41:B:701:HOH:O	45.56	0.55
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	1.91	0.55
24:A:404:CLA:HBB1	24:A:404:CLA:HMB1	1.88	0.55
24:B:603:CLA:C3D	24:B:605:CLA:H2	4.51	0.55
2:B:216:HIS:HE1	24:B:609:CLA:C1A	2.21	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.87	0.55
24:D:403:CLA:HHC	24:D:403:CLA:HBB1	1.89	0.55
24:C:507:CLA:H62	34:I:101:LMT:H91	1.89	0.54
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.88	0.54
24:A:406:CLA:H152	31:A:416[A]:PL9:H252	1.88	0.54
24:C:511:CLA:H192	24:C:511:CLA:HBC3	1.89	0.54
36:C:519:DGD:HB52	33:C:521:LMG:H362	35.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:E:101:LHG:O2	6:F:19:ARG:NH1	2.40	0.54
5:E:56:TYR:O	16:V:1:ALA:N	2.53	0.54
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.18	0.54
24:B:602:CLA:HHC	24:B:602:CLA:HBB1	1.91	0.53
3:C:409[A]:GLY:O	41:C:601:HOH:O	23.23	0.53
4:D:141:TYR:OH	38:D:406:LHG:O4	18.58	0.53
13:O:58:ASN:HD21	13:O:61:GLN:HB2	3.90	0.53
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.52	0.53
24:A:409:CLA:H193	24:C:507:CLA:H101	1.91	0.53
3:C:41:ARG:NH1	24:C:513:CLA:HMD1	19.63	0.53
24:D:403:CLA:H162	7:H:37:LEU:HD21	8.55	0.53
24:C:510:CLA:H203	36:C:519:DGD:HA92	39.12	0.53
4:D:14:TRP:CD1	35:D:410:HTG:H61	2.43	0.52
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.90	0.52
10:K:24:VAL:HG11	18:Y:25:ILE:HB	1.92	0.52
10:K:16:ALA:O	10:K:19:ASP:HB2	2.22	0.52
2:B:173:GLY:HA3	2:B:265:ILE:HD11	2.20	0.52
2:B:36[A]:SER:OG	26:B:618:BCR:H362	2.09	0.52
3:C:146:PHE:HZ	24:C:514:CLA:HBB2	10.91	0.52
16:V:85:GLU:OE2	41:V:301:HOH:O	13.45	0.52
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.90	0.52
16:V:12:LEU:HD12	16:V:69:ILE:HB	2.34	0.52
3:C:148:GLY:O	3:C:156:LYS:NZ	2.39	0.52
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.11	0.52
1:A:310:LYS:HD2	16:V:1:ALA:HB1	2.01	0.51
1:A:274[B]:PHE:HD1	27:A:411:SQD:H101	1.74	0.51
3:C:437:PHE:CZ	24:C:512:CLA:HMB3	14.13	0.51
24:A:406:CLA:HMD3	4:D:182:LEU:HD11	1.91	0.51
2:B:162:PHE:O	24:B:606:CLA:HHD	2.17	0.51
3:C:42:LEU:HD21	24:C:513:CLA:H2A	18.81	0.51
5:E:18:ARG:H	9:J:2:SER:N	2.08	0.51
24:B:602:CLA:H101	24:B:609:CLA:H193	1.93	0.51
36:C:518:DGD:HG11	41:C:607:HOH:O	38.15	0.51
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.54	0.51
3:C:41:ARG:NH1	24:C:512:CLA:HMD1	2.26	0.50
31:A:416[A]:PL9:H262	38:E:101:LHG:H223	1.93	0.50
4:D:13:GLY:HA3	35:D:410:HTG:H62	1.92	0.50
24:B:610:CLA:H122	24:B:615:CLA:HAA1	1.93	0.50
4:D:244:TYR:OH	4:D:264[B]:LYS:HE2	2.12	0.50
10:K:23:ASP:OD2	18:Y:21:GLN:NE2	2.45	0.50
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:C:507:CLA:H2	26:C:516:BCR:H10C	1.93	0.50
1:A:72:LEU:HD11	34:A:359:LMT:H51	4.17	0.50
24:B:607:CLA:H122	33:B:621:LMG:H242	3.93	0.50
3:C:437:PHE:CZ	24:C:511:CLA:HMB3	2.47	0.50
38:D:406:LHG:H322	14:T:21:ILE:HD11	1.93	0.50
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.94	0.50
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.14	0.50
2:B:233:ASN:O	2:B:236:THR:HG22	2.37	0.49
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.93	0.49
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.49
11:L:9:PRO:HA	34:M:101:LMT:H6D	17.22	0.49
6:F:30:THR:HG21	33:J:101:LMG:H412	1.93	0.49
10:K:17:ILE:H	10:K:17:ILE:HD13	1.85	0.49
2:B:13:ILE:HG12	24:B:612:CLA:HAC2	1.95	0.49
2:B:30:VAL:HG12	24:B:605:CLA:HHD	1.97	0.49
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.00	0.49
24:C:503:CLA:C3D	24:C:505:CLA:H2	18.24	0.49
24:C:506:CLA:HMD2	24:C:508:CLA:HAB	1.94	0.49
2:B:149:LEU:HD13	24:B:604:CLA:H171	1.95	0.49
24:C:502:CLA:HMD2	24:C:503:CLA:H101	1.95	0.49
3:C:56:HIS:HB2	24:C:511:CLA:HMB2	8.66	0.49
13:O:51:LEU:HD12	13:O:234:LYS:HG2	1.94	0.49
3:C:38:GLY:HA3	24:C:512:CLA:HMD3	1.93	0.49
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.48	0.49
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.95	0.48
38:D:407:LHG:HC62	11:L:15:THR:HG23	27.50	0.48
1:A:240:GLY:HA3	14:T:29:ILE:HG23	1.96	0.48
2:B:185:TRP:CD1	35:B:625:HTG:H2	2.90	0.48
3:C:38:GLY:HA3	24:C:513:CLA:HMD3	17.36	0.48
24:C:510:CLA:HBB1	24:C:510:CLA:HMB1	2.06	0.48
3:C:437:PHE:CE1	24:C:511:CLA:HMB3	2.48	0.48
5:E:8:ARG:HG3	5:E:9:PRO:HD2	2.35	0.48
34:M:103:LMT:O2B	34:M:103:LMT:O3'	2.21	0.48
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.06	0.48
13:O:40:ILE:HG12	13:O:243:ILE:HD13	2.17	0.48
31:A:416[A]:PL9:H171	31:A:416[A]:PL9:H151	1.52	0.48
33:C:521:LMG:H292	33:C:521:LMG:H152	3.77	0.48
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.02	0.48
2:B:489:GLU:HB3	2:B:495:PHE:CG	2.49	0.48
4:D:85:MET:CE	4:D:96:GLU:HG2	2.43	0.48
24:A:404:CLA:CBD	24:A:405:CLA:HAC2	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:GLU:HB3	2:B:495:PHE:CD1	2.48	0.48
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.95	0.48
13:O:32:ILE:HG21	13:O:93:LEU:HD21	2.08	0.48
2:B:299:GLU:HG3	41:B:831:HOH:O	2.14	0.47
2:B:98:LEU:HB2	35:B:623:HTG:H7'1	2.41	0.47
4:D:199:MET:HG2	31:D:405:PL9:H321	1.96	0.47
5:E:77:GLU:O	5:E:81:GLU:HG2	2.13	0.47
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.54	0.47
2:B:363:PHE:HB3	2:B:365:SER:O	2.15	0.47
3:C:174:LEU:HD22	24:C:504:CLA:H203	19.39	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.96	0.47
24:A:406:CLA:HED1	36:C:519:DGD:HAE2	1.95	0.47
2:B:413:ASP:O	2:B:417:VAL:HG23	2.68	0.47
2:B:124:ARG:HD2	2:B:129:GLY:O	2.44	0.47
3:C:338:GLY:HA3	3:C:341:LEU:O	2.26	0.47
24:D:403:CLA:H112	24:D:403:CLA:H142	2.38	0.47
2:B:245:VAL:HG22	24:B:612:CLA:H202	2.21	0.47
15:U:86:GLU:HG3	41:U:217:HOH:O	14.92	0.47
1:A:105:TRP:CE2	1:A:110:GLY:HA3	2.64	0.47
41:E:204:HOH:O	9:J:6:ARG:HG3	2.15	0.47
24:B:614:CLA:H41	24:B:614:CLA:H62	1.64	0.47
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.97	0.47
2:B:341:LYS:HE2	41:B:704:HOH:O	17.62	0.47
2:B:201:HIS:HB2	24:B:602:CLA:C1B	2.53	0.47
24:B:606:CLA:H162	24:B:606:CLA:H122	3.25	0.47
3:C:429:SER:HA	36:C:519:DGD:HBW1	13.89	0.47
31:A:416[B]:PL9:H262	38:E:101:LHG:H223	1.97	0.46
24:C:512:CLA:HMB1	24:C:512:CLA:HBB1	2.35	0.46
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.46
24:C:507:CLA:HBD	24:C:507:CLA:HAA1	2.12	0.46
36:C:518:DGD:HA81	36:C:518:DGD:HAE2	1.68	0.46
24:B:601:CLA:H111	24:B:601:CLA:H93	3.44	0.46
36:C:519:DGD:HAF1	36:C:519:DGD:HA81	6.68	0.46
4:D:185:PHE:CG	24:D:402:CLA:HMD3	2.50	0.46
3:C:127:PHE:HZ	33:Z:101:LMG:H121	1.80	0.46
2:B:160:GLY:HA2	2:B:163:GLY:O	2.15	0.46
24:C:502:CLA:C4D	24:C:504:CLA:H2	2.46	0.46
24:C:508:CLA:HMC2	24:C:509:CLA:H102	28.37	0.46
24:C:513:CLA:H101	24:C:514:CLA:H141	1.98	0.46
4:D:210:LEU:HA	4:D:213:ILE:HG22	1.98	0.46
24:A:404:CLA:H191	38:D:406:LHG:H332	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.98	0.46
24:C:505:CLA:H41	24:C:505:CLA:H62	1.75	0.46
1:A:187:GLN:HB2	24:A:404:CLA:HAC2	1.96	0.46
2:B:423:LYS:HD3	2:B:423:LYS:HA	1.79	0.46
3:C:42:LEU:HD21	24:C:512:CLA:H2A	1.98	0.46
3:C:53:HIS:CB	24:C:513:CLA:HMD1	2.45	0.46
34:B:622:LMT:H6E	4:D:16:ASP:OD2	2.15	0.46
24:A:404:CLA:H112	33:J:101:LMG:H231	32.99	0.46
2:B:145:LEU:HD22	24:B:604:CLA:H162	1.98	0.46
26:B:619:BCR:C8	26:B:619:BCR:H331	2.47	0.46
35:B:624:HTG:H62	41:O:405:HOH:O	43.04	0.46
26:D:404:BCR:H383	33:J:101:LMG:H171	3.49	0.46
1:A:131:TRP:CH2	24:C:507:CLA:HAA2	16.56	0.46
24:B:605:CLA:HHC	24:B:605:CLA:CBB	2.67	0.46
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.97	0.46
24:B:605:CLA:HBD	24:B:605:CLA:HAA1	2.04	0.45
24:C:509:CLA:H92	38:D:407:LHG:H371	1.98	0.45
38:D:406:LHG:HC62	11:L:15:THR:HG23	1.98	0.45
24:B:611:CLA:HBB1	24:B:611:CLA:HHC	4.49	0.45
24:B:612:CLA:CMB	24:B:614:CLA:HBB1	2.70	0.45
27:A:411:SQD:H81	27:A:411:SQD:H112	1.66	0.45
4:D:54:PHE:O	5:E:49:THR:OG1	2.31	0.45
19:Z:26:ALA:HB1	19:Z:36:SER:HB3	2.17	0.45
24:C:509:CLA:H142	24:C:509:CLA:H112	3.15	0.45
33:C:521:LMG:H152	35:C:522:HTG:H4'2	1.98	0.45
24:D:403:CLA:H61	24:D:403:CLA:H41	2.29	0.45
38:D:407:LHG:H332	38:D:407:LHG:H302	1.81	0.45
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.99	0.45
1:A:274[B]:PHE:CD1	27:A:411:SQD:H101	2.52	0.45
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.99	0.45
24:B:605:CLA:H41	24:B:612:CLA:H161	4.93	0.45
3:C:48:LYS:HD2	3:C:138:GLU:HG3	1.99	0.45
4:D:83:ASN:ND2	4:D:166:SER:OG	2.78	0.45
5:E:36:LEU:HA	5:E:39:SER:OG	2.16	0.45
13:O:92:SER:HB3	13:O:131:PRO:HA	1.98	0.45
20:R:29:LYS:HE2	20:R:29:LYS:HB3	1.76	0.45
31:D:405:PL9:C33	38:L:101:LHG:H222	2.45	0.45
5:E:14:ILE:O	5:E:20:TRP:NE1	2.92	0.45
26:K:102:BCR:H371	26:K:102:BCR:H24C	1.60	0.45
26:B:617:BCR:H371	26:B:617:BCR:H24C	1.92	0.45
3:C:95:LEU:HD21	24:C:502:CLA:OBD	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:67:THR:N	5:E:75:GLN:HE22	3.19	0.45
24:A:404:CLA:H203	33:J:101:LMG:H412	47.22	0.45
24:B:602:CLA:H162	24:B:602:CLA:H203	1.70	0.45
24:B:605:CLA:H192	24:B:609:CLA:HBB2	1.99	0.45
24:B:613:CLA:H151	24:B:613:CLA:H112	3.73	0.45
24:C:502:CLA:H42	24:C:503:CLA:HMD1	1.98	0.45
16:V:61:LEU:HA	16:V:61:LEU:HD23	2.00	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.17	0.44
24:A:409:CLA:H171	24:C:507:CLA:H112	1.99	0.44
4:D:186:GLN:HB2	24:D:402:CLA:HBC1	2.04	0.44
7:H:43:LEU:HD12	7:H:43:LEU:HA	1.76	0.44
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.52	0.44
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.99	0.44
24:B:602:CLA:HMD2	7:H:38:PHE:HZ	1.82	0.44
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.99	0.44
26:D:404:BCR:H351	26:D:404:BCR:H15C	1.86	0.44
24:C:512:CLA:HED2	24:C:512:CLA:H2	10.80	0.44
14:T:2:GLU:CD	14:T:2:GLU:H	2.19	0.44
18:Y:22:LEU:HA	18:Y:25:ILE:HG22	1.99	0.44
2:B:26:HIS:HB2	24:B:612:CLA:HMB2	2.05	0.44
26:C:516:BCR:H11C	26:C:516:BCR:H341	1.79	0.44
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.72	0.44
35:B:624:HTG:H3	13:O:178:LYS:HE3	1.99	0.44
1:A:183:MET:HB3	24:A:404:CLA:HBC2	1.99	0.44
2:B:224:ARG:HD2	41:D:501:HOH:O	2.15	0.44
26:B:619:BCR:H351	26:B:619:BCR:H15C	1.96	0.44
2:B:98:LEU:HD13	35:B:623:HTG:H7'1	2.06	0.44
34:B:622:LMT:H5'	32:D:409:UNL:O9	2.17	0.44
8:I:2:GLU:O	8:I:6:ILE:HG12	2.28	0.44
24:B:609:CLA:HMD1	7:H:27:THR:HB	1.98	0.44
24:B:616:CLA:H62	24:B:616:CLA:H92	2.46	0.44
24:C:502:CLA:C3D	24:C:504:CLA:H2	2.48	0.44
3:C:166:ILE:HG21	24:C:514:CLA:H171	13.09	0.44
26:H:101:BCR:C8	26:H:101:BCR:H331	2.47	0.44
9:J:17:GLY:HA3	26:Y:101:BCR:H371	2.19	0.44
16:V:6:GLU:OE2	16:V:6:GLU:N	2.46	0.44
2:B:499:VAL:HG12	4:D:135:LEU:HB3	1.99	0.44
26:C:516:BCR:H15C	26:C:516:BCR:H351	1.88	0.44
4:D:244:TYR:OH	4:D:264[A]:LYS:HE2	2.28	0.44
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.00	0.44
24:D:403:CLA:H2	17:X:17:GLY:HA3	2.36	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASP:OD2	13:O:69:LYS:HE3	4.45	0.44
3:C:171:GLY:O	3:C:174:LEU:HB2	2.31	0.44
3:C:52:ALA:HA	24:C:512:CLA:HMB3	1.99	0.44
2:B:143:LEU:HA	24:B:610:CLA:HED1	2.00	0.44
24:B:606:CLA:H151	24:B:616:CLA:H122	1.98	0.44
3:C:199:ILE:HG21	3:C:234:VAL:HG21	2.37	0.44
4:D:55:VAL:O	4:D:66:SER:HB3	2.34	0.44
34:E:102:LMT:O3'	34:E:102:LMT:O2B	2.32	0.44
8:I:17:LEU:HD22	8:I:21:PHE:HE2	2.16	0.44
13:O:81:ILE:HA	13:O:100:GLY:HA3	2.00	0.44
1:A:82:VAL:HB	1:A:174:LEU:HB2	2.06	0.43
34:A:359:LMT:H21	35:B:623:HTG:H1	50.27	0.43
3:C:276:LEU:HD23	24:C:510:CLA:HED1	2.00	0.43
5:E:14:ILE:HD12	9:J:12:VAL:HG11	2.00	0.43
1:A:26:ASN:OD1	27:A:413:SQD:O2	2.32	0.43
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.87	0.43
24:B:601:CLA:H2	24:B:601:CLA:H72	4.47	0.43
1:A:63:ILE:HB	3:C:335:THR:HG21	2.00	0.43
36:C:517:DGD:HG11	41:C:601:HOH:O	2.18	0.43
3:C:60:ILE:HG22	24:C:504:CLA:HHD	1.99	0.43
31:D:405:PL9:H422	31:D:405:PL9:H401	1.54	0.43
24:B:602:CLA:H92	36:H:102:DGD:HB71	1.99	0.43
26:Y:101:BCR:H351	26:Y:101:BCR:H15C	1.93	0.43
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.53	0.43
3:C:213:LEU:HG	24:C:507:CLA:H202	2.00	0.43
26:T:101:BCR:H371	26:T:101:BCR:H24C	1.83	0.43
16:V:106:ASN:N	16:V:106:ASN:OD1	2.85	0.43
18:Y:39:LEU:HA	18:Y:39:LEU:HD23	1.85	0.43
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.87	0.43
24:C:509:CLA:H142	24:C:509:CLA:H111	1.82	0.43
3:C:56:HIS:HB2	24:C:510:CLA:HMB2	1.99	0.43
4:D:24:ARG:NH2	27:F:101:SQD:O4	2.51	0.43
5:E:60:GLN:HE21	5:E:61:ARG:H	4.77	0.43
13:O:30:TYR:HA	13:O:31:PRO:HD3	1.81	0.43
16:V:64:PRO:HD2	16:V:66:ARG:NH2	2.56	0.43
27:B:620:SQD:H62	11:L:7:ARG:NH1	4.88	0.43
13:O:81:ILE:HG23	13:O:97:GLU:HG3	2.27	0.43
4:D:20:ASP:HB3	17:X:37:VAL:HG21	2.42	0.43
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.84	0.43
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.43
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:D:405:PL9:H28	31:D:405:PL9:H322	1.79	0.43
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.43
10:K:15:TYR:CE1	19:Z:5:PHE:HZ	2.37	0.43
15:U:48:LEU:HA	15:U:48:LEU:HD23	1.86	0.43
33:Z:101:LMG:H141	33:Z:101:LMG:H111	1.90	0.43
24:B:614:CLA:H162	24:B:614:CLA:H122	4.62	0.43
26:B:618:BCR:H351	26:B:618:BCR:H15C	1.86	0.43
3:C:60:ILE:HG22	24:C:505:CLA:HHD	13.26	0.43
24:C:512:CLA:H61	24:C:512:CLA:H102	2.30	0.43
24:C:514:CLA:H92	24:C:514:CLA:H62	2.20	0.43
12:M:18:PRO:O	12:M:21:PHE:HB3	2.18	0.43
26:T:101:BCR:HC8	26:T:101:BCR:H321	2.01	0.43
25:A:407:PHO:HAB	4:D:205:LEU:HD13	2.01	0.43
3:C:61:VAL:HG12	3:C:118:HIS:O	2.25	0.43
24:C:512:CLA:H161	24:C:512:CLA:H122	4.53	0.43
24:C:514:CLA:HHC	24:C:514:CLA:HBB1	3.15	0.43
5:E:42:LEU:HA	20:R:4:ARG:NH2	2.34	0.43
3:C:127:PHE:CE1	33:Z:101:LMG:H142	2.54	0.43
1:A:12:ASN:ND2	1:A:15:GLU:HB2	2.34	0.43
1:A:272[B]:HIS:CD2	4:D:218:VAL:HG21	2.54	0.43
2:B:237:VAL:HG12	24:B:612:CLA:HMD1	2.01	0.43
24:B:615:CLA:H152	24:B:615:CLA:H112	1.56	0.43
34:B:622:LMT:H91	34:B:622:LMT:H62	1.69	0.43
3:C:24:THR:HB	3:C:138:GLU:OE1	2.19	0.43
5:E:20:TRP:HZ2	9:J:12:VAL:HG13	2.50	0.43
2:B:191:ASN:ND2	7:H:59:ASN:O	2.72	0.43
8:I:17:LEU:HD23	8:I:17:LEU:HA	2.14	0.42
38:D:357:LHG:H152	11:L:23:LEU:HD21	2.00	0.42
24:B:614:CLA:H203	33:B:621:LMG:H421	2.00	0.42
24:B:606:CLA:H192	24:B:616:CLA:H101	2.01	0.42
15:U:70:ARG:HH21	15:U:73:GLN:HE21	1.66	0.42
19:Z:36:SER:O	19:Z:40:ILE:HG13	2.18	0.42
24:B:613:CLA:H111	24:B:613:CLA:H72	2.14	0.42
2:B:266:GLU:HB3	28:B:627:GOL:H12	2.02	0.42
3:C:230:LEU:HA	3:C:230:LEU:HD23	1.87	0.42
26:B:618:BCR:H363	26:T:101:BCR:H19C	35.25	0.42
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.92	0.42
13:O:234:LYS:HE2	13:O:234:LYS:HB2	1.86	0.42
26:T:101:BCR:HC7	26:T:101:BCR:H331	1.56	0.42
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.69	0.42
2:B:159:THR:HA	2:B:181:VAL:O	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.01	0.42
2:B:489:GLU:HG2	2:B:495:PHE:CE2	2.54	0.42
3:C:275:SER:HB3	24:C:510:CLA:HED3	2.00	0.42
24:C:507:CLA:H112	24:C:507:CLA:H72	4.38	0.42
24:C:512:CLA:H111	24:C:512:CLA:H142	4.56	0.42
4:D:24:ARG:NH2	17:X:37:VAL:HG22	5.55	0.42
9:J:7:ILE:HA	9:J:8:PRO:HD3	1.93	0.42
3:C:47:GLY:HA3	3:C:137:PRO:O	2.23	0.42
3:C:415:ASN:O	3:C:416[B]:SER:HB2	2.32	0.42
24:C:503:CLA:H42	24:C:504:CLA:HMD1	7.32	0.42
33:J:101:LMG:H191	33:J:101:LMG:H241	5.14	0.42
31:A:416[B]:PL9:H171	31:A:416[B]:PL9:H151	1.59	0.42
3:C:45:LEU:HA	3:C:139:THR:HG22	2.14	0.42
3:C:459:ILE:HG21	3:C:464:GLU:HG3	2.11	0.42
24:C:509:CLA:H162	24:C:509:CLA:H122	1.87	0.42
3:C:146:PHE:HZ	24:C:513:CLA:HBB2	1.84	0.42
5:E:17:VAL:O	5:E:21:VAL:HG23	2.20	0.42
2:B:216:HIS:CE1	24:B:609:CLA:NA	2.87	0.42
2:B:149:LEU:HG	24:B:606:CLA:HBB2	2.16	0.42
3:C:230:LEU:O	3:C:234:VAL:HG23	2.38	0.42
4:D:90:LEU:HA	4:D:90:LEU:HD23	1.82	0.42
39:E:103:HEM:CAC	6:F:27:ALA:HB1	2.50	0.42
26:H:101:BCR:H341	26:H:101:BCR:H11C	1.82	0.42
24:A:404:CLA:HBD	24:A:405:CLA:HAC2	2.02	0.42
24:C:502:CLA:H192	24:C:507:CLA:C1B	2.50	0.42
24:C:504:CLA:H102	24:C:505:CLA:CHB	17.40	0.42
13:O:15:LEU:HD23	13:O:15:LEU:HA	1.82	0.42
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.50	0.42
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.66	0.42
2:B:445:THR:HA	41:B:707:HOH:O	2.18	0.42
24:B:613:CLA:H141	24:B:613:CLA:H162	4.45	0.42
26:B:618:BCR:H371	26:B:618:BCR:H24C	1.79	0.42
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.58	0.42
26:T:101:BCR:HC8	26:T:101:BCR:H311	2.01	0.42
24:A:406:CLA:H191	38:E:101:LHG:H142	2.02	0.41
26:A:410:BCR:H371	26:A:410:BCR:H24C	1.74	0.41
27:A:411:SQD:H381	9:J:21:ILE:HD11	2.01	0.41
31:A:416[B]:PL9:H121	31:A:416[B]:PL9:HC8	1.79	0.41
24:B:604:CLA:HBD	24:B:604:CLA:HAA1	2.07	0.41
2:B:221:PRO:HA	24:B:609:CLA:HED3	2.15	0.41
24:B:614:CLA:H72	24:B:614:CLA:H112	3.16	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:619:BCR:H321	26:B:619:BCR:HC7	2.07	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.02	0.41
26:D:404:BCR:H11C	26:D:404:BCR:H341	2.03	0.41
24:B:614:CLA:H101	26:B:617:BCR:H362	2.53	0.41
3:C:433:LEU:HD13	24:C:503:CLA:CHC	2.50	0.41
24:C:504:CLA:HBB1	24:C:504:CLA:CHC	2.50	0.41
24:C:508:CLA:H122	24:C:508:CLA:H162	4.22	0.41
24:C:506:CLA:HMD3	24:C:508:CLA:HAB	1.96	0.41
26:D:404:BCR:H20C	26:D:404:BCR:H361	1.89	0.41
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.86	0.41
10:K:25:LEU:HD22	26:Y:101:BCR:H332	2.01	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.89	0.41
4:D:146:PHE:O	4:D:149:PRO:HD2	2.19	0.41
24:D:402:CLA:HBD	24:D:402:CLA:HAA2	2.01	0.41
26:D:404:BCR:H381	33:J:101:LMG:H231	2.03	0.41
26:T:101:BCR:H341	26:T:101:BCR:H11C	1.81	0.41
27:A:411:SQD:H122	27:A:411:SQD:H152	1.81	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.39	0.41
24:B:606:CLA:H161	24:B:606:CLA:H192	3.29	0.41
24:B:614:CLA:HAA1	24:B:614:CLA:HBD	2.01	0.41
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.82	0.41
12:M:5:GLN:HG3	12:M:5:GLN:OE1	3.15	0.41
25:A:408:PHO:H112	25:A:408:PHO:H72	1.92	0.41
24:B:603:CLA:CGA	24:B:603:CLA:H3A	2.53	0.41
26:B:617:BCR:H351	26:B:617:BCR:H15C	1.91	0.41
5:E:9:PRO:HA	38:E:101:LHG:HC31	2.03	0.41
13:O:83:GLY:HA2	13:O:98:GLU:HG3	2.35	0.41
2:B:76[A]:SER:HB2	35:B:623:HTG:H2	2.34	0.41
13:O:49[A]:THR:OG1	13:O:236:GLN:HB2	2.20	0.41
33:Z:101:LMG:H142	33:Z:101:LMG:H111	2.81	0.41
1:A:272[A]:HIS:CD2	4:D:218:VAL:HG21	2.62	0.41
2:B:413:ASP:HA	2:B:414:PRO:HD3	1.98	0.41
24:B:616:CLA:H193	26:B:619:BCR:H331	2.02	0.41
24:C:514:CLA:HBB1	26:C:515:BCR:H371	2.01	0.41
4:D:24:ARG:HD3	17:X:37:VAL:HG22	2.02	0.41
8:I:18:LEU:HA	8:I:18:LEU:HD23	1.93	0.41
27:A:413:SQD:H261	2:B:109:LEU:HD13	58.82	0.41
26:B:619:BCR:H341	26:B:619:BCR:H11C	1.92	0.41
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.06	0.41
24:C:512:CLA:HBA1	24:C:512:CLA:H3A	2.31	0.41
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:33:LYS:HB3	8:I:34:ARG:H	1.67	0.41
16:V:41:HIS:HA	16:V:45:ILE:O	2.21	0.41
24:C:506:CLA:H62	24:C:506:CLA:H41	4.30	0.41
24:C:506:CLA:HBD	24:C:506:CLA:HAA1	2.03	0.41
24:C:507:CLA:H3A	24:C:507:CLA:HBA1	1.79	0.41
15:U:17:LEU:HD23	15:U:17:LEU:HA	2.17	0.41
4:D:343:GLU:HG2	16:V:135:VAL:HG11	2.19	0.41
25:A:408:PHO:ND	25:A:408:PHO:NC	2.68	0.41
2:B:133:LEU:HB3	2:B:138:MET:SD	2.67	0.41
4:D:261:PHE:CZ	38:D:407:LHG:HC81	24.99	0.41
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.86	0.41
3:C:262:ARG:HG2	8:I:38:GLU:HG2	2.02	0.41
13:O:54:GLU:HG2	13:O:64:GLU:O	2.21	0.41
18:Y:39:LEU:HD21	19:Z:25:VAL:HA	2.51	0.41
2:B:285:ASN:O	2:B:289:GLN:HG2	2.21	0.41
2:B:464:PHE:HD2	24:B:611:CLA:HAC2	1.85	0.41
2:B:497:GLN:HE22	17:X:38:GLN:HB2	1.85	0.41
2:B:201:HIS:HB2	24:B:602:CLA:CHB	2.51	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.63	0.41
24:C:503:CLA:HMD2	24:C:504:CLA:H101	3.82	0.41
1:A:269:ARG:NE	4:D:222:LEU:HD22	2.49	0.40
1:A:270[A]:SER:HA	4:D:232:PHE:CE2	2.85	0.40
25:A:408:PHO:HBC2	25:A:408:PHO:HHD	2.03	0.40
1:A:40:THR:HG21	1:A:121[A]:LEU:HD23	5.75	0.40
4:D:40:CYS:HB3	4:D:117:HIS:O	2.33	0.40
13:O:124:ASN:ND2	13:O:147:ASN:HD22	2.18	0.40
24:B:609:CLA:HBA1	24:B:609:CLA:H3A	1.86	0.40
3:C:52:ALA:HB2	24:C:513:CLA:HMA1	17.44	0.40
14:T:20:ALA:O	14:T:24:ARG:HB3	2.23	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.86	0.40
24:B:613:CLA:H161	24:B:613:CLA:H192	1.75	0.40
18:Y:30:ILE:HD12	18:Y:30:ILE:HA	1.91	0.40
1:A:132:GLU:O	1:A:136:ARG:HG2	2.24	0.40
1:A:197:PHE:HB3	1:A:285:PHE:O	2.33	0.40
26:A:410:BCR:H15C	26:A:410:BCR:H351	1.88	0.40
3:C:48:LYS:HG3	3:C:138:GLU:HG3	2.03	0.40
3:C:375:LEU:HA	3:C:375:LEU:HD23	2.06	0.40
24:C:514:CLA:CBB	26:C:515:BCR:H371	2.51	0.40
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.05	0.40
1:A:213:ALA:HB2	4:D:275:PRO:HG2	2.09	0.40
38:E:101:LHG:H291	38:E:101:LHG:H261	1.82	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:407:PHO:ND	25:A:407:PHO:NC	2.67	0.40
24:B:615:CLA:H72	26:B:619:BCR:C11	2.91	0.40
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/344 (104%)	355 (99%)	3 (1%)	1 (0%)	44	53
1	a	360/344 (105%)	355 (99%)	4 (1%)	1 (0%)	44	53
2	B	510/505 (101%)	506 (99%)	4 (1%)	0	100	100
2	b	506/505 (100%)	497 (98%)	9 (2%)	0	100	100
3	C	459/455 (101%)	447 (97%)	10 (2%)	2 (0%)	38	44
3	c	463/455 (102%)	449 (97%)	12 (3%)	2 (0%)	38	44
4	D	343/342 (100%)	333 (97%)	10 (3%)	0	100	100
4	d	342/342 (100%)	336 (98%)	6 (2%)	0	100	100
5	E	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
5	e	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	29/44 (66%)	29 (100%)	0	0	100	100
7	H	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
7	h	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	11	9
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	3
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	32/36 (89%)	30 (94%)	2 (6%)	0	100	100
13	O	246/244 (101%)	237 (96%)	9 (4%)	0	100	100
13	o	243/244 (100%)	238 (98%)	5 (2%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	94/104 (90%)	92 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	27 (100%)	0	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	8
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	11	8
20	R	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5316/5384 (99%)	5202 (98%)	104 (2%)	10 (0%)	51	61

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	i	36	ASP
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
19	z	30	PRO
1	a	259	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	h	63	LYS
19	Z	30	PRO
1	A	259	ILE

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	295/279 (106%)	295 (100%)	0	100	100
1	a	296/279 (106%)	295 (100%)	1 (0%)	94	97
2	B	410/403 (102%)	405 (99%)	5 (1%)	75	86
2	b	406/403 (101%)	398 (98%)	8 (2%)	60	73
3	C	360/356 (101%)	357 (99%)	3 (1%)	85	91
3	c	364/356 (102%)	358 (98%)	6 (2%)	68	79
4	D	280/277 (101%)	279 (100%)	1 (0%)	93	96
4	d	279/277 (101%)	278 (100%)	1 (0%)	93	96
5	E	73/73 (100%)	73 (100%)	0	100	100
5	e	70/73 (96%)	70 (100%)	0	100	100
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	25/38 (66%)	24 (96%)	1 (4%)	36	46
7	H	55/54 (102%)	51 (93%)	4 (7%)	16	18
7	h	54/54 (100%)	53 (98%)	1 (2%)	62	75
8	I	34/34 (100%)	33 (97%)	1 (3%)	48	60
8	i	34/34 (100%)	32 (94%)	2 (6%)	23	26
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	26/27 (96%)	25 (96%)	1 (4%)	38	48
10	K	30/30 (100%)	28 (93%)	2 (7%)	19	21
10	k	30/30 (100%)	27 (90%)	3 (10%)	9	8
11	L	35/35 (100%)	35 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	l	35/35 (100%)	34 (97%)	1 (3%)	48	60
12	M	30/32 (94%)	30 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	43	54
13	O	211/207 (102%)	205 (97%)	6 (3%)	49	61
13	o	208/207 (100%)	207 (100%)	1 (0%)	91	95
14	T	26/28 (93%)	26 (100%)	0	100	100
14	t	26/28 (93%)	25 (96%)	1 (4%)	38	48
15	U	83/89 (93%)	81 (98%)	2 (2%)	54	67
15	u	84/89 (94%)	82 (98%)	2 (2%)	54	67
16	V	117/117 (100%)	116 (99%)	1 (1%)	82	90
16	v	117/117 (100%)	116 (99%)	1 (1%)	82	90
17	X	31/33 (94%)	31 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	32	40
18	y	22/23 (96%)	21 (96%)	1 (4%)	32	40
19	Z	52/52 (100%)	50 (96%)	2 (4%)	38	48
19	z	52/52 (100%)	49 (94%)	3 (6%)	23	27
20	R	29/29 (100%)	29 (100%)	0	100	100
All	All	4416/4403 (100%)	4353 (99%)	63 (1%)	71	82

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	223	GLN
2	B	362	PHE
2	B	489	GLU
2	B	505	ARG
3	C	78	GLU
3	C	289	PHE
3	C	315	MET
4	D	180	ARG
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	23	PRO
7	H	49	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	I	36	ASP
10	K	17	ILE
10	K	19	ASP
13	O	4	THR
13	O	18	LYS
13	O	24	ASP
13	O	69	LYS
13	O	118	LEU
13	O	234	LYS
15	U	16	LYS
15	U	70	ARG
16	V	110	LYS
18	Y	30	ILE
19	Z	3	ILE
19	Z	4	LEU
1	a	12	ASN
2	b	63	LEU
2	b	223	GLN
2	b	298	LEU
2	b	352	GLU
2	b	362	PHE
2	b	472	ARG
2	b	485	GLU
2	b	505	ARG
3	c	24	THR
3	c	142	GLU
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	180	ARG
6	f	15	ILE
7	h	49	TYR
8	i	33	LYS
8	i	36	ASP
9	j	9	LEU
10	k	17	ILE
10	k	19	ASP
10	k	24	VAL
11	l	2	GLU
12	m	5	GLN
13	o	118	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	t	2	GLU
15	u	16	LYS
15	u	86	GLU
16	v	106	ASN
18	y	45	ASN
19	z	3	ILE
19	z	4	LEU
19	z	41	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	75	ASN
2	B	53	ASN
2	B	331	ASN
4	D	61	HIS
4	D	83	ASN
4	D	142	ASN
5	E	60	GLN
13	O	124	ASN
15	U	73	GLN
15	U	78	ASN
15	U	81	HIS
19	Z	58	ASN
2	b	53	ASN
2	b	223	GLN
2	b	289	GLN
2	b	331	ASN
3	c	201	ASN
4	d	83	ASN
5	e	60	GLN
5	e	75	GLN
6	f	44	GLN
12	m	5	GLN
13	o	124	ASN
13	o	130	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	I	1	8	9,9,10	0.57	0	7,9,11	1.22	1 (14%)
12	FME	M	1	12	9,9,10	0.62	0	7,9,11	1.47	1 (14%)
14	FME	T	1	14	9,9,10	0.63	0	7,9,11	1.36	1 (14%)
8	FME	i	1	8	9,9,10	0.60	0	7,9,11	1.50	2 (28%)
12	FME	m	1	12	9,9,10	0.72	0	7,9,11	1.26	0
14	FME	t	1	14	9,9,10	0.62	0	7,9,11	1.46	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
12	FME	M	1	12	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
12	FME	m	1	12	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-3.22	117.64	125.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	1	FME	O-C-CA	-2.51	119.30	125.15
8	I	1	FME	O-C-CA	-2.47	119.39	125.15
8	i	1	FME	O-C-CA	-2.44	119.46	125.15
14	T	1	FME	O-C-CA	-2.22	119.97	125.15
8	i	1	FME	CB-CA-C	-2.11	108.17	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 227 ligands modelled in this entry, 18 are unknown and 18 are monoatomic - leaving 191 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$
34	LMT	A	359	-	36,36,36	0.55	1 (2%)	47,47,47	0.90	1 (2%)
23	BCT	A	403[A]	21	0,3,3	0.00	-	0,3,3	0.00	-
23	BCT	A	403[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	A	404	1	56,73,73	1.94	12 (21%)	65,113,113	2.38	22 (33%)
24	CLA	A	405	41	56,73,73	1.91	10 (17%)	65,113,113	2.32	23 (35%)
24	CLA	A	406	41	56,73,73	1.90	12 (21%)	65,113,113	2.15	23 (35%)
25	PHO	A	407	-	67,69,69	2.04	17 (25%)	87,99,99	1.98	24 (27%)
25	PHO	A	408	-	67,69,69	2.07	15 (22%)	87,99,99	2.12	25 (28%)
24	CLA	A	409	1	56,73,73	1.90	12 (21%)	65,113,113	2.27	23 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	A	410	-	41,41,41	1.00	1 (2%)	56,56,56	1.63	11 (19%)
27	SQD	A	411	-	53,54,54	0.91	3 (5%)	63,65,65	1.97	16 (25%)
28	GOL	A	412	-	5,5,5	0.38	0	5,5,5	0.30	0
27	SQD	A	413	-	53,54,54	0.99	3 (5%)	63,65,65	1.27	7 (11%)
29	OEX	A	414[A]	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
30	OXY	A	415[B]	1,3,41	1,17,17	1.13	0	0,39,39	0.00	-
31	PL9	A	416[A]	-	55,55,55	0.62	1 (1%)	69,69,69	1.94	23 (33%)
31	PL9	A	416[B]	-	55,55,55	0.62	1 (1%)	69,69,69	1.81	18 (26%)
33	LMG	A	418	-	51,51,55	0.89	2 (3%)	59,59,63	1.22	5 (8%)
24	CLA	B	601	41	56,73,73	1.96	11 (19%)	65,113,113	2.18	22 (33%)
24	CLA	B	602	2	56,73,73	1.92	12 (21%)	65,113,113	2.19	23 (35%)
24	CLA	B	603	2	56,73,73	1.90	12 (21%)	65,113,113	2.50	25 (38%)
24	CLA	B	604	2	56,73,73	1.88	11 (19%)	65,113,113	2.40	19 (29%)
24	CLA	B	605	2	56,73,73	1.86	11 (19%)	65,113,113	2.35	20 (30%)
24	CLA	B	606	2	56,73,73	1.81	10 (17%)	65,113,113	2.33	22 (33%)
24	CLA	B	607	41	56,73,73	1.87	12 (21%)	65,113,113	2.32	20 (30%)
24	CLA	B	608	2	56,73,73	1.90	10 (17%)	65,113,113	2.32	22 (33%)
24	CLA	B	609	2	56,73,73	1.87	11 (19%)	65,113,113	2.25	18 (27%)
24	CLA	B	610	41	56,73,73	1.96	11 (19%)	65,113,113	2.27	23 (35%)
24	CLA	B	611	2	56,73,73	1.84	11 (19%)	65,113,113	2.38	22 (33%)
24	CLA	B	612	2	56,73,73	1.90	12 (21%)	65,113,113	2.46	21 (32%)
24	CLA	B	613	2	56,73,73	1.94	12 (21%)	65,113,113	2.37	23 (35%)
24	CLA	B	614	2	56,73,73	1.86	12 (21%)	65,113,113	2.40	22 (33%)
24	CLA	B	615	2	56,73,73	1.83	10 (17%)	65,113,113	2.20	21 (32%)
24	CLA	B	616	2	56,73,73	1.90	11 (19%)	65,113,113	2.16	19 (29%)
26	BCR	B	617	-	41,41,41	0.99	2 (4%)	56,56,56	1.53	10 (17%)
26	BCR	B	618	-	41,41,41	0.95	1 (2%)	56,56,56	1.56	14 (25%)
26	BCR	B	619	-	41,41,41	1.07	2 (4%)	56,56,56	1.48	14 (25%)
27	SQD	B	620	-	53,54,54	1.00	3 (5%)	63,65,65	1.55	11 (17%)
33	LMG	B	621	-	51,51,55	0.89	2 (3%)	59,59,63	1.13	3 (5%)
34	LMT	B	622	-	36,36,36	0.42	0	47,47,47	1.12	4 (8%)
35	HTG	B	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.41	4 (17%)
35	HTG	B	624	-	19,19,19	0.88	1 (5%)	23,24,24	1.59	1 (4%)
35	HTG	B	625	-	19,19,19	0.97	1 (5%)	23,24,24	1.83	2 (8%)
28	GOL	B	626	-	5,5,5	0.36	0	5,5,5	0.44	0
28	GOL	B	627	-	5,5,5	0.44	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	HTG	B	628	-	19,19,19	0.95	2 (10%)	23,24,24	1.46	3 (13%)
34	LMT	B	630	-	25,25,36	0.43	0	30,30,47	0.73	1 (3%)
24	CLA	C	502	3	56,73,73	1.89	12 (21%)	65,113,113	2.23	21 (32%)
24	CLA	C	503	3	56,73,73	1.90	11 (19%)	65,113,113	2.22	18 (27%)
24	CLA	C	504	3	56,73,73	1.85	12 (21%)	65,113,113	2.09	16 (24%)
24	CLA	C	505	41	56,73,73	1.89	12 (21%)	65,113,113	2.33	25 (38%)
24	CLA	C	506	3	56,73,73	1.87	12 (21%)	65,113,113	2.29	18 (27%)
24	CLA	C	507	3	56,73,73	1.87	12 (21%)	65,113,113	2.31	23 (35%)
24	CLA	C	508	41	56,73,73	1.88	12 (21%)	65,113,113	2.28	19 (29%)
24	CLA	C	509	3	56,73,73	1.99	12 (21%)	65,113,113	2.41	21 (32%)
24	CLA	C	510	3	56,73,73	2.01	12 (21%)	65,113,113	2.26	20 (30%)
24	CLA	C	511	3	56,73,73	1.91	12 (21%)	65,113,113	2.27	22 (33%)
24	CLA	C	512	3	56,73,73	1.96	12 (21%)	65,113,113	2.22	18 (27%)
24	CLA	C	513	3	56,73,73	1.92	12 (21%)	65,113,113	2.29	21 (32%)
24	CLA	C	514	3	56,73,73	1.92	12 (21%)	65,113,113	2.18	18 (27%)
26	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.49	8 (14%)
26	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.62	12 (21%)
36	DGD	C	517	-	63,63,67	0.80	2 (3%)	77,77,81	1.19	5 (6%)
36	DGD	C	518	-	63,63,67	0.84	2 (3%)	77,77,81	1.04	6 (7%)
36	DGD	C	519	-	63,63,67	0.81	3 (4%)	77,77,81	0.96	4 (5%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.16	4 (6%)
33	LMG	C	521	-	51,51,55	0.99	3 (5%)	59,59,63	1.21	4 (6%)
35	HTG	C	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.60	2 (8%)
35	HTG	C	523	-	19,19,19	1.03	2 (10%)	23,24,24	1.91	5 (21%)
28	GOL	C	525	-	5,5,5	0.40	0	5,5,5	0.12	0
38	LHG	D	357	-	48,48,48	0.87	2 (4%)	49,54,54	1.26	5 (10%)
24	CLA	D	402	4	56,73,73	1.86	12 (21%)	65,113,113	2.31	23 (35%)
24	CLA	D	403	4	56,73,73	1.89	11 (19%)	65,113,113	2.16	22 (33%)
26	BCR	D	404	-	41,41,41	1.02	1 (2%)	56,56,56	1.84	18 (32%)
31	PL9	D	405	-	55,55,55	0.65	2 (3%)	69,69,69	1.69	19 (27%)
38	LHG	D	406	-	48,48,48	0.87	3 (6%)	49,54,54	1.03	3 (6%)
38	LHG	D	407	-	48,48,48	0.89	2 (4%)	49,54,54	1.03	3 (6%)
35	HTG	D	410	-	16,16,19	1.06	2 (12%)	20,21,24	1.63	1 (5%)
38	LHG	E	101	-	41,41,48	1.00	2 (4%)	42,47,54	1.16	4 (9%)
34	LMT	E	102	-	36,36,36	0.47	0	47,47,47	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	HEM	E	103	5,6	28,50,50	0.89	1 (3%)	17,82,82	2.33	3 (17%)
27	SQD	F	101	-	42,43,54	1.13	3 (7%)	52,54,65	1.76	8 (15%)
26	BCR	H	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.47	10 (17%)
36	DGD	H	102	-	63,63,67	0.81	3 (4%)	77,77,81	0.96	4 (5%)
34	LMT	I	101	-	36,36,36	0.48	0	47,47,47	1.14	3 (6%)
33	LMG	J	101	40	51,51,55	0.87	2 (3%)	59,59,63	0.92	3 (5%)
26	BCR	K	102	-	41,41,41	1.01	1 (2%)	56,56,56	1.61	12 (21%)
38	LHG	L	101	-	48,48,48	0.89	2 (4%)	49,54,54	1.12	4 (8%)
34	LMT	M	101	-	36,36,36	0.50	0	47,47,47	1.12	3 (6%)
34	LMT	M	103	-	36,36,36	0.42	0	47,47,47	0.99	3 (6%)
26	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.74	13 (23%)
28	GOL	V	202	-	5,5,5	0.33	0	5,5,5	0.35	0
39	HEM	V	203	16	28,50,50	0.97	3 (10%)	17,82,82	1.52	3 (17%)
35	HTG	V	204	-	11,11,19	0.23	0	13,15,24	1.07	1 (7%)
26	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.74	14 (25%)
33	LMG	Z	101	-	37,37,55	0.98	3 (8%)	45,45,63	1.53	7 (15%)
24	CLA	a	350	41	56,73,73	1.92	11 (19%)	65,113,113	2.18	18 (27%)
34	LMT	a	359	-	36,36,36	0.50	1 (2%)	47,47,47	0.94	2 (4%)
24	CLA	a	403	1	56,73,73	1.92	12 (21%)	65,113,113	2.44	25 (38%)
24	CLA	a	404	41	56,73,73	1.90	12 (21%)	65,113,113	2.14	20 (30%)
25	PHO	a	405	-	67,69,69	2.01	17 (25%)	87,99,99	2.03	25 (28%)
25	PHO	a	406	-	67,69,69	2.15	15 (22%)	87,99,99	2.00	25 (28%)
24	CLA	a	407	1	56,73,73	1.88	12 (21%)	65,113,113	2.35	24 (36%)
26	BCR	a	408	-	41,41,41	0.95	1 (2%)	56,56,56	1.55	10 (17%)
27	SQD	a	409	-	53,54,54	0.93	3 (5%)	63,65,65	1.92	14 (22%)
28	GOL	a	410	-	5,5,5	0.34	0	5,5,5	0.34	0
27	SQD	a	411	-	53,54,54	1.02	3 (5%)	63,65,65	1.40	10 (15%)
29	OEX	a	412[A]	1,3,41	0,15,15	0.00	-	0,32,32	0.00	-
30	OEY	a	413[B]	1,3,41	1,17,17	4.21	1 (100%)	0,39,39	0.00	-
31	PL9	a	414[A]	-	55,55,55	0.61	1 (1%)	69,69,69	1.91	20 (28%)
31	PL9	a	414[B]	-	55,55,55	0.62	1 (1%)	69,69,69	1.82	19 (27%)
28	GOL	a	416	-	5,5,5	0.30	0	5,5,5	0.64	0
33	LMG	a	417	-	51,51,55	0.91	2 (3%)	59,59,63	1.20	6 (10%)
34	LMT	a	418	-	36,36,36	0.49	1 (2%)	47,47,47	0.88	0
38	LHG	a	419	-	41,41,48	1.02	2 (4%)	42,47,54	0.94	2 (4%)
23	BCT	a	420[A]	21	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCT	a	420[B]	21	0,3,3	0.00	-	0,3,3	0.00	-
24	CLA	b	601	41	56,73,73	1.96	12 (21%)	65,113,113	2.21	19 (29%)
24	CLA	b	602	2	56,73,73	1.95	12 (21%)	65,113,113	2.17	24 (36%)
24	CLA	b	603	2	56,73,73	1.95	12 (21%)	65,113,113	2.37	21 (32%)
24	CLA	b	604	2	56,73,73	1.85	11 (19%)	65,113,113	2.32	20 (30%)
24	CLA	b	605	2	56,73,73	1.84	12 (21%)	65,113,113	2.28	18 (27%)
24	CLA	b	606	2	56,73,73	1.84	11 (19%)	65,113,113	2.26	22 (33%)
24	CLA	b	607	41	56,73,73	1.85	11 (19%)	65,113,113	2.26	20 (30%)
24	CLA	b	608	2	56,73,73	1.92	12 (21%)	65,113,113	2.24	22 (33%)
24	CLA	b	609	2	56,73,73	1.90	12 (21%)	65,113,113	2.28	20 (30%)
24	CLA	b	610	41	56,73,73	1.94	12 (21%)	65,113,113	2.33	21 (32%)
24	CLA	b	611	2	56,73,73	1.86	12 (21%)	65,113,113	2.20	17 (26%)
24	CLA	b	612	2	56,73,73	1.90	12 (21%)	65,113,113	2.35	22 (33%)
24	CLA	b	613	2	56,73,73	1.96	11 (19%)	65,113,113	2.27	19 (29%)
24	CLA	b	614	2	56,73,73	1.89	12 (21%)	65,113,113	2.31	19 (29%)
24	CLA	b	615	2	56,73,73	1.88	11 (19%)	65,113,113	2.16	20 (30%)
24	CLA	b	616	2	56,73,73	1.87	11 (19%)	65,113,113	2.27	22 (33%)
26	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.55	11 (19%)
26	BCR	b	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	16 (28%)
26	BCR	b	619	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	12 (21%)
27	SQD	b	620	-	53,54,54	1.00	3 (5%)	63,65,65	1.60	11 (17%)
33	LMG	b	621	-	51,51,55	0.85	2 (3%)	59,59,63	1.31	6 (10%)
34	LMT	b	622	-	25,25,36	0.45	0	30,30,47	0.74	0
35	HTG	b	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.58	3 (13%)
35	HTG	b	624	-	19,19,19	1.00	1 (5%)	23,24,24	1.61	1 (4%)
35	HTG	b	625	-	19,19,19	1.07	2 (10%)	23,24,24	2.01	2 (8%)
28	GOL	b	627	-	5,5,5	0.30	0	5,5,5	0.36	0
35	HTG	b	628	-	19,19,19	0.89	2 (10%)	23,24,24	1.36	3 (13%)
34	LMT	b	630	-	25,25,36	0.51	1 (4%)	30,30,47	0.89	0
28	GOL	c	502	-	5,5,5	0.38	0	5,5,5	0.32	0
24	CLA	c	503	3	56,73,73	1.91	12 (21%)	65,113,113	2.14	20 (30%)
24	CLA	c	504	3	56,73,73	1.86	11 (19%)	65,113,113	2.23	20 (30%)
24	CLA	c	505	3	56,73,73	1.86	12 (21%)	65,113,113	2.19	17 (26%)
24	CLA	c	506	41	56,73,73	1.96	12 (21%)	65,113,113	2.16	23 (35%)
24	CLA	c	507	3	56,73,73	1.89	12 (21%)	65,113,113	2.32	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	508	3	56,73,73	1.94	11 (19%)	65,113,113	2.21	23 (35%)
24	CLA	c	509	41	56,73,73	1.88	11 (19%)	65,113,113	2.18	17 (26%)
24	CLA	c	510	3	56,73,73	1.99	12 (21%)	65,113,113	2.34	19 (29%)
24	CLA	c	511	3	56,73,73	1.94	12 (21%)	65,113,113	2.26	21 (32%)
24	CLA	c	512	3	56,73,73	1.90	12 (21%)	65,113,113	2.28	21 (32%)
24	CLA	c	513	3	56,73,73	1.93	12 (21%)	65,113,113	2.15	20 (30%)
24	CLA	c	514	3	56,73,73	1.90	12 (21%)	65,113,113	2.27	22 (33%)
24	CLA	c	515	3	56,73,73	1.92	12 (21%)	65,113,113	2.19	20 (30%)
26	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.76	12 (21%)
26	BCR	c	517	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	11 (19%)
36	DGD	c	518	-	63,63,67	0.82	2 (3%)	77,77,81	1.13	5 (6%)
36	DGD	c	519	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	4 (5%)
36	DGD	c	520	-	63,63,67	0.81	2 (3%)	77,77,81	1.12	3 (3%)
33	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.10	5 (8%)
33	LMG	c	522	-	51,51,55	0.95	2 (3%)	59,59,63	1.16	6 (10%)
35	HTG	c	523	-	19,19,19	0.95	1 (5%)	23,24,24	1.55	1 (4%)
35	HTG	c	526	-	19,19,19	1.01	2 (10%)	23,24,24	1.66	3 (13%)
24	CLA	d	402	4	56,73,73	1.88	12 (21%)	65,113,113	2.36	23 (35%)
24	CLA	d	403	4	56,73,73	1.91	11 (19%)	65,113,113	2.09	24 (36%)
26	BCR	d	404	-	41,41,41	1.12	2 (4%)	56,56,56	1.83	14 (25%)
31	PL9	d	405	-	55,55,55	0.60	1 (1%)	69,69,69	1.67	17 (24%)
38	LHG	d	406	-	48,48,48	0.88	3 (6%)	49,54,54	1.13	5 (10%)
38	LHG	d	407	-	48,48,48	0.87	2 (4%)	49,54,54	0.94	3 (6%)
38	LHG	d	408	-	48,48,48	0.89	2 (4%)	49,54,54	1.16	5 (10%)
34	LMT	e	101	-	36,36,36	0.47	0	47,47,47	0.84	2 (4%)
39	HEM	e	102	5,6	28,50,50	0.88	1 (3%)	17,82,82	1.84	3 (17%)
27	SQD	f	101	-	42,43,54	1.14	3 (7%)	52,54,65	1.56	10 (19%)
35	HTG	h	101	-	16,16,19	1.13	2 (12%)	20,21,24	1.87	2 (10%)
26	BCR	h	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.48	11 (19%)
36	DGD	h	103	-	63,63,67	0.84	3 (4%)	77,77,81	0.99	3 (3%)
33	LMG	j	101	40	51,51,55	0.87	2 (3%)	59,59,63	1.16	5 (8%)
26	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	10 (17%)
38	LHG	l	101	-	48,48,48	0.89	2 (4%)	49,54,54	1.14	3 (6%)
34	LMT	m	102	-	36,36,36	0.43	0	47,47,47	0.92	1 (2%)
34	LMT	t	101	-	26,26,36	0.55	1 (3%)	31,31,47	1.17	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	t	102	-	41,41,41	0.99	1 (2%)	56,56,56	1.70	15 (26%)
28	GOL	v	202	-	5,5,5	0.34	0	5,5,5	0.28	0
39	HEM	v	203	16	28,50,50	0.95	3 (10%)	17,82,82	1.53	2 (11%)
26	BCR	y	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.68	11 (19%)
33	LMG	z	101	-	39,39,55	1.06	2 (5%)	47,47,63	1.13	4 (8%)

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
34	LMT	A	359	-	-	0/21/61/61	0/2/2/2
23	BCT	A	403[A]	21	-	0/0/0/0	0/0/0/0
23	BCT	A	403[B]	21	-	0/0/0/0	0/0/0/0
24	CLA	A	404	1	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	405	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	A	406	41	3/3/20/25	0/37/135/135	0/0/9/9
25	PHO	A	407	-	-	0/53/103/103	0/1/6/6
25	PHO	A	408	-	-	0/53/103/103	0/1/6/6
24	CLA	A	409	1	2/2/20/25	0/37/135/135	0/0/9/9
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
27	SQD	A	411	-	-	0/49/69/69	0/1/1/1
28	GOL	A	412	-	-	0/4/4/4	0/0/0/0
27	SQD	A	413	-	-	0/49/69/69	0/1/1/1
29	OEX	A	414[A]	1,3,41	-	0/0/68/68	0/0/6/6
30	OXY	A	415[B]	1,3,41	-	0/0/86/86	0/0/7/7
31	PL9	A	416[A]	-	-	0/53/73/73	0/1/1/1
31	PL9	A	416[B]	-	-	0/53/73/73	0/1/1/1
33	LMG	A	418	-	-	0/46/66/70	0/1/1/1
24	CLA	B	601	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	602	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	603	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	604	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	605	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	606	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	607	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	608	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	B	609	2	2/2/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	610	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	611	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	612	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	613	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	614	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	615	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	B	616	2	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	B	617	-	-	0/29/63/63	0/2/2/2
26	BCR	B	618	-	-	0/29/63/63	0/2/2/2
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	B	620	-	-	0/49/69/69	0/1/1/1
33	LMG	B	621	-	-	0/46/66/70	0/1/1/1
34	LMT	B	622	-	-	0/21/61/61	0/2/2/2
35	HTG	B	623	-	-	0/10/30/30	0/1/1/1
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
35	HTG	B	625	-	-	0/10/30/30	0/1/1/1
28	GOL	B	626	-	-	0/4/4/4	0/0/0/0
28	GOL	B	627	-	-	0/4/4/4	0/0/0/0
35	HTG	B	628	-	-	0/10/30/30	0/1/1/1
34	LMT	B	630	-	-	0/17/37/61	0/1/1/2
24	CLA	C	502	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	503	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	504	3	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	C	505	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	506	3	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	C	507	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	508	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	509	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	510	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	512	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	513	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	C	514	3	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	C	515	-	-	0/29/63/63	0/2/2/2
26	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2
36	DGD	C	518	-	-	0/51/91/95	0/2/2/2
36	DGD	C	519	-	-	0/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	520	-	-	0/46/66/70	0/1/1/1
33	LMG	C	521	-	-	0/46/66/70	0/1/1/1
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
35	HTG	C	523	-	-	0/10/30/30	0/1/1/1
28	GOL	C	525	-	-	0/4/4/4	0/0/0/0
38	LHG	D	357	-	-	0/53/53/53	0/0/0/0
24	CLA	D	402	4	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	D	403	4	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	D	404	-	-	0/29/63/63	0/2/2/2
31	PL9	D	405	-	-	0/53/73/73	0/1/1/1
38	LHG	D	406	-	-	0/53/53/53	0/0/0/0
38	LHG	D	407	-	-	0/53/53/53	0/0/0/0
35	HTG	D	410	-	-	0/7/27/30	0/1/1/1
38	LHG	E	101	-	-	0/46/46/53	0/0/0/0
34	LMT	E	102	-	-	0/21/61/61	0/2/2/2
39	HEM	E	103	5,6	-	0/6/54/54	0/0/8/8
27	SQD	F	101	-	-	2/38/58/69	0/1/1/1
26	BCR	H	101	-	-	0/29/63/63	0/2/2/2
36	DGD	H	102	-	-	0/51/91/95	0/2/2/2
34	LMT	I	101	-	-	0/21/61/61	0/2/2/2
33	LMG	J	101	40	-	0/46/66/70	0/1/1/1
26	BCR	K	102	-	-	0/29/63/63	0/2/2/2
38	LHG	L	101	-	-	0/53/53/53	0/0/0/0
34	LMT	M	101	-	-	0/21/61/61	0/2/2/2
34	LMT	M	103	-	-	0/21/61/61	0/2/2/2
26	BCR	T	101	-	-	0/29/63/63	0/2/2/2
28	GOL	V	202	-	-	0/4/4/4	0/0/0/0
39	HEM	V	203	16	-	0/6/54/54	0/0/8/8
35	HTG	V	204	-	-	0/2/19/30	0/1/1/1
26	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
33	LMG	Z	101	-	-	2/31/51/70	0/1/1/1
24	CLA	a	350	41	3/3/20/25	0/37/135/135	0/0/9/9
34	LMT	a	359	-	-	0/21/61/61	0/2/2/2
24	CLA	a	403	1	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	a	404	41	2/2/20/25	0/37/135/135	0/0/9/9
25	PHO	a	405	-	-	0/53/103/103	0/1/6/6
25	PHO	a	406	-	-	0/53/103/103	0/1/6/6
24	CLA	a	407	1	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	a	408	-	-	0/29/63/63	0/2/2/2
27	SQD	a	409	-	-	0/49/69/69	0/1/1/1
28	GOL	a	410	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	a	411	-	-	0/49/69/69	0/1/1/1
29	OEX	a	412[A]	1,3,41	-	0/0/68/68	0/0/6/6
30	OXY	a	413[B]	1,3,41	-	0/0/86/86	0/0/7/7
31	PL9	a	414[A]	-	-	0/53/73/73	0/1/1/1
31	PL9	a	414[B]	-	-	0/53/73/73	0/1/1/1
28	GOL	a	416	-	-	0/4/4/4	0/0/0/0
33	LMG	a	417	-	-	0/46/66/70	0/1/1/1
34	LMT	a	418	-	-	0/21/61/61	0/2/2/2
38	LHG	a	419	-	-	0/46/46/53	0/0/0/0
23	BCT	a	420[A]	21	-	0/0/0/0	0/0/0/0
23	BCT	a	420[B]	21	-	0/0/0/0	0/0/0/0
24	CLA	b	601	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	602	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	603	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	604	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	605	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	606	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	607	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	608	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	609	2	2/2/20/25	0/37/135/135	0/0/9/9
24	CLA	b	610	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	611	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	612	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	613	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	614	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	615	2	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	b	616	2	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	b	617	-	-	0/29/63/63	0/2/2/2
26	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
27	SQD	b	620	-	-	0/49/69/69	0/1/1/1
33	LMG	b	621	-	-	0/46/66/70	0/1/1/1
34	LMT	b	622	-	-	0/17/37/61	0/1/1/2
35	HTG	b	623	-	-	0/10/30/30	0/1/1/1
35	HTG	b	624	-	-	0/10/30/30	0/1/1/1
35	HTG	b	625	-	-	0/10/30/30	0/1/1/1
28	GOL	b	627	-	-	0/4/4/4	0/0/0/0
35	HTG	b	628	-	-	0/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	b	630	-	-	0/17/37/61	0/1/1/2
28	GOL	c	502	-	-	0/4/4/4	0/0/0/0
24	CLA	c	503	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	504	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	505	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	506	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	507	3	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	c	508	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	509	41	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	510	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	511	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	512	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	513	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	514	3	3/3/20/25	0/37/135/135	0/0/9/9
24	CLA	c	515	3	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	c	516	-	-	0/29/63/63	0/2/2/2
26	BCR	c	517	-	-	0/29/63/63	0/2/2/2
36	DGD	c	518	-	-	0/51/91/95	0/2/2/2
36	DGD	c	519	-	-	0/51/91/95	0/2/2/2
36	DGD	c	520	-	-	0/51/91/95	0/2/2/2
33	LMG	c	521	-	-	0/46/66/70	0/1/1/1
33	LMG	c	522	-	-	0/46/66/70	0/1/1/1
35	HTG	c	523	-	-	0/10/30/30	0/1/1/1
35	HTG	c	526	-	-	0/10/30/30	0/1/1/1
24	CLA	d	402	4	1/1/20/25	0/37/135/135	0/0/9/9
24	CLA	d	403	4	3/3/20/25	0/37/135/135	0/0/9/9
26	BCR	d	404	-	-	0/29/63/63	0/2/2/2
31	PL9	d	405	-	-	0/53/73/73	0/1/1/1
38	LHG	d	406	-	-	0/53/53/53	0/0/0/0
38	LHG	d	407	-	-	0/53/53/53	0/0/0/0
38	LHG	d	408	-	-	0/53/53/53	0/0/0/0
34	LMT	e	101	-	-	0/21/61/61	0/2/2/2
39	HEM	e	102	5,6	-	0/6/54/54	0/0/8/8
27	SQD	f	101	-	-	2/38/58/69	0/1/1/1
35	HTG	h	101	-	-	0/7/27/30	0/1/1/1
26	BCR	h	102	-	-	0/29/63/63	0/2/2/2
36	DGD	h	103	-	-	0/51/91/95	0/2/2/2
33	LMG	j	101	40	-	0/46/66/70	0/1/1/1
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LHG	l	101	-	-	0/53/53/53	0/0/0/0
34	LMT	m	102	-	-	0/21/61/61	0/2/2/2
34	LMT	t	101	-	-	0/17/38/61	0/1/1/2
26	BCR	t	102	-	-	0/29/63/63	0/2/2/2
28	GOL	v	202	-	-	0/4/4/4	0/0/0/0
39	HEM	v	203	16	-	0/6/54/54	0/0/8/8
26	BCR	y	101	-	-	0/29/63/63	0/2/2/2
33	LMG	z	101	-	-	0/34/54/70	0/1/1/1

All (1034) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	404	BCR	C23-C22	-5.30	1.34	1.45
26	K	102	BCR	C23-C22	-5.21	1.34	1.45
26	B	619	BCR	C23-C22	-5.17	1.34	1.45
26	k	101	BCR	C23-C22	-5.06	1.34	1.45
26	C	516	BCR	C23-C22	-5.06	1.34	1.45
26	C	515	BCR	C23-C22	-4.95	1.35	1.45
26	c	517	BCR	C23-C22	-4.94	1.35	1.45
26	c	516	BCR	C23-C22	-4.92	1.35	1.45
26	t	102	BCR	C23-C22	-4.88	1.35	1.45
26	y	101	BCR	C23-C22	-4.87	1.35	1.45
26	T	101	BCR	C23-C22	-4.82	1.35	1.45
26	b	617	BCR	C23-C22	-4.81	1.35	1.45
26	A	410	BCR	C23-C22	-4.77	1.35	1.45
26	D	404	BCR	C23-C22	-4.77	1.35	1.45
26	b	619	BCR	C23-C22	-4.71	1.35	1.45
26	h	102	BCR	C23-C22	-4.69	1.35	1.45
26	b	618	BCR	C23-C22	-4.67	1.35	1.45
26	H	101	BCR	C23-C22	-4.61	1.35	1.45
26	a	408	BCR	C23-C22	-4.57	1.36	1.45
26	Y	101	BCR	C23-C22	-4.52	1.36	1.45
26	B	617	BCR	C23-C22	-4.50	1.36	1.45
26	B	618	BCR	C23-C22	-4.35	1.36	1.45
35	b	623	HTG	C1'-S1	-3.91	1.76	1.81
35	b	625	HTG	C1'-S1	-3.83	1.76	1.81
35	B	623	HTG	C1'-S1	-3.72	1.76	1.81
35	h	101	HTG	C1'-S1	-3.66	1.76	1.81
25	A	407	PHO	C4A-NA	-3.61	1.26	1.35
35	C	523	HTG	C1'-S1	-3.60	1.76	1.81
35	c	526	HTG	C1'-S1	-3.56	1.76	1.81
35	b	624	HTG	C1'-S1	-3.56	1.76	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C4A-NA	-3.49	1.26	1.35
35	B	625	HTG	C1'-S1	-3.42	1.77	1.81
35	C	522	HTG	C1'-S1	-3.40	1.77	1.81
35	c	523	HTG	C1'-S1	-3.34	1.77	1.81
25	a	405	PHO	C4A-NA	-3.33	1.27	1.35
35	D	410	HTG	C1'-S1	-3.20	1.77	1.81
35	B	628	HTG	C1'-S1	-3.20	1.77	1.81
25	a	406	PHO	C4A-NA	-3.18	1.27	1.35
35	B	624	HTG	C1'-S1	-3.06	1.77	1.81
39	e	102	HEM	C3B-C2B	-3.01	1.36	1.40
35	b	628	HTG	C1'-S1	-2.96	1.77	1.81
27	A	413	SQD	C6-S	-2.62	1.66	1.77
27	f	101	SQD	C6-S	-2.60	1.66	1.77
39	V	203	HEM	C4D-ND	-2.59	1.33	1.36
27	a	409	SQD	C6-S	-2.56	1.67	1.77
25	A	407	PHO	C1A-NA	-2.55	1.32	1.37
27	a	411	SQD	C6-S	-2.53	1.67	1.77
27	b	620	SQD	C6-S	-2.52	1.67	1.77
27	F	101	SQD	C6-S	-2.48	1.67	1.77
27	B	620	SQD	C6-S	-2.47	1.67	1.77
27	A	411	SQD	C6-S	-2.44	1.67	1.77
35	D	410	HTG	C1-S1	-2.43	1.76	1.80
39	v	203	HEM	C4D-ND	-2.39	1.33	1.36
35	B	628	HTG	C1-S1	-2.36	1.77	1.80
39	v	203	HEM	C1B-NB	-2.36	1.34	1.36
39	V	203	HEM	C3B-C2B	-2.33	1.37	1.40
25	a	406	PHO	C1A-NA	-2.31	1.32	1.37
39	V	203	HEM	C1B-NB	-2.29	1.34	1.36
39	E	103	HEM	C3B-C2B	-2.28	1.37	1.40
25	A	408	PHO	C1A-NA	-2.27	1.32	1.37
35	h	101	HTG	C1-S1	-2.25	1.77	1.80
26	B	619	BCR	C30-C25	-2.21	1.50	1.53
35	b	625	HTG	C1-S1	-2.19	1.77	1.80
26	B	617	BCR	C1-C6	-2.19	1.50	1.53
25	a	405	PHO	C1A-NA	-2.18	1.32	1.37
24	A	409	CLA	C1C-NC	-2.18	1.34	1.37
35	c	526	HTG	C1-S1	-2.18	1.77	1.80
35	b	628	HTG	C1-S1	-2.14	1.77	1.80
24	B	612	CLA	C1C-NC	-2.10	1.34	1.37
38	d	406	LHG	O7-C5	-2.09	1.41	1.46
36	C	519	DGD	O2G-C2G	-2.08	1.41	1.46
38	D	406	LHG	O7-C5	-2.06	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	v	203	HEM	C3B-C2B	-2.05	1.37	1.40
35	C	523	HTG	C1-S1	-2.04	1.77	1.80
24	b	601	CLA	C1C-NC	-2.04	1.34	1.37
26	d	404	BCR	C30-C25	-2.02	1.51	1.53
34	b	630	LMT	O1'-C1'	2.02	1.43	1.40
24	C	508	CLA	C4C-C3C	2.02	1.48	1.45
36	h	103	DGD	O5D-C1E	2.03	1.43	1.40
24	C	514	CLA	C4C-C3C	2.03	1.48	1.45
24	B	605	CLA	CHD-C4C	2.04	1.47	1.41
24	d	402	CLA	CHD-C4C	2.04	1.47	1.41
24	c	507	CLA	CHD-C4C	2.04	1.47	1.41
25	A	407	PHO	C4D-CHA	2.04	1.49	1.44
24	b	616	CLA	CHD-C4C	2.05	1.47	1.41
33	Z	101	LMG	O1-C1	2.05	1.43	1.40
34	a	418	LMT	O1'-C1'	2.05	1.43	1.40
24	b	603	CLA	CHD-C4C	2.06	1.47	1.41
24	C	513	CLA	C4C-C3C	2.07	1.48	1.45
33	C	521	LMG	O1-C1	2.07	1.43	1.40
25	a	405	PHO	C4D-CHA	2.08	1.49	1.44
24	b	602	CLA	C4C-C3C	2.08	1.48	1.45
24	a	404	CLA	C4C-C3C	2.08	1.48	1.45
36	H	102	DGD	O5D-C1E	2.09	1.43	1.40
25	a	405	PHO	C4C-C3C	2.09	1.49	1.45
24	b	605	CLA	C1C-C2C	2.09	1.48	1.44
24	B	613	CLA	CHD-C4C	2.09	1.47	1.41
24	b	611	CLA	C4C-C3C	2.10	1.48	1.45
24	B	611	CLA	CHD-C4C	2.10	1.47	1.41
34	a	359	LMT	O1'-C1'	2.10	1.43	1.40
24	B	616	CLA	CHD-C4C	2.10	1.47	1.41
24	C	509	CLA	CHD-C4C	2.10	1.47	1.41
24	c	510	CLA	CHD-C4C	2.10	1.47	1.41
34	t	101	LMT	O1'-C1'	2.10	1.43	1.40
24	A	406	CLA	C4C-C3C	2.10	1.48	1.45
24	B	609	CLA	CHD-C4C	2.10	1.47	1.41
24	B	601	CLA	CHD-C4C	2.11	1.47	1.41
24	C	511	CLA	C4C-C3C	2.11	1.48	1.45
24	b	614	CLA	C4C-C3C	2.12	1.48	1.45
24	c	513	CLA	C4C-C3C	2.12	1.48	1.45
24	B	604	CLA	CHD-C4C	2.12	1.47	1.41
24	c	514	CLA	C4C-C3C	2.12	1.48	1.45
24	C	507	CLA	C1C-C2C	2.13	1.48	1.44
24	b	605	CLA	CHD-C4C	2.14	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608	CLA	C4C-C3C	2.14	1.48	1.45
24	c	504	CLA	CHD-C4C	2.14	1.47	1.41
24	A	404	CLA	CHD-C4C	2.14	1.47	1.41
24	B	612	CLA	C4C-C3C	2.15	1.48	1.45
24	c	507	CLA	C4C-C3C	2.15	1.48	1.45
24	b	612	CLA	CHD-C4C	2.15	1.47	1.41
24	d	402	CLA	C4C-C3C	2.15	1.48	1.45
24	B	603	CLA	C4C-C3C	2.16	1.48	1.45
31	D	405	PL9	C2-C3	2.16	1.40	1.34
25	A	407	PHO	C4C-C3C	2.16	1.49	1.45
24	b	606	CLA	CHD-C4C	2.16	1.47	1.41
24	b	613	CLA	CHD-C4C	2.16	1.47	1.41
24	a	407	CLA	CHD-C4C	2.16	1.47	1.41
24	b	611	CLA	CHD-C4C	2.16	1.47	1.41
24	C	503	CLA	C1C-C2C	2.17	1.48	1.44
24	b	614	CLA	CHD-C4C	2.17	1.47	1.41
24	c	506	CLA	CHD-C4C	2.17	1.47	1.41
24	C	505	CLA	CHD-C4C	2.17	1.47	1.41
24	C	502	CLA	C4C-C3C	2.18	1.48	1.45
24	D	402	CLA	CHD-C4C	2.19	1.47	1.41
24	C	508	CLA	CHD-C4C	2.19	1.47	1.41
24	B	611	CLA	C1C-C2C	2.19	1.48	1.44
24	D	403	CLA	CHD-C4C	2.20	1.47	1.41
24	B	610	CLA	CHD-C4C	2.20	1.47	1.41
24	a	350	CLA	CHD-C4C	2.20	1.47	1.41
24	a	407	CLA	C4C-C3C	2.20	1.48	1.45
24	D	402	CLA	C4B-CHC	2.22	1.46	1.40
24	b	605	CLA	C4C-C3C	2.22	1.49	1.45
24	B	614	CLA	CHD-C4C	2.22	1.47	1.41
24	a	403	CLA	C4C-C3C	2.22	1.49	1.45
24	b	601	CLA	C1C-C2C	2.23	1.48	1.44
24	B	603	CLA	CHD-C4C	2.23	1.47	1.41
24	b	616	CLA	C1C-C2C	2.24	1.48	1.44
24	c	512	CLA	C4C-C3C	2.24	1.49	1.45
24	b	608	CLA	CHD-C4C	2.24	1.47	1.41
24	C	503	CLA	CHD-C4C	2.25	1.47	1.41
24	a	350	CLA	C1C-C2C	2.26	1.48	1.44
24	C	513	CLA	CHD-C4C	2.26	1.47	1.41
24	a	403	CLA	C1C-C2C	2.26	1.48	1.44
24	A	409	CLA	CHD-C4C	2.26	1.48	1.41
24	a	403	CLA	C4B-CHC	2.27	1.46	1.40
24	c	503	CLA	C4C-C3C	2.27	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	CHD-C4C	2.28	1.48	1.41
24	C	502	CLA	CHD-C4C	2.28	1.48	1.41
24	C	506	CLA	CHD-C4C	2.28	1.48	1.41
24	c	511	CLA	C1C-C2C	2.28	1.48	1.44
24	C	506	CLA	C4C-C3C	2.28	1.49	1.45
24	c	508	CLA	C4C-C3C	2.28	1.49	1.45
24	c	514	CLA	CHD-C4C	2.29	1.48	1.41
24	C	512	CLA	C4C-C3C	2.29	1.49	1.45
24	C	505	CLA	C4C-C3C	2.29	1.49	1.45
24	c	513	CLA	CHD-C4C	2.29	1.48	1.41
24	b	610	CLA	CHD-C4C	2.30	1.48	1.41
24	b	604	CLA	CHD-C4C	2.30	1.48	1.41
24	c	511	CLA	CHD-C4C	2.30	1.48	1.41
24	C	512	CLA	CHD-C4C	2.30	1.48	1.41
24	C	509	CLA	C4C-C3C	2.30	1.49	1.45
24	b	606	CLA	C1B-CHB	2.31	1.46	1.40
24	c	510	CLA	C4C-C3C	2.31	1.49	1.45
24	c	506	CLA	C4C-C3C	2.32	1.49	1.45
24	b	607	CLA	C4C-C3C	2.32	1.49	1.45
24	b	615	CLA	CHD-C4C	2.32	1.48	1.41
24	b	607	CLA	C4B-CHC	2.32	1.46	1.40
24	c	505	CLA	CHD-C4C	2.32	1.48	1.41
24	B	608	CLA	C1C-C2C	2.33	1.49	1.44
24	A	409	CLA	C1C-C2C	2.33	1.49	1.44
24	b	615	CLA	C4C-C3C	2.33	1.49	1.45
24	a	404	CLA	C1C-C2C	2.33	1.49	1.44
24	C	511	CLA	CHD-C4C	2.34	1.48	1.41
24	c	514	CLA	C1C-C2C	2.34	1.49	1.44
24	C	504	CLA	C1C-C2C	2.35	1.49	1.44
24	B	607	CLA	CHD-C4C	2.35	1.48	1.41
24	d	402	CLA	C1C-C2C	2.35	1.49	1.44
24	B	611	CLA	C4B-CHC	2.36	1.46	1.40
24	b	603	CLA	C4C-C3C	2.37	1.49	1.45
24	B	612	CLA	C1C-C2C	2.37	1.49	1.44
24	c	503	CLA	CHD-C4C	2.37	1.48	1.41
24	a	404	CLA	CHD-C4C	2.37	1.48	1.41
24	b	601	CLA	CHD-C4C	2.37	1.48	1.41
24	b	609	CLA	C4C-C3C	2.38	1.49	1.45
24	c	504	CLA	C1C-C2C	2.38	1.49	1.44
24	C	504	CLA	CHD-C4C	2.38	1.48	1.41
24	c	509	CLA	C1C-C2C	2.39	1.49	1.44
24	c	512	CLA	C1C-C2C	2.40	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C1C-C2C	2.40	1.49	1.44
24	C	507	CLA	CHD-C4C	2.41	1.48	1.41
24	c	505	CLA	C4C-C3C	2.41	1.49	1.45
24	b	612	CLA	C4C-C3C	2.41	1.49	1.45
24	c	512	CLA	CHD-C4C	2.41	1.48	1.41
24	B	616	CLA	C1C-C2C	2.41	1.49	1.44
24	C	514	CLA	CHD-C4C	2.41	1.48	1.41
24	b	609	CLA	C1C-C2C	2.42	1.49	1.44
34	A	359	LMT	O1'-C1'	2.42	1.44	1.40
24	b	602	CLA	CHD-C4C	2.43	1.48	1.41
24	B	602	CLA	CHD-C4C	2.43	1.48	1.41
24	B	610	CLA	C1C-C2C	2.44	1.49	1.44
24	c	505	CLA	C1C-C2C	2.44	1.49	1.44
24	c	515	CLA	CHD-C4C	2.44	1.48	1.41
24	d	403	CLA	CHD-C4C	2.44	1.48	1.41
24	a	403	CLA	CHD-C4C	2.45	1.48	1.41
24	A	409	CLA	C4B-CHC	2.45	1.46	1.40
24	b	606	CLA	C1C-C2C	2.46	1.49	1.44
24	c	504	CLA	C4B-CHC	2.46	1.46	1.40
24	C	510	CLA	CHD-C4C	2.47	1.48	1.41
24	b	612	CLA	C1C-C2C	2.48	1.49	1.44
24	b	611	CLA	C1C-C2C	2.48	1.49	1.44
24	b	610	CLA	C4C-C3C	2.48	1.49	1.45
24	B	602	CLA	C4C-C3C	2.48	1.49	1.45
24	C	510	CLA	C4C-C3C	2.48	1.49	1.45
24	b	615	CLA	C1B-CHB	2.48	1.46	1.40
24	c	508	CLA	CHD-C4C	2.48	1.48	1.41
24	D	402	CLA	C1C-C2C	2.49	1.49	1.44
24	B	614	CLA	C4C-C3C	2.49	1.49	1.45
24	c	515	CLA	C4C-C3C	2.49	1.49	1.45
24	B	607	CLA	C4C-C3C	2.49	1.49	1.45
24	A	404	CLA	C4C-C3C	2.50	1.49	1.45
24	a	404	CLA	C4B-CHC	2.50	1.46	1.40
24	b	607	CLA	C1C-C2C	2.50	1.49	1.44
25	A	407	PHO	CHB-C4A	2.50	1.46	1.40
24	b	608	CLA	C1C-C2C	2.50	1.49	1.44
24	B	603	CLA	C1B-CHB	2.50	1.46	1.40
24	a	350	CLA	C1B-CHB	2.51	1.46	1.40
24	B	602	CLA	C1B-CHB	2.51	1.46	1.40
24	B	608	CLA	C4B-CHC	2.52	1.46	1.40
24	A	406	CLA	CHD-C4C	2.53	1.48	1.41
31	d	405	PL9	C6-C5	2.53	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C1C-C2C	2.53	1.49	1.44
24	A	404	CLA	C1B-CHB	2.53	1.46	1.40
24	C	513	CLA	C1B-CHB	2.53	1.46	1.40
24	b	603	CLA	C1B-CHB	2.54	1.46	1.40
33	Z	101	LMG	O8-C28	2.54	1.46	1.33
25	a	405	PHO	CHD-C4C	2.55	1.46	1.40
24	c	513	CLA	C1C-C2C	2.55	1.49	1.44
24	b	609	CLA	C4B-CHC	2.55	1.46	1.40
24	b	616	CLA	C1B-CHB	2.55	1.46	1.40
31	D	405	PL9	C6-C5	2.55	1.48	1.35
24	A	406	CLA	C1C-C2C	2.55	1.49	1.44
24	D	402	CLA	C4C-C3C	2.56	1.49	1.45
24	c	509	CLA	CHD-C4C	2.56	1.48	1.41
24	c	514	CLA	C1B-CHB	2.57	1.47	1.40
24	B	606	CLA	C1B-CHB	2.57	1.47	1.40
24	C	502	CLA	C1C-C2C	2.57	1.49	1.44
24	A	406	CLA	C1B-CHB	2.58	1.47	1.40
24	c	506	CLA	C4B-CHC	2.58	1.47	1.40
24	c	506	CLA	C1C-C2C	2.58	1.49	1.44
24	b	614	CLA	C1C-C2C	2.59	1.49	1.44
24	C	505	CLA	C1C-C2C	2.59	1.49	1.44
24	B	614	CLA	C1C-C2C	2.59	1.49	1.44
24	c	510	CLA	C1C-C2C	2.60	1.49	1.44
24	C	505	CLA	C4B-CHC	2.60	1.47	1.40
24	B	615	CLA	C1B-CHB	2.60	1.47	1.40
24	b	610	CLA	C1C-C2C	2.60	1.49	1.44
24	d	403	CLA	C1C-C2C	2.60	1.49	1.44
25	A	407	PHO	C3B-C4B	2.60	1.48	1.43
24	C	508	CLA	C1C-C2C	2.61	1.49	1.44
31	A	416[B]	PL9	C6-C5	2.61	1.49	1.35
24	c	511	CLA	C4C-C3C	2.61	1.49	1.45
24	B	613	CLA	C4B-CHC	2.61	1.47	1.40
24	a	407	CLA	C1C-C2C	2.61	1.49	1.44
24	C	509	CLA	C4B-CHC	2.61	1.47	1.40
24	b	605	CLA	C4B-CHC	2.61	1.47	1.40
24	B	601	CLA	C1B-CHB	2.61	1.47	1.40
24	a	407	CLA	C1B-CHB	2.61	1.47	1.40
24	C	504	CLA	C4C-C3C	2.61	1.49	1.45
24	c	511	CLA	C4B-CHC	2.62	1.47	1.40
24	a	407	CLA	C4B-CHC	2.62	1.47	1.40
24	C	507	CLA	C1B-CHB	2.62	1.47	1.40
24	C	504	CLA	C1B-CHB	2.63	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C1C-C2C	2.63	1.49	1.44
24	c	509	CLA	C1B-CHB	2.63	1.47	1.40
24	C	512	CLA	C1C-C2C	2.63	1.49	1.44
24	C	512	CLA	C4B-CHC	2.63	1.47	1.40
24	C	507	CLA	C4B-CHC	2.63	1.47	1.40
24	B	609	CLA	C1C-C2C	2.63	1.49	1.44
31	a	414[B]	PL9	C6-C5	2.64	1.49	1.35
24	B	613	CLA	C4C-C3C	2.64	1.49	1.45
24	B	615	CLA	C1C-C2C	2.64	1.49	1.44
24	C	507	CLA	C4C-C3C	2.64	1.49	1.45
24	c	512	CLA	C4B-CHC	2.64	1.47	1.40
24	C	514	CLA	C4B-CHC	2.65	1.47	1.40
24	c	515	CLA	C1C-C2C	2.65	1.49	1.44
24	C	511	CLA	C1C-C2C	2.65	1.49	1.44
24	B	614	CLA	C1B-CHB	2.65	1.47	1.40
24	B	607	CLA	C4B-CHC	2.66	1.47	1.40
24	b	602	CLA	C1B-CHB	2.66	1.47	1.40
24	b	616	CLA	C4B-CHC	2.66	1.47	1.40
24	D	403	CLA	C1C-C2C	2.67	1.49	1.44
24	B	612	CLA	C4B-CHC	2.67	1.47	1.40
24	B	604	CLA	C4B-CHC	2.68	1.47	1.40
24	b	615	CLA	C4B-CHC	2.68	1.47	1.40
24	c	515	CLA	C1B-CHB	2.68	1.47	1.40
31	A	416[A]	PL9	C6-C5	2.68	1.49	1.35
24	C	508	CLA	C1B-CHB	2.69	1.47	1.40
24	C	503	CLA	C1B-CHB	2.69	1.47	1.40
24	B	616	CLA	C1B-CHB	2.69	1.47	1.40
24	B	609	CLA	C1B-CHB	2.70	1.47	1.40
24	b	601	CLA	C4B-CHC	2.70	1.47	1.40
24	B	603	CLA	C1C-C2C	2.70	1.49	1.44
24	d	403	CLA	C1B-CHB	2.70	1.47	1.40
31	a	414[A]	PL9	C6-C5	2.70	1.49	1.35
24	b	604	CLA	C1C-C2C	2.71	1.49	1.44
24	b	614	CLA	C4B-CHC	2.71	1.47	1.40
24	b	606	CLA	C4B-CHC	2.71	1.47	1.40
24	c	515	CLA	C4B-CHC	2.71	1.47	1.40
25	a	405	PHO	C3B-C4B	2.71	1.49	1.43
24	B	606	CLA	C4B-CHC	2.72	1.47	1.40
24	b	608	CLA	C4B-CHC	2.72	1.47	1.40
24	c	505	CLA	C1B-CHB	2.72	1.47	1.40
24	C	506	CLA	C4B-CHC	2.72	1.47	1.40
24	B	609	CLA	C4B-CHC	2.73	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	403	CLA	C1B-CHB	2.73	1.47	1.40
24	b	603	CLA	C4B-CHC	2.73	1.47	1.40
25	a	405	PHO	CHB-C4A	2.74	1.46	1.40
24	D	402	CLA	C1B-CHB	2.74	1.47	1.40
24	C	514	CLA	C1C-C2C	2.74	1.49	1.44
24	C	510	CLA	C4B-CHC	2.75	1.47	1.40
24	c	510	CLA	C1B-CHB	2.75	1.47	1.40
24	b	613	CLA	C1B-CHB	2.75	1.47	1.40
24	C	504	CLA	C4B-CHC	2.75	1.47	1.40
24	B	601	CLA	C1C-C2C	2.75	1.49	1.44
24	b	608	CLA	C1B-CHB	2.76	1.47	1.40
25	A	408	PHO	CHD-C4C	2.76	1.47	1.40
24	A	405	CLA	C1B-CHB	2.76	1.47	1.40
24	b	601	CLA	C1B-CHB	2.76	1.47	1.40
24	c	506	CLA	C1B-CHB	2.76	1.47	1.40
25	A	408	PHO	CHB-C4A	2.77	1.47	1.40
24	c	513	CLA	C4B-CHC	2.77	1.47	1.40
24	B	616	CLA	C4B-CHC	2.77	1.47	1.40
24	b	604	CLA	C4B-CHC	2.77	1.47	1.40
24	B	613	CLA	C1C-C2C	2.77	1.49	1.44
24	A	409	CLA	C1B-CHB	2.77	1.47	1.40
24	C	503	CLA	C4B-CHC	2.77	1.47	1.40
24	B	607	CLA	C1C-C2C	2.78	1.49	1.44
24	B	605	CLA	C1C-C2C	2.78	1.49	1.44
24	a	404	CLA	C1B-CHB	2.78	1.47	1.40
24	C	510	CLA	C1C-C2C	2.78	1.49	1.44
24	A	406	CLA	C4B-CHC	2.78	1.47	1.40
24	B	613	CLA	C1B-CHB	2.79	1.47	1.40
25	a	406	PHO	CHD-C4C	2.79	1.47	1.40
24	B	614	CLA	C4B-CHC	2.79	1.47	1.40
24	c	503	CLA	C1B-CHB	2.79	1.47	1.40
24	b	604	CLA	C1B-CHB	2.80	1.47	1.40
24	C	502	CLA	C1B-CHB	2.80	1.47	1.40
24	B	606	CLA	C1C-C2C	2.80	1.49	1.44
24	c	508	CLA	C4B-CHC	2.80	1.47	1.40
25	a	406	PHO	C3B-C4B	2.80	1.49	1.43
24	B	607	CLA	C1B-CHB	2.80	1.47	1.40
24	b	613	CLA	C1C-C2C	2.80	1.50	1.44
24	C	512	CLA	C1B-CHB	2.81	1.47	1.40
24	A	404	CLA	C1C-C2C	2.82	1.50	1.44
24	C	513	CLA	C1C-C2C	2.82	1.50	1.44
24	C	508	CLA	C4B-CHC	2.82	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	C1B-CHB	2.83	1.47	1.40
24	c	509	CLA	C4B-CHC	2.83	1.47	1.40
24	C	514	CLA	C1B-CHB	2.83	1.47	1.40
24	b	614	CLA	C1B-CHB	2.83	1.47	1.40
24	c	504	CLA	C1B-CHB	2.84	1.47	1.40
24	c	510	CLA	C4B-CHC	2.84	1.47	1.40
25	A	407	PHO	OBD-CAD	2.84	1.27	1.22
24	C	511	CLA	C4B-CHC	2.84	1.47	1.40
24	b	612	CLA	C4B-CHC	2.84	1.47	1.40
24	c	503	CLA	C4B-CHC	2.85	1.47	1.40
24	b	610	CLA	C1B-CHB	2.85	1.47	1.40
25	A	407	PHO	CHC-C4B	2.86	1.47	1.40
25	a	406	PHO	CHB-C4A	2.86	1.47	1.40
24	D	403	CLA	C1B-CHB	2.86	1.47	1.40
24	b	611	CLA	C1B-CHB	2.86	1.47	1.40
24	c	505	CLA	C4B-CHC	2.88	1.47	1.40
24	c	508	CLA	C1B-CHB	2.88	1.47	1.40
24	b	603	CLA	C1C-C2C	2.88	1.50	1.44
24	A	405	CLA	C1C-C2C	2.88	1.50	1.44
24	d	402	CLA	C1B-CHB	2.88	1.47	1.40
24	b	605	CLA	C1B-CHB	2.88	1.47	1.40
24	b	607	CLA	C1B-CHB	2.89	1.47	1.40
24	B	608	CLA	C1B-CHB	2.90	1.47	1.40
24	B	603	CLA	C4B-CHC	2.91	1.47	1.40
24	b	602	CLA	C1C-C2C	2.91	1.50	1.44
24	a	350	CLA	C4B-CHC	2.91	1.47	1.40
24	C	513	CLA	C4B-CHC	2.92	1.47	1.40
24	B	602	CLA	C1C-C2C	2.93	1.50	1.44
24	C	510	CLA	C1B-CHB	2.94	1.47	1.40
24	B	615	CLA	C4B-CHC	2.94	1.47	1.40
24	C	505	CLA	C1B-CHB	2.94	1.47	1.40
25	A	408	PHO	C3B-C4B	2.96	1.49	1.43
24	B	605	CLA	C1B-CHB	2.96	1.48	1.40
24	B	605	CLA	C4B-CHC	2.96	1.48	1.40
24	b	613	CLA	C4B-CHC	2.97	1.48	1.40
24	c	514	CLA	C4B-CHC	2.97	1.48	1.40
24	b	611	CLA	C4B-CHC	2.97	1.48	1.40
24	C	506	CLA	C1B-CHB	2.98	1.48	1.40
24	c	507	CLA	C1B-CHB	2.98	1.48	1.40
24	c	511	CLA	C1B-CHB	2.99	1.48	1.40
24	C	511	CLA	C1B-CHB	3.00	1.48	1.40
24	c	507	CLA	C1C-C2C	3.01	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	C4B-CHC	3.01	1.48	1.40
24	B	610	CLA	C1B-CHB	3.01	1.48	1.40
24	d	402	CLA	C4B-CHC	3.01	1.48	1.40
24	C	509	CLA	C1B-CHB	3.01	1.48	1.40
24	A	404	CLA	C4B-CHC	3.02	1.48	1.40
24	b	609	CLA	C1B-CHB	3.03	1.48	1.40
24	B	601	CLA	C4B-CHC	3.03	1.48	1.40
25	a	405	PHO	CHC-C4B	3.04	1.47	1.40
24	B	610	CLA	C4B-CHC	3.04	1.48	1.40
24	B	602	CLA	C4B-CHC	3.06	1.48	1.40
24	D	403	CLA	C4B-CHC	3.06	1.48	1.40
24	B	612	CLA	C1B-CHB	3.07	1.48	1.40
24	C	502	CLA	C4B-CHC	3.08	1.48	1.40
24	b	612	CLA	C1B-CHB	3.08	1.48	1.40
24	c	512	CLA	C1B-CHB	3.09	1.48	1.40
24	c	513	CLA	C1B-CHB	3.11	1.48	1.40
24	A	405	CLA	C4B-CHC	3.13	1.48	1.40
24	b	602	CLA	C4B-CHC	3.14	1.48	1.40
25	A	407	PHO	CHD-C4C	3.15	1.48	1.40
25	a	405	PHO	OBD-CAD	3.17	1.28	1.22
24	B	604	CLA	C1B-CHB	3.19	1.48	1.40
24	C	506	CLA	C1C-C2C	3.20	1.50	1.44
24	d	403	CLA	C4B-CHC	3.24	1.48	1.40
25	A	408	PHO	CHC-C4B	3.28	1.48	1.40
25	a	406	PHO	CHC-C4B	3.35	1.48	1.40
36	H	102	DGD	O2G-C1B	3.37	1.44	1.34
25	a	405	PHO	O2A-CGA	3.39	1.43	1.33
25	A	408	PHO	O2A-CGA	3.40	1.43	1.33
24	b	610	CLA	C4B-CHC	3.40	1.49	1.40
33	b	621	LMG	O7-C10	3.40	1.44	1.34
24	B	605	CLA	OBD-CAD	3.42	1.27	1.22
27	A	411	SQD	O47-C7	3.43	1.44	1.34
24	A	404	CLA	O2A-CGA	3.44	1.43	1.33
24	B	611	CLA	O2A-CGA	3.47	1.43	1.33
38	d	407	LHG	O7-C7	3.47	1.44	1.34
38	d	406	LHG	O7-C7	3.49	1.44	1.34
24	b	606	CLA	OBD-CAD	3.50	1.27	1.22
36	C	519	DGD	O2G-C1B	3.50	1.44	1.34
38	D	357	LHG	O7-C7	3.54	1.44	1.34
24	b	610	CLA	O2A-CGA	3.55	1.43	1.33
24	a	403	CLA	O2A-CGA	3.57	1.43	1.33
25	a	405	PHO	C3D-C2D	3.58	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	D	406	LHG	O7-C7	3.58	1.44	1.34
36	c	520	DGD	O2G-C1B	3.58	1.44	1.34
38	D	406	LHG	O8-C23	3.58	1.43	1.33
24	b	612	CLA	OBD-CAD	3.59	1.27	1.22
24	B	606	CLA	OBD-CAD	3.61	1.27	1.22
24	D	402	CLA	OBD-CAD	3.61	1.27	1.22
38	L	101	LHG	O7-C7	3.61	1.44	1.34
36	c	519	DGD	O2G-C1B	3.62	1.44	1.34
33	J	101	LMG	O7-C10	3.62	1.44	1.34
24	B	610	CLA	O2A-CGA	3.63	1.44	1.33
36	C	517	DGD	O1G-C1A	3.64	1.44	1.33
24	B	604	CLA	O2A-CGA	3.65	1.44	1.33
24	B	609	CLA	OBD-CAD	3.65	1.27	1.22
24	a	407	CLA	OBD-CAD	3.66	1.27	1.22
38	D	407	LHG	O7-C7	3.68	1.45	1.34
24	C	506	CLA	C3D-C2D	3.69	1.47	1.39
24	B	602	CLA	O2A-CGA	3.69	1.44	1.33
24	b	605	CLA	O2A-CGA	3.69	1.44	1.33
24	B	612	CLA	O2A-CGA	3.69	1.44	1.33
38	l	101	LHG	O7-C7	3.70	1.45	1.34
36	c	518	DGD	O2G-C1B	3.70	1.45	1.34
25	A	407	PHO	C3D-C2D	3.70	1.48	1.38
24	B	605	CLA	O2A-CGA	3.71	1.44	1.33
24	A	406	CLA	O2A-CGA	3.71	1.44	1.33
25	a	406	PHO	OBD-CAD	3.71	1.29	1.22
36	C	518	DGD	O2G-C1B	3.71	1.45	1.34
38	d	407	LHG	O8-C23	3.72	1.44	1.33
25	A	408	PHO	OBD-CAD	3.74	1.29	1.22
24	C	504	CLA	O2A-CGA	3.75	1.44	1.33
36	C	517	DGD	O2G-C1B	3.76	1.45	1.34
24	b	611	CLA	OBD-CAD	3.76	1.27	1.22
24	C	505	CLA	O2A-CGA	3.76	1.44	1.33
24	B	614	CLA	O2A-CGA	3.76	1.44	1.33
24	D	403	CLA	O2A-CGA	3.77	1.44	1.33
25	A	408	PHO	C3D-C2D	3.77	1.48	1.38
33	B	621	LMG	O7-C10	3.78	1.45	1.34
24	c	512	CLA	O2A-CGA	3.78	1.44	1.33
24	b	603	CLA	O2A-CGA	3.78	1.44	1.33
38	d	406	LHG	O8-C23	3.79	1.44	1.33
24	B	614	CLA	OBD-CAD	3.79	1.27	1.22
24	b	613	CLA	OBD-CAD	3.80	1.27	1.22
36	h	103	DGD	O2G-C1B	3.80	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	407	PHO	O2A-CGA	3.81	1.44	1.33
24	C	506	CLA	O2A-CGA	3.81	1.44	1.33
24	b	612	CLA	CHC-C1C	3.82	1.46	1.35
38	D	357	LHG	O8-C23	3.83	1.44	1.33
38	d	408	LHG	O8-C23	3.83	1.44	1.33
27	a	409	SQD	O47-C7	3.83	1.45	1.34
33	j	101	LMG	O7-C10	3.83	1.45	1.34
33	J	101	LMG	O8-C28	3.84	1.44	1.33
24	C	510	CLA	O2A-CGA	3.84	1.44	1.33
24	D	402	CLA	O2A-CGA	3.85	1.44	1.33
24	B	608	CLA	O2A-CGA	3.86	1.44	1.33
24	b	610	CLA	C3D-C2D	3.86	1.48	1.39
24	b	605	CLA	CHC-C1C	3.86	1.46	1.35
38	E	101	LHG	O7-C7	3.87	1.45	1.34
24	b	604	CLA	O2A-CGA	3.87	1.44	1.33
33	c	521	LMG	O7-C10	3.88	1.45	1.34
36	H	102	DGD	O1G-C1A	3.88	1.44	1.33
24	B	604	CLA	C3D-C2D	3.89	1.48	1.39
24	B	608	CLA	OBD-CAD	3.89	1.28	1.22
24	A	405	CLA	OBD-CAD	3.89	1.28	1.22
24	C	505	CLA	OBD-CAD	3.90	1.28	1.22
38	D	407	LHG	O8-C23	3.90	1.44	1.33
24	c	504	CLA	O2A-CGA	3.90	1.44	1.33
24	C	511	CLA	O2A-CGA	3.90	1.44	1.33
25	a	406	PHO	C3D-C2D	3.90	1.49	1.38
24	B	603	CLA	OBD-CAD	3.90	1.28	1.22
24	C	507	CLA	CHC-C1C	3.90	1.46	1.35
24	b	612	CLA	O2A-CGA	3.91	1.44	1.33
24	a	404	CLA	O2A-CGA	3.91	1.44	1.33
33	z	101	LMG	O7-C10	3.91	1.45	1.34
24	c	505	CLA	O2A-CGA	3.91	1.44	1.33
33	A	418	LMG	O7-C10	3.91	1.45	1.34
33	a	417	LMG	O7-C10	3.92	1.45	1.34
24	D	402	CLA	CHC-C1C	3.92	1.46	1.35
24	B	603	CLA	O2A-CGA	3.93	1.44	1.33
33	j	101	LMG	O8-C28	3.93	1.44	1.33
24	c	508	CLA	O2A-CGA	3.93	1.44	1.33
24	B	613	CLA	O2A-CGA	3.93	1.44	1.33
24	b	607	CLA	O2A-CGA	3.94	1.44	1.33
24	d	402	CLA	O2A-CGA	3.94	1.44	1.33
24	B	616	CLA	O2A-CGA	3.94	1.44	1.33
24	c	507	CLA	C3D-C2D	3.94	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	OBD-CAD	3.94	1.28	1.22
24	b	616	CLA	OBD-CAD	3.95	1.28	1.22
27	a	411	SQD	O47-C7	3.95	1.45	1.34
24	b	605	CLA	OBD-CAD	3.96	1.28	1.22
36	C	519	DGD	O1G-C1A	3.97	1.45	1.33
24	A	409	CLA	OBD-CAD	3.97	1.28	1.22
24	c	507	CLA	O2A-CGA	3.97	1.45	1.33
24	b	607	CLA	CHC-C1C	3.97	1.46	1.35
24	c	507	CLA	OBD-CAD	3.97	1.28	1.22
27	a	409	SQD	O48-C23	3.98	1.45	1.33
24	C	507	CLA	OBD-CAD	3.98	1.28	1.22
27	F	101	SQD	O48-C23	3.99	1.45	1.33
24	b	609	CLA	O2A-CGA	3.99	1.45	1.33
24	D	402	CLA	C3D-C2D	3.99	1.48	1.39
24	B	606	CLA	O2A-CGA	3.99	1.45	1.33
36	C	518	DGD	O1G-C1A	3.99	1.45	1.33
33	C	520	LMG	O7-C10	3.99	1.45	1.34
24	C	506	CLA	OBD-CAD	4.00	1.28	1.22
24	b	613	CLA	O2A-CGA	4.00	1.45	1.33
36	c	520	DGD	O1G-C1A	4.01	1.45	1.33
25	a	406	PHO	O2A-CGA	4.01	1.45	1.33
24	d	402	CLA	OBD-CAD	4.01	1.28	1.22
24	c	506	CLA	O2A-CGA	4.02	1.45	1.33
24	A	409	CLA	O2A-CGA	4.02	1.45	1.33
24	b	607	CLA	OBD-CAD	4.02	1.28	1.22
24	c	505	CLA	OBD-CAD	4.03	1.28	1.22
27	A	413	SQD	O47-C7	4.03	1.46	1.34
24	C	503	CLA	O2A-CGA	4.04	1.45	1.33
24	b	616	CLA	O2A-CGA	4.04	1.45	1.33
24	B	607	CLA	O2A-CGA	4.04	1.45	1.33
38	d	408	LHG	O7-C7	4.04	1.46	1.34
24	C	511	CLA	C3D-C2D	4.04	1.48	1.39
36	c	518	DGD	O1G-C1A	4.05	1.45	1.33
27	B	620	SQD	O47-C7	4.05	1.46	1.34
38	L	101	LHG	O8-C23	4.05	1.45	1.33
24	B	614	CLA	C3D-C2D	4.06	1.48	1.39
24	c	506	CLA	CHC-C1C	4.06	1.47	1.35
24	B	612	CLA	CHC-C1C	4.06	1.47	1.35
24	B	613	CLA	OBD-CAD	4.07	1.28	1.22
24	b	606	CLA	O2A-CGA	4.07	1.45	1.33
24	b	611	CLA	O2A-CGA	4.07	1.45	1.33
24	C	507	CLA	O2A-CGA	4.07	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	CHC-C1C	4.07	1.47	1.35
24	b	608	CLA	O2A-CGA	4.07	1.45	1.33
27	b	620	SQD	O47-C7	4.08	1.46	1.34
24	C	502	CLA	O2D-CGD	4.08	1.43	1.33
38	l	101	LHG	O8-C23	4.08	1.45	1.33
24	b	601	CLA	CHC-C1C	4.09	1.47	1.35
24	B	608	CLA	CHC-C1C	4.09	1.47	1.35
24	B	615	CLA	O2A-CGA	4.09	1.45	1.33
24	B	607	CLA	C3D-C2D	4.09	1.48	1.39
24	B	607	CLA	CHC-C1C	4.09	1.47	1.35
24	B	612	CLA	OBD-CAD	4.09	1.28	1.22
38	a	419	LHG	O7-C7	4.09	1.46	1.34
24	d	403	CLA	O2D-CGD	4.09	1.43	1.33
33	A	418	LMG	O8-C28	4.09	1.45	1.33
24	B	613	CLA	CHC-C1C	4.09	1.47	1.35
24	C	509	CLA	O2A-CGA	4.10	1.45	1.33
24	B	603	CLA	CHC-C1C	4.10	1.47	1.35
24	a	403	CLA	OBD-CAD	4.10	1.28	1.22
27	b	620	SQD	O48-C23	4.10	1.45	1.33
24	a	403	CLA	CHC-C1C	4.11	1.47	1.35
24	b	602	CLA	O2A-CGA	4.11	1.45	1.33
24	C	508	CLA	O2A-CGA	4.11	1.45	1.33
33	b	621	LMG	O8-C28	4.11	1.45	1.33
24	B	603	CLA	C3D-C2D	4.12	1.48	1.39
36	c	519	DGD	O1G-C1A	4.12	1.45	1.33
36	h	103	DGD	O1G-C1A	4.12	1.45	1.33
24	A	409	CLA	CHC-C1C	4.12	1.47	1.35
33	a	417	LMG	O8-C28	4.12	1.45	1.33
24	b	604	CLA	OBD-CAD	4.13	1.28	1.22
27	A	411	SQD	O48-C23	4.13	1.45	1.33
24	c	510	CLA	O2A-CGA	4.13	1.45	1.33
24	c	503	CLA	O2A-CGA	4.13	1.45	1.33
24	B	614	CLA	CHC-C1C	4.14	1.47	1.35
24	c	504	CLA	C3D-C2D	4.14	1.48	1.39
24	C	502	CLA	O2A-CGA	4.14	1.45	1.33
27	f	101	SQD	O48-C23	4.15	1.45	1.33
24	C	511	CLA	OBD-CAD	4.15	1.28	1.22
24	A	405	CLA	O2A-CGA	4.15	1.45	1.33
24	B	607	CLA	O2D-CGD	4.15	1.43	1.33
24	c	511	CLA	OBD-CAD	4.15	1.28	1.22
24	c	509	CLA	O2A-CGA	4.15	1.45	1.33
24	C	505	CLA	CHC-C1C	4.16	1.47	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	OBD-CAD	4.16	1.28	1.22
24	C	507	CLA	C3D-C2D	4.16	1.48	1.39
27	B	620	SQD	O48-C23	4.16	1.45	1.33
24	b	607	CLA	C3D-C2D	4.16	1.48	1.39
24	a	407	CLA	O2A-CGA	4.16	1.45	1.33
24	C	504	CLA	C3D-C2D	4.16	1.48	1.39
24	b	614	CLA	O2A-CGA	4.17	1.45	1.33
24	b	608	CLA	CHC-C1C	4.17	1.47	1.35
24	a	350	CLA	OBD-CAD	4.17	1.28	1.22
24	b	602	CLA	OBD-CAD	4.17	1.28	1.22
24	B	611	CLA	CHC-C1C	4.17	1.47	1.35
33	Z	101	LMG	O7-C10	4.17	1.46	1.34
24	c	504	CLA	CHC-C1C	4.18	1.47	1.35
24	b	606	CLA	CHC-C1C	4.18	1.47	1.35
24	c	503	CLA	OBD-CAD	4.18	1.28	1.22
24	c	513	CLA	O2A-CGA	4.18	1.45	1.33
24	c	512	CLA	CHC-C1C	4.18	1.47	1.35
24	B	602	CLA	OBD-CAD	4.18	1.28	1.22
24	c	511	CLA	O2A-CGA	4.19	1.45	1.33
24	C	512	CLA	O2A-CGA	4.19	1.45	1.33
24	C	504	CLA	OBD-CAD	4.19	1.28	1.22
24	c	507	CLA	CHC-C1C	4.20	1.47	1.35
24	B	615	CLA	CHC-C1C	4.20	1.47	1.35
24	b	613	CLA	CHC-C1C	4.21	1.47	1.35
24	a	350	CLA	O2A-CGA	4.21	1.45	1.33
24	b	614	CLA	CHC-C1C	4.21	1.47	1.35
24	c	514	CLA	O2A-CGA	4.21	1.45	1.33
30	a	413[B]	OEY	O4-MN3	4.21	1.99	1.90
24	b	614	CLA	OBD-CAD	4.21	1.28	1.22
24	b	606	CLA	O2D-CGD	4.21	1.43	1.33
24	c	515	CLA	CHC-C1C	4.21	1.47	1.35
24	c	515	CLA	O2A-CGA	4.22	1.45	1.33
24	b	604	CLA	O2D-CGD	4.22	1.43	1.33
24	c	512	CLA	C3D-C2D	4.22	1.49	1.39
24	c	515	CLA	OBD-CAD	4.22	1.28	1.22
24	C	505	CLA	C3D-C2D	4.22	1.49	1.39
33	B	621	LMG	O8-C28	4.22	1.45	1.33
24	b	604	CLA	C3D-C2D	4.23	1.49	1.39
24	d	403	CLA	O2A-CGA	4.23	1.45	1.33
33	c	522	LMG	O7-C10	4.23	1.46	1.34
24	C	508	CLA	OBD-CAD	4.23	1.28	1.22
24	C	514	CLA	O2A-CGA	4.23	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	O2A-CGA	4.23	1.45	1.33
24	b	609	CLA	C3D-C2D	4.23	1.49	1.39
24	b	605	CLA	C3D-C2D	4.23	1.49	1.39
24	b	609	CLA	CHC-C1C	4.24	1.47	1.35
24	c	512	CLA	OBD-CAD	4.24	1.28	1.22
24	B	606	CLA	O2D-CGD	4.24	1.43	1.33
24	B	612	CLA	C3D-C2D	4.24	1.49	1.39
24	C	510	CLA	CHC-C1C	4.24	1.47	1.35
24	c	509	CLA	CHC-C1C	4.24	1.47	1.35
24	c	511	CLA	CHC-C1C	4.25	1.47	1.35
24	C	509	CLA	CHC-C1C	4.25	1.47	1.35
24	c	508	CLA	CHC-C1C	4.25	1.47	1.35
24	d	402	CLA	CHC-C1C	4.25	1.47	1.35
24	b	603	CLA	CHC-C1C	4.25	1.47	1.35
24	a	407	CLA	CHC-C1C	4.25	1.47	1.35
24	A	404	CLA	CHC-C1C	4.26	1.47	1.35
24	C	502	CLA	C3D-C2D	4.26	1.49	1.39
33	C	520	LMG	O8-C28	4.26	1.45	1.33
27	A	413	SQD	O48-C23	4.26	1.45	1.33
24	C	510	CLA	C3D-C2D	4.27	1.49	1.39
24	b	610	CLA	O2D-CGD	4.27	1.44	1.33
33	c	522	LMG	O8-C28	4.27	1.45	1.33
33	c	521	LMG	O8-C28	4.27	1.45	1.33
24	C	504	CLA	CHC-C1C	4.27	1.47	1.35
24	D	403	CLA	C3D-C2D	4.27	1.49	1.39
24	b	611	CLA	CHC-C1C	4.27	1.47	1.35
33	C	521	LMG	O7-C10	4.28	1.46	1.34
24	C	512	CLA	CHC-C1C	4.28	1.47	1.35
24	B	609	CLA	O2A-CGA	4.28	1.45	1.33
38	a	419	LHG	O8-C23	4.28	1.45	1.33
38	E	101	LHG	O8-C23	4.28	1.45	1.33
27	f	101	SQD	O47-C7	4.29	1.46	1.34
24	c	505	CLA	C3D-C2D	4.29	1.49	1.39
24	B	614	CLA	O2D-CGD	4.29	1.44	1.33
24	b	615	CLA	CHC-C1C	4.29	1.47	1.35
24	A	404	CLA	OBD-CAD	4.29	1.28	1.22
24	D	403	CLA	OBD-CAD	4.29	1.28	1.22
24	b	606	CLA	C3D-C2D	4.29	1.49	1.39
24	B	601	CLA	OBD-CAD	4.30	1.28	1.22
24	A	404	CLA	C3D-C2D	4.30	1.49	1.39
25	A	408	PHO	CHD-C1D	4.30	1.47	1.38
24	c	513	CLA	C3D-C2D	4.30	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	O2D-CGD	4.31	1.44	1.33
24	B	609	CLA	CHC-C1C	4.31	1.47	1.35
24	c	513	CLA	CHC-C1C	4.32	1.47	1.35
24	B	606	CLA	CHC-C1C	4.32	1.47	1.35
24	C	512	CLA	OBD-CAD	4.32	1.28	1.22
25	a	405	PHO	O2D-CGD	4.32	1.44	1.33
24	B	604	CLA	OBD-CAD	4.32	1.28	1.22
24	B	606	CLA	C3D-C2D	4.33	1.49	1.39
24	a	350	CLA	CHC-C1C	4.33	1.48	1.35
24	b	603	CLA	C3D-C2D	4.33	1.49	1.39
24	c	510	CLA	CHC-C1C	4.33	1.48	1.35
25	a	405	PHO	CHD-C1D	4.34	1.47	1.38
24	C	508	CLA	O2D-CGD	4.34	1.44	1.33
24	B	611	CLA	OBD-CAD	4.34	1.28	1.22
24	b	611	CLA	C3D-C2D	4.34	1.49	1.39
24	B	616	CLA	OBD-CAD	4.34	1.28	1.22
24	a	403	CLA	C3D-C2D	4.34	1.49	1.39
24	c	503	CLA	CHC-C1C	4.34	1.48	1.35
24	B	604	CLA	CHC-C1C	4.35	1.48	1.35
24	B	603	CLA	O2D-CGD	4.35	1.44	1.33
24	b	610	CLA	OBD-CAD	4.35	1.28	1.22
24	A	409	CLA	C3D-C2D	4.35	1.49	1.39
24	c	505	CLA	CHC-C1C	4.36	1.48	1.35
24	b	612	CLA	C3D-C2D	4.36	1.49	1.39
24	C	509	CLA	OBD-CAD	4.36	1.28	1.22
25	a	405	PHO	CHC-C1C	4.36	1.47	1.38
24	A	406	CLA	OBD-CAD	4.36	1.28	1.22
24	C	514	CLA	OBD-CAD	4.36	1.28	1.22
24	c	514	CLA	OBD-CAD	4.37	1.28	1.22
24	C	502	CLA	CHC-C1C	4.37	1.48	1.35
24	A	405	CLA	CHC-C1C	4.37	1.48	1.35
24	A	404	CLA	O2D-CGD	4.38	1.44	1.33
24	C	514	CLA	CHC-C1C	4.38	1.48	1.35
27	a	411	SQD	O48-C23	4.38	1.46	1.33
24	a	404	CLA	CHC-C1C	4.38	1.48	1.35
24	b	615	CLA	C3D-C2D	4.38	1.49	1.39
24	d	402	CLA	C3D-C2D	4.39	1.49	1.39
24	B	610	CLA	O2D-CGD	4.39	1.44	1.33
24	b	602	CLA	C3D-C2D	4.39	1.49	1.39
25	A	408	PHO	CHB-C1B	4.39	1.47	1.38
24	B	610	CLA	CHC-C1C	4.39	1.48	1.35
24	b	604	CLA	CHC-C1C	4.39	1.48	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	503	CLA	CHC-C1C	4.39	1.48	1.35
24	b	601	CLA	OBD-CAD	4.40	1.28	1.22
24	c	514	CLA	CHC-C1C	4.40	1.48	1.35
24	B	613	CLA	C3D-C2D	4.40	1.49	1.39
24	B	608	CLA	C3D-C2D	4.40	1.49	1.39
24	B	616	CLA	O2D-CGD	4.40	1.44	1.33
24	b	616	CLA	C3D-C2D	4.41	1.49	1.39
24	b	615	CLA	O2A-CGA	4.41	1.46	1.33
33	C	521	LMG	O8-C28	4.42	1.46	1.33
24	C	503	CLA	OBD-CAD	4.42	1.28	1.22
24	b	610	CLA	CHC-C1C	4.42	1.48	1.35
24	b	614	CLA	C3D-C2D	4.42	1.49	1.39
24	A	406	CLA	CHC-C1C	4.43	1.48	1.35
24	C	504	CLA	O2D-CGD	4.43	1.44	1.33
24	c	509	CLA	C3D-C2D	4.43	1.49	1.39
24	b	616	CLA	CHC-C1C	4.44	1.48	1.35
24	C	513	CLA	OBD-CAD	4.44	1.28	1.22
24	C	503	CLA	C3D-C2D	4.45	1.49	1.39
24	B	615	CLA	OBD-CAD	4.45	1.28	1.22
24	C	506	CLA	CHC-C1C	4.45	1.48	1.35
24	b	615	CLA	O2D-CGD	4.45	1.44	1.33
24	d	403	CLA	OBD-CAD	4.45	1.28	1.22
33	z	101	LMG	O8-C28	4.45	1.46	1.33
24	B	612	CLA	O2D-CGD	4.45	1.44	1.33
24	c	510	CLA	OBD-CAD	4.46	1.28	1.22
24	B	604	CLA	O2D-CGD	4.46	1.44	1.33
24	a	404	CLA	OBD-CAD	4.46	1.28	1.22
24	B	601	CLA	CHC-C1C	4.46	1.48	1.35
24	B	611	CLA	C3D-C2D	4.47	1.49	1.39
24	c	506	CLA	C3D-C2D	4.47	1.49	1.39
27	F	101	SQD	O47-C7	4.47	1.47	1.34
24	b	607	CLA	O2D-CGD	4.47	1.44	1.33
24	C	513	CLA	CHC-C1C	4.48	1.48	1.35
24	B	615	CLA	C3D-C2D	4.48	1.49	1.39
24	d	403	CLA	C3D-C2D	4.49	1.49	1.39
24	B	605	CLA	C3D-C2D	4.49	1.49	1.39
24	b	608	CLA	C3D-C2D	4.49	1.49	1.39
24	c	513	CLA	O2D-CGD	4.49	1.44	1.33
24	c	503	CLA	C3D-C2D	4.49	1.49	1.39
24	C	513	CLA	C3D-C2D	4.50	1.49	1.39
24	D	403	CLA	CHC-C1C	4.50	1.48	1.35
24	b	608	CLA	OBD-CAD	4.50	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	OBD-CAD	4.50	1.28	1.22
24	C	510	CLA	O2D-CGD	4.51	1.44	1.33
24	B	601	CLA	C3D-C2D	4.51	1.49	1.39
24	b	615	CLA	OBD-CAD	4.51	1.28	1.22
24	B	601	CLA	O2A-CGA	4.51	1.46	1.33
24	D	402	CLA	O2D-CGD	4.51	1.44	1.33
24	C	513	CLA	O2D-CGD	4.51	1.44	1.33
24	c	509	CLA	OBD-CAD	4.51	1.28	1.22
24	d	402	CLA	O2D-CGD	4.51	1.44	1.33
24	B	616	CLA	C3D-C2D	4.52	1.49	1.39
24	c	505	CLA	O2D-CGD	4.52	1.44	1.33
24	a	407	CLA	O2D-CGD	4.52	1.44	1.33
24	c	503	CLA	O2D-CGD	4.52	1.44	1.33
24	a	404	CLA	O2D-CGD	4.53	1.44	1.33
24	c	511	CLA	C3D-C2D	4.55	1.49	1.39
24	b	609	CLA	OBD-CAD	4.56	1.28	1.22
24	a	407	CLA	C3D-C2D	4.56	1.49	1.39
24	C	509	CLA	O2D-CGD	4.56	1.44	1.33
24	b	611	CLA	O2D-CGD	4.56	1.44	1.33
24	b	612	CLA	O2D-CGD	4.56	1.44	1.33
24	C	511	CLA	CHC-C1C	4.56	1.48	1.35
24	C	508	CLA	C3D-C2D	4.57	1.49	1.39
24	b	614	CLA	O2D-CGD	4.57	1.44	1.33
25	A	408	PHO	O2D-CGD	4.57	1.44	1.33
24	B	616	CLA	CHC-C1C	4.58	1.48	1.35
24	A	405	CLA	O2D-CGD	4.58	1.44	1.33
24	B	602	CLA	C3D-C2D	4.58	1.49	1.39
24	b	601	CLA	O2A-CGA	4.58	1.46	1.33
24	B	609	CLA	C3D-C2D	4.58	1.49	1.39
24	C	514	CLA	O2D-CGD	4.59	1.44	1.33
24	c	514	CLA	O2D-CGD	4.59	1.44	1.33
25	A	407	PHO	CHC-C1C	4.60	1.47	1.38
25	a	405	PHO	CHB-C1B	4.61	1.47	1.38
24	C	514	CLA	C3D-C2D	4.61	1.49	1.39
24	a	404	CLA	C3D-C2D	4.61	1.49	1.39
24	B	615	CLA	O2D-CGD	4.62	1.44	1.33
24	c	515	CLA	C3D-C2D	4.62	1.49	1.39
24	c	514	CLA	C3D-C2D	4.62	1.49	1.39
24	C	506	CLA	O2D-CGD	4.62	1.44	1.33
24	B	605	CLA	CHC-C1C	4.62	1.48	1.35
24	c	510	CLA	C3D-C2D	4.62	1.49	1.39
24	b	608	CLA	O2D-CGD	4.63	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	513	CLA	OBD-CAD	4.63	1.29	1.22
24	A	406	CLA	C3D-C2D	4.64	1.49	1.39
25	A	407	PHO	O2D-CGD	4.64	1.45	1.33
24	c	512	CLA	O2D-CGD	4.65	1.45	1.33
24	d	403	CLA	CHC-C1C	4.66	1.48	1.35
24	c	509	CLA	O2D-CGD	4.66	1.45	1.33
24	B	610	CLA	C3D-C2D	4.67	1.50	1.39
24	B	608	CLA	O2D-CGD	4.67	1.45	1.33
24	b	603	CLA	O2D-CGD	4.67	1.45	1.33
25	A	407	PHO	CHD-C1D	4.69	1.47	1.38
24	c	508	CLA	OBD-CAD	4.69	1.29	1.22
24	b	602	CLA	O2D-CGD	4.69	1.45	1.33
24	B	602	CLA	O2D-CGD	4.70	1.45	1.33
24	C	512	CLA	C3C-C2C	4.70	1.46	1.36
24	c	515	CLA	O2D-CGD	4.70	1.45	1.33
24	C	503	CLA	O2D-CGD	4.70	1.45	1.33
24	b	605	CLA	O2D-CGD	4.71	1.45	1.33
24	a	350	CLA	C3D-C2D	4.71	1.50	1.39
24	D	403	CLA	O2D-CGD	4.71	1.45	1.33
24	C	505	CLA	O2D-CGD	4.71	1.45	1.33
24	C	509	CLA	C3D-C2D	4.72	1.50	1.39
24	C	510	CLA	OBD-CAD	4.72	1.29	1.22
24	B	602	CLA	CHC-C1C	4.73	1.49	1.35
25	A	407	PHO	CHB-C1B	4.73	1.48	1.38
24	c	504	CLA	O2D-CGD	4.75	1.45	1.33
24	c	508	CLA	C3D-C2D	4.75	1.50	1.39
24	B	613	CLA	C3C-C2C	4.76	1.46	1.36
24	b	601	CLA	C3D-C2D	4.76	1.50	1.39
24	B	605	CLA	O2D-CGD	4.76	1.45	1.33
24	A	405	CLA	C3D-C2D	4.77	1.50	1.39
24	b	602	CLA	CHC-C1C	4.77	1.49	1.35
24	b	603	CLA	OBD-CAD	4.78	1.29	1.22
24	C	511	CLA	O2D-CGD	4.79	1.45	1.33
24	b	613	CLA	C3D-C2D	4.79	1.50	1.39
24	C	512	CLA	C3D-C2D	4.80	1.50	1.39
24	B	612	CLA	C3C-C2C	4.80	1.47	1.36
24	A	409	CLA	O2D-CGD	4.80	1.45	1.33
24	b	609	CLA	C3C-C2C	4.81	1.47	1.36
24	A	406	CLA	O2D-CGD	4.82	1.45	1.33
25	A	408	PHO	CHC-C1C	4.82	1.48	1.38
24	b	609	CLA	O2D-CGD	4.83	1.45	1.33
24	c	506	CLA	OBD-CAD	4.83	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	350	CLA	O2D-CGD	4.84	1.45	1.33
24	d	402	CLA	C3C-C2C	4.84	1.47	1.36
24	B	613	CLA	O2D-CGD	4.84	1.45	1.33
24	c	506	CLA	O2D-CGD	4.85	1.45	1.33
24	B	606	CLA	C3C-C2C	4.85	1.47	1.36
24	a	403	CLA	O2D-CGD	4.86	1.45	1.33
24	b	601	CLA	O2D-CGD	4.86	1.45	1.33
24	B	610	CLA	OBD-CAD	4.88	1.29	1.22
24	b	614	CLA	C3C-C2C	4.88	1.47	1.36
24	C	512	CLA	O2D-CGD	4.88	1.45	1.33
24	C	507	CLA	O2D-CGD	4.89	1.45	1.33
24	c	508	CLA	O2D-CGD	4.89	1.45	1.33
24	a	403	CLA	C3C-C2C	4.93	1.47	1.36
24	B	609	CLA	O2D-CGD	4.93	1.45	1.33
24	b	616	CLA	O2D-CGD	4.95	1.45	1.33
24	C	506	CLA	C3C-C2C	4.95	1.47	1.36
24	c	511	CLA	O2D-CGD	4.95	1.45	1.33
24	B	601	CLA	O2D-CGD	4.95	1.45	1.33
24	c	507	CLA	O2D-CGD	4.95	1.45	1.33
24	c	506	CLA	C3C-C2C	4.95	1.47	1.36
24	b	613	CLA	O2D-CGD	4.96	1.45	1.33
25	a	406	PHO	O2D-CGD	4.97	1.45	1.33
24	C	503	CLA	C3C-C2C	4.97	1.47	1.36
25	a	406	PHO	CHD-C1D	4.99	1.48	1.38
24	B	614	CLA	C3C-C2C	5.00	1.47	1.36
24	A	404	CLA	C3C-C2C	5.01	1.47	1.36
24	B	615	CLA	C3B-C2B	5.01	1.47	1.40
24	B	609	CLA	C3C-C2C	5.01	1.47	1.36
25	a	406	PHO	CHB-C1B	5.01	1.48	1.38
24	C	507	CLA	C3C-C2C	5.02	1.47	1.36
24	b	604	CLA	C3C-C2C	5.03	1.47	1.36
24	d	403	CLA	C3C-C2C	5.04	1.47	1.36
24	C	505	CLA	C3C-C2C	5.05	1.47	1.36
24	C	504	CLA	C3C-C2C	5.07	1.47	1.36
24	B	607	CLA	C3C-C2C	5.07	1.47	1.36
24	c	504	CLA	C3C-C2C	5.07	1.47	1.36
24	A	405	CLA	C3C-C2C	5.08	1.47	1.36
24	D	402	CLA	C3C-C2C	5.08	1.47	1.36
24	a	407	CLA	C3C-C2C	5.10	1.47	1.36
24	B	604	CLA	C3C-C2C	5.11	1.47	1.36
24	D	403	CLA	C3C-C2C	5.11	1.47	1.36
24	c	507	CLA	C3C-C2C	5.13	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3C-C2C	5.13	1.47	1.36
24	c	505	CLA	C3C-C2C	5.14	1.47	1.36
24	B	611	CLA	C3C-C2C	5.15	1.47	1.36
24	B	605	CLA	C3C-C2C	5.16	1.47	1.36
24	B	615	CLA	C3C-C2C	5.16	1.47	1.36
24	a	404	CLA	C3C-C2C	5.18	1.47	1.36
24	c	512	CLA	C3C-C2C	5.19	1.47	1.36
24	C	514	CLA	C3C-C2C	5.19	1.47	1.36
24	B	603	CLA	C3C-C2C	5.19	1.47	1.36
24	c	510	CLA	O2D-CGD	5.20	1.46	1.33
24	c	509	CLA	C3C-C2C	5.22	1.47	1.36
24	b	607	CLA	C3C-C2C	5.22	1.47	1.36
24	c	511	CLA	C3C-C2C	5.23	1.47	1.36
24	c	515	CLA	C3C-C2C	5.23	1.48	1.36
24	B	602	CLA	C3C-C2C	5.23	1.48	1.36
24	c	513	CLA	C3C-C2C	5.24	1.48	1.36
24	b	608	CLA	C3C-C2C	5.27	1.48	1.36
25	A	407	PHO	C3C-C2C	5.29	1.48	1.36
25	a	406	PHO	CHC-C1C	5.29	1.49	1.38
24	A	409	CLA	C3C-C2C	5.29	1.48	1.36
24	C	511	CLA	C3C-C2C	5.29	1.48	1.36
24	b	601	CLA	C3C-C2C	5.30	1.48	1.36
24	B	608	CLA	C3C-C2C	5.30	1.48	1.36
24	C	508	CLA	C3C-C2C	5.30	1.48	1.36
24	A	406	CLA	C3C-C2C	5.30	1.48	1.36
24	b	612	CLA	C3C-C2C	5.30	1.48	1.36
24	C	510	CLA	C3C-C2C	5.32	1.48	1.36
24	c	508	CLA	C3C-C2C	5.32	1.48	1.36
24	b	611	CLA	C3C-C2C	5.32	1.48	1.36
24	C	502	CLA	C3C-C2C	5.34	1.48	1.36
24	b	602	CLA	C3C-C2C	5.34	1.48	1.36
24	B	607	CLA	C3B-C2B	5.35	1.47	1.40
24	A	406	CLA	C3B-C2B	5.35	1.47	1.40
24	B	605	CLA	C3B-C2B	5.35	1.47	1.40
24	B	616	CLA	C3C-C2C	5.35	1.48	1.36
24	b	606	CLA	C3C-C2C	5.37	1.48	1.36
24	b	605	CLA	C3C-C2C	5.39	1.48	1.36
24	B	601	CLA	C3C-C2C	5.40	1.48	1.36
24	C	504	CLA	C3B-C2B	5.41	1.47	1.40
24	c	510	CLA	C3C-C2C	5.41	1.48	1.36
24	c	503	CLA	C3C-C2C	5.42	1.48	1.36
24	C	509	CLA	C3C-C2C	5.44	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	C3C-C2C	5.45	1.48	1.36
24	b	603	CLA	C3C-C2C	5.45	1.48	1.36
24	a	350	CLA	C3C-C2C	5.45	1.48	1.36
24	b	610	CLA	C3C-C2C	5.46	1.48	1.36
24	c	514	CLA	C3B-C2B	5.46	1.47	1.40
24	b	615	CLA	C3C-C2C	5.48	1.48	1.36
24	b	611	CLA	C3B-C2B	5.50	1.47	1.40
24	B	609	CLA	C3B-C2B	5.50	1.47	1.40
24	b	613	CLA	C3C-C2C	5.51	1.48	1.36
24	C	513	CLA	C3C-C2C	5.51	1.48	1.36
24	B	602	CLA	C3B-C2B	5.55	1.47	1.40
25	a	405	PHO	C3C-C2C	5.59	1.48	1.36
24	b	615	CLA	C3B-C2B	5.59	1.47	1.40
24	b	604	CLA	C3B-C2B	5.62	1.47	1.40
24	c	505	CLA	C3B-C2B	5.62	1.47	1.40
24	b	605	CLA	C3B-C2B	5.65	1.47	1.40
24	a	350	CLA	C3B-C2B	5.66	1.47	1.40
24	d	403	CLA	C3B-C2B	5.67	1.47	1.40
24	c	509	CLA	C3B-C2B	5.68	1.47	1.40
24	b	616	CLA	C3B-C2B	5.69	1.47	1.40
24	D	403	CLA	C3B-C2B	5.69	1.47	1.40
24	B	610	CLA	C3C-C2C	5.71	1.49	1.36
24	a	404	CLA	C3B-C2B	5.73	1.47	1.40
24	b	607	CLA	C3B-C2B	5.74	1.47	1.40
24	c	515	CLA	C3B-C2B	5.78	1.48	1.40
24	C	513	CLA	C3B-C2B	5.78	1.48	1.40
24	B	606	CLA	C3B-C2B	5.79	1.48	1.40
24	c	508	CLA	C3B-C2B	5.82	1.48	1.40
24	c	507	CLA	C3B-C2B	5.83	1.48	1.40
24	a	407	CLA	C3B-C2B	5.84	1.48	1.40
24	C	507	CLA	C3B-C2B	5.85	1.48	1.40
24	C	508	CLA	C3B-C2B	5.85	1.48	1.40
24	B	610	CLA	C3B-C2B	5.88	1.48	1.40
24	b	609	CLA	C3B-C2B	5.90	1.48	1.40
25	A	408	PHO	C3C-C2C	5.92	1.49	1.36
24	c	503	CLA	C3B-C2B	5.92	1.48	1.40
24	C	514	CLA	C3B-C2B	5.95	1.48	1.40
24	c	504	CLA	C3B-C2B	5.96	1.48	1.40
24	C	506	CLA	C3B-C2B	5.96	1.48	1.40
25	a	406	PHO	C3C-C2C	5.96	1.49	1.36
24	b	608	CLA	C3B-C2B	6.00	1.48	1.40
24	B	601	CLA	C3B-C2B	6.01	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	602	CLA	C3B-C2B	6.03	1.48	1.40
24	b	603	CLA	C3B-C2B	6.03	1.48	1.40
24	B	616	CLA	C3B-C2B	6.05	1.48	1.40
24	B	604	CLA	C3B-C2B	6.06	1.48	1.40
24	A	409	CLA	C3B-C2B	6.06	1.48	1.40
24	C	511	CLA	C3B-C2B	6.06	1.48	1.40
24	B	611	CLA	C3B-C2B	6.07	1.48	1.40
24	A	405	CLA	C3B-C2B	6.07	1.48	1.40
24	b	606	CLA	C3B-C2B	6.07	1.48	1.40
25	a	406	PHO	C3B-C2B	6.13	1.48	1.37
24	b	614	CLA	C3B-C2B	6.14	1.48	1.40
24	c	513	CLA	C3B-C2B	6.14	1.48	1.40
24	c	511	CLA	C3B-C2B	6.17	1.48	1.40
24	d	402	CLA	C3B-C2B	6.17	1.48	1.40
24	C	502	CLA	C3B-C2B	6.18	1.48	1.40
24	c	512	CLA	C3B-C2B	6.20	1.48	1.40
25	A	407	PHO	C3B-C2B	6.26	1.49	1.37
24	b	601	CLA	C3B-C2B	6.29	1.48	1.40
24	C	503	CLA	C3B-C2B	6.31	1.48	1.40
25	a	405	PHO	C3B-C2B	6.31	1.49	1.37
24	B	614	CLA	C3B-C2B	6.33	1.48	1.40
24	C	505	CLA	C3B-C2B	6.37	1.48	1.40
24	c	510	CLA	C3B-C2B	6.40	1.48	1.40
24	B	608	CLA	C3B-C2B	6.41	1.48	1.40
24	D	402	CLA	C3B-C2B	6.42	1.48	1.40
25	A	408	PHO	C3B-C2B	6.45	1.49	1.37
24	b	613	CLA	C3B-C2B	6.50	1.48	1.40
24	c	506	CLA	C3B-C2B	6.56	1.49	1.40
24	B	603	CLA	C3B-C2B	6.57	1.49	1.40
24	b	612	CLA	C3B-C2B	6.57	1.49	1.40
24	a	403	CLA	C3B-C2B	6.58	1.49	1.40
24	b	610	CLA	C3B-C2B	6.73	1.49	1.40
24	C	512	CLA	C3B-C2B	6.74	1.49	1.40
24	C	509	CLA	C3B-C2B	6.80	1.49	1.40
24	A	404	CLA	C3B-C2B	6.80	1.49	1.40
24	B	612	CLA	C3B-C2B	6.87	1.49	1.40
24	B	613	CLA	C3B-C2B	6.96	1.49	1.40
24	C	510	CLA	C3B-C2B	7.33	1.50	1.40

All (2226) bond angle outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
-----	-------	-----	------	-------	---	-------------	----------

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	405	CLA	CHD-C4C-C3C	-6.95	114.44	124.92
24	B	615	CLA	CHD-C4C-C3C	-6.91	114.51	124.92
24	B	605	CLA	CHD-C4C-C3C	-6.83	114.62	124.92
24	B	606	CLA	CHD-C4C-C3C	-6.74	114.77	124.92
24	c	507	CLA	C1C-NC-C4C	-6.56	103.28	107.06
24	B	604	CLA	CHD-C4C-C3C	-6.56	115.04	124.92
24	B	616	CLA	CHD-C4C-C3C	-6.51	115.11	124.92
24	b	613	CLA	CHD-C4C-C3C	-6.44	115.21	124.92
24	B	601	CLA	CHD-C4C-C3C	-6.42	115.25	124.92
24	b	616	CLA	CHD-C4C-C3C	-6.41	115.27	124.92
24	B	609	CLA	CHD-C4C-C3C	-6.39	115.28	124.92
24	B	611	CLA	CHD-C4C-C3C	-6.39	115.29	124.92
24	a	350	CLA	CHD-C4C-C3C	-6.38	115.31	124.92
24	c	507	CLA	CHD-C4C-C3C	-6.34	115.36	124.92
24	C	513	CLA	CHD-C4C-C3C	-6.33	115.38	124.92
24	d	402	CLA	C1C-NC-C4C	-6.33	103.42	107.06
24	B	612	CLA	C1C-NC-C4C	-6.31	103.42	107.06
24	c	513	CLA	CHD-C4C-C3C	-6.29	115.43	124.92
24	C	506	CLA	CHD-C4C-C3C	-6.25	115.50	124.92
24	D	403	CLA	CHD-C4C-C3C	-6.24	115.51	124.92
24	B	608	CLA	CHD-C4C-C3C	-6.23	115.54	124.92
24	C	509	CLA	C1C-NC-C4C	-6.21	103.48	107.06
24	C	511	CLA	CHD-C4C-C3C	-6.20	115.58	124.92
24	b	605	CLA	CHD-C4C-C3C	-6.18	115.61	124.92
24	c	504	CLA	CHD-C4C-C3C	-6.18	115.61	124.92
24	b	601	CLA	CHD-C4C-C3C	-6.17	115.62	124.92
24	B	604	CLA	C1C-NC-C4C	-6.15	103.52	107.06
24	B	613	CLA	C1C-NC-C4C	-6.13	103.53	107.06
24	C	503	CLA	CHD-C4C-C3C	-6.13	115.68	124.92
24	B	610	CLA	CHD-C4C-C3C	-6.12	115.69	124.92
24	B	603	CLA	CHD-C4C-C3C	-6.12	115.70	124.92
24	b	606	CLA	CHD-C4C-C3C	-6.10	115.73	124.92
24	b	611	CLA	CHD-C4C-C3C	-6.10	115.73	124.92
24	c	510	CLA	CHD-C4C-C3C	-6.10	115.73	124.92
24	b	604	CLA	CHD-C4C-C3C	-6.05	115.80	124.92
24	a	404	CLA	CHD-C4C-C3C	-6.04	115.81	124.92
24	B	612	CLA	CHD-C4C-C3C	-6.01	115.86	124.92
24	b	602	CLA	CHD-C4C-C3C	-6.01	115.86	124.92
24	B	609	CLA	C1C-NC-C4C	-5.93	103.64	107.06
24	b	603	CLA	CHD-C4C-C3C	-5.93	115.98	124.92
24	b	608	CLA	CHD-C4C-C3C	-5.93	115.98	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CHD-C4C-C3C	-5.92	115.99	124.92
24	b	612	CLA	C1C-NC-C4C	-5.92	103.65	107.06
24	C	506	CLA	C1C-NC-C4C	-5.86	103.68	107.06
24	C	502	CLA	CHD-C4C-C3C	-5.86	116.09	124.92
24	b	604	CLA	C1C-NC-C4C	-5.85	103.69	107.06
24	A	409	CLA	CHD-C4C-C3C	-5.82	116.14	124.92
24	b	607	CLA	CHD-C4C-C3C	-5.82	116.15	124.92
24	B	614	CLA	CHD-C4C-C3C	-5.81	116.16	124.92
24	c	505	CLA	C1C-NC-C4C	-5.80	103.72	107.06
24	A	406	CLA	CHD-C4C-C3C	-5.80	116.17	124.92
24	b	614	CLA	CHD-C4C-C3C	-5.79	116.19	124.92
24	A	404	CLA	CHD-C4C-C3C	-5.76	116.24	124.92
24	C	508	CLA	CHD-C4C-C3C	-5.75	116.25	124.92
24	C	514	CLA	CHD-C4C-C3C	-5.75	116.26	124.92
24	c	505	CLA	CHD-C4C-C3C	-5.74	116.27	124.92
24	c	509	CLA	CHD-C4C-C3C	-5.73	116.28	124.92
24	D	402	CLA	C1C-NC-C4C	-5.72	103.77	107.06
24	c	514	CLA	CHD-C4C-C3C	-5.72	116.30	124.92
24	A	404	CLA	C1C-NC-C4C	-5.71	103.77	107.06
24	d	402	CLA	CHD-C4C-C3C	-5.71	116.31	124.92
24	b	614	CLA	C1C-NC-C4C	-5.70	103.78	107.06
24	C	512	CLA	CHD-C4C-C3C	-5.69	116.35	124.92
24	d	403	CLA	CHD-C4C-C3C	-5.68	116.35	124.92
24	B	602	CLA	CHD-C4C-C3C	-5.65	116.41	124.92
24	b	607	CLA	C1C-NC-C4C	-5.64	103.81	107.06
26	D	404	BCR	C7-C8-C9	-5.64	117.74	126.21
24	C	510	CLA	CHD-C4C-C3C	-5.63	116.44	124.92
24	b	612	CLA	CHD-C4C-C3C	-5.58	116.51	124.92
24	b	609	CLA	CHD-C4C-C3C	-5.57	116.52	124.92
24	b	610	CLA	CHD-C4C-C3C	-5.57	116.52	124.92
25	A	407	PHO	C3D-C2D-C1D	-5.55	97.59	105.82
24	c	512	CLA	CHD-C4C-C3C	-5.54	116.57	124.92
24	B	607	CLA	CHD-C4C-C3C	-5.53	116.59	124.92
24	a	407	CLA	CHD-C4C-C3C	-5.51	116.61	124.92
24	b	609	CLA	C1C-NC-C4C	-5.51	103.89	107.06
24	c	510	CLA	C1C-NC-C4C	-5.50	103.89	107.06
24	c	506	CLA	CHD-C4C-C3C	-5.50	116.63	124.92
24	B	603	CLA	C1C-NC-C4C	-5.49	103.90	107.06
25	A	408	PHO	C3D-C2D-C1D	-5.48	97.70	105.82
24	C	505	CLA	C1C-NC-C4C	-5.47	103.91	107.06
24	b	615	CLA	CHD-C4C-C3C	-5.44	116.73	124.92
24	C	508	CLA	C1C-NC-C4C	-5.43	103.93	107.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	C1C-NC-C4C	-5.40	103.95	107.06
24	C	512	CLA	C1C-NC-C4C	-5.36	103.97	107.06
24	c	503	CLA	CHD-C4C-C3C	-5.35	116.86	124.92
25	a	405	PHO	C3D-C2D-C1D	-5.34	97.89	105.82
31	A	416[A]	PL9	C7-C8-C9	-5.34	117.78	126.71
24	b	613	CLA	C1C-NC-C4C	-5.33	103.99	107.06
24	a	403	CLA	C1C-NC-C4C	-5.33	103.99	107.06
26	Y	101	BCR	C33-C5-C6	-5.32	118.55	124.51
24	B	614	CLA	C1C-NC-C4C	-5.32	103.99	107.06
24	C	504	CLA	CHD-C4C-C3C	-5.31	116.91	124.92
24	B	613	CLA	CHD-C4C-C3C	-5.31	116.92	124.92
24	b	603	CLA	C1C-NC-C4C	-5.27	104.02	107.06
24	c	515	CLA	CHD-C4C-C3C	-5.22	117.05	124.92
24	B	611	CLA	C1C-NC-C4C	-5.20	104.07	107.06
24	B	608	CLA	C1C-NC-C4C	-5.18	104.08	107.06
24	B	615	CLA	C1C-NC-C4C	-5.18	104.08	107.06
24	C	505	CLA	CHD-C4C-C3C	-5.16	117.14	124.92
24	B	605	CLA	C1C-NC-C4C	-5.16	104.09	107.06
24	c	508	CLA	CHD-C4C-C3C	-5.16	117.15	124.92
24	D	402	CLA	CHD-C4C-C3C	-5.10	117.23	124.92
24	C	504	CLA	C1C-NC-C4C	-5.09	104.13	107.06
26	b	617	BCR	C7-C8-C9	-5.07	118.60	126.21
24	C	503	CLA	C1C-NC-C4C	-5.04	104.16	107.06
24	c	511	CLA	CHD-C4C-C3C	-5.02	117.34	124.92
24	a	407	CLA	C1C-NC-C4C	-5.02	104.17	107.06
24	c	504	CLA	C1C-NC-C4C	-5.02	104.17	107.06
25	a	406	PHO	C3D-C2D-C1D	-5.01	98.38	105.82
24	C	507	CLA	C1C-NC-C4C	-4.99	104.18	107.06
39	E	103	HEM	CBD-CAD-C3D	-4.94	103.04	112.47
26	y	101	BCR	C33-C5-C6	-4.91	119.01	124.51
24	a	403	CLA	CHD-C4C-C3C	-4.90	117.54	124.92
25	A	408	PHO	C1-C2-C3	-4.86	117.00	125.96
24	C	510	CLA	C1C-NC-C4C	-4.86	104.26	107.06
24	B	606	CLA	C1C-NC-C4C	-4.85	104.26	107.06
24	B	604	CLA	C1-C2-C3	-4.84	117.03	125.96
24	b	610	CLA	C1C-NC-C4C	-4.81	104.29	107.06
24	C	507	CLA	CHD-C4C-C3C	-4.80	117.68	124.92
24	c	508	CLA	C1C-NC-C4C	-4.80	104.29	107.06
24	b	606	CLA	C1C-NC-C4C	-4.78	104.30	107.06
24	b	615	CLA	C1C-NC-C4C	-4.78	104.31	107.06
26	t	102	BCR	C33-C5-C6	-4.76	119.18	124.51
24	A	404	CLA	CAA-C2A-C3A	-4.76	99.77	112.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	PHO	C1-C2-C3	-4.73	117.23	125.96
24	A	409	CLA	C1C-NC-C4C	-4.73	104.33	107.06
27	A	411	SQD	C1-C2-C3	-4.72	101.20	109.98
24	C	514	CLA	C1C-NC-C4C	-4.71	104.34	107.06
26	H	101	BCR	C11-C10-C9	-4.71	120.59	127.31
27	a	409	SQD	C1-O5-C5	-4.68	104.91	113.72
26	d	404	BCR	C15-C14-C13	-4.67	120.64	127.31
24	B	613	CLA	C1-C2-C3	-4.67	117.35	125.96
24	c	515	CLA	C1C-NC-C4C	-4.67	104.37	107.06
24	c	512	CLA	C1C-NC-C4C	-4.63	104.39	107.06
26	c	517	BCR	C7-C8-C9	-4.63	119.26	126.21
24	C	513	CLA	C1C-NC-C4C	-4.62	104.39	107.06
24	c	511	CLA	C1-C2-C3	-4.61	117.46	125.96
24	a	403	CLA	CAA-C2A-C3A	-4.58	100.26	112.81
24	B	607	CLA	C1C-C2C-C3C	-4.58	101.84	106.92
27	A	411	SQD	C1-O5-C5	-4.57	105.11	113.72
24	b	608	CLA	C1C-NC-C4C	-4.54	104.44	107.06
24	b	605	CLA	C1C-NC-C4C	-4.53	104.45	107.06
24	c	511	CLA	C1C-NC-C4C	-4.51	104.46	107.06
24	c	505	CLA	C1D-CHD-C4C	-4.49	116.34	122.48
24	B	602	CLA	C1C-NC-C4C	-4.49	104.47	107.06
24	C	511	CLA	C1C-NC-C4C	-4.49	104.47	107.06
24	b	610	CLA	C1-C2-C3	-4.46	117.73	125.96
24	b	611	CLA	C1C-NC-C4C	-4.41	104.52	107.06
24	C	502	CLA	C1C-NC-C4C	-4.41	104.52	107.06
24	b	601	CLA	C1C-NC-C4C	-4.40	104.52	107.06
24	a	403	CLA	C1C-C2C-C3C	-4.39	102.05	106.92
24	c	513	CLA	C1C-NC-C4C	-4.35	104.55	107.06
24	A	405	CLA	C1C-NC-C4C	-4.35	104.55	107.06
24	b	616	CLA	C1C-NC-C4C	-4.35	104.55	107.06
25	A	408	PHO	C4C-C3C-C2C	-4.32	101.96	106.81
26	b	617	BCR	C33-C5-C6	-4.31	119.68	124.51
24	c	506	CLA	C1C-NC-C4C	-4.30	104.58	107.06
24	B	612	CLA	C1-C2-C3	-4.30	118.03	125.96
26	d	404	BCR	C38-C26-C25	-4.30	119.69	124.51
24	B	605	CLA	C1D-CHD-C4C	-4.29	116.61	122.48
24	D	403	CLA	C1C-NC-C4C	-4.28	104.59	107.06
24	c	509	CLA	C1C-NC-C4C	-4.27	104.60	107.06
26	T	101	BCR	C15-C16-C17	-4.25	114.38	123.46
27	a	409	SQD	C1-C2-C3	-4.25	102.08	109.98
24	B	610	CLA	C1C-NC-C4C	-4.24	104.62	107.06
26	K	102	BCR	C24-C23-C22	-4.23	119.85	126.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C1D-CHD-C4C	-4.23	116.70	122.48
26	B	617	BCR	C7-C8-C9	-4.22	119.86	126.21
24	B	615	CLA	C1D-CHD-C4C	-4.22	116.71	122.48
24	a	403	CLA	C1D-CHD-C4C	-4.21	116.72	122.48
31	D	405	PL9	C37-C38-C39	-4.20	117.12	127.68
26	c	516	BCR	C15-C14-C13	-4.19	121.33	127.31
24	C	507	CLA	C1C-C2C-C3C	-4.18	102.28	106.92
24	B	611	CLA	C1D-CHD-C4C	-4.18	116.77	122.48
24	B	614	CLA	O2D-CGD-O1D	-4.18	115.41	123.82
24	D	402	CLA	C1C-C2C-C3C	-4.18	102.29	106.92
24	C	513	CLA	C1D-CHD-C4C	-4.17	116.79	122.48
24	a	404	CLA	C1C-NC-C4C	-4.15	104.67	107.06
24	c	510	CLA	C1C-C2C-C3C	-4.13	102.34	106.92
24	B	616	CLA	C1C-NC-C4C	-4.12	104.68	107.06
24	c	514	CLA	C1C-NC-C4C	-4.08	104.71	107.06
24	B	614	CLA	C1C-C2C-C3C	-4.08	102.40	106.92
24	b	616	CLA	C1D-CHD-C4C	-4.07	116.92	122.48
26	B	617	BCR	C33-C5-C6	-4.06	119.96	124.51
26	K	102	BCR	C3-C4-C5	-4.05	106.82	113.78
24	C	502	CLA	O2D-CGD-O1D	-4.04	115.70	123.82
26	c	516	BCR	C11-C10-C9	-4.03	121.56	127.31
26	C	515	BCR	C7-C8-C9	-4.02	120.18	126.21
24	b	601	CLA	C1D-CHD-C4C	-4.01	117.00	122.48
31	A	416[B]	PL9	C7-C8-C9	-4.01	120.01	126.71
24	B	601	CLA	C1C-NC-C4C	-4.00	104.76	107.06
26	D	404	BCR	C24-C23-C22	-3.99	120.22	126.21
24	c	509	CLA	C1C-C2C-C3C	-3.97	102.51	106.92
24	C	505	CLA	C1C-C2C-C3C	-3.97	102.52	106.92
24	B	611	CLA	C1-C2-C3	-3.97	118.65	125.96
25	a	405	PHO	C4C-C3C-C2C	-3.97	102.36	106.81
26	c	516	BCR	C20-C21-C22	-3.95	121.67	127.31
27	a	409	SQD	C45-O47-C7	-3.95	108.54	117.88
24	A	405	CLA	C1D-CHD-C4C	-3.95	117.09	122.48
26	D	404	BCR	C38-C26-C25	-3.94	120.09	124.51
24	C	511	CLA	C1-C2-C3	-3.93	118.71	125.96
24	C	511	CLA	C1D-CHD-C4C	-3.90	117.16	122.48
24	B	603	CLA	C1C-C2C-C3C	-3.89	102.60	106.92
24	c	512	CLA	C1C-C2C-C3C	-3.89	102.60	106.92
24	c	503	CLA	O2D-CGD-O1D	-3.89	116.00	123.82
24	c	503	CLA	C1C-NC-C4C	-3.88	104.82	107.06
24	D	402	CLA	C1-C2-C3	-3.88	118.81	125.96
24	B	601	CLA	C1D-CHD-C4C	-3.88	117.19	122.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C1-C2-C3	-3.88	118.81	125.96
31	a	414[A]	PL9	C7-C8-C9	-3.88	120.23	126.71
24	B	604	CLA	C1D-CHD-C4C	-3.87	117.19	122.48
24	C	510	CLA	C1-C2-C3	-3.87	118.83	125.96
24	B	606	CLA	O2D-CGD-O1D	-3.86	116.05	123.82
25	a	406	PHO	C4C-C3C-C2C	-3.86	102.48	106.81
24	c	512	CLA	C1-C2-C3	-3.84	118.88	125.96
26	T	101	BCR	C11-C10-C9	-3.84	121.83	127.31
24	c	506	CLA	C1C-C2C-C3C	-3.84	102.66	106.92
24	b	604	CLA	C1-C2-C3	-3.84	118.89	125.96
24	b	611	CLA	C1-C2-C3	-3.84	118.89	125.96
24	b	612	CLA	C1D-CHD-C4C	-3.83	117.24	122.48
26	b	619	BCR	C15-C14-C13	-3.83	121.84	127.31
26	C	515	BCR	C15-C14-C13	-3.81	121.87	127.31
24	a	350	CLA	C1C-C2C-C3C	-3.79	102.71	106.92
24	B	612	CLA	O2D-CGD-O1D	-3.79	116.20	123.82
24	A	404	CLA	C1D-CHD-C4C	-3.78	117.32	122.48
24	b	613	CLA	C1C-C2C-C3C	-3.78	102.73	106.92
26	t	102	BCR	C11-C10-C9	-3.77	121.92	127.31
24	C	509	CLA	C1D-CHD-C4C	-3.77	117.34	122.48
26	K	102	BCR	C7-C8-C9	-3.77	120.55	126.21
26	A	410	BCR	C15-C14-C13	-3.76	121.94	127.31
24	B	611	CLA	O2D-CGD-O1D	-3.76	116.26	123.82
26	y	101	BCR	C38-C26-C25	-3.75	120.31	124.51
31	a	414[A]	PL9	C32-C33-C34	-3.75	118.26	127.68
24	a	350	CLA	CBC-CAC-C3C	-3.75	101.76	112.41
24	b	602	CLA	C1C-NC-C4C	-3.74	104.90	107.06
24	b	605	CLA	O2D-CGD-O1D	-3.74	116.29	123.82
24	c	508	CLA	C1C-C2C-C3C	-3.73	102.78	106.92
24	b	605	CLA	C1C-C2C-C3C	-3.73	102.78	106.92
24	B	606	CLA	C1D-CHD-C4C	-3.73	117.39	122.48
24	c	504	CLA	C1C-C2C-C3C	-3.72	102.79	106.92
26	C	516	BCR	C11-C10-C9	-3.72	122.01	127.31
24	b	614	CLA	O2D-CGD-O1D	-3.71	116.35	123.82
31	A	416[A]	PL9	C37-C38-C39	-3.70	118.38	127.68
24	A	405	CLA	C1C-C2C-C3C	-3.69	102.83	106.92
24	a	407	CLA	CAA-C2A-C3A	-3.67	102.74	112.81
24	B	608	CLA	C1C-C2C-C3C	-3.67	102.85	106.92
24	C	508	CLA	C1D-CHD-C4C	-3.67	117.47	122.48
24	B	605	CLA	O2A-CGA-O1A	-3.66	114.45	123.55
24	B	613	CLA	C1C-C2C-C3C	-3.66	102.86	106.92
26	h	102	BCR	C7-C8-C9	-3.66	120.72	126.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C20-C21-C22	-3.66	122.09	127.31
26	C	516	BCR	C7-C8-C9	-3.66	120.72	126.21
24	a	350	CLA	C1D-CHD-C4C	-3.65	117.49	122.48
26	Y	101	BCR	C16-C17-C18	-3.65	122.10	127.31
26	b	619	BCR	C7-C8-C9	-3.64	120.75	126.21
24	b	608	CLA	C1-C2-C3	-3.63	119.27	125.96
31	a	414[A]	PL9	C22-C23-C24	-3.63	118.57	127.68
24	b	608	CLA	C1C-C2C-C3C	-3.62	102.90	106.92
24	B	605	CLA	O2D-CGD-O1D	-3.62	116.53	123.82
24	B	603	CLA	C1D-CHD-C4C	-3.62	117.54	122.48
24	b	606	CLA	C1D-CHD-C4C	-3.61	117.55	122.48
26	a	408	BCR	C7-C8-C9	-3.61	120.79	126.21
24	a	407	CLA	C1D-CHD-C4C	-3.60	117.56	122.48
24	C	509	CLA	O2D-CGD-O1D	-3.60	116.57	123.82
24	A	405	CLA	CBC-CAC-C3C	-3.60	102.18	112.41
24	C	508	CLA	O2D-CGD-O1D	-3.60	116.58	123.82
24	B	604	CLA	C1C-C2C-C3C	-3.59	102.94	106.92
26	h	102	BCR	C16-C17-C18	-3.59	122.19	127.31
24	C	502	CLA	C1D-CHD-C4C	-3.59	117.58	122.48
24	b	604	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
24	C	508	CLA	C1C-C2C-C3C	-3.58	102.95	106.92
24	B	616	CLA	C1D-CHD-C4C	-3.57	117.60	122.48
33	A	418	LMG	C7-O1-C1	-3.56	106.45	113.76
24	C	503	CLA	C1C-C2C-C3C	-3.56	102.97	106.92
27	A	413	SQD	C5-C6-S	-3.56	109.38	114.34
24	B	604	CLA	O2A-CGA-O1A	-3.56	114.72	123.55
31	D	405	PL9	C42-C43-C44	-3.55	118.76	127.68
24	C	503	CLA	C1D-CHD-C4C	-3.55	117.63	122.48
24	d	403	CLA	O2D-CGD-O1D	-3.55	116.68	123.82
24	C	504	CLA	C1D-CHD-C4C	-3.55	117.64	122.48
24	B	612	CLA	C4C-C3C-C2C	-3.54	101.48	106.91
24	A	406	CLA	C1-C2-C3	-3.53	119.45	125.96
26	d	404	BCR	C24-C23-C22	-3.53	120.91	126.21
24	C	506	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
24	c	507	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
24	c	514	CLA	C1D-CHD-C4C	-3.53	117.66	122.48
26	B	617	BCR	C16-C17-C18	-3.52	122.29	127.31
24	B	603	CLA	O2D-CGD-O1D	-3.52	116.74	123.82
24	c	512	CLA	C1D-CHD-C4C	-3.52	117.67	122.48
24	b	609	CLA	C1-C2-C3	-3.52	119.47	125.96
25	A	408	PHO	O2D-CGD-O1D	-3.52	116.74	123.82
24	B	611	CLA	C1C-C2C-C3C	-3.52	103.02	106.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C1C-C2C-C3C	-3.52	103.02	106.92
26	D	404	BCR	C15-C14-C13	-3.51	122.29	127.31
24	b	603	CLA	CAA-C2A-C3A	-3.51	103.17	112.81
24	A	405	CLA	CAA-C2A-C3A	-3.51	103.18	112.81
24	B	602	CLA	CAA-C2A-C3A	-3.51	103.18	112.81
24	A	404	CLA	O2A-CGA-O1A	-3.51	114.84	123.55
27	b	620	SQD	C5-C6-S	-3.51	109.45	114.34
24	A	409	CLA	C1-C2-C3	-3.51	119.50	125.96
24	b	609	CLA	C1C-C2C-C3C	-3.49	103.05	106.92
31	A	416[A]	PL9	C32-C33-C34	-3.48	118.94	127.68
24	B	608	CLA	C1D-CHD-C4C	-3.48	117.73	122.48
24	c	507	CLA	C4C-C3C-C2C	-3.47	101.58	106.91
24	c	515	CLA	C1D-CHD-C4C	-3.47	117.74	122.48
24	c	514	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
24	c	503	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
24	C	502	CLA	C1C-C2C-C3C	-3.46	103.08	106.92
24	a	407	CLA	O2D-CGD-O1D	-3.46	116.86	123.82
24	B	610	CLA	CMA-C3A-C4A	-3.45	102.50	111.77
25	a	405	PHO	CHC-C1C-C2C	-3.45	117.71	125.62
25	A	407	PHO	C4C-C3C-C2C	-3.44	102.94	106.81
24	C	509	CLA	C1-C2-C3	-3.44	119.62	125.96
24	b	606	CLA	O2D-CGD-O1D	-3.43	116.91	123.82
24	a	404	CLA	C1D-CHD-C4C	-3.43	117.80	122.48
24	b	612	CLA	C1-C2-C3	-3.43	119.64	125.96
24	A	409	CLA	C1C-C2C-C3C	-3.43	103.12	106.92
24	C	511	CLA	C1C-C2C-C3C	-3.43	103.12	106.92
24	c	515	CLA	C1C-C2C-C3C	-3.42	103.12	106.92
27	a	409	SQD	C5-C6-S	-3.42	109.57	114.34
26	A	410	BCR	C16-C17-C18	-3.42	122.42	127.31
24	A	406	CLA	C1C-C2C-C3C	-3.42	103.12	106.92
26	b	618	BCR	C15-C14-C13	-3.42	122.43	127.31
26	c	516	BCR	C16-C17-C18	-3.42	122.43	127.31
24	c	508	CLA	C1D-CHD-C4C	-3.41	117.82	122.48
25	A	407	PHO	CHC-C1C-C2C	-3.41	117.80	125.62
24	B	616	CLA	C4C-C3C-C2C	-3.41	101.68	106.91
24	a	350	CLA	C1C-NC-C4C	-3.41	105.09	107.06
24	a	407	CLA	CMA-C3A-C2A	-3.41	99.95	113.77
26	B	618	BCR	C15-C14-C13	-3.40	122.45	127.31
24	c	511	CLA	C1D-CHD-C4C	-3.40	117.84	122.48
24	b	606	CLA	C1C-C2C-C3C	-3.40	103.15	106.92
26	A	410	BCR	C33-C5-C6	-3.40	120.70	124.51
24	b	613	CLA	C1D-CHD-C4C	-3.40	117.84	122.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	CAA-C2A-C3A	-3.40	103.50	112.81
24	B	610	CLA	CAA-C2A-C3A	-3.40	103.50	112.81
24	A	404	CLA	C1C-C2C-C3C	-3.40	103.15	106.92
31	a	414[A]	PL9	C37-C38-C39	-3.39	119.15	127.68
31	a	414[B]	PL9	C27-C28-C29	-3.39	119.16	127.68
24	B	616	CLA	O2D-CGD-O1D	-3.39	117.00	123.82
26	a	408	BCR	C20-C21-C22	-3.39	122.47	127.31
24	c	508	CLA	C1-C2-C3	-3.39	119.72	125.96
24	b	607	CLA	C1C-C2C-C3C	-3.38	103.17	106.92
24	a	404	CLA	CAA-C2A-C3A	-3.38	103.55	112.81
24	C	509	CLA	C4C-C3C-C2C	-3.38	101.73	106.91
31	a	414[B]	PL9	C32-C33-C34	-3.38	119.20	127.68
27	A	411	SQD	C44-O6-C1	-3.37	106.84	113.76
26	t	102	BCR	C7-C8-C9	-3.37	121.15	126.21
24	B	607	CLA	O2D-CGD-O1D	-3.37	117.04	123.82
24	d	402	CLA	C1-C2-C3	-3.37	119.75	125.96
24	C	514	CLA	C1-C2-C3	-3.37	119.75	125.96
24	c	513	CLA	O2D-CGD-O1D	-3.37	117.04	123.82
24	b	601	CLA	O2D-CGD-O1D	-3.37	117.05	123.82
24	B	603	CLA	O2A-CGA-O1A	-3.37	115.19	123.55
24	b	616	CLA	C4C-C3C-C2C	-3.37	101.75	106.91
24	a	407	CLA	C1C-C2C-C3C	-3.36	103.19	106.92
24	B	610	CLA	C1C-C2C-C3C	-3.36	103.19	106.92
31	d	405	PL9	C42-C43-C44	-3.36	119.23	127.68
24	b	615	CLA	C1C-C2C-C3C	-3.36	103.19	106.92
24	c	504	CLA	C1D-CHD-C4C	-3.35	117.90	122.48
24	B	614	CLA	C1D-CHD-C4C	-3.35	117.91	122.48
24	a	403	CLA	CHC-C1C-C2C	-3.34	117.53	126.65
24	C	507	CLA	CHC-C1C-C2C	-3.34	117.55	126.65
24	b	602	CLA	CAA-C2A-C3A	-3.33	103.67	112.81
24	B	609	CLA	C1C-C2C-C3C	-3.33	103.22	106.92
36	C	517	DGD	C3G-C2G-C1G	-3.33	104.34	111.86
26	C	515	BCR	C33-C5-C6	-3.33	120.78	124.51
24	b	605	CLA	C1D-CHD-C4C	-3.33	117.93	122.48
24	B	612	CLA	C1D-CHD-C4C	-3.33	117.94	122.48
31	a	414[B]	PL9	C7-C3-C2	-3.33	118.50	123.23
26	k	101	BCR	C24-C23-C22	-3.32	121.22	126.21
24	C	510	CLA	C1C-C2C-C3C	-3.32	103.23	106.92
24	b	611	CLA	O2D-CGD-O1D	-3.32	117.14	123.82
24	b	610	CLA	O2A-CGA-O1A	-3.32	115.31	123.55
24	a	404	CLA	C1C-C2C-C3C	-3.32	103.24	106.92
26	C	516	BCR	C33-C5-C6	-3.32	120.80	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	611	CLA	C1D-CHD-C4C	-3.31	117.95	122.48
26	Y	101	BCR	C15-C14-C13	-3.31	122.58	127.31
31	A	416[A]	PL9	C17-C18-C19	-3.31	119.36	127.68
24	B	603	CLA	C5-C3-C2	-3.31	114.33	121.10
24	b	612	CLA	C1C-C2C-C3C	-3.31	103.25	106.92
24	C	509	CLA	C1C-C2C-C3C	-3.29	103.27	106.92
24	A	409	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
24	c	510	CLA	C1D-CHD-C4C	-3.29	117.98	122.48
26	y	101	BCR	C15-C14-C13	-3.29	122.62	127.31
31	A	416[B]	PL9	C7-C3-C2	-3.28	118.56	123.23
24	C	512	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
31	a	414[B]	PL9	C42-C43-C44	-3.28	119.43	127.68
24	b	615	CLA	C1D-CHD-C4C	-3.28	118.00	122.48
26	T	101	BCR	C33-C5-C6	-3.28	120.84	124.51
26	h	102	BCR	C38-C26-C25	-3.28	120.84	124.51
24	c	508	CLA	CHC-C1C-C2C	-3.28	117.71	126.65
24	C	504	CLA	C1C-C2C-C3C	-3.27	103.29	106.92
31	d	405	PL9	C37-C38-C39	-3.27	119.46	127.68
26	T	101	BCR	C7-C8-C9	-3.27	121.30	126.21
26	A	410	BCR	C11-C10-C9	-3.27	122.65	127.31
26	a	408	BCR	C11-C10-C9	-3.27	122.65	127.31
24	B	605	CLA	C4C-C3C-C2C	-3.26	101.90	106.91
24	A	406	CLA	C1C-NC-C4C	-3.26	105.18	107.06
24	C	514	CLA	C1D-CHD-C4C	-3.26	118.03	122.48
31	a	414[B]	PL9	C37-C38-C39	-3.25	119.51	127.68
24	C	505	CLA	C1D-CHD-C4C	-3.25	118.04	122.48
24	c	511	CLA	C1C-C2C-C3C	-3.25	103.31	106.92
24	c	514	CLA	C1-C2-C3	-3.25	119.97	125.96
38	D	357	LHG	C5-O7-C7	-3.25	110.20	117.88
24	b	605	CLA	O2A-CGA-O1A	-3.25	115.48	123.55
31	A	416[A]	PL9	C27-C28-C29	-3.25	119.52	127.68
24	C	513	CLA	C1-C2-C3	-3.25	119.97	125.96
24	b	615	CLA	CHC-C1C-C2C	-3.24	117.81	126.65
24	b	610	CLA	C1D-CHD-C4C	-3.24	118.05	122.48
36	c	518	DGD	C2G-O2G-C1B	-3.24	110.22	117.88
31	a	414[A]	PL9	C42-C43-C44	-3.24	119.55	127.68
24	c	505	CLA	C1C-C2C-C3C	-3.24	103.33	106.92
24	b	610	CLA	C1C-C2C-C3C	-3.22	103.34	106.92
24	d	402	CLA	C1D-CHD-C4C	-3.22	118.08	122.48
24	C	507	CLA	CBC-CAC-C3C	-3.22	103.28	112.41
26	T	101	BCR	C12-C13-C14	-3.21	114.01	118.94
24	d	402	CLA	C1C-C2C-C3C	-3.21	103.36	106.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	416[B]	PL9	C17-C18-C19	-3.21	119.61	127.68
31	A	416[A]	PL9	C7-C3-C2	-3.21	118.67	123.23
24	B	610	CLA	C1D-CHD-C4C	-3.21	118.10	122.48
24	C	506	CLA	C4C-C3C-C2C	-3.21	101.99	106.91
24	c	513	CLA	C1-C2-C3	-3.21	120.05	125.96
31	a	414[A]	PL9	C7-C3-C2	-3.20	118.67	123.23
24	b	601	CLA	C1C-C2C-C3C	-3.20	103.37	106.92
38	d	406	LHG	O8-C23-O10	-3.20	115.61	123.55
24	c	512	CLA	CBC-CAC-C3C	-3.19	103.34	112.41
24	b	604	CLA	C1D-CHD-C4C	-3.19	118.12	122.48
27	A	411	SQD	C5-C6-S	-3.19	109.89	114.34
26	k	101	BCR	C15-C14-C13	-3.19	122.76	127.31
24	b	614	CLA	C1D-CHD-C4C	-3.19	118.13	122.48
24	b	613	CLA	C1-C2-C3	-3.18	120.09	125.96
24	B	606	CLA	C1C-C2C-C3C	-3.18	103.39	106.92
24	b	607	CLA	C4C-C3C-C2C	-3.18	102.03	106.91
24	a	404	CLA	C1-C2-C3	-3.17	120.11	125.96
24	c	513	CLA	C1D-CHD-C4C	-3.17	118.15	122.48
31	a	414[B]	PL9	C22-C23-C24	-3.17	119.72	127.68
24	b	603	CLA	O2A-CGA-O1A	-3.17	115.68	123.55
24	b	614	CLA	C1C-C2C-C3C	-3.17	103.41	106.92
25	A	407	PHO	C1C-C2C-C3C	-3.17	102.84	106.51
26	D	404	BCR	C28-C27-C26	-3.17	108.34	113.78
38	D	357	LHG	O8-C23-O10	-3.16	115.69	123.55
24	C	507	CLA	O2D-CGD-O1D	-3.16	117.46	123.82
24	a	350	CLA	CAA-C2A-C3A	-3.16	104.15	112.81
26	d	404	BCR	C7-C8-C9	-3.16	121.47	126.21
26	b	619	BCR	C38-C26-C25	-3.16	120.97	124.51
25	a	406	PHO	O2D-CGD-O1D	-3.15	117.48	123.82
24	c	514	CLA	O2D-CGD-O1D	-3.15	117.48	123.82
31	A	416[B]	PL9	C42-C43-C44	-3.15	119.76	127.68
24	B	608	CLA	CMA-C3A-C4A	-3.15	103.30	111.77
26	B	619	BCR	C24-C23-C22	-3.15	121.48	126.21
25	a	406	PHO	CHC-C1C-C2C	-3.15	118.39	125.62
24	c	504	CLA	C1-C2-C3	-3.15	120.16	125.96
24	B	602	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
24	A	409	CLA	CAA-C2A-C3A	-3.14	104.19	112.81
24	d	402	CLA	C4C-C3C-C2C	-3.14	102.09	106.91
24	b	602	CLA	O2D-CGD-O1D	-3.14	117.50	123.82
24	D	403	CLA	C1D-CHD-C4C	-3.14	118.19	122.48
26	c	517	BCR	C21-C20-C19	-3.14	113.61	123.23
24	b	616	CLA	OBD-CAD-C3D	-3.13	122.25	128.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	517	DGD	O3G-C3G-C2G	-3.13	103.54	110.99
24	C	512	CLA	C1C-C2C-C3C	-3.13	103.45	106.92
31	a	414[A]	PL9	C27-C28-C29	-3.13	119.83	127.68
31	a	414[B]	PL9	C17-C18-C19	-3.12	119.83	127.68
24	B	614	CLA	O2A-CGA-O1A	-3.12	115.80	123.55
24	C	504	CLA	CHC-C1C-C2C	-3.12	118.14	126.65
24	A	405	CLA	O2D-CGD-O1D	-3.12	117.55	123.82
26	c	517	BCR	C33-C5-C6	-3.11	121.02	124.51
24	D	402	CLA	CHC-C1C-C2C	-3.11	118.16	126.65
24	b	605	CLA	CHC-C1C-C2C	-3.11	118.17	126.65
24	B	615	CLA	C1C-C2C-C3C	-3.11	103.48	106.92
24	C	514	CLA	C4C-C3C-C2C	-3.10	102.15	106.91
31	A	416[B]	PL9	C37-C38-C39	-3.10	119.89	127.68
24	b	612	CLA	CHC-C1C-C2C	-3.10	118.19	126.65
24	a	403	CLA	CAA-C2A-C1A	-3.10	101.83	111.97
25	A	408	PHO	CHD-C1D-C2D	-3.09	118.52	125.62
24	c	511	CLA	CHC-C1C-C2C	-3.09	118.21	126.65
24	D	403	CLA	C4C-C3C-C2C	-3.09	102.17	106.91
24	b	612	CLA	C4C-C3C-C2C	-3.09	102.17	106.91
31	A	416[B]	PL9	C32-C33-C34	-3.09	119.92	127.68
24	C	513	CLA	C4C-C3C-C2C	-3.09	102.17	106.91
24	b	609	CLA	C1D-CHD-C4C	-3.09	118.27	122.48
24	C	505	CLA	C1-C2-C3	-3.08	120.28	125.96
24	C	514	CLA	O2D-CGD-O1D	-3.08	117.62	123.82
24	B	603	CLA	CBC-CAC-C3C	-3.08	103.67	112.41
24	b	611	CLA	C4C-C3C-C2C	-3.08	102.19	106.91
24	B	611	CLA	OBD-CAD-C3D	-3.08	122.36	128.03
24	A	409	CLA	C4C-C3C-C2C	-3.07	102.20	106.91
26	A	410	BCR	C38-C26-C25	-3.07	121.07	124.51
24	B	610	CLA	C4C-C3C-C2C	-3.07	102.20	106.91
36	c	520	DGD	O3G-C3G-C2G	-3.07	103.69	110.99
24	B	614	CLA	CHC-C1C-C2C	-3.06	118.29	126.65
24	c	513	CLA	C1C-C2C-C3C	-3.06	103.53	106.92
24	d	403	CLA	C1D-CHD-C4C	-3.05	118.31	122.48
39	v	203	HEM	CBA-CAA-C2A	-3.05	106.66	112.48
24	C	506	CLA	C1C-C2C-C3C	-3.04	103.54	106.92
24	B	602	CLA	C4C-C3C-C2C	-3.04	102.24	106.91
24	B	601	CLA	O2D-CGD-O1D	-3.04	117.69	123.82
24	C	513	CLA	O1D-CGD-CBD	-3.04	119.14	124.60
25	a	405	PHO	O2D-CGD-O1D	-3.04	117.70	123.82
24	B	609	CLA	C4C-C3C-C2C	-3.04	102.25	106.91
26	K	102	BCR	C20-C21-C22	-3.04	122.97	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CHC-C1C-C2C	-3.04	118.36	126.65
24	C	510	CLA	O2D-CGD-O1D	-3.04	117.71	123.82
24	d	403	CLA	C1-C2-C3	-3.03	120.37	125.96
24	C	513	CLA	C1C-C2C-C3C	-3.03	103.56	106.92
24	C	504	CLA	C1-C2-C3	-3.03	120.37	125.96
24	B	601	CLA	C4C-C3C-C2C	-3.03	102.26	106.91
26	c	517	BCR	C38-C26-C25	-3.03	121.11	124.51
24	b	610	CLA	C4C-C3C-C2C	-3.03	102.26	106.91
24	B	602	CLA	O2D-CGD-O1D	-3.03	117.73	123.82
26	D	404	BCR	C10-C11-C12	-3.03	113.95	123.23
24	A	406	CLA	O2A-CGA-O1A	-3.03	116.04	123.55
26	b	619	BCR	C10-C11-C12	-3.02	113.95	123.23
24	B	608	CLA	O2A-CGA-O1A	-3.02	116.04	123.55
25	A	408	PHO	C4D-ND-C1D	-3.02	101.52	106.98
24	B	615	CLA	C4C-C3C-C2C	-3.02	102.27	106.91
39	e	102	HEM	CBD-CAD-C3D	-3.02	106.70	112.47
24	D	403	CLA	O2D-CGD-O1D	-3.02	117.75	123.82
24	c	510	CLA	C1-C2-C3	-3.02	120.40	125.96
24	B	608	CLA	C1-C2-C3	-3.01	120.41	125.96
24	c	509	CLA	C1D-CHD-C4C	-3.01	118.37	122.48
24	d	402	CLA	O2D-CGD-O1D	-3.01	117.77	123.82
24	a	350	CLA	C1-C2-C3	-3.01	120.42	125.96
25	A	407	PHO	CHD-C1D-C2D	-3.00	118.73	125.62
24	C	514	CLA	C1C-C2C-C3C	-3.00	103.59	106.92
24	b	615	CLA	C4C-C3C-C2C	-3.00	102.30	106.91
24	B	603	CLA	CAA-C2A-C3A	-3.00	104.58	112.81
24	C	510	CLA	C4C-C3C-C2C	-3.00	102.31	106.91
38	D	407	LHG	O8-C23-O10	-3.00	116.10	123.55
24	B	604	CLA	C4C-C3C-C2C	-3.00	102.31	106.91
24	c	505	CLA	C4C-C3C-C2C	-3.00	102.31	106.91
24	b	611	CLA	C1C-C2C-C3C	-2.99	103.60	106.92
24	b	605	CLA	C2A-C1A-CHA	-2.99	118.62	123.92
39	V	203	HEM	CBD-CAD-C3D	-2.99	106.76	112.47
24	b	608	CLA	C1D-CHD-C4C	-2.99	118.40	122.48
24	b	614	CLA	C1-C2-C3	-2.98	120.46	125.96
24	c	507	CLA	C1C-C2C-C3C	-2.98	103.61	106.92
24	C	503	CLA	O2D-CGD-O1D	-2.98	117.82	123.82
24	c	503	CLA	C1D-CHD-C4C	-2.98	118.41	122.48
24	b	607	CLA	C1D-CHD-C4C	-2.98	118.41	122.48
24	b	614	CLA	C4C-C3C-C2C	-2.98	102.34	106.91
24	c	508	CLA	CAA-C2A-C3A	-2.98	104.65	112.81
25	a	405	PHO	C4D-ND-C1D	-2.97	101.61	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C4C-C3C-C2C	-2.97	102.35	106.91
24	b	613	CLA	C4C-C3C-C2C	-2.97	102.35	106.91
24	B	606	CLA	C4C-C3C-C2C	-2.97	102.35	106.91
24	b	602	CLA	C4C-C3C-C2C	-2.97	102.36	106.91
31	A	416[B]	PL9	C10-C9-C8	-2.97	115.78	123.69
24	b	602	CLA	C2A-C1A-CHA	-2.97	118.66	123.92
24	c	504	CLA	O2D-CGD-O1D	-2.96	117.86	123.82
24	b	601	CLA	C4C-C3C-C2C	-2.96	102.37	106.91
24	A	406	CLA	C2A-C1A-CHA	-2.96	118.67	123.92
24	b	603	CLA	O2D-CGD-O1D	-2.96	117.87	123.82
24	b	602	CLA	C1C-C2C-C3C	-2.96	103.64	106.92
24	b	609	CLA	O2D-CGD-O1D	-2.95	117.88	123.82
36	C	517	DGD	C2G-O2G-C1B	-2.95	110.89	117.88
26	Y	101	BCR	C28-C27-C26	-2.95	108.70	113.78
24	d	403	CLA	C1C-NC-C4C	-2.95	105.36	107.06
24	b	611	CLA	CHC-C1C-C2C	-2.95	118.60	126.65
24	C	512	CLA	C4C-C3C-C2C	-2.95	102.38	106.91
24	c	504	CLA	CBC-CAC-C3C	-2.95	104.04	112.41
24	B	601	CLA	C1C-C2C-C3C	-2.94	103.66	106.92
24	C	505	CLA	CHC-C1C-C2C	-2.94	118.62	126.65
24	B	608	CLA	CHC-C1C-C2C	-2.94	118.63	126.65
24	c	506	CLA	C1D-CHD-C4C	-2.93	118.48	122.48
26	B	619	BCR	C38-C26-C25	-2.93	121.23	124.51
24	c	515	CLA	CAA-C2A-C3A	-2.93	104.78	112.81
26	H	101	BCR	C38-C26-C25	-2.93	121.23	124.51
24	b	607	CLA	CHC-C1C-C2C	-2.93	118.67	126.65
24	c	510	CLA	CHC-C1C-C2C	-2.92	118.67	126.65
26	C	516	BCR	C38-C26-C25	-2.92	121.23	124.51
24	c	515	CLA	C1-C2-C3	-2.92	120.58	125.96
24	b	604	CLA	C4C-C3C-C2C	-2.92	102.43	106.91
24	C	510	CLA	C1D-CHD-C4C	-2.92	118.49	122.48
24	A	404	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
31	a	414[A]	PL9	C17-C18-C19	-2.92	120.35	127.68
24	b	615	CLA	C11-C10-C8	-2.91	106.18	115.73
24	b	606	CLA	C4C-C3C-C2C	-2.91	102.44	106.91
26	T	101	BCR	C21-C20-C19	-2.91	114.31	123.23
24	c	513	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
24	C	504	CLA	C4C-C3C-C2C	-2.91	102.45	106.91
24	B	612	CLA	C1C-C2C-C3C	-2.91	103.70	106.92
26	d	404	BCR	C33-C5-C6	-2.90	121.26	124.51
24	B	605	CLA	C1C-C2C-C3C	-2.90	103.70	106.92
24	a	407	CLA	C4C-C3C-C2C	-2.90	102.46	106.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	609	CLA	CBC-CAC-C3C	-2.90	104.18	112.41
24	a	404	CLA	C4C-C3C-C2C	-2.90	102.46	106.91
24	C	508	CLA	C4C-C3C-C2C	-2.89	102.47	106.91
24	B	611	CLA	C4C-C3C-C2C	-2.89	102.48	106.91
24	A	406	CLA	CMA-C3A-C2A	-2.89	102.05	113.77
24	B	607	CLA	CHC-C1C-C2C	-2.89	118.77	126.65
24	B	607	CLA	CBC-CAC-C3C	-2.89	104.21	112.41
24	c	503	CLA	CHC-C1C-C2C	-2.88	118.79	126.65
24	c	509	CLA	O2D-CGD-O1D	-2.88	118.03	123.82
24	c	504	CLA	O2A-CGA-O1A	-2.88	116.41	123.55
26	k	101	BCR	C10-C11-C12	-2.87	114.41	123.23
25	A	408	PHO	C4D-CHA-C1A	-2.87	118.68	125.06
27	a	409	SQD	O47-C7-O49	-2.87	116.52	123.68
33	b	621	LMG	C8-O7-C10	-2.87	111.11	117.88
25	A	407	PHO	O1D-CGD-CBD	-2.87	119.45	124.60
24	a	404	CLA	CHC-C1C-C2C	-2.86	118.84	126.65
24	B	608	CLA	C4C-C3C-C2C	-2.86	102.52	106.91
24	C	502	CLA	CHC-C1C-C2C	-2.86	118.84	126.65
24	B	603	CLA	C2A-C1A-CHA	-2.86	118.85	123.92
24	C	507	CLA	C1-C2-C3	-2.86	120.69	125.96
24	b	609	CLA	CHC-C1C-C2C	-2.86	118.86	126.65
24	C	503	CLA	CBC-CAC-C3C	-2.86	104.30	112.41
25	A	408	PHO	CHC-C1C-C2C	-2.85	119.07	125.62
26	T	101	BCR	C16-C17-C18	-2.85	123.24	127.31
24	B	611	CLA	CHC-C1C-C2C	-2.85	118.87	126.65
24	b	616	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
24	c	503	CLA	C1-C2-C3	-2.85	120.71	125.96
26	K	102	BCR	C11-C10-C9	-2.85	123.25	127.31
24	A	404	CLA	C4C-C3C-C2C	-2.85	102.54	106.91
24	b	610	CLA	O2D-CGD-O1D	-2.85	118.09	123.82
24	c	515	CLA	C4C-C3C-C2C	-2.85	102.54	106.91
26	A	410	BCR	C24-C23-C22	-2.85	121.94	126.21
24	b	606	CLA	CHC-C1C-C2C	-2.85	118.89	126.65
24	c	506	CLA	CHC-C1C-C2C	-2.84	118.89	126.65
31	A	416[B]	PL9	C27-C28-C29	-2.84	120.54	127.68
25	A	407	PHO	C4D-ND-C1D	-2.84	101.85	106.98
24	b	608	CLA	C4C-C3C-C2C	-2.84	102.55	106.91
24	b	612	CLA	C2A-C1A-CHA	-2.84	118.88	123.92
33	z	101	LMG	C8-O7-C10	-2.84	111.17	117.88
24	a	350	CLA	CHC-C1C-C2C	-2.84	118.91	126.65
24	c	504	CLA	CHC-C1C-C2C	-2.84	118.91	126.65
24	c	510	CLA	O2D-CGD-O1D	-2.84	118.11	123.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	514	CLA	CHC-C1C-C2C	-2.84	118.91	126.65
24	A	409	CLA	CHC-C1C-C2C	-2.84	118.92	126.65
24	C	507	CLA	O2A-CGA-O1A	-2.84	116.51	123.55
31	A	416[A]	PL9	C42-C43-C44	-2.84	120.56	127.68
24	b	604	CLA	O2D-CGD-O1D	-2.84	118.11	123.82
24	c	509	CLA	CHC-C1C-C2C	-2.83	118.92	126.65
24	B	602	CLA	C1-C2-C3	-2.83	120.74	125.96
24	C	509	CLA	C2A-C1A-CHA	-2.83	118.90	123.92
24	D	403	CLA	C1C-C2C-C3C	-2.83	103.78	106.92
24	b	601	CLA	CHC-C1C-C2C	-2.83	118.94	126.65
24	C	514	CLA	C2A-C1A-CHA	-2.83	118.90	123.92
31	A	416[A]	PL9	C22-C23-C24	-2.83	120.58	127.68
26	t	102	BCR	C7-C6-C5	-2.83	114.80	121.54
24	B	603	CLA	CHC-C1C-C2C	-2.83	118.94	126.65
24	b	602	CLA	C1D-CHD-C4C	-2.82	118.62	122.48
24	b	609	CLA	C4C-C3C-C2C	-2.82	102.58	106.91
24	C	509	CLA	CHC-C1C-C2C	-2.82	118.95	126.65
24	B	602	CLA	C1C-C2C-C3C	-2.82	103.79	106.92
31	d	405	PL9	C12-C13-C14	-2.82	120.60	127.68
24	C	508	CLA	CHC-C1C-C2C	-2.82	118.96	126.65
26	c	516	BCR	C37-C22-C21	-2.82	118.97	122.92
25	a	405	PHO	C1C-C2C-C3C	-2.82	103.24	106.51
33	j	101	LMG	C8-O7-C10	-2.82	111.22	117.88
24	d	403	CLA	CAA-C2A-C3A	-2.81	105.10	112.81
24	a	403	CLA	C2A-C1A-CHA	-2.81	118.93	123.92
24	B	602	CLA	C4A-NA-C1A	-2.81	102.97	106.45
26	d	404	BCR	C28-C27-C26	-2.81	108.95	113.78
26	B	617	BCR	C15-C14-C13	-2.81	123.30	127.31
26	b	619	BCR	C3-C4-C5	-2.81	108.95	113.78
24	d	403	CLA	C4C-C3C-C2C	-2.81	102.61	106.91
25	A	408	PHO	C6-C5-C3	-2.80	106.31	112.66
24	C	507	CLA	CAA-C2A-C3A	-2.80	105.13	112.81
24	B	610	CLA	CHC-C1C-C2C	-2.80	119.01	126.65
24	c	511	CLA	C4C-C3C-C2C	-2.80	102.61	106.91
24	c	505	CLA	CHC-C1C-C2C	-2.80	119.02	126.65
24	D	403	CLA	CAA-C2A-C3A	-2.80	105.15	112.81
24	B	609	CLA	C1D-CHD-C4C	-2.79	118.67	122.48
31	a	414[B]	PL9	C7-C8-C9	-2.79	122.05	126.71
24	A	406	CLA	C1D-CHD-C4C	-2.79	118.67	122.48
24	b	614	CLA	CHC-C1C-C2C	-2.78	119.07	126.65
24	c	506	CLA	C2A-C1A-CHA	-2.78	118.99	123.92
24	C	510	CLA	O2A-CGA-O1A	-2.78	116.65	123.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	O2A-CGA-O1A	-2.78	116.65	123.55
24	B	613	CLA	C1D-CHD-C4C	-2.78	118.69	122.48
25	a	406	PHO	CHD-C1D-C2D	-2.78	119.25	125.62
24	b	610	CLA	CAA-C2A-C3A	-2.77	105.20	112.81
38	d	408	LHG	O8-C23-O10	-2.77	116.66	123.55
24	c	514	CLA	CMA-C3A-C4A	-2.77	104.32	111.77
26	c	516	BCR	C38-C26-C25	-2.77	121.40	124.51
24	b	605	CLA	C4C-C3C-C2C	-2.77	102.65	106.91
26	h	102	BCR	C37-C22-C21	-2.77	119.04	122.92
24	C	502	CLA	C4C-C3C-C2C	-2.77	102.66	106.91
24	b	614	CLA	C2A-C1A-CHA	-2.77	119.01	123.92
24	c	513	CLA	CHC-C1C-C2C	-2.77	119.10	126.65
24	a	350	CLA	C2A-C1A-CHA	-2.77	119.02	123.92
24	B	609	CLA	CHC-C1C-C2C	-2.77	119.11	126.65
24	c	503	CLA	C4C-C3C-C2C	-2.76	102.67	106.91
31	A	416[B]	PL9	C22-C23-C24	-2.76	120.75	127.68
24	a	407	CLA	CHC-C1C-C2C	-2.76	119.13	126.65
24	C	512	CLA	CHC-C1C-C2C	-2.76	119.13	126.65
25	a	406	PHO	C4D-CHA-C1A	-2.76	118.94	125.06
26	C	516	BCR	C15-C14-C13	-2.75	123.38	127.31
33	j	101	LMG	O8-C28-O10	-2.75	116.72	123.55
24	B	612	CLA	C2A-C1A-CHA	-2.75	119.05	123.92
26	a	408	BCR	C37-C22-C21	-2.75	119.08	122.92
24	c	509	CLA	O1D-CGD-CBD	-2.75	119.67	124.60
24	a	403	CLA	C1-C2-C3	-2.74	120.90	125.96
26	c	516	BCR	C28-C27-C26	-2.74	109.06	113.78
24	d	403	CLA	C1C-C2C-C3C	-2.74	103.88	106.92
26	a	408	BCR	C38-C26-C25	-2.74	121.44	124.51
24	B	613	CLA	C7-C6-C5	-2.74	105.49	113.11
24	b	608	CLA	CHC-C1C-C2C	-2.74	119.17	126.65
24	c	504	CLA	C4C-C3C-C2C	-2.74	102.70	106.91
24	B	612	CLA	CHC-C1C-C2C	-2.74	119.18	126.65
24	B	610	CLA	O2A-CGA-O1A	-2.74	116.75	123.55
24	C	503	CLA	C4C-C3C-C2C	-2.74	102.71	106.91
26	C	515	BCR	C16-C17-C18	-2.74	123.41	127.31
25	a	405	PHO	CHD-C1D-C2D	-2.73	119.35	125.62
24	C	505	CLA	CBC-CAC-C3C	-2.73	104.65	112.41
24	C	507	CLA	C1D-CHD-C4C	-2.73	118.75	122.48
24	D	402	CLA	O2A-CGA-O1A	-2.73	116.77	123.55
24	c	514	CLA	C4C-C3C-C2C	-2.73	102.72	106.91
24	C	511	CLA	CHC-C1C-C2C	-2.73	119.20	126.65
24	B	614	CLA	CBC-CAC-C3C	-2.73	104.66	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	O2D-CGD-O1D	-2.73	118.33	123.82
33	c	521	LMG	C8-O7-C10	-2.73	111.43	117.88
24	B	615	CLA	O2D-CGD-O1D	-2.73	118.33	123.82
31	D	405	PL9	C32-C33-C34	-2.72	120.84	127.68
26	B	618	BCR	C28-C27-C26	-2.72	109.10	113.78
26	A	410	BCR	C8-C7-C6	-2.72	119.64	127.25
24	b	608	CLA	O2D-CGD-O1D	-2.72	118.35	123.82
26	k	101	BCR	C11-C10-C9	-2.71	123.44	127.31
24	C	512	CLA	C1-C2-C3	-2.71	120.96	125.96
24	C	512	CLA	O2D-CGD-O1D	-2.71	118.36	123.82
39	E	103	HEM	CBA-CAA-C2A	-2.71	107.30	112.48
24	B	613	CLA	CHC-C1C-C2C	-2.71	119.25	126.65
24	c	515	CLA	C2A-C1A-CHA	-2.71	119.11	123.92
24	b	610	CLA	CHC-C1C-C2C	-2.71	119.26	126.65
24	D	402	CLA	C4C-C3C-C2C	-2.71	102.75	106.91
24	b	603	CLA	CHC-C1C-C2C	-2.71	119.26	126.65
24	d	403	CLA	C2A-C1A-CHA	-2.70	119.12	123.92
24	c	515	CLA	CHC-C1C-C2C	-2.70	119.28	126.65
24	B	611	CLA	O2A-CGA-O1A	-2.70	116.84	123.55
31	D	405	PL9	C12-C13-C14	-2.70	120.90	127.68
24	b	603	CLA	C2A-C1A-CHA	-2.69	119.14	123.92
24	b	612	CLA	O2D-CGD-O1D	-2.69	118.40	123.82
36	C	518	DGD	O1G-C1A-O1A	-2.69	116.86	123.55
24	C	503	CLA	CHC-C1C-C2C	-2.69	119.31	126.65
24	B	607	CLA	C1D-CHD-C4C	-2.69	118.81	122.48
26	Y	101	BCR	C38-C26-C25	-2.69	121.50	124.51
26	d	404	BCR	C40-C30-C25	-2.69	105.94	110.31
24	B	613	CLA	C4C-C3C-C2C	-2.69	102.78	106.91
36	c	518	DGD	O3G-C3G-C2G	-2.69	104.59	110.99
35	B	623	HTG	O2-C2-C3	-2.69	104.51	110.36
26	D	404	BCR	C33-C5-C6	-2.69	121.50	124.51
26	b	618	BCR	C28-C27-C26	-2.68	109.17	113.78
26	H	101	BCR	C16-C17-C18	-2.68	123.48	127.31
24	B	610	CLA	O2D-CGD-O1D	-2.68	118.42	123.82
24	C	513	CLA	CHC-C1C-C2C	-2.67	119.36	126.65
24	C	511	CLA	CBC-CAC-C3C	-2.67	104.82	112.41
24	C	506	CLA	O2D-CGD-O1D	-2.67	118.44	123.82
24	B	614	CLA	C2A-C1A-CHA	-2.67	119.19	123.92
24	b	608	CLA	CMA-C3A-C4A	-2.67	104.60	111.77
24	c	510	CLA	C4C-C3C-C2C	-2.67	102.82	106.91
33	b	621	LMG	O8-C28-O10	-2.67	116.93	123.55
24	C	510	CLA	CHC-C1C-C2C	-2.66	119.38	126.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	CLA	CMA-C3A-C2A	-2.66	102.97	113.77
24	B	616	CLA	CHC-C1C-C2C	-2.66	119.39	126.65
25	a	406	PHO	C4D-ND-C1D	-2.66	102.18	106.98
31	A	416[B]	PL9	C12-C13-C14	-2.66	121.00	127.68
24	A	406	CLA	C4C-C3C-C2C	-2.66	102.83	106.91
24	c	511	CLA	O2D-CGD-O1D	-2.66	118.47	123.82
24	D	403	CLA	CBC-CAC-C3C	-2.66	104.86	112.41
24	B	611	CLA	CBC-CAC-C3C	-2.66	104.87	112.41
26	c	517	BCR	C11-C10-C9	-2.65	123.52	127.31
33	Z	101	LMG	C9-C8-C7	-2.65	105.87	111.86
24	b	616	CLA	CHC-C1C-C2C	-2.65	119.42	126.65
24	b	604	CLA	CHC-C1C-C2C	-2.65	119.42	126.65
24	b	611	CLA	C2A-C1A-CHA	-2.65	119.22	123.92
24	D	403	CLA	C2A-C1A-CHA	-2.65	119.22	123.92
24	B	606	CLA	CBC-CAC-C3C	-2.65	104.89	112.41
24	c	512	CLA	O2A-CGA-O1A	-2.65	116.97	123.55
24	A	405	CLA	CMA-C3A-C2A	-2.65	103.03	113.77
24	A	404	CLA	C2A-C1A-CHA	-2.65	119.23	123.92
26	y	101	BCR	C10-C11-C12	-2.65	115.11	123.23
24	d	402	CLA	CHC-C1C-C2C	-2.64	119.45	126.65
24	D	402	CLA	O2D-CGD-O1D	-2.64	118.51	123.82
24	b	604	CLA	O2A-CGA-O1A	-2.64	117.00	123.55
26	c	517	BCR	C20-C21-C22	-2.64	123.54	127.31
26	D	404	BCR	C16-C17-C18	-2.64	123.55	127.31
25	a	405	PHO	O1D-CGD-CBD	-2.64	119.87	124.60
24	A	409	CLA	C2A-C1A-CHA	-2.63	119.25	123.92
24	b	607	CLA	CAA-C2A-C3A	-2.63	105.59	112.81
24	b	611	CLA	O2A-CGA-O1A	-2.63	117.01	123.55
26	b	619	BCR	C16-C17-C18	-2.63	123.55	127.31
26	B	618	BCR	C7-C8-C9	-2.63	122.26	126.21
24	d	402	CLA	O2A-CGA-O1A	-2.63	117.01	123.55
24	B	610	CLA	CAA-CBA-CGA	-2.63	105.42	113.35
26	b	619	BCR	C31-C1-C6	-2.63	106.05	110.31
24	C	513	CLA	CBA-CAA-C2A	-2.62	105.95	113.80
24	C	511	CLA	O1D-CGD-CBD	-2.62	119.90	124.60
24	c	508	CLA	CBC-CAC-C3C	-2.62	104.98	112.41
24	C	511	CLA	C4C-C3C-C2C	-2.62	102.90	106.91
24	b	601	CLA	CBC-CAC-C3C	-2.62	104.99	112.41
25	a	405	PHO	C4D-CHA-C1A	-2.61	119.25	125.06
38	D	406	LHG	O8-C23-O10	-2.61	117.06	123.55
24	b	612	CLA	O2A-CGA-O1A	-2.61	117.07	123.55
24	A	404	CLA	CHC-C1C-C2C	-2.61	119.54	126.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	V	203	HEM	CBA-CAA-C2A	-2.60	107.50	112.48
24	b	613	CLA	CHC-C1C-C2C	-2.60	119.56	126.65
24	B	602	CLA	CHC-C1C-C2C	-2.60	119.56	126.65
26	h	102	BCR	C10-C11-C12	-2.60	115.26	123.23
24	c	508	CLA	O2A-CGA-O1A	-2.60	117.10	123.55
24	B	605	CLA	CHC-C1C-C2C	-2.60	119.57	126.65
24	C	514	CLA	CHC-C1C-C2C	-2.60	119.57	126.65
24	B	604	CLA	O1D-CGD-CBD	-2.59	119.94	124.60
24	a	407	CLA	C1-C2-C3	-2.59	121.18	125.96
24	C	502	CLA	C2A-C1A-CHA	-2.59	119.32	123.92
24	A	406	CLA	O2D-CGD-O1D	-2.59	118.60	123.82
24	C	502	CLA	C1-C2-C3	-2.59	121.18	125.96
24	b	606	CLA	CAA-C2A-C3A	-2.59	105.71	112.81
26	T	101	BCR	C3-C4-C5	-2.59	109.33	113.78
27	b	620	SQD	C1-O5-C5	-2.59	108.84	113.72
26	k	101	BCR	C7-C8-C9	-2.58	122.33	126.21
26	Y	101	BCR	C10-C11-C12	-2.58	115.30	123.23
24	B	613	CLA	O2D-CGD-O1D	-2.58	118.62	123.82
26	B	618	BCR	C24-C23-C22	-2.58	122.33	126.21
24	C	505	CLA	C2A-C1A-CHA	-2.58	119.34	123.92
24	c	508	CLA	C4C-C3C-C2C	-2.58	102.95	106.91
24	B	601	CLA	C1-C2-C3	-2.58	121.20	125.96
24	C	507	CLA	C2A-C1A-CHA	-2.58	119.35	123.92
24	c	507	CLA	O1D-CGD-CBD	-2.57	119.98	124.60
38	l	101	LHG	O8-C23-O10	-2.57	117.17	123.55
24	b	607	CLA	O2A-CGA-O1A	-2.57	117.18	123.55
38	d	406	LHG	C5-O7-C7	-2.56	111.82	117.88
24	C	505	CLA	C4C-C3C-C2C	-2.56	102.98	106.91
26	B	618	BCR	C37-C22-C21	-2.56	119.34	122.92
26	d	404	BCR	C21-C20-C19	-2.56	115.38	123.23
24	b	616	CLA	CBC-CAC-C3C	-2.56	105.14	112.41
26	c	516	BCR	C33-C5-C6	-2.56	121.65	124.51
24	C	513	CLA	O2D-CGD-O1D	-2.55	118.69	123.82
24	A	405	CLA	C4C-C3C-C2C	-2.55	103.00	106.91
24	c	508	CLA	O2D-CGD-O1D	-2.55	118.70	123.82
26	y	101	BCR	C21-C20-C19	-2.55	115.42	123.23
24	B	611	CLA	C2A-C1A-CHA	-2.55	119.41	123.92
24	B	603	CLA	C4C-C3C-C2C	-2.54	103.01	106.91
26	d	404	BCR	C16-C17-C18	-2.54	123.69	127.31
24	c	503	CLA	CBC-CAC-C3C	-2.54	105.21	112.41
24	B	607	CLA	CAA-C2A-C3A	-2.53	105.86	112.81
27	b	620	SQD	C1-C2-C3	-2.53	105.27	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C3-C4-C5	-2.53	109.43	113.78
24	b	616	CLA	C1C-C2C-C3C	-2.53	104.12	106.92
31	d	405	PL9	C22-C23-C24	-2.52	121.34	127.68
24	b	607	CLA	C2A-C1A-CHA	-2.52	119.44	123.92
26	C	516	BCR	C15-C16-C17	-2.52	118.08	123.46
24	A	409	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
31	D	405	PL9	C27-C28-C29	-2.52	121.35	127.68
26	b	618	BCR	C24-C23-C22	-2.52	122.43	126.21
24	C	502	CLA	CBC-CAC-C3C	-2.52	105.26	112.41
26	C	515	BCR	C11-C10-C9	-2.52	123.72	127.31
27	F	101	SQD	C44-O6-C1	-2.52	108.60	113.76
24	c	514	CLA	CBC-CAC-C3C	-2.52	105.27	112.41
24	b	606	CLA	OBD-CAD-C3D	-2.51	123.40	128.03
26	B	618	BCR	C33-C5-C6	-2.51	121.70	124.51
24	B	613	CLA	C2A-C1A-CHA	-2.51	119.47	123.92
24	b	616	CLA	O2A-CGA-O1A	-2.51	117.32	123.55
26	B	619	BCR	C7-C8-C9	-2.51	122.44	126.21
24	a	403	CLA	O2A-CGA-O1A	-2.51	117.32	123.55
33	a	417	LMG	C8-O7-C10	-2.50	111.96	117.88
26	c	517	BCR	C24-C23-C22	-2.50	122.45	126.21
24	A	405	CLA	O2A-CGA-O1A	-2.50	117.34	123.55
31	D	405	PL9	C17-C18-C19	-2.50	121.40	127.68
24	B	604	CLA	CHC-C1C-C2C	-2.50	119.83	126.65
24	C	505	CLA	O2D-CGD-O1D	-2.50	118.79	123.82
26	H	101	BCR	C3-C4-C5	-2.50	109.48	113.78
27	a	411	SQD	C5-C6-S	-2.50	110.86	114.34
24	A	404	CLA	CAA-CBA-CGA	-2.49	105.83	113.35
24	c	514	CLA	O1D-CGD-CBD	-2.49	120.12	124.60
24	b	607	CLA	CBC-CAC-C3C	-2.49	105.33	112.41
26	B	617	BCR	C31-C1-C6	-2.49	106.27	110.31
24	c	512	CLA	O1D-CGD-CBD	-2.49	120.13	124.60
24	D	403	CLA	CHC-C1C-C2C	-2.49	119.87	126.65
24	c	506	CLA	C4C-C3C-C2C	-2.49	103.09	106.91
24	B	607	CLA	C1-C2-C3	-2.49	121.38	125.96
26	y	101	BCR	C40-C30-C25	-2.49	106.28	110.31
26	B	619	BCR	C21-C20-C19	-2.49	115.61	123.23
26	c	516	BCR	C24-C23-C22	-2.48	122.48	126.21
24	d	402	CLA	CAA-C2A-C3A	-2.48	106.00	112.81
26	a	408	BCR	C33-C5-C6	-2.48	121.73	124.51
26	b	618	BCR	C16-C17-C18	-2.48	123.77	127.31
24	b	605	CLA	C1-C2-C3	-2.48	121.39	125.96
24	b	606	CLA	O2A-CGA-O1A	-2.48	117.40	123.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	OBD-CAD-C3D	-2.48	123.46	128.03
24	a	350	CLA	C4C-C3C-C2C	-2.48	103.11	106.91
24	B	601	CLA	CHC-C1C-C2C	-2.48	119.89	126.65
27	f	101	SQD	C5-C6-S	-2.47	110.89	114.34
24	A	406	CLA	CHC-C1C-C2C	-2.47	119.91	126.65
24	b	616	CLA	C4A-NA-C1A	-2.47	103.39	106.45
24	C	505	CLA	OBD-CAD-C3D	-2.47	123.48	128.03
27	b	620	SQD	C44-O6-C1	-2.47	108.70	113.76
24	A	405	CLA	C1-C2-C3	-2.47	121.41	125.96
26	c	517	BCR	C15-C14-C13	-2.47	123.79	127.31
27	A	411	SQD	O48-C23-O10	-2.47	117.43	123.55
24	B	605	CLA	C2A-C1A-CHA	-2.47	119.55	123.92
24	B	603	CLA	C7-C6-C5	-2.46	106.26	113.11
24	C	504	CLA	C4A-NA-C1A	-2.46	103.39	106.45
24	C	506	CLA	CHC-C1C-C2C	-2.46	119.93	126.65
36	c	519	DGD	C2G-O2G-C1B	-2.46	112.06	117.88
24	b	616	CLA	O1D-CGD-CBD	-2.46	120.18	124.60
24	B	606	CLA	C4A-NA-C1A	-2.46	103.40	106.45
24	C	505	CLA	O1D-CGD-CBD	-2.46	120.19	124.60
24	b	602	CLA	C11-C10-C8	-2.46	107.67	115.73
36	h	103	DGD	O1G-C1A-O1A	-2.45	117.45	123.55
25	A	408	PHO	C4A-NA-C1A	-2.45	106.18	108.16
24	a	407	CLA	O2A-CGA-O1A	-2.45	117.46	123.55
26	K	102	BCR	C10-C11-C12	-2.45	115.71	123.23
24	b	611	CLA	C4A-NA-C1A	-2.45	103.41	106.45
24	B	616	CLA	C1C-C2C-C3C	-2.45	104.21	106.92
24	d	402	CLA	C2A-C1A-CHA	-2.45	119.58	123.92
24	b	608	CLA	OBD-CAD-C3D	-2.44	123.52	128.03
24	B	614	CLA	C4C-C3C-C2C	-2.44	103.16	106.91
24	D	402	CLA	C2A-C1A-CHA	-2.44	119.59	123.92
26	C	516	BCR	C16-C17-C18	-2.44	123.83	127.31
24	b	602	CLA	CHC-C1C-C2C	-2.43	120.02	126.65
24	c	510	CLA	C2A-C1A-CHA	-2.43	119.61	123.92
24	C	511	CLA	O2D-CGD-O1D	-2.43	118.94	123.82
24	C	504	CLA	O2A-CGA-O1A	-2.43	117.53	123.55
24	C	511	CLA	O2A-CGA-O1A	-2.43	117.53	123.55
24	A	409	CLA	O2D-CGD-O1D	-2.42	118.94	123.82
24	B	602	CLA	C2A-C1A-CHA	-2.42	119.62	123.92
38	d	407	LHG	O8-C23-O10	-2.42	117.54	123.55
26	C	516	BCR	C3-C4-C5	-2.42	109.62	113.78
24	c	507	CLA	O2D-CGD-O1D	-2.42	118.96	123.82
34	M	101	LMT	C1-O1'-C1'	-2.41	109.72	113.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	403	CLA	C17-C16-C15	-2.41	101.59	113.25
24	B	615	CLA	O2A-CGA-O1A	-2.41	117.57	123.55
26	b	617	BCR	C24-C23-C22	-2.41	122.59	126.21
25	a	405	PHO	C3B-C2B-C1B	-2.41	101.44	106.30
27	B	620	SQD	O48-C23-O10	-2.41	117.57	123.55
26	t	102	BCR	C21-C20-C19	-2.40	115.87	123.23
24	B	604	CLA	O2D-CGD-O1D	-2.40	118.99	123.82
24	b	605	CLA	CBC-CAC-C3C	-2.40	105.60	112.41
36	C	518	DGD	C2G-O2G-C1B	-2.40	112.21	117.88
24	b	604	CLA	O1D-CGD-CBD	-2.40	120.30	124.60
26	H	101	BCR	C7-C8-C9	-2.40	122.61	126.21
27	f	101	SQD	O47-C7-O49	-2.40	117.70	123.68
27	A	413	SQD	O48-C23-O10	-2.39	117.61	123.55
34	B	630	LMT	C1-O1'-C1'	-2.39	109.76	113.87
24	c	513	CLA	CBC-CAC-C3C	-2.39	105.62	112.41
24	b	608	CLA	O2A-CGA-O1A	-2.39	117.62	123.55
24	c	504	CLA	C2A-C1A-CHA	-2.39	119.68	123.92
26	b	619	BCR	C24-C23-C22	-2.38	122.63	126.21
26	C	516	BCR	C21-C20-C19	-2.38	115.92	123.23
26	b	619	BCR	C21-C20-C19	-2.38	115.92	123.23
24	a	403	CLA	CMA-C3A-C2A	-2.38	104.11	113.77
24	C	514	CLA	CAA-C2A-C3A	-2.38	106.28	112.81
26	H	101	BCR	C34-C9-C10	-2.38	119.59	122.92
24	c	510	CLA	O1D-CGD-CBD	-2.38	120.33	124.60
26	B	617	BCR	C11-C10-C9	-2.38	123.92	127.31
24	c	508	CLA	C2A-C1A-CHA	-2.38	119.70	123.92
24	B	615	CLA	CHC-C1C-C2C	-2.38	120.16	126.65
24	B	616	CLA	C4A-NA-C1A	-2.38	103.50	106.45
27	F	101	SQD	O47-C7-O49	-2.38	117.75	123.68
24	b	602	CLA	C4A-NA-C1A	-2.38	103.50	106.45
26	c	516	BCR	C34-C9-C10	-2.37	119.60	122.92
24	A	409	CLA	CBC-CAC-C3C	-2.37	105.67	112.41
33	C	520	LMG	O8-C28-O10	-2.37	117.66	123.55
24	b	614	CLA	O2A-CGA-O1A	-2.37	117.67	123.55
24	B	607	CLA	C2A-C1A-CHA	-2.37	119.72	123.92
26	k	101	BCR	C16-C17-C18	-2.37	123.93	127.31
24	C	503	CLA	C2A-C1A-CHA	-2.37	119.72	123.92
24	c	511	CLA	CBC-CAC-C3C	-2.37	105.69	112.41
34	m	102	LMT	C1-O1'-C1'	-2.36	109.81	113.87
36	C	519	DGD	O3G-C3G-C2G	-2.36	105.36	110.99
26	K	102	BCR	C15-C14-C13	-2.36	123.94	127.31
26	H	101	BCR	C24-C23-C22	-2.36	122.66	126.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	407	PHO	C3B-C2B-C1B	-2.36	101.53	106.30
24	b	616	CLA	C1-C2-C3	-2.36	121.61	125.96
24	B	616	CLA	O1D-CGD-CBD	-2.36	120.36	124.60
26	A	410	BCR	C20-C21-C22	-2.36	123.94	127.31
24	c	507	CLA	CHC-C1C-C2C	-2.36	120.21	126.65
31	A	416[B]	PL9	C47-C48-C49	-2.36	119.38	127.80
24	C	507	CLA	C4C-C3C-C2C	-2.36	103.29	106.91
31	D	405	PL9	C22-C23-C24	-2.36	121.76	127.68
36	H	102	DGD	C2G-O2G-C1B	-2.36	112.31	117.88
24	A	404	CLA	C4A-NA-C1A	-2.36	103.53	106.45
24	b	601	CLA	C2A-C1A-CHA	-2.36	119.74	123.92
24	C	511	CLA	C2A-C1A-CHA	-2.36	119.74	123.92
24	B	609	CLA	CBC-CAC-C3C	-2.35	105.73	112.41
24	B	606	CLA	C2A-C1A-CHA	-2.35	119.74	123.92
24	c	506	CLA	CBC-CAC-C3C	-2.35	105.73	112.41
31	d	405	PL9	C36-C37-C38	-2.35	103.89	111.97
24	a	407	CLA	OBD-CAD-C3D	-2.35	123.69	128.03
24	C	506	CLA	O1D-CGD-CBD	-2.35	120.38	124.60
25	A	407	PHO	C4D-CHA-C1A	-2.35	119.84	125.06
24	c	509	CLA	CBC-CAC-C3C	-2.34	105.76	112.41
26	B	619	BCR	C20-C21-C22	-2.34	123.97	127.31
25	a	405	PHO	CBA-CAA-C2A	-2.34	106.79	113.80
24	b	606	CLA	C4A-NA-C1A	-2.34	103.55	106.45
31	d	405	PL9	C17-C18-C19	-2.34	121.81	127.68
24	a	404	CLA	O2A-CGA-O1A	-2.34	117.75	123.55
26	b	618	BCR	C38-C26-C25	-2.34	121.89	124.51
24	C	506	CLA	C1-C2-C3	-2.34	121.65	125.96
24	C	509	CLA	O2A-CGA-O1A	-2.33	117.76	123.55
27	a	409	SQD	O4-C4-C3	-2.33	105.28	110.36
24	B	612	CLA	C11-C12-C13	-2.33	108.08	115.73
26	h	102	BCR	C36-C18-C17	-2.33	119.66	122.92
24	B	601	CLA	C2A-C1A-CHA	-2.33	119.80	123.92
24	B	610	CLA	C2A-C1A-CHA	-2.33	119.80	123.92
24	c	512	CLA	C4C-C3C-C2C	-2.32	103.34	106.91
26	B	619	BCR	C16-C15-C14	-2.32	118.50	123.46
24	c	510	CLA	CAA-C2A-C3A	-2.32	106.45	112.81
25	a	406	PHO	C3B-C2B-C1B	-2.32	101.61	106.30
24	b	602	CLA	CMA-C3A-C2A	-2.32	104.37	113.77
24	b	601	CLA	CAA-C2A-C3A	-2.32	106.45	112.81
27	A	411	SQD	C45-O47-C7	-2.32	112.40	117.88
24	b	610	CLA	C2A-C1A-CHA	-2.32	119.81	123.92
24	b	615	CLA	C11-C12-C13	-2.32	108.13	115.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C16-C15-C14	-2.32	118.52	123.46
24	C	508	CLA	C6-C7-C8	-2.32	108.13	115.73
26	H	101	BCR	C16-C15-C14	-2.31	118.52	123.46
27	a	409	SQD	O48-C23-O10	-2.31	117.81	123.55
24	a	350	CLA	O2A-CGA-O1A	-2.31	117.81	123.55
24	c	514	CLA	CBA-CAA-C2A	-2.31	106.88	113.80
24	B	607	CLA	C4C-C3C-C2C	-2.31	103.36	106.91
24	B	614	CLA	C1-C2-C3	-2.31	121.70	125.96
24	b	615	CLA	CBC-CAC-C3C	-2.31	105.85	112.41
31	D	405	PL9	C7-C8-C9	-2.31	122.85	126.71
24	b	603	CLA	O1D-CGD-CBD	-2.31	120.45	124.60
24	b	604	CLA	C2A-C1A-CHA	-2.31	119.83	123.92
26	T	101	BCR	C7-C6-C5	-2.31	116.04	121.54
24	B	609	CLA	O2D-CGD-O1D	-2.30	119.18	123.82
24	B	613	CLA	O2A-CGA-O1A	-2.30	117.83	123.55
24	B	606	CLA	OBD-CAD-C3D	-2.30	123.78	128.03
24	c	503	CLA	O2A-CGA-O1A	-2.30	117.84	123.55
24	A	405	CLA	CHC-C1C-C2C	-2.30	120.38	126.65
24	C	509	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
24	A	404	CLA	OBD-CAD-C3D	-2.29	123.80	128.03
24	B	615	CLA	CBC-CAC-C3C	-2.29	105.90	112.41
25	A	408	PHO	O2A-CGA-O1A	-2.29	117.86	123.55
24	a	407	CLA	CBC-CAC-C3C	-2.29	105.91	112.41
24	b	613	CLA	O2D-CGD-O1D	-2.29	119.21	123.82
25	A	408	PHO	C1C-C2C-C3C	-2.29	103.85	106.51
24	d	403	CLA	CHC-C1C-C2C	-2.29	120.41	126.65
31	D	405	PL9	C40-C39-C38	-2.29	117.59	123.69
24	a	404	CLA	C2A-C1A-CHA	-2.29	119.87	123.92
26	Y	101	BCR	C40-C30-C25	-2.28	106.60	110.31
26	c	516	BCR	C21-C20-C19	-2.28	116.22	123.23
26	b	617	BCR	C15-C16-C17	-2.28	118.59	123.46
31	d	405	PL9	C32-C33-C34	-2.28	121.95	127.68
26	Y	101	BCR	C21-C20-C19	-2.28	116.23	123.23
24	c	512	CLA	C2A-C1A-CHA	-2.28	119.87	123.92
24	B	606	CLA	CHC-C1C-C2C	-2.28	120.43	126.65
24	a	350	CLA	CMA-C3A-C2A	-2.28	104.52	113.77
24	B	606	CLA	O2A-CGA-O1A	-2.28	117.89	123.55
31	d	405	PL9	C27-C28-C29	-2.28	121.96	127.68
27	A	413	SQD	O6-C44-C45	-2.28	105.57	110.99
34	B	622	LMT	C1-O1'-C1'	-2.28	109.96	113.87
38	d	408	LHG	C6-C5-C4	-2.28	106.72	111.86
36	H	102	DGD	O1G-C1A-O1A	-2.28	117.90	123.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	CBC-CAC-C3C	-2.27	105.95	112.41
24	a	407	CLA	C2A-C1A-CHA	-2.27	119.89	123.92
26	y	101	BCR	C11-C10-C9	-2.27	124.07	127.31
38	d	406	LHG	O7-C7-O9	-2.27	118.01	123.68
25	a	405	PHO	O2A-CGA-O1A	-2.27	117.91	123.55
26	h	102	BCR	C20-C21-C22	-2.27	124.07	127.31
24	D	402	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
24	B	605	CLA	OBD-CAD-C3D	-2.27	123.85	128.03
24	D	403	CLA	O2A-CGA-O1A	-2.27	117.92	123.55
26	y	101	BCR	C23-C24-C25	-2.26	120.91	127.25
24	A	405	CLA	OBD-CAD-C3D	-2.26	123.86	128.03
36	c	519	DGD	O1G-C1A-O1A	-2.26	117.94	123.55
26	Y	101	BCR	C36-C18-C17	-2.26	119.76	122.92
25	A	407	PHO	C4A-NA-C1A	-2.26	106.34	108.16
36	C	518	DGD	C3G-O3G-C1D	-2.26	109.13	113.76
25	A	408	PHO	C3B-C2B-C1B	-2.25	101.75	106.30
24	b	606	CLA	C6-C7-C8	-2.25	108.33	115.73
24	a	404	CLA	CBC-CAC-C3C	-2.25	106.01	112.41
24	C	510	CLA	C2A-C1A-CHA	-2.25	119.92	123.92
25	A	407	PHO	CBA-CAA-C2A	-2.25	107.06	113.80
24	d	403	CLA	CBC-CAC-C3C	-2.25	106.02	112.41
24	c	515	CLA	O2D-CGD-O1D	-2.25	119.30	123.82
26	b	618	BCR	C37-C22-C21	-2.25	119.78	122.92
38	E	101	LHG	C5-O7-C7	-2.25	112.57	117.88
24	C	505	CLA	O2A-CGA-O1A	-2.24	117.98	123.55
26	c	516	BCR	C7-C8-C9	-2.24	122.84	126.21
31	A	416[A]	PL9	C37-C36-C34	-2.24	105.34	112.93
26	B	619	BCR	C10-C11-C12	-2.24	116.36	123.23
33	c	522	LMG	O8-C28-O10	-2.24	117.99	123.55
33	J	101	LMG	O8-C28-O10	-2.24	117.99	123.55
24	c	506	CLA	O1D-CGD-CBD	-2.24	120.58	124.60
26	d	404	BCR	C16-C15-C14	-2.24	118.69	123.46
24	a	404	CLA	O2D-CGD-O1D	-2.24	119.32	123.82
26	a	408	BCR	C15-C16-C17	-2.24	118.69	123.46
24	D	403	CLA	C1-C2-C3	-2.24	121.84	125.96
24	c	506	CLA	O2A-CGA-O1A	-2.24	118.00	123.55
24	b	606	CLA	C2A-C1A-CHA	-2.24	119.95	123.92
27	B	620	SQD	C1-C2-C3	-2.24	105.82	109.98
39	e	102	HEM	C3C-C4C-NC	-2.23	106.73	110.94
26	B	618	BCR	C10-C11-C12	-2.23	116.38	123.23
26	H	101	BCR	C31-C1-C6	-2.23	106.69	110.31
24	b	616	CLA	C2A-C1A-CHA	-2.23	119.96	123.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C39-C30-C25	-2.23	106.69	110.31
26	t	102	BCR	C15-C16-C17	-2.23	118.70	123.46
24	B	605	CLA	C7-C6-C5	-2.23	106.92	113.11
26	C	515	BCR	C20-C21-C22	-2.23	124.13	127.31
24	B	614	CLA	OBD-CAD-C3D	-2.22	123.93	128.03
38	D	357	LHG	O7-C7-O9	-2.22	118.13	123.68
24	A	404	CLA	CMA-C3A-C2A	-2.22	104.75	113.77
24	A	405	CLA	C2A-C1A-CHA	-2.22	119.98	123.92
24	C	508	CLA	O2A-CGA-O1A	-2.22	118.05	123.55
24	c	513	CLA	CAA-CBA-CGA	-2.22	106.67	113.35
24	c	503	CLA	C2A-C1A-CHA	-2.22	119.99	123.92
24	C	511	CLA	C4-C3-C2	-2.22	117.78	123.69
31	d	405	PL9	C7-C8-C9	-2.22	123.01	126.71
26	b	617	BCR	C16-C17-C18	-2.21	124.15	127.31
26	t	102	BCR	C10-C11-C12	-2.21	116.44	123.23
31	a	414[B]	PL9	C12-C13-C14	-2.21	122.13	127.68
31	d	405	PL9	C20-C19-C18	-2.21	117.80	123.69
24	B	610	CLA	C1-C2-C3	-2.21	121.89	125.96
24	B	616	CLA	C2A-C1A-CHA	-2.21	120.01	123.92
24	B	608	CLA	C2A-C1A-CHA	-2.21	120.01	123.92
24	d	402	CLA	CBC-CAC-C3C	-2.21	106.15	112.41
26	A	410	BCR	C31-C1-C6	-2.20	106.74	110.31
24	d	403	CLA	O2A-CGA-O1A	-2.20	118.08	123.55
24	C	508	CLA	C1-C2-C3	-2.20	121.90	125.96
38	L	101	LHG	C6-C5-C4	-2.20	106.89	111.86
26	B	618	BCR	C38-C26-C25	-2.20	122.05	124.51
33	z	101	LMG	C7-O1-C1	-2.20	109.25	113.76
26	D	404	BCR	C40-C30-C25	-2.20	106.75	110.31
24	c	512	CLA	CMA-C3A-C4A	-2.19	105.87	111.77
31	a	414[A]	PL9	C47-C48-C49	-2.19	119.97	127.80
33	j	101	LMG	O7-C10-O9	-2.19	118.20	123.68
24	b	608	CLA	C6-C7-C8	-2.19	108.53	115.73
24	B	608	CLA	O2D-CGD-O1D	-2.19	119.41	123.82
27	f	101	SQD	C4-C3-C2	-2.19	106.97	110.84
24	c	511	CLA	C2A-C1A-CHA	-2.19	120.03	123.92
33	A	418	LMG	C8-O7-C10	-2.19	112.70	117.88
24	b	604	CLA	C6-C7-C8	-2.19	108.54	115.73
24	b	602	CLA	C11-C12-C13	-2.19	108.54	115.73
34	t	101	LMT	C3'-C4'-C5'	-2.19	106.22	110.88
24	B	613	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
26	K	102	BCR	C16-C17-C18	-2.19	124.18	127.31
25	a	406	PHO	CBA-CAA-C2A	-2.19	107.24	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	517	BCR	C15-C16-C17	-2.19	118.79	123.46
24	b	608	CLA	C2A-C1A-CHA	-2.19	120.04	123.92
26	B	619	BCR	C11-C10-C9	-2.19	124.19	127.31
26	k	101	BCR	C39-C30-C25	-2.19	106.76	110.31
26	k	101	BCR	C15-C16-C17	-2.18	118.81	123.46
26	b	619	BCR	C16-C15-C14	-2.18	118.81	123.46
26	K	102	BCR	C38-C26-C25	-2.18	122.07	124.51
24	B	610	CLA	C6-C7-C8	-2.18	108.57	115.73
24	c	507	CLA	C1-C2-C3	-2.18	121.94	125.96
24	C	510	CLA	C16-C15-C13	-2.18	108.58	115.73
24	B	601	CLA	O1D-CGD-CBD	-2.18	120.69	124.60
38	E	101	LHG	O8-C23-O10	-2.17	118.15	123.55
24	B	602	CLA	C11-C12-C13	-2.17	108.60	115.73
26	a	408	BCR	C10-C11-C12	-2.17	116.57	123.23
36	C	517	DGD	O1G-C1A-O1A	-2.17	118.16	123.55
24	c	508	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
24	B	601	CLA	CBC-CAC-C3C	-2.17	106.25	112.41
24	c	509	CLA	C4C-C3C-C2C	-2.17	103.58	106.91
27	A	411	SQD	O9-S-O7	-2.17	106.35	113.86
24	a	407	CLA	C4A-NA-C1A	-2.17	103.76	106.45
26	h	102	BCR	C16-C15-C14	-2.17	118.84	123.46
26	b	618	BCR	C11-C10-C9	-2.17	124.22	127.31
24	c	514	CLA	CAA-C2A-C3A	-2.16	106.88	112.81
24	D	403	CLA	CMA-C3A-C2A	-2.16	105.00	113.77
33	c	522	LMG	C9-C8-C7	-2.16	106.98	111.86
24	b	607	CLA	C6-C7-C8	-2.16	108.64	115.73
24	b	615	CLA	O2D-CGD-O1D	-2.16	119.47	123.82
24	A	406	CLA	CMA-C3A-C4A	-2.16	105.97	111.77
24	B	604	CLA	C6-C7-C8	-2.16	108.64	115.73
25	a	406	PHO	C1C-C2C-C3C	-2.16	104.01	106.51
25	a	405	PHO	C3A-C4A-CHB	-2.16	118.11	121.75
26	t	102	BCR	C23-C22-C21	-2.16	115.63	118.94
24	b	613	CLA	C2A-C1A-CHA	-2.16	120.10	123.92
24	D	403	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
24	b	603	CLA	C4A-NA-C1A	-2.15	103.79	106.45
26	A	410	BCR	C40-C30-C25	-2.14	106.83	110.31
24	b	609	CLA	CMA-C3A-C4A	-2.14	106.02	111.77
26	c	517	BCR	C3-C4-C5	-2.14	110.10	113.78
26	t	102	BCR	C3-C4-C5	-2.14	110.10	113.78
27	A	411	SQD	O47-C7-O49	-2.14	118.33	123.68
25	a	406	PHO	C4A-NA-C1A	-2.14	106.43	108.16
26	B	618	BCR	C21-C20-C19	-2.14	116.67	123.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	403	CLA	CAA-CBA-CGA	-2.14	106.90	113.35
26	B	618	BCR	C3-C4-C5	-2.14	110.10	113.78
24	B	602	CLA	CMA-C3A-C4A	-2.14	106.03	111.77
31	d	405	PL9	C40-C39-C38	-2.14	117.99	123.69
33	B	621	LMG	O8-C28-O10	-2.14	118.25	123.55
24	B	605	CLA	CAA-C2A-C3A	-2.13	106.96	112.81
24	B	602	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
26	b	617	BCR	C20-C21-C22	-2.13	124.27	127.31
26	A	410	BCR	C10-C11-C12	-2.13	116.69	123.23
24	B	612	CLA	O2A-CGA-O1A	-2.13	118.26	123.55
24	D	402	CLA	CAA-C2A-C3A	-2.13	106.97	112.81
24	a	403	CLA	C4C-C3C-C2C	-2.13	103.64	106.91
26	t	102	BCR	C12-C13-C14	-2.13	115.68	118.94
24	b	609	CLA	C4A-NA-C1A	-2.13	103.81	106.45
27	B	620	SQD	C5-C6-S	-2.13	111.38	114.34
24	B	610	CLA	CMA-C3A-C2A	-2.13	105.15	113.77
24	A	409	CLA	O2A-CGA-O1A	-2.13	118.27	123.55
24	b	610	CLA	O1D-CGD-CBD	-2.12	120.79	124.60
27	B	620	SQD	O47-C7-O49	-2.12	118.38	123.68
31	A	416[A]	PL9	C47-C48-C49	-2.12	120.22	127.80
24	b	604	CLA	C4A-NA-C1A	-2.12	103.82	106.45
26	D	404	BCR	C3-C4-C5	-2.12	110.14	113.78
26	c	517	BCR	C37-C22-C21	-2.12	119.96	122.92
24	B	603	CLA	OBD-CAD-C3D	-2.12	124.12	128.03
24	a	403	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
24	c	511	CLA	CAA-C2A-C3A	-2.12	107.01	112.81
31	a	414[B]	PL9	C47-C48-C49	-2.11	120.25	127.80
38	d	408	LHG	C5-O7-C7	-2.11	112.89	117.88
24	b	608	CLA	CBC-CAC-C3C	-2.11	106.42	112.41
24	B	603	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
31	d	405	PL9	C31-C29-C28	-2.11	116.78	121.10
25	a	406	PHO	C3A-C4A-CHB	-2.11	118.19	121.75
26	D	404	BCR	C24-C25-C26	-2.11	116.51	121.54
24	B	610	CLA	O1D-CGD-CBD	-2.11	120.81	124.60
39	V	203	HEM	C1D-C2D-C3D	-2.11	105.53	107.00
26	b	618	BCR	C39-C30-C25	-2.11	106.89	110.31
24	D	402	CLA	CBC-CAC-C3C	-2.11	106.42	112.41
24	B	611	CLA	C4A-NA-C1A	-2.11	103.83	106.45
26	b	618	BCR	C21-C20-C19	-2.10	116.78	123.23
24	b	612	CLA	OBD-CAD-C3D	-2.10	124.15	128.03
26	b	618	BCR	C8-C7-C6	-2.10	121.37	127.25
33	c	521	LMG	O8-C28-O10	-2.10	118.34	123.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	617	BCR	C21-C20-C19	-2.10	116.79	123.23
24	c	505	CLA	C2A-C1A-CHA	-2.10	120.20	123.92
24	C	502	CLA	O2A-CGA-O1A	-2.10	118.34	123.55
24	B	603	CLA	C16-C15-C13	-2.10	108.84	115.73
27	a	409	SQD	C44-O6-C1	-2.10	109.46	113.76
26	b	617	BCR	C36-C18-C17	-2.09	119.99	122.92
31	D	405	PL9	C45-C44-C43	-2.09	118.10	123.69
26	D	404	BCR	C21-C20-C19	-2.09	116.81	123.23
24	C	502	CLA	C11-C12-C13	-2.09	108.86	115.73
24	b	615	CLA	C2A-C1A-CHA	-2.09	120.21	123.92
26	d	404	BCR	C35-C13-C14	-2.09	120.00	122.92
24	B	606	CLA	CAA-C2A-C3A	-2.09	107.09	112.81
33	c	521	LMG	O7-C10-O9	-2.09	118.47	123.68
26	D	404	BCR	C15-C16-C17	-2.08	119.02	123.46
24	c	504	CLA	OBD-CAD-C3D	-2.08	124.19	128.03
26	B	618	BCR	C15-C16-C17	-2.08	119.02	123.46
33	a	417	LMG	C30-C29-C28	-2.08	105.99	113.58
24	d	402	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
24	B	603	CLA	C4A-NA-C1A	-2.08	103.87	106.45
31	D	405	PL9	C42-C41-C39	-2.08	105.91	112.93
24	B	609	CLA	C2A-C1A-CHA	-2.07	120.24	123.92
24	c	506	CLA	CAA-C2A-C3A	-2.07	107.12	112.81
24	B	608	CLA	CBC-CAC-C3C	-2.07	106.53	112.41
24	C	512	CLA	C2A-C1A-CHA	-2.07	120.25	123.92
26	b	618	BCR	C10-C11-C12	-2.07	116.88	123.23
26	C	516	BCR	C34-C9-C10	-2.07	120.02	122.92
24	B	612	CLA	C6-C5-C3	-2.07	107.97	112.66
24	a	403	CLA	CBC-CAC-C3C	-2.07	106.54	112.41
26	C	515	BCR	C21-C20-C19	-2.07	116.89	123.23
24	D	402	CLA	C4A-NA-C1A	-2.07	103.89	106.45
31	A	416[B]	PL9	C35-C34-C33	-2.06	118.18	123.69
24	b	611	CLA	CAA-C2A-C3A	-2.06	107.15	112.81
26	B	617	BCR	C38-C26-C25	-2.06	122.20	124.51
24	B	602	CLA	CMA-C3A-C2A	-2.06	105.41	113.77
24	b	606	CLA	CBC-CAC-C3C	-2.06	106.56	112.41
24	C	506	CLA	C11-C10-C8	-2.06	108.97	115.73
36	C	519	DGD	O1G-C1A-O1A	-2.06	118.44	123.55
24	B	613	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
31	A	416[A]	PL9	C12-C13-C14	-2.06	122.51	127.68
24	b	612	CLA	C4A-NA-C1A	-2.06	103.90	106.45
24	b	614	CLA	CAA-C2A-C3A	-2.05	107.18	112.81
25	A	407	PHO	C1-C2-C3	-2.05	122.17	125.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C11-C10-C8	-2.05	108.99	115.73
24	C	509	CLA	CAA-C2A-C3A	-2.05	107.18	112.81
26	B	619	BCR	C37-C22-C21	-2.05	120.05	122.92
26	Y	101	BCR	C16-C15-C14	-2.05	119.08	123.46
24	C	513	CLA	C4A-NA-C1A	-2.05	103.91	106.45
27	a	411	SQD	O6-C44-C45	-2.05	106.11	110.99
24	b	615	CLA	O2A-CGA-O1A	-2.05	118.46	123.55
24	B	615	CLA	C2A-C1A-CHA	-2.05	120.28	123.92
24	d	403	CLA	C11-C10-C8	-2.05	109.01	115.73
24	d	403	CLA	C4A-NA-C1A	-2.05	103.91	106.45
24	c	513	CLA	C2A-C1A-CHA	-2.05	120.29	123.92
38	L	101	LHG	O8-C23-O10	-2.04	118.47	123.55
24	B	604	CLA	C2A-C1A-CHA	-2.04	120.29	123.92
24	c	506	CLA	O2D-CGD-O1D	-2.04	119.71	123.82
27	A	411	SQD	O4-C4-C3	-2.04	105.92	110.36
24	c	509	CLA	O2A-CGA-O1A	-2.04	118.50	123.55
26	b	617	BCR	C11-C10-C9	-2.04	124.41	127.31
26	D	404	BCR	C37-C22-C21	-2.04	120.07	122.92
24	B	609	CLA	OBD-CAD-C3D	-2.03	124.28	128.03
24	b	612	CLA	C11-C12-C13	-2.03	109.06	115.73
26	b	618	BCR	C33-C5-C6	-2.03	122.23	124.51
26	B	619	BCR	C2-C3-C4	-2.03	106.50	111.34
24	b	607	CLA	O1D-CGD-CBD	-2.03	120.96	124.60
26	h	102	BCR	C24-C23-C22	-2.03	123.17	126.21
24	b	602	CLA	C1-C2-C3	-2.03	122.22	125.96
24	B	608	CLA	OBD-CAD-C3D	-2.03	124.29	128.03
24	C	513	CLA	CBC-CAC-C3C	-2.02	106.67	112.41
26	t	102	BCR	C34-C9-C10	-2.02	120.09	122.92
26	B	619	BCR	C15-C14-C13	-2.02	124.43	127.31
36	c	518	DGD	C3G-C2G-C1G	-2.02	107.30	111.86
24	D	402	CLA	OBD-CAD-C3D	-2.02	124.31	128.03
24	C	503	CLA	O2A-CGA-O1A	-2.02	118.55	123.55
34	B	622	LMT	O1B-C4'-C5'	-2.01	104.39	109.34
24	b	609	CLA	C2A-C1A-CHA	-2.01	120.35	123.92
24	B	609	CLA	C1-C2-C3	-2.01	122.25	125.96
24	C	511	CLA	OBD-CAD-C3D	-2.01	124.32	128.03
27	a	411	SQD	O48-C23-O10	-2.01	118.56	123.55
24	C	507	CLA	CGD-CBD-CAD	-2.01	103.98	110.71
24	c	505	CLA	C4A-NA-C1A	-2.01	103.96	106.45
26	b	618	BCR	C7-C8-C9	-2.00	123.20	126.21
24	B	601	CLA	OBD-CAD-C3D	-2.00	124.33	128.03
24	c	508	CLA	CGD-CBD-CAD	-2.00	104.01	110.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	O1D-CGD-CBD	-2.00	121.01	124.60
26	C	516	BCR	C36-C18-C19	2.00	121.29	118.10
26	B	617	BCR	C37-C22-C23	2.01	121.30	118.10
25	A	407	PHO	C1-O2A-CGA	2.01	121.59	116.77
31	D	405	PL9	C15-C14-C16	2.01	118.78	115.29
24	b	602	CLA	CMB-C2B-C3B	2.01	128.63	124.89
24	B	615	CLA	CHB-C4A-NA	2.01	127.30	124.51
33	b	621	LMG	C3-C4-C5	2.02	113.77	110.22
24	C	505	CLA	CHB-C4A-NA	2.02	127.31	124.51
24	b	607	CLA	CMC-C2C-C1C	2.02	128.09	125.02
24	b	616	CLA	CMC-C2C-C1C	2.03	128.09	125.02
24	C	509	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	A	406	CLA	CMB-C2B-C1B	2.03	131.58	128.46
24	b	603	CLA	CMB-C2B-C3B	2.03	128.66	124.89
26	h	102	BCR	C36-C18-C19	2.03	121.33	118.10
24	c	507	CLA	CMB-C2B-C1B	2.04	131.60	128.46
24	A	405	CLA	C3D-CAD-CBD	2.04	110.48	107.60
31	A	416[B]	PL9	C35-C34-C36	2.04	118.83	115.29
27	a	409	SQD	C3-C4-C5	2.04	113.81	110.22
24	A	409	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	B	615	CLA	CMB-C2B-C1B	2.04	131.60	128.46
26	Y	101	BCR	C36-C18-C19	2.04	121.35	118.10
24	b	603	CLA	CAC-C3C-C4C	2.05	127.72	124.83
24	D	402	CLA	CMB-C2B-C3B	2.05	128.69	124.89
24	b	615	CLA	C1-O2A-CGA	2.05	121.69	116.77
24	B	601	CLA	CHB-C4A-NA	2.05	127.35	124.51
24	C	507	CLA	CMB-C2B-C3B	2.05	128.70	124.89
25	A	407	PHO	CMC-C2C-C1C	2.05	128.24	125.04
31	a	414[B]	PL9	C51-C49-C50	2.06	119.41	114.60
24	c	513	CLA	CAC-C3C-C4C	2.07	127.74	124.83
24	C	505	CLA	C1-O2A-CGA	2.07	121.73	116.77
35	B	628	HTG	O5-C5-C4	2.07	113.48	109.66
24	c	508	CLA	CMB-C2B-C3B	2.07	128.74	124.89
24	C	505	CLA	CED-O2D-CGD	2.08	120.84	115.97
24	A	406	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	B	614	CLA	CHB-C4A-NA	2.08	127.39	124.51
24	c	515	CLA	CED-O2D-CGD	2.09	120.87	115.97
24	C	513	CLA	CHB-C4A-NA	2.09	127.41	124.51
24	C	513	CLA	CMB-C2B-C3B	2.09	128.78	124.89
26	b	617	BCR	C33-C5-C4	2.09	117.42	113.45
26	K	102	BCR	C29-C30-C25	2.10	113.76	110.48
26	b	618	BCR	C37-C22-C23	2.10	121.44	118.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CMC-C2C-C1C	2.10	128.21	125.02
24	C	505	CLA	CMB-C2B-C3B	2.10	128.80	124.89
24	c	504	CLA	C4-C3-C5	2.11	118.95	115.29
24	c	506	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	B	605	CLA	CAC-C3C-C2C	2.11	131.16	127.49
27	B	620	SQD	O8-S-C6	2.12	108.59	106.01
24	B	615	CLA	CAC-C3C-C4C	2.12	127.82	124.83
24	c	513	CLA	CMB-C2B-C3B	2.12	128.83	124.89
24	C	513	CLA	CMC-C2C-C1C	2.12	128.24	125.02
27	A	411	SQD	C3-C4-C5	2.12	113.96	110.22
33	b	621	LMG	O6-C1-C2	2.12	114.39	110.30
24	a	404	CLA	CMC-C2C-C1C	2.13	128.24	125.02
26	B	618	BCR	C2-C1-C6	2.13	113.81	110.48
24	c	514	CLA	CMB-C2B-C3B	2.13	128.84	124.89
31	a	414[B]	PL9	C25-C24-C26	2.13	118.99	115.29
24	c	504	CLA	CAC-C3C-C4C	2.14	127.84	124.83
26	b	618	BCR	C2-C1-C6	2.14	113.82	110.48
24	C	508	CLA	CAC-C3C-C4C	2.14	127.85	124.83
24	B	611	CLA	CAC-C3C-C4C	2.14	127.85	124.83
35	C	523	HTG	C3-C4-C5	2.14	113.99	110.22
24	B	602	CLA	C3B-C4B-NB	2.14	111.98	109.21
35	h	101	HTG	C1-O5-C5	2.14	116.82	112.69
24	A	409	CLA	CAC-C3C-C4C	2.15	127.86	124.83
26	Y	101	BCR	C34-C9-C8	2.16	121.53	118.10
24	B	607	CLA	O2A-CGA-CBA	2.16	118.18	111.90
34	e	101	LMT	O1B-C1B-C2B	2.16	112.97	108.11
27	a	411	SQD	C3-C4-C5	2.16	114.02	110.22
24	b	614	CLA	C4-C3-C5	2.16	119.04	115.29
24	C	508	CLA	C1-O2A-CGA	2.16	121.97	116.77
26	t	102	BCR	C36-C18-C19	2.17	121.55	118.10
24	b	613	CLA	CMC-C2C-C1C	2.17	128.31	125.02
24	C	505	CLA	O2A-CGA-CBA	2.17	118.23	111.90
34	B	622	LMT	O1B-C4'-C3'	2.18	112.43	107.19
24	B	616	CLA	CAC-C3C-C4C	2.18	127.90	124.83
31	a	414[B]	PL9	C10-C9-C11	2.18	119.07	115.29
31	a	414[A]	PL9	C51-C49-C50	2.18	119.69	114.60
34	A	359	LMT	O1B-C1B-C2B	2.18	113.02	108.11
24	B	611	CLA	C4-C3-C5	2.19	119.08	115.29
24	c	508	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	h	102	BCR	C35-C13-C12	2.19	121.59	118.10
24	B	607	CLA	CMB-C2B-C1B	2.19	131.84	128.46
34	e	101	LMT	O5'-C5'-C4'	2.20	114.25	109.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	CMB-C2B-C3B	2.20	128.97	124.89
26	T	101	BCR	C15-C14-C13	2.20	130.45	127.31
31	A	416[A]	PL9	C51-C49-C50	2.20	119.73	114.60
24	d	403	CLA	C4-C3-C5	2.20	119.11	115.29
24	b	601	CLA	CMC-C2C-C1C	2.20	128.36	125.02
24	B	610	CLA	CMB-C2B-C3B	2.21	128.99	124.89
24	a	350	CLA	CED-O2D-CGD	2.21	121.14	115.97
25	A	408	PHO	CBD-CHA-C1A	2.21	131.56	126.36
25	a	406	PHO	C3C-C4C-NC	2.21	113.81	110.19
26	C	515	BCR	C37-C22-C23	2.21	121.62	118.10
35	c	526	HTG	O5-C5-C4	2.21	113.73	109.66
34	a	359	LMT	C1B-O5B-C5B	2.21	117.88	113.72
26	D	404	BCR	C38-C26-C27	2.21	117.65	113.45
24	b	601	CLA	CMB-C2B-C3B	2.22	129.00	124.89
25	a	405	PHO	C4D-C3D-CAD	2.22	109.52	105.41
24	B	608	CLA	C4-C3-C5	2.22	119.14	115.29
25	a	406	PHO	C4D-C3D-CAD	2.22	109.53	105.41
24	b	601	CLA	C1-O2A-CGA	2.22	122.11	116.77
24	b	610	CLA	C3B-C4B-NB	2.23	112.09	109.21
24	b	602	CLA	CAC-C3C-C4C	2.23	127.97	124.83
34	M	103	LMT	O1B-C1B-C2B	2.23	113.14	108.11
36	C	518	DGD	O6E-C5E-C6E	2.23	111.76	106.41
24	a	407	CLA	CMB-C2B-C3B	2.23	129.04	124.89
24	b	609	CLA	C4-C3-C5	2.24	119.17	115.29
33	a	417	LMG	O8-C28-C29	2.24	118.41	111.90
31	A	416[A]	PL9	C2-C3-C4	2.24	121.92	118.81
31	d	405	PL9	C35-C34-C36	2.25	119.18	115.29
25	A	407	PHO	CMB-C2B-C1B	2.25	128.54	125.04
24	C	510	CLA	C4-C3-C5	2.25	119.19	115.29
24	b	604	CLA	C4-C3-C5	2.25	119.19	115.29
34	a	359	LMT	O5'-C5'-C4'	2.25	114.36	109.75
24	c	503	CLA	C4-C3-C5	2.25	119.20	115.29
36	c	518	DGD	O1G-C1A-C2A	2.25	118.46	111.90
24	c	512	CLA	CAC-C3C-C4C	2.25	128.01	124.83
25	a	406	PHO	CBD-CHA-C1A	2.26	131.69	126.36
31	D	405	PL9	C2-C1-C6	2.26	121.62	117.82
26	K	102	BCR	C36-C18-C19	2.26	121.71	118.10
24	b	613	CLA	CAC-C3C-C2C	2.26	131.42	127.49
24	B	615	CLA	CED-O2D-CGD	2.27	121.28	115.97
24	B	607	CLA	C1-O2A-CGA	2.27	122.21	116.77
24	B	601	CLA	CAC-C3C-C4C	2.27	128.03	124.83
24	b	607	CLA	O2A-CGA-CBA	2.27	118.50	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C4-C3-C5	2.27	119.23	115.29
24	c	506	CLA	C1-O2A-CGA	2.27	122.22	116.77
26	K	102	BCR	C2-C1-C6	2.27	114.03	110.48
24	A	405	CLA	CMB-C2B-C3B	2.28	129.12	124.89
24	d	403	CLA	CMB-C2B-C3B	2.28	129.12	124.89
24	c	514	CLA	CMC-C2C-C1C	2.28	128.47	125.02
31	D	405	PL9	C20-C19-C21	2.29	119.26	115.29
26	a	408	BCR	C37-C22-C23	2.29	121.74	118.10
24	b	602	CLA	C3B-C4B-NB	2.29	112.17	109.21
24	C	502	CLA	CAC-C3C-C4C	2.30	128.07	124.83
24	d	402	CLA	CHB-C4A-NA	2.30	127.69	124.51
33	Z	101	LMG	C1-O6-C5	2.30	118.05	113.72
24	b	612	CLA	CMC-C2C-C1C	2.30	128.51	125.02
24	B	601	CLA	CMB-C2B-C3B	2.30	129.17	124.89
24	B	615	CLA	C4-C3-C5	2.30	119.29	115.29
34	B	622	LMT	O5'-C5'-C4'	2.31	114.47	109.75
24	A	406	CLA	C4-C3-C5	2.31	119.29	115.29
26	B	619	BCR	C34-C9-C8	2.31	121.78	118.10
26	D	404	BCR	C30-C25-C24	2.31	122.22	115.73
24	c	506	CLA	CMB-C2B-C3B	2.32	129.19	124.89
24	c	506	CLA	C4-C3-C5	2.32	119.31	115.29
24	c	510	CLA	CMC-C2C-C1C	2.32	128.53	125.02
24	B	602	CLA	O2A-CGA-CBA	2.32	118.64	111.90
24	b	608	CLA	CMB-C2B-C3B	2.32	129.20	124.89
24	a	404	CLA	CMB-C2B-C3B	2.32	129.20	124.89
25	a	406	PHO	C2A-C1A-NA	2.33	114.73	111.91
25	a	406	PHO	O2A-CGA-CBA	2.33	118.67	111.90
26	b	617	BCR	C36-C18-C19	2.33	121.81	118.10
24	b	616	CLA	CAC-C3C-C4C	2.33	128.12	124.83
31	A	416[B]	PL9	C40-C39-C41	2.33	119.33	115.29
24	c	505	CLA	O2A-CGA-CBA	2.33	118.68	111.90
27	b	620	SQD	O9-S-C6	2.33	108.82	106.83
31	A	416[A]	PL9	C40-C39-C41	2.34	119.34	115.29
35	B	623	HTG	O5-C1-C2	2.34	113.48	110.28
35	C	522	HTG	C1-O5-C5	2.34	117.19	112.69
24	c	505	CLA	CMC-C2C-C1C	2.34	128.57	125.02
24	B	605	CLA	CMC-C2C-C1C	2.34	128.57	125.02
31	A	416[B]	PL9	C20-C19-C21	2.35	119.36	115.29
24	A	404	CLA	O2D-CGD-CBD	2.35	115.50	111.30
25	a	406	PHO	CAC-C3C-C4C	2.35	127.97	125.21
25	A	408	PHO	O2A-CGA-CBA	2.35	118.75	111.90
26	Y	101	BCR	C29-C30-C25	2.35	114.16	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	414[B]	PL9	C30-C29-C31	2.36	119.38	115.29
35	C	523	HTG	O5-C1-C2	2.36	113.51	110.28
35	B	623	HTG	C1-O5-C5	2.36	117.23	112.69
24	C	503	CLA	C4-C3-C5	2.36	119.38	115.29
24	B	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
27	f	101	SQD	O5-C5-C4	2.36	114.02	109.66
24	c	511	CLA	CMC-C2C-C1C	2.37	128.61	125.02
26	d	404	BCR	C37-C22-C23	2.37	121.87	118.10
35	b	623	HTG	O5-C5-C4	2.37	114.02	109.66
24	A	409	CLA	CMB-C2B-C3B	2.37	129.28	124.89
24	B	611	CLA	CMB-C2B-C3B	2.37	129.29	124.89
25	A	407	PHO	O2A-CGA-CBA	2.37	118.80	111.90
24	b	602	CLA	O2A-CGA-CBA	2.37	118.81	111.90
31	a	414[A]	PL9	C20-C19-C21	2.38	119.41	115.29
25	a	405	PHO	CAC-C3C-C4C	2.38	128.00	125.21
24	B	602	CLA	CED-O2D-CGD	2.38	121.55	115.97
24	B	616	CLA	C1-O2A-CGA	2.39	122.50	116.77
33	A	418	LMG	O1-C1-C2	2.39	112.13	108.23
31	a	414[A]	PL9	C45-C44-C46	2.40	119.44	115.29
26	d	404	BCR	C38-C26-C27	2.40	118.00	113.45
26	T	101	BCR	C1-C6-C7	2.40	122.49	115.73
24	c	508	CLA	CAC-C3C-C4C	2.41	128.22	124.83
34	I	101	LMT	O5'-C5'-C4'	2.41	114.67	109.75
26	a	408	BCR	C29-C30-C25	2.41	114.24	110.48
24	b	602	CLA	C4-C3-C5	2.41	119.47	115.29
24	C	504	CLA	O2A-CGA-CBA	2.41	118.91	111.90
24	C	506	CLA	O2A-CGA-CBA	2.41	118.91	111.90
26	y	101	BCR	C35-C13-C12	2.41	121.94	118.10
26	T	101	BCR	C2-C1-C6	2.41	114.25	110.48
24	d	402	CLA	CMB-C2B-C3B	2.41	129.37	124.89
38	d	407	LHG	O8-C23-C24	2.42	118.93	111.90
24	B	604	CLA	C4-C3-C5	2.42	119.49	115.29
24	B	611	CLA	O2A-CGA-CBA	2.42	118.95	111.90
25	a	405	PHO	CBD-CHA-C1A	2.42	132.07	126.36
35	B	628	HTG	C1-O5-C5	2.43	117.36	112.69
27	a	411	SQD	O5-C5-C4	2.43	114.14	109.66
31	a	414[A]	PL9	C53-C6-C1	2.43	120.00	114.84
31	a	414[B]	PL9	C15-C14-C16	2.43	119.51	115.29
24	D	402	CLA	CMC-C2C-C1C	2.43	128.71	125.02
24	c	509	CLA	O2A-CGA-CBA	2.43	118.98	111.90
25	a	406	PHO	CMB-C2B-C1B	2.44	128.84	125.04
35	b	628	HTG	O5-C5-C4	2.44	114.15	109.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	503	CLA	CMC-C2C-C1C	2.44	128.72	125.02
26	H	101	BCR	C2-C1-C6	2.44	114.29	110.48
34	M	103	LMT	C1'-O5'-C5'	2.44	118.32	113.72
26	C	516	BCR	C37-C22-C23	2.44	121.99	118.10
33	C	520	LMG	O6-C5-C6	2.45	112.29	106.41
31	A	416[A]	PL9	C45-C44-C46	2.46	119.55	115.29
24	C	511	CLA	CMB-C2B-C3B	2.46	129.46	124.89
24	B	601	CLA	C4-C3-C5	2.46	119.56	115.29
24	B	608	CLA	CMC-C2C-C1C	2.46	128.75	125.02
24	c	513	CLA	CMC-C2C-C1C	2.47	128.77	125.02
26	D	404	BCR	C29-C30-C25	2.47	114.34	110.48
24	b	605	CLA	O2A-CGA-CBA	2.48	119.11	111.90
31	D	405	PL9	C10-C9-C11	2.48	119.59	115.29
24	D	403	CLA	O2A-CGA-CBA	2.48	119.11	111.90
24	B	602	CLA	CMC-C2C-C1C	2.48	128.78	125.02
24	b	602	CLA	C1-O2A-CGA	2.48	122.72	116.77
38	D	406	LHG	O8-C23-C24	2.48	119.12	111.90
33	J	101	LMG	O8-C28-C29	2.48	119.13	111.90
24	B	609	CLA	CMC-C2C-C1C	2.48	128.79	125.02
25	A	408	PHO	C4D-C3D-CAD	2.49	110.02	105.41
31	d	405	PL9	C25-C24-C26	2.49	119.60	115.29
24	b	615	CLA	CAC-C3C-C4C	2.50	128.35	124.83
24	c	512	CLA	CMB-C2B-C3B	2.50	129.53	124.89
24	C	509	CLA	CMB-C2B-C3B	2.50	129.53	124.89
26	Y	101	BCR	C37-C22-C23	2.50	122.09	118.10
38	d	407	LHG	O7-C7-C8	2.50	116.75	111.55
24	C	502	CLA	CMC-C2C-C1C	2.51	128.82	125.02
24	b	606	CLA	O2A-CGA-CBA	2.51	119.21	111.90
24	b	609	CLA	O2A-CGA-CBA	2.51	119.21	111.90
24	D	402	CLA	CAC-C3C-C4C	2.51	128.38	124.83
33	Z	101	LMG	C4-C3-C2	2.51	115.27	110.84
24	B	612	CLA	O2A-CGA-CBA	2.51	119.22	111.90
24	A	405	CLA	O2A-CGA-CBA	2.52	119.23	111.90
24	C	503	CLA	CMC-C2C-C1C	2.52	128.84	125.02
24	d	403	CLA	C3B-C4B-NB	2.52	112.47	109.21
24	c	515	CLA	CMB-C2B-C3B	2.52	129.57	124.89
24	C	502	CLA	C1-O2A-CGA	2.53	122.83	116.77
26	d	404	BCR	C29-C30-C25	2.53	114.43	110.48
25	A	408	PHO	C2C-C1C-NC	2.53	113.56	109.82
24	C	509	CLA	C4-C3-C5	2.53	119.68	115.29
25	a	405	PHO	C2A-C1A-NA	2.53	114.98	111.91
34	M	101	LMT	O1B-C1B-C2B	2.54	113.84	108.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	CLA	C4-C3-C5	2.54	119.70	115.29
24	C	507	CLA	CMC-C2C-C1C	2.55	128.88	125.02
24	b	601	CLA	O2A-CGA-CBA	2.55	119.32	111.90
24	b	616	CLA	C4-C3-C5	2.55	119.71	115.29
36	h	103	DGD	O2G-C1B-C2B	2.55	116.85	111.55
24	b	607	CLA	CAC-C3C-C4C	2.55	128.43	124.83
24	c	510	CLA	O2A-CGA-CBA	2.55	119.33	111.90
24	c	507	CLA	C4-C3-C5	2.56	119.72	115.29
24	C	506	CLA	CAC-C3C-C4C	2.56	128.44	124.83
24	B	605	CLA	O2A-CGA-CBA	2.56	119.36	111.90
31	D	405	PL9	C25-C24-C26	2.56	119.73	115.29
24	c	514	CLA	CHB-C4A-NA	2.57	128.06	124.51
27	a	411	SQD	O8-S-C6	2.57	109.15	106.01
24	C	508	CLA	CMC-C2C-C1C	2.58	128.93	125.02
24	c	511	CLA	CMB-C2B-C3B	2.58	129.67	124.89
24	c	506	CLA	O2A-CGA-CBA	2.58	119.42	111.90
24	C	508	CLA	O2A-CGA-CBA	2.58	119.42	111.90
31	A	416[A]	PL9	C53-C6-C1	2.59	120.33	114.84
31	a	414[B]	PL9	C40-C39-C41	2.59	119.78	115.29
24	C	509	CLA	CAC-C3C-C4C	2.59	128.49	124.83
25	a	405	PHO	O2A-CGA-CBA	2.59	119.45	111.90
25	a	405	PHO	CMB-C2B-C1B	2.60	129.08	125.04
33	a	417	LMG	C3-C4-C5	2.60	114.79	110.22
26	B	617	BCR	C29-C30-C25	2.60	114.54	110.48
24	C	512	CLA	CMB-C2B-C3B	2.60	129.72	124.89
24	c	507	CLA	C3B-C4B-NB	2.61	112.58	109.21
26	T	101	BCR	C35-C13-C12	2.61	122.26	118.10
27	b	620	SQD	O48-C23-C24	2.62	119.51	111.90
31	a	414[B]	PL9	C53-C6-C1	2.62	120.40	114.84
33	A	418	LMG	O8-C28-C29	2.62	119.52	111.90
38	L	101	LHG	O8-C23-C24	2.62	119.53	111.90
38	D	406	LHG	O7-C7-C8	2.63	117.01	111.55
24	b	606	CLA	CMC-C2C-C1C	2.63	129.00	125.02
24	A	405	CLA	C3B-C4B-NB	2.63	112.61	109.21
24	a	403	CLA	CMC-C2C-C1C	2.63	129.01	125.02
24	b	603	CLA	C4-C3-C5	2.63	119.85	115.29
24	B	608	CLA	CHB-C4A-NA	2.63	128.16	124.51
26	b	617	BCR	C29-C30-C25	2.63	114.60	110.48
24	C	511	CLA	CMC-C2C-C1C	2.64	129.02	125.02
35	B	625	HTG	O5-C1-C2	2.64	113.89	110.28
24	B	613	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	d	403	CLA	O2A-CGA-CBA	2.64	119.57	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	CED-O2D-CGD	2.64	122.16	115.97
24	C	514	CLA	O2A-CGA-CBA	2.64	119.58	111.90
24	B	612	CLA	CMC-C2C-C1C	2.64	129.03	125.02
24	C	514	CLA	C4-C3-C5	2.64	119.88	115.29
31	A	416[A]	PL9	C25-C24-C26	2.64	119.88	115.29
24	b	608	CLA	CMC-C2C-C1C	2.64	129.03	125.02
24	D	402	CLA	C4-C3-C5	2.64	119.88	115.29
24	b	615	CLA	O2A-CGA-CBA	2.65	119.60	111.90
26	t	102	BCR	C35-C13-C12	2.65	122.32	118.10
24	B	615	CLA	O2A-CGA-CBA	2.65	119.62	111.90
38	a	419	LHG	O8-C23-C24	2.65	119.62	111.90
35	B	623	HTG	C1'-S1-C1	2.66	104.22	100.28
26	b	619	BCR	C37-C22-C23	2.66	122.33	118.10
31	a	414[A]	PL9	C40-C39-C41	2.66	119.90	115.29
24	C	512	CLA	O2A-CGA-CBA	2.66	119.64	111.90
36	c	519	DGD	O1G-C1A-C2A	2.67	119.66	111.90
33	Z	101	LMG	C3-C4-C5	2.67	114.92	110.22
36	C	519	DGD	O2G-C1B-C2B	2.68	117.12	111.55
24	C	505	CLA	C4-C3-C5	2.68	119.94	115.29
24	C	502	CLA	O2A-CGA-CBA	2.68	119.71	111.90
35	b	625	HTG	O5-C1-C2	2.69	113.96	110.28
24	c	510	CLA	C4-C3-C5	2.69	119.96	115.29
24	b	603	CLA	CMC-C2C-C1C	2.69	129.10	125.02
26	y	101	BCR	C37-C22-C23	2.69	122.39	118.10
24	a	404	CLA	O2A-CGA-CBA	2.69	119.74	111.90
33	c	522	LMG	C3-C4-C5	2.70	114.97	110.22
24	B	603	CLA	CMB-C2B-C3B	2.70	129.90	124.89
24	a	350	CLA	O2A-CGA-CBA	2.70	119.75	111.90
24	A	405	CLA	C4-C3-C5	2.70	119.97	115.29
24	C	509	CLA	O2A-CGA-CBA	2.70	119.75	111.90
27	F	101	SQD	O48-C23-C24	2.70	119.77	111.90
24	c	515	CLA	O2A-CGA-CBA	2.70	119.77	111.90
31	A	416[A]	PL9	C30-C29-C31	2.71	119.98	115.29
25	A	407	PHO	C3C-C4C-NC	2.71	114.62	110.19
24	a	403	CLA	C4-C3-C5	2.71	119.99	115.29
24	C	504	CLA	CAC-C3C-C4C	2.71	128.66	124.83
33	j	101	LMG	O8-C28-C29	2.71	119.80	111.90
31	a	414[A]	PL9	C25-C24-C26	2.71	120.00	115.29
24	c	511	CLA	C4-C3-C5	2.72	120.00	115.29
24	c	505	CLA	CAC-C3C-C4C	2.72	128.67	124.83
27	A	411	SQD	O8-S-C6	2.72	109.33	106.01
25	A	407	PHO	CAC-C3C-C4C	2.72	128.41	125.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	C4-C3-C5	2.72	120.02	115.29
24	B	614	CLA	CAC-C3C-C4C	2.73	128.67	124.83
35	b	628	HTG	C1-O5-C5	2.73	117.94	112.69
26	B	618	BCR	C37-C22-C23	2.73	122.45	118.10
31	A	416[B]	PL9	C25-C24-C26	2.73	120.03	115.29
24	c	507	CLA	O2A-CGA-CBA	2.73	119.85	111.90
27	f	101	SQD	O5-C1-C2	2.74	115.57	110.30
24	c	503	CLA	CAC-C3C-C4C	2.74	128.69	124.83
31	a	414[A]	PL9	C35-C34-C36	2.74	120.04	115.29
24	c	508	CLA	O2A-CGA-CBA	2.75	119.90	111.90
24	A	409	CLA	O2A-CGA-CBA	2.76	119.92	111.90
24	B	607	CLA	C4-C3-C5	2.76	120.07	115.29
24	c	511	CLA	C1-O2A-CGA	2.76	123.40	116.77
24	c	506	CLA	CAC-C3C-C4C	2.76	128.73	124.83
26	b	618	BCR	C29-C30-C25	2.77	114.80	110.48
36	H	102	DGD	O2G-C1B-C2B	2.77	117.30	111.55
24	C	513	CLA	C4-C3-C5	2.77	120.09	115.29
24	b	610	CLA	CAC-C3C-C4C	2.77	128.73	124.83
27	A	411	SQD	O7-S-C6	2.77	109.19	106.83
24	b	602	CLA	CMC-C2C-C1C	2.77	129.22	125.02
24	C	507	CLA	C4-C3-C5	2.77	120.09	115.29
35	V	204	HTG	C1-O5-C5	2.77	115.99	112.17
27	a	411	SQD	C1-O5-C5	2.77	118.94	113.72
27	f	101	SQD	O48-C23-C24	2.77	119.97	111.90
24	c	503	CLA	O2A-CGA-CBA	2.77	119.97	111.90
27	F	101	SQD	C3-C4-C5	2.78	115.11	110.22
24	b	611	CLA	O2A-CGA-CBA	2.78	119.99	111.90
24	A	406	CLA	C3B-C4B-NB	2.78	112.81	109.21
27	b	620	SQD	C3-C4-C5	2.79	115.14	110.22
24	B	606	CLA	O2A-CGA-CBA	2.80	120.04	111.90
24	c	512	CLA	CMC-C2C-C1C	2.80	129.26	125.02
27	B	620	SQD	C3-C4-C5	2.80	115.15	110.22
36	C	519	DGD	O1G-C1A-C2A	2.81	120.07	111.90
24	C	513	CLA	C3B-C4B-NB	2.81	112.84	109.21
24	b	610	CLA	CMC-C2C-C1C	2.82	129.29	125.02
24	B	612	CLA	CMB-C2B-C3B	2.82	130.12	124.89
36	H	102	DGD	O1G-C1A-C2A	2.82	120.10	111.90
31	a	414[B]	PL9	C35-C34-C36	2.82	120.18	115.29
24	B	616	CLA	O2A-CGA-CBA	2.82	120.11	111.90
33	Z	101	LMG	O6-C1-C2	2.82	115.74	110.30
24	C	502	CLA	C3B-C4B-NB	2.82	112.86	109.21
24	B	606	CLA	C3B-C4B-NB	2.83	112.86	109.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	v	203	HEM	CAD-CBD-CGD	2.83	117.49	112.66
31	D	405	PL9	C45-C44-C46	2.83	120.20	115.29
24	b	604	CLA	CMC-C2C-C1C	2.84	129.33	125.02
24	c	504	CLA	CMC-C2C-C1C	2.84	129.33	125.02
24	C	510	CLA	CAC-C3C-C4C	2.84	128.84	124.83
24	C	502	CLA	C4-C3-C5	2.84	120.22	115.29
24	d	403	CLA	C1-O2A-CGA	2.84	123.59	116.77
24	b	606	CLA	CMB-C2B-C3B	2.85	130.18	124.89
24	c	510	CLA	CMB-C2B-C3B	2.85	130.19	124.89
24	B	609	CLA	O2A-CGA-CBA	2.86	120.21	111.90
24	C	508	CLA	C3B-C4B-NB	2.86	112.91	109.21
24	D	402	CLA	O2A-CGA-CBA	2.86	120.23	111.90
24	c	511	CLA	O2A-CGA-CBA	2.86	120.23	111.90
31	A	416[A]	PL9	C20-C19-C21	2.86	120.26	115.29
24	a	404	CLA	C4-C3-C5	2.87	120.26	115.29
24	b	607	CLA	C4-C3-C5	2.87	120.26	115.29
26	t	102	BCR	C1-C6-C7	2.87	123.79	115.73
24	b	612	CLA	CMB-C2B-C3B	2.87	130.22	124.89
26	t	102	BCR	C37-C22-C23	2.87	122.68	118.10
24	B	611	CLA	CMC-C2C-C1C	2.87	129.38	125.02
33	C	521	LMG	O8-C28-C29	2.88	120.29	111.90
24	C	506	CLA	C4-C3-C5	2.89	120.29	115.29
24	B	601	CLA	C3B-C4B-NB	2.89	112.94	109.21
24	B	613	CLA	CMB-C2B-C3B	2.89	130.25	124.89
24	B	604	CLA	CMC-C2C-C1C	2.89	129.41	125.02
24	b	613	CLA	C4-C3-C5	2.90	120.31	115.29
24	C	512	CLA	C4-C3-C5	2.90	120.31	115.29
27	B	620	SQD	O9-S-C6	2.90	109.30	106.83
31	D	405	PL9	C53-C6-C1	2.90	121.00	114.84
24	c	504	CLA	O2A-CGA-CBA	2.90	120.34	111.90
24	B	615	CLA	C3B-C4B-NB	2.90	112.96	109.21
31	D	405	PL9	C40-C39-C41	2.90	120.33	115.29
24	b	610	CLA	C4-C3-C5	2.90	120.33	115.29
25	A	408	PHO	C3C-C4C-NC	2.91	114.94	110.19
24	B	606	CLA	C4-C3-C5	2.91	120.33	115.29
24	c	505	CLA	C4-C3-C5	2.91	120.33	115.29
24	B	601	CLA	CMC-C2C-C1C	2.91	129.44	125.02
31	A	416[B]	PL9	C53-C6-C1	2.92	121.03	114.84
25	a	406	PHO	C2B-C1B-NB	2.93	114.15	109.82
24	C	514	CLA	CMC-C2C-C1C	2.93	129.46	125.02
24	C	503	CLA	C3B-C4B-NB	2.93	113.00	109.21
25	A	408	PHO	C2A-C1A-NA	2.93	115.46	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C4-C3-C5	2.93	120.38	115.29
24	B	608	CLA	O2A-CGA-CBA	2.94	120.45	111.90
24	C	505	CLA	CMC-C2C-C1C	2.94	129.48	125.02
24	B	603	CLA	C3B-C4B-NB	2.94	113.01	109.21
26	D	404	BCR	C37-C22-C23	2.95	122.79	118.10
24	d	402	CLA	CMC-C2C-C1C	2.95	129.49	125.02
31	d	405	PL9	C40-C39-C41	2.96	120.42	115.29
24	a	403	CLA	CAC-C3C-C4C	2.96	129.00	124.83
24	c	509	CLA	C3B-C4B-NB	2.96	113.04	109.21
24	A	404	CLA	CMB-C2B-C3B	2.96	130.38	124.89
24	A	409	CLA	C4-C3-C5	2.96	120.42	115.29
24	b	609	CLA	CMC-C2C-C1C	2.96	129.51	125.02
24	a	407	CLA	CMC-C2C-C1C	2.96	129.51	125.02
24	c	507	CLA	CAC-C3C-C4C	2.96	129.01	124.83
36	c	520	DGD	O1G-C1A-C2A	2.96	120.52	111.90
24	c	514	CLA	C3B-C4B-NB	2.97	113.05	109.21
24	b	614	CLA	O2A-CGA-CBA	2.97	120.54	111.90
24	c	515	CLA	CMC-C2C-C1C	2.97	129.52	125.02
24	B	616	CLA	C3B-C4B-NB	2.97	113.05	109.21
25	A	407	PHO	C2A-C1A-NA	2.97	115.52	111.91
24	C	514	CLA	CAC-C3C-C4C	2.98	129.03	124.83
38	a	419	LHG	O7-C7-C8	2.98	117.74	111.55
31	a	414[A]	PL9	C10-C9-C11	2.98	120.46	115.29
24	B	603	CLA	CMC-C2C-C1C	2.98	129.55	125.02
24	b	615	CLA	C4-C3-C5	2.99	120.47	115.29
25	a	405	PHO	C3C-C4C-NC	2.99	115.07	110.19
24	c	503	CLA	C3B-C4B-NB	2.99	113.08	109.21
24	b	612	CLA	CAC-C3C-C4C	2.99	129.05	124.83
24	b	610	CLA	CMB-C2B-C3B	3.00	130.45	124.89
24	C	508	CLA	C4-C3-C5	3.00	120.49	115.29
25	A	408	PHO	C4-C3-C5	3.00	120.50	115.29
24	C	510	CLA	CMB-C2B-C3B	3.01	130.48	124.89
24	B	613	CLA	O2A-CGA-CBA	3.01	120.67	111.90
27	f	101	SQD	O8-S-C6	3.02	109.69	106.01
24	C	510	CLA	CMC-C2C-C1C	3.02	129.59	125.02
24	A	406	CLA	CMC-C2C-C1C	3.02	129.59	125.02
24	B	610	CLA	C3B-C4B-NB	3.02	113.11	109.21
33	c	522	LMG	O8-C28-C29	3.02	120.68	111.90
31	A	416[A]	PL9	C35-C34-C36	3.02	120.53	115.29
24	B	602	CLA	CAC-C3C-C4C	3.02	129.09	124.83
24	C	503	CLA	O2A-CGA-CBA	3.02	120.69	111.90
24	B	614	CLA	O2A-CGA-CBA	3.02	120.70	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	CMB-C2B-C3B	3.03	130.51	124.89
24	c	509	CLA	CMC-C2C-C1C	3.03	129.62	125.02
24	C	507	CLA	O2A-CGA-CBA	3.04	120.73	111.90
24	C	510	CLA	O2A-CGA-CBA	3.04	120.74	111.90
24	c	514	CLA	O2A-CGA-CBA	3.04	120.75	111.90
26	b	619	BCR	C2-C1-C6	3.04	115.23	110.48
24	B	613	CLA	C4-C3-C5	3.05	120.57	115.29
33	a	417	LMG	O6-C5-C4	3.05	115.27	109.66
38	d	408	LHG	O8-C23-C24	3.05	120.78	111.90
24	c	513	CLA	O2A-CGA-CBA	3.05	120.78	111.90
24	b	611	CLA	C3B-C4B-NB	3.06	113.16	109.21
24	C	504	CLA	O2D-CGD-CBD	3.06	116.77	111.30
24	d	403	CLA	CAC-C3C-C4C	3.06	129.15	124.83
24	a	407	CLA	O2A-CGA-CBA	3.07	120.83	111.90
24	C	505	CLA	CAC-C3C-C4C	3.08	129.18	124.83
33	C	521	LMG	O6-C5-C4	3.09	115.35	109.66
24	c	508	CLA	C4-C3-C5	3.09	120.65	115.29
24	C	506	CLA	C3B-C4B-NB	3.09	113.20	109.21
24	b	606	CLA	C3B-C4B-NB	3.09	113.20	109.21
34	M	103	LMT	O5'-C5'-C4'	3.09	116.08	109.75
35	c	526	HTG	C1-O5-C5	3.09	118.64	112.69
33	c	522	LMG	O6-C5-C4	3.10	115.36	109.66
27	a	409	SQD	O48-C23-C24	3.10	120.92	111.90
27	a	411	SQD	O48-C23-C24	3.10	120.93	111.90
24	a	350	CLA	C3B-C4B-NB	3.10	113.22	109.21
33	z	101	LMG	O8-C28-C29	3.10	120.93	111.90
38	E	101	LHG	O8-C23-C24	3.11	120.94	111.90
24	b	604	CLA	C3B-C4B-NB	3.11	113.23	109.21
38	D	407	LHG	O8-C23-C24	3.11	120.95	111.90
31	A	416[A]	PL9	C7-C3-C4	3.11	119.40	116.88
24	B	605	CLA	C3B-C4B-NB	3.11	113.23	109.21
24	D	403	CLA	C3B-C4B-NB	3.11	113.23	109.21
33	J	101	LMG	O7-C10-C11	3.11	118.02	111.55
24	C	513	CLA	O2A-CGA-CBA	3.12	120.97	111.90
27	b	620	SQD	O8-S-C6	3.12	109.82	106.01
24	c	509	CLA	C4-C3-C5	3.13	120.71	115.29
24	C	511	CLA	O2A-CGA-CBA	3.13	121.00	111.90
24	a	407	CLA	CAC-C3C-C4C	3.13	129.24	124.83
24	b	608	CLA	O2A-CGA-CBA	3.13	121.02	111.90
24	b	613	CLA	CMB-C2B-C3B	3.13	130.71	124.89
24	b	616	CLA	C3B-C4B-NB	3.14	113.27	109.21
24	C	506	CLA	CMC-C2C-C1C	3.14	129.79	125.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	407	PHO	C2C-C1C-NC	3.15	114.48	109.82
31	d	405	PL9	C45-C44-C46	3.15	120.76	115.29
24	C	507	CLA	CAC-C3C-C4C	3.15	129.28	124.83
24	B	606	CLA	CMB-C2B-C3B	3.16	130.75	124.89
24	d	402	CLA	CAC-C3C-C4C	3.16	129.29	124.83
24	B	612	CLA	C4-C3-C5	3.16	120.77	115.29
24	B	607	CLA	CMC-C2C-C1C	3.17	129.82	125.02
24	D	403	CLA	CAC-C3C-C4C	3.17	129.30	124.83
27	A	411	SQD	O48-C23-C24	3.18	121.14	111.90
24	C	504	CLA	C3B-C4B-NB	3.19	113.33	109.21
24	a	403	CLA	CMB-C2B-C3B	3.19	130.81	124.89
24	b	609	CLA	C3B-C4B-NB	3.19	113.33	109.21
24	c	507	CLA	CMC-C2C-C1C	3.19	129.86	125.02
24	b	612	CLA	O2A-CGA-CBA	3.19	121.19	111.90
25	a	405	PHO	C2C-C1C-NC	3.19	114.55	109.82
31	A	416[A]	PL9	C15-C14-C16	3.20	120.83	115.29
24	c	512	CLA	O2A-CGA-CBA	3.20	121.20	111.90
24	c	513	CLA	C4-C3-C5	3.20	120.84	115.29
27	A	413	SQD	O48-C23-C24	3.20	121.20	111.90
24	C	514	CLA	C3B-C4B-NB	3.20	113.35	109.21
24	b	613	CLA	O2A-CGA-CBA	3.21	121.24	111.90
25	a	405	PHO	C2B-C1B-NB	3.21	114.57	109.82
25	A	408	PHO	CAC-C3C-C4C	3.21	128.98	125.21
24	c	515	CLA	CAC-C3C-C4C	3.23	129.38	124.83
24	c	512	CLA	C4-C3-C5	3.23	120.89	115.29
24	A	406	CLA	O2A-CGA-CBA	3.23	121.30	111.90
24	b	614	CLA	C3B-C4B-NB	3.23	113.39	109.21
24	c	505	CLA	C3B-C4B-NB	3.24	113.40	109.21
36	C	518	DGD	O1G-C1A-C2A	3.24	121.33	111.90
24	A	404	CLA	CAC-C3C-C4C	3.25	129.41	124.83
24	B	615	CLA	CMC-C2C-C1C	3.25	129.96	125.02
27	A	413	SQD	O7-S-C6	3.26	109.61	106.83
24	B	609	CLA	C3B-C4B-NB	3.26	113.43	109.21
24	B	614	CLA	C4-C3-C5	3.27	120.95	115.29
25	A	408	PHO	C2B-C1B-NB	3.27	114.66	109.82
24	B	604	CLA	O2A-CGA-CBA	3.27	121.41	111.90
24	B	609	CLA	C1-O2A-CGA	3.27	124.62	116.77
27	B	620	SQD	O48-C23-C24	3.28	121.43	111.90
33	C	521	LMG	C3-C4-C5	3.28	115.99	110.22
34	M	101	LMT	O1'-C1'-C2'	3.28	113.58	108.23
24	b	612	CLA	C4-C3-C5	3.28	120.98	115.29
24	b	605	CLA	C4-C3-C5	3.28	120.98	115.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	CLA	C3B-C4B-NB	3.28	113.45	109.21
24	B	612	CLA	CAC-C3C-C4C	3.29	129.47	124.83
24	B	601	CLA	O2A-CGA-CBA	3.29	121.47	111.90
24	c	506	CLA	CMC-C2C-C1C	3.29	130.01	125.02
24	c	513	CLA	C3B-C4B-NB	3.29	113.47	109.21
24	C	511	CLA	C3B-C4B-NB	3.29	113.47	109.21
25	A	407	PHO	C2B-C1B-NB	3.29	114.70	109.82
34	t	101	LMT	C1'-O5'-C5'	3.30	119.92	113.72
24	c	514	CLA	C4-C3-C5	3.30	121.01	115.29
38	d	406	LHG	O8-C23-C24	3.30	121.50	111.90
24	a	403	CLA	O2A-CGA-CBA	3.31	121.53	111.90
24	B	614	CLA	CMB-C2B-C3B	3.31	131.04	124.89
24	B	604	CLA	C3B-C4B-NB	3.32	113.50	109.21
27	A	413	SQD	O47-C7-C8	3.32	118.44	111.55
33	c	521	LMG	O8-C28-C29	3.32	121.55	111.90
24	C	510	CLA	C3B-C4B-NB	3.32	113.50	109.21
31	d	405	PL9	C10-C9-C11	3.32	121.06	115.29
24	b	601	CLA	C4-C3-C5	3.34	121.08	115.29
24	a	404	CLA	C3B-C4B-NB	3.34	113.53	109.21
31	a	414[A]	PL9	C30-C29-C31	3.35	121.10	115.29
24	b	601	CLA	C3B-C4B-NB	3.35	113.54	109.21
24	d	402	CLA	C4-C3-C5	3.35	121.11	115.29
24	c	504	CLA	C3B-C4B-NB	3.35	113.55	109.21
24	B	603	CLA	O2A-CGA-CBA	3.36	121.67	111.90
24	b	603	CLA	O2A-CGA-CBA	3.36	121.69	111.90
36	h	103	DGD	O1G-C1A-C2A	3.37	121.71	111.90
24	b	608	CLA	C3B-C4B-NB	3.37	113.57	109.21
24	b	614	CLA	CAC-C3C-C4C	3.38	129.60	124.83
24	b	605	CLA	C3B-C4B-NB	3.38	113.58	109.21
24	A	404	CLA	C3B-C4B-NB	3.39	113.59	109.21
24	c	510	CLA	C3B-C4B-NB	3.40	113.60	109.21
24	b	609	CLA	CAC-C3C-C4C	3.40	129.62	124.83
24	B	614	CLA	CMC-C2C-C1C	3.40	130.17	125.02
24	b	604	CLA	O2A-CGA-CBA	3.40	121.79	111.90
26	B	618	BCR	C29-C30-C25	3.40	115.80	110.48
24	d	402	CLA	O2A-CGA-CBA	3.41	121.81	111.90
38	d	406	LHG	O7-C7-C8	3.41	118.63	111.55
24	B	614	CLA	C3B-C4B-NB	3.41	113.62	109.21
24	D	403	CLA	CMC-C2C-C1C	3.42	130.21	125.02
36	c	519	DGD	O2G-C1B-C2B	3.43	118.68	111.55
36	C	518	DGD	O2G-C1B-C2B	3.43	118.68	111.55
27	A	413	SQD	O8-S-C6	3.43	110.20	106.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C3B-C4B-NB	3.44	113.65	109.21
27	f	101	SQD	O7-S-C6	3.44	109.76	106.83
24	b	613	CLA	C3B-C4B-NB	3.44	113.66	109.21
33	z	101	LMG	O7-C10-C11	3.45	118.71	111.55
24	b	615	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	B	613	CLA	O2D-CGD-CBD	3.45	117.47	111.30
33	B	621	LMG	O8-C28-C29	3.46	121.96	111.90
24	d	402	CLA	C3B-C4B-NB	3.46	113.68	109.21
38	D	357	LHG	O8-C23-C24	3.46	121.97	111.90
36	c	520	DGD	O2G-C1B-C2B	3.46	118.74	111.55
35	C	523	HTG	O5-C5-C4	3.46	116.04	109.66
24	C	511	CLA	C4-C3-C5	3.47	121.31	115.29
27	b	620	SQD	O7-S-C6	3.48	109.80	106.83
24	b	613	CLA	O2D-CGD-CBD	3.48	117.51	111.30
38	l	101	LHG	O8-C23-C24	3.48	122.03	111.90
24	a	403	CLA	O2D-CGD-CBD	3.48	117.52	111.30
24	C	504	CLA	C4-C3-C5	3.49	121.34	115.29
24	d	403	CLA	CMC-C2C-C1C	3.50	130.32	125.02
24	A	404	CLA	CMC-C2C-C1C	3.51	130.34	125.02
31	a	414[A]	PL9	C15-C14-C16	3.52	121.39	115.29
31	A	416[A]	PL9	C10-C9-C11	3.53	121.41	115.29
24	C	509	CLA	C3B-C4B-NB	3.53	113.78	109.21
33	C	520	LMG	O8-C28-C29	3.55	122.22	111.90
24	C	512	CLA	C3B-C4B-NB	3.55	113.80	109.21
24	C	507	CLA	C3B-C4B-NB	3.55	113.80	109.21
25	a	406	PHO	C4-C3-C5	3.55	121.45	115.29
38	D	407	LHG	O7-C7-C8	3.56	118.94	111.55
35	b	623	HTG	C1-O5-C5	3.56	119.54	112.69
24	B	607	CLA	C3B-C4B-NB	3.59	113.85	109.21
24	b	616	CLA	O2A-CGA-CBA	3.60	122.36	111.90
34	I	101	LMT	O1B-C4'-C3'	3.61	115.87	107.19
24	c	511	CLA	CAC-C3C-C4C	3.61	129.92	124.83
24	b	614	CLA	CMC-C2C-C1C	3.62	130.50	125.02
33	b	621	LMG	O8-C28-C29	3.62	122.44	111.90
24	a	407	CLA	C3B-C4B-NB	3.63	113.91	109.21
24	B	606	CLA	CMC-C2C-C1C	3.65	130.55	125.02
24	B	613	CLA	C3B-C4B-NB	3.68	113.96	109.21
24	c	506	CLA	C3B-C4B-NB	3.68	113.97	109.21
24	C	512	CLA	CMC-C2C-C1C	3.69	130.61	125.02
38	L	101	LHG	O7-C7-C8	3.69	119.22	111.55
38	l	101	LHG	O7-C7-C8	3.71	119.25	111.55
24	B	610	CLA	O2A-CGA-CBA	3.72	122.72	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	D	402	CLA	C3B-C4B-NB	3.74	114.05	109.21
24	a	407	CLA	C4-C3-C5	3.75	121.79	115.29
27	f	101	SQD	C1-O5-C5	3.78	120.84	113.72
24	B	612	CLA	C3B-C4B-NB	3.79	114.11	109.21
24	c	511	CLA	C3B-C4B-NB	3.79	114.11	109.21
27	a	409	SQD	O9-S-C6	3.80	110.07	106.83
24	D	402	CLA	O2D-CGD-CBD	3.80	118.09	111.30
24	A	409	CLA	C3B-C4B-NB	3.80	114.12	109.21
24	c	508	CLA	C3B-C4B-NB	3.81	114.13	109.21
24	b	615	CLA	O2D-CGD-CBD	3.82	118.12	111.30
33	Z	101	LMG	C1-C2-C3	3.84	117.11	109.98
27	F	101	SQD	O7-S-C6	3.84	110.11	106.83
24	C	512	CLA	CAC-C3C-C4C	3.84	130.24	124.83
27	a	411	SQD	O47-C7-C8	3.84	119.53	111.55
33	b	621	LMG	O7-C10-C11	3.86	119.57	111.55
24	c	508	CLA	O2D-CGD-CBD	3.86	118.20	111.30
24	C	505	CLA	C3B-C4B-NB	3.87	114.21	109.21
24	b	612	CLA	C3B-C4B-NB	3.88	114.23	109.21
36	c	518	DGD	O2G-C1B-C2B	3.89	119.62	111.55
26	k	101	BCR	C29-C30-C25	3.89	116.56	110.48
24	c	512	CLA	C3B-C4B-NB	3.90	114.26	109.21
33	B	621	LMG	O7-C10-C11	3.91	119.67	111.55
36	C	517	DGD	O2G-C1B-C2B	3.94	119.73	111.55
24	B	613	CLA	CMC-C2C-C1C	3.96	131.02	125.02
24	b	607	CLA	C3B-C4B-NB	3.97	114.35	109.21
27	F	101	SQD	O8-S-C6	3.98	110.87	106.01
24	B	611	CLA	C3B-C4B-NB	3.98	114.36	109.21
33	a	417	LMG	O7-C10-C11	4.01	119.88	111.55
24	a	404	CLA	O2D-CGD-CBD	4.02	118.49	111.30
24	A	405	CLA	CMC-C2C-C1C	4.04	131.15	125.02
24	a	350	CLA	O2D-CGD-CBD	4.05	118.54	111.30
33	c	521	LMG	O7-C10-C11	4.06	119.97	111.55
33	c	522	LMG	O7-C10-C11	4.06	119.98	111.55
35	b	628	HTG	C1'-S1-C1	4.06	106.30	100.28
24	B	603	CLA	C4-C3-C5	4.09	122.38	115.29
24	C	507	CLA	C3C-C4C-NC	4.09	114.35	110.21
38	d	408	LHG	O7-C7-C8	4.09	120.05	111.55
34	I	101	LMT	C1'-O5'-C5'	4.10	121.44	113.72
38	D	357	LHG	O7-C7-C8	4.12	120.11	111.55
27	B	620	SQD	O6-C1-C2	4.12	114.96	108.23
24	b	607	CLA	O2D-CGD-CBD	4.13	118.68	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	403	CLA	C3C-C4C-NC	4.15	114.41	110.21
24	c	505	CLA	O2D-CGD-CBD	4.16	118.73	111.30
24	B	605	CLA	C4-C3-C5	4.18	122.55	115.29
24	b	610	CLA	O2A-CGA-CBA	4.20	124.11	111.90
24	c	509	CLA	C3C-C4C-NC	4.20	114.47	110.21
24	B	609	CLA	O2D-CGD-CBD	4.22	118.83	111.30
24	A	404	CLA	O2A-CGA-CBA	4.24	124.24	111.90
24	c	512	CLA	O2D-CGD-CBD	4.24	118.88	111.30
24	c	512	CLA	C3C-C4C-NC	4.25	114.51	110.21
24	B	613	CLA	CAC-C3C-C4C	4.28	130.86	124.83
33	C	521	LMG	O7-C10-C11	4.28	120.44	111.55
24	c	508	CLA	C3C-C4C-NC	4.29	114.56	110.21
24	a	403	CLA	C3B-C4B-NB	4.31	114.78	109.21
35	b	623	HTG	C1'-S1-C1	4.33	106.70	100.28
24	c	515	CLA	O2D-CGD-CBD	4.34	119.06	111.30
24	d	403	CLA	C3C-C4C-NC	4.35	114.61	110.21
24	A	406	CLA	C3C-C4C-NC	4.38	114.65	110.21
24	c	511	CLA	C3C-C4C-NC	4.39	114.65	110.21
24	c	506	CLA	C3C-C4C-NC	4.39	114.66	110.21
24	B	615	CLA	O2D-CGD-CBD	4.41	119.18	111.30
24	B	602	CLA	O2D-CGD-CBD	4.43	119.22	111.30
38	E	101	LHG	O7-C7-C8	4.43	120.76	111.55
24	C	512	CLA	O2D-CGD-CBD	4.44	119.23	111.30
24	a	350	CLA	C3C-C4C-NC	4.46	114.73	110.21
24	A	409	CLA	O2D-CGD-CBD	4.46	119.27	111.30
31	A	416[B]	PL9	C7-C3-C4	4.48	120.52	116.88
24	d	402	CLA	O2D-CGD-CBD	4.48	119.31	111.30
27	B	620	SQD	O47-C7-C8	4.51	120.92	111.55
24	c	503	CLA	C3C-C4C-NC	4.52	114.79	110.21
33	C	520	LMG	O7-C10-C11	4.53	120.97	111.55
27	A	411	SQD	O47-C7-C8	4.54	120.98	111.55
24	c	514	CLA	C3C-C4C-NC	4.56	114.83	110.21
24	C	514	CLA	O2D-CGD-CBD	4.56	119.44	111.30
24	B	608	CLA	O2D-CGD-CBD	4.56	119.45	111.30
24	b	605	CLA	C3C-C4C-NC	4.57	114.84	110.21
31	a	414[A]	PL9	C7-C3-C4	4.62	120.63	116.88
24	D	403	CLA	O2D-CGD-CBD	4.65	119.60	111.30
24	c	515	CLA	C3C-C4C-NC	4.66	114.94	110.21
24	b	612	CLA	O2D-CGD-CBD	4.67	119.64	111.30
24	C	511	CLA	C3C-C4C-NC	4.67	114.94	110.21
24	c	506	CLA	O2D-CGD-CBD	4.70	119.70	111.30
24	b	615	CLA	C3C-C4C-NC	4.71	114.98	110.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	507	CLA	O2D-CGD-CBD	4.71	119.71	111.30
35	C	523	HTG	C1-O5-C5	4.71	121.76	112.69
24	b	601	CLA	C3C-C4C-NC	4.72	114.99	110.21
24	B	607	CLA	C3C-C4C-NC	4.72	114.99	110.21
24	a	404	CLA	C3C-C4C-NC	4.72	115.00	110.21
33	A	418	LMG	O7-C10-C11	4.74	121.39	111.55
24	b	609	CLA	O2D-CGD-CBD	4.74	119.77	111.30
33	Z	101	LMG	O7-C10-C11	4.75	121.41	111.55
24	C	504	CLA	C3C-C4C-NC	4.75	115.02	110.21
24	b	608	CLA	O2D-CGD-CBD	4.76	119.81	111.30
24	A	406	CLA	O2D-CGD-CBD	4.77	119.81	111.30
24	C	502	CLA	C3C-C4C-NC	4.77	115.05	110.21
24	B	614	CLA	C3C-C4C-NC	4.79	115.06	110.21
25	A	407	PHO	O2D-CGD-CBD	4.83	119.92	111.30
24	d	403	CLA	C2C-C1C-NC	4.83	113.55	110.22
24	C	505	CLA	C3C-C4C-NC	4.84	115.11	110.21
24	c	513	CLA	C3C-C4C-NC	4.85	115.12	110.21
24	c	513	CLA	O2D-CGD-CBD	4.85	119.96	111.30
25	a	406	PHO	C2D-C1D-ND	4.85	117.00	109.82
33	j	101	LMG	O7-C10-C11	4.87	121.65	111.55
27	F	101	SQD	O6-C1-C2	4.87	116.19	108.23
24	B	611	CLA	O2D-CGD-CBD	4.89	120.04	111.30
27	b	620	SQD	O47-C7-C8	4.93	121.79	111.55
24	b	608	CLA	C3C-C4C-NC	4.94	115.21	110.21
24	c	504	CLA	C3C-C4C-NC	4.94	115.22	110.21
24	b	609	CLA	C3C-C4C-NC	4.94	115.22	110.21
24	D	402	CLA	C3C-C4C-NC	4.95	115.22	110.21
24	C	503	CLA	O2D-CGD-CBD	4.95	120.14	111.30
24	C	510	CLA	C3C-C4C-NC	4.97	115.25	110.21
24	c	511	CLA	O2D-CGD-CBD	4.98	120.19	111.30
24	b	602	CLA	C3C-C4C-NC	4.98	115.25	110.21
27	a	409	SQD	O8-S-C6	4.98	112.09	106.01
24	B	602	CLA	C3C-C4C-NC	4.98	115.26	110.21
24	A	405	CLA	O2D-CGD-CBD	4.99	120.22	111.30
24	a	407	CLA	O2D-CGD-CBD	5.01	120.26	111.30
24	C	512	CLA	C3C-C4C-NC	5.03	115.31	110.21
24	b	611	CLA	C3C-C4C-NC	5.03	115.31	110.21
24	b	610	CLA	C3C-C4C-NC	5.04	115.31	110.21
31	a	414[B]	PL9	C7-C3-C4	5.05	120.98	116.88
24	A	409	CLA	C3C-C4C-NC	5.05	115.33	110.21
24	B	607	CLA	O2D-CGD-CBD	5.07	120.36	111.30
24	B	601	CLA	C3C-C4C-NC	5.07	115.35	110.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C3C-C4C-NC	5.08	115.36	110.21
24	A	405	CLA	C3C-C4C-NC	5.09	115.36	110.21
24	B	603	CLA	C3C-C4C-NC	5.09	115.37	110.21
24	B	610	CLA	C3C-C4C-NC	5.10	115.37	110.21
24	a	407	CLA	C3C-C4C-NC	5.10	115.38	110.21
27	b	620	SQD	O6-C1-C2	5.11	116.57	108.23
24	c	505	CLA	C3C-C4C-NC	5.13	115.40	110.21
24	c	504	CLA	O2D-CGD-CBD	5.14	120.48	111.30
27	a	411	SQD	O7-S-C6	5.14	111.22	106.83
24	B	613	CLA	C3C-C4C-NC	5.14	115.42	110.21
24	A	404	CLA	C3C-C4C-NC	5.14	115.42	110.21
24	B	605	CLA	O2D-CGD-CBD	5.17	120.54	111.30
24	d	403	CLA	O2D-CGD-CBD	5.18	120.55	111.30
24	b	606	CLA	C3C-C4C-NC	5.18	115.46	110.21
24	C	514	CLA	C3C-C4C-NC	5.19	115.47	110.21
24	B	608	CLA	C3C-C4C-NC	5.22	115.50	110.21
24	B	611	CLA	C3C-C4C-NC	5.22	115.50	110.21
24	c	510	CLA	C3C-C4C-NC	5.23	115.51	110.21
24	b	605	CLA	O2D-CGD-CBD	5.24	120.66	111.30
35	B	628	HTG	C1'-S1-C1	5.25	108.07	100.28
24	b	612	CLA	C3C-C4C-NC	5.26	115.54	110.21
24	b	602	CLA	C2C-C1C-NC	5.26	113.84	110.22
24	B	616	CLA	C2C-C1C-NC	5.27	113.85	110.22
24	C	508	CLA	C3C-C4C-NC	5.28	115.56	110.21
24	C	513	CLA	C3C-C4C-NC	5.28	115.56	110.21
24	D	403	CLA	C3C-C4C-NC	5.29	115.57	110.21
24	B	610	CLA	O2D-CGD-CBD	5.29	120.76	111.30
24	B	616	CLA	C3C-C4C-NC	5.30	115.58	110.21
24	C	510	CLA	O2D-CGD-CBD	5.30	120.77	111.30
24	b	616	CLA	C3C-C4C-NC	5.32	115.60	110.21
24	D	403	CLA	C2C-C1C-NC	5.32	113.88	110.22
24	b	614	CLA	C3C-C4C-NC	5.38	115.66	110.21
24	b	603	CLA	C3C-C4C-NC	5.38	115.66	110.21
27	f	101	SQD	O47-C7-C8	5.38	122.73	111.55
24	b	606	CLA	O2D-CGD-CBD	5.39	120.93	111.30
27	a	409	SQD	O6-C1-C2	5.40	117.04	108.23
39	e	102	HEM	CAD-CBD-CGD	5.40	121.89	112.66
24	C	505	CLA	O2D-CGD-CBD	5.44	121.02	111.30
27	B	620	SQD	O7-S-C6	5.44	111.48	106.83
24	B	604	CLA	O2D-CGD-CBD	5.44	121.03	111.30
24	b	607	CLA	C3C-C4C-NC	5.44	115.73	110.21
25	A	408	PHO	O2D-CGD-CBD	5.45	121.05	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	O2D-CGD-CBD	5.46	121.05	111.30
24	B	601	CLA	C2C-C1C-NC	5.46	113.98	110.22
24	b	616	CLA	C2C-C1C-NC	5.47	113.98	110.22
24	C	509	CLA	O2D-CGD-CBD	5.48	121.10	111.30
24	b	610	CLA	O2D-CGD-CBD	5.49	121.11	111.30
25	A	408	PHO	C2D-C1D-ND	5.50	117.96	109.82
24	C	506	CLA	O2D-CGD-CBD	5.51	121.15	111.30
24	C	511	CLA	O2D-CGD-CBD	5.52	121.16	111.30
27	a	409	SQD	O47-C7-C8	5.53	123.03	111.55
25	A	407	PHO	C2D-C1D-ND	5.54	118.02	109.82
24	b	613	CLA	C3C-C4C-NC	5.55	115.83	110.21
24	B	606	CLA	C2C-C1C-NC	5.55	114.04	110.22
24	b	611	CLA	O2D-CGD-CBD	5.57	121.25	111.30
25	a	405	PHO	C2D-C1D-ND	5.59	118.09	109.82
24	b	602	CLA	O2D-CGD-CBD	5.61	121.32	111.30
24	B	615	CLA	C3C-C4C-NC	5.62	115.90	110.21
24	b	604	CLA	C3C-C4C-NC	5.63	115.91	110.21
24	d	402	CLA	C3C-C4C-NC	5.63	115.92	110.21
25	a	406	PHO	O2D-CGD-CBD	5.64	121.37	111.30
24	C	502	CLA	O2D-CGD-CBD	5.64	121.38	111.30
24	B	605	CLA	C3C-C4C-NC	5.66	115.94	110.21
24	B	606	CLA	C3C-C4C-NC	5.66	115.95	110.21
24	b	604	CLA	O2D-CGD-CBD	5.73	121.53	111.30
24	c	503	CLA	O2D-CGD-CBD	5.73	121.54	111.30
24	B	609	CLA	C3C-C4C-NC	5.73	116.02	110.21
24	c	510	CLA	O2D-CGD-CBD	5.74	121.56	111.30
24	B	601	CLA	O2D-CGD-CBD	5.77	121.61	111.30
24	C	509	CLA	C3C-C4C-NC	5.77	116.06	110.21
24	b	603	CLA	O2D-CGD-CBD	5.78	121.64	111.30
24	A	406	CLA	C2C-C1C-NC	5.80	114.21	110.22
24	C	506	CLA	C3C-C4C-NC	5.80	116.09	110.21
27	F	101	SQD	O47-C7-C8	5.81	123.61	111.55
24	b	601	CLA	O2D-CGD-CBD	5.81	121.68	111.30
27	A	411	SQD	O9-S-C6	5.82	111.80	106.83
24	B	602	CLA	C2C-C1C-NC	5.83	114.23	110.22
35	C	523	HTG	C1'-S1-C1	5.83	108.94	100.28
24	b	616	CLA	O2D-CGD-CBD	5.84	121.73	111.30
24	A	405	CLA	C2C-C1C-NC	5.84	114.24	110.22
24	B	615	CLA	C2C-C1C-NC	5.89	114.27	110.22
24	C	513	CLA	C2C-C1C-NC	5.94	114.31	110.22
24	C	508	CLA	O2D-CGD-CBD	5.96	121.95	111.30
24	B	614	CLA	O2D-CGD-CBD	5.98	121.99	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C2C-C1C-NC	6.00	114.35	110.22
24	B	612	CLA	C3C-C4C-NC	6.00	116.29	110.21
24	a	350	CLA	C2C-C1C-NC	6.01	114.36	110.22
24	B	604	CLA	C3C-C4C-NC	6.02	116.31	110.21
24	B	605	CLA	C2C-C1C-NC	6.03	114.37	110.22
24	b	611	CLA	C2C-C1C-NC	6.05	114.38	110.22
24	C	513	CLA	O2D-CGD-CBD	6.08	122.17	111.30
24	b	614	CLA	O2D-CGD-CBD	6.09	122.19	111.30
24	C	514	CLA	C2C-C1C-NC	6.12	114.43	110.22
24	c	509	CLA	O2D-CGD-CBD	6.15	122.29	111.30
27	A	411	SQD	O6-C1-C2	6.16	118.29	108.23
24	c	514	CLA	O2D-CGD-CBD	6.21	122.40	111.30
24	B	603	CLA	O2D-CGD-CBD	6.22	122.42	111.30
25	a	405	PHO	O2D-CGD-CBD	6.23	122.43	111.30
24	B	612	CLA	O2D-CGD-CBD	6.28	122.52	111.30
35	C	522	HTG	C1'-S1-C1	6.28	109.60	100.28
24	c	507	CLA	C3C-C4C-NC	6.31	116.61	110.21
24	C	511	CLA	C2C-C1C-NC	6.31	114.56	110.22
35	c	526	HTG	C1'-S1-C1	6.33	109.66	100.28
24	B	616	CLA	O2D-CGD-CBD	6.35	122.64	111.30
25	a	406	PHO	CMD-C2D-C1D	6.35	134.94	125.04
24	B	610	CLA	C2C-C1C-NC	6.38	114.61	110.22
24	a	404	CLA	C2C-C1C-NC	6.40	114.62	110.22
24	c	503	CLA	C2C-C1C-NC	6.41	114.63	110.22
35	c	523	HTG	C1'-S1-C1	6.42	109.80	100.28
24	b	606	CLA	C2C-C1C-NC	6.43	114.64	110.22
24	c	514	CLA	C2C-C1C-NC	6.46	114.67	110.22
24	C	506	CLA	C2C-C1C-NC	6.47	114.67	110.22
25	A	407	PHO	CMD-C2D-C1D	6.48	135.13	125.04
24	C	502	CLA	C2C-C1C-NC	6.50	114.69	110.22
24	B	606	CLA	O2D-CGD-CBD	6.51	122.93	111.30
24	b	601	CLA	C2C-C1C-NC	6.57	114.74	110.22
35	B	624	HTG	C1'-S1-C1	6.59	110.05	100.28
25	a	405	PHO	CMD-C2D-C1D	6.64	135.38	125.04
24	b	610	CLA	C2C-C1C-NC	6.64	114.79	110.22
24	C	503	CLA	C2C-C1C-NC	6.65	114.80	110.22
24	a	407	CLA	C2C-C1C-NC	6.67	114.81	110.22
24	b	614	CLA	C2C-C1C-NC	6.68	114.81	110.22
24	c	509	CLA	C2C-C1C-NC	6.70	114.83	110.22
24	B	609	CLA	C2C-C1C-NC	6.75	114.87	110.22
24	C	512	CLA	C2C-C1C-NC	6.79	114.89	110.22
24	b	608	CLA	C2C-C1C-NC	6.79	114.89	110.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C2C-C1C-NC	6.83	114.92	110.22
24	B	604	CLA	C2C-C1C-NC	6.83	114.92	110.22
24	B	611	CLA	C2C-C1C-NC	6.85	114.93	110.22
35	D	410	HTG	C1'-S1-C1	6.85	110.44	100.28
24	b	603	CLA	C2C-C1C-NC	6.86	114.94	110.22
24	C	510	CLA	C2C-C1C-NC	6.87	114.95	110.22
24	c	511	CLA	C2C-C1C-NC	6.88	114.96	110.22
39	E	103	HEM	CAD-CBD-CGD	6.92	124.48	112.66
24	c	506	CLA	C2C-C1C-NC	6.95	115.00	110.22
24	c	515	CLA	C2C-C1C-NC	6.96	115.01	110.22
24	b	604	CLA	C2C-C1C-NC	6.97	115.01	110.22
24	A	409	CLA	C2C-C1C-NC	6.98	115.02	110.22
35	b	624	HTG	C1'-S1-C1	6.99	110.65	100.28
24	B	608	CLA	C2C-C1C-NC	7.03	115.06	110.22
24	C	508	CLA	C2C-C1C-NC	7.06	115.08	110.22
24	b	613	CLA	C2C-C1C-NC	7.08	115.09	110.22
24	B	612	CLA	C2C-C1C-NC	7.09	115.10	110.22
24	A	404	CLA	C2C-C1C-NC	7.10	115.10	110.22
24	C	504	CLA	C2C-C1C-NC	7.10	115.10	110.22
24	c	504	CLA	C2C-C1C-NC	7.11	115.11	110.22
24	B	603	CLA	C2C-C1C-NC	7.12	115.12	110.22
24	c	512	CLA	C2C-C1C-NC	7.16	115.15	110.22
35	h	101	HTG	C1'-S1-C1	7.22	110.99	100.28
24	d	402	CLA	C2C-C1C-NC	7.23	115.20	110.22
24	b	615	CLA	C2C-C1C-NC	7.26	115.22	110.22
24	c	505	CLA	C2C-C1C-NC	7.28	115.23	110.22
25	A	408	PHO	CMD-C2D-C1D	7.31	136.43	125.04
24	b	609	CLA	C2C-C1C-NC	7.33	115.26	110.22
24	b	607	CLA	C2C-C1C-NC	7.33	115.26	110.22
24	b	605	CLA	C2C-C1C-NC	7.33	115.27	110.22
24	b	612	CLA	C2C-C1C-NC	7.49	115.37	110.22
24	B	614	CLA	C2C-C1C-NC	7.51	115.39	110.22
24	B	613	CLA	C2C-C1C-NC	7.54	115.41	110.22
24	c	508	CLA	C2C-C1C-NC	7.56	115.42	110.22
35	B	625	HTG	C1'-S1-C1	7.57	111.51	100.28
24	c	510	CLA	C2C-C1C-NC	7.60	115.45	110.22
24	C	509	CLA	C2C-C1C-NC	7.62	115.46	110.22
24	C	505	CLA	C2C-C1C-NC	7.65	115.49	110.22
24	B	607	CLA	C2C-C1C-NC	8.19	115.86	110.22
24	C	507	CLA	C2C-C1C-NC	8.24	115.89	110.22
24	a	403	CLA	C2C-C1C-NC	8.25	115.89	110.22
35	b	625	HTG	C1'-S1-C1	8.28	112.56	100.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	CLA	C2C-C1C-NC	8.33	115.95	110.22

All (191) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	C	508	CLA	NC
24	C	508	CLA	ND
24	C	508	CLA	NA
24	b	609	CLA	NC
24	b	609	CLA	ND
24	B	615	CLA	NA
24	B	615	CLA	NC
24	B	615	CLA	ND
24	C	506	CLA	ND
24	D	403	CLA	NC
24	D	403	CLA	ND
24	D	403	CLA	NA
24	B	610	CLA	NC
24	B	610	CLA	ND
24	B	610	CLA	NA
24	b	601	CLA	NC
24	b	601	CLA	ND
24	b	601	CLA	NA
24	d	402	CLA	ND
24	d	403	CLA	NC
24	d	403	CLA	ND
24	d	403	CLA	NA
24	C	514	CLA	NC
24	C	514	CLA	ND
24	C	514	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	ND
24	c	505	CLA	NA
24	b	613	CLA	NC
24	b	613	CLA	ND
24	b	613	CLA	NA
24	a	403	CLA	NC
24	a	403	CLA	ND
24	C	503	CLA	NC
24	C	503	CLA	ND
24	C	503	CLA	NA
24	a	404	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	a	404	CLA	NA
24	c	512	CLA	NC
24	c	512	CLA	ND
24	c	512	CLA	NA
24	a	350	CLA	NC
24	a	350	CLA	ND
24	a	350	CLA	NA
24	B	614	CLA	NC
24	B	614	CLA	ND
24	B	614	CLA	NA
24	C	502	CLA	NC
24	C	502	CLA	ND
24	C	502	CLA	NA
24	C	510	CLA	NC
24	C	510	CLA	ND
24	C	510	CLA	NA
24	c	508	CLA	NC
24	c	508	CLA	ND
24	c	508	CLA	NA
24	c	506	CLA	NC
24	c	506	CLA	ND
24	c	506	CLA	NA
24	A	405	CLA	NC
24	A	405	CLA	ND
24	A	405	CLA	NA
24	B	603	CLA	NC
24	B	603	CLA	ND
24	b	616	CLA	NA
24	b	616	CLA	NC
24	b	616	CLA	ND
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	606	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	604	CLA	NA
24	A	404	CLA	NC
24	A	404	CLA	ND
24	A	404	CLA	NA
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	616	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	a	407	CLA	NC
24	a	407	CLA	ND
24	a	407	CLA	NA
24	A	406	CLA	NC
24	A	406	CLA	ND
24	A	406	CLA	NA
24	c	511	CLA	NC
24	c	511	CLA	ND
24	c	511	CLA	NA
24	C	509	CLA	NC
24	C	509	CLA	ND
24	C	509	CLA	NA
24	b	610	CLA	NC
24	b	610	CLA	ND
24	b	610	CLA	NA
24	D	402	CLA	ND
24	b	602	CLA	NC
24	b	602	CLA	ND
24	b	602	CLA	NA
24	B	612	CLA	NC
24	B	612	CLA	ND
24	B	612	CLA	NA
24	A	409	CLA	NC
24	A	409	CLA	NA
24	C	505	CLA	NC
24	C	505	CLA	ND
24	C	505	CLA	NA
24	B	605	CLA	NC
24	B	605	CLA	ND
24	B	605	CLA	NA
24	B	602	CLA	NC
24	B	602	CLA	ND
24	b	608	CLA	NC
24	b	608	CLA	NA
24	C	507	CLA	NC
24	C	507	CLA	ND
24	C	507	CLA	NA
24	c	504	CLA	NC
24	c	504	CLA	ND
24	c	504	CLA	NA
24	B	601	CLA	NC
24	B	601	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	B	601	CLA	NA
24	b	605	CLA	NC
24	b	605	CLA	ND
24	b	605	CLA	NA
24	C	513	CLA	NC
24	C	513	CLA	ND
24	C	513	CLA	NA
24	b	615	CLA	NA
24	b	615	CLA	NC
24	b	615	CLA	ND
24	B	606	CLA	NC
24	B	606	CLA	ND
24	B	606	CLA	NA
24	c	515	CLA	NC
24	c	515	CLA	ND
24	c	515	CLA	NA
24	B	607	CLA	NC
24	B	607	CLA	ND
24	B	607	CLA	NA
24	c	507	CLA	ND
24	c	513	CLA	NC
24	c	513	CLA	ND
24	c	513	CLA	NA
24	b	612	CLA	NC
24	b	612	CLA	ND
24	b	612	CLA	NA
24	B	611	CLA	NC
24	B	611	CLA	ND
24	B	611	CLA	NA
24	b	603	CLA	NC
24	b	603	CLA	ND
24	c	503	CLA	NC
24	c	503	CLA	ND
24	c	503	CLA	NA
24	c	509	CLA	NC
24	c	509	CLA	ND
24	c	509	CLA	NA
24	C	504	CLA	NC
24	C	504	CLA	NA
24	B	609	CLA	NC
24	B	609	CLA	ND
24	c	510	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	c	510	CLA	ND
24	c	510	CLA	NA
24	b	604	CLA	NC
24	b	604	CLA	ND
24	b	604	CLA	NA
24	C	511	CLA	NC
24	C	511	CLA	ND
24	C	511	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	b	607	CLA	NA
24	B	608	CLA	NC
24	B	608	CLA	NA
24	c	514	CLA	NC
24	c	514	CLA	ND
24	c	514	CLA	NA
24	C	512	CLA	NC
24	C	512	CLA	ND
24	C	512	CLA	NA
24	b	611	CLA	NC
24	b	611	CLA	ND
24	b	611	CLA	NA
24	b	614	CLA	NC
24	b	614	CLA	ND
24	b	614	CLA	NA
24	B	613	CLA	NC
24	B	613	CLA	ND
24	B	613	CLA	NA

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C8-O7-C10-O9
33	Z	101	LMG	C8-O7-C10-C11
27	f	101	SQD	C45-O47-C7-O49
27	F	101	SQD	C45-O47-C7-O49
27	f	101	SQD	C45-O47-C7-C8
27	F	101	SQD	C45-O47-C7-C8

There are no ring outliers.

81 monomers are involved in 302 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	A	359	LMT	4	0
24	A	404	CLA	10	0
24	A	405	CLA	3	0
24	A	406	CLA	5	0
25	A	407	PHO	2	0
25	A	408	PHO	4	0
24	A	409	CLA	3	0
26	A	410	BCR	2	0
27	A	411	SQD	6	0
27	A	413	SQD	2	0
31	A	416[A]	PL9	4	0
31	A	416[B]	PL9	5	0
33	A	418	LMG	1	0
24	B	601	CLA	3	0
24	B	602	CLA	7	0
24	B	603	CLA	3	0
24	B	604	CLA	4	0
24	B	605	CLA	10	0
24	B	606	CLA	7	0
24	B	607	CLA	1	0
24	B	609	CLA	7	0
24	B	610	CLA	2	0
24	B	611	CLA	2	0
24	B	612	CLA	8	0
24	B	613	CLA	7	0
24	B	614	CLA	8	0
24	B	615	CLA	4	0
24	B	616	CLA	6	0
26	B	617	BCR	3	0
26	B	618	BCR	4	0
26	B	619	BCR	6	0
27	B	620	SQD	3	0
33	B	621	LMG	2	0
34	B	622	LMT	3	0
35	B	623	HTG	5	0
35	B	624	HTG	3	0
35	B	625	HTG	1	0
28	B	627	GOL	1	0
24	C	502	CLA	7	0
24	C	503	CLA	8	0
24	C	504	CLA	10	0
24	C	505	CLA	6	0
24	C	506	CLA	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	507	CLA	15	0
24	C	508	CLA	6	0
24	C	509	CLA	8	0
24	C	510	CLA	8	0
24	C	511	CLA	8	0
24	C	512	CLA	12	0
24	C	513	CLA	8	0
24	C	514	CLA	11	0
26	C	515	BCR	4	0
26	C	516	BCR	3	0
36	C	517	DGD	2	0
36	C	518	DGD	2	0
36	C	519	DGD	6	0
33	C	521	LMG	5	0
35	C	522	HTG	2	0
38	D	357	LHG	2	0
24	D	402	CLA	7	0
24	D	403	CLA	5	0
26	D	404	BCR	5	0
31	D	405	PL9	5	0
38	D	406	LHG	5	0
38	D	407	LHG	7	0
35	D	410	HTG	2	0
38	E	101	LHG	6	0
34	E	102	LMT	1	0
39	E	103	HEM	2	0
27	F	101	SQD	1	0
26	H	101	BCR	3	0
36	H	102	DGD	2	0
34	I	101	LMT	1	0
33	J	101	LMG	6	0
26	K	102	BCR	1	0
38	L	101	LHG	2	0
34	M	101	LMT	1	0
34	M	103	LMT	2	0
26	T	101	BCR	6	0
26	Y	101	BCR	4	0
33	Z	101	LMG	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/344 (97%)	1.54	82 (24%) 1 1	40, 48, 69, 120	1 (0%)
1	a	334/344 (97%)	1.80	113 (33%) 0 0	41, 52, 84, 120	0
2	B	504/505 (99%)	1.68	151 (29%) 1 0	41, 53, 83, 128	0
2	b	504/505 (99%)	1.86	172 (34%) 0 0	44, 57, 97, 149	0
3	C	451/455 (99%)	1.87	171 (37%) 0 0	43, 59, 81, 142	0
3	c	455/455 (100%)	2.02	188 (41%) 0 0	48, 67, 90, 129	0
4	D	342/342 (100%)	1.48	90 (26%) 1 1	38, 49, 68, 139	0
4	d	341/342 (99%)	1.66	108 (31%) 0 0	43, 55, 78, 147	0
5	E	81/84 (96%)	2.39	40 (49%) 0 0	53, 70, 100, 151	0
5	e	79/84 (94%)	3.56	61 (77%) 0 0	62, 78, 122, 140	0
6	F	34/44 (77%)	1.51	9 (26%) 1 1	52, 63, 90, 117	0
6	f	31/44 (70%)	2.78	19 (61%) 0 0	62, 68, 100, 140	0
7	H	64/65 (98%)	1.99	25 (39%) 0 0	49, 62, 81, 129	0
7	h	64/65 (98%)	2.26	31 (48%) 0 0	58, 69, 95, 147	0
8	I	37/38 (97%)	2.06	13 (35%) 0 0	55, 62, 127, 147	0
8	i	37/38 (97%)	2.07	15 (40%) 0 0	57, 66, 123, 138	0
9	J	38/39 (97%)	2.17	16 (42%) 0 0	51, 71, 129, 175	0
9	j	39/39 (100%)	2.88	23 (58%) 0 0	56, 80, 149, 175	0
10	K	37/37 (100%)	1.77	14 (37%) 0 0	60, 67, 89, 101	0
10	k	37/37 (100%)	2.45	24 (64%) 0 0	70, 77, 101, 117	0
11	L	36/37 (97%)	1.90	10 (27%) 1 1	41, 47, 109, 162	0
11	l	36/37 (97%)	1.51	7 (19%) 1 2	43, 48, 103, 152	0
12	M	32/36 (88%)	1.41	6 (18%) 1 2	43, 49, 74, 134	0
12	m	33/36 (91%)	1.59	5 (15%) 2 4	43, 50, 86, 140	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	1.94	77 (31%) 0 0	40, 63, 115, 176	0
13	o	243/244 (99%)	2.07	100 (41%) 0 0	44, 65, 121, 161	0
14	T	29/32 (90%)	1.23	3 (10%) 7 11	42, 49, 81, 115	0
14	t	29/32 (90%)	1.18	2 (6%) 18 25	43, 50, 81, 130	0
15	U	96/104 (92%)	1.84	33 (34%) 0 0	47, 60, 90, 101	0
15	u	97/104 (93%)	1.38	22 (22%) 1 1	51, 62, 84, 121	0
16	V	137/137 (100%)	1.57	33 (24%) 1 1	46, 57, 82, 112	0
16	v	137/137 (100%)	2.43	74 (54%) 0 0	52, 71, 104, 137	0
17	X	38/40 (95%)	2.51	23 (60%) 0 0	59, 71, 96, 126	0
17	x	38/40 (95%)	3.16	25 (65%) 0 0	65, 78, 117, 154	0
18	Y	29/30 (96%)	4.46	24 (82%) 0 0	73, 87, 140, 155	0
18	y	29/30 (96%)	4.10	25 (86%) 0 0	79, 97, 126, 136	0
19	Z	62/62 (100%)	3.99	52 (83%) 0 0	67, 84, 131, 173	0
19	z	62/62 (100%)	4.84	56 (90%) 0 0	83, 99, 148, 185	0
20	R	34/34 (100%)	6.60	34 (100%) 0 0	97, 125, 149, 154	0
All	All	5283/5384 (98%)	1.98	1976 (37%) 0 0	38, 59, 104, 185	1 (0%)

All (1976) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	494	GLY	15.0
6	f	15	ILE	12.4
11	L	2	GLU	12.3
19	z	33	TRP	12.3
18	Y	19	ILE	11.8
18	Y	20	ALA	11.5
13	O	61	GLN	11.4
2	b	504	THR	11.0
2	B	494	GLY	11.0
19	z	3	ILE	11.0
19	z	30	PRO	10.0
2	b	487	SER	10.0
20	R	23	ILE	9.7
20	R	18	TRP	9.7
17	x	2	THR	9.6
18	y	41	VAL	9.5
1	a	11	ALA	9.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Z	31	GLN	9.4
17	x	38	GLN	9.3
12	M	33	GLN	8.9
20	R	24	LEU	8.8
20	R	7	VAL	8.8
20	R	28	VAL	8.8
3	c	200	THR	8.7
19	z	2	THR	8.7
19	Z	42	LEU	8.6
2	b	295	GLY	8.6
19	Z	33	TRP	8.5
2	b	496	TYR	8.5
2	b	503	THR	8.4
7	h	65	LEU	8.3
20	R	6	LEU	8.3
8	i	36	ASP	8.3
20	R	31	VAL	8.2
2	b	493	TRP	8.2
19	z	31	GLN	8.2
20	R	27	ALA	8.2
19	z	39	LEU	8.1
2	b	293	ALA	8.1
2	B	496	TYR	8.1
19	z	34	ASP	8.1
2	b	502	VAL	8.1
13	O	133	VAL	8.1
19	z	61	VAL	8.0
2	b	495	PHE	8.0
18	Y	18	VAL	8.0
4	d	14	TRP	7.9
19	Z	38	GLN	7.8
19	Z	34	ASP	7.8
19	z	7	LEU	7.8
19	Z	30	PRO	7.7
13	o	140	THR	7.7
18	y	19	ILE	7.7
9	j	6	ARG	7.7
2	B	293	ALA	7.6
18	Y	23	THR	7.6
20	R	3	TRP	7.5
1	A	13	LEU	7.5
5	e	20	TRP	7.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	R	13	LEU	7.5
16	V	16	GLY	7.5
16	v	16	GLY	7.5
5	E	84	LYS	7.4
3	c	203	THR	7.4
19	z	50	LEU	7.4
5	E	4	THR	7.4
13	o	134	THR	7.4
13	O	27	ARG	7.4
19	Z	35	ARG	7.3
20	R	35	LEU	7.3
3	c	24	THR	7.3
12	m	33	GLN	7.3
19	z	60	PHE	7.3
9	j	4	GLY	7.3
20	R	32	GLN	7.3
13	o	133	VAL	7.2
16	v	14	SER	7.2
19	Z	41	PHE	7.2
19	Z	1	MET	7.2
20	R	25	PRO	7.2
5	e	19	TYR	7.2
9	J	3	GLU	7.2
8	I	36	ASP	7.2
3	C	155	ASN	7.1
5	E	17	VAL	7.1
20	R	26	TYR	7.1
4	D	11	GLU	7.1
13	o	58	ASN	7.1
3	c	143	TYR	7.1
13	O	139	SER	7.0
11	l	3	PRO	7.0
20	R	11	PRO	7.0
8	I	38	GLU	7.0
4	D	238	THR	7.0
9	J	4	GLY	7.0
3	C	30	SER	6.9
7	h	64	ALA	6.9
5	e	79	PHE	6.9
16	v	19	ILE	6.9
13	o	139	SER	6.9
3	C	257	PHE	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	i	37	LEU	6.9
18	y	22	LEU	6.9
3	C	193	GLY	6.8
13	o	132	ASN	6.8
17	x	37	VAL	6.8
20	R	2	ASP	6.8
19	z	10	ALA	6.8
2	b	497	GLN	6.8
19	Z	3	ILE	6.8
5	e	34	GLY	6.8
13	o	208	THR	6.8
5	e	39	SER	6.8
19	z	46	LEU	6.8
19	z	38	GLN	6.8
13	o	35	SER	6.7
2	B	295	GLY	6.7
3	C	207	ARG	6.7
3	c	101	PRO	6.7
20	R	14	LEU	6.7
2	B	487	SER	6.6
4	d	17	ILE	6.6
19	z	35	ARG	6.6
5	e	21	VAL	6.6
2	b	129	GLY	6.6
5	e	15	THR	6.6
19	z	41	PHE	6.6
19	Z	4	LEU	6.6
20	R	33	LYS	6.6
13	O	23	ASP	6.6
19	z	5	PHE	6.6
2	B	495	PHE	6.5
13	o	33	ASP	6.5
2	B	290	ALA	6.5
2	b	296	ALA	6.5
20	R	21	ARG	6.5
20	R	22	ASN	6.5
13	O	131	PRO	6.5
19	z	32	ASP	6.5
5	e	6	GLY	6.4
9	J	7	ILE	6.4
5	e	74	GLN	6.4
13	O	208	THR	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	z	25	VAL	6.4
13	O	59	LYS	6.4
2	b	482	ILE	6.4
9	j	9	LEU	6.4
19	z	29	SER	6.4
13	o	207	ARG	6.3
18	Y	26	ALA	6.3
13	o	27	ARG	6.3
18	y	37	PHE	6.3
19	Z	32	ASP	6.2
3	c	258	GLY	6.2
13	o	209	GLY	6.2
13	O	137	THR	6.2
16	v	15	GLU	6.2
13	o	246	ALA	6.2
7	H	65	LEU	6.2
13	o	37	THR	6.2
18	y	23	THR	6.2
2	b	491	VAL	6.2
3	c	426	LEU	6.1
13	o	21	THR	6.1
3	c	201	ASN	6.1
1	A	11	ALA	6.1
17	X	38	GLN	6.1
20	R	10	LEU	6.1
13	O	130	GLN	6.1
19	z	1	MET	6.1
4	d	12	ARG	6.1
5	E	5	THR	6.1
13	o	4	THR	6.1
3	C	433	LEU	6.1
5	E	83	LEU	6.1
3	c	23	ALA	6.0
1	A	12	ASN	6.0
3	c	433	LEU	6.0
13	o	36	GLN	6.0
13	O	26	ALA	6.0
16	v	22	THR	6.0
12	m	34	LYS	6.0
2	b	294	SER	6.0
6	F	14	PRO	6.0
9	j	3	GLU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	25	THR	5.9
4	d	159	ILE	5.9
5	E	25	ILE	5.9
3	c	205	ASP	5.9
17	x	9	GLY	5.9
19	Z	26	ALA	5.9
13	o	31	PRO	5.9
18	y	20	ALA	5.9
20	R	34	LEU	5.9
3	c	193	GLY	5.9
4	d	13	GLY	5.8
2	b	290	ALA	5.8
13	o	24	ASP	5.8
2	B	297	THR	5.8
7	h	23	PRO	5.8
16	v	108	THR	5.8
3	c	181	PHE	5.7
6	f	16	PHE	5.7
10	k	14	ALA	5.7
5	e	84	LYS	5.7
8	i	38	GLU	5.7
3	C	438	LEU	5.7
5	e	24	SER	5.7
3	c	248	GLY	5.7
5	e	71	GLU	5.7
19	z	59	PHE	5.7
7	H	6	TRP	5.7
2	B	502	VAL	5.7
20	R	4	ARG	5.7
9	J	6	ARG	5.6
13	O	91	GLY	5.6
16	v	13	ASN	5.6
17	X	2	THR	5.6
13	o	32	ILE	5.6
19	z	40	ILE	5.6
6	f	20	TRP	5.6
19	z	57	LEU	5.6
3	c	182	PHE	5.6
13	O	132	ASN	5.6
13	o	59	LYS	5.5
3	C	285	ILE	5.5
3	C	201	ASN	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	Z	61	VAL	5.5
3	c	438	LEU	5.5
13	O	24	ASP	5.5
20	R	15	ALA	5.5
3	c	250	TRP	5.5
20	R	8	VAL	5.5
20	R	12	VAL	5.5
1	a	326	LEU	5.5
3	C	437	PHE	5.5
1	a	15	GLU	5.5
5	E	22	ILE	5.5
3	c	144	SER	5.5
7	H	64	ALA	5.5
16	v	17	LYS	5.4
2	B	294	SER	5.4
19	z	43	GLY	5.4
9	j	7	ILE	5.4
15	U	102	LEU	5.4
13	O	89	SER	5.4
16	v	5	PRO	5.4
7	h	6	TRP	5.4
20	R	29	LYS	5.4
2	B	292	LEU	5.4
13	O	58	ASN	5.4
19	Z	36	SER	5.4
18	Y	24	MET	5.4
2	b	483	ASP	5.3
19	Z	37	LYS	5.3
3	C	131	TYR	5.3
19	z	36	SER	5.3
3	C	279	LEU	5.3
19	Z	45	GLY	5.3
5	e	29	ALA	5.3
17	x	3	ILE	5.3
2	b	505	ARG	5.3
1	A	339	PHE	5.3
13	o	25	THR	5.3
13	o	204	VAL	5.3
3	C	258	GLY	5.3
9	j	5	GLY	5.3
13	o	91	GLY	5.3
3	C	181	PHE	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	162	GLY	5.3
19	z	42	LEU	5.3
11	L	7	ARG	5.3
13	o	29	ALA	5.3
16	v	4	THR	5.3
18	Y	22	LEU	5.3
9	j	12	VAL	5.2
18	y	24	MET	5.2
3	c	142	GLU	5.2
16	v	6	GLU	5.2
13	o	41	ALA	5.2
13	o	63	ALA	5.2
13	O	138	THR	5.2
5	e	17	VAL	5.2
19	z	49	ALA	5.2
13	O	90	ASP	5.2
5	E	21	VAL	5.2
18	Y	41	VAL	5.2
2	b	501	ASP	5.2
3	c	257	PHE	5.2
9	J	2	SER	5.2
1	a	14	TRP	5.2
18	y	18	VAL	5.2
5	e	33	ALA	5.2
2	B	247	PHE	5.1
1	A	326	LEU	5.1
2	b	288	VAL	5.1
13	o	137	THR	5.1
1	a	297	LEU	5.1
3	c	202	PRO	5.1
1	a	228	THR	5.1
2	B	504	THR	5.1
2	b	186	GLY	5.1
2	B	497	GLN	5.1
2	b	489	GLU	5.1
13	O	36	GLN	5.1
19	Z	15	LEU	5.1
3	c	159	THR	5.1
3	c	260	ALA	5.1
19	Z	62	VAL	5.1
5	e	22	ILE	5.1
17	x	33	GLN	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	341	LEU	5.1
13	O	141	ASP	5.1
18	Y	43	ARG	5.1
20	R	19	ALA	5.1
2	b	488	PRO	5.0
16	v	107	LEU	5.0
17	X	15	LEU	5.0
7	H	5	THR	5.0
13	O	134	THR	5.0
19	Z	25	VAL	5.0
15	U	73	GLN	5.0
3	c	190	ALA	5.0
17	x	34	ILE	5.0
1	A	341	LEU	5.0
2	B	296	ALA	5.0
15	u	68	THR	5.0
2	B	245	VAL	5.0
2	B	488	PRO	5.0
3	C	317	PHE	5.0
2	B	289	GLN	5.0
3	c	206	PRO	5.0
19	z	4	LEU	5.0
5	e	60	GLN	5.0
4	d	158	LEU	4.9
13	O	28	GLY	4.9
3	c	255	THR	4.9
6	F	13	TYR	4.9
2	B	486	LEU	4.9
2	b	463	PHE	4.9
8	I	37	LEU	4.9
4	d	16	ASP	4.9
13	o	6	THR	4.9
17	x	15	LEU	4.9
1	a	12	ASN	4.9
3	C	439	VAL	4.9
4	D	352	LEU	4.9
19	z	45	GLY	4.9
20	R	17	GLY	4.9
2	b	245	VAL	4.9
2	b	252	VAL	4.9
2	b	301	ALA	4.8
6	f	19	ARG	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	O	21	THR	4.8
13	O	140	THR	4.8
17	x	4	THR	4.8
3	C	200	THR	4.8
18	Y	21	GLN	4.8
5	e	25	ILE	4.8
2	b	460	LEU	4.8
4	D	159	ILE	4.8
6	f	37	ILE	4.8
18	Y	34	MET	4.8
19	Z	23	VAL	4.8
11	L	6	ASN	4.8
3	c	279	LEU	4.8
4	d	352	LEU	4.8
2	b	128	THR	4.8
2	b	297	THR	4.8
12	m	31	SER	4.8
8	i	2	GLU	4.8
7	h	46	LEU	4.8
17	x	36	LYS	4.8
5	e	14	ILE	4.8
2	b	249	ALA	4.7
10	k	16	ALA	4.7
5	e	42	LEU	4.7
3	c	60	ILE	4.7
19	z	8	ALA	4.7
4	d	154	VAL	4.7
19	Z	52	LEU	4.7
3	C	281	MET	4.7
2	b	251	VAL	4.7
3	c	194	GLY	4.7
2	b	291	SER	4.7
3	c	145	SER	4.7
13	o	205	ASP	4.7
18	y	40	ALA	4.7
20	R	5	VAL	4.7
3	C	28	GLN	4.7
4	D	346	LEU	4.7
3	c	251	HIS	4.7
2	b	250	PHE	4.7
13	o	38	TYR	4.7
18	y	34	MET	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	t	29	ILE	4.7
2	b	247	PHE	4.7
15	U	68	THR	4.6
3	c	207	ARG	4.6
5	e	81	GLU	4.6
5	e	57	ALA	4.6
2	B	250	PHE	4.6
20	R	20	VAL	4.6
15	U	80	GLU	4.6
3	C	442	LEU	4.6
19	Z	60	PHE	4.6
2	b	485	GLU	4.6
16	V	6	GLU	4.6
11	l	5	PRO	4.6
16	v	9	THR	4.6
2	B	458	PHE	4.6
3	c	261	ARG	4.6
13	O	60	ARG	4.6
13	o	60	ARG	4.6
5	e	36	LEU	4.6
5	e	83	LEU	4.6
1	a	248	ILE	4.5
7	h	13	PRO	4.5
3	c	158	THR	4.5
3	C	253	LEU	4.5
3	C	341	LEU	4.5
19	Z	29	SER	4.5
19	Z	39	LEU	4.5
8	I	6	ILE	4.5
15	u	66	GLY	4.5
5	e	10	PHE	4.5
18	y	27	MET	4.5
4	D	14	TRP	4.5
16	v	113	VAL	4.5
16	v	135	VAL	4.5
2	b	486	LEU	4.5
5	E	12	ASP	4.5
2	B	242	ILE	4.5
13	O	62	GLU	4.5
18	Y	42	ARG	4.5
4	d	122	LEU	4.5
2	B	248	ALA	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	o	202	ALA	4.5
18	Y	37	PHE	4.5
4	D	17	ILE	4.5
1	A	343[A]	LEU	4.5
4	d	325	ILE	4.5
3	C	25	ASN	4.4
13	O	88	ASN	4.4
19	Z	2	THR	4.4
15	U	101	GLY	4.4
3	c	442	LEU	4.4
5	E	36	LEU	4.4
13	O	63	ALA	4.4
3	C	143	TYR	4.4
4	d	20	ASP	4.4
17	x	26	ALA	4.4
13	o	130	GLN	4.4
16	v	78	ASN	4.4
16	v	20	THR	4.4
3	c	147	PHE	4.4
5	e	11	SER	4.4
13	o	241	ALA	4.4
4	d	346	LEU	4.4
3	C	145[A]	SER	4.4
13	O	4	THR	4.4
10	K	16	ALA	4.4
11	L	3	PRO	4.4
7	h	42	LEU	4.4
16	v	23	GLU	4.4
5	e	26	THR	4.4
9	j	14	THR	4.4
1	a	120	LEU	4.3
2	b	246	PHE	4.3
5	e	16	SER	4.3
3	C	23	ALA	4.3
1	a	258	LEU	4.3
2	B	505	ARG	4.3
14	t	30	THR	4.3
1	a	262	TYR	4.3
2	b	458	PHE	4.3
13	O	22	LEU	4.3
1	a	330	VAL	4.3
3	c	87	ILE	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	286	ARG	4.3
1	a	295	PHE	4.3
13	O	30	TYR	4.3
19	Z	46	LEU	4.3
2	B	490	GLN	4.3
5	E	81	GLU	4.3
19	z	6	GLN	4.3
15	U	104	LYS	4.3
3	C	435	PHE	4.3
4	d	27	PHE	4.3
3	C	153	ASP	4.3
13	O	32	ILE	4.2
5	e	78	THR	4.2
5	E	20	TRP	4.2
9	j	10	TRP	4.2
18	y	30	ILE	4.2
3	C	276	LEU	4.2
3	c	401	LEU	4.2
18	Y	38	LEU	4.2
13	o	206	GLY	4.2
20	R	30	GLN	4.2
9	J	8	PRO	4.2
17	x	39	ARG	4.2
2	B	350	GLU	4.2
1	a	13	LEU	4.2
2	b	498	LYS	4.2
9	j	2	SER	4.2
5	e	23	HIS	4.2
11	L	5	PRO	4.2
17	X	37	VAL	4.2
2	b	467	ILE	4.2
3	c	21	ILE	4.2
3	C	27	ASP	4.2
2	B	485	GLU	4.2
13	o	64	GLU	4.2
1	a	343[A]	LEU	4.2
2	B	161	LEU	4.2
17	X	23	LEU	4.2
19	z	54	VAL	4.2
2	b	456	ALA	4.2
16	v	69	ILE	4.2
18	Y	36	ILE	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	o	61	GLN	4.1
2	B	288	VAL	4.1
1	a	188	ALA	4.1
13	o	90	ASP	4.1
13	o	34	SER	4.1
3	c	191	PRO	4.1
2	B	461	LEU	4.1
2	b	292	LEU	4.1
16	v	28	GLU	4.1
3	C	60	ILE	4.1
1	a	261	GLN	4.1
2	b	130[A]	GLU	4.1
3	c	254	THR	4.1
17	X	28	LEU	4.1
19	Z	7	LEU	4.1
18	Y	44	GLY	4.1
3	C	262	ARG	4.1
8	I	34	ARG	4.1
18	y	21	GLN	4.1
3	C	282	MET	4.1
5	e	40	THR	4.1
16	v	99	ASP	4.1
18	Y	30	ILE	4.1
4	d	238	THR	4.1
14	T	30	THR	4.1
2	b	298	LEU	4.1
2	B	249	ALA	4.0
1	a	321	ILE	4.0
3	c	166	ILE	4.0
2	b	461	LEU	4.0
3	c	404	LEU	4.0
3	c	22	PHE	4.0
3	c	431	PHE	4.0
2	b	243	ALA	4.0
16	v	114	ALA	4.0
3	C	432	VAL	4.0
13	O	200	ASN	4.0
3	C	192	GLY	4.0
2	b	244	ALA	4.0
13	O	31	PRO	4.0
3	C	100	GLY	4.0
3	c	148	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	251	VAL	4.0
16	V	7	VAL	4.0
8	I	10	ILE	4.0
5	E	23	HIS	4.0
5	E	79	PHE	4.0
9	j	8	PRO	4.0
20	R	16	ALA	4.0
13	O	205	ASP	4.0
13	o	198	SER	4.0
16	V	14	SER	4.0
2	b	242	ILE	4.0
3	C	288	CYS	4.0
17	X	36	LYS	4.0
4	D	90	LEU	4.0
5	E	57	ALA	4.0
3	C	436	PHE	4.0
2	B	300	GLU	4.0
1	a	320	ILE	3.9
3	c	282	MET	3.9
19	z	27	TYR	3.9
16	V	99	ASP	3.9
19	z	52	LEU	3.9
19	Z	17	PHE	3.9
15	U	64	ILE	3.9
18	y	43	ARG	3.9
2	B	298	LEU	3.9
16	V	52	LEU	3.9
1	A	228	THR	3.9
3	C	210	PHE	3.9
8	I	3	THR	3.9
3	c	285	ILE	3.9
10	K	33	LEU	3.9
16	v	8	LEU	3.9
5	e	28	PRO	3.9
16	V	50	PRO	3.9
4	d	321	LEU	3.9
5	e	59	GLU	3.9
17	x	30	ALA	3.9
15	U	63	ASN	3.9
1	A	160	ILE	3.9
13	o	56	PRO	3.9
18	y	33	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	c	119	LEU	3.9
7	H	2	ALA	3.9
10	k	41	ALA	3.9
2	B	383	PHE	3.9
11	l	7	ARG	3.9
18	Y	25	ILE	3.9
17	X	32	SER	3.9
19	z	37	LYS	3.8
5	e	58	GLN	3.8
13	O	56	PRO	3.8
1	a	63	ILE	3.8
1	a	160	ILE	3.8
2	b	499	VAL	3.8
7	h	56	ASP	3.8
3	c	249	ILE	3.8
5	e	27	ILE	3.8
16	v	7	VAL	3.8
19	z	62	VAL	3.8
2	b	248	ALA	3.8
5	e	72	ALA	3.8
5	E	15	THR	3.8
19	Z	27	TYR	3.8
3	c	437	PHE	3.8
17	x	5	PRO	3.8
3	c	384	ILE	3.8
4	d	119	ALA	3.8
16	v	27	LEU	3.8
13	O	35	SER	3.8
1	a	184	ILE	3.8
3	C	43	ILE	3.8
19	z	58	ASN	3.8
3	c	153	ASP	3.8
10	k	20	PRO	3.8
3	C	426	LEU	3.8
4	d	162	LEU	3.8
18	y	38	LEU	3.8
3	C	251	HIS	3.8
1	A	16	ARG	3.8
2	b	462	PHE	3.8
8	i	6	ILE	3.8
3	C	401	LEU	3.8
5	E	16	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	e	7	GLU	3.8
5	e	82	GLN	3.8
15	u	103	TYR	3.8
3	c	25	ASN	3.7
15	U	65	PRO	3.7
2	b	162	PHE	3.7
16	v	25	GLN	3.7
3	c	95	LEU	3.7
3	C	206	PRO	3.7
13	o	245	PRO	3.7
4	d	21	TRP	3.7
13	o	138	THR	3.7
10	k	17	ILE	3.7
13	o	89	SER	3.7
13	o	237	GLY	3.7
3	c	427	ALA	3.7
13	O	34	SER	3.7
4	d	287	VAL	3.7
9	j	15	VAL	3.7
13	O	203	LYS	3.7
16	v	72	LEU	3.7
1	a	16	ARG	3.7
2	b	348	ASN	3.7
2	b	350	GLU	3.7
2	B	410	THR	3.7
16	V	45	ILE	3.7
4	d	320	LEU	3.7
4	D	351	ALA	3.7
2	b	127	ARG	3.7
5	E	78	THR	3.7
3	C	32	GLY	3.7
4	D	89	LEU	3.6
4	d	127	LEU	3.6
3	c	424	SER	3.6
3	C	139	THR	3.6
4	D	151	ALA	3.6
18	y	26	ALA	3.6
18	y	31	ALA	3.6
1	A	15	GLU	3.6
1	a	89	ILE	3.6
2	b	256	MET	3.6
13	o	10	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	e	65	LEU	3.6
3	C	142	GLU	3.6
3	c	429	SER	3.6
2	B	454	ALA	3.6
1	A	295	PHE	3.6
19	Z	5	PHE	3.6
5	E	13	ILE	3.6
13	o	211	ILE	3.6
1	A	120	LEU	3.6
16	v	79	PRO	3.6
7	h	10	ILE	3.6
3	C	95	LEU	3.6
7	H	42	LEU	3.6
13	O	87	VAL	3.6
16	V	135	VAL	3.6
3	c	20	SER	3.6
9	j	19	GLY	3.6
17	X	4	THR	3.6
4	d	284	ILE	3.6
9	j	18	MET	3.6
3	c	59	LEU	3.6
3	c	198	VAL	3.6
15	U	103	TYR	3.6
3	C	135	ARG	3.6
3	c	378	ASN	3.6
15	U	59	GLU	3.6
6	f	36	ALA	3.6
1	a	259	ILE	3.6
1	A	121[A]	LEU	3.6
1	A	145	VAL	3.6
3	c	410[A]	VAL	3.6
15	U	57	SER	3.6
15	u	101	GLY	3.6
2	B	301	ALA	3.5
2	b	454	ALA	3.5
8	i	3	THR	3.6
15	U	60	ASP	3.5
2	B	452	THR	3.5
2	B	503	THR	3.5
3	C	254	THR	3.5
3	c	259	TRP	3.5
9	J	10	TRP	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	V	18	THR	3.5
5	e	12	ASP	3.5
5	e	18	ARG	3.5
13	o	57	LYS	3.5
1	A	331	MET	3.5
3	c	170	ILE	3.5
2	B	460	LEU	3.5
3	c	117	VAL	3.5
4	D	287	VAL	3.5
13	O	201	VAL	3.5
2	b	484	PRO	3.5
9	J	14	THR	3.5
5	e	8	ARG	3.5
15	u	73	GLN	3.5
3	c	284	PHE	3.5
4	d	169	PHE	3.5
1	A	151	LEU	3.5
1	a	163	ILE	3.5
16	v	136	TYR	3.5
1	A	14	TRP	3.5
1	a	331	MET	3.5
2	b	383	PHE	3.5
3	C	284	PHE	3.5
4	d	120	PHE	3.5
8	i	21	PHE	3.5
1	A	159	LEU	3.5
1	A	163	ILE	3.5
6	f	28	VAL	3.5
2	b	452	THR	3.5
13	O	129	THR	3.5
3	C	427	ALA	3.5
4	d	151	ALA	3.5
18	y	44	GLY	3.5
5	e	53	ASP	3.5
2	b	300	GLU	3.5
15	u	8	GLU	3.5
1	A	330	VAL	3.5
2	B	252	VAL	3.5
10	k	38	VAL	3.5
13	o	200	ASN	3.5
18	Y	40	ALA	3.5
13	O	92	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	126	PRO	3.4
1	a	224	ILE	3.4
13	o	22	LEU	3.4
1	a	238	LYS	3.4
3	C	158	THR	3.4
2	b	163	GLY	3.4
4	D	233	ARG	3.4
17	X	33	GLN	3.4
2	b	479	PHE	3.4
5	E	35	TRP	3.4
3	C	159	THR	3.4
3	c	88	LEU	3.4
15	u	64	ILE	3.4
1	a	231	GLU	3.4
3	C	286	ALA	3.4
10	k	15	TYR	3.4
4	d	123	ILE	3.4
4	d	157	PHE	3.4
4	d	188	PHE	3.4
19	z	47	TRP	3.4
1	a	294	ALA	3.4
16	v	98	ALA	3.4
16	v	64	PRO	3.4
13	o	28	GLY	3.4
2	b	289	GLN	3.4
2	b	398	THR	3.4
3	C	59	LEU	3.4
4	D	144	ILE	3.4
18	Y	35	ILE	3.4
13	o	96	VAL	3.4
7	h	18	TYR	3.4
13	o	131	PRO	3.4
6	f	24	HIS	3.4
7	h	51	SER	3.4
1	a	286	ALA	3.4
2	B	456	ALA	3.4
2	B	464	PHE	3.4
8	I	2	GLU	3.4
13	O	55	GLU	3.4
16	V	15	GLU	3.4
3	c	208	VAL	3.4
4	D	12	ARG	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	492	GLU	3.4
2	B	65	PHE	3.4
2	B	366	PHE	3.4
3	C	431	PHE	3.4
3	c	317	PHE	3.4
4	d	144	ILE	3.4
4	D	154	VAL	3.3
16	v	137	TYR	3.3
18	Y	45	ASN	3.3
13	O	202	ALA	3.3
3	C	42	LEU	3.3
2	B	462	PHE	3.3
7	H	10	ILE	3.3
14	T	14	ILE	3.3
3	c	141	GLU	3.3
1	a	67	VAL	3.3
3	c	54	VAL	3.3
3	C	283	GLY	3.3
1	a	232	SER	3.3
1	a	19	ASN	3.3
5	E	26	THR	3.3
13	O	240	TYR	3.3
2	b	238	LEU	3.3
4	D	158	LEU	3.3
17	x	35	ASP	3.3
1	a	290	ILE	3.3
7	H	54	ILE	3.3
15	U	32	ILE	3.3
1	a	340	PRO	3.3
3	c	64	ALA	3.3
4	d	115	ALA	3.3
3	c	253	LEU	3.3
2	B	463	PHE	3.3
2	b	464	PHE	3.3
3	c	92	ILE	3.3
3	c	235	GLY	3.3
15	u	65	PRO	3.3
3	c	439	VAL	3.3
3	C	24	THR	3.3
5	E	40	THR	3.3
13	O	37	THR	3.3
2	B	493	TRP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	328	MET	3.3
15	U	70	ARG	3.3
1	a	252	HIS	3.3
3	C	318	LEU	3.3
1	A	63	ILE	3.3
2	b	268	PHE	3.3
18	y	28	ILE	3.3
15	u	28	ASN	3.3
2	B	483	ASP	3.3
16	V	81	THR	3.3
1	a	242	GLU	3.3
9	j	34	GLY	3.3
10	k	39	TRP	3.3
2	B	256	MET	3.3
1	A	338	ASN	3.3
4	D	210	LEU	3.3
7	H	46	LEU	3.3
18	Y	39	LEU	3.3
2	b	241	SER	3.3
4	d	146	PHE	3.3
19	z	14	ILE	3.3
15	U	58	VAL	3.3
19	z	18	VAL	3.3
7	h	5	THR	3.3
3	c	19	ASN	3.2
8	I	4	LEU	3.2
16	V	94	SER	3.2
20	R	9	LEU	3.2
3	C	104	GLU	3.2
4	D	270	PHE	3.2
15	U	86	GLU	3.2
19	z	51	VAL	3.2
2	b	373	LYS	3.2
3	C	144	SER	3.2
4	d	25	ASP	3.2
13	O	135	SER	3.2
3	c	199	ILE	3.2
4	D	276	VAL	3.2
2	b	206	GLY	3.2
2	b	121	GLU	3.2
3	C	101	PRO	3.2
2	B	265	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	c	425	TRP	3.2
6	F	15	ILE	3.2
9	j	11	ILE	3.2
16	v	110	LYS	3.2
16	v	26	TYR	3.2
2	B	453	PHE	3.2
16	V	63	THR	3.2
2	B	413	ASP	3.2
3	c	197	ARG	3.2
1	A	336	ALA	3.2
3	c	86	LEU	3.2
3	c	276	LEU	3.2
15	U	56	GLU	3.2
2	b	449	GLY	3.2
3	c	350	ILE	3.2
3	c	414	ILE	3.2
7	H	18	TYR	3.2
13	o	83	GLY	3.2
2	b	30	VAL	3.2
13	o	39	ARG	3.2
2	b	490	GLN	3.2
5	E	74	GLN	3.2
3	C	404	LEU	3.2
3	c	204	LEU	3.2
4	d	18	LEU	3.2
2	b	413	ASP	3.2
3	c	43	ILE	3.2
13	o	243	ILE	3.2
19	Z	48	ILE	3.2
1	A	123	ALA	3.2
1	a	336	ALA	3.2
4	D	36	LEU	3.2
4	D	321	LEU	3.2
4	d	183	LEU	3.2
3	C	29	GLU	3.1
3	c	29	GLU	3.1
4	D	123	ILE	3.1
11	l	2	GLU	3.1
17	X	34	ILE	3.1
4	d	153	PHE	3.1
4	D	28	VAL	3.1
19	z	13	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	57	ALA	3.1
5	e	45	ASP	3.1
8	I	35	LYS	3.1
1	a	288	LEU	3.1
3	C	414	ILE	3.1
16	v	18	THR	3.1
2	b	65	PHE	3.1
4	d	15	PHE	3.1
6	F	42	PHE	3.1
2	B	258	TYR	3.1
1	a	309	ALA	3.1
3	c	246	ALA	3.1
19	z	11	ALA	3.1
3	c	171	GLY	3.1
12	m	32	GLN	3.1
2	B	474	LEU	3.1
3	C	272	LEU	3.1
3	C	337	LEU	3.1
13	O	93	LEU	3.1
15	U	75	LEU	3.1
5	E	24	SER	3.1
1	a	243	GLU	3.1
5	E	59	GLU	3.1
17	X	35	ASP	3.1
17	x	11	PHE	3.1
3	c	227	VAL	3.1
4	D	234	ALA	3.1
5	e	43	ALA	3.1
10	K	24	VAL	3.1
13	o	201	VAL	3.1
3	C	35	TRP	3.1
11	L	19	LEU	3.1
3	c	240	ILE	3.1
15	U	74	ILE	3.1
16	v	106	ASN	3.1
2	B	253	ALA	3.1
2	B	489	GLU	3.1
2	B	501	ASP	3.1
3	C	88	LEU	3.1
4	D	162	LEU	3.1
3	C	256	PRO	3.1
3	c	209	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	150	ILE	3.1
3	c	136	GLY	3.1
3	C	331	ALA	3.1
13	o	227	ALA	3.1
4	d	345	VAL	3.1
16	V	96	ARG	3.1
3	c	242	LEU	3.1
4	D	116	LEU	3.1
4	d	116	LEU	3.1
2	B	396	GLY	3.1
10	k	28	ILE	3.1
1	A	33	PHE	3.1
10	K	14	ALA	3.1
10	k	34	ALA	3.1
2	B	457	VAL	3.0
3	c	420	VAL	3.0
17	x	27	VAL	3.0
3	c	187	ASP	3.0
4	D	291	LEU	3.0
13	o	157	LEU	3.0
5	E	29	ALA	3.0
9	j	13	ALA	3.0
1	a	339	PHE	3.0
1	a	311	GLY	3.0
3	c	356	MET	3.0
3	c	428	THR	3.0
4	d	279	LEU	3.0
3	C	63	TRP	3.0
1	a	116	ILE	3.0
4	d	178	ILE	3.0
13	o	62	GLU	3.0
3	C	358	PHE	3.0
4	D	130	PHE	3.0
6	f	18	VAL	3.0
7	H	8	GLY	3.0
8	i	26	GLY	3.0
3	C	255	THR	3.0
2	B	179	GLN	3.0
2	b	87	ASP	3.0
4	d	74	LEU	3.0
7	H	30	LEU	3.0
7	h	9	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	v	21	LEU	3.0
4	d	143	ALA	3.0
2	B	62	VAL	3.0
19	z	53	VAL	3.0
2	B	449	GLY	3.0
16	v	132	GLY	3.0
11	L	23	LEU	3.0
13	o	5	LEU	3.0
16	v	12	LEU	3.0
3	C	92	ILE	3.0
13	O	128	SER	3.0
1	A	285	PHE	3.0
1	A	281	VAL	3.0
2	B	30	VAL	3.0
2	b	457	VAL	3.0
4	D	324	GLY	3.0
4	D	19	ASP	3.0
3	C	26	ARG	3.0
3	C	263	ALA	3.0
3	C	280	SER	3.0
4	d	259	ILE	3.0
16	v	45	ILE	3.0
3	c	385	GLN	3.0
2	B	254	GLY	3.0
13	o	9	ASP	3.0
2	B	162	PHE	3.0
6	F	20	TRP	3.0
1	a	283	VAL	3.0
2	B	478	VAL	3.0
16	v	10	VAL	3.0
11	l	6	ASN	3.0
2	B	267	LEU	2.9
2	B	402	TYR	2.9
3	c	168	LEU	2.9
5	e	77	GLU	2.9
17	X	13	GLY	2.9
4	d	204	VAL	2.9
7	H	12[A]	ARG	2.9
17	X	11	PHE	2.9
19	Z	56	VAL	2.9
2	B	128	THR	2.9
3	C	204	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	c	157	MET	2.9
4	d	182	LEU	2.9
13	O	33	ASP	2.9
5	e	13	ILE	2.9
13	O	204	VAL	2.9
1	A	218	LEU	2.9
1	a	42	LEU	2.9
3	C	140	LEU	2.9
13	o	92	SER	2.9
13	o	30	TYR	2.9
13	o	226	GLY	2.9
16	v	70	GLU	2.9
17	X	22	GLY	2.9
3	C	224	ILE	2.9
3	c	358	PHE	2.9
1	a	281	VAL	2.9
3	C	225	VAL	2.9
16	v	42	VAL	2.9
19	Z	18	VAL	2.9
2	B	241	SER	2.9
15	u	86	GLU	2.9
1	A	258	LEU	2.9
3	c	353	GLY	2.9
5	e	41	GLY	2.9
2	B	304	ALA	2.9
3	c	131	TYR	2.9
16	v	116	ALA	2.9
1	A	38	ILE	2.9
4	D	213	ILE	2.9
16	V	64	PRO	2.9
16	v	11	PRO	2.9
16	v	24	LYS	2.9
15	U	19	THR	2.9
1	a	158	PHE	2.9
2	B	246	PHE	2.9
2	b	411	PHE	2.9
2	b	399	VAL	2.9
3	C	463	SER	2.9
17	x	32	SER	2.9
2	b	39	LEU	2.9
2	b	109	LEU	2.9
3	c	50	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	d	229	ALA	2.9
4	d	160	TYR	2.9
2	B	484	PRO	2.9
6	F	17	THR	2.9
10	k	18	PHE	2.9
16	V	13	ASN	2.9
2	b	223	GLN	2.9
1	a	200	LEU	2.9
4	d	329	MET	2.9
2	b	185	TRP	2.9
4	d	100	ASP	2.9
3	C	137	PRO	2.9
1	a	46	ILE	2.8
2	B	268	PHE	2.8
17	X	20	VAL	2.8
1	a	28	LEU	2.8
4	d	147	SER	2.8
15	U	85	THR	2.8
17	x	31	ILE	2.8
1	a	327	GLY	2.8
3	C	184	GLY	2.8
3	C	205	ASP	2.8
13	O	5	LEU	2.8
16	v	2	GLU	2.8
2	B	403	GLY	2.8
2	B	465	GLY	2.8
3	C	277	GLY	2.8
1	A	53	ILE	2.8
1	a	176	ILE	2.8
3	c	340	TYR	2.8
4	d	163	GLY	2.8
11	L	4	ASN	2.8
4	D	284	ILE	2.8
7	h	28	THR	2.8
1	a	225	ARG	2.8
4	d	130	PHE	2.8
3	C	196	VAL	2.8
16	v	121	VAL	2.8
17	x	8	LYS	2.8
2	B	244	ALA	2.8
16	v	62	ALA	2.8
2	b	29	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	168	LEU	2.8
3	c	28	GLN	2.8
19	Z	6	GLN	2.8
3	C	383	ASP	2.8
1	A	143	ILE	2.8
2	B	467	ILE	2.8
19	Z	40	ILE	2.8
13	o	55	GLU	2.8
3	C	182	PHE	2.8
4	d	156	VAL	2.8
11	l	8	GLN	2.8
1	A	324	ALA	2.8
1	A	200	LEU	2.8
2	B	39	LEU	2.8
19	Z	12	LEU	2.8
19	Z	24	PRO	2.8
3	C	396	MET	2.8
7	h	57	GLY	2.8
2	B	373	LYS	2.8
3	C	428	THR	2.8
13	o	229	GLU	2.8
16	V	48	THR	2.8
1	A	321	ILE	2.8
1	a	143	ILE	2.8
3	C	252	ILE	2.8
4	D	259	ILE	2.8
4	d	286	VAL	2.8
6	f	38	ALA	2.8
13	O	127	ALA	2.8
17	X	26	ALA	2.8
1	a	218	LEU	2.8
2	B	120	LEU	2.8
3	C	429	SER	2.8
4	D	209	LEU	2.8
4	D	293	LEU	2.8
13	O	85	LEU	2.8
13	o	93	LEU	2.8
16	V	97	SER	2.8
4	d	150	ILE	2.8
4	d	256	ILE	2.8
2	B	285	ASN	2.8
4	D	257	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	h	22	ALA	2.7
3	C	148	GLY	2.7
16	v	71	GLY	2.7
1	A	288	LEU	2.7
3	c	213[A]	LEU	2.7
15	U	79	LEU	2.7
17	x	7	LEU	2.7
2	b	435	GLU	2.7
10	K	28	ILE	2.7
13	o	136	ILE	2.7
14	T	21	ILE	2.7
7	h	12	ARG	2.7
13	o	141	ASP	2.7
3	C	309	ALA	2.7
3	C	352	GLY	2.7
3	c	314	ALA	2.7
15	U	18	GLY	2.7
19	Z	49	ALA	2.7
3	C	208	VAL	2.7
9	J	24	VAL	2.7
2	B	238	LEU	2.7
2	b	324	LEU	2.7
3	C	165	LEU	2.7
19	Z	50	LEU	2.7
1	A	242	GLU	2.7
3	c	412[A]	THR	2.7
2	b	425	ILE	2.7
2	b	189	GLY	2.7
3	C	211	GLY	2.7
13	O	237	GLY	2.7
1	A	152	ALA	2.7
2	b	320	ALA	2.7
4	d	327	ALA	2.7
4	D	328	TRP	2.7
7	H	25	TRP	2.7
7	H	58	VAL	2.7
10	k	13	GLU	2.7
2	b	63	LEU	2.7
4	D	49	LEU	2.7
4	d	293	LEU	2.7
13	O	157	LEU	2.7
10	K	46	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	372	ASP	2.7
4	d	227	GLU	2.7
10	k	10	LYS	2.7
1	A	49	VAL	2.7
1	A	280	VAL	2.7
1	a	18	CYS	2.7
1	a	197	PHE	2.7
2	b	61	PHE	2.7
5	E	42	LEU	2.7
10	K	25	LEU	2.7
1	A	127	MET	2.7
2	b	410	THR	2.7
4	D	277	THR	2.7
2	B	425	ILE	2.7
5	E	39	SER	2.7
19	z	16	SER	2.7
19	z	48	ILE	2.7
1	a	324	ALA	2.7
10	k	42	ALA	2.7
19	Z	10	ALA	2.7
2	b	402	TYR	2.7
16	v	74	ASP	2.7
1	A	205	VAL	2.7
2	b	412	THR	2.7
3	c	173	LEU	2.7
3	c	175	LEU	2.7
7	h	30	LEU	2.7
5	E	71	GLU	2.7
13	o	54	GLU	2.7
2	B	185	TRP	2.7
5	e	32	ILE	2.7
16	v	88	ILE	2.7
18	y	35	ILE	2.7
4	D	20	ASP	2.7
4	D	115	ALA	2.7
19	z	26	ALA	2.7
16	v	134	LYS	2.7
1	A	158	PHE	2.7
2	B	219	VAL	2.7
2	b	218	LEU	2.7
2	b	363	PHE	2.7
4	d	49	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	144	CYS	2.6
3	C	259	TRP	2.6
3	c	63	TRP	2.6
3	c	291	TRP	2.6
2	b	125	ASP	2.6
13	O	64	GLU	2.6
3	c	286	ALA	2.6
1	a	121[A]	LEU	2.6
1	a	300	PHE	2.6
2	B	12	LEU	2.6
2	B	129	GLY	2.6
2	b	351	GLY	2.6
15	U	13	VAL	2.6
19	Z	53	VAL	2.6
7	H	45	ILE	2.6
9	j	16	ALA	2.6
19	Z	14	ILE	2.6
9	J	5	GLY	2.6
9	j	25	GLY	2.6
16	v	84	GLY	2.6
1	a	186	PHE	2.6
1	a	306	VAL	2.6
2	B	349	LYS	2.6
3	c	436	PHE	2.6
4	d	185	PHE	2.6
4	d	339	PHE	2.6
8	i	35	LYS	2.6
16	V	126	LEU	2.6
19	Z	59	PHE	2.6
13	o	23	ASP	2.6
13	o	135	SER	2.6
17	X	6	SER	2.6
5	E	82	GLN	2.6
2	B	450	TRP	2.6
1	a	149	ALA	2.6
2	B	101	ILE	2.6
2	B	124	ARG	2.6
4	D	325	ILE	2.6
3	c	462[A]	GLU	2.6
3	C	86	LEU	2.6
3	c	272	LEU	2.6
3	c	337	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	328	MET	2.6
2	b	62	VAL	2.6
5	E	58	GLN	2.6
13	o	199	LEU	2.6
19	z	12	LEU	2.6
8	i	34	ARG	2.6
3	C	87	ILE	2.6
2	B	481	GLY	2.6
4	D	280	TRP	2.6
4	d	228	GLY	2.6
5	e	48	GLY	2.6
19	Z	22	GLY	2.6
13	O	217[A]	SER	2.6
1	A	114	LEU	2.6
1	a	159	LEU	2.6
2	b	103	LEU	2.6
7	H	43	LEU	2.6
1	a	49	VAL	2.6
3	C	261	ARG	2.6
3	c	396	MET	2.6
9	j	1	MET	2.6
7	h	63	LYS	2.6
2	b	253	ALA	2.6
2	b	304	ALA	2.6
4	D	170	ALA	2.6
1	a	38	ILE	2.6
1	a	227	THR	2.6
2	B	255	THR	2.6
1	A	229	GLU	2.6
2	b	303	SER	2.6
3	C	424	SER	2.6
12	M	29	THR	2.6
13	O	153	THR	2.6
6	f	29	PRO	2.6
16	v	123	PRO	2.6
2	B	356	VAL	2.6
3	C	109	PHE	2.6
3	c	281	MET	2.6
2	b	459	ALA	2.6
3	C	450	ALA	2.6
5	E	34	GLY	2.6
13	o	210	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	37	ILE	2.6
8	I	33	LYS	2.6
2	b	239[A]	SER	2.5
2	b	415	PRO	2.5
3	c	137	PRO	2.5
4	d	171	PRO	2.5
3	c	341	LEU	2.5
11	L	17	LEU	2.5
13	o	78	LEU	2.5
1	A	197	PHE	2.5
6	f	41	GLN	2.5
3	C	339	LYS	2.5
1	A	287	ALA	2.5
3	C	270	ALA	2.5
3	C	445	ALA	2.5
3	c	450	ALA	2.5
13	o	183	ALA	2.5
16	v	68	ASN	2.5
1	a	307[A]	ILE	2.5
3	c	459	ILE	2.5
4	D	256	ILE	2.5
16	v	100	ILE	2.5
19	Z	44	SER	2.5
1	a	196	PRO	2.5
3	c	90	PRO	2.5
1	A	231	GLU	2.5
2	B	63	LEU	2.5
2	B	130[A]	GLU	2.5
4	D	122	LEU	2.5
4	d	48	TRP	2.5
3	c	430	HIS	2.5
1	a	145	VAL	2.5
1	a	285	PHE	2.5
2	b	362	PHE	2.5
3	C	407	VAL	2.5
4	d	126	MET	2.5
5	e	31	PHE	2.5
6	F	16	PHE	2.5
10	k	44	GLY	2.5
1	a	323	ARG	2.5
3	c	212	TYR	2.5
2	b	155	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	434	ALA	2.5
3	c	270	ALA	2.5
13	o	26	ALA	2.5
18	Y	31	ALA	2.5
3	C	249	ILE	2.5
3	C	287	THR	2.5
13	o	193	THR	2.5
1	A	340	PRO	2.5
16	v	102	PRO	2.5
2	B	163	GLY	2.5
3	C	161	LEU	2.5
3	c	409[A]	GLY	2.5
4	d	24	ARG	2.5
10	k	35	LEU	2.5
11	L	22	LEU	2.5
19	z	9	LEU	2.5
1	a	280	VAL	2.5
3	c	130	VAL	2.5
3	c	167	VAL	2.5
5	e	37	PHE	2.5
3	c	288	CYS	2.5
3	c	302	TYR	2.5
3	c	309	ALA	2.5
5	E	19	TYR	2.5
3	c	188	THR	2.5
13	o	94	THR	2.5
10	k	46	ARG	2.5
1	A	19	ASN	2.5
2	b	375	GLY	2.5
3	c	192	GLY	2.5
4	d	89	LEU	2.5
3	C	157	MET	2.5
3	C	250	TRP	2.5
3	C	443	TRP	2.5
4	D	120	PHE	2.5
4	d	196	PHE	2.5
7	H	63	LYS	2.5
2	B	97	ALA	2.5
3	C	278	ALA	2.5
1	a	245	THR	2.5
3	C	141	GLU	2.5
4	d	241	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	370	LEU	2.5
15	u	104	LYS	2.5
2	b	366	PHE	2.5
3	c	176	VAL	2.5
4	D	156	VAL	2.5
2	B	243	ALA	2.5
1	a	230	THR	2.5
4	D	141	TYR	2.5
4	d	75	THR	2.5
5	E	28	PRO	2.5
2	B	482	ILE	2.5
3	C	459	ILE	2.5
3	C	125	LEU	2.5
3	c	49	LEU	2.5
3	c	467	LEU	2.5
4	D	289	LEU	2.5
13	o	125	LEU	2.5
17	x	28	LEU	2.5
3	c	31	SER	2.4
15	U	76	ARG	2.4
1	a	152	ALA	2.4
2	B	387	GLU	2.4
3	C	190	ALA	2.4
3	C	292	PHE	2.4
4	d	44	ALA	2.4
5	E	33	ALA	2.4
3	c	397	THR	2.4
13	o	88	ASN	2.4
2	b	89	GLY	2.4
1	a	60	ILE	2.4
2	B	384	ARG	2.4
3	c	30	SER	2.4
5	e	61	ARG	2.4
16	v	96	ARG	2.4
1	A	209	ALA	2.4
2	b	212	ALA	2.4
2	b	471	ALA	2.4
3	c	278	ALA	2.4
9	J	13	ALA	2.4
19	z	20	VAL	2.4
8	i	28	PRO	2.4
3	C	47	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	V	4	THR	2.4
16	V	46	THR	2.4
2	B	125	ASP	2.4
2	b	119	ASP	2.4
7	H	17	GLU	2.4
16	V	24	LYS	2.4
1	A	41	LEU	2.4
2	b	214	LEU	2.4
3	c	161	LEU	2.4
3	c	244	CYS	2.4
13	O	70	LEU	2.4
15	u	102	LEU	2.4
1	a	296	ASN	2.4
2	b	407	ASN	2.4
19	Z	19	MET	2.4
1	A	185[A]	VAL	2.4
1	a	33	PHE	2.4
2	B	237	VAL	2.4
2	B	376	VAL	2.4
2	b	131	PRO	2.4
3	c	237	HIS	2.4
3	c	289	PHE	2.4
5	e	38	VAL	2.4
9	J	20	VAL	2.4
13	O	66	VAL	2.4
13	o	87	VAL	2.4
7	H	28	THR	2.4
17	x	24	THR	2.4
2	B	286	ARG	2.4
2	b	283	GLU	2.4
1	A	147	TYR	2.4
2	B	273	TYR	2.4
13	O	38	TYR	2.4
1	A	259	ILE	2.4
4	D	319	LEU	2.4
4	D	320	LEU	2.4
8	i	4	LEU	2.4
10	k	21	LEU	2.4
1	a	168	PHE	2.4
2	B	399	VAL	2.4
3	C	61	VAL	2.4
17	X	39	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	291	SER	2.4
2	b	258	TYR	2.4
4	d	155	SER	2.4
3	C	199	ILE	2.4
1	a	315	ASN	2.4
5	e	35	TRP	2.4
15	U	71	GLN	2.4
2	B	109	LEU	2.4
4	d	289	LEU	2.4
1	a	318	ALA	2.4
2	B	224	ARG	2.4
4	d	330	ALA	2.4
13	o	213	GLY	2.4
3	c	67	MET	2.4
16	V	92	HIS	2.4
1	a	185[A]	VAL	2.4
2	B	451	PHE	2.4
3	C	146	PHE	2.4
7	h	58	VAL	2.4
8	i	8	VAL	2.4
10	k	43	VAL	2.4
11	l	10	VAL	2.4
1	a	221[A]	SER	2.4
2	b	240	SER	2.4
12	M	31	SER	2.4
13	o	128	SER	2.4
1	A	238[A]	LYS	2.4
1	A	290	ILE	2.4
7	H	26	GLY	2.4
7	h	8	GLY	2.4
4	d	92	LEU	2.4
5	e	80	LEU	2.4
9	J	35	LEU	2.4
18	y	39	LEU	2.4
1	a	233	ALA	2.4
2	b	187	PRO	2.4
10	k	12	PRO	2.4
19	Z	28	ALA	2.4
13	O	6	THR	2.4
3	c	196	VAL	2.4
4	D	341	PHE	2.4
7	h	17	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	K	27	VAL	2.4
3	C	275	SER	2.4
5	e	73	LYS	2.3
3	c	102	GLY	2.3
2	B	447	PRO	2.3
2	b	222	PRO	2.3
2	b	450	TRP	2.3
2	b	474	LEU	2.3
4	d	283	ALA	2.3
4	d	291	LEU	2.3
13	o	20	PRO	2.3
15	u	17	LEU	2.3
1	A	230	THR	2.3
1	a	325	ASN	2.3
2	B	139	PHE	2.3
2	B	426	PHE	2.3
4	D	30	VAL	2.3
7	h	60	VAL	2.3
2	b	68	ARG	2.3
4	D	348	ARG	2.3
16	V	51	SER	2.3
1	A	337[A]	HIS	2.3
4	d	213	ILE	2.3
13	o	197	ILE	2.3
4	d	347	PRO	2.3
7	h	29	PRO	2.3
3	c	172	ALA	2.3
4	D	119	ALA	2.3
4	D	279	LEU	2.3
15	u	9	LEU	2.3
17	X	30	ALA	2.3
1	a	127	MET	2.3
4	D	236	ASN	2.3
4	d	175	VAL	2.3
10	k	19	ASP	2.3
2	B	61	PHE	2.3
2	b	215	PHE	2.3
2	b	451	PHE	2.3
15	u	23	GLU	2.3
3	C	136	GLY	2.3
3	c	162	GLY	2.3
13	O	226	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
16	V	47	LYS	2.3
2	b	80	ILE	2.3
3	C	384	ILE	2.3
3	c	120	ILE	2.3
13	O	172	ILE	2.3
15	U	36	ILE	2.3
1	a	193	LEU	2.3
3	C	340	TYR	2.3
4	d	63	LEU	2.3
16	v	38	ALA	2.3
3	c	195	ASP	2.3
6	f	40	MET	2.3
15	u	44	THR	2.3
3	C	425	TRP	2.3
16	v	90	GLU	2.3
1	A	249	VAL	2.3
2	B	397	VAL	2.3
4	D	136	VAL	2.3
10	K	22	VAL	2.3
2	B	186	GLY	2.3
2	B	374	ASN	2.3
3	c	155	ASN	2.3
7	H	32	ALA	2.3
2	b	98	LEU	2.3
2	b	225	LEU	2.3
4	D	160	TYR	2.3
4	d	209	LEU	2.3
7	H	49	TYR	2.3
12	M	22	LEU	2.3
15	u	85	THR	2.3
16	V	107	LEU	2.3
2	B	351	GLY	2.3
2	b	254	GLY	2.3
2	b	500	GLY	2.3
1	A	155	PHE	2.3
2	b	417	VAL	2.3
3	C	296	VAL	2.3
3	c	61	VAL	2.3
3	c	114	VAL	2.3
3	C	138	GLU	2.3
2	B	270	PRO	2.3
2	b	374	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	60	ILE	2.3
8	i	10	ILE	2.3
9	j	23	ILE	2.3
16	v	115	ILE	2.3
1	a	123	ALA	2.3
2	B	38	ALA	2.3
2	b	480	SER	2.3
4	D	205	LEU	2.3
5	e	30	LEU	2.3
6	F	12	SER	2.3
3	C	297	TYR	2.3
13	O	196	GLN	2.3
16	V	40	CYS	2.3
3	C	440	GLY	2.3
4	D	271	MET	2.3
2	b	455	HIS	2.3
5	E	8	ARG	2.3
15	U	77	GLU	2.3
3	C	54	VAL	2.3
3	C	351	PHE	2.3
3	c	225	VAL	2.3
4	d	328	TRP	2.3
9	j	24	VAL	2.3
2	b	88	PRO	2.3
5	e	9	PRO	2.3
16	v	50	PRO	2.3
2	B	381	ILE	2.3
2	b	315	ILE	2.3
3	C	260	ALA	2.3
3	C	314	ALA	2.3
3	C	319	ILE	2.3
19	Z	8	ALA	2.3
19	z	44	SER	2.3
1	A	28	LEU	2.2
2	b	255	THR	2.2
3	c	42	LEU	2.2
4	D	91	LEU	2.2
4	d	36	LEU	2.2
5	e	49	THR	2.2
7	h	7	LEU	2.2
19	Z	9	LEU	2.2
2	B	330	MET	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	342	MET	2.2
4	D	126	MET	2.2
1	A	125	CYS	2.2
3	c	56	HIS	2.2
4	D	105	CYS	2.2
4	d	40	CYS	2.2
15	U	81	HIS	2.2
2	b	194	ASN	2.2
1	a	206	PHE	2.2
3	c	435	PHE	2.2
15	u	10	VAL	2.2
2	B	88	PRO	2.2
12	M	32	GLN	2.2
3	c	226	SER	2.2
2	B	369	ILE	2.2
2	b	207	ILE	2.2
4	D	148	ALA	2.2
18	y	36	ILE	2.2
7	h	27	THR	2.2
1	a	223	LEU	2.2
2	b	133	LEU	2.2
3	C	377	LEU	2.2
6	f	26	LEU	2.2
4	D	281	MET	2.2
3	C	290	VAL	2.2
4	D	152	VAL	2.2
7	H	29	PRO	2.2
10	k	30	VAL	2.2
8	i	19	PHE	2.2
19	z	17	PHE	2.2
2	B	257	TRP	2.2
2	B	468	TRP	2.2
18	y	42	ARG	2.2
19	Z	47	TRP	2.2
1	A	320	ILE	2.2
2	b	416	THR	2.2
3	C	134	ILE	2.2
3	c	58	GLY	2.2
3	c	283	GLY	2.2
4	d	46	GLY	2.2
13	O	29	ALA	2.2
13	O	214	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	o	129	THR	2.2
17	X	9	GLY	2.2
1	a	275	LEU	2.2
2	B	29	LEU	2.2
3	c	69	LEU	2.2
4	D	182	LEU	2.2
4	D	272	LEU	2.2
4	d	37	LEU	2.2
13	o	182	LEU	2.2
1	a	214[A]	MET	2.2
4	D	227	GLU	2.2
10	K	15	TYR	2.2
2	B	180	PRO	2.2
3	c	290	VAL	2.2
4	d	276	VAL	2.2
10	K	30	VAL	2.2
4	d	38	PHE	2.2
1	A	50	ILE	2.2
1	A	245	THR	2.2
2	b	271	THR	2.2
2	b	371	THR	2.2
3	C	430	HIS	2.2
5	E	27	ILE	2.2
17	X	31	ILE	2.2
13	o	244	GLU	2.2
3	C	175	LEU	2.2
19	Z	57	LEU	2.2
1	a	293	MET	2.2
4	d	180	ARG	2.2
16	v	47	LYS	2.2
1	a	58	VAL	2.2
6	f	21	VAL	2.2
16	v	97	SER	2.2
2	b	160	GLY	2.2
8	I	26	GLY	2.2
13	o	65	PHE	2.2
2	B	361	ALA	2.2
2	B	455	HIS	2.2
3	c	37	ALA	2.2
3	c	57	ALA	2.2
3	c	118	HIS	2.2
3	c	139	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	216	ALA	2.2
4	D	283	ALA	2.2
4	d	148	ALA	2.2
15	U	34	ALA	2.2
16	V	49	ASN	2.2
6	f	17	THR	2.2
6	f	25	THR	2.2
13	o	172	ILE	2.2
1	A	297	LEU	2.2
1	a	174	LEU	2.2
3	c	185	LEU	2.2
4	d	43	LEU	2.2
1	A	124	SER	2.2
4	D	147	SER	2.2
2	B	119	ASP	2.2
2	b	397	VAL	2.2
4	D	286	VAL	2.2
17	x	22	GLY	2.2
18	y	32	GLY	2.2
2	B	411	PHE	2.2
5	e	75	GLN	2.2
3	C	399	ALA	2.2
13	O	19	CYS	2.2
2	B	324	LEU	2.2
2	b	468	TRP	2.2
4	d	253	TRP	2.2
13	o	84	GLU	2.2
13	o	181	GLU	2.2
3	C	152	LYS	2.1
4	d	187	GLY	2.2
2	B	178	VAL	2.1
4	D	204	VAL	2.1
15	U	50	VAL	2.1
7	h	38	PHE	2.1
2	B	111	ALA	2.1
10	k	36	ALA	2.1
13	O	154	ALA	2.1
1	a	229	GLU	2.1
2	b	217	ILE	2.1
9	J	11	ILE	2.1
15	u	74	ILE	2.1
17	x	29	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	149	LEU	2.1
3	C	444	HIS	2.1
15	u	81	HIS	2.1
16	v	92	HIS	2.1
3	c	113	VAL	2.1
3	c	233	VAL	2.1
1	A	146	ALA	2.1
3	C	94	THR	2.1
4	d	217	THR	2.1
16	V	134	LYS	2.1
2	b	414	PRO	2.1
3	C	422	PRO	2.1
2	B	127	ARG	2.1
2	B	165	GLY	2.1
3	C	197	ARG	2.1
4	D	163	GLY	2.1
4	D	350	ASN	2.1
7	h	55	LEU	2.1
10	K	35	LEU	2.1
15	u	79	LEU	2.1
4	d	215	GLY	2.1
3	C	356	MET	2.1
13	O	225	MET	2.1
1	A	149	ALA	2.1
1	a	156	ALA	2.1
3	c	271	TYR	2.1
2	b	151	PHE	2.1
4	D	249	ALA	2.1
4	d	173	PHE	2.1
4	d	184	PHE	2.1
6	f	27	ALA	2.1
13	o	11	VAL	2.1
16	V	136	TYR	2.1
16	v	56	THR	2.1
4	D	16	ASP	2.1
13	O	224	ASP	2.1
2	b	224	ARG	2.1
3	c	310	SER	2.1
1	a	137	LEU	2.1
2	b	465	GLY	2.1
4	d	135	LEU	2.1
5	E	6	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	30	LEU	2.1
7	h	39	LEU	2.1
9	J	34	GLY	2.1
15	u	18	GLY	2.1
16	v	29	GLY	2.1
16	v	94	SER	2.1
4	D	329	MET	2.1
16	v	40	CYS	2.1
1	A	97	TRP	2.1
3	C	410[A]	VAL	2.1
3	c	177	ALA	2.1
3	c	312	ALA	2.1
13	o	71	VAL	2.1
3	c	351	PHE	2.1
4	D	146	PHE	2.1
4	D	235	PHE	2.1
1	A	164	GLY	2.1
1	a	289	GLY	2.1
3	c	256	PRO	2.1
16	v	93	PRO	2.1
1	a	151	LEU	2.1
13	o	118	LEU	2.1
2	b	60	MET	2.1
13	o	180	GLU	2.1
1	a	154	ALA	2.1
2	b	27	THR	2.1
2	b	228	ALA	2.1
3	C	66	ALA	2.1
4	D	143	ALA	2.1
16	v	130	TRP	2.1
10	K	38	VAL	2.1
3	C	163	PHE	2.1
19	z	55	GLY	2.1
1	A	184	ILE	2.1
4	D	35	ILE	2.1
13	O	136	ILE	2.1
16	V	69	ILE	2.1
18	Y	46	LEU	2.1
2	B	448	ARG	2.1
19	z	19	MET	2.1
7	h	20	LYS	2.1
2	B	118	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	237	VAL	2.1
3	C	105	VAL	2.1
3	c	128	GLY	2.1
3	c	239	TRP	2.1
3	c	352	GLY	2.1
4	D	206	GLY	2.1
13	o	19	CYS	2.1
16	V	132	GLY	2.1
1	A	300	PHE	2.1
1	a	265[A]	PHE	2.1
3	c	292	PHE	2.1
4	d	237	PRO	2.1
6	f	42	PHE	2.1
15	U	55	TYR	2.1
12	m	28	GLN	2.0
2	B	19	LEU	2.0
2	B	103	LEU	2.0
3	C	240	ILE	2.0
17	X	3	ILE	2.0
1	A	250	ALA	2.0
3	C	329	GLY	2.0
4	D	121	GLY	2.0
2	B	126	PRO	2.0
2	b	181	VAL	2.0
8	I	20	VAL	2.0
10	k	26	PRO	2.0
1	a	182	PHE	2.0
3	c	218	PHE	2.0
4	D	153	PHE	2.0
4	d	167	TRP	2.0
7	h	4	ARG	2.0
10	K	37	PHE	2.0
1	a	41	LEU	2.0
3	C	119	LEU	2.0
3	C	185	LEU	2.0
16	v	112	LEU	2.0
1	a	267[A]	ASN	2.0
3	C	67	MET	2.0
2	B	85	GLY	2.0
3	c	94	THR	2.0
13	O	161	GLY	2.0
1	A	148	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	b	21	ALA	2.0
3	C	310	SER	2.0
4	d	230	SER	2.0
5	E	18	ARG	2.0
7	H	13	PRO	2.0
1	A	283	VAL	2.0
2	b	311	PHE	2.0
2	b	453	PHE	2.0
3	C	419	PHE	2.0
4	d	341	PHE	2.0
4	d	322	ASN	2.0
2	b	161	LEU	2.0
2	b	299	GLU	2.0
3	c	125	LEU	2.0
12	M	23	ILE	2.0
13	O	10	ILE	2.0
1	A	327	GLY	2.0
19	z	22	GLY	2.0
1	a	220	THR	2.0
1	a	264	SER	2.0
2	B	239[A]	SER	2.0
2	b	159	THR	2.0
4	d	102	THR	2.0
16	v	48	THR	2.0
4	d	351	ALA	2.0
9	J	16	ALA	2.0
9	j	33	ALA	2.0

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

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
12	FME	M	1	10/11	0.85	0.24	-	34,56,91,100	0
12	FME	m	1	10/11	0.89	0.18	-	47,60,91,103	0
8	FME	I	1	10/11	0.80	0.25	-	46,65,76,76	0
14	FME	t	1	10/11	0.89	0.17	-	43,51,75,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	FME	i	1	10/11	0.81	0.28	-	59,64,77,78	0
14	FME	T	1	10/11	0.86	0.19	-	44,50,74,88	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
32	UNL	K	101	34/-	0.28	0.61	10.03	83,119,134,150	0
32	UNL	j	102	10/-	0.52	0.59	9.94	87,106,117,118	0
34	LMT	B	630	25/35	0.43	0.47	8.47	54,89,147,148	0
28	GOL	v	202	6/6	0.71	0.78	8.46	75,86,94,96	0
32	UNL	d	410	36/-	0.44	0.59	7.81	73,100,136,140	0
32	UNL	d	409	17/-	0.80	0.66	7.49	68,83,111,114	0
35	HTG	B	624	19/19	0.57	0.35	7.25	71,103,114,115	0
34	LMT	a	359	35/35	0.31	0.49	6.47	65,144,151,154	0
35	HTG	D	410	16/19	0.21	0.51	6.19	82,121,136,138	0
34	LMT	A	359	35/35	0.30	0.52	6.06	73,134,144,148	0
34	LMT	b	630	25/35	0.50	0.43	5.83	57,81,151,153	0
32	UNL	D	408	17/-	0.83	0.58	5.56	66,85,107,110	0
28	GOL	a	416	6/6	0.65	0.35	5.45	55,82,84,86	0
38	LHG	D	357	49/49	0.75	0.49	5.21	49,64,86,102	0
34	LMT	M	103	35/35	0.44	0.37	5.07	68,146,169,171	0
28	GOL	V	202	6/6	0.78	0.74	5.03	64,74,85,92	0
35	HTG	b	624	19/19	0.47	0.43	4.51	114,128,145,170	0
35	HTG	b	623	19/19	0.47	0.41	4.50	68,88,130,131	0
28	GOL	a	410	6/6	0.73	0.31	4.38	79,81,90,95	0
27	SQD	A	413	54/54	0.52	0.42	4.37	63,91,128,137	0
28	GOL	c	502	6/6	0.91	0.54	4.30	68,70,71,75	0
38	LHG	D	407	49/49	0.79	0.42	4.15	53,61,120,125	0
28	GOL	B	626	6/6	0.94	0.32	4.14	85,88,90,95	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	PL9	A	416[A]	55/55	0.72	0.39	4.13	66,93,107,111	55
34	LMT	e	101	35/35	0.30	0.67	4.03	121,166,181,186	0
34	LMT	E	102	35/35	0.55	0.46	4.02	119,145,171,173	0
33	LMG	c	522	51/55	0.20	0.54	3.99	80,127,154,158	0
27	SQD	b	620	54/54	0.39	0.44	3.98	68,93,144,152	0
31	PL9	A	416[B]	55/55	0.72	0.39	3.89	66,93,108,113	55
33	LMG	a	417	51/55	0.41	0.52	3.86	76,100,122,129	0
38	LHG	D	406	49/49	0.83	0.40	3.84	47,57,76,93	0
32	UNL	D	409	40/-	0.58	0.43	3.76	67,93,136,140	0
31	PL9	a	414[A]	55/55	0.65	0.43	3.76	97,107,120,124	55
31	PL9	a	414[B]	55/55	0.65	0.43	3.75	97,107,120,124	55
27	SQD	a	411	54/54	0.49	0.43	3.67	72,95,139,149	0
35	HTG	B	623	19/19	0.60	0.35	3.64	70,88,128,128	0
33	LMG	C	521	51/55	0.28	0.46	3.49	68,121,155,157	0
26	BCR	B	618	40/40	0.83	0.34	3.42	44,57,70,77	0
38	LHG	d	407	49/49	0.78	0.36	3.38	48,59,73,85	0
22	CL	a	402	1/1	0.98	0.40	3.35	51,51,51,51	0
36	DGD	H	102	62/66	0.64	0.48	3.31	46,63,76,78	0
26	BCR	b	618	40/40	0.84	0.35	3.26	44,60,73,75	0
28	GOL	B	627	6/6	0.88	0.34	3.15	58,77,85,87	0
26	BCR	t	102	40/40	0.88	0.32	3.12	45,60,76,80	0
34	LMT	t	101	26/35	0.67	0.28	3.06	71,110,152,153	0
32	UNL	i	101	40/-	0.19	0.45	3.03	77,109,164,165	0
38	LHG	L	101	49/49	0.78	0.36	2.99	45,55,67,96	0
34	LMT	B	622	35/35	0.22	0.45	2.91	78,125,142,144	0
38	LHG	d	408	49/49	0.80	0.34	2.88	53,68,121,125	0
36	DGD	h	103	62/66	0.47	0.51	2.76	52,66,78,86	0
27	SQD	B	620	54/54	0.48	0.42	2.75	65,93,132,134	0
26	BCR	B	617	40/40	0.89	0.29	2.70	44,52,59,65	0
33	LMG	A	418	51/55	0.46	0.50	2.69	61,97,118,121	0
38	LHG	l	101	49/49	0.70	0.32	2.66	50,60,74,91	0
34	LMT	b	622	25/35	0.04	0.59	2.64	88,117,159,160	0
33	LMG	B	621	51/55	0.60	0.42	2.61	53,72,94,108	0
24	CLA	B	605	65/65	0.74	0.33	2.54	39,48,65,68	0
27	SQD	A	411	54/54	0.64	0.41	2.52	55,86,123,126	0
22	CL	A	402	1/1	0.98	0.33	2.48	44,44,44,44	0
38	LHG	d	406	49/49	0.79	0.38	2.47	50,66,90,106	0
26	BCR	T	101	40/40	0.84	0.33	2.46	46,57,68,72	0
24	CLA	B	601	65/65	0.78	0.30	2.45	53,77,112,132	0
36	DGD	C	518	62/66	0.67	0.37	2.43	48,67,127,131	0
31	PL9	D	405	55/55	0.92	0.34	2.41	37,49,62,78	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	HTG	C	523	19/19	0.48	0.54	2.40	84,153,166,186	0
35	HTG	b	625	19/19	0.15	0.45	2.34	91,138,154,196	0
32	UNL	I	102	40/-	0.47	0.39	2.32	66,113,156,158	0
33	LMG	J	101	51/55	0.76	0.30	2.22	48,73,119,126	0
38	LHG	E	101	42/49	0.36	0.45	2.10	72,118,132,132	0
31	PL9	d	405	55/55	0.89	0.29	2.09	41,50,66,85	0
24	CLA	b	608	65/65	0.76	0.40	2.00	46,58,81,84	0
33	LMG	b	621	51/55	0.62	0.36	1.97	53,74,105,124	0
25	PHO	a	405	64/64	0.89	0.31	1.95	41,49,56,64	0
24	CLA	C	505	65/65	0.69	0.40	1.88	42,56,103,113	0
34	LMT	I	101	35/35	0.21	0.49	1.86	110,145,160,162	0
24	CLA	b	605	65/65	0.79	0.34	1.84	43,52,70,74	0
35	HTG	V	204	11/19	0.83	0.44	1.84	104,117,122,125	0
36	DGD	c	518	62/66	0.73	0.37	1.82	49,67,95,103	0
24	CLA	c	505	65/65	0.68	0.41	1.82	58,67,77,83	0
38	LHG	a	419	42/49	0.25	0.51	1.80	78,141,167,179	0
36	DGD	C	517	62/66	0.73	0.40	1.79	43,63,104,106	0
24	CLA	B	608	65/65	0.77	0.35	1.75	41,54,68,71	0
24	CLA	C	504	65/65	0.70	0.40	1.71	47,58,76,85	0
28	GOL	C	525	6/6	0.83	0.40	1.68	66,73,76,78	0
27	SQD	a	409	54/54	0.74	0.30	1.64	63,85,127,131	0
35	HTG	c	526	19/19	0.12	0.58	1.64	114,161,170,200	0
25	PHO	A	407	64/64	0.86	0.31	1.61	35,45,54,58	0
24	CLA	b	610	65/65	0.79	0.34	1.60	47,58,73,75	0
36	DGD	C	519	62/66	0.78	0.28	1.57	43,60,94,116	0
34	LMT	a	418	35/35	0.35	0.50	1.55	113,136,151,151	0
24	CLA	b	603	65/65	0.74	0.38	1.55	46,56,85,92	0
24	CLA	C	506	65/65	0.75	0.36	1.50	49,57,92,100	0
24	CLA	B	604	65/65	0.80	0.38	1.48	34,46,123,127	0
24	CLA	b	607	65/65	0.81	0.30	1.47	35,49,77,87	0
35	HTG	b	628	19/19	0.50	0.31	1.45	61,82,106,112	0
28	GOL	b	627	6/6	0.74	0.29	1.45	97,106,113,116	0
32	UNL	X	101	18/-	0.75	0.27	1.39	57,76,100,100	0
33	LMG	c	521	51/55	0.62	0.39	1.37	68,101,145,156	0
36	DGD	c	519	62/66	0.73	0.34	1.37	56,73,136,145	0
24	CLA	B	609	65/65	0.63	0.30	1.34	47,57,73,80	0
24	CLA	B	614	65/65	0.80	0.25	1.34	38,49,103,113	0
24	CLA	B	610	65/65	0.84	0.31	1.34	43,53,64,80	0
32	UNL	x	101	18/-	0.69	0.27	1.33	70,85,105,106	0
22	CL	A	347	1/1	0.98	0.37	1.31	49,49,49,49	0
35	HTG	h	101	16/19	0.24	0.51	1.28	98,133,140,163	0
24	CLA	c	510	65/65	0.76	0.30	1.27	53,63,141,145	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	DGD	c	520	62/66	0.84	0.28	1.27	55,64,100,116	0
27	SQD	f	101	43/54	0.25	0.51	1.25	118,136,170,175	0
24	CLA	B	603	65/65	0.83	0.34	1.23	42,52,69,76	0
24	CLA	b	612	65/65	0.78	0.34	1.20	43,54,64,75	0
24	CLA	B	607	65/65	0.81	0.30	1.18	32,45,71,78	0
24	CLA	B	611	65/65	0.76	0.34	1.17	37,47,63,73	0
25	PHO	A	408	64/64	0.86	0.27	1.16	37,49,57,60	0
34	LMT	m	102	35/35	0.19	0.45	1.16	63,95,117,121	0
24	CLA	C	511	65/65	0.81	0.42	1.15	49,61,74,88	0
24	CLA	a	350	65/65	0.76	0.27	1.15	36,46,63,77	0
33	LMG	C	520	51/55	0.65	0.42	1.13	56,90,127,140	0
24	CLA	c	512	65/65	0.71	0.39	1.07	50,65,81,92	0
24	CLA	b	602	65/65	0.61	0.38	1.04	51,62,79,88	0
24	CLA	c	507	65/65	0.71	0.30	1.04	49,61,91,95	0
24	CLA	B	602	65/65	0.71	0.34	1.04	45,55,80,84	0
26	BCR	C	516	40/40	0.88	0.30	1.04	53,62,72,81	0
24	CLA	C	509	65/65	0.76	0.35	1.03	44,57,115,131	0
24	CLA	B	613	65/65	0.80	0.36	1.02	37,47,94,103	0
26	BCR	b	617	40/40	0.88	0.25	0.98	45,52,63,63	0
33	LMG	Z	101	37/55	0.33	0.45	0.98	77,129,150,151	0
23	BCT	a	420[A]	4/4	0.92	0.22	0.97	58,63,63,68	4
23	BCT	a	420[B]	4/4	0.92	0.22	0.97	54,63,64,72	4
24	CLA	C	503	65/65	0.84	0.37	0.97	47,55,78,95	0
24	CLA	A	404	65/65	0.79	0.27	0.95	36,43,66,80	0
24	CLA	a	403	65/65	0.81	0.29	0.94	36,48,69,86	0
24	CLA	c	503	65/65	0.82	0.32	0.92	56,66,79,86	0
24	CLA	c	511	65/65	0.80	0.32	0.90	51,69,82,89	0
24	CLA	C	510	65/65	0.87	0.34	0.89	49,60,81,91	0
24	CLA	B	612	65/65	0.78	0.32	0.86	35,47,57,74	0
24	CLA	B	606	65/65	0.76	0.25	0.86	41,52,104,114	0
24	CLA	C	502	65/65	0.78	0.33	0.86	48,59,73,83	0
24	CLA	b	604	65/65	0.84	0.36	0.85	37,50,122,128	0
24	CLA	A	406	65/65	0.81	0.24	0.84	36,47,110,116	0
24	CLA	A	405	65/65	0.78	0.26	0.82	34,45,54,63	0
39	HEM	e	102	43/43	0.81	0.42	0.80	67,93,128,137	0
24	CLA	b	609	65/65	0.70	0.30	0.76	50,61,83,99	0
24	CLA	b	614	65/65	0.77	0.25	0.74	41,49,116,120	0
33	LMG	j	101	51/55	0.78	0.27	0.73	60,70,121,138	0
24	CLA	c	506	65/65	0.81	0.34	0.72	51,66,116,125	0
24	CLA	c	504	65/65	0.78	0.36	0.71	45,65,86,89	0
24	CLA	b	601	65/65	0.73	0.30	0.70	58,85,115,130	0
34	LMT	M	101	35/35	0.29	0.42	0.70	61,99,123,126	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	c	515	65/65	0.65	0.34	0.68	70,91,134,138	0
24	CLA	C	514	65/65	0.61	0.31	0.67	60,81,122,127	0
24	CLA	b	606	65/65	0.75	0.26	0.67	45,58,114,129	0
23	BCT	A	403[B]	4/4	0.88	0.24	0.65	55,61,62,78	4
22	CL	a	347	1/1	0.97	0.29	0.65	53,53,53,53	0
23	BCT	A	403[A]	4/4	0.88	0.24	0.65	58,60,60,69	4
24	CLA	d	402	65/65	0.82	0.29	0.65	39,48,74,86	0
25	PHO	a	406	64/64	0.82	0.28	0.62	41,55,63,65	0
33	LMG	z	101	39/55	0.39	0.42	0.60	84,133,148,153	0
24	CLA	b	613	65/65	0.84	0.33	0.59	42,49,101,106	0
24	CLA	a	404	65/65	0.80	0.27	0.57	42,53,126,133	0
35	HTG	B	628	19/19	0.68	0.25	0.55	65,80,89,95	0
24	CLA	C	508	65/65	0.80	0.30	0.54	49,60,80,82	0
26	BCR	a	408	40/40	0.87	0.23	0.46	42,52,65,68	0
24	CLA	b	611	65/65	0.81	0.28	0.36	41,52,73,82	0
26	BCR	A	410	40/40	0.91	0.22	0.34	42,51,61,62	0
24	CLA	D	402	65/65	0.81	0.24	0.31	31,45,68,82	0
29	OEX	A	414[A]	10/10	0.92	0.24	0.25	44,48,55,59	10
30	OEY	A	415[B]	11/11	0.92	0.23	0.21	43,49,55,56	11
30	OEY	a	413[B]	11/11	0.93	0.24	0.21	50,54,58,74	11
27	SQD	F	101	43/54	0.67	0.33	0.19	81,114,134,137	0
26	BCR	K	102	40/40	0.86	0.23	0.19	56,67,74,81	0
26	BCR	D	404	40/40	0.87	0.22	0.18	46,61,94,95	0
24	CLA	c	513	65/65	0.74	0.24	0.10	57,71,91,97	0
24	CLA	C	507	65/65	0.76	0.27	0.09	53,69,137,141	0
29	OEX	a	412[A]	10/10	0.92	0.24	0.04	50,55,61,74	10
24	CLA	C	513	65/65	0.76	0.24	-0.02	60,73,118,123	0
26	BCR	b	619	40/40	0.88	0.20	-0.05	51,62,81,84	0
24	CLA	c	514	65/65	0.77	0.26	-0.09	59,80,123,128	0
26	BCR	k	101	40/40	0.83	0.26	-0.10	58,73,84,90	0
24	CLA	A	409	65/65	0.87	0.21	-0.10	42,53,136,144	0
24	CLA	b	615	65/65	0.75	0.23	-0.10	46,59,81,86	0
24	CLA	c	509	65/65	0.81	0.25	-0.15	56,70,86,92	0
24	CLA	B	615	65/65	0.80	0.20	-0.16	37,52,74,83	0
24	CLA	d	403	65/65	0.82	0.20	-0.24	46,64,132,137	0
26	BCR	h	102	40/40	0.71	0.24	-0.26	56,70,80,81	0
40	MG	J	103	1/1	0.86	0.18	-0.32	61,61,61,61	0
24	CLA	C	512	65/65	0.72	0.23	-0.34	52,63,79,86	0
24	CLA	c	508	65/65	0.75	0.26	-0.34	60,72,120,133	0
26	BCR	H	101	40/40	0.79	0.21	-0.38	50,65,77,82	0
39	HEM	E	103	43/43	0.77	0.26	-0.39	60,70,80,93	0
24	CLA	D	403	65/65	0.85	0.21	-0.40	44,58,139,144	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
24	CLA	b	616	65/65	0.80	0.21	-0.40	50,60,124,127	0
24	CLA	a	407	65/65	0.90	0.19	-0.46	44,57,134,140	0
26	BCR	d	404	40/40	0.84	0.20	-0.61	53,67,96,98	0
26	BCR	B	619	40/40	0.87	0.18	-0.63	45,57,80,87	0
24	CLA	B	616	65/65	0.86	0.19	-0.66	45,58,147,153	0
39	HEM	V	203	43/43	0.84	0.19	-0.69	39,52,58,60	0
26	BCR	c	517	40/40	0.89	0.20	-0.70	56,67,80,81	0
26	BCR	Y	101	40/40	0.89	0.18	-0.92	57,68,74,81	0
26	BCR	C	515	40/40	0.86	0.16	-1.04	63,75,82,85	0
40	MG	j	103	1/1	0.91	0.17	-1.10	64,64,64,64	0
26	BCR	c	516	40/40	0.83	0.22	-1.23	77,86,93,96	0
39	HEM	v	203	43/43	0.86	0.17	-1.27	51,64,72,78	0
28	GOL	A	412	6/6	0.88	0.17	-1.56	80,82,86,98	0
37	CA	O	301	1/1	0.66	0.32	-1.59	119,119,119,119	0
37	CA	c	525	1/1	0.83	0.17	-1.69	92,92,92,92	0
37	CA	o	301	1/1	0.85	0.25	-1.69	108,108,108,108	0
37	CA	C	524	1/1	0.99	0.20	-1.78	72,72,72,72	0
37	CA	c	524	1/1	0.94	0.20	-2.37	78,78,78,78	0
26	BCR	y	101	40/40	0.83	0.16	-2.39	58,74,88,88	0
21	FE2	a	401[B]	1/1	0.99	0.07	-4.31	60,60,60,60	1
21	FE2	a	401[A]	1/1	0.99	0.07	-4.31	60,60,60,60	1
21	FE2	A	401[B]	1/1	0.99	0.05	-8.02	60,60,60,60	1
21	FE2	A	401[A]	1/1	0.99	0.05	-8.02	62,62,62,62	1
32	UNL	c	527	32/-	0.48	0.38	-	93,125,140,143	0
32	UNL	a	415	30/-	0.33	0.41	-	98,115,136,146	0
35	HTG	B	625	19/19	0.28	0.36	-	82,167,178,238	0
32	UNL	b	629	33/-	0.22	0.40	-	72,108,162,162	0
32	UNL	m	101	10/-	0.69	0.55	-	69,78,80,84	0
35	HTG	c	523	19/19	-0.05	0.61	-	118,144,148,169	0
37	CA	v	201	1/1	0.84	0.20	-	123,123,123,123	0
32	UNL	J	102	10/-	0.82	0.49	-	77,81,99,104	0
35	HTG	C	522	19/19	0.39	0.39	-	112,123,133,150	0
32	UNL	B	629	33/-	0.30	0.44	-	57,103,166,173	0
37	CA	V	201	1/1	0.09	0.21	-	141,141,141,141	0
32	UNL	A	417	28/-	0.24	0.44	-	98,110,128,144	0
32	UNL	M	102	10/-	0.82	0.47	-	62,72,86,92	0
37	CA	b	626	1/1	0.80	0.53	-	151,151,151,151	0

6.5 Other polymers ⓘ

There are no such residues in this entry.