Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:06 PM GMT

PDB ID	:	1RWT
Title	:	Crystal Structure of Spinach Major Light-harvesting complex at 2.72 Angstrom Resolution
Authors	:	Liu, Z.; Yan, H.; Wang, K.; Kuang, T.; Zhang, J.; Gui, L.; An, X.; Chang, W.
Deposited on	:	2003-12-17
Resolution	:	2.72 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

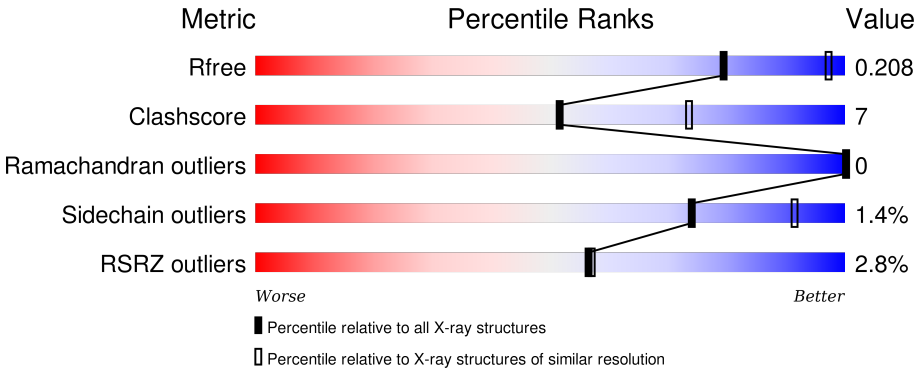
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	232	2% 78% 16% 6%
1	B	232	2% 74% 20% 6%
1	C	232	3% 79% 15% 6%
1	D	232	2% 80% 14% 6%
1	E	232	2% 78% 16% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	232	3% 76% 18% 6%
1	G	232	4% 80% 14% 6%
1	H	232	3% 76% 18% 6%
1	I	232	3% 78% 16% 6%
1	J	232	2% 83% 11% 6%

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
10	CLA	A	602	X	-	-	-
10	CLA	A	603	X	-	-	-
10	CLA	A	604	X	-	-	X
10	CLA	A	610	X	-	-	-
10	CLA	A	611	X	-	-	X
10	CLA	A	612	X	-	-	-
10	CLA	A	613	X	-	-	-
10	CLA	A	614	X	-	-	-
10	CLA	B	602	X	-	-	-
10	CLA	B	603	X	-	-	-
10	CLA	B	604	X	-	-	X
10	CLA	B	610	X	-	-	-
10	CLA	B	611	X	-	-	X
10	CLA	B	612	X	-	-	-
10	CLA	B	613	X	-	-	-
10	CLA	B	614	X	-	-	-
10	CLA	C	602	X	-	-	-
10	CLA	C	603	X	-	-	-
10	CLA	C	604	X	-	-	-
10	CLA	C	610	X	-	-	-
10	CLA	C	611	X	-	-	X
10	CLA	C	612	X	-	-	-
10	CLA	C	613	X	-	-	-
10	CLA	C	614	X	-	-	-
10	CLA	D	602	X	-	-	-
10	CLA	D	603	X	-	-	-
10	CLA	D	604	X	-	-	-
10	CLA	D	610	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	D	611	X	-	-	X
10	CLA	D	612	X	-	-	-
10	CLA	D	613	X	-	-	-
10	CLA	D	614	X	-	-	-
10	CLA	E	602	X	-	-	-
10	CLA	E	603	X	-	-	-
10	CLA	E	604	X	-	-	-
10	CLA	E	610	X	-	-	-
10	CLA	E	611	X	-	-	-
10	CLA	E	612	X	-	-	-
10	CLA	E	613	X	-	-	-
10	CLA	E	614	X	-	-	X
10	CLA	F	602	X	-	-	-
10	CLA	F	603	X	-	-	-
10	CLA	F	604	X	-	-	X
10	CLA	F	610	X	-	-	-
10	CLA	F	611	X	-	-	-
10	CLA	F	612	X	-	-	-
10	CLA	F	613	X	-	-	-
10	CLA	F	614	X	-	-	-
10	CLA	G	602	X	-	-	-
10	CLA	G	603	X	-	-	X
10	CLA	G	604	X	-	-	-
10	CLA	G	610	X	-	-	-
10	CLA	G	611	X	-	-	-
10	CLA	G	612	X	-	-	-
10	CLA	G	613	X	-	-	-
10	CLA	G	614	X	-	-	-
10	CLA	H	602	X	-	-	-
10	CLA	H	603	X	-	-	-
10	CLA	H	604	X	-	-	-
10	CLA	H	610	X	-	-	-
10	CLA	H	611	X	-	-	-
10	CLA	H	612	X	-	-	-
10	CLA	H	613	X	-	-	-
10	CLA	H	614	X	-	-	-
10	CLA	I	602	X	-	-	-
10	CLA	I	603	X	-	-	-
10	CLA	I	604	X	-	-	-
10	CLA	I	610	X	-	-	-
10	CLA	I	611	X	-	-	-
10	CLA	I	612	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	I	613	X	-	-	-
10	CLA	I	614	X	-	-	-
10	CLA	J	602	X	-	-	-
10	CLA	J	603	X	-	-	-
10	CLA	J	604	X	-	-	-
10	CLA	J	610	X	-	-	-
10	CLA	J	611	X	-	-	-
10	CLA	J	612	X	-	-	-
10	CLA	J	613	X	-	-	-
10	CLA	J	614	X	-	-	-
4	LUT	A	621	-	-	-	X
4	LUT	B	1621	-	-	-	X
4	LUT	D	3621	-	-	-	X
4	LUT	G	6621	-	-	-	X
4	LUT	H	7621	-	-	-	X
4	LUT	I	8621	-	-	-	X
4	LUT	J	9621	-	-	-	X
6	NEX	A	623	-	-	-	X
6	NEX	B	1623	-	-	-	X
6	NEX	C	2623	-	-	-	X
6	NEX	D	3623	-	-	-	X
6	NEX	E	4623	-	-	-	X
6	NEX	F	5623	-	-	-	X
6	NEX	G	6623	-	-	-	X
6	NEX	H	7623	-	-	-	X
6	NEX	I	8623	-	-	-	X
6	NEX	J	9623	-	-	-	X
7	LHG	A	630	-	-	-	X
7	LHG	B	1630	-	-	-	X
7	LHG	D	3630	-	-	-	X
7	LHG	E	4630	-	-	-	X
7	LHG	J	9630	-	-	-	X
8	DGD	A	632	X	-	-	X
8	DGD	B	1632	X	-	-	X
8	DGD	B	2632	X	-	-	X
8	DGD	D	3632	X	-	-	X
8	DGD	D	5632	X	-	-	X
8	DGD	E	4632	X	-	-	X
8	DGD	G	9632	X	-	-	X
8	DGD	H	6632	X	-	-	X
8	DGD	H	7632	X	-	-	X
8	DGD	I	8632	X	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	CHL	A	601	X	-	-	-
9	CHL	A	606	-	-	-	X
9	CHL	A	607	X	-	-	-
9	CHL	A	609	X	-	-	-
9	CHL	B	607	X	-	-	-
9	CHL	B	609	X	-	-	-
9	CHL	C	607	X	-	-	-
9	CHL	C	609	X	-	-	-
9	CHL	D	607	X	-	-	-
9	CHL	D	609	X	-	-	-
9	CHL	E	607	X	-	-	-
9	CHL	E	609	X	-	-	-
9	CHL	F	607	X	-	-	-
9	CHL	F	609	X	-	-	-
9	CHL	G	607	X	-	-	-
9	CHL	G	609	X	-	-	-
9	CHL	H	607	X	-	-	-
9	CHL	H	609	X	-	-	-
9	CHL	I	607	X	-	-	-
9	CHL	I	609	X	-	-	-
9	CHL	J	606	-	-	-	X
9	CHL	J	607	X	-	-	-
9	CHL	J	609	X	-	-	-

2 Entry composition

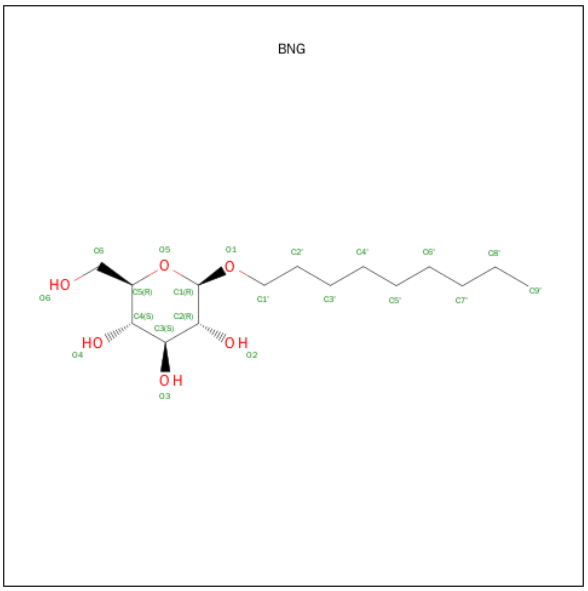
There are 11 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Chlorophyll A-B binding protein, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	B	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	C	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	D	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	E	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	F	219	Total	C	N	O	S	0	0	0
			1670	1085	272	306	7			
1	G	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	H	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	I	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			
1	J	218	Total	C	N	O	S	0	0	0
			1661	1079	270	305	7			

- Molecule 2 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



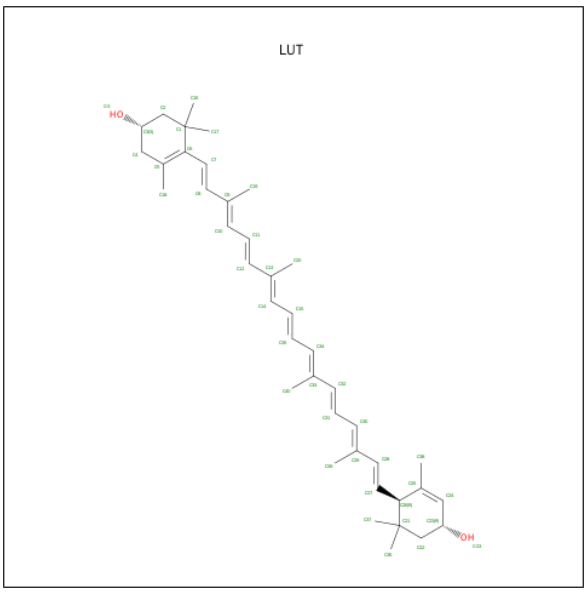
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0
2	D	1	Total C O 21 15 6	0	0
2	E	1	Total C O 21 15 6	0	0
2	F	1	Total C O 21 15 6	0	0
2	G	1	Total C O 21 15 6	0	0
2	H	1	Total C O 21 15 6	0	0
2	I	1	Total C O 21 15 6	0	0
2	J	1	Total C O 21 15 6	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,

3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



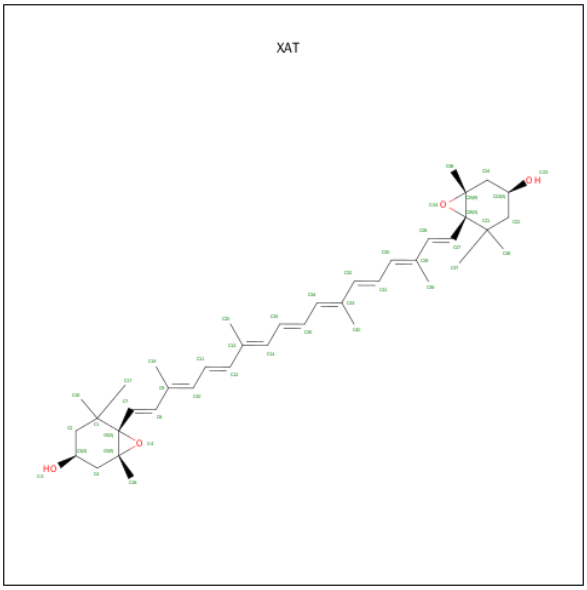
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 42 40 2	0	0
4	A	1	Total C O 42 40 2	0	0
4	B	1	Total C O 42 40 2	0	0
4	B	1	Total C O 42 40 2	0	0
4	C	1	Total C O 42 40 2	0	0
4	C	1	Total C O 42 40 2	0	0
4	D	1	Total C O 42 40 2	0	0
4	D	1	Total C O 42 40 2	0	0
4	E	1	Total C O 42 40 2	0	0
4	E	1	Total C O 42 40 2	0	0
4	F	1	Total C O 42 40 2	0	0
4	F	1	Total C O 42 40 2	0	0
4	G	1	Total C O 42 40 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 42 40 2	0	0
4	H	1	Total C O 42 40 2	0	0
4	H	1	Total C O 42 40 2	0	0
4	I	1	Total C O 42 40 2	0	0
4	I	1	Total C O 42 40 2	0	0
4	J	1	Total C O 42 40 2	0	0
4	J	1	Total C O 42 40 2	0	0

- Molecule 5 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



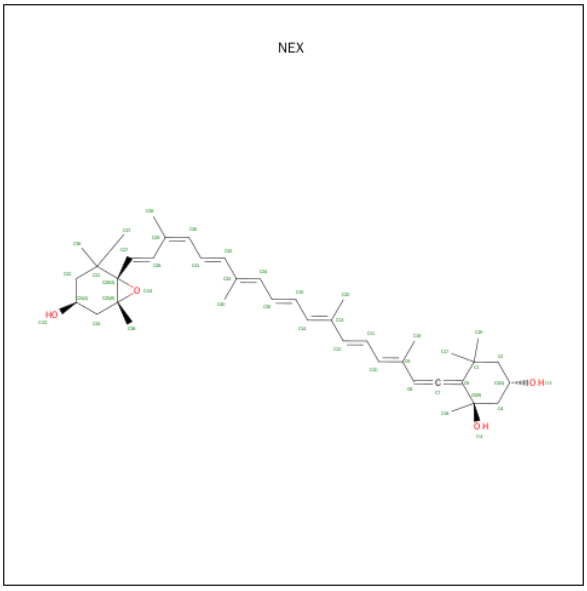
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 44 40 4	0	0
5	B	1	Total C O 44 40 4	0	0
5	E	1	Total C O 44 40 4	0	0
5	J	1	Total C O 44 40 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 44 40 4	0	0
5	B	1	Total C O 44 40 4	0	0
5	F	1	Total C O 44 40 4	0	0
5	C	1	Total C O 44 40 4	0	0
5	D	1	Total C O 44 40 4	0	0
5	I	1	Total C O 44 40 4	0	0

- Molecule 6 is (1R,3R)-6-{(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: $C_{40}H_{56}O_4$).



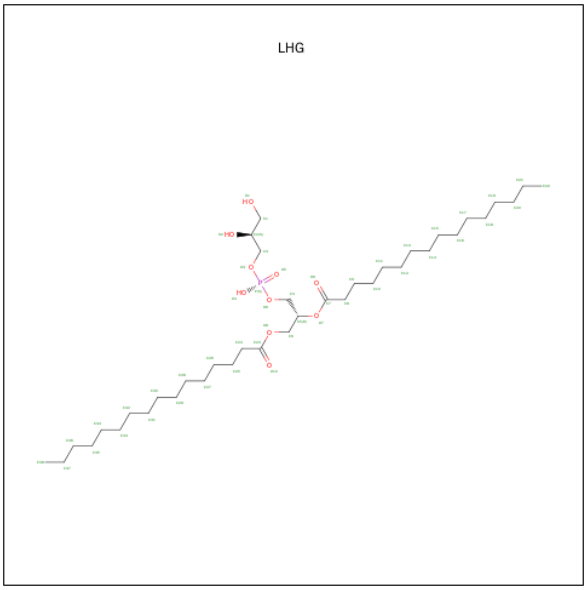
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 44 40 4	0	0
6	B	1	Total C O 44 40 4	0	0
6	C	1	Total C O 44 40 4	0	0
6	D	1	Total C O 44 40 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 44 40 4	0	0
6	F	1	Total C O 44 40 4	0	0
6	G	1	Total C O 44 40 4	0	0
6	H	1	Total C O 44 40 4	0	0
6	I	1	Total C O 44 40 4	0	0
6	J	1	Total C O 44 40 4	0	0

- Molecule 7 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



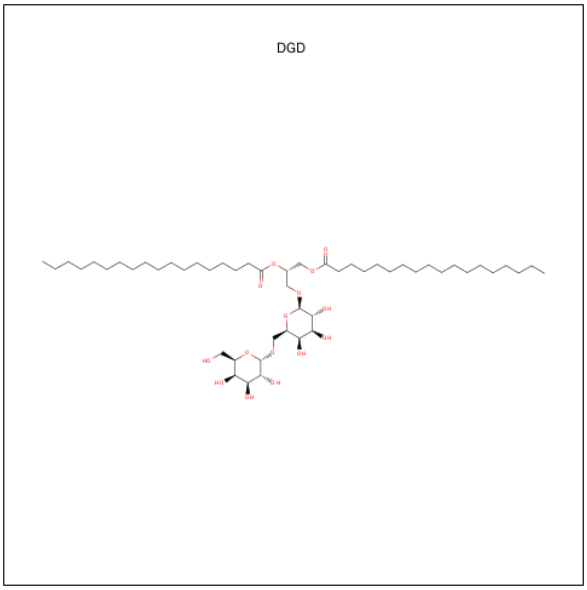
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O P 49 38 10 1	0	0
7	B	1	Total C O P 49 38 10 1	0	0
7	C	1	Total C O P 49 38 10 1	0	0
7	D	1	Total C O P 49 38 10 1	0	0
7	E	1	Total C O P 49 38 10 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	O	P	0	0
			49	38	10	1		
7	G	1	Total	C	O	P	0	0
			49	38	10	1		
7	H	1	Total	C	O	P	0	0
			49	38	10	1		
7	I	1	Total	C	O	P	0	0
			49	38	10	1		
7	J	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 8 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



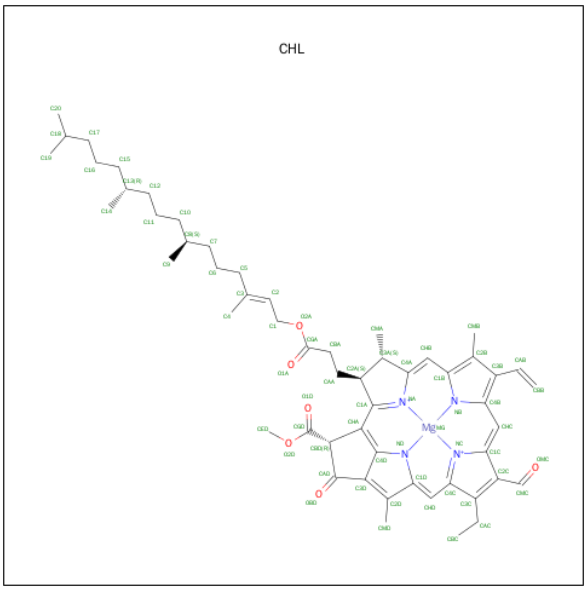
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	B	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		
8	E	1	Total	C	O	0	0
			66	51	15		
8	D	1	Total	C	O	0	0
			66	51	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 66 51 15	0	0
8	H	1	Total C O 66 51 15	0	0
8	I	1	Total C O 66 51 15	0	0
8	G	1	Total C O 66 51 15	0	0

- Molecule 9 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	A	1	Total C Mg N O 48 37 1 4 6	0	0
9	A	1	Total C Mg N O 51 40 1 4 6	0	0
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	A	1	Total C Mg N O 66 55 1 4 6	0	0
9	B	1	Total C Mg N O 66 55 1 4 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	D	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

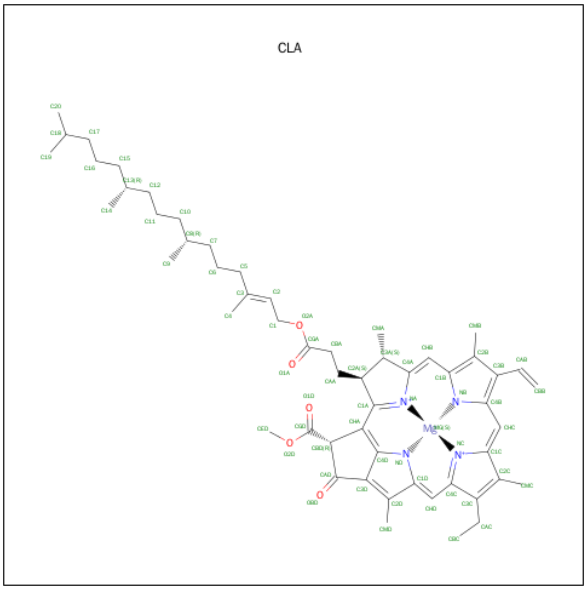
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	E	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	F	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	G	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	H	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	I	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	A	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	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
10	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	C	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	D	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	E	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	F	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	G	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	H	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	I	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
10	J	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	60	Total	O	0	0
			60	60		
11	B	78	Total	O	0	0
			78	78		
11	C	69	Total	O	0	0
			69	69		

Continued on next page...

Continued from previous page...

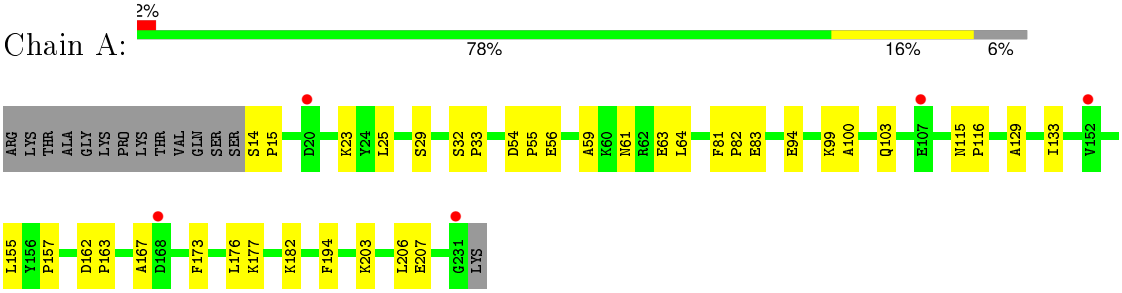
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	77	Total O 77 77	0	0
11	E	67	Total O 67 67	0	0
11	F	73	Total O 73 73	0	0
11	G	71	Total O 71 71	0	0
11	H	70	Total O 70 70	0	0
11	I	68	Total O 68 68	0	0
11	J	66	Total O 66 66	0	0

3 Residue-property plots (i)

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

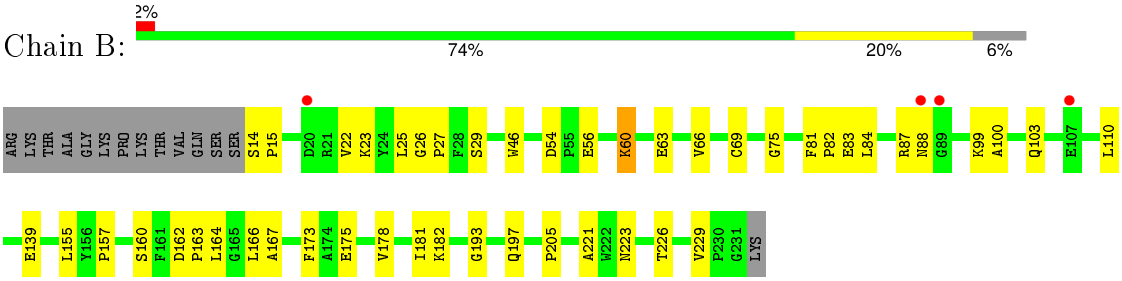
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain A:



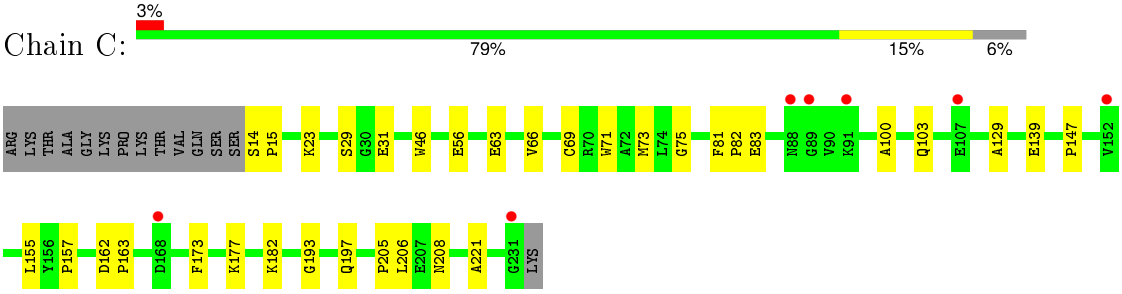
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain B:



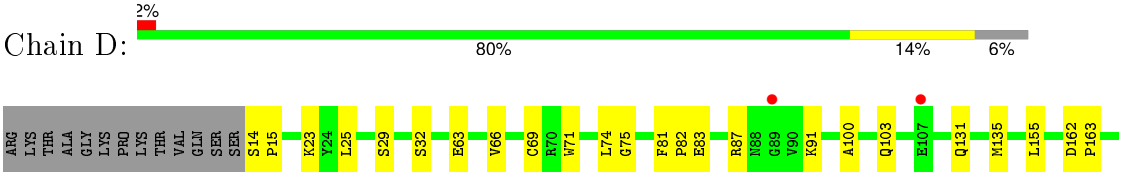
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

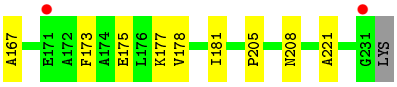
Chain C:



- Molecule 1: Chlorophyll A-B binding protein, chloroplast

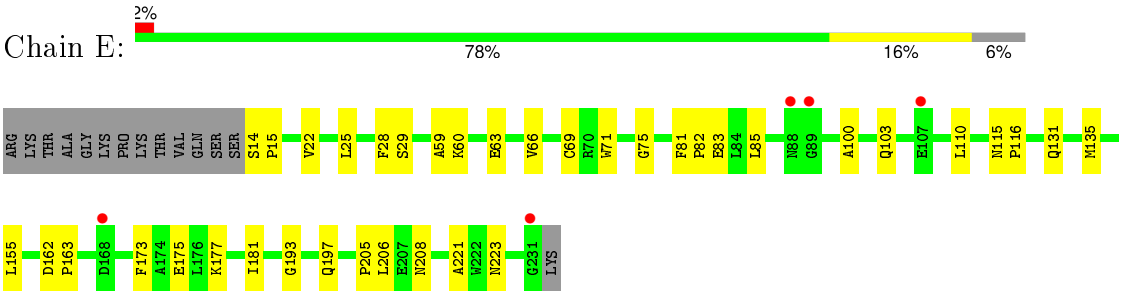
Chain D:





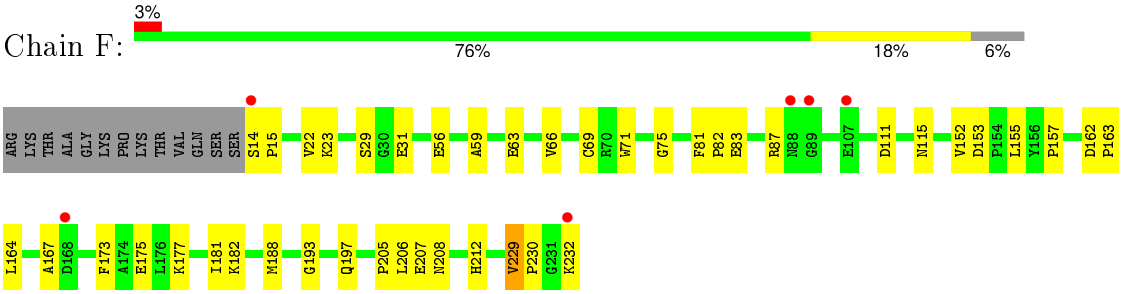
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain E:



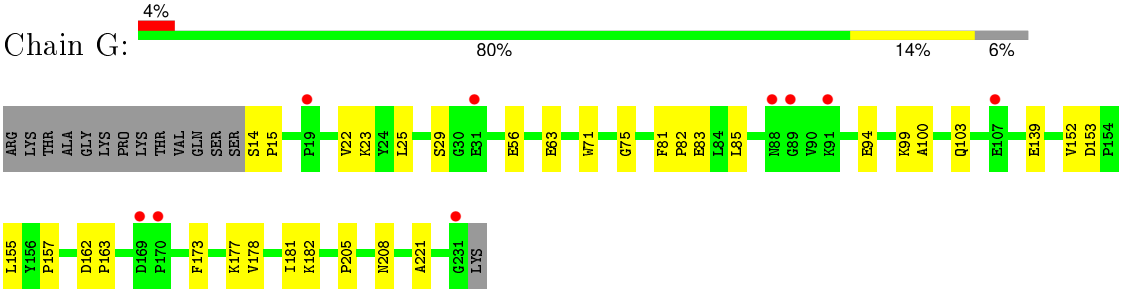
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain F:



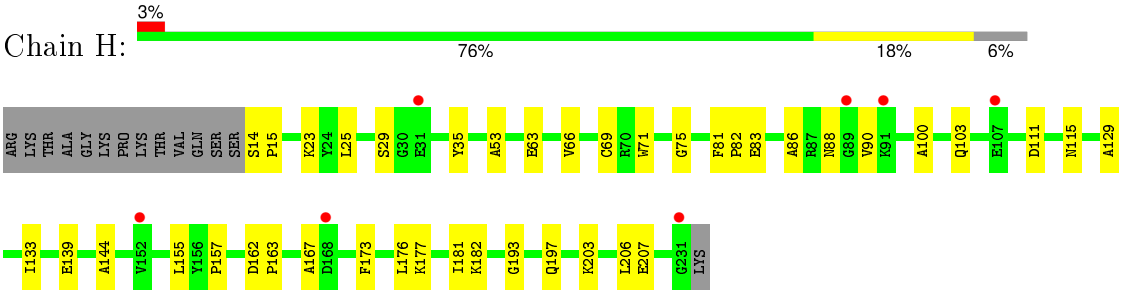
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain G:



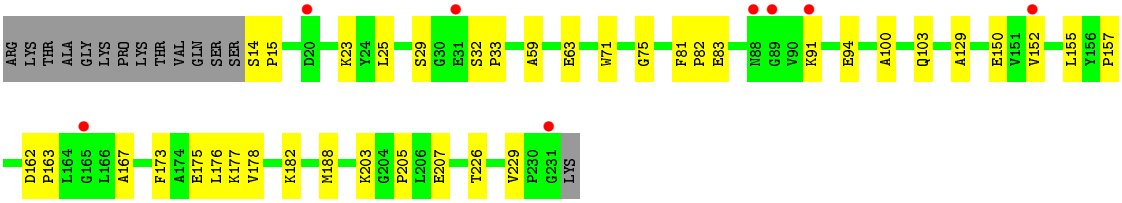
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain H:

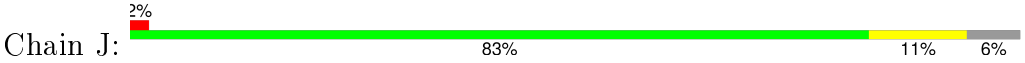


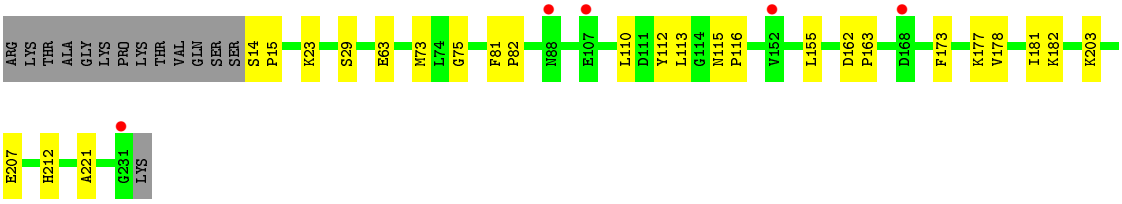
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain I:



- Molecule 1: Chlorophyll A-B binding protein, chloroplast





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	261.79Å 261.79Å 660.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.72 25.07 – 2.71	Depositor EDS
% Data completeness (in resolution range)	83.0 (10.00-2.72) 82.8 (25.07-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.04 (at 2.72Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.221 0.184 , 0.208	Depositor DCC
R_{free} test set	9326 reflections (5.21%)	DCC
Wilson B-factor (Å^2)	31.5	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 66.6	EDS
Estimated twinning fraction	0.003 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.008 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.005 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	3 of 211079 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29039	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LUT, DGD, XAT, CHL, CLA, NEX, NA, BNG

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	0.35	0/1713	0.55	0/2333
1	B	0.37	0/1713	0.58	0/2333
1	C	0.37	0/1713	0.58	0/2333
1	D	0.37	0/1713	0.58	0/2333
1	E	0.36	0/1713	0.57	0/2333
1	F	0.37	0/1722	0.58	0/2344
1	G	0.37	0/1713	0.58	0/2333
1	H	0.36	0/1713	0.56	0/2333
1	I	0.36	0/1713	0.57	0/2333
1	J	0.36	0/1713	0.56	0/2333
All	All	0.36	0/17139	0.57	0/23341

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1661	0	1592	27	0
1	B	1661	0	1592	35	0
1	C	1661	0	1592	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1661	0	1592	21	0
1	E	1661	0	1592	26	0
1	F	1670	0	1605	30	0
1	G	1661	0	1592	27	0
1	H	1661	0	1592	32	0
1	I	1661	0	1592	28	0
1	J	1661	0	1592	17	0
2	A	21	0	30	0	0
2	B	21	0	30	0	0
2	C	21	0	30	0	0
2	D	21	0	30	1	0
2	E	21	0	30	0	0
2	F	21	0	30	0	0
2	G	21	0	30	0	0
2	H	21	0	30	0	0
2	I	21	0	30	0	0
2	J	21	0	30	0	0
3	A	1	0	0	0	0
4	A	84	0	112	3	0
4	B	84	0	112	4	0
4	C	84	0	112	2	0
4	D	84	0	112	1	0
4	E	84	0	112	3	0
4	F	84	0	112	2	0
4	G	84	0	112	1	0
4	H	84	0	112	2	0
4	I	84	0	112	3	0
4	J	84	0	112	1	0
5	A	44	0	56	0	0
5	B	88	0	112	1	0
5	C	44	0	56	0	0
5	D	44	0	56	0	0
5	E	44	0	56	2	0
5	F	44	0	56	1	0
5	H	44	0	56	1	0
5	I	44	0	56	1	0
5	J	44	0	56	1	0
6	A	44	0	56	0	0
6	B	44	0	56	0	0
6	C	44	0	56	0	0
6	D	44	0	56	0	0
6	E	44	0	56	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	44	0	56	0	0
6	G	44	0	56	1	0
6	H	44	0	56	0	0
6	I	44	0	56	0	0
6	J	44	0	56	0	0
7	A	49	0	74	2	0
7	B	49	0	74	3	0
7	C	49	0	74	1	0
7	D	49	0	74	1	0
7	E	49	0	74	1	0
7	F	49	0	74	3	0
7	G	49	0	74	2	0
7	H	49	0	74	2	0
7	I	49	0	74	3	0
7	J	49	0	74	0	0
8	A	66	0	96	1	0
8	B	132	0	192	0	0
8	D	132	0	192	1	0
8	E	66	0	96	0	0
8	G	66	0	96	0	0
8	H	132	0	192	1	0
8	I	66	0	96	1	0
9	A	363	0	349	4	0
9	B	363	0	349	8	0
9	C	363	0	350	5	0
9	D	363	0	349	2	0
9	E	363	0	350	3	0
9	F	363	0	350	5	0
9	G	363	0	349	9	0
9	H	363	0	350	5	0
9	I	363	0	350	5	0
9	J	363	0	350	2	0
10	A	501	0	534	12	0
10	B	501	0	532	13	0
10	C	501	0	533	14	0
10	D	501	0	532	9	0
10	E	501	0	534	10	0
10	F	501	0	534	10	0
10	G	501	0	532	12	0
10	H	501	0	534	13	0
10	I	501	0	532	10	0
10	J	501	0	533	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	60	0	0	1	0
11	B	78	0	0	1	0
11	C	69	0	0	0	0
11	D	77	0	0	2	0
11	E	67	0	0	0	0
11	F	73	0	0	0	0
11	G	71	0	0	1	0
11	H	70	0	0	0	0
11	I	68	0	0	1	0
11	J	66	0	0	0	0
All	All	29039	0	28999	388	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 7.

All (388) 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)
1:I:14:SER:HB2	1:I:15:PRO:HD2	1.56	0.85
1:F:152:VAL:HG23	1:F:153:ASP:H	1.44	0.82
1:B:14:SER:HB2	1:B:15:PRO:HD2	1.65	0.79
1:H:14:SER:HB2	1:H:15:PRO:HD2	1.64	0.78
1:E:60:LYS:HA	1:E:60:LYS:HE2	1.66	0.77
1:B:99:LYS:HE2	1:F:232:LYS:HE3	1.68	0.76
6:G:6623:NEX:H403	9:G:606:CHL:HBA1	1.67	0.75
4:A:621:LUT:H32	10:A:602:CLA:HBB1	1.68	0.74
1:D:83:GLU:O	1:D:87:ARG:HG3	1.87	0.73
1:I:173:PHE:CZ	1:I:177:LYS:HE3	2.24	0.73
1:C:14:SER:HB2	1:C:15:PRO:HD2	1.70	0.72
1:G:81:PHE:HB3	1:G:82:PRO:HD3	1.72	0.71
1:A:167:ALA:HB1	1:A:173:PHE:CD1	2.26	0.71
10:G:604:CLA:HMB1	10:G:604:CLA:HBB1	1.72	0.71
1:B:83:GLU:O	1:B:87:ARG:HG2	1.92	0.70
10:C:604:CLA:HBB1	10:C:604:CLA:HMB1	1.74	0.70
1:F:81:PHE:HB3	1:F:82:PRO:HD3	1.74	0.69
10:E:602:CLA:H92	10:H:603:CLA:H52	1.75	0.69
1:I:81:PHE:HB3	1:I:82:PRO:HD3	1.75	0.69
1:G:14:SER:HB2	1:G:15:PRO:HD2	1.77	0.67
1:E:14:SER:HB2	1:E:15:PRO:HD2	1.77	0.67
10:B:602:CLA:H93	10:B:603:CLA:HMA1	1.76	0.67
4:B:1620:LUT:H32	10:B:610:CLA:HBB1	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:604:CLA:HBB1	10:J:604:CLA:HMB1	1.76	0.66
1:J:162:ASP:N	1:J:163:PRO:HD3	2.11	0.66
1:B:60:LYS:HA	1:B:60:LYS:HE3	1.78	0.65
10:H:613:CLA:HMB1	10:H:613:CLA:HBB1	1.79	0.65
1:G:173:PHE:CZ	1:G:177:LYS:HE3	2.31	0.65
10:D:604:CLA:HBB1	10:D:604:CLA:HMB1	1.79	0.65
1:C:83:GLU:HG2	1:C:206:LEU:HD12	1.79	0.65
10:C:603:CLA:H52	10:H:602:CLA:H92	1.80	0.64
10:B:604:CLA:HMB1	10:B:604:CLA:HBB1	1.80	0.64
7:B:1630:LHG:H152	9:B:601:CHL:H41	1.80	0.64
1:G:162:ASP:N	1:G:163:PRO:HD3	2.13	0.63
10:C:613:CLA:HBB1	10:C:613:CLA:HMB1	1.79	0.63
10:F:604:CLA:HBB1	10:F:604:CLA:HMB1	1.81	0.63
1:I:14:SER:HB2	1:I:15:PRO:CD	2.29	0.63
10:F:613:CLA:HBB1	10:F:613:CLA:HMB1	1.79	0.63
10:I:602:CLA:H93	10:I:603:CLA:HMA1	1.80	0.63
1:F:162:ASP:N	1:F:163:PRO:HD3	2.14	0.63
1:J:81:PHE:HB3	1:J:82:PRO:HD3	1.79	0.63
10:B:603:CLA:H52	10:F:602:CLA:H92	1.81	0.62
1:A:162:ASP:N	1:A:163:PRO:HD3	2.14	0.62
10:G:613:CLA:HMB1	10:G:613:CLA:HBB1	1.82	0.62
1:A:81:PHE:HB3	1:A:82:PRO:HD3	1.82	0.62
1:E:81:PHE:HB3	1:E:82:PRO:HD3	1.80	0.62
1:B:81:PHE:HB3	1:B:82:PRO:HD3	1.81	0.62
1:D:14:SER:HB2	1:D:15:PRO:HD2	1.81	0.61
10:I:604:CLA:HBB1	10:I:604:CLA:HMB1	1.82	0.61
1:A:25:LEU:HB2	1:A:29:SER:HA	1.82	0.61
1:C:162:ASP:N	1:C:163:PRO:HD3	2.15	0.61
1:H:25:LEU:HB2	1:H:29:SER:HA	1.83	0.60
1:F:63:GLU:HA	1:F:155:LEU:HD11	1.83	0.60
10:I:613:CLA:HMB1	10:I:613:CLA:HBB1	1.82	0.60
9:B:606:CHL:HBA2	9:B:606:CHL:HBD	1.83	0.60
1:B:205:PRO:HG3	11:B:5623:HOH:O	2.00	0.60
1:F:59:ALA:O	1:F:63:GLU:HG3	2.02	0.60
1:A:100:ALA:O	1:A:103:GLN:HG3	2.02	0.60
1:A:173:PHE:CZ	1:A:177:LYS:HE3	2.37	0.59
1:B:63:GLU:HA	1:B:155:LEU:HD11	1.83	0.59
1:C:23:LYS:HB2	1:C:29:SER:OG	2.02	0.59
10:C:602:CLA:H92	10:E:603:CLA:H52	1.85	0.59
1:E:162:ASP:N	1:E:163:PRO:HD3	2.17	0.59
1:C:81:PHE:HB3	1:C:82:PRO:HD3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:GLU:OE1	1:D:205:PRO:HD2	2.01	0.59
10:G:602:CLA:H93	10:G:603:CLA:HMA1	1.85	0.59
1:J:182:LYS:HE2	10:J:611:CLA:O1D	2.01	0.59
10:A:602:CLA:H93	10:A:603:CLA:HMA1	1.85	0.59
1:J:14:SER:HB2	1:J:15:PRO:HD2	1.85	0.59
10:A:604:CLA:HBB1	10:A:604:CLA:HMB1	1.85	0.59
1:B:193:GLY:O	1:B:197:GLN:HG3	2.03	0.58
1:H:81:PHE:HB3	1:H:82:PRO:HD3	1.84	0.58
1:F:173:PHE:CZ	1:F:177:LYS:HE3	2.39	0.58
1:E:173:PHE:CZ	1:E:177:LYS:HE3	2.39	0.58
1:I:63:GLU:HA	1:I:155:LEU:HD11	1.86	0.58
1:I:203:LYS:HD3	1:I:207:GLU:OE2	2.04	0.58
1:H:162:ASP:N	1:H:163:PRO:HD3	2.18	0.57
1:F:75:GLY:HA2	4:F:5621:LUT:H181	1.86	0.57
10:E:604:CLA:HMB1	10:E:604:CLA:HBB1	1.86	0.57
1:D:25:LEU:HB2	1:D:29:SER:HA	1.84	0.57
1:F:182:LYS:HE2	10:F:611:CLA:O1D	2.05	0.57
1:E:173:PHE:CE1	1:E:177:LYS:HE3	2.40	0.57
1:I:162:ASP:N	1:I:163:PRO:HD3	2.19	0.57
1:A:83:GLU:HG2	1:A:206:LEU:HD12	1.87	0.57
1:D:23:LYS:HB2	1:D:29:SER:OG	2.05	0.57
10:I:611:CLA:HBA2	10:I:612:CLA:OBD	2.05	0.57
1:A:63:GLU:HA	1:A:155:LEU:HD11	1.86	0.56
1:G:100:ALA:O	1:G:103:GLN:HG3	2.05	0.56
1:E:63:GLU:HA	1:E:155:LEU:HD21	1.85	0.56
1:H:14:SER:HB2	1:H:15:PRO:CD	2.36	0.56
7:C:2630:LHG:H212	10:E:603:CLA:H191	1.88	0.56
10:D:613:CLA:HBB1	10:D:613:CLA:HMB1	1.87	0.56
10:C:611:CLA:HBA1	10:C:612:CLA:OBD	2.05	0.56
1:H:173:PHE:CZ	1:H:177:LYS:HE3	2.40	0.55
1:F:83:GLU:HG2	1:F:206:LEU:HD12	1.89	0.55
1:H:75:GLY:HA2	4:H:7621:LUT:H181	1.88	0.55
7:G:6630:LHG:H262	7:G:6630:LHG:HC62	1.89	0.55
1:D:173:PHE:CZ	1:D:177:LYS:HE3	2.42	0.55
1:H:203:LYS:HD3	1:H:207:GLU:OE2	2.06	0.55
1:D:75:GLY:HA2	4:D:3621:LUT:H181	1.88	0.55
1:J:63:GLU:HA	1:J:155:LEU:HD11	1.87	0.55
1:I:23:LYS:HB2	1:I:29:SER:OG	2.07	0.55
1:F:66:VAL:O	1:F:69:CYS:HB2	2.07	0.54
1:E:100:ALA:O	1:E:103:GLN:HG3	2.06	0.54
1:A:94:GLU:HG2	1:A:99:LYS:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:602:CLA:H93	10:D:603:CLA:HMA1	1.90	0.54
1:I:59:ALA:O	1:I:63:GLU:HG3	2.08	0.54
1:D:205:PRO:HG3	11:D:8623:HOH:O	2.07	0.54
1:B:182:LYS:HE2	10:B:611:CLA:O1D	2.09	0.53
10:E:611:CLA:HBA1	10:E:612:CLA:OBD	2.09	0.53
1:C:75:GLY:HA2	4:C:2621:LUT:H181	1.91	0.53
1:C:71:TRP:CD1	9:C:609:CHL:HMD3	2.43	0.53
1:D:205:PRO:O	1:D:208:ASN:HB2	2.08	0.53
1:I:100:ALA:O	1:I:103:GLN:HG3	2.08	0.53
1:A:182:LYS:HE2	10:A:611:CLA:O1D	2.08	0.53
10:F:602:CLA:H93	10:F:603:CLA:HMA1	1.91	0.53
1:J:75:GLY:HA2	4:J:9621:LUT:H181	1.91	0.53
10:E:602:CLA:H93	10:E:603:CLA:HMA1	1.90	0.52
1:H:167:ALA:HB1	1:H:173:PHE:CD1	2.44	0.52
1:I:25:LEU:HB2	1:I:29:SER:HA	1.91	0.52
1:C:147:PRO:HB2	9:C:608:CHL:HBB2	1.91	0.52
1:D:81:PHE:HB3	1:D:82:PRO:HD3	1.90	0.52
10:G:611:CLA:HBA1	10:G:612:CLA:OBD	2.09	0.52
10:H:602:CLA:H93	10:H:603:CLA:HMA1	1.92	0.52
1:B:162:ASP:N	1:B:163:PRO:CD	2.72	0.52
1:E:75:GLY:HA2	4:E:4621:LUT:H181	1.91	0.52
1:E:83:GLU:OE1	1:E:205:PRO:HD2	2.09	0.52
1:J:23:LYS:HB2	1:J:29:SER:OG	2.10	0.52
1:G:25:LEU:HB2	1:G:29:SER:HA	1.92	0.52
1:B:14:SER:HB2	1:B:15:PRO:CD	2.38	0.51
1:D:71:TRP:CD1	9:D:609:CHL:HMD3	2.45	0.51
1:F:193:GLY:O	1:F:197:GLN:HG3	2.09	0.51
1:F:205:PRO:O	1:F:208:ASN:HB2	2.10	0.51
1:B:100:ALA:O	1:B:103:GLN:HG3	2.10	0.51
1:C:193:GLY:O	1:C:197:GLN:HG3	2.10	0.51
10:D:611:CLA:HBA1	10:D:612:CLA:OBD	2.10	0.51
9:I:601:CHL:HBB1	9:I:601:CHL:HHC	1.92	0.51
1:E:28:PHE:O	1:H:144:ALA:HB2	2.11	0.51
1:I:167:ALA:HB1	1:I:173:PHE:CD1	2.47	0.50
1:A:64:LEU:HD13	10:A:603:CLA:HBA2	1.92	0.50
7:I:8630:LHG:H152	9:I:601:CHL:H41	1.93	0.50
1:B:75:GLY:HA2	4:B:1621:LUT:H181	1.92	0.50
8:D:5632:DGD:HD2	11:D:8628:HOH:O	2.11	0.50
1:B:54:ASP:OD1	1:B:56:GLU:N	2.44	0.50
1:C:182:LYS:HE2	10:C:611:CLA:O1D	2.12	0.50
10:A:603:CLA:HHC	10:A:603:CLA:HBB1	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:613:CLA:HBB1	10:B:613:CLA:HMB1	1.94	0.50
10:A:611:CLA:HBA1	10:A:612:CLA:OBD	2.12	0.49
1:C:14:SER:HB2	1:C:15:PRO:CD	2.42	0.49
7:I:8630:LHG:H262	7:I:8630:LHG:HC62	1.93	0.49
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.95	0.49
10:D:602:CLA:H92	10:J:603:CLA:H52	1.95	0.49
7:A:630:LHG:HC62	7:A:630:LHG:H262	1.94	0.49
1:C:205:PRO:O	1:C:208:ASN:HB2	2.13	0.49
1:F:71:TRP:CD1	9:F:609:CHL:HMD3	2.47	0.49
1:G:83:GLU:OE1	1:G:205:PRO:HD2	2.13	0.49
1:D:178:VAL:O	1:D:181:ILE:HG22	2.12	0.49
10:H:611:CLA:HBA1	10:H:612:CLA:OBD	2.13	0.49
1:B:25:LEU:HB2	1:B:29:SER:HA	1.95	0.48
10:B:603:CLA:HBB1	10:B:603:CLA:HHC	1.94	0.48
1:I:182:LYS:HE2	10:I:611:CLA:O1D	2.13	0.48
1:E:193:GLY:O	1:E:197:GLN:HG3	2.13	0.48
1:E:205:PRO:O	1:E:208:ASN:HB2	2.13	0.48
1:J:203:LYS:HD3	1:J:207:GLU:OE2	2.13	0.48
1:H:176:LEU:HD13	10:H:610:CLA:O1A	2.13	0.48
10:C:602:CLA:H93	10:C:603:CLA:HMA1	1.93	0.48
1:A:176:LEU:HD13	10:A:610:CLA:O1A	2.12	0.48
4:E:4620:LUT:H32	10:E:610:CLA:HBB1	1.95	0.48
1:C:147:PRO:HB2	9:C:608:CHL:CBB	2.44	0.48
1:G:71:TRP:CD1	9:G:609:CHL:HMD3	2.49	0.48
1:G:75:GLY:HA2	4:G:6621:LUT:H181	1.95	0.48
1:H:23:LYS:HB2	1:H:29:SER:OG	2.14	0.48
1:H:182:LYS:HE2	10:H:611:CLA:O1D	2.14	0.48
7:A:630:LHG:H152	9:A:601:CHL:H41	1.95	0.48
1:B:23:LYS:HB2	1:B:29:SER:OG	2.14	0.48
1:H:129:ALA:O	1:H:133:ILE:HG12	2.13	0.47
10:J:602:CLA:H93	10:J:603:CLA:HMA1	1.96	0.47
10:H:603:CLA:HHC	10:H:603:CLA:HBB1	1.96	0.47
10:H:612:CLA:HHC	10:H:612:CLA:HBB1	1.94	0.47
1:A:129:ALA:HB1	8:I:8632:DGD:HAE2	1.95	0.47
10:B:603:CLA:H201	7:F:5630:LHG:H212	1.96	0.47
10:I:603:CLA:HHC	10:I:603:CLA:HBB1	1.96	0.47
1:E:83:GLU:HG2	1:E:206:LEU:HD12	1.95	0.47
1:A:203:LYS:HD3	1:A:207:GLU:OE2	2.14	0.47
1:F:23:LYS:HB2	1:F:29:SER:OG	2.15	0.47
10:I:603:CLA:H52	10:J:602:CLA:H92	1.97	0.47
10:F:603:CLA:H52	10:G:602:CLA:H92	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:601:CHL:HBB1	9:A:601:CHL:HHC	1.96	0.47
1:D:162:ASP:N	1:D:163:PRO:CD	2.77	0.47
1:H:63:GLU:HA	1:H:155:LEU:HD21	1.95	0.47
10:H:611:CLA:HBB1	10:H:611:CLA:HHC	1.95	0.47
1:H:193:GLY:O	1:H:197:GLN:HG3	2.15	0.47
1:D:100:ALA:O	1:D:103:GLN:HG3	2.14	0.47
8:A:632:DGD:HAE2	1:I:129:ALA:HB1	1.95	0.46
1:F:229:VAL:HA	1:F:230:PRO:HD3	1.85	0.46
1:E:221:ALA:CB	5:H:4622:XAT:H193	2.45	0.46
1:J:178:VAL:O	1:J:182:LYS:HG3	2.15	0.46
1:B:164:LEU:HD12	4:B:1620:LUT:H222	1.97	0.46
10:A:611:CLA:HBB1	10:A:611:CLA:HHC	1.96	0.46
1:E:25:LEU:HB2	1:E:29:SER:HA	1.97	0.46
1:I:173:PHE:CE1	1:I:177:LYS:HE3	2.49	0.46
7:F:5630:LHG:H152	9:F:601:CHL:H41	1.98	0.46
10:G:611:CLA:HBB1	10:G:611:CLA:HHC	1.96	0.46
1:F:14:SER:HB2	1:F:15:PRO:CD	2.45	0.46
1:A:162:ASP:N	1:A:163:PRO:CD	2.79	0.46
1:C:221:ALA:CB	5:E:2622:XAT:H193	2.46	0.46
9:I:606:CHL:HBA1	9:I:606:CHL:HBD	1.98	0.46
1:C:14:SER:CB	1:C:15:PRO:HD2	2.43	0.46
1:D:63:GLU:HA	1:D:155:LEU:HD11	1.97	0.46
1:B:229:VAL:HG21	9:G:607:CHL:HED1	1.98	0.45
1:A:59:ALA:O	1:A:63:GLU:HG3	2.16	0.45
1:E:71:TRP:CD1	9:E:609:CHL:HMD3	2.52	0.45
1:H:203:LYS:HD3	1:H:207:GLU:CD	2.36	0.45
1:A:157:PRO:HD2	10:A:610:CLA:OBD	2.16	0.45
10:B:611:CLA:HBA1	10:B:612:CLA:OBD	2.17	0.45
1:F:162:ASP:N	1:F:163:PRO:CD	2.80	0.45
9:D:601:CHL:HBB1	9:D:601:CHL:HHC	1.98	0.45
1:J:173:PHE:CZ	1:J:177:LYS:HE3	2.52	0.45
1:B:178:VAL:O	1:B:181:ILE:HG22	2.17	0.45
1:B:157:PRO:CG	9:B:608:CHL:HMD2	2.47	0.45
1:C:100:ALA:O	1:C:103:GLN:HG3	2.17	0.45
1:J:162:ASP:N	1:J:163:PRO:CD	2.79	0.45
1:I:75:GLY:HA2	4:I:8621:LUT:H181	1.98	0.45
1:E:110:LEU:HD23	1:E:110:LEU:C	2.38	0.45
1:C:63:GLU:HA	1:C:155:LEU:HD21	1.99	0.45
9:A:605:CHL:HHC	9:A:605:CHL:HBB1	1.99	0.45
9:H:605:CHL:HBB1	9:H:605:CHL:HHC	1.98	0.45
10:E:603:CLA:HHC	10:E:603:CLA:HBB1	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:4630:LHG:H212	10:H:603:CLA:H191	1.99	0.44
7:B:1630:LHG:H262	7:B:1630:LHG:HC62	1.99	0.44
1:A:163:PRO:HD2	4:A:620:LUT:H23	1.99	0.44
1:E:163:PRO:HD2	4:E:4620:LUT:H23	1.97	0.44
1:B:46:TRP:CE3	4:B:1621:LUT:H383	2.52	0.44
1:D:167:ALA:HB1	1:D:173:PHE:CD1	2.53	0.44
1:C:46:TRP:CE3	4:C:2621:LUT:H383	2.51	0.44
1:D:131:GLN:O	1:D:135:MET:HB2	2.17	0.44
1:J:212:HIS:CG	10:J:613:CLA:HAA2	2.52	0.44
1:B:84:LEU:O	1:B:88:ASN:ND2	2.49	0.44
1:G:162:ASP:N	1:G:163:PRO:CD	2.79	0.44
1:I:157:PRO:HD2	10:I:610:CLA:OBD	2.17	0.44
1:I:176:LEU:HD13	10:I:610:CLA:O1A	2.17	0.44
9:B:601:CHL:HHC	9:B:601:CHL:HBB1	1.99	0.44
9:H:601:CHL:HBB1	9:H:601:CHL:HHC	1.98	0.44
1:F:66:VAL:HG22	1:F:181:ILE:HD11	1.99	0.44
2:D:3633:BNG:H1'1	10:D:611:CLA:O1A	2.17	0.44
1:I:94:GLU:HG3	11:I:9626:HOH:O	2.17	0.44
1:D:74:LEU:HB3	10:D:604:CLA:HAB	2.00	0.44
1:A:94:GLU:HG3	11:A:638:HOH:O	2.18	0.44
1:H:157:PRO:HD2	10:H:610:CLA:OBD	2.17	0.44
1:F:22:VAL:HB	9:F:601:CHL:CBC	2.48	0.44
1:B:182:LYS:NZ	7:B:1630:LHG:O5	2.51	0.44
1:B:167:ALA:HB1	1:B:173:PHE:CD1	2.52	0.44
1:B:26:GLY:HA3	1:B:27:PRO:HD3	1.86	0.44
1:H:173:PHE:CE2	1:H:177:LYS:HE3	2.53	0.44
1:G:182:LYS:HE2	10:G:611:CLA:O1D	2.18	0.44
9:I:605:CHL:HBB1	9:I:605:CHL:HHC	1.99	0.44
1:F:152:VAL:HG23	1:F:153:ASP:N	2.22	0.43
7:H:7630:LHG:HC62	7:H:7630:LHG:H262	1.99	0.43
10:B:612:CLA:HHC	10:B:612:CLA:HBB1	1.99	0.43
10:J:603:CLA:HHC	10:J:603:CLA:HBB1	2.00	0.43
1:I:32:SER:HB2	1:I:33:PRO:CD	2.48	0.43
10:J:614:CLA:HHC	10:J:614:CLA:HBB1	1.99	0.43
1:H:139:GLU:HA	1:H:139:GLU:OE2	2.18	0.43
10:B:611:CLA:HBB1	10:B:611:CLA:HHC	1.99	0.43
10:J:611:CLA:HBA1	10:J:612:CLA:OBD	2.18	0.43
1:I:163:PRO:HD2	4:I:8620:LUT:H23	1.99	0.43
1:C:221:ALA:HB1	5:E:2622:XAT:H193	2.01	0.43
1:I:226:THR:O	1:I:229:VAL:HG23	2.18	0.43
1:B:160:SER:O	1:B:163:PRO:HD3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:8630:LHG:H282	7:I:8630:LHG:HC92	2.00	0.43
1:H:139:GLU:HG3	9:H:609:CHL:C4B	2.49	0.43
1:J:110:LEU:C	1:J:110:LEU:HD23	2.39	0.43
7:F:5630:LHG:H262	7:F:5630:LHG:HC62	2.00	0.43
10:F:603:CLA:HHC	10:F:603:CLA:HBB1	2.00	0.43
10:C:603:CLA:H192	7:H:7630:LHG:H212	1.99	0.43
10:J:611:CLA:HHC	10:J:611:CLA:HBB1	2.01	0.43
10:J:612:CLA:HBB1	10:J:612:CLA:HHC	2.00	0.43
1:C:173:PHE:CZ	1:C:177:LYS:HE3	2.53	0.43
10:E:612:CLA:HBB1	10:E:612:CLA:HHC	2.00	0.43
1:G:23:LYS:HE2	11:G:9702:HOH:O	2.18	0.43
1:G:205:PRO:O	1:G:208:ASN:HB2	2.19	0.43
1:E:131:GLN:O	1:E:135:MET:HB2	2.18	0.43
1:C:66:VAL:O	1:C:69:CYS:HB2	2.18	0.43
1:F:229:VAL:CG2	1:F:232:LYS:HD2	2.48	0.43
5:I:9622:XAT:H193	1:J:221:ALA:CB	2.49	0.43
1:G:63:GLU:HA	1:G:155:LEU:HD11	2.01	0.43
10:C:603:CLA:HHC	10:C:603:CLA:HBB1	2.00	0.43
10:G:612:CLA:HHC	10:G:612:CLA:HBB1	2.01	0.43
1:G:23:LYS:HB2	1:G:29:SER:OG	2.19	0.43
9:C:601:CHL:HHC	9:C:601:CHL:HBB1	2.00	0.43
1:H:100:ALA:O	1:H:103:GLN:HG3	2.19	0.43
10:A:602:CLA:HMB1	10:A:602:CLA:HAB	1.85	0.42
1:H:71:TRP:CD1	9:H:609:CHL:HMD3	2.54	0.42
9:B:605:CHL:HHC	9:B:605:CHL:HBB1	2.00	0.42
1:F:164:LEU:HD12	4:F:5620:LUT:H222	2.01	0.42
4:H:7621:LUT:H382	10:H:602:CLA:HBA1	2.01	0.42
1:I:188:MET:HB2	10:I:602:CLA:HMC3	2.02	0.42
1:C:162:ASP:N	1:C:163:PRO:CD	2.81	0.42
1:D:173:PHE:CE1	1:D:177:LYS:HE3	2.55	0.42
9:B:605:CHL:HAB	9:B:605:CHL:HMB1	1.87	0.42
1:H:86:ALA:C	1:H:88:ASN:H	2.22	0.42
1:C:139:GLU:HG3	9:C:609:CHL:NB	2.35	0.42
1:J:112:TYR:O	1:J:113:LEU:HB2	2.19	0.42
1:G:63:GLU:HA	1:G:155:LEU:HD21	2.01	0.42
1:F:87:ARG:NH2	1:F:207:GLU:HA	2.34	0.42
1:G:22:VAL:HB	9:G:601:CHL:HBC1	2.01	0.42
1:H:157:PRO:CG	9:H:608:CHL:HMD2	2.50	0.42
9:F:601:CHL:HBB1	9:F:601:CHL:HHC	2.01	0.42
10:C:611:CLA:HBB1	10:C:611:CLA:HHC	2.00	0.42
1:I:71:TRP:CD1	9:I:609:CHL:HMD3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:MET:SD	10:J:610:CLA:HBB1	2.60	0.42
1:G:173:PHE:CE1	1:G:177:LYS:HE3	2.55	0.42
7:D:3630:LHG:HC62	7:D:3630:LHG:H262	2.01	0.42
9:J:605:CHL:HHC	9:J:605:CHL:HBB1	2.01	0.42
1:C:129:ALA:HB1	8:H:6632:DGD:HAE2	2.01	0.42
1:G:157:PRO:CG	9:G:608:CHL:HMD2	2.50	0.42
10:A:612:CLA:HHC	10:A:612:CLA:HBB1	2.01	0.42
1:I:178:VAL:O	1:I:182:LYS:HG3	2.20	0.42
1:A:23:LYS:HB2	1:A:29:SER:OG	2.20	0.41
1:G:178:VAL:O	1:G:182:LYS:HG3	2.19	0.41
1:I:83:GLU:OE1	1:I:205:PRO:HD2	2.20	0.41
1:F:155:LEU:C	1:F:157:PRO:HD3	2.40	0.41
1:G:22:VAL:HB	9:G:601:CHL:CBC	2.50	0.41
1:H:83:GLU:HG2	1:H:206:LEU:HD12	2.03	0.41
1:H:111:ASP:HB3	1:H:115:ASN:O	2.20	0.41
9:E:605:CHL:HBB1	9:E:605:CHL:HHC	2.02	0.41
1:G:94:GLU:HG2	1:G:99:LYS:HB3	2.02	0.41
1:D:66:VAL:O	1:D:69:CYS:HB2	2.20	0.41
1:H:162:ASP:N	1:H:163:PRO:CD	2.82	0.41
7:G:6630:LHG:H152	9:G:601:CHL:H41	2.01	0.41
1:H:66:VAL:O	1:H:69:CYS:HB2	2.20	0.41
1:B:66:VAL:O	1:B:69:CYS:HB2	2.20	0.41
1:A:61:ASN:HA	1:A:64:LEU:HD12	2.01	0.41
1:E:81:PHE:CE2	1:E:85:LEU:HD11	2.55	0.41
1:C:173:PHE:CE1	1:C:177:LYS:HE3	2.56	0.41
1:B:221:ALA:CB	5:B:1622:XAT:H193	2.50	0.41
10:E:613:CLA:H8	10:E:614:CLA:HMD1	2.01	0.41
1:C:14:SER:CB	1:C:15:PRO:CD	2.98	0.41
1:F:188:MET:HB2	10:F:602:CLA:HMC3	2.02	0.41
1:E:115:ASN:HA	1:E:116:PRO:HD3	1.92	0.41
1:B:110:LEU:HD23	1:B:110:LEU:C	2.41	0.41
10:B:602:CLA:H92	10:G:603:CLA:H52	2.02	0.41
1:B:166:LEU:HD12	10:B:610:CLA:CGA	2.51	0.41
1:A:194:PHE:HE2	4:A:620:LUT:H41	1.85	0.41
1:H:86:ALA:HA	1:H:90:VAL:O	2.20	0.41
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.94	0.41
1:H:35:TYR:CE2	1:H:53:ALA:HA	2.56	0.41
1:A:115:ASN:HA	1:A:116:PRO:HD3	1.89	0.41
10:G:603:CLA:HBB1	10:G:603:CLA:HHC	2.02	0.41
1:F:83:GLU:OE1	1:F:205:PRO:HD2	2.21	0.41
1:G:25:LEU:HD23	1:G:25:LEU:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:610:CLA:HAB	10:G:610:CLA:HMB1	1.90	0.41
1:E:162:ASP:N	1:E:163:PRO:CD	2.84	0.41
10:F:610:CLA:HMB1	10:F:610:CLA:HAB	1.90	0.41
9:A:608:CHL:HBB1	9:A:608:CHL:HHC	2.03	0.41
1:G:81:PHE:CE2	1:G:85:LEU:HD11	2.56	0.41
10:C:602:CLA:HAB	10:C:602:CLA:HMB1	1.90	0.41
1:B:178:VAL:O	1:B:182:LYS:HG3	2.21	0.41
1:B:155:LEU:C	1:B:157:PRO:HD3	2.42	0.41
1:G:139:GLU:HG3	9:G:609:CHL:NB	2.36	0.41
9:J:605:CHL:HMB1	9:J:605:CHL:HAB	1.90	0.41
1:A:32:SER:HB2	1:A:33:PRO:CD	2.51	0.41
1:D:221:ALA:CB	5:J:3622:XAT:H193	2.51	0.41
1:A:129:ALA:O	1:A:133:ILE:HG12	2.21	0.41
1:H:23:LYS:HB2	1:H:29:SER:CB	2.51	0.40
10:D:610:CLA:HAB	10:D:610:CLA:HMB1	1.91	0.40
1:F:212:HIS:CG	10:F:613:CLA:HAA2	2.56	0.40
1:I:163:PRO:HD2	4:I:8620:LUT:C23	2.51	0.40
1:E:59:ALA:O	1:E:63:GLU:HG3	2.22	0.40
10:D:612:CLA:HHC	10:D:612:CLA:HBB1	2.02	0.40
1:C:155:LEU:C	1:C:157:PRO:HD3	2.41	0.40
1:E:22:VAL:HB	9:E:601:CHL:CBC	2.51	0.40
1:J:115:ASN:HA	1:J:116:PRO:HD3	1.90	0.40
1:B:139:GLU:HG3	9:B:609:CHL:C4B	2.51	0.40
1:B:22:VAL:HB	9:B:601:CHL:CBC	2.52	0.40
10:C:612:CLA:HBB1	10:C:612:CLA:HHC	2.04	0.40
10:G:611:CLA:HMB1	10:G:611:CLA:HAB	1.93	0.40
1:B:226:THR:O	1:B:229:VAL:HG23	2.21	0.40
1:E:66:VAL:O	1:E:69:CYS:HB2	2.22	0.40
1:G:152:VAL:HB	1:G:153:ASP:H	1.69	0.40
9:G:608:CHL:HBA1	9:G:608:CHL:H151	2.01	0.40
1:F:111:ASP:HB3	1:F:115:ASN:O	2.22	0.40
1:I:150:GLU:HA	1:I:150:GLU:OE2	2.21	0.40
10:C:614:CLA:HHC	10:C:614:CLA:HBB1	2.04	0.40
1:F:167:ALA:HB1	1:F:173:PHE:CD1	2.56	0.40
9:F:608:CHL:HHC	9:F:608:CHL:HBB1	2.02	0.40
5:F:6622:XAT:H193	1:G:221:ALA:CB	2.52	0.40
1:C:73:MET:SD	10:C:610:CLA:HBB1	2.62	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	216/232 (93%)	207 (96%)	9 (4%)	0	100	100
1	B	216/232 (93%)	210 (97%)	6 (3%)	0	100	100
1	C	216/232 (93%)	209 (97%)	7 (3%)	0	100	100
1	D	216/232 (93%)	208 (96%)	8 (4%)	0	100	100
1	E	216/232 (93%)	208 (96%)	8 (4%)	0	100	100
1	F	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	G	216/232 (93%)	209 (97%)	7 (3%)	0	100	100
1	H	216/232 (93%)	206 (95%)	10 (5%)	0	100	100
1	I	216/232 (93%)	209 (97%)	7 (3%)	0	100	100
1	J	216/232 (93%)	207 (96%)	9 (4%)	0	100	100
All	All	2161/2320 (93%)	2084 (96%)	77 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	168/180 (93%)	167 (99%)	1 (1%)	90	97
1	B	168/180 (93%)	165 (98%)	3 (2%)	66	88
1	C	168/180 (93%)	166 (99%)	2 (1%)	78	93
1	D	168/180 (93%)	165 (98%)	3 (2%)	66	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	168/180 (93%)	165 (98%)	3 (2%)	66 88
1	F	169/180 (94%)	165 (98%)	4 (2%)	57 84
1	G	168/180 (93%)	166 (99%)	2 (1%)	78 93
1	H	168/180 (93%)	167 (99%)	1 (1%)	90 97
1	I	168/180 (93%)	165 (98%)	3 (2%)	66 88
1	J	168/180 (93%)	167 (99%)	1 (1%)	90 97
All	All	1681/1800 (93%)	1658 (99%)	23 (1%)	74 91

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	B	60	LYS
1	B	175	GLU
1	B	223	ASN
1	C	31	GLU
1	C	56	GLU
1	D	32	SER
1	D	91	LYS
1	D	175	GLU
1	E	175	GLU
1	E	181	ILE
1	E	223	ASN
1	F	31	GLU
1	F	56	GLU
1	F	175	GLU
1	F	229	VAL
1	G	56	GLU
1	G	181	ILE
1	H	181	ILE
1	I	91	LYS
1	I	152	VAL
1	I	175	GLU
1	J	181	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	223	ASN
1	B	223	ASN
1	D	223	ASN
1	E	88	ASN
1	E	223	ASN
1	F	88	ASN
1	G	223	ASN
1	H	88	ASN
1	H	223	ASN
1	I	88	ASN
1	I	223	ASN
1	J	223	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 211 ligands modelled in this entry, 1 is monoatomic - leaving 210 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	$\#\|Z\| > 2$
9	CHL	A	601	1	57,74,74	1.37	7 (12%)	56,114,114	1.81	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CLA	A	602	1	55,73,73	1.27	6 (10%)	61,113,113	2.07	20 (32%)
10	CLA	A	603	1	55,73,73	1.24	7 (12%)	61,113,113	1.99	14 (22%)
10	CLA	A	604	11	52,70,73	1.32	5 (9%)	56,109,113	2.19	12 (21%)
9	CHL	A	605	1	39,56,74	1.64	6 (15%)	37,92,114	1.79	10 (27%)
9	CHL	A	606	11	42,59,74	1.71	6 (14%)	39,96,114	2.23	13 (33%)
9	CHL	A	607	11	57,74,74	1.36	7 (12%)	56,114,114	1.95	14 (25%)
9	CHL	A	608	11	57,74,74	1.43	7 (12%)	56,114,114	1.87	14 (25%)
9	CHL	A	609	1	57,74,74	1.42	7 (12%)	56,114,114	1.65	11 (19%)
10	CLA	A	610	1	55,73,73	1.36	8 (14%)	61,113,113	1.71	14 (22%)
10	CLA	A	611	7	55,73,73	1.27	6 (10%)	61,113,113	1.90	18 (29%)
10	CLA	A	612	1	55,73,73	1.24	6 (10%)	61,113,113	1.77	15 (24%)
10	CLA	A	613	1	55,73,73	1.28	6 (10%)	61,113,113	1.72	12 (19%)
10	CLA	A	614	1	39,57,73	1.32	5 (12%)	43,93,113	2.42	10 (23%)
4	LUT	A	620	-	41,43,43	1.06	2 (4%)	51,60,60	1.96	9 (17%)
4	LUT	A	621	-	41,43,43	1.28	4 (9%)	51,60,60	1.95	12 (23%)
5	XAT	A	622	-	41,47,47	0.62	1 (2%)	48,74,74	1.20	3 (6%)
6	NEX	A	623	-	39,46,46	0.95	2 (5%)	48,70,70	1.02	4 (8%)
7	LHG	A	630	10	48,48,48	0.89	3 (6%)	49,54,54	1.43	5 (10%)
8	DGD	A	632	-	67,67,67	0.91	2 (2%)	81,81,81	0.98	7 (8%)
2	BNG	A	633	-	21,21,21	0.55	0	26,26,26	0.81	2 (7%)
4	LUT	B	1620	-	41,43,43	1.13	3 (7%)	51,60,60	1.78	8 (15%)
4	LUT	B	1621	-	41,43,43	1.15	4 (9%)	51,60,60	1.87	8 (15%)
5	XAT	B	1622	-	41,47,47	0.67	0	48,74,74	1.31	3 (6%)
6	NEX	B	1623	-	39,46,46	0.84	1 (2%)	48,70,70	0.98	5 (10%)
7	LHG	B	1630	10	48,48,48	0.99	3 (6%)	49,54,54	1.33	5 (10%)
8	DGD	B	1632	-	67,67,67	0.92	2 (2%)	81,81,81	1.05	7 (8%)
2	BNG	B	1633	-	21,21,21	0.48	0	26,26,26	0.82	2 (7%)
8	DGD	B	2632	-	67,67,67	0.88	1 (1%)	81,81,81	1.07	7 (8%)
5	XAT	B	5622	-	41,47,47	0.72	0	48,74,74	1.22	5 (10%)
9	CHL	B	601	1	57,74,74	1.31	6 (10%)	56,114,114	1.76	14 (25%)
10	CLA	B	602	1	55,73,73	1.29	9 (16%)	61,113,113	2.19	18 (29%)
10	CLA	B	603	1	55,73,73	1.26	7 (12%)	61,113,113	1.97	14 (22%)
10	CLA	B	604	11	52,70,73	1.29	4 (7%)	56,109,113	2.42	17 (30%)
9	CHL	B	605	1	39,56,74	1.55	7 (17%)	37,92,114	1.78	10 (27%)
9	CHL	B	606	11	42,59,74	1.68	7 (16%)	39,96,114	2.12	12 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CHL	B	607	11	57,74,74	1.43	7 (12%)	56,114,114	1.99	16 (28%)
9	CHL	B	608	11	57,74,74	1.39	7 (12%)	56,114,114	1.95	13 (23%)
9	CHL	B	609	1	57,74,74	1.48	9 (15%)	56,114,114	1.55	10 (17%)
10	CLA	B	610	1	55,73,73	1.32	7 (12%)	61,113,113	1.62	12 (19%)
10	CLA	B	611	7	55,73,73	1.22	6 (10%)	61,113,113	2.04	16 (26%)
10	CLA	B	612	1	55,73,73	1.32	8 (14%)	61,113,113	1.72	13 (21%)
10	CLA	B	613	1	55,73,73	1.29	7 (12%)	61,113,113	1.95	11 (18%)
10	CLA	B	614	1	39,57,73	1.33	5 (12%)	43,93,113	2.53	11 (25%)
4	LUT	C	2620	-	41,43,43	1.07	3 (7%)	51,60,60	1.75	8 (15%)
4	LUT	C	2621	-	41,43,43	1.41	5 (12%)	51,60,60	1.69	11 (21%)
6	NEX	C	2623	-	39,46,46	0.95	2 (5%)	48,70,70	0.94	3 (6%)
7	LHG	C	2630	10	48,48,48	0.91	3 (6%)	49,54,54	1.34	5 (10%)
2	BNG	C	2633	-	21,21,21	0.53	0	26,26,26	0.81	2 (7%)
9	CHL	C	601	1	57,74,74	1.38	7 (12%)	56,114,114	1.71	12 (21%)
10	CLA	C	602	1	55,73,73	1.27	6 (10%)	61,113,113	2.08	18 (29%)
10	CLA	C	603	1	55,73,73	1.18	5 (9%)	61,113,113	1.99	15 (24%)
10	CLA	C	604	11	52,70,73	1.30	5 (9%)	56,109,113	2.36	14 (25%)
9	CHL	C	605	1	39,56,74	1.60	7 (17%)	37,92,114	1.88	10 (27%)
9	CHL	C	606	11	42,59,74	1.74	6 (14%)	39,96,114	2.33	14 (35%)
9	CHL	C	607	11	57,74,74	1.41	8 (14%)	56,114,114	2.02	18 (32%)
9	CHL	C	608	11	57,74,74	1.42	9 (15%)	56,114,114	1.89	13 (23%)
9	CHL	C	609	1	57,74,74	1.40	7 (12%)	56,114,114	1.62	9 (16%)
10	CLA	C	610	1	55,73,73	1.42	9 (16%)	61,113,113	1.64	14 (22%)
10	CLA	C	611	7	55,73,73	1.21	6 (10%)	61,113,113	1.90	14 (22%)
10	CLA	C	612	1	55,73,73	1.20	6 (10%)	61,113,113	1.84	14 (22%)
10	CLA	C	613	1	55,73,73	1.20	6 (10%)	61,113,113	1.86	12 (19%)
10	CLA	C	614	1	39,57,73	1.31	6 (15%)	43,93,113	2.57	12 (27%)
5	XAT	C	7622	-	41,47,47	0.77	1 (2%)	48,74,74	1.37	7 (14%)
4	LUT	D	3620	-	41,43,43	1.03	3 (7%)	51,60,60	1.96	9 (17%)
4	LUT	D	3621	-	41,43,43	1.24	4 (9%)	51,60,60	1.78	13 (25%)
6	NEX	D	3623	-	39,46,46	0.92	2 (5%)	48,70,70	1.00	5 (10%)
7	LHG	D	3630	10	48,48,48	0.82	3 (6%)	49,54,54	1.26	5 (10%)
8	DGD	D	3632	-	67,67,67	0.93	2 (2%)	81,81,81	1.01	7 (8%)
2	BNG	D	3633	-	21,21,21	0.50	0	26,26,26	0.86	2 (7%)
8	DGD	D	5632	-	67,67,67	0.91	1 (1%)	81,81,81	1.10	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CHL	D	601	1	57,74,74	1.38	7 (12%)	56,114,114	1.82	13 (23%)
10	CLA	D	602	1	55,73,73	1.34	9 (16%)	61,113,113	2.04	19 (31%)
10	CLA	D	603	1	55,73,73	1.13	5 (9%)	61,113,113	1.77	15 (24%)
10	CLA	D	604	11	52,70,73	1.30	5 (9%)	56,109,113	2.49	17 (30%)
9	CHL	D	605	1	39,56,74	1.63	7 (17%)	37,92,114	1.84	8 (21%)
9	CHL	D	606	11	42,59,74	1.73	9 (21%)	39,96,114	2.39	14 (35%)
9	CHL	D	607	11	57,74,74	1.44	8 (14%)	56,114,114	1.84	14 (25%)
9	CHL	D	608	11	57,74,74	1.39	9 (15%)	56,114,114	1.79	11 (19%)
9	CHL	D	609	1	57,74,74	1.42	8 (14%)	56,114,114	1.68	12 (21%)
10	CLA	D	610	1	55,73,73	1.35	6 (10%)	61,113,113	1.69	13 (21%)
10	CLA	D	611	7	55,73,73	1.19	4 (7%)	61,113,113	1.96	16 (26%)
10	CLA	D	612	1	55,73,73	1.29	7 (12%)	61,113,113	1.89	15 (24%)
10	CLA	D	613	1	55,73,73	1.37	6 (10%)	61,113,113	1.99	10 (16%)
10	CLA	D	614	1	39,57,73	1.33	5 (12%)	43,93,113	2.36	9 (20%)
5	XAT	D	8622	-	41,47,47	0.72	1 (2%)	48,74,74	1.27	7 (14%)
5	XAT	E	2622	-	41,47,47	0.70	1 (2%)	48,74,74	1.14	5 (10%)
4	LUT	E	4620	-	41,43,43	1.20	4 (9%)	51,60,60	1.89	6 (11%)
4	LUT	E	4621	-	41,43,43	1.24	4 (9%)	51,60,60	1.73	9 (17%)
6	NEX	E	4623	-	39,46,46	0.90	1 (2%)	48,70,70	0.94	4 (8%)
7	LHG	E	4630	10	48,48,48	0.87	3 (6%)	49,54,54	1.33	5 (10%)
8	DGD	E	4632	-	67,67,67	0.92	1 (1%)	81,81,81	1.07	8 (9%)
2	BNG	E	4633	-	21,21,21	0.52	0	26,26,26	0.76	2 (7%)
9	CHL	E	601	1	57,74,74	1.44	8 (14%)	56,114,114	1.85	13 (23%)
10	CLA	E	602	1	55,73,73	1.32	8 (14%)	61,113,113	2.03	17 (27%)
10	CLA	E	603	1	55,73,73	1.26	7 (12%)	61,113,113	1.85	16 (26%)
10	CLA	E	604	11	52,70,73	1.30	5 (9%)	56,109,113	2.15	12 (21%)
9	CHL	E	605	1	39,56,74	1.53	7 (17%)	37,92,114	1.79	9 (24%)
9	CHL	E	606	11	42,59,74	1.67	8 (19%)	39,96,114	2.36	13 (33%)
9	CHL	E	607	11	57,74,74	1.40	7 (12%)	56,114,114	1.97	17 (30%)
9	CHL	E	608	11	57,74,74	1.41	9 (15%)	56,114,114	1.83	12 (21%)
9	CHL	E	609	1	57,74,74	1.41	8 (14%)	56,114,114	1.59	9 (16%)
10	CLA	E	610	1	55,73,73	1.40	7 (12%)	61,113,113	1.61	12 (19%)
10	CLA	E	611	7	55,73,73	1.28	6 (10%)	61,113,113	1.85	16 (26%)
10	CLA	E	612	1	55,73,73	1.32	7 (12%)	61,113,113	1.75	14 (22%)
10	CLA	E	613	1	55,73,73	1.27	6 (10%)	61,113,113	1.83	13 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CLA	E	614	1	39,57,73	1.34	6 (15%)	43,93,113	2.47	11 (25%)
4	LUT	F	5620	-	41,43,43	0.99	3 (7%)	51,60,60	1.83	10 (19%)
4	LUT	F	5621	-	41,43,43	1.19	4 (9%)	51,60,60	2.02	12 (23%)
6	NEX	F	5623	-	39,46,46	0.89	2 (5%)	48,70,70	1.02	5 (10%)
7	LHG	F	5630	10	48,48,48	0.99	3 (6%)	49,54,54	1.32	5 (10%)
2	BNG	F	5633	-	21,21,21	0.53	0	26,26,26	0.82	2 (7%)
9	CHL	F	601	1	57,74,74	1.33	7 (12%)	56,114,114	1.76	11 (19%)
10	CLA	F	602	1	55,73,73	1.27	9 (16%)	61,113,113	2.08	21 (34%)
10	CLA	F	603	1	55,73,73	1.28	6 (10%)	61,113,113	1.91	14 (22%)
10	CLA	F	604	11	52,70,73	1.20	6 (11%)	56,109,113	2.30	19 (33%)
9	CHL	F	605	1	39,56,74	1.62	5 (12%)	37,92,114	1.81	10 (27%)
9	CHL	F	606	11	42,59,74	1.80	7 (16%)	39,96,114	2.17	14 (35%)
9	CHL	F	607	11	57,74,74	1.50	6 (10%)	56,114,114	2.10	19 (33%)
9	CHL	F	608	11	57,74,74	1.43	7 (12%)	56,114,114	1.91	15 (26%)
9	CHL	F	609	1	57,74,74	1.41	8 (14%)	56,114,114	1.70	13 (23%)
10	CLA	F	610	1	55,73,73	1.39	7 (12%)	61,113,113	1.61	12 (19%)
10	CLA	F	611	7	55,73,73	1.21	5 (9%)	61,113,113	1.84	17 (27%)
10	CLA	F	612	1	55,73,73	1.28	6 (10%)	61,113,113	1.84	14 (22%)
10	CLA	F	613	1	55,73,73	1.28	6 (10%)	61,113,113	1.85	11 (18%)
10	CLA	F	614	1	39,57,73	1.37	4 (10%)	43,93,113	2.32	11 (25%)
5	XAT	F	6622	-	41,47,47	0.67	1 (2%)	48,74,74	1.23	6 (12%)
9	CHL	G	601	1	57,74,74	1.38	7 (12%)	56,114,114	1.80	11 (19%)
10	CLA	G	602	1	55,73,73	1.30	9 (16%)	61,113,113	2.14	22 (36%)
10	CLA	G	603	1	55,73,73	1.23	7 (12%)	61,113,113	1.94	12 (19%)
10	CLA	G	604	11	52,70,73	1.23	7 (13%)	56,109,113	2.25	14 (25%)
9	CHL	G	605	1	39,56,74	1.61	7 (17%)	37,92,114	1.68	8 (21%)
9	CHL	G	606	11	42,59,74	1.81	8 (19%)	39,96,114	2.08	10 (25%)
9	CHL	G	607	11	57,74,74	1.40	7 (12%)	56,114,114	1.99	16 (28%)
9	CHL	G	608	11	57,74,74	1.48	8 (14%)	56,114,114	1.71	13 (23%)
9	CHL	G	609	1	57,74,74	1.40	8 (14%)	56,114,114	1.54	11 (19%)
10	CLA	G	610	1	55,73,73	1.36	8 (14%)	61,113,113	1.72	15 (24%)
10	CLA	G	611	7	55,73,73	1.22	5 (9%)	61,113,113	1.93	17 (27%)
10	CLA	G	612	1	55,73,73	1.24	7 (12%)	61,113,113	1.89	14 (22%)
10	CLA	G	613	1	55,73,73	1.25	7 (12%)	61,113,113	1.97	11 (18%)
10	CLA	G	614	1	39,57,73	1.39	6 (15%)	43,93,113	2.32	13 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	LUT	G	6620	-	41,43,43	1.08	3 (7%)	51,60,60	1.88	10 (19%)
4	LUT	G	6621	-	41,43,43	1.12	3 (7%)	51,60,60	1.75	11 (21%)
6	NEX	G	6623	-	39,46,46	0.92	2 (5%)	48,70,70	1.06	4 (8%)
7	LHG	G	6630	10	48,48,48	0.95	3 (6%)	49,54,54	1.41	5 (10%)
2	BNG	G	6633	-	21,21,21	0.52	0	26,26,26	0.82	2 (7%)
8	DGD	G	9632	-	67,67,67	1.01	2 (2%)	81,81,81	1.08	7 (8%)
5	XAT	H	4622	-	41,47,47	0.73	1 (2%)	48,74,74	1.34	4 (8%)
9	CHL	H	601	1	57,74,74	1.39	7 (12%)	56,114,114	1.80	13 (23%)
10	CLA	H	602	1	55,73,73	1.34	8 (14%)	61,113,113	2.10	22 (36%)
10	CLA	H	603	1	55,73,73	1.20	6 (10%)	61,113,113	1.80	11 (18%)
10	CLA	H	604	11	52,70,73	1.24	5 (9%)	56,109,113	2.33	16 (28%)
9	CHL	H	605	1	39,56,74	1.64	7 (17%)	37,92,114	1.68	9 (24%)
9	CHL	H	606	11	42,59,74	1.68	7 (16%)	39,96,114	2.13	10 (25%)
9	CHL	H	607	11	57,74,74	1.43	7 (12%)	56,114,114	1.92	15 (26%)
9	CHL	H	608	11	57,74,74	1.45	7 (12%)	56,114,114	1.90	13 (23%)
9	CHL	H	609	1	57,74,74	1.39	8 (14%)	56,114,114	1.59	12 (21%)
10	CLA	H	610	1	55,73,73	1.42	7 (12%)	61,113,113	1.66	15 (24%)
10	CLA	H	611	7	55,73,73	1.24	5 (9%)	61,113,113	1.87	16 (26%)
10	CLA	H	612	1	55,73,73	1.27	7 (12%)	61,113,113	1.83	14 (22%)
10	CLA	H	613	1	55,73,73	1.21	4 (7%)	61,113,113	1.99	13 (21%)
10	CLA	H	614	1	39,57,73	1.27	4 (10%)	43,93,113	2.51	14 (32%)
8	DGD	H	6632	-	67,67,67	0.82	1 (1%)	81,81,81	1.02	7 (8%)
4	LUT	H	7620	-	41,43,43	0.96	2 (4%)	51,60,60	2.11	7 (13%)
4	LUT	H	7621	-	41,43,43	1.13	4 (9%)	51,60,60	1.88	10 (19%)
6	NEX	H	7623	-	39,46,46	0.89	2 (5%)	48,70,70	1.01	5 (10%)
7	LHG	H	7630	10	48,48,48	0.89	3 (6%)	49,54,54	1.33	5 (10%)
8	DGD	H	7632	-	67,67,67	0.90	2 (2%)	81,81,81	1.02	8 (9%)
2	BNG	H	7633	-	21,21,21	0.50	0	26,26,26	0.81	2 (7%)
9	CHL	I	601	1	57,74,74	1.35	8 (14%)	56,114,114	1.75	12 (21%)
10	CLA	I	602	1	55,73,73	1.30	9 (16%)	61,113,113	2.27	21 (34%)
10	CLA	I	603	1	55,73,73	1.21	6 (10%)	61,113,113	1.77	15 (24%)
10	CLA	I	604	11	52,70,73	1.25	5 (9%)	56,109,113	2.30	16 (28%)
9	CHL	I	605	1	39,56,74	1.62	7 (17%)	37,92,114	1.76	9 (24%)
9	CHL	I	606	11	42,59,74	1.70	7 (16%)	39,96,114	2.16	11 (28%)
9	CHL	I	607	11	57,74,74	1.51	7 (12%)	56,114,114	1.99	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CHL	I	608	11	57,74,74	1.42	8 (14%)	56,114,114	1.64	13 (23%)
9	CHL	I	609	1	57,74,74	1.47	7 (12%)	56,114,114	1.69	11 (19%)
10	CLA	I	610	1	55,73,73	1.39	7 (12%)	61,113,113	1.54	12 (19%)
10	CLA	I	611	7	55,73,73	1.26	5 (9%)	61,113,113	1.84	17 (27%)
10	CLA	I	612	1	55,73,73	1.24	7 (12%)	61,113,113	1.89	15 (24%)
10	CLA	I	613	1	55,73,73	1.21	4 (7%)	61,113,113	1.97	11 (18%)
10	CLA	I	614	1	39,57,73	1.36	6 (15%)	43,93,113	2.41	11 (25%)
4	LUT	I	8620	-	41,43,43	1.01	3 (7%)	51,60,60	1.93	9 (17%)
4	LUT	I	8621	-	41,43,43	1.06	4 (9%)	51,60,60	1.93	10 (19%)
6	NEX	I	8623	-	39,46,46	0.91	2 (5%)	48,70,70	0.99	5 (10%)
7	LHG	I	8630	10	48,48,48	0.99	3 (6%)	49,54,54	1.39	5 (10%)
8	DGD	I	8632	-	67,67,67	0.88	1 (1%)	81,81,81	1.02	8 (9%)
2	BNG	I	8633	-	21,21,21	0.52	0	26,26,26	0.77	2 (7%)
5	XAT	I	9622	-	41,47,47	0.75	1 (2%)	48,74,74	1.24	4 (8%)
5	XAT	J	3622	-	41,47,47	0.72	1 (2%)	48,74,74	1.19	5 (10%)
9	CHL	J	601	1	57,74,74	1.44	9 (15%)	56,114,114	1.67	11 (19%)
10	CLA	J	602	1	55,73,73	1.25	9 (16%)	61,113,113	2.23	20 (32%)
10	CLA	J	603	1	55,73,73	1.35	6 (10%)	61,113,113	1.99	15 (24%)
10	CLA	J	604	11	52,70,73	1.28	6 (11%)	56,109,113	2.29	15 (26%)
9	CHL	J	605	1	39,56,74	1.57	7 (17%)	37,92,114	1.83	9 (24%)
9	CHL	J	606	11	42,59,74	1.76	8 (19%)	39,96,114	2.07	9 (23%)
9	CHL	J	607	11	57,74,74	1.36	6 (10%)	56,114,114	1.88	15 (26%)
9	CHL	J	608	11	57,74,74	1.50	9 (15%)	56,114,114	1.68	10 (17%)
9	CHL	J	609	1	57,74,74	1.44	8 (14%)	56,114,114	1.57	12 (21%)
10	CLA	J	610	1	55,73,73	1.35	8 (14%)	61,113,113	1.65	14 (22%)
10	CLA	J	611	7	55,73,73	1.18	5 (9%)	61,113,113	1.86	16 (26%)
10	CLA	J	612	1	55,73,73	1.22	6 (10%)	61,113,113	1.82	17 (27%)
10	CLA	J	613	1	55,73,73	1.31	7 (12%)	61,113,113	1.78	12 (19%)
10	CLA	J	614	1	39,57,73	1.33	4 (10%)	43,93,113	2.27	10 (23%)
4	LUT	J	9620	-	41,43,43	1.08	3 (7%)	51,60,60	1.99	6 (11%)
4	LUT	J	9621	-	41,43,43	1.13	4 (9%)	51,60,60	1.94	11 (21%)
6	NEX	J	9623	-	39,46,46	0.94	2 (5%)	48,70,70	1.03	5 (10%)
7	LHG	J	9630	10	48,48,48	0.93	3 (6%)	49,54,54	1.33	5 (10%)
2	BNG	J	9633	-	21,21,21	0.51	0	26,26,26	0.81	2 (7%)

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
9	CHL	A	601	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	A	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	A	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	A	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	A	605	1	-	0/18/116/137	0/0/9/9
9	CHL	A	606	11	-	0/21/119/137	0/0/9/9
9	CHL	A	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	A	608	11	-	0/39/137/137	0/0/9/9
9	CHL	A	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	A	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	A	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	A	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	A	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	A	614	1	3/3/16/25	0/18/116/135	0/0/9/9
4	LUT	A	620	-	-	0/29/67/67	0/2/2/2
4	LUT	A	621	-	-	0/29/67/67	0/2/2/2
5	XAT	A	622	-	-	0/31/93/93	0/2/4/4
6	NEX	A	623	-	-	0/27/83/83	0/2/3/3
7	LHG	A	630	10	-	0/53/53/53	0/0/0/0
8	DGD	A	632	-	2/2/13/13	0/55/95/95	0/2/2/2
2	BNG	A	633	-	-	0/12/32/32	0/1/1/1
4	LUT	B	1620	-	-	0/29/67/67	0/2/2/2
4	LUT	B	1621	-	-	0/29/67/67	0/2/2/2
5	XAT	B	1622	-	-	0/31/93/93	0/2/4/4
6	NEX	B	1623	-	-	0/27/83/83	0/2/3/3
7	LHG	B	1630	10	-	0/53/53/53	0/0/0/0
8	DGD	B	1632	-	2/2/13/13	0/55/95/95	0/2/2/2
2	BNG	B	1633	-	-	0/12/32/32	0/1/1/1
8	DGD	B	2632	-	2/2/13/13	0/55/95/95	0/2/2/2
5	XAT	B	5622	-	-	0/31/93/93	0/2/4/4
9	CHL	B	601	1	-	0/39/137/137	0/0/9/9
10	CLA	B	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	B	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	B	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	B	605	1	-	0/18/116/137	0/0/9/9
9	CHL	B	606	11	-	0/21/119/137	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CHL	B	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	B	608	11	-	0/39/137/137	0/0/9/9
9	CHL	B	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	B	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	B	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	B	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	B	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	B	614	1	3/3/16/25	0/18/116/135	0/0/9/9
4	LUT	C	2620	-	-	0/29/67/67	0/2/2/2
4	LUT	C	2621	-	-	0/29/67/67	0/2/2/2
6	NEX	C	2623	-	-	0/27/83/83	0/2/3/3
7	LHG	C	2630	10	-	0/53/53/53	0/0/0/0
2	BNG	C	2633	-	-	0/12/32/32	0/1/1/1
9	CHL	C	601	1	-	0/39/137/137	0/0/9/9
10	CLA	C	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	C	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	C	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	C	605	1	-	0/18/116/137	0/0/9/9
9	CHL	C	606	11	-	0/21/119/137	0/0/9/9
9	CHL	C	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	C	608	11	-	0/39/137/137	0/0/9/9
9	CHL	C	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	C	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	C	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	C	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	C	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	C	614	1	3/3/16/25	0/18/116/135	0/0/9/9
5	XAT	C	7622	-	-	0/31/93/93	0/2/4/4
4	LUT	D	3620	-	-	0/29/67/67	0/2/2/2
4	LUT	D	3621	-	-	0/29/67/67	0/2/2/2
6	NEX	D	3623	-	-	0/27/83/83	0/2/3/3
7	LHG	D	3630	10	-	0/53/53/53	0/0/0/0
8	DGD	D	3632	-	2/2/13/13	0/55/95/95	0/2/2/2
2	BNG	D	3633	-	-	0/12/32/32	0/1/1/1
8	DGD	D	5632	-	2/2/13/13	0/55/95/95	0/2/2/2
9	CHL	D	601	1	-	0/39/137/137	0/0/9/9
10	CLA	D	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	D	603	1	4/4/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	D	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	D	605	1	-	0/18/116/137	0/0/9/9
9	CHL	D	606	11	-	0/21/119/137	0/0/9/9
9	CHL	D	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	D	608	11	-	0/39/137/137	0/0/9/9
9	CHL	D	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	D	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	D	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	D	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	D	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	D	614	1	3/3/16/25	0/18/116/135	0/0/9/9
5	XAT	D	8622	-	-	0/31/93/93	0/2/4/4
5	XAT	E	2622	-	-	0/31/93/93	0/2/4/4
4	LUT	E	4620	-	-	0/29/67/67	0/2/2/2
4	LUT	E	4621	-	-	0/29/67/67	0/2/2/2
6	NEX	E	4623	-	-	0/27/83/83	0/2/3/3
7	LHG	E	4630	10	-	0/53/53/53	0/0/0/0
8	DGD	E	4632	-	2/2/13/13	0/55/95/95	0/2/2/2
2	BNG	E	4633	-	-	0/12/32/32	0/1/1/1
9	CHL	E	601	1	-	0/39/137/137	0/0/9/9
10	CLA	E	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	E	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	E	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	E	605	1	-	0/18/116/137	0/0/9/9
9	CHL	E	606	11	-	0/21/119/137	0/0/9/9
9	CHL	E	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	E	608	11	-	0/39/137/137	0/0/9/9
9	CHL	E	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	E	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	E	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	E	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	E	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	E	614	1	3/3/16/25	0/18/116/135	0/0/9/9
4	LUT	F	5620	-	-	0/29/67/67	0/2/2/2
4	LUT	F	5621	-	-	0/29/67/67	0/2/2/2
6	NEX	F	5623	-	-	0/27/83/83	0/2/3/3
7	LHG	F	5630	10	-	0/53/53/53	0/0/0/0
2	BNG	F	5633	-	-	0/12/32/32	0/1/1/1
9	CHL	F	601	1	-	0/39/137/137	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	F	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	F	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	F	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	F	605	1	-	0/18/116/137	0/0/9/9
9	CHL	F	606	11	-	0/21/119/137	0/0/9/9
9	CHL	F	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	F	608	11	-	0/39/137/137	0/0/9/9
9	CHL	F	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	F	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	F	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	F	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	F	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	F	614	1	3/3/16/25	0/18/116/135	0/0/9/9
5	XAT	F	6622	-	-	0/31/93/93	0/2/4/4
9	CHL	G	601	1	-	0/39/137/137	0/0/9/9
10	CLA	G	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	G	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	G	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	G	605	1	-	0/18/116/137	0/0/9/9
9	CHL	G	606	11	-	0/21/119/137	0/0/9/9
9	CHL	G	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	G	608	11	-	0/39/137/137	0/0/9/9
9	CHL	G	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	G	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	G	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	G	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	G	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	G	614	1	3/3/16/25	0/18/116/135	0/0/9/9
4	LUT	G	6620	-	-	0/29/67/67	0/2/2/2
4	LUT	G	6621	-	-	0/29/67/67	0/2/2/2
6	NEX	G	6623	-	-	0/27/83/83	0/2/3/3
7	LHG	G	6630	10	-	0/53/53/53	0/0/0/0
2	BNG	G	6633	-	-	0/12/32/32	0/1/1/1
8	DGD	G	9632	-	2/2/13/13	0/55/95/95	0/2/2/2
5	XAT	H	4622	-	-	0/31/93/93	0/2/4/4
9	CHL	H	601	1	-	0/39/137/137	0/0/9/9
10	CLA	H	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	H	603	1	4/4/20/25	0/37/135/135	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	H	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	H	605	1	-	0/18/116/137	0/0/9/9
9	CHL	H	606	11	-	0/21/119/137	0/0/9/9
9	CHL	H	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	H	608	11	-	0/39/137/137	0/0/9/9
9	CHL	H	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	H	610	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	H	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	H	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	H	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	H	614	1	3/3/16/25	0/18/116/135	0/0/9/9
8	DGD	H	6632	-	2/2/13/13	0/55/95/95	0/2/2/2
4	LUT	H	7620	-	-	0/29/67/67	0/2/2/2
4	LUT	H	7621	-	-	0/29/67/67	0/2/2/2
6	NEX	H	7623	-	-	0/27/83/83	0/2/3/3
7	LHG	H	7630	10	-	0/53/53/53	0/0/0/0
8	DGD	H	7632	-	2/2/13/13	0/55/95/95	0/2/2/2
2	BNG	H	7633	-	-	0/12/32/32	0/1/1/1
9	CHL	I	601	1	-	0/39/137/137	0/0/9/9
10	CLA	I	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	I	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	I	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	I	605	1	-	0/18/116/137	0/0/9/9
9	CHL	I	606	11	-	0/21/119/137	0/0/9/9
9	CHL	I	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	I	608	11	-	0/39/137/137	0/0/9/9
9	CHL	I	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	I	610	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	I	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	I	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	I	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	I	614	1	3/3/16/25	0/18/116/135	0/0/9/9
4	LUT	I	8620	-	-	0/29/67/67	0/2/2/2
4	LUT	I	8621	-	-	0/29/67/67	0/2/2/2
6	NEX	I	8623	-	-	0/27/83/83	0/2/3/3
7	LHG	I	8630	10	-	0/53/53/53	0/0/0/0
8	DGD	I	8632	-	2/2/13/13	0/55/95/95	0/2/2/2
2	BNG	I	8633	-	-	0/12/32/32	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	XAT	I	9622	-	-	0/31/93/93	0/2/4/4
5	XAT	J	3622	-	-	0/31/93/93	0/2/4/4
9	CHL	J	601	1	-	0/39/137/137	0/0/9/9
10	CLA	J	602	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	J	603	1	4/4/20/25	0/37/135/135	0/0/9/9
10	CLA	J	604	11	3/3/19/25	0/34/132/135	0/0/9/9
9	CHL	J	605	1	-	0/18/116/137	0/0/9/9
9	CHL	J	606	11	-	0/21/119/137	0/0/9/9
9	CHL	J	607	11	1/1/20/26	0/39/137/137	0/0/9/9
9	CHL	J	608	11	-	0/39/137/137	0/0/9/9
9	CHL	J	609	1	1/1/20/26	0/39/137/137	0/0/9/9
10	CLA	J	610	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	J	611	7	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	J	612	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	J	613	1	3/3/20/25	0/37/135/135	0/0/9/9
10	CLA	J	614	1	3/3/16/25	0/18/116/135	0/0/9/9
4	LUT	J	9620	-	-	0/29/67/67	0/2/2/2
4	LUT	J	9621	-	-	0/29/67/67	0/2/2/2
6	NEX	J	9623	-	-	0/27/83/83	0/2/3/3
7	LHG	J	9630	10	-	0/53/53/53	0/0/0/0
2	BNG	J	9633	-	-	0/12/32/32	0/1/1/1

All (1082) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	608	CHL	C4D-CHA	-5.89	1.37	1.45
9	H	608	CHL	C4D-CHA	-5.37	1.38	1.45
9	F	606	CHL	C4D-CHA	-5.30	1.38	1.45
9	I	606	CHL	C4D-CHA	-5.30	1.38	1.45
9	G	606	CHL	C4D-CHA	-5.19	1.38	1.45
9	I	609	CHL	C4D-CHA	-5.11	1.38	1.45
9	C	601	CHL	C4D-CHA	-5.10	1.38	1.45
9	E	609	CHL	C4D-CHA	-5.04	1.38	1.45
9	A	601	CHL	C4D-CHA	-4.97	1.38	1.45
9	D	607	CHL	C4D-CHA	-4.97	1.38	1.45
9	F	601	CHL	C4D-CHA	-4.95	1.38	1.45
9	H	606	CHL	C4D-CHA	-4.91	1.38	1.45
9	I	608	CHL	C4D-CHA	-4.89	1.38	1.45
9	G	608	CHL	C4D-CHA	-4.87	1.39	1.45
9	A	609	CHL	C4D-CHA	-4.86	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	608	CHL	C4D-CHA	-4.80	1.39	1.45
9	H	601	CHL	C4D-CHA	-4.80	1.39	1.45
9	H	609	CHL	C4D-CHA	-4.78	1.39	1.45
9	B	607	CHL	C4D-CHA	-4.76	1.39	1.45
9	B	606	CHL	C4D-CHA	-4.75	1.39	1.45
9	G	605	CHL	C4D-CHA	-4.75	1.39	1.45
9	G	601	CHL	C4D-CHA	-4.73	1.39	1.45
9	D	601	CHL	C4D-CHA	-4.73	1.39	1.45
9	I	601	CHL	C4D-CHA	-4.72	1.39	1.45
9	A	605	CHL	C4D-CHA	-4.71	1.39	1.45
9	D	609	CHL	C4D-CHA	-4.70	1.39	1.45
9	F	608	CHL	C4D-CHA	-4.68	1.39	1.45
9	B	609	CHL	C4D-CHA	-4.68	1.39	1.45
9	D	606	CHL	C4D-CHA	-4.63	1.39	1.45
9	C	606	CHL	C4D-CHA	-4.62	1.39	1.45
9	J	601	CHL	C4D-CHA	-4.61	1.39	1.45
9	E	601	CHL	C4D-CHA	-4.61	1.39	1.45
9	C	608	CHL	C4D-CHA	-4.58	1.39	1.45
9	G	609	CHL	C4D-CHA	-4.56	1.39	1.45
9	J	609	CHL	C4D-CHA	-4.56	1.39	1.45
9	F	609	CHL	C4D-CHA	-4.55	1.39	1.45
9	A	608	CHL	C4D-CHA	-4.54	1.39	1.45
9	I	607	CHL	C4D-CHA	-4.53	1.39	1.45
9	F	605	CHL	C4D-CHA	-4.48	1.39	1.45
9	J	606	CHL	C4D-CHA	-4.46	1.39	1.45
9	D	605	CHL	C4D-CHA	-4.46	1.39	1.45
9	E	606	CHL	C4D-CHA	-4.44	1.39	1.45
9	E	608	CHL	C4D-CHA	-4.38	1.39	1.45
9	E	607	CHL	C4D-CHA	-4.38	1.39	1.45
9	J	607	CHL	C4D-CHA	-4.34	1.39	1.45
9	B	608	CHL	C4D-CHA	-4.32	1.39	1.45
9	B	601	CHL	C4D-CHA	-4.32	1.39	1.45
9	E	605	CHL	C4D-CHA	-4.32	1.39	1.45
9	C	609	CHL	C4D-CHA	-4.31	1.39	1.45
9	J	605	CHL	C4D-CHA	-4.29	1.39	1.45
9	C	605	CHL	C4D-CHA	-4.28	1.39	1.45
9	H	605	CHL	C4D-CHA	-4.28	1.39	1.45
9	I	605	CHL	C4D-CHA	-4.26	1.39	1.45
9	A	606	CHL	C4D-CHA	-4.20	1.39	1.45
9	H	607	CHL	C4D-CHA	-4.19	1.39	1.45
9	G	607	CHL	C4D-CHA	-4.16	1.39	1.45
9	B	605	CHL	C4D-CHA	-4.12	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	607	CHL	C4D-CHA	-3.93	1.40	1.45
9	C	607	CHL	C4D-CHA	-3.89	1.40	1.45
9	F	607	CHL	C4D-CHA	-3.85	1.40	1.45
10	I	612	CLA	O2D-CED	-3.43	1.36	1.45
9	G	601	CHL	O2D-CED	-3.39	1.37	1.45
9	H	608	CHL	O2D-CED	-3.35	1.37	1.45
10	F	603	CLA	O2D-CED	-3.32	1.37	1.45
10	A	612	CLA	O2D-CED	-3.30	1.37	1.45
10	C	604	CLA	O2D-CED	-3.20	1.37	1.45
9	G	608	CHL	O2D-CED	-3.20	1.37	1.45
9	I	608	CHL	O2D-CED	-3.16	1.37	1.45
10	B	603	CLA	C3B-C2B	-3.07	1.36	1.40
10	D	612	CLA	O2D-CED	-3.06	1.37	1.45
10	G	612	CLA	O2D-CED	-3.06	1.37	1.45
10	B	603	CLA	O2D-CED	-3.01	1.38	1.45
10	E	611	CLA	O2D-CED	-3.00	1.38	1.45
10	F	612	CLA	O2D-CED	-3.00	1.38	1.45
9	J	608	CHL	O2D-CED	-2.99	1.38	1.45
10	C	612	CLA	O2D-CED	-2.97	1.38	1.45
9	B	608	CHL	O2D-CED	-2.94	1.38	1.45
9	C	608	CHL	O2D-CED	-2.93	1.38	1.45
9	A	608	CHL	O2D-CED	-2.93	1.38	1.45
10	I	604	CLA	O2D-CED	-2.93	1.38	1.45
10	F	604	CLA	O2D-CED	-2.92	1.38	1.45
10	E	612	CLA	C3B-C2B	-2.92	1.36	1.40
10	H	612	CLA	O2D-CED	-2.91	1.38	1.45
9	A	609	CHL	C3B-C2B	-2.90	1.36	1.40
9	B	606	CHL	O2D-CED	-2.89	1.38	1.45
9	F	608	CHL	O2D-CED	-2.88	1.38	1.45
10	H	602	CLA	O2D-CED	-2.84	1.38	1.45
10	G	602	CLA	O2D-CED	-2.83	1.38	1.45
9	I	605	CHL	O2D-CED	-2.82	1.38	1.45
9	C	609	CHL	O2D-CED	-2.81	1.38	1.45
10	D	604	CLA	O2D-CED	-2.80	1.38	1.45
9	D	609	CHL	O2D-CED	-2.80	1.38	1.45
9	I	609	CHL	C3B-C2B	-2.79	1.36	1.40
10	H	610	CLA	O2D-CED	-2.79	1.38	1.45
9	J	609	CHL	C3B-C2B	-2.79	1.36	1.40
10	I	612	CLA	C3B-C2B	-2.77	1.36	1.40
9	A	608	CHL	C3B-C2B	-2.77	1.36	1.40
9	B	607	CHL	O2D-CED	-2.77	1.38	1.45
10	J	603	CLA	O2D-CED	-2.76	1.38	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	602	CLA	C3B-C2B	-2.76	1.36	1.40
9	G	609	CHL	O2D-CED	-2.76	1.38	1.45
9	C	605	CHL	O2D-CED	-2.75	1.38	1.45
10	B	604	CLA	O2D-CED	-2.75	1.38	1.45
10	E	604	CLA	O2D-CED	-2.75	1.38	1.45
9	C	609	CHL	C3B-C2B	-2.75	1.36	1.40
9	B	609	CHL	O2D-CED	-2.74	1.38	1.45
10	A	603	CLA	O2D-CED	-2.74	1.38	1.45
9	J	609	CHL	O2D-CED	-2.73	1.38	1.45
10	H	610	CLA	C3B-C2B	-2.73	1.36	1.40
10	A	604	CLA	O2D-CED	-2.73	1.38	1.45
9	E	609	CHL	C3B-C2B	-2.71	1.36	1.40
10	E	602	CLA	C3B-C2B	-2.71	1.36	1.40
9	D	609	CHL	C3B-C2B	-2.71	1.36	1.40
10	E	610	CLA	O2D-CED	-2.70	1.38	1.45
10	J	612	CLA	O2D-CED	-2.70	1.38	1.45
10	F	603	CLA	C3B-C2B	-2.70	1.36	1.40
10	B	610	CLA	C3B-C2B	-2.70	1.36	1.40
10	H	602	CLA	C3B-C2B	-2.69	1.36	1.40
10	D	602	CLA	O2D-CED	-2.68	1.38	1.45
10	G	602	CLA	C1-C2	-2.68	1.40	1.49
10	H	612	CLA	C3B-C2B	-2.68	1.36	1.40
10	I	602	CLA	C1-C2	-2.67	1.40	1.49
9	D	608	CHL	O2D-CED	-2.66	1.38	1.45
9	A	601	CHL	O2D-CED	-2.66	1.38	1.45
10	E	603	CLA	O2D-CED	-2.66	1.38	1.45
10	E	603	CLA	C3B-C2B	-2.65	1.36	1.40
10	D	602	CLA	C1-C2	-2.65	1.40	1.49
9	A	609	CHL	O2D-CED	-2.65	1.38	1.45
10	D	602	CLA	C3B-C2B	-2.65	1.36	1.40
10	A	602	CLA	C3B-C2B	-2.65	1.36	1.40
9	J	608	CHL	C3B-C2B	-2.65	1.36	1.40
9	I	608	CHL	C3B-C2B	-2.64	1.36	1.40
10	A	610	CLA	C3B-C2B	-2.64	1.36	1.40
10	J	604	CLA	O2D-CED	-2.63	1.38	1.45
10	G	612	CLA	C3B-C2B	-2.63	1.36	1.40
10	G	613	CLA	O2D-CED	-2.63	1.38	1.45
10	D	603	CLA	O2D-CED	-2.62	1.38	1.45
10	J	613	CLA	O2D-CED	-2.61	1.38	1.45
9	H	607	CHL	O2D-CED	-2.61	1.38	1.45
10	J	602	CLA	O2D-CED	-2.61	1.39	1.45
9	J	601	CHL	O2D-CED	-2.60	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	609	CHL	C3B-C2B	-2.60	1.36	1.40
10	G	604	CLA	O2D-CED	-2.60	1.39	1.45
7	B	1630	LHG	C26-C25	-2.58	1.36	1.51
9	D	607	CHL	O2D-CED	-2.58	1.39	1.45
9	D	608	CHL	C3B-C2B	-2.58	1.36	1.40
10	F	612	CLA	C3B-C2B	-2.58	1.36	1.40
10	I	603	CLA	C3B-C2B	-2.58	1.36	1.40
10	I	603	CLA	O2D-CED	-2.57	1.39	1.45
9	F	609	CHL	O2D-CED	-2.57	1.39	1.45
10	B	612	CLA	O2D-CED	-2.57	1.39	1.45
10	C	602	CLA	C1-C2	-2.57	1.40	1.49
10	I	613	CLA	O2D-CED	-2.57	1.39	1.45
7	I	8630	LHG	C26-C25	-2.57	1.36	1.51
10	H	614	CLA	C3B-C2B	-2.56	1.36	1.40
10	I	611	CLA	C3B-C2B	-2.56	1.36	1.40
7	J	9630	LHG	C26-C25	-2.56	1.36	1.51
9	G	609	CHL	C3B-C2B	-2.56	1.37	1.40
10	A	611	CLA	O2D-CED	-2.56	1.39	1.45
10	C	612	CLA	C3B-C2B	-2.54	1.37	1.40
10	C	603	CLA	C3B-C2B	-2.54	1.37	1.40
10	D	612	CLA	C3B-C2B	-2.54	1.37	1.40
10	G	610	CLA	C3B-C2B	-2.54	1.37	1.40
9	J	605	CHL	O2D-CED	-2.53	1.39	1.45
10	A	603	CLA	C3B-C2B	-2.53	1.37	1.40
9	F	601	CHL	O2D-CED	-2.53	1.39	1.45
9	E	608	CHL	O2D-CED	-2.53	1.39	1.45
10	D	614	CLA	C3B-C2B	-2.53	1.37	1.40
7	D	3630	LHG	C26-C25	-2.52	1.37	1.51
9	G	608	CHL	C3B-C2B	-2.52	1.37	1.40
9	I	601	CHL	O2D-CED	-2.52	1.39	1.45
9	H	608	CHL	C3B-C2B	-2.52	1.37	1.40
9	H	601	CHL	O2D-CED	-2.51	1.39	1.45
9	C	608	CHL	C3B-C2B	-2.51	1.37	1.40
9	F	608	CHL	C3B-C2B	-2.51	1.37	1.40
10	H	603	CLA	C3B-C2B	-2.50	1.37	1.40
10	A	602	CLA	O2D-CED	-2.50	1.39	1.45
9	B	609	CHL	C3B-C2B	-2.49	1.37	1.40
10	C	602	CLA	C3B-C2B	-2.49	1.37	1.40
10	J	603	CLA	C3B-C2B	-2.49	1.37	1.40
7	G	6630	LHG	C26-C25	-2.49	1.37	1.51
7	E	4630	LHG	C26-C25	-2.48	1.37	1.51
10	H	611	CLA	C3B-C2B	-2.48	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	603	CLA	C3B-C2B	-2.48	1.37	1.40
10	I	602	CLA	O2D-CED	-2.48	1.39	1.45
10	C	611	CLA	O2D-CED	-2.48	1.39	1.45
10	B	602	CLA	O2D-CED	-2.47	1.39	1.45
10	J	610	CLA	C3B-C2B	-2.47	1.37	1.40
9	E	609	CHL	O2D-CED	-2.46	1.39	1.45
10	C	610	CLA	O2D-CED	-2.46	1.39	1.45
9	E	608	CHL	C3B-C2B	-2.46	1.37	1.40
10	J	612	CLA	C3B-C2B	-2.45	1.37	1.40
9	B	605	CHL	C3B-C2B	-2.45	1.37	1.40
9	B	608	CHL	C3B-C2B	-2.45	1.37	1.40
10	D	610	CLA	C3B-C2B	-2.45	1.37	1.40
10	F	614	CLA	C3B-C2B	-2.45	1.37	1.40
10	C	611	CLA	C3B-C2B	-2.45	1.37	1.40
9	D	605	CHL	O2D-CED	-2.45	1.39	1.45
10	H	603	CLA	O2D-CED	-2.44	1.39	1.45
9	J	601	CHL	C3B-C2B	-2.44	1.37	1.40
10	B	602	CLA	C3B-C2B	-2.43	1.37	1.40
9	A	605	CHL	C3B-C2B	-2.43	1.37	1.40
9	E	607	CHL	O2D-CED	-2.43	1.39	1.45
10	D	611	CLA	C3B-C2B	-2.42	1.37	1.40
9	I	607	CHL	O2D-CED	-2.41	1.39	1.45
9	G	605	CHL	O2D-CED	-2.40	1.39	1.45
10	G	614	CLA	C3B-C2B	-2.40	1.37	1.40
9	E	606	CHL	O2D-CED	-2.40	1.39	1.45
10	H	604	CLA	O2D-CED	-2.40	1.39	1.45
9	H	606	CHL	O2D-CED	-2.39	1.39	1.45
10	B	612	CLA	C3B-C2B	-2.38	1.37	1.40
9	E	601	CHL	C3B-C2B	-2.38	1.37	1.40
7	F	5630	LHG	C26-C25	-2.37	1.37	1.51
9	H	601	CHL	C3B-C2B	-2.37	1.37	1.40
10	G	603	CLA	C3B-C2B	-2.37	1.37	1.40
10	I	614	CLA	C3B-C2B	-2.37	1.37	1.40
9	C	601	CHL	O2D-CED	-2.37	1.39	1.45
7	C	2630	LHG	C26-C25	-2.37	1.37	1.51
10	J	613	CLA	C3B-C2B	-2.37	1.37	1.40
10	D	613	CLA	O2D-CED	-2.36	1.39	1.45
9	H	609	CHL	C3B-C2B	-2.36	1.37	1.40
10	C	610	CLA	C3B-C2B	-2.36	1.37	1.40
9	H	609	CHL	O2D-CED	-2.36	1.39	1.45
9	I	606	CHL	O2D-CED	-2.36	1.39	1.45
10	E	610	CLA	C3B-C2B	-2.36	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	602	CLA	C3B-C2B	-2.35	1.37	1.40
9	J	605	CHL	C3B-C2B	-2.35	1.37	1.40
9	C	601	CHL	C3B-C2B	-2.35	1.37	1.40
10	J	602	CLA	C3B-C2B	-2.35	1.37	1.40
10	J	602	CLA	C1-C2	-2.34	1.41	1.49
9	D	601	CHL	C3B-C2B	-2.34	1.37	1.40
10	F	602	CLA	C3B-C2B	-2.33	1.37	1.40
10	J	611	CLA	C3B-C2B	-2.33	1.37	1.40
10	E	611	CLA	C3B-C2B	-2.32	1.37	1.40
10	F	610	CLA	C3B-C2B	-2.31	1.37	1.40
10	G	611	CLA	C3B-C2B	-2.30	1.37	1.40
7	A	630	LHG	C26-C25	-2.30	1.38	1.51
9	E	609	CHL	C1-C2	-2.30	1.41	1.49
9	B	601	CHL	C3B-C2B	-2.29	1.37	1.40
10	D	610	CLA	O2D-CED	-2.29	1.39	1.45
9	G	607	CHL	O2D-CED	-2.29	1.39	1.45
9	A	607	CHL	O2D-CED	-2.29	1.39	1.45
7	H	7630	LHG	C26-C25	-2.28	1.38	1.51
10	H	602	CLA	C1-C2	-2.28	1.41	1.49
9	G	605	CHL	C3B-C2B	-2.27	1.37	1.40
10	A	612	CLA	C3B-C2B	-2.27	1.37	1.40
10	A	614	CLA	C3B-C2B	-2.26	1.37	1.40
10	B	611	CLA	O2D-CED	-2.25	1.39	1.45
10	B	610	CLA	O2D-CED	-2.25	1.39	1.45
10	G	603	CLA	O2D-CED	-2.25	1.39	1.45
10	C	614	CLA	C3B-C2B	-2.25	1.37	1.40
9	G	601	CHL	C3B-C2B	-2.25	1.37	1.40
9	C	605	CHL	C3B-C2B	-2.25	1.37	1.40
9	A	605	CHL	O2D-CED	-2.24	1.39	1.45
10	B	614	CLA	C3B-C2B	-2.23	1.37	1.40
9	A	601	CHL	C3B-C2B	-2.23	1.37	1.40
10	F	613	CLA	O2D-CED	-2.23	1.39	1.45
10	E	613	CLA	C3B-C2B	-2.23	1.37	1.40
10	B	602	CLA	C1-C2	-2.23	1.41	1.49
10	J	610	CLA	O2D-CED	-2.23	1.39	1.45
10	J	611	CLA	O2D-CED	-2.23	1.39	1.45
9	F	605	CHL	C3B-C2B	-2.23	1.37	1.40
10	B	614	CLA	O2D-CED	-2.22	1.39	1.45
10	F	602	CLA	C1-C2	-2.22	1.41	1.49
10	F	610	CLA	O2D-CED	-2.21	1.39	1.45
9	C	607	CHL	O2D-CED	-2.21	1.39	1.45
10	J	614	CLA	C3B-C2B	-2.19	1.37	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	610	CLA	O2D-CED	-2.19	1.40	1.45
9	F	601	CHL	C3B-C2B	-2.19	1.37	1.40
10	G	611	CLA	O2D-CED	-2.19	1.40	1.45
9	C	608	CHL	C1-C2	-2.18	1.41	1.49
9	J	609	CHL	C1-C2	-2.17	1.41	1.49
9	E	605	CHL	O2D-CED	-2.17	1.40	1.45
10	A	611	CLA	C3B-C2B	-2.17	1.37	1.40
10	F	611	CLA	C3B-C2B	-2.17	1.37	1.40
9	E	601	CHL	O2D-CED	-2.16	1.40	1.45
10	E	612	CLA	O2D-CED	-2.14	1.40	1.45
10	C	614	CLA	O2D-CED	-2.11	1.40	1.45
10	B	613	CLA	O2D-CED	-2.09	1.40	1.45
9	I	601	CHL	C3B-C2B	-2.09	1.37	1.40
9	I	609	CHL	O2D-CED	-2.08	1.40	1.45
10	I	614	CLA	O2D-CED	-2.08	1.40	1.45
9	E	605	CHL	C3B-C2B	-2.08	1.37	1.40
9	D	606	CHL	O2D-CED	-2.08	1.40	1.45
10	I	610	CLA	C3B-C2B	-2.08	1.37	1.40
10	F	602	CLA	O2D-CED	-2.07	1.40	1.45
9	H	605	CHL	O2D-CED	-2.07	1.40	1.45
9	B	609	CHL	C1-C2	-2.06	1.42	1.49
10	F	611	CLA	O2D-CED	-2.06	1.40	1.45
9	H	605	CHL	C3B-C2B	-2.06	1.37	1.40
9	D	605	CHL	C3B-C2B	-2.05	1.37	1.40
10	E	614	CLA	C3B-C2B	-2.05	1.37	1.40
9	I	605	CHL	C3B-C2B	-2.04	1.37	1.40
10	H	611	CLA	O2D-CED	-2.02	1.40	1.45
10	B	611	CLA	C3B-C2B	-2.00	1.37	1.40
10	J	610	CLA	C4-C3	2.00	1.55	1.50
4	I	8620	LUT	C24-C25	2.01	1.35	1.33
9	I	608	CHL	C4-C3	2.01	1.55	1.50
10	I	612	CLA	C4-C3	2.01	1.55	1.50
10	C	610	CLA	C4-C3	2.01	1.55	1.50
10	I	614	CLA	CMC-C2C	2.01	1.55	1.50
9	D	606	CHL	C4-C3	2.01	1.56	1.50
5	A	622	XAT	C28-C27	2.01	1.36	1.32
10	J	613	CLA	CMC-C2C	2.01	1.55	1.50
9	D	608	CHL	CMB-C2B	2.01	1.56	1.51
10	A	610	CLA	CAC-C3C	2.01	1.56	1.51
9	H	609	CHL	CMB-C2B	2.02	1.56	1.51
10	E	613	CLA	CMB-C2B	2.02	1.55	1.51
10	D	602	CLA	CMB-C2B	2.02	1.55	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	614	CLA	CMC-C2C	2.02	1.55	1.50
4	G	6620	LUT	C24-C25	2.02	1.35	1.33
10	C	613	CLA	CBD-CGD	2.02	1.59	1.52
4	G	6621	LUT	C5-C6	2.02	1.37	1.34
10	A	610	CLA	C4-C3	2.02	1.55	1.50
9	A	607	CHL	CMB-C2B	2.02	1.56	1.51
4	D	3620	LUT	C24-C25	2.02	1.35	1.33
9	A	609	CHL	C4-C3	2.02	1.55	1.50
10	A	614	CLA	CMC-C2C	2.02	1.55	1.50
10	F	613	CLA	CMC-C2C	2.02	1.55	1.50
6	H	7623	NEX	C1-C6	2.03	1.57	1.54
4	C	2620	LUT	C1-C6	2.03	1.56	1.53
6	F	5623	NEX	C1-C6	2.03	1.57	1.54
10	F	614	CLA	CHC-C1C	2.03	1.41	1.35
10	G	614	CLA	CAC-C3C	2.03	1.56	1.51
10	E	614	CLA	CHC-C1C	2.03	1.41	1.35
9	E	606	CHL	C4-C3	2.03	1.56	1.50
10	G	610	CLA	C4-C3	2.04	1.55	1.50
10	G	614	CLA	CHC-C1C	2.04	1.41	1.35
10	F	604	CLA	C4-C3	2.04	1.55	1.50
4	F	5620	LUT	C1-C6	2.04	1.56	1.53
5	H	4622	XAT	C28-C27	2.05	1.36	1.32
10	D	614	CLA	CHC-C1C	2.05	1.41	1.35
10	G	604	CLA	C5-C3	2.05	1.55	1.51
6	D	3623	NEX	C1-C6	2.05	1.58	1.54
10	I	602	CLA	CMC-C2C	2.05	1.55	1.50
9	J	606	CHL	C5-C3	2.05	1.56	1.50
10	E	603	CLA	CAC-C3C	2.05	1.56	1.51
9	J	608	CHL	CMB-C2B	2.05	1.56	1.51
9	I	609	CHL	C1A-CHA	2.05	1.41	1.37
10	C	610	CLA	CMC-C2C	2.05	1.55	1.50
10	E	612	CLA	C4-C3	2.06	1.55	1.50
10	J	604	CLA	C4-C3	2.06	1.55	1.50
9	D	606	CHL	C5-C3	2.06	1.56	1.50
9	G	606	CHL	C5-C3	2.06	1.56	1.50
9	G	606	CHL	CMB-C2B	2.06	1.56	1.51
10	J	604	CLA	CMC-C2C	2.07	1.55	1.50
9	B	605	CHL	CBD-CGD	2.07	1.59	1.52
9	E	605	CHL	CMB-C2B	2.07	1.56	1.51
10	C	612	CLA	C4-C3	2.07	1.55	1.50
10	D	602	CLA	CHC-C1C	2.07	1.41	1.35
9	J	609	CHL	C1A-CHA	2.07	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	614	CLA	CMC-C2C	2.07	1.55	1.50
10	G	612	CLA	CMB-C2B	2.07	1.55	1.51
10	H	603	CLA	CMB-C2B	2.07	1.55	1.51
10	G	602	CLA	CMB-C2B	2.08	1.55	1.51
9	E	608	CHL	C4-C3	2.08	1.55	1.50
10	H	602	CLA	C4-C3	2.08	1.55	1.50
9	J	606	CHL	C4-C3	2.08	1.56	1.50
4	C	2621	LUT	C26-C27	2.08	1.53	1.50
10	J	602	CLA	C4-C3	2.09	1.55	1.50
9	C	607	CHL	CMD-C2D	2.09	1.55	1.51
9	F	606	CHL	C5-C3	2.09	1.56	1.50
5	E	2622	XAT	C28-C27	2.09	1.36	1.32
10	F	613	CLA	CMB-C2B	2.09	1.56	1.51
10	A	612	CLA	CMB-C2B	2.09	1.56	1.51
9	G	606	CHL	C4-C3	2.09	1.56	1.50
10	A	603	CLA	CMC-C2C	2.10	1.55	1.50
6	G	6623	NEX	C1-C6	2.10	1.58	1.54
10	A	614	CLA	CMB-C2B	2.10	1.56	1.51
9	I	606	CHL	C4-C3	2.10	1.56	1.50
4	F	5621	LUT	C1-C6	2.10	1.56	1.53
10	C	603	CLA	CMB-C2B	2.10	1.56	1.51
10	A	611	CLA	CMB-C2B	2.11	1.56	1.51
9	D	601	CHL	CMB-C2B	2.11	1.56	1.51
4	I	8621	LUT	C24-C25	2.11	1.35	1.33
10	G	603	CLA	CMC-C2C	2.11	1.55	1.50
4	H	7621	LUT	C1-C6	2.11	1.56	1.53
9	B	608	CHL	C1A-CHA	2.12	1.42	1.37
9	J	608	CHL	C4-C3	2.12	1.55	1.50
9	F	609	CHL	C1A-CHA	2.12	1.42	1.37
4	B	1621	LUT	C1-C6	2.12	1.56	1.53
10	G	613	CLA	C5-C3	2.13	1.56	1.51
10	D	610	CLA	CHC-C1C	2.13	1.42	1.35
10	G	610	CLA	CAC-C3C	2.13	1.57	1.51
10	G	612	CLA	C4-C3	2.13	1.55	1.50
10	B	612	CLA	C4-C3	2.13	1.55	1.50
4	D	3621	LUT	C26-C27	2.13	1.53	1.50
10	D	614	CLA	CMB-C2B	2.13	1.56	1.51
10	F	604	CLA	C5-C3	2.13	1.56	1.51
10	I	614	CLA	CMB-C2B	2.14	1.56	1.51
10	J	610	CLA	CHC-C1C	2.14	1.42	1.35
4	E	4621	LUT	C26-C27	2.14	1.53	1.50
10	H	610	CLA	CHC-C1C	2.14	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	602	CLA	C4-C3	2.14	1.55	1.50
9	D	608	CHL	C4-C3	2.14	1.55	1.50
10	B	613	CLA	CMB-C2B	2.14	1.56	1.51
10	J	612	CLA	C4-C3	2.14	1.55	1.50
9	J	605	CHL	CMB-C2B	2.15	1.56	1.51
10	E	602	CLA	CMB-C2B	2.15	1.56	1.51
9	D	609	CHL	C1A-CHA	2.16	1.42	1.37
10	H	614	CLA	CHC-C1C	2.16	1.42	1.35
10	A	610	CLA	CHC-C1C	2.16	1.42	1.35
10	C	610	CLA	CBD-CGD	2.16	1.59	1.52
10	A	604	CLA	C4-C3	2.16	1.56	1.50
9	F	609	CHL	C4-C3	2.17	1.56	1.50
10	D	612	CLA	C4-C3	2.17	1.56	1.50
9	G	608	CHL	CMB-C2B	2.17	1.56	1.51
10	H	614	CLA	O2D-CGD	2.17	1.38	1.33
9	I	601	CHL	CMB-C2B	2.17	1.56	1.51
10	C	604	CLA	C4-C3	2.17	1.56	1.50
10	D	604	CLA	C4-C3	2.18	1.56	1.50
10	F	603	CLA	CBD-CGD	2.18	1.59	1.52
10	B	612	CLA	CBD-CGD	2.18	1.59	1.52
9	E	608	CHL	CMB-C2B	2.18	1.56	1.51
10	B	602	CLA	CHC-C1C	2.18	1.42	1.35
6	A	623	NEX	C1-C6	2.18	1.58	1.54
4	E	4620	LUT	C1-C6	2.19	1.56	1.53
10	E	611	CLA	CMB-C2B	2.19	1.56	1.51
9	G	605	CHL	C1A-CHA	2.19	1.42	1.37
9	G	608	CHL	C1A-CHA	2.20	1.42	1.37
10	F	612	CLA	C4-C3	2.20	1.56	1.50
10	B	610	CLA	CHC-C1C	2.20	1.42	1.35
10	E	613	CLA	CMC-C2C	2.20	1.55	1.50
9	H	607	CHL	CMB-C2B	2.20	1.56	1.51
10	G	610	CLA	CHC-C1C	2.20	1.42	1.35
10	H	612	CLA	C4-C3	2.21	1.56	1.50
10	J	613	CLA	C4-C3	2.21	1.56	1.50
10	J	602	CLA	CMB-C2B	2.21	1.56	1.51
10	C	611	CLA	CMB-C2B	2.22	1.56	1.51
4	H	7621	LUT	C24-C25	2.22	1.36	1.33
10	B	613	CLA	C4-C3	2.22	1.56	1.50
10	B	602	CLA	CMB-C2B	2.23	1.56	1.51
6	J	9623	NEX	C1-C6	2.23	1.58	1.54
10	C	602	CLA	CHC-C1C	2.23	1.42	1.35
8	H	7632	DGD	O1G-C1A	2.23	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	605	CHL	CMB-C2B	2.23	1.56	1.51
4	B	1620	LUT	C24-C25	2.23	1.36	1.33
4	J	9620	LUT	C26-C27	2.23	1.54	1.50
9	B	607	CHL	CMB-C2B	2.23	1.56	1.51
9	C	605	CHL	CMB-C2B	2.23	1.56	1.51
10	B	602	CLA	C4-C3	2.24	1.56	1.50
9	J	601	CHL	CMB-C2B	2.24	1.56	1.51
10	E	602	CLA	CHC-C1C	2.25	1.42	1.35
9	G	609	CHL	C4-C3	2.25	1.56	1.50
5	F	6622	XAT	C28-C27	2.25	1.36	1.32
10	E	610	CLA	CMB-C2B	2.25	1.56	1.51
10	H	612	CLA	CMB-C2B	2.25	1.56	1.51
10	H	602	CLA	CHC-C1C	2.25	1.42	1.35
10	C	610	CLA	CHC-C1C	2.26	1.42	1.35
9	D	605	CHL	CMB-C2B	2.26	1.56	1.51
10	H	604	CLA	C4-C3	2.27	1.56	1.50
9	C	608	CHL	CMB-C2B	2.27	1.56	1.51
10	A	613	CLA	C4-C3	2.27	1.56	1.50
8	D	3632	DGD	O1G-C1A	2.27	1.40	1.33
10	B	613	CLA	C5-C3	2.28	1.56	1.51
10	I	602	CLA	CHC-C1C	2.28	1.42	1.35
10	A	610	CLA	CMB-C2B	2.28	1.56	1.51
9	C	607	CHL	CMB-C2B	2.28	1.56	1.51
10	I	602	CLA	CMB-C2B	2.28	1.56	1.51
10	H	610	CLA	CMB-C2B	2.28	1.56	1.51
4	J	9621	LUT	C24-C25	2.29	1.36	1.33
9	F	601	CHL	C1A-CHA	2.29	1.42	1.37
6	C	2623	NEX	C1-C6	2.29	1.58	1.54
10	I	610	CLA	CMB-C2B	2.29	1.56	1.51
9	H	608	CHL	CMB-C2B	2.29	1.56	1.51
4	I	8621	LUT	C1-C6	2.29	1.57	1.53
8	A	632	DGD	O1G-C1A	2.29	1.40	1.33
10	G	602	CLA	C4-C3	2.30	1.56	1.50
6	I	8623	NEX	C1-C6	2.30	1.58	1.54
10	A	602	CLA	CHC-C1C	2.30	1.42	1.35
10	F	602	CLA	CMB-C2B	2.30	1.56	1.51
10	I	610	CLA	C4-C3	2.30	1.56	1.50
4	I	8620	LUT	C5-C6	2.30	1.38	1.34
10	F	610	CLA	C4-C3	2.31	1.56	1.50
9	A	608	CHL	C1A-CHA	2.31	1.42	1.37
10	F	602	CLA	CMC-C2C	2.32	1.55	1.50
10	F	602	CLA	CHC-C1C	2.32	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	607	CHL	C4-C3	2.32	1.56	1.50
10	J	610	CLA	CMB-C2B	2.32	1.56	1.51
4	C	2620	LUT	C5-C6	2.32	1.38	1.34
10	G	604	CLA	CMC-C2C	2.33	1.55	1.50
10	F	610	CLA	CHC-C1C	2.33	1.42	1.35
10	I	610	CLA	CHC-C1C	2.33	1.42	1.35
10	E	603	CLA	CMB-C2B	2.33	1.56	1.51
10	B	611	CLA	CMB-C2B	2.33	1.56	1.51
10	E	610	CLA	CHC-C1C	2.33	1.42	1.35
4	B	1621	LUT	C24-C25	2.33	1.36	1.33
4	F	5621	LUT	C24-C25	2.33	1.36	1.33
10	H	613	CLA	CMB-C2B	2.33	1.56	1.51
10	E	604	CLA	C4-C3	2.33	1.56	1.50
10	A	603	CLA	CMB-C2B	2.34	1.56	1.51
10	G	613	CLA	CMC-C2C	2.34	1.55	1.50
5	J	3622	XAT	C28-C27	2.34	1.37	1.32
9	J	608	CHL	C1A-CHA	2.35	1.42	1.37
10	A	613	CLA	CMB-C2B	2.35	1.56	1.51
10	B	603	CLA	CMB-C2B	2.36	1.56	1.51
9	I	608	CHL	C1A-CHA	2.36	1.42	1.37
10	A	613	CLA	CMC-C2C	2.37	1.55	1.50
4	J	9621	LUT	C5-C6	2.37	1.38	1.34
10	G	602	CLA	CHC-C1C	2.37	1.42	1.35
9	I	605	CHL	CMB-C2B	2.37	1.56	1.51
10	J	602	CLA	CHC-C1C	2.38	1.42	1.35
10	E	612	CLA	CMB-C2B	2.38	1.56	1.51
4	D	3621	LUT	C24-C25	2.39	1.36	1.33
10	D	613	CLA	CMC-C2C	2.39	1.55	1.50
9	E	601	CHL	CMB-C2B	2.39	1.56	1.51
9	J	601	CHL	C4-C3	2.39	1.56	1.50
10	B	603	CLA	CMC-C2C	2.39	1.55	1.50
9	H	606	CHL	CMB-C2B	2.40	1.56	1.51
9	E	608	CHL	C1A-CHA	2.40	1.42	1.37
10	G	614	CLA	CMB-C2B	2.40	1.56	1.51
9	B	609	CHL	C4-C3	2.40	1.56	1.50
10	G	613	CLA	CMB-C2B	2.41	1.56	1.51
9	B	606	CHL	CMB-C2B	2.41	1.56	1.51
10	E	602	CLA	CMC-C2C	2.42	1.56	1.50
10	D	602	CLA	CMC-C2C	2.42	1.56	1.50
4	H	7621	LUT	C5-C6	2.42	1.38	1.34
4	G	6621	LUT	C24-C25	2.42	1.36	1.33
9	C	601	CHL	C1A-CHA	2.42	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	605	CHL	C1A-CHA	2.42	1.42	1.37
9	E	609	CHL	CMB-C2B	2.43	1.56	1.51
10	C	613	CLA	CMB-C2B	2.43	1.56	1.51
4	C	2621	LUT	C5-C6	2.43	1.38	1.34
9	C	609	CHL	C4-C3	2.43	1.56	1.50
4	E	4621	LUT	C1-C6	2.43	1.57	1.53
9	A	605	CHL	C1A-CHA	2.44	1.42	1.37
9	C	606	CHL	C1A-CHA	2.45	1.42	1.37
10	I	611	CLA	CMB-C2B	2.45	1.56	1.51
9	C	605	CHL	C1A-CHA	2.46	1.42	1.37
4	E	4620	LUT	C24-C25	2.47	1.36	1.33
10	E	614	CLA	CMB-C2B	2.47	1.56	1.51
9	D	609	CHL	C4-C3	2.47	1.56	1.50
10	I	603	CLA	CMB-C2B	2.47	1.56	1.51
9	H	605	CHL	CMB-C2B	2.48	1.57	1.51
10	I	604	CLA	C4-C3	2.48	1.56	1.50
9	G	609	CHL	C1A-CHA	2.49	1.42	1.37
10	C	614	CLA	CMB-C2B	2.50	1.56	1.51
10	B	614	CLA	CMB-C2B	2.50	1.56	1.51
8	G	9632	DGD	O1G-C1A	2.51	1.40	1.33
10	J	614	CLA	CMB-C2B	2.51	1.56	1.51
5	I	9622	XAT	C28-C27	2.52	1.37	1.32
9	D	606	CHL	CMB-C2B	2.53	1.57	1.51
4	C	2621	LUT	C1-C6	2.54	1.57	1.53
9	C	608	CHL	C1A-CHA	2.55	1.42	1.37
9	E	607	CHL	CMB-C2B	2.55	1.57	1.51
4	H	7620	LUT	C5-C6	2.55	1.38	1.34
10	I	612	CLA	CMB-C2B	2.55	1.56	1.51
4	I	8621	LUT	C5-C6	2.55	1.38	1.34
4	A	620	LUT	C5-C6	2.57	1.38	1.34
4	E	4621	LUT	C24-C25	2.57	1.36	1.33
10	C	613	CLA	CMC-C2C	2.57	1.56	1.50
9	E	601	CHL	C1A-CHA	2.58	1.42	1.37
9	H	609	CHL	C1A-CHA	2.58	1.42	1.37
5	D	8622	XAT	C28-C27	2.59	1.37	1.32
9	D	608	CHL	C1A-CHA	2.59	1.43	1.37
7	E	4630	LHG	O7-C7	2.60	1.42	1.34
4	A	621	LUT	C5-C6	2.60	1.38	1.34
7	D	3630	LHG	O7-C7	2.61	1.42	1.34
9	D	607	CHL	O2A-CGA	2.61	1.41	1.33
5	C	7622	XAT	C28-C27	2.61	1.37	1.32
4	A	621	LUT	C24-C25	2.62	1.36	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	610	CLA	CMB-C2B	2.62	1.57	1.51
10	G	604	CLA	C4-C3	2.62	1.57	1.50
9	F	609	CHL	O2D-CGD	2.63	1.39	1.33
4	C	2621	LUT	C24-C25	2.63	1.36	1.33
4	F	5620	LUT	C5-C6	2.64	1.38	1.34
9	B	606	CHL	C2-C3	2.65	1.40	1.32
9	C	606	CHL	CMB-C2B	2.66	1.57	1.51
4	D	3621	LUT	C5-C6	2.66	1.38	1.34
9	J	606	CHL	C2-C3	2.66	1.40	1.32
4	B	1620	LUT	C5-C6	2.67	1.38	1.34
9	I	606	CHL	C2-C3	2.68	1.40	1.32
9	E	606	CHL	C2-C3	2.68	1.40	1.32
9	G	605	CHL	CMB-C2B	2.68	1.57	1.51
8	B	1632	DGD	O1G-C1A	2.70	1.41	1.33
9	G	601	CHL	C1A-CHA	2.70	1.43	1.37
9	F	605	CHL	C1A-CHA	2.70	1.43	1.37
9	E	609	CHL	O2D-CGD	2.70	1.40	1.33
4	B	1621	LUT	C5-C6	2.70	1.38	1.34
9	D	606	CHL	C2-C3	2.71	1.40	1.32
4	F	5621	LUT	C5-C6	2.72	1.38	1.34
9	F	608	CHL	C1A-CHA	2.72	1.43	1.37
9	H	606	CHL	C2-C3	2.72	1.40	1.32
7	B	1630	LHG	O7-C7	2.73	1.42	1.34
9	I	601	CHL	C1A-CHA	2.73	1.43	1.37
9	H	605	CHL	C1A-CHA	2.74	1.43	1.37
4	D	3620	LUT	C5-C6	2.74	1.38	1.34
9	A	601	CHL	C1A-CHA	2.75	1.43	1.37
10	B	612	CLA	CMB-C2B	2.76	1.57	1.51
9	B	605	CHL	C1A-CHA	2.77	1.43	1.37
9	A	606	CHL	C2-C3	2.77	1.40	1.32
9	E	606	CHL	CMB-C2B	2.79	1.57	1.51
9	H	601	CHL	C1A-CHA	2.79	1.43	1.37
9	C	606	CHL	C2-C3	2.79	1.40	1.32
9	G	606	CHL	C2-C3	2.80	1.40	1.32
9	J	606	CHL	CMB-C2B	2.80	1.57	1.51
7	A	630	LHG	O7-C7	2.80	1.42	1.34
10	D	612	CLA	CMB-C2B	2.81	1.57	1.51
9	F	606	CHL	CMB-C2B	2.81	1.57	1.51
9	D	601	CHL	C1A-CHA	2.82	1.43	1.37
9	A	606	CHL	CMB-C2B	2.82	1.57	1.51
10	J	602	CLA	C2-C3	2.83	1.38	1.33
9	J	607	CHL	O2A-CGA	2.84	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	G	603	CLA	CMB-C2B	2.86	1.57	1.51
10	I	602	CLA	C2-C3	2.86	1.38	1.33
9	F	606	CHL	C2-C3	2.86	1.41	1.32
9	B	609	CHL	C1A-CHA	2.88	1.43	1.37
9	G	606	CHL	C1A-CHA	2.88	1.43	1.37
9	C	601	CHL	O2A-CGA	2.88	1.42	1.33
10	H	602	CLA	C2-C3	2.89	1.38	1.33
10	F	602	CLA	C2-C3	2.89	1.38	1.33
10	J	603	CLA	CMB-C2B	2.89	1.57	1.51
9	J	608	CHL	O2D-CGD	2.89	1.40	1.33
10	G	602	CLA	C2-C3	2.90	1.38	1.33
9	D	606	CHL	C1A-CHA	2.90	1.43	1.37
9	G	607	CHL	CMB-C2B	2.91	1.57	1.51
7	C	2630	LHG	O7-C7	2.91	1.43	1.34
10	C	603	CLA	O2D-CGD	2.93	1.40	1.33
9	H	609	CHL	O2D-CGD	2.93	1.40	1.33
7	G	6630	LHG	O7-C7	2.94	1.43	1.34
10	H	613	CLA	O2A-CGA	2.94	1.42	1.33
9	J	605	CHL	C1A-CHA	2.94	1.43	1.37
10	D	613	CLA	CMB-C2B	2.94	1.57	1.51
9	D	607	CHL	CMB-C2B	2.96	1.58	1.51
7	I	8630	LHG	O7-C7	2.96	1.43	1.34
10	D	602	CLA	C2-C3	2.97	1.38	1.33
9	I	606	CHL	C1A-CHA	2.97	1.43	1.37
4	J	9621	LUT	C1-C6	2.97	1.58	1.53
9	F	601	CHL	O2D-CGD	2.98	1.40	1.33
7	J	9630	LHG	O8-C23	2.98	1.42	1.33
10	G	602	CLA	O2A-CGA	2.98	1.42	1.33
10	C	613	CLA	O2A-CGA	2.99	1.42	1.33
10	D	603	CLA	O2D-CGD	3.00	1.40	1.33
9	H	608	CHL	O2D-CGD	3.00	1.40	1.33
7	D	3630	LHG	O8-C23	3.01	1.42	1.33
6	B	1623	NEX	C7-C8	3.01	1.37	1.32
9	I	605	CHL	C1A-CHA	3.02	1.43	1.37
9	B	601	CHL	C1A-CHA	3.02	1.43	1.37
10	J	602	CLA	O2A-CGA	3.03	1.42	1.33
9	F	607	CHL	CMB-C2B	3.04	1.58	1.51
9	J	607	CHL	C1A-CHA	3.04	1.43	1.37
10	B	602	CLA	C2-C3	3.04	1.38	1.33
9	E	606	CHL	C1A-CHA	3.05	1.43	1.37
9	A	606	CHL	O2D-CGD	3.06	1.41	1.33
10	A	612	CLA	O2A-CGA	3.07	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4620	LUT	C5-C6	3.08	1.39	1.34
10	C	612	CLA	O2A-CGA	3.10	1.42	1.33
9	J	601	CHL	C1A-CHA	3.11	1.44	1.37
9	H	606	CHL	C1A-CHA	3.11	1.44	1.37
9	A	609	CHL	C2-C3	3.13	1.39	1.33
9	J	607	CHL	CMB-C2B	3.14	1.58	1.51
10	C	602	CLA	C2-C3	3.15	1.39	1.33
9	H	607	CHL	C1A-CHA	3.16	1.44	1.37
7	H	7630	LHG	O7-C7	3.17	1.43	1.34
9	C	608	CHL	C2-C3	3.18	1.39	1.33
10	A	603	CLA	C2-C3	3.18	1.39	1.33
4	G	6620	LUT	C5-C6	3.18	1.39	1.34
9	E	605	CHL	C1A-CHA	3.19	1.44	1.37
10	A	602	CLA	C2-C3	3.19	1.39	1.33
9	I	606	CHL	O2D-CGD	3.19	1.41	1.33
9	F	601	CHL	C2-C3	3.20	1.39	1.33
9	D	608	CHL	O2D-CGD	3.20	1.41	1.33
10	A	614	CLA	O2D-CGD	3.20	1.41	1.33
10	J	612	CLA	O2A-CGA	3.20	1.43	1.33
9	J	609	CHL	C2-C3	3.21	1.39	1.33
4	A	621	LUT	C1-C6	3.21	1.58	1.53
10	B	610	CLA	C2-C3	3.22	1.39	1.33
10	B	603	CLA	O2D-CGD	3.22	1.41	1.33
4	J	9620	LUT	C5-C6	3.23	1.39	1.34
9	A	601	CHL	C2-C3	3.23	1.39	1.33
9	D	601	CHL	C2-C3	3.23	1.39	1.33
9	I	601	CHL	C2-C3	3.24	1.39	1.33
9	D	608	CHL	C2-C3	3.24	1.39	1.33
10	F	604	CLA	O2D-CGD	3.24	1.41	1.33
10	A	610	CLA	C2-C3	3.24	1.39	1.33
10	I	603	CLA	O2D-CGD	3.25	1.41	1.33
9	G	601	CHL	O2D-CGD	3.25	1.41	1.33
9	C	601	CHL	C2-C3	3.25	1.39	1.33
10	G	603	CLA	C2-C3	3.26	1.39	1.33
9	B	601	CHL	C2-C3	3.26	1.39	1.33
10	D	603	CLA	C2-C3	3.26	1.39	1.33
9	B	606	CHL	C1A-CHA	3.26	1.44	1.37
9	B	608	CHL	O2A-CGA	3.27	1.43	1.33
9	E	607	CHL	C2-C3	3.27	1.39	1.33
9	D	607	CHL	O2D-CGD	3.27	1.41	1.33
10	I	610	CLA	C2-C3	3.28	1.39	1.33
10	B	603	CLA	C2-C3	3.28	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	613	CLA	C2-C3	3.28	1.39	1.33
10	I	612	CLA	O2D-CGD	3.29	1.41	1.33
4	H	7620	LUT	C23-C24	3.29	1.53	1.50
10	H	612	CLA	O2D-CGD	3.30	1.41	1.33
10	F	602	CLA	O2A-CGA	3.30	1.43	1.33
9	D	609	CHL	C2-C3	3.31	1.39	1.33
9	G	608	CHL	C2-C3	3.32	1.39	1.33
9	I	608	CHL	O2D-CGD	3.32	1.41	1.33
10	G	612	CLA	O2A-CGA	3.32	1.43	1.33
9	E	607	CHL	C1A-CHA	3.32	1.44	1.37
10	I	603	CLA	C2-C3	3.33	1.39	1.33
10	H	603	CLA	C2-C3	3.33	1.39	1.33
9	I	601	CHL	O2D-CGD	3.33	1.41	1.33
10	E	604	CLA	O2A-CGA	3.33	1.43	1.33
10	I	612	CLA	O2A-CGA	3.34	1.43	1.33
9	G	601	CHL	C2-C3	3.34	1.39	1.33
10	J	604	CLA	C2-C3	3.35	1.39	1.33
10	C	603	CLA	C2-C3	3.35	1.39	1.33
9	D	606	CHL	O2D-CGD	3.35	1.41	1.33
10	E	604	CLA	C2-C3	3.35	1.39	1.33
9	I	609	CHL	C2-C3	3.35	1.39	1.33
9	C	609	CHL	C2-C3	3.35	1.39	1.33
9	C	607	CHL	C2-C3	3.35	1.39	1.33
9	J	607	CHL	C2-C3	3.36	1.39	1.33
9	A	609	CHL	O2D-CGD	3.36	1.41	1.33
10	G	604	CLA	O2A-CGA	3.36	1.43	1.33
10	E	603	CLA	C2-C3	3.36	1.39	1.33
9	F	609	CHL	C2-C3	3.36	1.39	1.33
10	I	602	CLA	O2A-CGA	3.36	1.43	1.33
9	G	609	CHL	C2-C3	3.37	1.39	1.33
9	D	607	CHL	C2-C3	3.37	1.39	1.33
9	I	607	CHL	CMB-C2B	3.37	1.58	1.51
10	I	611	CLA	C2-C3	3.38	1.39	1.33
10	F	611	CLA	C2-C3	3.38	1.39	1.33
10	E	602	CLA	C2-C3	3.38	1.39	1.33
7	E	4630	LHG	O8-C23	3.39	1.43	1.33
9	E	608	CHL	O2A-CGA	3.39	1.43	1.33
9	J	601	CHL	C2-C3	3.39	1.39	1.33
9	E	601	CHL	C2-C3	3.40	1.39	1.33
10	B	614	CLA	O2D-CGD	3.40	1.41	1.33
10	C	614	CLA	O2A-CGA	3.40	1.43	1.33
9	F	601	CHL	O2A-CGA	3.41	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	607	CHL	C2-C3	3.41	1.39	1.33
9	G	609	CHL	O2D-CGD	3.41	1.41	1.33
10	H	602	CLA	O2A-CGA	3.43	1.43	1.33
10	C	612	CLA	C2-C3	3.43	1.39	1.33
9	G	607	CHL	C2-C3	3.43	1.39	1.33
9	I	607	CHL	C2-C3	3.43	1.39	1.33
9	E	608	CHL	C2-C3	3.44	1.39	1.33
10	C	604	CLA	C2-C3	3.44	1.39	1.33
10	D	610	CLA	C2-C3	3.44	1.39	1.33
10	F	604	CLA	C2-C3	3.44	1.39	1.33
10	J	611	CLA	O2A-CGA	3.44	1.43	1.33
9	J	601	CHL	O2D-CGD	3.44	1.42	1.33
10	C	611	CLA	O2A-CGA	3.44	1.43	1.33
10	J	603	CLA	C2-C3	3.44	1.39	1.33
10	H	610	CLA	C2-C3	3.44	1.39	1.33
9	B	607	CHL	C1A-CHA	3.45	1.44	1.37
9	B	609	CHL	C2-C3	3.45	1.39	1.33
9	E	609	CHL	C2-C3	3.45	1.39	1.33
6	G	6623	NEX	C7-C8	3.45	1.38	1.32
9	H	601	CHL	C2-C3	3.45	1.39	1.33
9	A	601	CHL	O2D-CGD	3.45	1.42	1.33
10	C	610	CLA	C2-C3	3.46	1.39	1.33
10	D	613	CLA	C2-C3	3.46	1.39	1.33
9	C	607	CHL	C1A-CHA	3.46	1.44	1.37
10	F	604	CLA	O2A-CGA	3.46	1.43	1.33
9	B	601	CHL	O2D-CGD	3.46	1.42	1.33
10	B	611	CLA	C2-C3	3.47	1.39	1.33
10	G	611	CLA	O2D-CGD	3.47	1.42	1.33
7	H	7630	LHG	O8-C23	3.47	1.43	1.33
9	C	608	CHL	O2D-CGD	3.47	1.42	1.33
10	E	613	CLA	C2-C3	3.47	1.39	1.33
9	A	608	CHL	C2-C3	3.48	1.39	1.33
9	F	607	CHL	C2-C3	3.48	1.39	1.33
9	H	607	CHL	C2-C3	3.48	1.39	1.33
9	H	609	CHL	C2-C3	3.48	1.39	1.33
6	C	2623	NEX	C7-C8	3.48	1.38	1.32
10	I	604	CLA	C2-C3	3.49	1.39	1.33
9	J	608	CHL	C2-C3	3.49	1.39	1.33
10	D	611	CLA	C2-C3	3.49	1.39	1.33
10	G	604	CLA	C2-C3	3.49	1.39	1.33
10	E	611	CLA	C2-C3	3.49	1.39	1.33
10	J	610	CLA	C2-C3	3.49	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	602	CLA	O2A-CGA	3.50	1.43	1.33
9	B	607	CHL	O2A-CGA	3.50	1.43	1.33
10	G	613	CLA	O2A-CGA	3.50	1.43	1.33
10	A	612	CLA	C2-C3	3.50	1.39	1.33
10	E	610	CLA	C2-C3	3.50	1.39	1.33
10	H	611	CLA	O2A-CGA	3.50	1.43	1.33
10	A	604	CLA	C2-C3	3.51	1.39	1.33
9	A	607	CHL	O2D-CGD	3.51	1.42	1.33
9	F	608	CHL	O2D-CGD	3.51	1.42	1.33
10	B	604	CLA	C2-C3	3.51	1.39	1.33
10	J	611	CLA	C2-C3	3.51	1.39	1.33
10	B	613	CLA	C2-C3	3.51	1.39	1.33
10	A	611	CLA	C2-C3	3.51	1.39	1.33
9	H	601	CHL	O2D-CGD	3.52	1.42	1.33
10	G	611	CLA	C2-C3	3.52	1.39	1.33
10	E	603	CLA	O2D-CGD	3.52	1.42	1.33
9	J	606	CHL	O2D-CGD	3.52	1.42	1.33
9	C	607	CHL	O2A-CGA	3.52	1.43	1.33
9	G	609	CHL	O2A-CGA	3.53	1.43	1.33
4	J	9620	LUT	C23-C24	3.53	1.53	1.50
10	E	614	CLA	O2D-CGD	3.53	1.42	1.33
9	J	606	CHL	C1A-CHA	3.53	1.44	1.37
9	H	608	CHL	C2-C3	3.53	1.39	1.33
9	J	609	CHL	O2D-CGD	3.53	1.42	1.33
9	F	606	CHL	C1A-CHA	3.53	1.44	1.37
9	F	606	CHL	O2D-CGD	3.53	1.42	1.33
9	I	605	CHL	O2D-CGD	3.54	1.42	1.33
6	F	5623	NEX	C7-C8	3.54	1.38	1.32
10	I	613	CLA	C2-C3	3.54	1.39	1.33
10	J	613	CLA	C2-C3	3.54	1.39	1.33
10	F	610	CLA	C2-C3	3.54	1.39	1.33
10	G	610	CLA	C2-C3	3.55	1.39	1.33
6	H	7623	NEX	C7-C8	3.55	1.38	1.32
9	B	606	CHL	O2D-CGD	3.55	1.42	1.33
10	H	604	CLA	C2-C3	3.55	1.39	1.33
9	I	608	CHL	C2-C3	3.56	1.39	1.33
10	H	603	CLA	O2A-CGA	3.57	1.44	1.33
9	F	608	CHL	C2-C3	3.57	1.40	1.33
10	F	603	CLA	C2-C3	3.57	1.40	1.33
10	A	613	CLA	O2A-CGA	3.57	1.44	1.33
10	A	613	CLA	C2-C3	3.57	1.40	1.33
10	C	611	CLA	C2-C3	3.58	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	607	CHL	C2-C3	3.58	1.40	1.33
10	E	612	CLA	C2-C3	3.58	1.40	1.33
10	F	613	CLA	O2A-CGA	3.59	1.44	1.33
9	E	607	CHL	O2A-CGA	3.59	1.44	1.33
10	D	604	CLA	C2-C3	3.59	1.40	1.33
10	H	611	CLA	C2-C3	3.60	1.40	1.33
9	I	607	CHL	C1A-CHA	3.60	1.44	1.37
10	H	613	CLA	C2-C3	3.60	1.40	1.33
10	D	612	CLA	C2-C3	3.61	1.40	1.33
10	E	613	CLA	O2A-CGA	3.62	1.44	1.33
9	B	609	CHL	O2D-CGD	3.62	1.42	1.33
10	F	613	CLA	C2-C3	3.62	1.40	1.33
10	C	611	CLA	O2D-CGD	3.63	1.42	1.33
6	J	9623	NEX	C7-C8	3.63	1.38	1.32
9	C	609	CHL	O2D-CGD	3.63	1.42	1.33
10	I	614	CLA	O2D-CGD	3.63	1.42	1.33
10	I	612	CLA	C2-C3	3.63	1.40	1.33
6	I	8623	NEX	C7-C8	3.64	1.38	1.32
10	A	603	CLA	O2A-CGA	3.64	1.44	1.33
10	C	612	CLA	O2D-CGD	3.64	1.42	1.33
7	A	630	LHG	O8-C23	3.65	1.44	1.33
9	E	605	CHL	O2A-CGA	3.66	1.44	1.33
10	G	612	CLA	C2-C3	3.66	1.40	1.33
9	D	609	CHL	O2D-CGD	3.66	1.42	1.33
6	E	4623	NEX	C7-C8	3.67	1.39	1.32
9	D	608	CHL	O2A-CGA	3.67	1.44	1.33
9	G	607	CHL	C1A-CHA	3.67	1.45	1.37
10	G	604	CLA	O2D-CGD	3.67	1.42	1.33
10	D	614	CLA	O2A-CGA	3.68	1.44	1.33
10	J	612	CLA	C2-C3	3.69	1.40	1.33
10	H	603	CLA	O2D-CGD	3.69	1.42	1.33
9	B	608	CHL	C2-C3	3.70	1.40	1.33
10	G	603	CLA	O2A-CGA	3.70	1.44	1.33
7	F	5630	LHG	O8-C23	3.72	1.44	1.33
9	G	607	CHL	O2A-CGA	3.72	1.44	1.33
10	I	611	CLA	O2D-CGD	3.72	1.42	1.33
10	G	603	CLA	O2D-CGD	3.73	1.42	1.33
10	C	602	CLA	O2A-CGA	3.73	1.44	1.33
10	J	612	CLA	O2D-CGD	3.73	1.42	1.33
9	G	601	CHL	O2A-CGA	3.73	1.44	1.33
9	A	607	CHL	O2A-CGA	3.73	1.44	1.33
9	B	607	CHL	O2D-CGD	3.74	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	613	CLA	O2A-CGA	3.74	1.44	1.33
10	F	612	CLA	O2A-CGA	3.74	1.44	1.33
10	J	613	CLA	O2A-CGA	3.74	1.44	1.33
9	G	606	CHL	O2D-CGD	3.75	1.42	1.33
10	J	611	CLA	O2D-CGD	3.77	1.42	1.33
10	B	612	CLA	C2-C3	3.77	1.40	1.33
9	A	608	CHL	O2A-CGA	3.77	1.44	1.33
10	B	613	CLA	O2A-CGA	3.77	1.44	1.33
10	E	612	CLA	O2A-CGA	3.78	1.44	1.33
10	C	604	CLA	O2D-CGD	3.78	1.42	1.33
9	F	607	CHL	O2A-CGA	3.78	1.44	1.33
9	J	605	CHL	O2D-CGD	3.78	1.42	1.33
10	D	611	CLA	O2A-CGA	3.79	1.44	1.33
9	I	601	CHL	O2A-CGA	3.79	1.44	1.33
10	G	613	CLA	C2-C3	3.79	1.40	1.33
10	B	612	CLA	O2A-CGA	3.80	1.44	1.33
10	H	612	CLA	C2-C3	3.80	1.40	1.33
10	A	613	CLA	O2D-CGD	3.81	1.42	1.33
9	C	609	CHL	O2A-CGA	3.81	1.44	1.33
9	H	607	CHL	O2A-CGA	3.81	1.44	1.33
9	B	605	CHL	O2D-CGD	3.81	1.42	1.33
10	G	614	CLA	O2D-CGD	3.82	1.42	1.33
9	A	601	CHL	O2A-CGA	3.82	1.44	1.33
10	J	614	CLA	O2D-CGD	3.82	1.43	1.33
10	F	603	CLA	O2D-CGD	3.82	1.43	1.33
10	F	612	CLA	C2-C3	3.83	1.40	1.33
9	D	601	CHL	O2D-CGD	3.83	1.43	1.33
6	A	623	NEX	C7-C8	3.84	1.39	1.32
9	I	609	CHL	O2D-CGD	3.84	1.43	1.33
10	D	612	CLA	O2D-CGD	3.85	1.43	1.33
9	G	607	CHL	O2D-CGD	3.85	1.43	1.33
10	D	612	CLA	O2A-CGA	3.86	1.44	1.33
10	I	603	CLA	O2A-CGA	3.86	1.45	1.33
10	A	611	CLA	O2D-CGD	3.86	1.43	1.33
9	A	606	CHL	C1A-CHA	3.87	1.45	1.37
10	I	604	CLA	O2A-CGA	3.87	1.45	1.33
10	A	602	CLA	O2A-CGA	3.87	1.45	1.33
10	C	613	CLA	O2D-CGD	3.87	1.43	1.33
10	D	611	CLA	O2D-CGD	3.88	1.43	1.33
9	C	606	CHL	O2D-CGD	3.88	1.43	1.33
10	F	611	CLA	O2A-CGA	3.88	1.45	1.33
9	J	601	CHL	O2A-CGA	3.88	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	607	CHL	C1A-CHA	3.89	1.45	1.37
10	G	612	CLA	O2D-CGD	3.89	1.43	1.33
10	D	614	CLA	O2D-CGD	3.89	1.43	1.33
9	I	608	CHL	O2A-CGA	3.89	1.45	1.33
10	E	611	CLA	O2A-CGA	3.90	1.45	1.33
9	E	607	CHL	O2D-CGD	3.90	1.43	1.33
9	G	608	CHL	O2D-CGD	3.91	1.43	1.33
10	A	612	CLA	O2D-CGD	3.91	1.43	1.33
10	F	612	CLA	O2D-CGD	3.91	1.43	1.33
10	H	604	CLA	O2D-CGD	3.92	1.43	1.33
10	H	612	CLA	O2A-CGA	3.92	1.45	1.33
10	B	611	CLA	O2D-CGD	3.92	1.43	1.33
10	J	604	CLA	O2A-CGA	3.93	1.45	1.33
10	E	603	CLA	O2A-CGA	3.93	1.45	1.33
9	I	607	CHL	O2A-CGA	3.93	1.45	1.33
10	A	604	CLA	O2D-CGD	3.93	1.43	1.33
4	I	8621	LUT	C23-C24	3.94	1.53	1.50
10	F	603	CLA	O2A-CGA	3.94	1.45	1.33
9	D	601	CHL	O2A-CGA	3.94	1.45	1.33
4	F	5620	LUT	C23-C24	3.94	1.53	1.50
10	B	611	CLA	O2A-CGA	3.94	1.45	1.33
9	C	601	CHL	O2D-CGD	3.95	1.43	1.33
9	C	608	CHL	O2A-CGA	3.95	1.45	1.33
10	I	613	CLA	O2D-CGD	3.95	1.43	1.33
7	J	9630	LHG	O7-C7	3.95	1.46	1.34
10	D	603	CLA	O2A-CGA	3.95	1.45	1.33
9	E	605	CHL	O2D-CGD	3.96	1.43	1.33
9	E	609	CHL	O2A-CGA	3.96	1.45	1.33
6	D	3623	NEX	C7-C8	3.96	1.39	1.32
9	J	607	CHL	O2D-CGD	3.97	1.43	1.33
10	G	613	CLA	O2D-CGD	3.97	1.43	1.33
10	A	611	CLA	O2A-CGA	3.98	1.45	1.33
7	C	2630	LHG	O8-C23	3.99	1.45	1.33
10	H	604	CLA	O2A-CGA	4.00	1.45	1.33
9	B	608	CHL	O2D-CGD	4.00	1.43	1.33
9	A	607	CHL	C1A-CHA	4.00	1.45	1.37
10	G	611	CLA	O2A-CGA	4.00	1.45	1.33
9	C	605	CHL	O2D-CGD	4.01	1.43	1.33
9	E	606	CHL	O2D-CGD	4.02	1.43	1.33
9	H	609	CHL	O2A-CGA	4.02	1.45	1.33
10	J	610	CLA	O2D-CGD	4.02	1.43	1.33
10	C	614	CLA	O2D-CGD	4.02	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	603	CLA	O2D-CGD	4.03	1.43	1.33
10	F	614	CLA	O2A-CGA	4.03	1.45	1.33
7	F	5630	LHG	O7-C7	4.04	1.46	1.34
4	D	3620	LUT	C23-C24	4.04	1.53	1.50
10	D	602	CLA	O2A-CGA	4.05	1.45	1.33
10	D	604	CLA	O2D-CGD	4.05	1.43	1.33
9	A	608	CHL	O2D-CGD	4.06	1.43	1.33
10	B	614	CLA	O2A-CGA	4.06	1.45	1.33
10	F	611	CLA	O2D-CGD	4.07	1.43	1.33
9	F	608	CHL	O2A-CGA	4.07	1.45	1.33
10	B	612	CLA	O2D-CGD	4.07	1.43	1.33
10	F	614	CLA	O2D-CGD	4.07	1.43	1.33
10	E	614	CLA	O2A-CGA	4.08	1.45	1.33
9	H	606	CHL	O2D-CGD	4.08	1.43	1.33
10	A	603	CLA	O2D-CGD	4.10	1.43	1.33
4	G	6620	LUT	C23-C24	4.10	1.53	1.50
9	H	608	CHL	O2A-CGA	4.10	1.45	1.33
9	B	605	CHL	O2A-CGA	4.12	1.45	1.33
9	H	605	CHL	O2D-CGD	4.12	1.43	1.33
10	E	611	CLA	O2D-CGD	4.12	1.43	1.33
10	B	604	CLA	O2D-CGD	4.13	1.43	1.33
9	B	609	CHL	O2A-CGA	4.13	1.45	1.33
10	G	614	CLA	O2A-CGA	4.14	1.45	1.33
7	G	6630	LHG	O8-C23	4.14	1.45	1.33
9	H	601	CHL	O2A-CGA	4.14	1.45	1.33
4	J	9621	LUT	C23-C24	4.14	1.53	1.50
10	F	602	CLA	O2D-CGD	4.15	1.43	1.33
9	E	601	CHL	O2D-CGD	4.15	1.43	1.33
10	J	614	CLA	O2A-CGA	4.15	1.45	1.33
9	G	605	CHL	O2A-CGA	4.16	1.45	1.33
4	A	620	LUT	C23-C24	4.16	1.53	1.50
10	C	603	CLA	O2A-CGA	4.17	1.45	1.33
10	I	602	CLA	O2D-CGD	4.18	1.43	1.33
9	F	607	CHL	C1A-CHA	4.19	1.46	1.37
9	D	609	CHL	O2A-CGA	4.20	1.46	1.33
10	H	614	CLA	O2A-CGA	4.20	1.46	1.33
10	I	604	CLA	O2D-CGD	4.21	1.43	1.33
9	B	601	CHL	O2A-CGA	4.22	1.46	1.33
10	B	603	CLA	O2A-CGA	4.22	1.46	1.33
9	J	608	CHL	O2A-CGA	4.25	1.46	1.33
9	A	605	CHL	O2D-CGD	4.26	1.44	1.33
10	E	602	CLA	O2A-CGA	4.27	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	613	CLA	O2D-CGD	4.27	1.44	1.33
10	B	610	CLA	O2D-CGD	4.27	1.44	1.33
9	G	605	CHL	O2D-CGD	4.28	1.44	1.33
10	B	604	CLA	O2A-CGA	4.28	1.46	1.33
9	A	609	CHL	O2A-CGA	4.29	1.46	1.33
10	C	604	CLA	O2A-CGA	4.30	1.46	1.33
4	I	8620	LUT	C23-C24	4.30	1.53	1.50
10	G	602	CLA	O2D-CGD	4.32	1.44	1.33
10	C	602	CLA	O2D-CGD	4.33	1.44	1.33
10	J	602	CLA	O2D-CGD	4.33	1.44	1.33
9	J	609	CHL	O2A-CGA	4.34	1.46	1.33
10	I	614	CLA	O2A-CGA	4.34	1.46	1.33
10	H	611	CLA	O2D-CGD	4.37	1.44	1.33
9	J	605	CHL	O2A-CGA	4.38	1.46	1.33
9	F	609	CHL	O2A-CGA	4.38	1.46	1.33
10	F	610	CLA	O2D-CGD	4.38	1.44	1.33
10	D	602	CLA	O2D-CGD	4.40	1.44	1.33
4	B	1621	LUT	C23-C24	4.41	1.54	1.50
10	A	614	CLA	O2A-CGA	4.41	1.46	1.33
9	G	608	CHL	O2A-CGA	4.41	1.46	1.33
10	I	611	CLA	O2A-CGA	4.42	1.46	1.33
10	E	602	CLA	O2D-CGD	4.45	1.44	1.33
10	B	602	CLA	O2D-CGD	4.46	1.44	1.33
4	C	2620	LUT	C23-C24	4.48	1.54	1.50
10	G	610	CLA	O2A-CGA	4.49	1.46	1.33
7	I	8630	LHG	O8-C23	4.50	1.46	1.33
10	H	610	CLA	O2A-CGA	4.54	1.47	1.33
10	J	603	CLA	O2A-CGA	4.55	1.47	1.33
9	H	607	CHL	O2D-CGD	4.55	1.44	1.33
10	D	604	CLA	O2A-CGA	4.56	1.47	1.33
9	D	605	CHL	O2A-CGA	4.56	1.47	1.33
10	J	604	CLA	O2D-CGD	4.56	1.44	1.33
10	E	613	CLA	O2D-CGD	4.56	1.44	1.33
10	D	613	CLA	O2A-CGA	4.58	1.47	1.33
10	G	610	CLA	O2D-CGD	4.58	1.44	1.33
10	A	610	CLA	O2D-CGD	4.58	1.44	1.33
10	I	610	CLA	O2A-CGA	4.59	1.47	1.33
10	D	613	CLA	O2D-CGD	4.59	1.44	1.33
9	C	607	CHL	O2D-CGD	4.60	1.44	1.33
10	E	612	CLA	O2D-CGD	4.61	1.45	1.33
7	B	1630	LHG	O8-C23	4.65	1.47	1.33
9	F	605	CHL	O2A-CGA	4.67	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	605	CHL	O2D-CGD	4.68	1.45	1.33
9	E	601	CHL	O2A-CGA	4.70	1.47	1.33
9	C	605	CHL	O2A-CGA	4.71	1.47	1.33
9	H	606	CHL	O2A-CGA	4.71	1.47	1.33
10	A	602	CLA	O2D-CGD	4.71	1.45	1.33
9	E	608	CHL	O2D-CGD	4.72	1.45	1.33
10	B	613	CLA	O2D-CGD	4.73	1.45	1.33
10	B	610	CLA	O2A-CGA	4.74	1.47	1.33
9	E	606	CHL	O2A-CGA	4.75	1.47	1.33
4	H	7621	LUT	C23-C24	4.76	1.54	1.50
9	D	605	CHL	O2D-CGD	4.76	1.45	1.33
9	I	609	CHL	O2A-CGA	4.76	1.47	1.33
10	A	610	CLA	O2A-CGA	4.76	1.47	1.33
10	C	610	CLA	O2A-CGA	4.77	1.47	1.33
10	D	610	CLA	O2A-CGA	4.78	1.47	1.33
4	F	5621	LUT	C23-C24	4.79	1.54	1.50
10	C	610	CLA	O2D-CGD	4.79	1.45	1.33
10	F	613	CLA	O2D-CGD	4.80	1.45	1.33
10	D	610	CLA	O2D-CGD	4.81	1.45	1.33
10	E	604	CLA	O2D-CGD	4.81	1.45	1.33
9	I	605	CHL	O2A-CGA	4.83	1.47	1.33
9	A	605	CHL	O2A-CGA	4.84	1.47	1.33
10	E	610	CLA	O2D-CGD	4.85	1.45	1.33
10	E	610	CLA	O2A-CGA	4.86	1.48	1.33
4	B	1620	LUT	C23-C24	4.88	1.54	1.50
4	A	621	LUT	C23-C24	4.90	1.54	1.50
10	H	613	CLA	O2D-CGD	4.90	1.45	1.33
10	A	604	CLA	O2A-CGA	4.95	1.48	1.33
4	E	4620	LUT	C23-C24	4.95	1.54	1.50
4	G	6621	LUT	C23-C24	4.98	1.54	1.50
9	B	606	CHL	O2A-CGA	5.00	1.48	1.33
9	F	607	CHL	O2D-CGD	5.03	1.46	1.33
9	I	607	CHL	O2D-CGD	5.06	1.46	1.33
4	D	3621	LUT	C23-C24	5.07	1.54	1.50
10	F	610	CLA	O2A-CGA	5.08	1.48	1.33
10	H	602	CLA	O2D-CGD	5.09	1.46	1.33
10	I	610	CLA	O2D-CGD	5.11	1.46	1.33
10	H	610	CLA	O2D-CGD	5.12	1.46	1.33
8	H	6632	DGD	O2G-C1B	5.17	1.49	1.34
9	H	605	CHL	O2A-CGA	5.18	1.48	1.33
10	J	610	CLA	O2A-CGA	5.19	1.49	1.33
4	E	4621	LUT	C23-C24	5.34	1.54	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	8632	DGD	O2G-C1B	5.67	1.51	1.34
9	I	606	CHL	O2A-CGA	5.73	1.50	1.33
8	A	632	DGD	O2G-C1B	5.75	1.51	1.34
8	B	2632	DGD	O2G-C1B	5.82	1.51	1.34
8	B	1632	DGD	O2G-C1B	5.86	1.51	1.34
8	H	7632	DGD	O2G-C1B	5.90	1.52	1.34
8	D	3632	DGD	O2G-C1B	5.91	1.52	1.34
9	J	606	CHL	O2A-CGA	5.93	1.51	1.33
8	D	5632	DGD	O2G-C1B	5.95	1.52	1.34
9	F	606	CHL	O2A-CGA	6.01	1.51	1.33
9	A	606	CHL	O2A-CGA	6.05	1.51	1.33
9	D	606	CHL	O2A-CGA	6.13	1.51	1.33
9	C	606	CHL	O2A-CGA	6.14	1.51	1.33
8	E	4632	DGD	O2G-C1B	6.24	1.53	1.34
4	C	2621	LUT	C23-C24	6.25	1.55	1.50
9	G	606	CHL	O2A-CGA	6.34	1.52	1.33
8	G	9632	DGD	O2G-C1B	6.70	1.54	1.34

All (2319) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	614	CLA	O1D-CGD-CBD	-9.15	111.51	124.62
10	B	614	CLA	O1D-CGD-CBD	-8.66	112.20	124.62
10	I	614	CLA	O1D-CGD-CBD	-8.25	112.79	124.62
10	H	614	CLA	O1D-CGD-CBD	-8.25	112.80	124.62
10	E	614	CLA	O1D-CGD-CBD	-8.24	112.82	124.62
10	A	614	CLA	O1D-CGD-CBD	-8.15	112.94	124.62
10	D	614	CLA	O1D-CGD-CBD	-7.72	113.56	124.62
10	F	614	CLA	O1D-CGD-CBD	-7.61	113.72	124.62
10	J	614	CLA	O1D-CGD-CBD	-7.58	113.76	124.62
10	G	614	CLA	O1D-CGD-CBD	-7.28	114.19	124.62
10	D	604	CLA	CMB-C2B-C1B	-7.21	116.43	128.36
10	G	613	CLA	CMB-C2B-C1B	-7.20	116.45	128.36
10	C	604	CLA	CMB-C2B-C1B	-7.20	116.46	128.36
10	A	604	CLA	CMB-C2B-C1B	-7.13	116.57	128.36
10	I	613	CLA	CMB-C2B-C1B	-7.10	116.62	128.36
10	D	613	CLA	CMB-C2B-C1B	-7.07	116.67	128.36
10	C	613	CLA	CMB-C2B-C1B	-6.91	116.93	128.36
9	E	606	CHL	CBA-CAA-C2A	-6.90	94.28	113.73
10	F	604	CLA	CMB-C2B-C1B	-6.86	117.02	128.36
10	B	613	CLA	CMB-C2B-C1B	-6.86	117.02	128.36
10	H	613	CLA	CMB-C2B-C1B	-6.85	117.03	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	604	CLA	CMB-C2B-C1B	-6.83	117.06	128.36
10	B	604	CLA	CMB-C2B-C1B	-6.69	117.29	128.36
10	F	613	CLA	CMB-C2B-C1B	-6.59	117.45	128.36
10	G	604	CLA	CMB-C2B-C1B	-6.58	117.47	128.36
10	I	602	CLA	O1D-CGD-CBD	-6.53	115.26	124.62
10	I	604	CLA	CMB-C2B-C1B	-6.51	117.59	128.36
10	J	611	CLA	CAA-C2A-C3A	-6.40	94.83	113.22
10	J	604	CLA	CMB-C2B-C1B	-6.37	117.83	128.36
10	G	612	CLA	O1D-CGD-CBD	-6.06	115.94	124.62
9	D	606	CHL	CBA-CAA-C2A	-5.99	96.84	113.73
10	H	604	CLA	CMB-C2B-C1B	-5.96	118.51	128.36
10	C	611	CLA	CAA-C2A-C3A	-5.93	96.16	113.22
9	I	606	CHL	CBA-CAA-C2A	-5.89	97.12	113.73
10	C	603	CLA	O1D-CGD-CBD	-5.85	116.24	124.62
10	H	604	CLA	O1D-CGD-CBD	-5.81	116.30	124.62
10	A	603	CLA	O1D-CGD-CBD	-5.77	116.35	124.62
10	F	611	CLA	CAA-C2A-C3A	-5.64	97.00	113.22
10	E	604	CLA	CAA-C2A-C3A	-5.51	97.37	113.22
10	D	612	CLA	O1D-CGD-CBD	-5.47	116.78	124.62
10	E	602	CLA	O1D-CGD-CBD	-5.43	116.85	124.62
10	I	612	CLA	O1D-CGD-CBD	-5.41	116.86	124.62
10	J	603	CLA	O1D-CGD-CBD	-5.39	116.90	124.62
10	B	603	CLA	O1D-CGD-CBD	-5.33	116.98	124.62
10	G	613	CLA	C4-C3-C5	-5.33	107.27	115.41
10	B	602	CLA	O1D-CGD-CBD	-5.31	117.01	124.62
4	H	7620	LUT	C38-C25-C24	-5.19	112.12	123.59
4	J	9620	LUT	C38-C25-C24	-5.18	112.15	123.59
10	D	604	CLA	CAA-C2A-C3A	-5.17	98.36	113.22
10	E	613	CLA	CMB-C2B-C1B	-5.14	119.86	128.36
10	C	612	CLA	O1D-CGD-CBD	-5.14	117.25	124.62
9	A	606	CHL	CBA-CAA-C2A	-5.08	99.40	113.73
10	D	604	CLA	O1D-CGD-CBD	-5.08	117.34	124.62
10	C	604	CLA	CAA-C2A-C3A	-5.01	98.82	113.22
10	B	611	CLA	CAA-C2A-C3A	-5.00	98.83	113.22
10	J	602	CLA	O1D-CGD-CBD	-4.99	117.47	124.62
9	C	606	CHL	CBA-CAA-C2A	-4.97	99.73	113.73
10	H	603	CLA	O1D-CGD-CBD	-4.91	117.59	124.62
10	I	604	CLA	O1D-CGD-CBD	-4.90	117.60	124.62
10	C	602	CLA	O1D-CGD-CBD	-4.86	117.65	124.62
9	F	607	CHL	C4-C3-C5	-4.82	108.04	115.41
10	J	612	CLA	O1D-CGD-CBD	-4.80	117.74	124.62
10	G	603	CLA	O1D-CGD-CBD	-4.80	117.74	124.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	604	CLA	O1D-CGD-CBD	-4.78	117.77	124.62
10	A	612	CLA	O1D-CGD-CBD	-4.78	117.77	124.62
10	J	613	CLA	CMB-C2B-C1B	-4.78	120.46	128.36
4	F	5621	LUT	C38-C25-C24	-4.77	113.06	123.59
10	F	612	CLA	O1D-CGD-CBD	-4.76	117.80	124.62
10	H	602	CLA	O1D-CGD-CBD	-4.75	117.81	124.62
4	I	8620	LUT	C38-C25-C24	-4.71	113.18	123.59
10	D	602	CLA	O1D-CGD-CBD	-4.71	117.87	124.62
4	B	1621	LUT	C38-C25-C24	-4.70	113.20	123.59
10	E	603	CLA	O1D-CGD-CBD	-4.69	117.90	124.62
10	B	604	CLA	CAA-C2A-C3A	-4.68	99.77	113.22
10	E	612	CLA	O1D-CGD-CBD	-4.67	117.94	124.62
10	I	603	CLA	O1D-CGD-CBD	-4.66	117.95	124.62
10	H	612	CLA	O1D-CGD-CBD	-4.65	117.96	124.62
10	G	602	CLA	O1D-CGD-CBD	-4.62	118.00	124.62
10	J	604	CLA	CAA-C2A-C3A	-4.60	99.99	113.22
10	A	602	CLA	O1D-CGD-CBD	-4.57	118.07	124.62
10	F	602	CLA	C5-C3-C2	-4.55	112.42	121.05
10	J	613	CLA	C4-C3-C5	-4.54	108.48	115.41
4	A	620	LUT	C38-C25-C24	-4.51	113.62	123.59
4	I	8621	LUT	C38-C25-C24	-4.51	113.63	123.59
4	G	6620	LUT	C38-C25-C24	-4.47	113.71	123.59
9	I	607	CHL	C4-C3-C5	-4.47	108.59	115.41
10	G	604	CLA	CAA-C2A-C3A	-4.44	100.44	113.22
10	F	604	CLA	O1D-CGD-CBD	-4.40	118.32	124.62
10	E	613	CLA	C4-C3-C5	-4.40	108.69	115.41
10	G	611	CLA	CAA-C2A-C3A	-4.37	100.64	113.22
10	J	602	CLA	C5-C3-C2	-4.37	112.76	121.05
4	D	3620	LUT	C38-C25-C24	-4.37	113.94	123.59
10	A	604	CLA	CAA-C2A-C3A	-4.34	100.73	113.22
10	H	613	CLA	C4-C3-C5	-4.34	108.78	115.41
10	D	603	CLA	O1D-CGD-CBD	-4.33	118.41	124.62
10	I	602	CLA	C5-C3-C2	-4.32	112.86	121.05
10	H	614	CLA	CMB-C2B-C1B	-4.31	121.23	128.36
10	B	611	CLA	CMB-C2B-C1B	-4.31	121.24	128.36
10	H	604	CLA	CAA-C2A-C3A	-4.30	100.85	113.22
10	A	614	CLA	CMB-C2B-C1B	-4.29	121.26	128.36
10	J	604	CLA	O1D-CGD-CBD	-4.29	118.48	124.62
4	F	5620	LUT	C38-C25-C24	-4.27	114.15	123.59
4	H	7621	LUT	C38-C25-C24	-4.26	114.18	123.59
10	G	602	CLA	C5-C3-C2	-4.23	113.02	121.05
10	H	612	CLA	C4-C3-C5	-4.23	108.95	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	603	CLA	O1D-CGD-CBD	-4.22	118.57	124.62
10	A	604	CLA	O1D-CGD-CBD	-4.21	118.58	124.62
10	A	610	CLA	CMB-C2B-C1B	-4.21	121.40	128.36
10	F	603	CLA	CMB-C2B-C1B	-4.21	121.40	128.36
4	J	9621	LUT	C38-C25-C24	-4.21	114.29	123.59
4	B	1620	LUT	C38-C25-C24	-4.18	114.35	123.59
9	E	607	CHL	C7-C6-C5	-4.18	100.72	113.06
10	I	612	CLA	OBD-CAD-CBD	-4.17	119.64	125.94
10	H	602	CLA	C5-C3-C2	-4.16	113.16	121.05
10	I	613	CLA	C4-C3-C5	-4.13	109.10	115.41
4	E	4620	LUT	C38-C25-C24	-4.13	114.47	123.59
4	C	2620	LUT	C38-C25-C24	-4.11	114.50	123.59
10	B	602	CLA	C5-C3-C2	-4.11	113.26	121.05
4	A	621	LUT	C38-C25-C24	-4.11	114.52	123.59
10	F	614	CLA	CMB-C2B-C1B	-4.10	121.58	128.36
10	G	614	CLA	CMB-C2B-C1B	-4.09	121.60	128.36
10	B	614	CLA	CMB-C2B-C1B	-4.09	121.60	128.36
10	F	610	CLA	CMB-C2B-C1B	-4.06	121.64	128.36
10	C	603	CLA	CMB-C2B-C1B	-4.05	121.66	128.36
10	A	613	CLA	C4-C3-C5	-4.05	109.22	115.41
4	J	9620	LUT	C18-C5-C4	-4.04	106.86	114.24
10	A	613	CLA	CMB-C2B-C1B	-4.04	121.69	128.36
10	I	612	CLA	C4-C3-C5	-4.03	109.25	115.41
10	D	611	CLA	CMB-C2B-C1B	-4.02	121.71	128.36
4	E	4620	LUT	C18-C5-C4	-3.98	106.97	114.24
10	J	603	CLA	C4-C3-C5	-3.97	109.34	115.41
10	J	610	CLA	CMB-C2B-C1B	-3.97	121.80	128.36
10	J	614	CLA	CMB-C2B-C1B	-3.97	121.80	128.36
10	C	604	CLA	O1D-CGD-CBD	-3.96	118.94	124.62
9	B	607	CHL	C4-C3-C5	-3.96	109.37	115.41
4	A	621	LUT	C23-C24-C25	-3.95	121.53	125.22
10	D	614	CLA	CMB-C2B-C1B	-3.95	121.83	128.36
10	C	602	CLA	C5-C3-C2	-3.94	113.58	121.05
10	F	612	CLA	CMB-C2B-C1B	-3.94	121.85	128.36
9	B	606	CHL	CAA-C2A-C3A	-3.90	102.00	113.22
10	A	611	CLA	CAA-C2A-C3A	-3.89	102.02	113.22
10	G	612	CLA	CMB-C2B-C1B	-3.89	121.93	128.36
10	F	613	CLA	C4-C3-C5	-3.88	109.48	115.41
10	B	612	CLA	O1D-CGD-CBD	-3.88	119.06	124.62
10	D	610	CLA	CMB-C2B-C1B	-3.88	121.95	128.36
10	H	611	CLA	CAA-C2A-C3A	-3.86	102.11	113.22
10	C	614	CLA	CMB-C2B-C1B	-3.85	122.00	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	7620	LUT	C18-C5-C4	-3.84	107.22	114.24
4	G	6620	LUT	C18-C5-C4	-3.83	107.25	114.24
10	H	612	CLA	OBD-CAD-CBD	-3.81	120.19	125.94
10	B	604	CLA	C4-C3-C5	-3.79	109.62	115.41
10	E	610	CLA	CMB-C2B-C1B	-3.78	122.11	128.36
10	J	611	CLA	CMB-C2B-C1B	-3.77	122.12	128.36
9	B	607	CHL	C7-C6-C5	-3.77	101.92	113.06
10	B	603	CLA	OBD-CAD-CBD	-3.75	120.28	125.94
4	D	3621	LUT	C38-C25-C24	-3.75	115.31	123.59
10	F	611	CLA	CMB-C2B-C1B	-3.75	122.17	128.36
10	F	602	CLA	O1D-CGD-CBD	-3.74	119.26	124.62
10	B	612	CLA	OBD-CAD-CBD	-3.73	120.30	125.94
9	E	601	CHL	C4-C3-C5	-3.73	109.71	115.41
4	D	3620	LUT	C18-C5-C4	-3.72	107.45	114.24
10	C	602	CLA	OBD-CAD-CBD	-3.71	120.34	125.94
10	I	614	CLA	CMB-C2B-C1B	-3.71	122.22	128.36
10	A	612	CLA	CMB-C2B-C1B	-3.71	122.22	128.36
10	H	612	CLA	CMB-C2B-C1B	-3.71	122.23	128.36
4	G	6621	LUT	C38-C25-C24	-3.71	115.41	123.59
10	E	612	CLA	CMB-C2B-C1B	-3.70	122.23	128.36
9	I	609	CHL	CAA-C2A-C3A	-3.70	102.57	113.22
10	C	612	CLA	CMB-C2B-C1B	-3.70	122.24	128.36
9	B	608	CHL	C4-C3-C5	-3.70	109.76	115.41
10	I	604	CLA	CAA-C2A-C3A	-3.69	102.61	113.22
10	C	611	CLA	CMB-C2B-C1B	-3.69	122.26	128.36
9	C	607	CHL	OBD-CAD-CBD	-3.68	120.38	125.94
4	A	620	LUT	C18-C5-C4	-3.68	107.51	114.24
10	I	611	CLA	OBD-CAD-CBD	-3.68	120.39	125.94
10	E	614	CLA	CMB-C2B-C1B	-3.67	122.29	128.36
10	I	611	CLA	CMB-C2B-C1B	-3.67	122.30	128.36
9	J	607	CHL	C4-C3-C5	-3.66	109.82	115.41
4	G	6621	LUT	C23-C24-C25	-3.66	121.80	125.22
10	B	604	CLA	O1D-CGD-CBD	-3.66	119.38	124.62
7	I	8630	LHG	O10-C23-C24	-3.66	109.09	123.72
10	J	602	CLA	OBD-CAD-CBD	-3.65	120.43	125.94
10	E	612	CLA	OBD-CAD-CBD	-3.64	120.45	125.94
9	H	608	CHL	C4-C3-C5	-3.63	109.86	115.41
10	E	611	CLA	CAA-C2A-C3A	-3.63	102.79	113.22
10	C	604	CLA	O1A-CGA-CBA	-3.63	109.22	123.72
10	G	602	CLA	CMB-C2B-C1B	-3.63	122.37	128.36
10	D	603	CLA	CMB-C2B-C1B	-3.62	122.37	128.36
10	A	602	CLA	CMB-C2B-C1B	-3.62	122.38	128.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	610	CLA	CMB-C2B-C1B	-3.62	122.38	128.36
4	D	3621	LUT	C23-C24-C25	-3.61	121.85	125.22
10	F	604	CLA	CAA-C2A-C3A	-3.60	102.86	113.22
10	A	612	CLA	OBD-CAD-CBD	-3.60	120.50	125.94
10	C	610	CLA	CMB-C2B-C1B	-3.60	122.41	128.36
10	D	603	CLA	OBD-CAD-CBD	-3.59	120.51	125.94
9	D	606	CHL	OBD-CAD-CBD	-3.59	120.52	125.94
10	C	612	CLA	OBD-CAD-CBD	-3.59	120.53	125.94
4	F	5621	LUT	C23-C24-C25	-3.59	121.87	125.22
10	J	612	CLA	CMB-C2B-C1B	-3.58	122.44	128.36
10	D	604	CLA	O1A-CGA-CBA	-3.58	109.39	123.72
10	B	604	CLA	O1A-CGA-CBA	-3.58	109.40	123.72
10	J	602	CLA	CMB-C2B-C1B	-3.58	122.44	128.36
10	F	603	CLA	OBD-CAD-CBD	-3.56	120.57	125.94
10	D	613	CLA	C4-C3-C5	-3.54	110.00	115.41
10	F	612	CLA	OBD-CAD-CBD	-3.53	120.62	125.94
4	E	4621	LUT	C38-C25-C24	-3.52	115.81	123.59
10	H	602	CLA	OBD-CAD-CBD	-3.51	120.64	125.94
4	H	7621	LUT	C23-C24-C25	-3.51	121.94	125.22
10	I	603	CLA	OBD-CAD-CBD	-3.50	120.65	125.94
10	A	603	CLA	OBD-CAD-CBD	-3.50	120.65	125.94
9	D	605	CHL	OBD-CAD-CBD	-3.50	120.66	125.94
9	C	608	CHL	OBD-CAD-CBD	-3.50	120.66	125.94
10	E	602	CLA	OBD-CAD-CBD	-3.50	120.66	125.94
9	F	608	CHL	C4-C3-C5	-3.50	110.07	115.41
10	D	611	CLA	O1D-CGD-CBD	-3.50	119.61	124.62
9	B	606	CHL	OBD-CAD-CBD	-3.50	120.66	125.94
10	B	602	CLA	OBD-CAD-CBD	-3.48	120.69	125.94
10	B	610	CLA	CMB-C2B-C1B	-3.46	122.63	128.36
9	G	605	CHL	OBD-CAD-CBD	-3.46	120.71	125.94
10	B	612	CLA	CMB-C2B-C1B	-3.46	122.64	128.36
10	G	610	CLA	CMB-C2B-C1B	-3.46	122.65	128.36
10	B	611	CLA	OBD-CAD-CBD	-3.46	120.72	125.94
9	E	608	CHL	OBD-CAD-CBD	-3.45	120.73	125.94
4	H	7621	LUT	C18-C5-C4	-3.44	107.95	114.24
9	J	608	CHL	OBD-CAD-CBD	-3.44	120.74	125.94
10	F	611	CLA	OBD-CAD-CBD	-3.44	120.75	125.94
10	A	603	CLA	C4-C3-C5	-3.44	110.16	115.41
10	G	603	CLA	OBD-CAD-CBD	-3.43	120.76	125.94
4	B	1620	LUT	C18-C5-C4	-3.43	107.97	114.24
9	H	607	CHL	C4-C3-C5	-3.42	110.18	115.41
10	C	613	CLA	C4-C3-C5	-3.42	110.18	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	607	CHL	OBD-CAD-CBD	-3.41	120.79	125.94
9	E	606	CHL	OBD-CAD-CBD	-3.41	120.79	125.94
10	I	604	CLA	OBD-CAD-CBD	-3.41	120.80	125.94
10	A	611	CLA	CMB-C2B-C1B	-3.41	122.73	128.36
10	C	603	CLA	OBD-CAD-CBD	-3.41	120.80	125.94
10	I	602	CLA	OBD-CAD-CBD	-3.40	120.80	125.94
10	H	602	CLA	C6-C7-C8	-3.40	104.20	115.49
10	H	611	CLA	CMB-C2B-C1B	-3.40	122.74	128.36
10	H	611	CLA	OBD-CAD-CBD	-3.39	120.81	125.94
9	F	608	CHL	OBD-CAD-CBD	-3.39	120.82	125.94
10	G	611	CLA	OBD-CAD-CBD	-3.39	120.82	125.94
9	F	605	CHL	OBD-CAD-CBD	-3.39	120.82	125.94
10	G	602	CLA	OBD-CAD-CBD	-3.39	120.83	125.94
10	D	602	CLA	OBD-CAD-CBD	-3.38	120.84	125.94
10	F	614	CLA	OBD-CAD-CBD	-3.38	120.84	125.94
10	D	602	CLA	CMB-C2B-C1B	-3.37	122.78	128.36
10	D	612	CLA	OBD-CAD-CBD	-3.37	120.86	125.94
9	C	605	CHL	OBD-CAD-CBD	-3.36	120.87	125.94
9	A	608	CHL	OBD-CAD-CBD	-3.36	120.87	125.94
10	C	604	CLA	OBD-CAD-CBD	-3.36	120.87	125.94
9	F	606	CHL	CBA-CAA-C2A	-3.34	104.30	113.73
9	A	607	CHL	OBD-CAD-CBD	-3.33	120.91	125.94
10	G	612	CLA	OBD-CAD-CBD	-3.33	120.91	125.94
7	A	630	LHG	O10-C23-C24	-3.33	110.39	123.72
9	G	607	CHL	C4-C3-C5	-3.33	110.32	115.41
10	G	611	CLA	CMB-C2B-C1B	-3.33	122.86	128.36
9	D	601	CHL	OBD-CAD-CBD	-3.32	120.93	125.94
4	C	2621	LUT	C38-C25-C24	-3.32	116.27	123.59
9	H	607	CHL	OBD-CAD-CBD	-3.32	120.94	125.94
10	E	604	CLA	OBD-CAD-CBD	-3.32	120.94	125.94
10	D	604	CLA	C4-C3-C5	-3.31	110.36	115.41
9	A	605	CHL	OBD-CAD-CBD	-3.31	120.95	125.94
10	A	611	CLA	OBD-CAD-CBD	-3.31	120.95	125.94
9	F	601	CHL	OBD-CAD-CBD	-3.30	120.95	125.94
10	A	602	CLA	C11-C10-C8	-3.30	104.55	115.49
10	D	611	CLA	OBD-CAD-CBD	-3.30	120.96	125.94
9	I	605	CHL	OBD-CAD-CBD	-3.29	120.97	125.94
10	I	612	CLA	CMB-C2B-C1B	-3.29	122.92	128.36
10	A	602	CLA	OBD-CAD-CBD	-3.29	120.98	125.94
10	J	612	CLA	OBD-CAD-CBD	-3.29	120.98	125.94
10	H	603	CLA	OBD-CAD-CBD	-3.28	120.99	125.94
10	D	604	CLA	OBD-CAD-CBD	-3.27	121.01	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	611	CLA	OBD-CAD-CBD	-3.27	121.01	125.94
10	H	604	CLA	OBD-CAD-CBD	-3.27	121.01	125.94
9	G	606	CHL	OBD-CAD-CBD	-3.26	121.02	125.94
10	I	611	CLA	CAA-C2A-C3A	-3.26	103.85	113.22
10	D	612	CLA	CMB-C2B-C1B	-3.26	122.98	128.36
4	I	8620	LUT	C18-C5-C4	-3.25	108.30	114.24
10	J	604	CLA	OBD-CAD-CBD	-3.25	121.03	125.94
9	B	608	CHL	OBD-CAD-CBD	-3.25	121.04	125.94
10	D	614	CLA	OBD-CAD-CBD	-3.25	121.04	125.94
9	J	605	CHL	OBD-CAD-CBD	-3.24	121.04	125.94
10	A	604	CLA	OBD-CAD-CBD	-3.24	121.05	125.94
10	E	602	CLA	CMB-C2B-C1B	-3.24	123.00	128.36
4	A	621	LUT	C18-C5-C4	-3.24	108.32	114.24
10	F	602	CLA	OBD-CAD-CBD	-3.24	121.05	125.94
7	G	6630	LHG	O10-C23-C24	-3.24	110.76	123.72
9	D	608	CHL	OBD-CAD-CBD	-3.24	121.05	125.94
10	J	602	CLA	C12-C11-C10	-3.24	96.94	112.99
9	I	606	CHL	OBD-CAD-CBD	-3.23	121.06	125.94
10	I	613	CLA	OBD-CAD-CBD	-3.23	121.06	125.94
10	B	611	CLA	O1D-CGD-CBD	-3.22	120.00	124.62
9	E	605	CHL	OBD-CAD-CBD	-3.22	121.07	125.94
9	D	607	CHL	OBD-CAD-CBD	-3.22	121.08	125.94
9	E	607	CHL	OBD-CAD-CBD	-3.22	121.08	125.94
10	E	611	CLA	OBD-CAD-CBD	-3.22	121.08	125.94
10	B	603	CLA	CMB-C2B-C1B	-3.22	123.04	128.36
10	H	610	CLA	CMB-C2B-C1B	-3.21	123.06	128.36
9	E	607	CHL	C4-C3-C5	-3.20	110.51	115.41
9	G	608	CHL	OBD-CAD-CBD	-3.20	121.11	125.94
4	E	4621	LUT	C23-C24-C25	-3.19	122.24	125.22
9	G	607	CHL	OBD-CAD-CBD	-3.18	121.13	125.94
10	F	602	CLA	C11-C10-C8	-3.18	104.93	115.49
10	B	604	CLA	OBD-CAD-CBD	-3.18	121.14	125.94
10	F	613	CLA	OBD-CAD-CBD	-3.17	121.15	125.94
10	A	603	CLA	CMB-C2B-C1B	-3.17	123.12	128.36
9	G	601	CHL	OBD-CAD-CBD	-3.17	121.16	125.94
10	B	602	CLA	C11-C10-C8	-3.17	104.98	115.49
7	B	1630	LHG	O10-C23-C24	-3.17	111.05	123.72
10	J	613	CLA	OBD-CAD-CBD	-3.16	121.16	125.94
9	D	608	CHL	C5-C3-C2	-3.16	115.05	121.05
10	D	612	CLA	C4-C3-C5	-3.16	110.58	115.41
10	C	611	CLA	C4-C3-C5	-3.16	110.58	115.41
9	C	606	CHL	OBD-CAD-CBD	-3.16	121.17	125.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	601	CHL	OBD-CAD-CBD	-3.16	121.17	125.94
9	F	606	CHL	C5-C3-C4	-3.16	106.87	114.64
10	J	602	CLA	C11-C10-C8	-3.16	105.02	115.49
10	F	602	CLA	CMB-C2B-C1B	-3.16	123.14	128.36
10	G	604	CLA	OBD-CAD-CBD	-3.15	121.18	125.94
10	B	610	CLA	OBD-CAD-CBD	-3.15	121.18	125.94
10	C	610	CLA	OBD-CAD-CBD	-3.14	121.19	125.94
7	C	2630	LHG	O10-C23-C24	-3.14	111.16	123.72
9	C	606	CHL	O1D-CGD-CBD	-3.14	120.12	124.62
10	B	613	CLA	C4-C3-C5	-3.14	110.61	115.41
9	J	606	CHL	OBD-CAD-CBD	-3.13	121.21	125.94
10	E	603	CLA	OBD-CAD-CBD	-3.13	121.21	125.94
9	I	608	CHL	OBD-CAD-CBD	-3.13	121.21	125.94
10	B	614	CLA	OBD-CAD-CBD	-3.13	121.22	125.94
9	H	609	CHL	CAA-C2A-C3A	-3.13	104.22	113.22
9	A	607	CHL	C4-C3-C5	-3.13	110.63	115.41
9	F	609	CHL	OBD-CAD-CBD	-3.12	121.22	125.94
9	A	609	CHL	OBD-CAD-CBD	-3.12	121.23	125.94
4	C	2620	LUT	C18-C5-C4	-3.12	108.54	114.24
9	H	606	CHL	OBD-CAD-CBD	-3.12	121.23	125.94
9	A	607	CHL	C12-C11-C10	-3.11	97.54	112.99
10	D	610	CLA	OBD-CAD-CBD	-3.11	121.24	125.94
10	G	611	CLA	C4-C3-C5	-3.09	110.68	115.41
10	B	612	CLA	C4-C3-C5	-3.09	110.69	115.41
9	D	609	CHL	OBD-CAD-CBD	-3.09	121.28	125.94
10	C	613	CLA	OBD-CAD-CBD	-3.08	121.29	125.94
9	I	607	CHL	C12-C11-C10	-3.08	97.70	112.99
10	F	603	CLA	C4-C3-C5	-3.08	110.71	115.41
9	F	606	CHL	OBD-CAD-CBD	-3.07	121.30	125.94
4	F	5621	LUT	C18-C5-C4	-3.07	108.63	114.24
10	I	614	CLA	OBD-CAD-CBD	-3.07	121.31	125.94
9	E	601	CHL	OBD-CAD-CBD	-3.07	121.31	125.94
10	I	602	CLA	C11-C10-C8	-3.06	105.33	115.49
10	C	614	CLA	OBD-CAD-CBD	-3.06	121.32	125.94
9	A	606	CHL	OBD-CAD-CBD	-3.06	121.32	125.94
7	E	4630	LHG	O10-C23-C24	-3.06	111.49	123.72
9	C	609	CHL	OBD-CAD-CBD	-3.06	121.33	125.94
10	D	602	CLA	C5-C3-C2	-3.05	115.27	121.05
10	E	611	CLA	CMB-C2B-C1B	-3.04	123.34	128.36
9	H	601	CHL	OBD-CAD-CBD	-3.04	121.36	125.94
10	E	613	CLA	OBD-CAD-CBD	-3.02	121.37	125.94
10	D	602	CLA	C11-C10-C8	-3.02	105.46	115.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	614	CLA	OBD-CAD-CBD	-3.02	121.38	125.94
10	E	610	CLA	OBD-CAD-CBD	-3.02	121.39	125.94
4	J	9621	LUT	C23-C24-C25	-3.01	122.41	125.22
10	A	614	CLA	OBD-CAD-CBD	-3.01	121.39	125.94
10	F	604	CLA	OBD-CAD-CBD	-3.01	121.40	125.94
10	B	602	CLA	CMB-C2B-C1B	-3.01	123.39	128.36
10	E	604	CLA	O1A-CGA-CBA	-3.01	111.70	123.72
10	E	603	CLA	CMB-C2B-C1B	-3.01	123.39	128.36
10	A	603	CLA	CAA-C2A-C3A	-3.00	104.59	113.22
7	J	9630	LHG	O10-C23-C24	-3.00	111.72	123.72
10	F	602	CLA	C12-C11-C10	-2.99	98.17	112.99
9	A	606	CHL	C5-C3-C4	-2.98	107.32	114.64
10	H	602	CLA	CMB-C2B-C1B	-2.98	123.44	128.36
9	C	601	CHL	OBD-CAD-CBD	-2.97	121.45	125.94
10	H	602	CLA	C12-C11-C10	-2.97	98.25	112.99
10	B	613	CLA	OBD-CAD-CBD	-2.97	121.46	125.94
10	F	612	CLA	C4-C3-C5	-2.96	110.88	115.41
9	A	608	CHL	O1D-CGD-CBD	-2.96	120.38	124.62
10	J	604	CLA	O1A-CGA-CBA	-2.96	111.90	123.72
10	J	603	CLA	OBD-CAD-CBD	-2.95	121.49	125.94
10	H	603	CLA	CMB-C2B-C1B	-2.95	123.49	128.36
10	B	611	CLA	C4-C3-C5	-2.95	110.91	115.41
4	J	9621	LUT	C18-C5-C4	-2.95	108.86	114.24
8	D	5632	DGD	C3G-C2G-C1G	-2.94	105.19	112.07
4	F	5620	LUT	C18-C5-C4	-2.94	108.87	114.24
9	H	607	CHL	C7-C6-C5	-2.94	104.38	113.06
10	E	604	CLA	O1D-CGD-CBD	-2.94	120.41	124.62
9	D	607	CHL	C7-C6-C5	-2.93	104.42	113.06
10	C	602	CLA	CMB-C2B-C1B	-2.92	123.53	128.36
10	I	603	CLA	CMB-C2B-C1B	-2.92	123.53	128.36
10	D	611	CLA	CAA-C2A-C3A	-2.92	104.81	113.22
10	H	610	CLA	OBD-CAD-CBD	-2.92	121.53	125.94
9	D	609	CHL	C7-C6-C5	-2.92	104.44	113.06
9	F	607	CHL	OBD-CAD-CBD	-2.91	121.54	125.94
10	C	611	CLA	OBD-CAD-CBD	-2.91	121.54	125.94
10	J	603	CLA	CMB-C2B-C1B	-2.90	123.56	128.36
10	H	604	CLA	O1A-CGA-CBA	-2.90	112.12	123.72
9	H	605	CHL	OBD-CAD-CBD	-2.89	121.58	125.94
10	G	610	CLA	OBD-CAD-CBD	-2.89	121.58	125.94
4	I	8621	LUT	C18-C5-C4	-2.88	108.97	114.24
8	H	7632	DGD	C3G-C2G-C1G	-2.88	105.33	112.07
7	H	7630	LHG	O10-C23-C24	-2.88	112.19	123.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	J	609	CHL	OBD-CAD-CBD	-2.88	121.59	125.94
10	J	614	CLA	OBD-CAD-CBD	-2.88	121.60	125.94
9	H	601	CHL	C12-C11-C10	-2.87	98.73	112.99
10	E	602	CLA	C5-C3-C2	-2.87	115.61	121.05
9	I	601	CHL	OBD-CAD-CBD	-2.86	121.62	125.94
9	J	607	CHL	C12-C11-C10	-2.86	98.80	112.99
10	H	613	CLA	OBD-CAD-CBD	-2.85	121.64	125.94
9	A	601	CHL	OBD-CAD-CBD	-2.85	121.64	125.94
9	B	605	CHL	OBD-CAD-CBD	-2.84	121.65	125.94
9	B	606	CHL	O1A-CGA-CBA	-2.84	112.36	123.72
10	G	613	CLA	OBD-CAD-CBD	-2.84	121.66	125.94
9	J	607	CHL	OBD-CAD-CBD	-2.84	121.66	125.94
10	E	614	CLA	OBD-CAD-CBD	-2.82	121.67	125.94
8	E	4632	DGD	C3G-C2G-C1G	-2.82	105.47	112.07
9	H	609	CHL	OBD-CAD-CBD	-2.82	121.68	125.94
9	B	607	CHL	OBD-CAD-CBD	-2.82	121.68	125.94
10	A	613	CLA	OBD-CAD-CBD	-2.82	121.69	125.94
10	F	604	CLA	O1A-CGA-CBA	-2.81	112.46	123.72
8	A	632	DGD	C3G-C2G-C1G	-2.81	105.49	112.07
9	J	601	CHL	OBD-CAD-CBD	-2.81	121.70	125.94
8	B	2632	DGD	C3G-C2G-C1G	-2.81	105.50	112.07
8	I	8632	DGD	C3G-C2G-C1G	-2.80	105.52	112.07
10	G	602	CLA	C11-C12-C13	-2.80	106.20	115.49
10	G	614	CLA	OBD-CAD-CBD	-2.80	121.71	125.94
10	F	610	CLA	OBD-CAD-CBD	-2.80	121.72	125.94
8	B	1632	DGD	C3G-C2G-C1G	-2.79	105.55	112.07
10	F	602	CLA	C11-C12-C13	-2.79	106.24	115.49
10	D	613	CLA	OBD-CAD-CBD	-2.78	121.74	125.94
10	H	611	CLA	O1D-CGD-CBD	-2.78	120.63	124.62
9	E	605	CHL	CAA-C2A-C3A	-2.78	105.22	113.22
4	B	1621	LUT	C23-C24-C25	-2.77	122.63	125.22
9	B	609	CHL	OBD-CAD-CBD	-2.77	121.76	125.94
10	I	604	CLA	O1A-CGA-CBA	-2.77	112.65	123.72
9	H	608	CHL	OBD-CAD-CBD	-2.76	121.77	125.94
4	D	3621	LUT	C18-C5-C4	-2.76	109.19	114.24
10	C	602	CLA	C12-C11-C10	-2.75	99.35	112.99
10	F	603	CLA	CAA-C2A-C3A	-2.75	105.32	113.22
10	A	610	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
8	D	3632	DGD	C3G-C2G-C1G	-2.72	105.71	112.07
10	I	611	CLA	C4-C3-C5	-2.72	111.25	115.41
10	F	611	CLA	C4-C3-C5	-2.71	111.26	115.41
9	F	607	CHL	C7-C6-C5	-2.71	105.05	113.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	607	CHL	C12-C11-C10	-2.71	99.53	112.99
9	G	609	CHL	OBD-CAD-CBD	-2.70	121.86	125.94
10	E	613	CLA	C12-C11-C10	-2.70	99.62	112.99
10	I	603	CLA	CAA-C2A-C3A	-2.70	105.47	113.22
9	E	609	CHL	OBD-CAD-CBD	-2.68	121.89	125.94
9	I	609	CHL	OBD-CAD-CBD	-2.67	121.90	125.94
8	G	9632	DGD	C3G-C2G-C1G	-2.66	105.84	112.07
9	H	601	CHL	C4-C3-C5	-2.66	111.34	115.41
9	C	606	CHL	C5-C3-C4	-2.66	108.09	114.64
10	H	602	CLA	C11-C10-C8	-2.66	106.67	115.49
9	E	607	CHL	C12-C11-C10	-2.65	99.82	112.99
9	F	605	CHL	O1D-CGD-CBD	-2.65	120.82	124.62
9	F	607	CHL	O2A-CGA-O1A	-2.65	116.65	123.49
10	E	611	CLA	C4-C3-C5	-2.65	111.36	115.41
10	J	602	CLA	C6-C7-C8	-2.64	106.72	115.49
10	J	610	CLA	OBD-CAD-CBD	-2.64	121.95	125.94
9	C	607	CHL	O2A-CGA-O1A	-2.64	116.68	123.49
9	B	601	CHL	C4-C3-C5	-2.64	111.38	115.41
10	B	603	CLA	C4-C3-C5	-2.64	111.38	115.41
10	F	602	CLA	C6-C7-C8	-2.63	106.75	115.49
6	D	3623	NEX	C18-C5-C4	-2.63	107.69	110.97
5	F	6622	XAT	C37-C21-C22	-2.63	104.24	108.94
9	A	609	CHL	CAA-C2A-C3A	-2.63	105.66	113.22
9	D	606	CHL	O1D-CGD-CBD	-2.63	120.86	124.62
10	G	602	CLA	C12-C11-C10	-2.62	99.97	112.99
9	D	607	CHL	O2A-CGA-O1A	-2.62	116.73	123.49
7	F	5630	LHG	O10-C23-C24	-2.62	113.25	123.72
9	G	607	CHL	O1D-CGD-CBD	-2.62	120.87	124.62
9	E	607	CHL	O2A-CGA-O1A	-2.60	116.78	123.49
10	C	602	CLA	C6-C7-C8	-2.59	106.89	115.49
9	J	606	CHL	O1A-CGA-CBA	-2.58	113.38	123.72
10	I	602	CLA	C12-C11-C10	-2.58	100.17	112.99
9	J	609	CHL	O1D-CGD-CBD	-2.57	120.94	124.62
4	C	2621	LUT	C18-C5-C4	-2.57	109.54	114.24
10	A	610	CLA	OBD-CAD-CBD	-2.56	122.07	125.94
9	C	605	CHL	O1D-CGD-CBD	-2.56	120.95	124.62
10	J	612	CLA	C4-C3-C5	-2.56	111.50	115.41
10	G	604	CLA	O1A-CGA-CBA	-2.56	113.50	123.72
9	I	607	CHL	O1D-CGD-CBD	-2.55	120.97	124.62
9	E	601	CHL	C12-C11-C10	-2.54	100.37	112.99
10	D	602	CLA	C9-C8-C10	-2.54	101.30	111.08
10	G	612	CLA	C4-C3-C5	-2.53	111.54	115.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	607	CHL	O2A-CGA-O1A	-2.53	116.97	123.49
10	B	603	CLA	C9-C8-C10	-2.53	101.37	111.08
8	H	6632	DGD	C3G-C2G-C1G	-2.53	106.16	112.07
10	I	610	CLA	OBD-CAD-CBD	-2.52	122.14	125.94
10	G	602	CLA	C6-C7-C8	-2.52	107.14	115.49
9	A	607	CHL	O2A-CGA-O1A	-2.50	117.04	123.49
10	E	602	CLA	C12-C11-C10	-2.50	100.59	112.99
10	E	610	CLA	C2C-C1C-NC	-2.49	108.39	110.24
9	J	607	CHL	O2A-CGA-O1A	-2.49	117.06	123.49
10	G	603	CLA	CMB-C2B-C1B	-2.49	124.25	128.36
10	A	612	CLA	C4-C3-C5	-2.47	111.63	115.41
4	D	3621	LUT	C1-C6-C5	-2.47	119.03	122.66
10	A	604	CLA	O1A-CGA-CBA	-2.47	113.84	123.72
5	D	8622	XAT	C37-C21-C22	-2.47	104.54	108.94
9	A	605	CHL	O1D-CGD-CBD	-2.45	121.11	124.62
10	J	612	CLA	C7-C6-C5	-2.45	105.83	113.06
9	F	607	CHL	O1D-CGD-CBD	-2.45	121.12	124.62
9	G	607	CHL	O2A-CGA-O1A	-2.44	117.19	123.49
4	G	6621	LUT	C18-C5-C4	-2.44	109.78	114.24
9	I	607	CHL	O2A-CGA-O1A	-2.44	117.20	123.49
9	B	607	CHL	O2A-CGA-O1A	-2.43	117.21	123.49
5	C	7622	XAT	C37-C21-C22	-2.43	104.60	108.94
9	C	607	CHL	C4-C3-C5	-2.42	111.71	115.41
9	D	601	CHL	C14-C13-C15	-2.42	101.77	111.08
10	I	611	CLA	O1D-CGD-CBD	-2.42	121.16	124.62
9	H	606	CHL	C5-C3-C4	-2.42	108.70	114.64
9	A	606	CHL	O1D-CGD-CBD	-2.41	121.16	124.62
9	G	607	CHL	C7-C6-C5	-2.41	105.93	113.06
9	I	605	CHL	CAA-C2A-C3A	-2.40	106.30	113.22
10	I	602	CLA	CMB-C2B-C1B	-2.40	124.39	128.36
10	D	611	CLA	C4-C3-C5	-2.40	111.74	115.41
10	I	610	CLA	C11-C10-C8	-2.40	107.53	115.49
10	C	602	CLA	C11-C12-C13	-2.40	107.54	115.49
9	D	606	CHL	C5-C3-C4	-2.39	108.78	114.64
6	E	4623	NEX	C18-C5-C4	-2.39	108.00	110.97
9	G	601	CHL	C7-C6-C5	-2.37	106.05	113.06
10	I	603	CLA	C7-C6-C5	-2.37	106.07	113.06
10	G	602	CLA	C11-C10-C8	-2.36	107.65	115.49
10	G	610	CLA	C2C-C1C-NC	-2.36	108.49	110.24
9	I	606	CHL	C5-C3-C4	-2.35	108.86	114.64
10	D	603	CLA	C4-C3-C5	-2.35	111.81	115.41
9	F	609	CHL	CAA-C2A-C3A	-2.34	106.48	113.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	603	CLA	C20-C18-C19	-2.34	98.75	110.55
7	D	3630	LHG	O10-C23-C24	-2.34	114.36	123.72
10	H	610	CLA	C11-C10-C8	-2.34	107.74	115.49
9	E	606	CHL	O1D-CGD-CBD	-2.33	121.28	124.62
10	C	602	CLA	C11-C10-C8	-2.33	107.76	115.49
9	J	605	CHL	CAA-C2A-C3A	-2.33	106.52	113.22
4	A	621	LUT	C1-C6-C5	-2.33	119.24	122.66
10	H	602	CLA	C11-C12-C13	-2.33	107.77	115.49
10	C	614	CLA	CAA-C2A-C3A	-2.32	106.55	113.22
9	G	606	CHL	C5-C3-C4	-2.32	108.94	114.64
10	A	602	CLA	C9-C8-C10	-2.31	102.18	111.08
10	G	602	CLA	C9-C8-C10	-2.29	102.25	111.08
10	A	602	CLA	C12-C11-C10	-2.29	101.61	112.99
9	B	606	CHL	O1D-CGD-CBD	-2.29	121.34	124.62
10	J	602	CLA	C2C-C1C-NC	-2.29	108.54	110.24
6	C	2623	NEX	C18-C5-C4	-2.29	108.11	110.97
4	G	6621	LUT	C1-C6-C5	-2.29	119.30	122.66
10	C	603	CLA	CAA-C2A-C3A	-2.28	106.65	113.22
10	I	603	CLA	C4-C3-C5	-2.28	111.92	115.41
6	B	1623	NEX	C18-C5-C4	-2.28	108.13	110.97
10	E	602	CLA	C11-C10-C8	-2.28	107.93	115.49
9	A	605	CHL	CAA-C2A-C3A	-2.28	106.67	113.22
5	B	5622	XAT	C37-C21-C22	-2.28	104.87	108.94
10	H	613	CLA	CAA-C2A-C3A	-2.28	106.67	113.22
10	G	611	CLA	O1D-CGD-CBD	-2.27	121.36	124.62
9	C	608	CHL	C6-C7-C8	-2.27	107.96	115.49
9	C	608	CHL	C5-C3-C2	-2.27	116.75	121.05
10	I	602	CLA	C9-C8-C10	-2.26	102.39	111.08
9	F	609	CHL	O1D-CGD-CBD	-2.26	121.39	124.62
6	I	8623	NEX	C18-C5-C4	-2.25	108.16	110.97
9	F	606	CHL	O1A-CGA-CBA	-2.25	114.72	123.72
9	E	607	CHL	O1D-CGD-CBD	-2.25	121.40	124.62
4	E	4621	LUT	C18-C5-C4	-2.25	110.13	114.24
4	F	5621	LUT	C1-C6-C5	-2.25	119.36	122.66
10	C	612	CLA	C4-C3-C5	-2.25	111.97	115.41
9	B	607	CHL	C16-C15-C13	-2.25	108.04	115.49
6	H	7623	NEX	C18-C5-C4	-2.25	108.17	110.97
9	F	607	CHL	C12-C11-C10	-2.24	101.86	112.99
10	F	611	CLA	O1D-CGD-CBD	-2.24	121.41	124.62
9	I	601	CHL	C4-C3-C5	-2.24	111.98	115.41
10	D	602	CLA	C11-C12-C13	-2.24	108.05	115.49
9	C	601	CHL	C7-C6-C5	-2.24	106.44	113.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	8622	XAT	C15-C35-C34	-2.23	118.46	123.39
9	D	607	CHL	C12-C11-C10	-2.23	101.92	112.99
5	H	4622	XAT	C37-C21-C22	-2.23	104.96	108.94
9	H	605	CHL	CAA-C2A-C3A	-2.23	106.82	113.22
9	E	606	CHL	C5-C3-C4	-2.22	109.18	114.64
10	C	611	CLA	O2A-CGA-O1A	-2.22	117.77	123.49
9	E	605	CHL	O2A-CGA-O1A	-2.21	117.78	123.49
9	G	605	CHL	O2A-CGA-O1A	-2.21	117.78	123.49
9	G	609	CHL	CAA-C2A-C3A	-2.21	106.85	113.22
10	H	614	CLA	C2C-C1C-NC	-2.21	108.60	110.24
10	I	610	CLA	C2C-C1C-NC	-2.20	108.60	110.24
10	E	612	CLA	C4-C3-C5	-2.20	112.04	115.41
9	J	605	CHL	O2A-CGA-O1A	-2.20	117.81	123.49
10	F	610	CLA	C2C-C1C-NC	-2.20	108.61	110.24
10	B	611	CLA	O2A-CGA-O1A	-2.20	117.82	123.49
9	D	609	CHL	O1D-CGD-CBD	-2.20	121.47	124.62
10	A	611	CLA	O2A-CGA-O1A	-2.19	117.83	123.49
10	I	612	CLA	O2A-CGA-O1A	-2.19	117.83	123.49
10	I	602	CLA	C6-C7-C8	-2.19	108.21	115.49
10	H	611	CLA	O2A-CGA-O1A	-2.19	117.83	123.49
10	H	611	CLA	C4-C3-C5	-2.19	112.06	115.41
9	I	608	CHL	O1D-CGD-CBD	-2.19	121.48	124.62
9	B	605	CHL	CAA-C2A-C3A	-2.19	106.92	113.22
10	I	602	CLA	C11-C12-C13	-2.19	108.22	115.49
4	C	2621	LUT	C23-C24-C25	-2.19	123.18	125.22
9	D	606	CHL	O2A-CGA-O1A	-2.19	117.84	123.49
10	B	610	CLA	C2C-C1C-NC	-2.19	108.61	110.24
9	C	607	CHL	C12-C11-C10	-2.18	102.16	112.99
6	J	9623	NEX	C18-C5-C4	-2.18	108.25	110.97
9	D	606	CHL	O1A-CGA-CBA	-2.17	115.03	123.72
9	C	605	CHL	O2A-CGA-O1A	-2.17	117.90	123.49
4	F	5620	LUT	C23-C24-C25	-2.16	123.20	125.22
10	C	611	CLA	O1D-CGD-CBD	-2.16	121.53	124.62
9	H	607	CHL	CMD-C2D-C1D	-2.16	124.80	128.36
5	J	3622	XAT	C36-C21-C22	-2.15	105.10	108.94
10	E	614	CLA	O2A-CGA-O1A	-2.15	117.95	123.49
10	B	602	CLA	C12-C11-C10	-2.14	102.36	112.99
9	G	601	CHL	C4-C3-C5	-2.14	112.14	115.41
10	E	611	CLA	O2A-CGA-O1A	-2.13	117.99	123.49
9	C	606	CHL	O2A-CGA-O1A	-2.13	117.99	123.49
9	F	606	CHL	O1D-CGD-CBD	-2.13	121.57	124.62
10	J	610	CLA	O1A-CGA-CBA	-2.12	115.23	123.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	603	CLA	C4-C3-C5	-2.12	112.17	115.41
10	E	603	CLA	C4-C3-C5	-2.12	112.17	115.41
9	F	606	CHL	O2A-CGA-O1A	-2.12	118.03	123.49
9	G	608	CHL	O1D-CGD-CBD	-2.11	121.60	124.62
10	J	611	CLA	O2A-CGA-O1A	-2.10	118.06	123.49
10	F	611	CLA	O2A-CGA-O1A	-2.10	118.07	123.49
10	I	602	CLA	C2C-C1C-NC	-2.10	108.68	110.24
9	J	601	CHL	C7-C6-C5	-2.09	106.88	113.06
5	E	2622	XAT	C37-C21-C22	-2.09	105.20	108.94
9	D	605	CHL	O2A-CGA-O1A	-2.09	118.09	123.49
10	E	603	CLA	C12-C11-C10	-2.09	102.61	112.99
10	H	614	CLA	O2A-CGA-O1A	-2.09	118.10	123.49
10	J	611	CLA	C12-C11-C10	-2.09	102.62	112.99
10	J	602	CLA	C9-C8-C10	-2.08	103.07	111.08
10	H	610	CLA	C2C-C1C-NC	-2.08	108.69	110.24
9	F	605	CHL	O2A-CGA-O1A	-2.08	118.12	123.49
10	H	602	CLA	C9-C8-C10	-2.08	103.09	111.08
8	D	5632	DGD	O1B-C1B-C2B	-2.08	115.42	123.72
10	D	611	CLA	O2A-CGA-O1A	-2.07	118.14	123.49
10	B	602	CLA	C11-C12-C13	-2.07	108.61	115.49
9	I	605	CHL	O2A-CGA-O1A	-2.07	118.14	123.49
10	C	610	CLA	C11-C10-C8	-2.07	108.62	115.49
9	E	608	CHL	CAA-C2A-C3A	-2.07	107.26	113.22
4	C	2621	LUT	C1-C6-C5	-2.07	119.62	122.66
10	A	602	CLA	C2C-C1C-NC	-2.06	108.71	110.24
10	C	612	CLA	O2A-CGA-O1A	-2.06	118.17	123.49
10	G	612	CLA	O2A-CGA-O1A	-2.06	118.18	123.49
10	C	614	CLA	O2A-CGA-O1A	-2.06	118.18	123.49
9	I	601	CHL	C12-C11-C10	-2.06	102.79	112.99
10	H	610	CLA	O1A-CGA-CBA	-2.06	115.50	123.72
9	B	605	CHL	O2A-CGA-O1A	-2.05	118.19	123.49
4	G	6620	LUT	C1-C6-C5	-2.05	119.65	122.66
6	F	5623	NEX	C18-C5-C4	-2.05	108.41	110.97
10	C	610	CLA	C2C-C1C-NC	-2.05	108.72	110.24
10	J	612	CLA	CAA-C2A-C3A	-2.04	107.34	113.22
10	I	614	CLA	O2A-CGA-O1A	-2.04	118.23	123.49
10	D	602	CLA	C12-C11-C10	-2.04	102.87	112.99
10	G	614	CLA	O2A-CGA-O1A	-2.04	118.23	123.49
10	G	611	CLA	O2A-CGA-O1A	-2.04	118.23	123.49
10	J	612	CLA	O2A-CGA-O1A	-2.03	118.25	123.49
9	D	601	CHL	C4-C3-C5	-2.03	112.31	115.41
9	H	606	CHL	O2A-CGA-O1A	-2.03	118.26	123.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	605	CHL	O1D-CGD-CBD	-2.03	121.72	124.62
10	D	610	CLA	C11-C10-C8	-2.02	108.78	115.49
9	A	606	CHL	O2A-CGA-O1A	-2.02	118.28	123.49
10	A	612	CLA	O2A-CGA-O1A	-2.02	118.29	123.49
10	F	602	CLA	C2C-C1C-NC	-2.01	108.74	110.24
10	G	602	CLA	C2C-C1C-NC	-2.01	108.75	110.24
10	C	611	CLA	C12-C11-C10	-2.01	103.02	112.99
10	F	604	CLA	O2A-CGA-O1A	-2.01	118.31	123.49
9	A	601	CHL	C4-C3-C5	-2.01	112.34	115.41
9	A	608	CHL	CAA-C2A-C3A	-2.00	107.46	113.22
10	A	610	CLA	C16-C15-C13	2.00	122.12	115.49
10	J	603	CLA	CMB-C2B-C3B	2.00	129.00	125.09
10	D	603	CLA	C16-C17-C18	2.00	125.96	115.87
10	B	611	CLA	CAA-CBA-CGA	2.00	119.18	113.32
10	E	611	CLA	CMB-C2B-C3B	2.01	129.01	125.09
10	F	611	CLA	C11-C10-C8	2.01	122.14	115.49
10	G	610	CLA	O2D-CGD-CBD	2.01	114.05	111.30
10	G	611	CLA	C6-C7-C8	2.01	122.15	115.49
9	I	605	CHL	CED-O2D-CGD	2.01	120.70	115.99
9	H	601	CHL	CAA-CBA-CGA	2.01	119.21	113.32
10	H	611	CLA	CAA-CBA-CGA	2.01	119.21	113.32
4	F	5621	LUT	C7-C8-C9	2.01	129.29	126.22
10	H	603	CLA	CMB-C2B-C3B	2.02	129.03	125.09
5	E	2622	XAT	C37-C21-C36	2.02	110.36	107.35
9	B	601	CHL	CAA-CBA-CGA	2.02	119.23	113.32
10	B	602	CLA	CMB-C2B-C3B	2.02	129.04	125.09
5	D	8622	XAT	C26-O24-C25	2.02	63.63	61.25
8	I	8632	DGD	C4D-C3D-C2D	2.02	114.56	110.79
9	D	607	CHL	CAC-C3C-C4C	2.02	127.77	124.83
9	F	606	CHL	CAA-C2A-C1A	2.02	119.61	112.47
10	F	614	CLA	CED-O2D-CGD	2.03	120.74	115.99
9	G	609	CHL	CAA-CBA-CGA	2.03	119.25	113.32
10	G	612	CLA	C4-C3-C2	2.03	127.49	123.50
9	F	601	CHL	CAC-C3C-C4C	2.03	127.78	124.83
9	E	607	CHL	O2D-CGD-CBD	2.03	114.08	111.30
10	I	603	CLA	CMB-C2B-C3B	2.03	129.07	125.09
10	A	612	CLA	C4-C3-C2	2.04	127.50	123.50
9	C	607	CHL	O2D-CGD-CBD	2.04	114.09	111.30
10	J	610	CLA	C14-C13-C12	2.04	118.91	111.08
9	B	606	CHL	CED-O2D-CGD	2.04	120.77	115.99
4	C	2621	LUT	C26-C25-C24	2.04	124.58	121.21
9	H	605	CHL	CMB-C2B-C3B	2.04	129.08	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	601	CHL	O2A-CGA-CBA	2.04	118.12	111.90
8	H	7632	DGD	C6D-C5D-C4D	2.04	116.65	112.03
10	F	611	CLA	CED-O2D-CGD	2.04	120.78	115.99
10	B	610	CLA	C16-C15-C13	2.04	122.27	115.49
10	I	612	CLA	CMD-C2D-C3D	2.04	129.09	125.09
8	I	8632	DGD	C6D-C5D-C4D	2.05	116.67	112.03
10	F	612	CLA	C4-C3-C2	2.05	127.53	123.50
9	I	608	CHL	C4-C3-C2	2.05	127.53	123.50
9	C	606	CHL	CMD-C2D-C3D	2.05	129.10	125.09
10	H	602	CLA	CMD-C2D-C3D	2.05	129.10	125.09
10	A	603	CLA	CAA-CBA-CGA	2.05	119.33	113.32
6	B	1623	NEX	C24-C23-C22	2.05	114.95	110.41
9	D	601	CHL	O2A-CGA-CBA	2.05	118.16	111.90
10	C	613	CLA	CMD-C2D-C3D	2.06	129.11	125.09
10	E	603	CLA	CMB-C2B-C3B	2.06	129.11	125.09
4	D	3620	LUT	C26-C25-C24	2.06	124.62	121.21
5	J	3622	XAT	C26-O24-C25	2.06	63.68	61.25
9	F	607	CHL	C11-C10-C8	2.06	122.33	115.49
10	C	610	CLA	C2A-C1A-CHA	2.06	127.69	123.89
2	E	4633	BNG	O1-C1-C2	2.06	110.65	108.04
5	F	6622	XAT	C26-O24-C25	2.06	63.69	61.25
6	D	3623	NEX	C21-C22-C23	2.07	118.50	115.02
2	B	1633	BNG	O1-C1-C2	2.07	110.65	108.04
9	H	601	CHL	O2A-CGA-CBA	2.07	118.19	111.90
10	J	611	CLA	C11-C12-C13	2.07	122.35	115.49
4	J	9621	LUT	C22-C23-C24	2.07	114.19	111.75
10	J	613	CLA	CAA-CBA-CGA	2.07	119.39	113.32
9	F	607	CHL	C14-C13-C12	2.07	119.05	111.08
8	A	632	DGD	C3D-C4D-C5D	2.08	113.82	110.20
9	B	608	CHL	C14-C13-C15	2.08	119.06	111.08
9	E	606	CHL	OMC-CMC-C2C	2.08	130.93	125.58
10	A	603	CLA	O2A-CGA-CBA	2.08	118.23	111.90
10	A	611	CLA	C6-C7-C8	2.08	122.39	115.49
5	C	7622	XAT	C26-O24-C25	2.08	63.70	61.25
10	H	610	CLA	C16-C15-C13	2.08	122.40	115.49
9	J	601	CHL	CMB-C2B-C3B	2.09	129.17	125.09
5	I	9622	XAT	C26-O24-C25	2.09	63.71	61.25
9	B	601	CHL	CAC-C3C-C4C	2.09	127.86	124.83
6	D	3623	NEX	C16-C1-C6	2.10	112.36	110.48
9	I	606	CHL	CMD-C2D-C3D	2.10	129.19	125.09
10	A	613	CLA	CAA-CBA-CGA	2.10	119.45	113.32
10	J	611	CLA	C6-C5-C3	2.10	117.08	112.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	602	CLA	C9-C8-C7	2.10	119.13	111.08
10	G	612	CLA	CMC-C2C-C1C	2.10	128.26	125.02
10	A	602	CLA	O2A-CGA-CBA	2.10	118.29	111.90
2	I	8633	BNG	O1-C1-C2	2.10	110.69	108.04
10	D	603	CLA	CAA-CBA-CGA	2.10	119.46	113.32
9	J	609	CHL	C6-C5-C3	2.10	117.09	112.48
4	H	7620	LUT	C26-C25-C24	2.10	124.69	121.21
9	A	608	CHL	CMB-C2B-C3B	2.10	129.19	125.09
10	H	610	CLA	CAA-CBA-CGA	2.10	119.47	113.32
9	A	607	CHL	C11-C12-C13	2.10	122.46	115.49
5	C	7622	XAT	C6-O4-C5	2.10	63.73	61.25
6	B	1623	NEX	C1-C2-C3	2.10	118.35	113.41
9	A	607	CHL	C5-C3-C2	2.11	125.04	121.05
10	I	604	CLA	CMD-C2D-C3D	2.11	129.21	125.09
9	E	608	CHL	C4-C3-C2	2.11	127.65	123.50
9	F	608	CHL	C6-C7-C8	2.11	122.49	115.49
9	I	609	CHL	C16-C15-C13	2.11	122.50	115.49
5	D	8622	XAT	C37-C21-C36	2.12	110.51	107.35
9	J	607	CHL	C6-C7-C8	2.12	122.52	115.49
9	C	601	CHL	C6-C5-C3	2.12	117.14	112.48
6	D	3623	NEX	C24-C23-C22	2.12	115.10	110.41
9	I	608	CHL	C14-C13-C15	2.12	119.23	111.08
4	A	620	LUT	C26-C25-C24	2.12	124.72	121.21
9	H	605	CHL	O2D-CGD-CBD	2.12	114.21	111.30
10	F	604	CLA	CAA-C2A-C1A	2.13	119.97	112.47
6	J	9623	NEX	C26-O24-C25	2.13	63.76	61.25
4	A	620	LUT	C2-C3-C4	2.13	114.08	110.32
9	A	605	CHL	CMB-C2B-C3B	2.13	129.25	125.09
8	A	632	DGD	C6D-C5D-C4D	2.13	116.84	112.03
10	E	603	CLA	C11-C10-C8	2.13	122.55	115.49
10	F	602	CLA	CMB-C2B-C3B	2.13	129.25	125.09
10	I	604	CLA	CAA-C2A-C1A	2.13	119.99	112.47
10	D	610	CLA	C16-C15-C13	2.13	122.56	115.49
5	B	5622	XAT	C37-C21-C36	2.13	110.53	107.35
6	J	9623	NEX	C1-C2-C3	2.14	118.42	113.41
9	E	607	CHL	C6-C7-C8	2.14	122.58	115.49
9	F	607	CHL	CAA-C2A-C1A	2.14	120.01	112.47
4	D	3621	LUT	C2-C3-C4	2.14	114.11	110.32
9	J	608	CHL	C14-C13-C15	2.14	119.30	111.08
6	E	4623	NEX	C1-C2-C3	2.14	118.43	113.41
10	F	611	CLA	C9-C8-C10	2.14	119.31	111.08
10	D	603	CLA	C16-C15-C13	2.14	122.59	115.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	609	CHL	CBA-CAA-C2A	2.14	119.78	113.73
9	G	608	CHL	C14-C13-C15	2.15	119.34	111.08
10	E	610	CLA	C2A-C1A-CHA	2.15	127.85	123.89
10	J	604	CLA	C6-C5-C3	2.15	117.21	112.48
9	H	608	CHL	C14-C13-C15	2.16	119.36	111.08
10	G	611	CLA	C16-C15-C13	2.16	122.64	115.49
9	E	601	CHL	C14-C13-C15	2.16	119.38	111.08
2	J	9633	BNG	O1-C1-C2	2.16	110.77	108.04
10	H	612	CLA	CBA-CAA-C2A	2.16	119.83	113.73
6	B	1623	NEX	C26-O24-C25	2.16	63.80	61.25
10	G	614	CLA	C1-C2-C3	2.16	137.05	124.86
9	I	607	CHL	O2D-CGD-CBD	2.16	114.27	111.30
8	D	5632	DGD	C4D-C3D-C2D	2.16	114.83	110.79
4	J	9621	LUT	C26-C25-C24	2.16	124.79	121.21
10	F	604	CLA	C9-C8-C10	2.16	119.39	111.08
10	A	611	CLA	C9-C8-C10	2.17	119.40	111.08
4	I	8620	LUT	C1-C2-C3	2.17	118.49	113.41
10	I	603	CLA	O2A-CGA-CBA	2.17	118.50	111.90
10	I	612	CLA	C14-C13-C15	2.17	119.40	111.08
4	G	6620	LUT	C2-C3-C4	2.17	114.16	110.32
10	C	612	CLA	C11-C10-C8	2.17	122.69	115.49
9	E	608	CHL	C14-C13-C15	2.17	119.42	111.08
10	J	604	CLA	C6-C7-C8	2.17	122.69	115.49
10	J	611	CLA	CAA-CBA-CGA	2.17	119.68	113.32
10	I	603	CLA	C16-C15-C13	2.17	122.69	115.49
9	G	608	CHL	C4-C3-C2	2.17	127.77	123.50
9	D	608	CHL	C4-C3-C2	2.18	127.78	123.50
9	B	609	CHL	C6-C5-C3	2.18	117.26	112.48
9	C	608	CHL	C11-C12-C13	2.18	122.71	115.49
10	F	604	CLA	C11-C10-C8	2.18	122.72	115.49
10	H	610	CLA	CMB-C2B-C3B	2.18	129.35	125.09
10	C	604	CLA	C6-C5-C3	2.18	117.27	112.48
4	B	1620	LUT	C26-C25-C24	2.18	124.82	121.21
10	B	610	CLA	C2A-C1A-CHA	2.18	127.90	123.89
5	E	2622	XAT	C6-O4-C5	2.18	63.83	61.25
8	D	5632	DGD	C6D-C5D-C4D	2.18	116.97	112.03
4	G	6620	LUT	C26-C25-C24	2.19	124.83	121.21
2	C	2633	BNG	O1-C1-C2	2.19	110.80	108.04
10	H	611	CLA	C6-C7-C8	2.19	122.74	115.49
10	E	612	CLA	C11-C12-C13	2.19	122.74	115.49
10	J	610	CLA	C2A-C1A-CHA	2.19	127.91	123.89
5	F	6622	XAT	C37-C21-C36	2.19	110.62	107.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	602	CLA	CMB-C2B-C3B	2.19	129.37	125.09
9	J	607	CHL	C14-C13-C12	2.19	119.49	111.08
9	B	601	CHL	CMB-C2B-C3B	2.19	129.37	125.09
10	E	612	CLA	CMC-C2C-C1C	2.19	128.41	125.02
10	H	610	CLA	C2A-C1A-CHA	2.19	127.92	123.89
10	D	610	CLA	C2A-C1A-CHA	2.19	127.92	123.89
9	B	609	CHL	O2A-CGA-CBA	2.20	118.59	111.90
9	J	609	CHL	CAA-CBA-CGA	2.20	119.76	113.32
10	G	614	CLA	CAA-CBA-CGA	2.20	119.76	113.32
8	I	8632	DGD	C3D-C4D-C5D	2.20	114.03	110.20
9	D	609	CHL	O2D-CGD-CBD	2.20	114.32	111.30
6	E	4623	NEX	C26-O24-C25	2.20	63.85	61.25
9	B	606	CHL	CMD-C2D-C3D	2.20	129.40	125.09
4	H	7621	LUT	C26-C25-C24	2.20	124.86	121.21
9	C	607	CHL	CED-O2D-CGD	2.20	121.16	115.99
10	C	603	CLA	CAC-C3C-C4C	2.21	128.03	124.83
9	F	608	CHL	CMB-C2B-C3B	2.21	129.41	125.09
9	F	601	CHL	C11-C10-C8	2.21	122.82	115.49
9	G	609	CHL	CMB-C2B-C3B	2.21	129.41	125.09
9	I	607	CHL	CAA-C2A-C1A	2.21	120.27	112.47
9	J	608	CHL	CMB-C2B-C3B	2.21	129.41	125.09
4	I	8620	LUT	C26-C25-C24	2.21	124.87	121.21
6	G	6623	NEX	C1-C2-C3	2.21	118.61	113.41
5	J	3622	XAT	C6-O4-C5	2.21	63.86	61.25
10	E	604	CLA	CBA-CAA-C2A	2.22	119.98	113.73
10	G	610	CLA	C14-C13-C12	2.22	119.61	111.08
9	I	601	CHL	C16-C15-C13	2.22	122.85	115.49
10	J	610	CLA	C16-C15-C13	2.22	122.86	115.49
10	G	610	CLA	C2A-C1A-CHA	2.22	127.98	123.89
9	C	608	CHL	CMB-C2B-C3B	2.22	129.43	125.09
10	A	611	CLA	C11-C10-C8	2.22	122.86	115.49
10	F	604	CLA	CED-O2D-CGD	2.22	121.20	115.99
4	D	3621	LUT	C22-C23-C24	2.22	114.37	111.75
4	I	8621	LUT	C22-C23-C24	2.22	114.37	111.75
9	C	605	CHL	CMB-C2B-C3B	2.23	129.44	125.09
9	H	607	CHL	C14-C13-C12	2.23	119.64	111.08
9	H	607	CHL	CAA-C2A-C1A	2.23	120.33	112.47
2	H	7633	BNG	O1-C1-C2	2.23	110.85	108.04
10	A	603	CLA	CMB-C2B-C3B	2.23	129.45	125.09
10	F	610	CLA	C2A-C1A-CHA	2.23	127.99	123.89
9	G	601	CHL	C6-C5-C3	2.24	117.39	112.48
10	D	604	CLA	CMD-C2D-C3D	2.24	129.46	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	6620	LUT	C1-C2-C3	2.24	118.66	113.41
10	D	612	CLA	CMB-C2B-C3B	2.24	129.47	125.09
9	C	608	CHL	C14-C13-C15	2.24	119.68	111.08
9	B	601	CHL	CMD-C2D-C3D	2.24	129.47	125.09
4	C	2621	LUT	C18-C5-C6	2.24	126.81	124.61
10	B	603	CLA	C11-C12-C13	2.24	122.92	115.49
9	C	607	CHL	CAA-C2A-C1A	2.24	120.38	112.47
9	C	601	CHL	C14-C13-C12	2.25	119.71	111.08
9	H	609	CHL	CBA-CAA-C2A	2.25	120.07	113.73
9	I	608	CHL	CMB-C2B-C3B	2.25	129.48	125.09
10	F	602	CLA	O2A-CGA-CBA	2.25	118.75	111.90
10	I	612	CLA	CMB-C2B-C3B	2.25	129.49	125.09
6	G	6623	NEX	C26-O24-C25	2.25	63.91	61.25
6	A	623	NEX	C24-C23-C22	2.26	115.40	110.41
10	B	603	CLA	C1D-CHD-C4C	2.26	126.02	122.60
5	H	4622	XAT	C6-O4-C5	2.26	63.91	61.25
9	C	607	CHL	C6-C5-C3	2.26	117.44	112.48
10	H	612	CLA	CED-O2D-CGD	2.26	121.28	115.99
6	D	3623	NEX	C26-O24-C25	2.26	63.91	61.25
10	G	614	CLA	CMC-C2C-C1C	2.26	128.51	125.02
9	H	607	CHL	CED-O2D-CGD	2.26	121.29	115.99
10	A	611	CLA	C16-C15-C13	2.26	122.98	115.49
10	D	604	CLA	C6-C5-C3	2.26	117.45	112.48
9	G	607	CHL	CED-O2D-CGD	2.26	121.29	115.99
6	A	623	NEX	C1-C2-C3	2.26	118.72	113.41
10	H	613	CLA	CAA-CBA-CGA	2.26	119.94	113.32
10	F	612	CLA	C11-C12-C13	2.27	123.01	115.49
9	B	609	CHL	CAA-CBA-CGA	2.27	119.96	113.32
5	D	8622	XAT	C6-O4-C5	2.27	63.93	61.25
10	G	611	CLA	CMB-C2B-C3B	2.27	129.53	125.09
10	E	611	CLA	C6-C7-C8	2.27	123.02	115.49
10	I	612	CLA	C4-C3-C2	2.27	127.96	123.50
4	F	5620	LUT	C1-C2-C3	2.28	118.75	113.41
5	C	7622	XAT	C37-C21-C36	2.28	110.75	107.35
9	I	607	CHL	CAC-C3C-C4C	2.28	128.14	124.83
10	D	602	CLA	CMB-C2B-C3B	2.28	129.55	125.09
6	F	5623	NEX	C26-O24-C25	2.28	63.94	61.25
6	I	8623	NEX	C26-O24-C25	2.29	63.95	61.25
2	A	633	BNG	O1-C1-C2	2.29	110.93	108.04
4	B	1620	LUT	C1-C2-C3	2.29	118.78	113.41
10	G	610	CLA	CMB-C2B-C3B	2.29	129.56	125.09
5	B	5622	XAT	C6-O4-C5	2.29	63.95	61.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	5623	NEX	C24-C23-C22	2.29	115.47	110.41
6	H	7623	NEX	C1-C2-C3	2.29	118.78	113.41
9	G	605	CHL	CED-O2D-CGD	2.29	121.36	115.99
10	B	603	CLA	CMB-C2B-C3B	2.29	129.57	125.09
6	A	623	NEX	C26-O24-C25	2.29	63.96	61.25
10	E	611	CLA	C9-C8-C10	2.30	119.90	111.08
10	J	612	CLA	CBA-CAA-C2A	2.30	120.21	113.73
10	J	611	CLA	C6-C7-C8	2.30	123.11	115.49
9	A	608	CHL	C4-C3-C2	2.30	128.01	123.50
10	B	611	CLA	C9-C8-C10	2.30	119.91	111.08
10	G	602	CLA	C7-C6-C5	2.30	119.85	113.06
9	G	607	CHL	C5-C3-C2	2.30	125.41	121.05
4	F	5620	LUT	C26-C25-C24	2.30	125.02	121.21
4	I	8621	LUT	C26-C25-C24	2.30	125.03	121.21
10	B	604	CLA	C9-C8-C10	2.30	119.93	111.08
6	I	8623	NEX	C1-C2-C3	2.31	118.82	113.41
10	A	610	CLA	C2A-C1A-CHA	2.31	128.13	123.89
9	I	608	CHL	O2D-CGD-CBD	2.31	114.46	111.30
6	C	2623	NEX	C16-C1-C6	2.31	112.55	110.48
9	C	607	CHL	CMD-C2D-C3D	2.31	129.60	125.09
8	H	6632	DGD	C4D-C3D-C2D	2.31	115.10	110.79
5	F	6622	XAT	C6-O4-C5	2.31	63.97	61.25
6	I	8623	NEX	C24-C23-C22	2.31	115.52	110.41
9	D	609	CHL	CAA-CBA-CGA	2.31	120.09	113.32
9	H	607	CHL	CMD-C2D-C3D	2.31	129.61	125.09
9	C	607	CHL	C5-C3-C2	2.32	125.44	121.05
10	I	611	CLA	CAA-C2A-C1A	2.32	120.64	112.47
9	F	608	CHL	C4-C3-C2	2.32	128.05	123.50
10	C	613	CLA	C5-C3-C2	2.32	125.45	121.05
10	H	602	CLA	C9-C8-C7	2.32	119.99	111.08
10	B	614	CLA	CED-O2D-CGD	2.32	121.43	115.99
10	I	610	CLA	C2A-C1A-CHA	2.32	128.16	123.89
4	A	620	LUT	C1-C2-C3	2.32	118.86	113.41
9	I	606	CHL	CED-O2D-CGD	2.32	121.44	115.99
10	D	612	CLA	C11-C12-C13	2.32	123.19	115.49
9	H	609	CHL	C6-C5-C3	2.32	117.58	112.48
10	H	611	CLA	CMB-C2B-C3B	2.33	129.64	125.09
9	H	605	CHL	CED-O2D-CGD	2.33	121.45	115.99
4	B	1621	LUT	C26-C25-C24	2.33	125.06	121.21
10	C	613	CLA	O2A-CGA-CBA	2.33	118.99	111.90
10	J	603	CLA	C1D-CHD-C4C	2.33	126.13	122.60
6	F	5623	NEX	C1-C2-C3	2.33	118.88	113.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	2623	NEX	C26-O24-C25	2.33	64.00	61.25
2	F	5633	BNG	O1-C1-C2	2.33	110.99	108.04
2	D	3633	BNG	O1-C1-C2	2.33	110.99	108.04
8	G	9632	DGD	C4D-C3D-C2D	2.33	115.15	110.79
9	G	609	CHL	C6-C5-C3	2.34	117.61	112.48
8	E	4632	DGD	C6D-C5D-C4D	2.34	117.32	112.03
10	A	614	CLA	CAA-CBA-CGA	2.34	120.16	113.32
10	I	611	CLA	CED-O2D-CGD	2.34	121.48	115.99
9	G	607	CHL	O2D-CGD-CBD	2.34	114.51	111.30
9	B	601	CHL	C16-C15-C13	2.34	123.26	115.49
9	D	601	CHL	CAC-C3C-C4C	2.34	128.23	124.83
4	G	6621	LUT	C18-C5-C6	2.34	126.91	124.61
9	J	609	CHL	C14-C13-C15	2.35	120.10	111.08
10	B	610	CLA	CMB-C2B-C3B	2.35	129.68	125.09
7	I	8630	LHG	O7-C7-C8	2.35	116.64	111.53
10	H	612	CLA	C14-C13-C15	2.35	120.11	111.08
9	E	607	CHL	CAA-C2A-C1A	2.35	120.77	112.47
10	D	603	CLA	O2A-CGA-CBA	2.35	119.07	111.90
5	A	622	XAT	C6-O4-C5	2.36	64.03	61.25
10	I	604	CLA	C11-C10-C8	2.36	123.31	115.49
10	B	613	CLA	C5-C3-C2	2.36	125.53	121.05
8	B	1632	DGD	C6D-C5D-C4D	2.36	117.38	112.03
10	E	613	CLA	C11-C10-C8	2.37	123.33	115.49
4	J	9620	LUT	C26-C25-C24	2.37	125.13	121.21
10	A	603	CLA	C1D-CHD-C4C	2.37	126.18	122.60
9	I	609	CHL	C14-C13-C15	2.37	120.17	111.08
10	I	611	CLA	CBA-CAA-C2A	2.37	120.42	113.73
9	J	605	CHL	CMB-C2B-C3B	2.37	129.73	125.09
10	D	612	CLA	C4-C3-C2	2.37	128.16	123.50
9	G	608	CHL	O2D-CGD-CBD	2.37	114.55	111.30
6	H	7623	NEX	C26-O24-C25	2.37	64.05	61.25
10	A	602	CLA	C14-C13-C15	2.38	120.21	111.08
10	E	611	CLA	CED-O2D-CGD	2.38	121.56	115.99
9	F	608	CHL	C14-C13-C15	2.38	120.23	111.08
4	C	2620	LUT	C2-C3-C4	2.38	114.54	110.32
9	A	609	CHL	CED-O2D-CGD	2.38	121.58	115.99
10	E	603	CLA	C1D-CHD-C4C	2.39	126.21	122.60
5	I	9622	XAT	C6-O4-C5	2.39	64.06	61.25
9	I	601	CHL	C6-C5-C3	2.39	117.72	112.48
9	A	607	CHL	C6-C5-C3	2.39	117.73	112.48
10	A	613	CLA	C5-C3-C2	2.39	125.59	121.05
10	E	603	CLA	C11-C12-C13	2.40	123.45	115.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	6633	BNG	O1-C1-C2	2.41	111.08	108.04
6	G	6623	NEX	C24-C23-C22	2.41	115.73	110.41
9	E	601	CHL	C5-C3-C2	2.41	125.62	121.05
10	F	613	CLA	C5-C3-C2	2.41	125.62	121.05
9	E	601	CHL	CMB-C2B-C3B	2.41	129.80	125.09
10	B	612	CLA	C4-C3-C2	2.41	128.24	123.50
9	E	607	CHL	C14-C13-C12	2.41	120.35	111.08
7	E	4630	LHG	O7-C7-C8	2.42	116.78	111.53
4	G	6621	LUT	C26-C25-C24	2.42	125.21	121.21
10	I	611	CLA	C11-C12-C13	2.42	123.51	115.49
10	D	603	CLA	C1D-CHD-C4C	2.42	126.27	122.60
10	I	611	CLA	C16-C15-C13	2.42	123.52	115.49
4	I	8620	LUT	C2-C3-C4	2.42	114.61	110.32
6	E	4623	NEX	C16-C1-C6	2.43	112.65	110.48
9	A	609	CHL	C6-C5-C3	2.43	117.81	112.48
9	G	605	CHL	CMB-C2B-C3B	2.43	129.84	125.09
10	H	604	CLA	CMD-C2D-C3D	2.43	129.84	125.09
10	A	612	CLA	CBA-CAA-C2A	2.43	120.58	113.73
10	A	611	CLA	CMB-C2B-C3B	2.43	129.84	125.09
10	J	602	CLA	CMB-C2B-C3B	2.43	129.85	125.09
9	F	609	CHL	C16-C15-C13	2.43	123.56	115.49
9	E	605	CHL	CMB-C2B-C3B	2.43	129.85	125.09
10	B	613	CLA	O2A-CGA-CBA	2.44	119.32	111.90
6	J	9623	NEX	C24-C23-C22	2.44	115.80	110.41
9	E	608	CHL	CMB-C2B-C3B	2.44	129.85	125.09
4	A	621	LUT	C26-C25-C24	2.44	125.25	121.21
10	C	611	CLA	O2D-CGD-CBD	2.44	114.65	111.30
4	C	2620	LUT	C26-C25-C24	2.44	125.25	121.21
10	B	604	CLA	C6-C5-C3	2.44	117.84	112.48
6	J	9623	NEX	C16-C1-C6	2.44	112.67	110.48
10	G	603	CLA	C1D-CHD-C4C	2.45	126.30	122.60
9	G	609	CHL	C14-C13-C15	2.45	120.48	111.08
10	J	614	CLA	O2A-CGA-CBA	2.45	119.37	111.90
4	G	6621	LUT	C2-C3-C4	2.45	114.67	110.32
4	G	6620	LUT	C3-C4-C5	2.46	116.91	111.86
10	F	612	CLA	CBA-CAA-C2A	2.46	120.67	113.73
10	C	611	CLA	CED-O2D-CGD	2.46	121.75	115.99
9	F	609	CHL	C14-C13-C15	2.46	120.52	111.08
10	I	603	CLA	C1D-CHD-C4C	2.46	126.33	122.60
9	H	609	CHL	C14-C13-C15	2.47	120.56	111.08
10	C	612	CLA	C11-C12-C13	2.47	123.68	115.49
9	D	608	CHL	CMB-C2B-C3B	2.47	129.92	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	610	CLA	CMB-C2B-C3B	2.47	129.92	125.09
4	D	3621	LUT	C18-C5-C6	2.48	127.04	124.61
6	B	1623	NEX	C16-C1-C6	2.48	112.70	110.48
9	B	601	CHL	C6-C5-C3	2.48	117.93	112.48
10	H	613	CLA	O2A-CGA-CBA	2.48	119.47	111.90
10	J	602	CLA	C14-C13-C15	2.48	120.62	111.08
10	A	613	CLA	O2A-CGA-CBA	2.48	119.47	111.90
10	J	612	CLA	CMB-C2B-C3B	2.49	129.95	125.09
9	D	605	CHL	CMB-C2B-C3B	2.49	129.95	125.09
10	C	614	CLA	CAA-CBA-CGA	2.49	120.60	113.32
9	D	607	CHL	C14-C13-C12	2.49	120.64	111.08
6	H	7623	NEX	C16-C1-C6	2.49	112.71	110.48
10	I	613	CLA	O2A-CGA-CBA	2.49	119.49	111.90
9	F	607	CHL	O2D-CGD-CBD	2.50	114.72	111.30
10	A	602	CLA	CMB-C2B-C3B	2.50	129.98	125.09
10	D	603	CLA	CMB-C2B-C3B	2.50	129.98	125.09
10	A	611	CLA	C11-C12-C13	2.50	123.79	115.49
10	B	612	CLA	CMB-C2B-C3B	2.50	129.98	125.09
10	B	614	CLA	CBA-CAA-C2A	2.51	120.80	113.73
9	G	601	CHL	C9-C8-C10	2.51	120.71	111.08
10	G	602	CLA	CMB-C2B-C3B	2.51	129.99	125.09
8	B	2632	DGD	C4D-C3D-C2D	2.51	115.47	110.79
10	C	603	CLA	C1D-CHD-C4C	2.51	126.40	122.60
10	H	614	CLA	CMC-C2C-C1C	2.51	128.91	125.02
8	D	5632	DGD	C3G-O3G-C1D	2.52	119.11	113.82
9	A	607	CHL	CED-O2D-CGD	2.52	121.89	115.99
9	J	607	CHL	CED-O2D-CGD	2.52	121.89	115.99
9	C	607	CHL	CAC-C3C-C4C	2.52	128.49	124.83
10	E	614	CLA	CMB-C2B-C3B	2.52	130.02	125.09
10	B	604	CLA	C6-C7-C8	2.52	123.85	115.49
5	C	7622	XAT	C1-C2-C3	2.53	119.28	115.02
10	I	614	CLA	CAA-CBA-CGA	2.53	120.73	113.32
9	G	601	CHL	CMB-C2B-C3B	2.53	130.04	125.09
10	J	610	CLA	CMC-C2C-C1C	2.53	128.94	125.02
10	E	610	CLA	C14-C13-C15	2.54	120.82	111.08
10	H	603	CLA	O2A-CGA-CBA	2.54	119.64	111.90
8	H	7632	DGD	O2G-C1B-C2B	2.54	117.05	111.53
10	F	614	CLA	C4A-NA-C1A	2.54	109.64	106.36
4	D	3621	LUT	C7-C8-C9	2.54	130.09	126.22
10	F	611	CLA	CAA-C2A-C1A	2.55	121.45	112.47
10	A	603	CLA	C16-C15-C13	2.55	123.94	115.49
10	G	604	CLA	C1D-CHD-C4C	2.55	126.46	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	610	CLA	CMC-C2C-C1C	2.55	128.96	125.02
10	D	612	CLA	C14-C13-C15	2.55	120.88	111.08
9	E	607	CHL	CED-O2D-CGD	2.55	121.97	115.99
9	C	601	CHL	CMB-C2B-C3B	2.56	130.09	125.09
10	F	613	CLA	O2A-CGA-CBA	2.56	119.69	111.90
10	E	610	CLA	CMB-C2B-C3B	2.56	130.09	125.09
8	H	7632	DGD	C3G-O3G-C1D	2.56	119.19	113.82
9	J	601	CHL	C14-C13-C12	2.56	120.91	111.08
10	D	610	CLA	CMC-C2C-C1C	2.56	128.98	125.02
10	C	614	CLA	C4A-NA-C1A	2.56	109.67	106.36
10	I	611	CLA	CMB-C2B-C3B	2.56	130.10	125.09
4	D	3621	LUT	C26-C25-C24	2.56	125.45	121.21
10	E	612	CLA	C14-C13-C15	2.56	120.93	111.08
5	B	1622	XAT	C6-O4-C5	2.56	64.27	61.25
10	I	610	CLA	CMB-C2B-C3B	2.56	130.10	125.09
8	B	2632	DGD	C6D-O5D-C1E	2.57	119.21	113.82
10	D	613	CLA	C5-C3-C2	2.57	125.92	121.05
9	C	601	CHL	C16-C15-C13	2.57	124.00	115.49
10	H	602	CLA	C7-C6-C5	2.57	120.65	113.06
10	I	614	CLA	CMB-C2B-C3B	2.57	130.11	125.09
10	C	610	CLA	C4A-NA-C1A	2.57	109.68	106.36
8	H	7632	DGD	C4D-C3D-C2D	2.57	115.59	110.79
9	D	607	CHL	CED-O2D-CGD	2.57	122.02	115.99
6	I	8623	NEX	C16-C1-C6	2.57	112.78	110.48
10	D	612	CLA	CED-O2D-CGD	2.58	122.03	115.99
10	A	602	CLA	C4-C3-C5	2.58	119.34	115.41
9	A	609	CHL	C14-C13-C15	2.58	121.00	111.08
10	H	614	CLA	CAA-CBA-CGA	2.58	120.88	113.32
8	B	1632	DGD	C3G-O3G-C1D	2.58	119.24	113.82
9	F	605	CHL	CMB-C2B-C3B	2.58	130.14	125.09
4	B	1621	LUT	C2-C3-C4	2.58	114.89	110.32
10	D	611	CLA	C6-C7-C8	2.59	124.06	115.49
10	C	611	CLA	CMB-C2B-C3B	2.59	130.16	125.09
10	F	611	CLA	C4A-NA-C1A	2.59	109.71	106.36
10	C	612	CLA	CMB-C2B-C3B	2.59	130.16	125.09
10	H	612	CLA	CMB-C2B-C3B	2.59	130.16	125.09
8	H	7632	DGD	C6D-O5D-C1E	2.59	119.27	113.82
10	C	604	CLA	C1D-CHD-C4C	2.60	126.53	122.60
9	A	605	CHL	O2D-CGD-CBD	2.60	114.86	111.30
2	E	4633	BNG	C1'-O1-C1	2.60	118.48	113.94
10	I	613	CLA	C5-C3-C2	2.60	125.98	121.05
9	I	605	CHL	CMB-C2B-C3B	2.60	130.17	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	5632	DGD	C3D-C4D-C5D	2.60	114.73	110.20
10	D	604	CLA	C6-C7-C8	2.60	124.11	115.49
4	D	3620	LUT	C1-C2-C3	2.60	119.52	113.41
9	F	606	CHL	O2D-CGD-CBD	2.60	114.87	111.30
10	A	613	CLA	C1D-CHD-C4C	2.61	126.54	122.60
8	D	3632	DGD	C4D-C3D-C2D	2.61	115.66	110.79
10	C	612	CLA	C4A-NA-C1A	2.61	109.73	106.36
9	F	608	CHL	C16-C15-C13	2.61	124.14	115.49
10	H	614	CLA	CED-O2D-CGD	2.61	122.11	115.99
7	J	9630	LHG	C27-C26-C25	2.61	128.01	114.53
10	G	602	CLA	C1D-CHD-C4C	2.61	126.56	122.60
6	A	623	NEX	C16-C1-C6	2.61	112.82	110.48
10	F	602	CLA	CED-O2D-CGD	2.62	122.12	115.99
10	G	611	CLA	CAA-CBA-CGA	2.62	120.98	113.32
10	I	611	CLA	C9-C8-C10	2.62	121.14	111.08
10	H	613	CLA	C1D-CHD-C4C	2.62	126.56	122.60
10	J	611	CLA	CED-O2D-CGD	2.62	122.14	115.99
10	F	610	CLA	C14-C13-C15	2.62	121.15	111.08
6	F	5623	NEX	C16-C1-C6	2.62	112.83	110.48
10	H	611	CLA	C4A-NA-C1A	2.62	109.75	106.36
10	F	611	CLA	CMB-C2B-C3B	2.62	130.22	125.09
9	D	601	CHL	C9-C8-C10	2.62	121.16	111.08
10	G	602	CLA	C4A-NA-C1A	2.62	109.75	106.36
9	B	609	CHL	CMB-C2B-C3B	2.63	130.22	125.09
9	G	607	CHL	C14-C13-C12	2.63	121.17	111.08
10	A	614	CLA	C4A-NA-C1A	2.63	109.75	106.36
10	H	604	CLA	CED-O2D-CGD	2.63	122.15	115.99
10	F	603	CLA	C1D-CHD-C4C	2.63	126.58	122.60
10	I	602	CLA	C1D-CHD-C4C	2.63	126.58	122.60
10	E	611	CLA	C6-C5-C3	2.63	118.25	112.48
10	H	604	CLA	C1D-CHD-C4C	2.63	126.58	122.60
10	I	604	CLA	C1D-CHD-C4C	2.63	126.58	122.60
10	J	613	CLA	C1D-CHD-C4C	2.63	126.58	122.60
10	B	614	CLA	O2A-CGA-CBA	2.63	119.92	111.90
10	D	604	CLA	C1D-CHD-C4C	2.63	126.58	122.60
9	E	609	CHL	C6-C5-C3	2.63	118.26	112.48
10	H	603	CLA	C1D-CHD-C4C	2.63	126.58	122.60
10	D	610	CLA	CMB-C2B-C3B	2.63	130.24	125.09
10	J	604	CLA	C1D-CHD-C4C	2.64	126.59	122.60
10	E	612	CLA	CMB-C2B-C3B	2.64	130.24	125.09
10	B	611	CLA	C4A-NA-C1A	2.64	109.77	106.36
10	A	612	CLA	CED-O2D-CGD	2.64	122.19	115.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	602	CLA	CED-O2D-CGD	2.64	122.19	115.99
9	D	606	CHL	O2D-CGD-CBD	2.64	114.92	111.30
10	B	613	CLA	C1D-CHD-C4C	2.64	126.60	122.60
10	H	602	CLA	C1D-CHD-C4C	2.64	126.60	122.60
6	G	6623	NEX	C16-C1-C6	2.65	112.85	110.48
10	D	604	CLA	C9-C8-C10	2.65	121.25	111.08
10	A	612	CLA	CMB-C2B-C3B	2.65	130.27	125.09
10	F	611	CLA	O2D-CGD-CBD	2.65	114.94	111.30
10	E	602	CLA	C14-C13-C15	2.66	121.29	111.08
10	I	612	CLA	C11-C12-C13	2.66	124.31	115.49
10	E	603	CLA	O2A-CGA-CBA	2.66	120.00	111.90
10	C	604	CLA	C6-C7-C8	2.66	124.31	115.49
10	F	613	CLA	C1D-CHD-C4C	2.66	126.63	122.60
10	A	611	CLA	C6-C5-C3	2.66	118.33	112.48
10	C	604	CLA	CBA-CAA-C2A	2.66	121.25	113.73
8	B	2632	DGD	C3G-O3G-C1D	2.66	119.41	113.82
9	F	609	CHL	O2D-CGD-CBD	2.67	114.96	111.30
10	I	611	CLA	C4A-NA-C1A	2.67	109.81	106.36
10	B	614	CLA	C1D-CHD-C4C	2.67	126.64	122.60
8	H	6632	DGD	C6D-O5D-C1E	2.67	119.43	113.82
10	B	614	CLA	C4A-NA-C1A	2.67	109.81	106.36
10	J	612	CLA	C1D-CHD-C4C	2.67	126.64	122.60
8	D	3632	DGD	C3G-O3G-C1D	2.67	119.43	113.82
10	E	603	CLA	CAA-CBA-CGA	2.67	121.13	113.32
9	F	607	CHL	CED-O2D-CGD	2.67	122.25	115.99
10	I	613	CLA	C1D-CHD-C4C	2.67	126.65	122.60
4	F	5621	LUT	C26-C25-C24	2.67	125.64	121.21
7	A	630	LHG	C27-C26-C25	2.67	128.34	114.53
10	C	610	CLA	C14-C13-C12	2.68	121.36	111.08
10	F	604	CLA	C1D-CHD-C4C	2.68	126.65	122.60
10	C	613	CLA	C1D-CHD-C4C	2.68	126.65	122.60
9	F	601	CHL	CMB-C2B-C3B	2.68	130.33	125.09
8	E	4632	DGD	C4D-C3D-C2D	2.68	115.79	110.79
10	J	603	CLA	O2A-CGA-CBA	2.68	120.07	111.90
4	A	621	LUT	C7-C8-C9	2.68	130.30	126.22
9	A	609	CHL	CAA-CBA-CGA	2.68	121.16	113.32
6	H	7623	NEX	C24-C23-C22	2.68	116.34	110.41
10	H	614	CLA	C4A-NA-C1A	2.68	109.83	106.36
10	H	602	CLA	C4A-NA-C1A	2.68	109.83	106.36
8	A	632	DGD	C3G-O3G-C1D	2.68	119.45	113.82
10	J	612	CLA	C14-C13-C15	2.68	121.39	111.08
10	C	614	CLA	CMB-C2B-C3B	2.68	130.34	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	612	CLA	O2A-CGA-CBA	2.69	120.08	111.90
10	F	604	CLA	C6-C7-C8	2.69	124.40	115.49
10	J	611	CLA	CMB-C2B-C3B	2.69	130.35	125.09
10	D	613	CLA	C1D-CHD-C4C	2.69	126.67	122.60
10	A	604	CLA	C1D-CHD-C4C	2.69	126.67	122.60
8	E	4632	DGD	C3G-O3G-C1D	2.69	119.47	113.82
10	B	612	CLA	C4A-NA-C1A	2.69	109.84	106.36
9	C	609	CHL	C14-C13-C15	2.69	121.42	111.08
10	D	614	CLA	C4A-NA-C1A	2.69	109.84	106.36
9	H	609	CHL	CAA-CBA-CGA	2.70	121.21	113.32
10	F	614	CLA	O2A-CGA-CBA	2.70	120.13	111.90
9	F	601	CHL	C9-C8-C10	2.70	121.46	111.08
10	G	602	CLA	C14-C13-C15	2.70	121.46	111.08
10	C	603	CLA	C4A-NA-C1A	2.70	109.85	106.36
8	A	632	DGD	C6D-O5D-C1E	2.70	119.50	113.82
8	D	3632	DGD	C6D-O5D-C1E	2.70	119.50	113.82
10	F	612	CLA	CMB-C2B-C3B	2.70	130.38	125.09
9	B	606	CHL	O2D-CGD-CBD	2.70	115.01	111.30
10	C	602	CLA	C4A-NA-C1A	2.71	109.86	106.36
10	C	603	CLA	O2A-CGA-CBA	2.71	120.15	111.90
10	E	602	CLA	C1D-CHD-C4C	2.71	126.70	122.60
10	A	612	CLA	C4A-NA-C1A	2.71	109.86	106.36
10	H	603	CLA	C6-C5-C3	2.71	118.42	112.48
2	I	8633	BNG	C1'-O1-C1	2.71	118.67	113.94
10	B	603	CLA	C4A-NA-C1A	2.71	109.86	106.36
10	H	604	CLA	C11-C10-C8	2.71	124.48	115.49
10	H	612	CLA	C4A-NA-C1A	2.71	109.86	106.36
10	B	610	CLA	C1D-CHD-C4C	2.71	126.70	122.60
10	E	610	CLA	CED-O2D-CGD	2.71	122.35	115.99
10	E	603	CLA	C4A-NA-C1A	2.71	109.87	106.36
10	J	614	CLA	C4A-NA-C1A	2.71	109.87	106.36
9	A	609	CHL	CMB-C2B-C3B	2.72	130.40	125.09
10	F	603	CLA	C4A-NA-C1A	2.72	109.87	106.36
8	B	1632	DGD	C6D-O5D-C1E	2.72	119.53	113.82
10	D	602	CLA	C1D-CHD-C4C	2.72	126.72	122.60
10	E	613	CLA	C1D-CHD-C4C	2.72	126.72	122.60
9	C	609	CHL	C6-C5-C3	2.72	118.46	112.48
9	J	609	CHL	CED-O2D-CGD	2.72	122.38	115.99
9	C	606	CHL	CED-O2D-CGD	2.73	122.38	115.99
9	C	607	CHL	C14-C13-C12	2.73	121.55	111.08
10	B	612	CLA	CED-O2D-CGD	2.73	122.38	115.99
10	G	613	CLA	C1D-CHD-C4C	2.73	126.73	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	G	612	CLA	C16-C15-C13	2.73	124.53	115.49
4	B	1621	LUT	C1-C2-C3	2.73	119.82	113.41
9	F	605	CHL	O2D-CGD-CBD	2.73	115.05	111.30
10	E	614	CLA	C1D-CHD-C4C	2.73	126.73	122.60
10	G	612	CLA	CED-O2D-CGD	2.73	122.40	115.99
10	D	614	CLA	CMB-C2B-C3B	2.73	130.43	125.09
9	I	609	CHL	CMB-C2B-C3B	2.73	130.43	125.09
8	D	3632	DGD	O2G-C1B-C2B	2.73	117.47	111.53
10	G	604	CLA	C6-C5-C3	2.74	118.49	112.48
10	E	602	CLA	C4A-NA-C1A	2.74	109.90	106.36
8	D	3632	DGD	C3D-C4D-C5D	2.74	114.97	110.20
10	I	604	CLA	CBA-CAA-C2A	2.74	121.46	113.73
8	I	8632	DGD	C6D-O5D-C1E	2.74	119.57	113.82
9	C	605	CHL	O2D-CGD-CBD	2.74	115.06	111.30
9	A	605	CHL	OMC-CMC-C2C	2.74	132.63	125.58
10	D	603	CLA	C4A-NA-C1A	2.74	109.90	106.36
9	D	607	CHL	CBA-CAA-C2A	2.74	121.47	113.73
10	G	610	CLA	CMC-C2C-C1C	2.74	129.27	125.02
8	D	3632	DGD	O3G-C1D-C2D	2.75	111.51	108.04
9	E	606	CHL	O2D-CGD-CBD	2.75	115.07	111.30
10	B	612	CLA	C1D-CHD-C4C	2.75	126.76	122.60
10	D	614	CLA	C1D-CHD-C4C	2.75	126.76	122.60
10	J	613	CLA	O2A-CGA-CBA	2.75	120.28	111.90
10	F	612	CLA	C4A-NA-C1A	2.75	109.92	106.36
10	F	611	CLA	C1D-CHD-C4C	2.75	126.77	122.60
8	A	632	DGD	O3G-C1D-C2D	2.75	111.52	108.04
9	A	608	CHL	C14-C13-C15	2.76	121.67	111.08
9	B	608	CHL	C16-C15-C13	2.76	124.63	115.49
7	H	7630	LHG	C27-C26-C25	2.76	128.77	114.53
10	A	602	CLA	C4A-NA-C1A	2.76	109.92	106.36
10	I	611	CLA	O2D-CGD-CBD	2.76	115.08	111.30
8	I	8632	DGD	C3G-O3G-C1D	2.76	119.62	113.82
10	J	612	CLA	C4A-NA-C1A	2.76	109.93	106.36
10	I	612	CLA	C4A-NA-C1A	2.76	109.93	106.36
10	D	610	CLA	C1D-CHD-C4C	2.76	126.78	122.60
10	F	610	CLA	CMB-C2B-C3B	2.76	130.49	125.09
10	I	603	CLA	CED-O2D-CGD	2.77	122.48	115.99
10	G	612	CLA	CMB-C2B-C3B	2.77	130.50	125.09
4	J	9621	LUT	C1-C2-C3	2.77	119.91	113.41
9	B	605	CHL	O2D-CGD-CBD	2.77	115.10	111.30
10	E	604	CLA	C1D-CHD-C4C	2.77	126.80	122.60
10	J	610	CLA	C1D-CHD-C4C	2.77	126.80	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	5630	LHG	C27-C26-C25	2.77	128.85	114.53
10	J	603	CLA	C16-C15-C13	2.77	124.69	115.49
10	D	611	CLA	C4A-NA-C1A	2.77	109.94	106.36
8	E	4632	DGD	C6D-O5D-C1E	2.77	119.65	113.82
10	E	610	CLA	C1D-CHD-C4C	2.78	126.80	122.60
10	E	612	CLA	C4A-NA-C1A	2.78	109.95	106.36
10	A	614	CLA	O2A-CGA-CBA	2.78	120.36	111.90
10	J	612	CLA	C4-C3-C2	2.78	128.96	123.50
10	G	611	CLA	O2D-CGD-CBD	2.78	115.11	111.30
10	A	612	CLA	C14-C13-C15	2.78	121.76	111.08
10	E	614	CLA	CAA-CBA-CGA	2.78	121.46	113.32
10	F	603	CLA	CED-O2D-CGD	2.78	122.52	115.99
8	G	9632	DGD	C6D-O5D-C1E	2.78	119.67	113.82
10	G	610	CLA	C16-C15-C13	2.78	124.72	115.49
10	J	612	CLA	CED-O2D-CGD	2.78	122.52	115.99
9	B	607	CHL	C6-C5-C3	2.79	118.60	112.48
10	F	602	CLA	C4A-NA-C1A	2.79	109.97	106.36
9	G	608	CHL	CMB-C2B-C3B	2.79	130.54	125.09
10	D	612	CLA	C1D-CHD-C4C	2.79	126.83	122.60
9	J	601	CHL	C6-C5-C3	2.79	118.61	112.48
10	J	610	CLA	CMB-C2B-C3B	2.79	130.55	125.09
10	F	614	CLA	CMB-C2B-C3B	2.79	130.55	125.09
10	G	612	CLA	C4A-NA-C1A	2.79	109.97	106.36
9	I	608	CHL	C16-C15-C13	2.79	124.76	115.49
10	I	602	CLA	C4A-NA-C1A	2.80	109.97	106.36
10	F	602	CLA	C9-C8-C7	2.80	121.83	111.08
10	J	602	CLA	C1D-CHD-C4C	2.80	126.84	122.60
10	A	612	CLA	C1D-CHD-C4C	2.80	126.84	122.60
10	H	613	CLA	C6-C5-C3	2.80	118.63	112.48
10	G	614	CLA	CMB-C2B-C3B	2.80	130.57	125.09
2	A	633	BNG	C1'-O1-C1	2.80	118.84	113.94
10	C	604	CLA	C4A-NA-C1A	2.80	109.98	106.36
10	B	610	CLA	C4A-NA-C1A	2.80	109.98	106.36
10	A	610	CLA	CMC-C2C-C1C	2.80	129.36	125.02
10	I	614	CLA	C4A-NA-C1A	2.81	109.99	106.36
10	D	610	CLA	C4A-NA-C1A	2.81	109.99	106.36
2	G	6633	BNG	C1'-O1-C1	2.81	118.85	113.94
7	D	3630	LHG	C27-C26-C25	2.81	129.04	114.53
9	H	601	CHL	CMB-C2B-C3B	2.81	130.59	125.09
10	A	610	CLA	C4A-NA-C1A	2.81	110.00	106.36
10	F	610	CLA	C1D-CHD-C4C	2.81	126.86	122.60
10	J	611	CLA	C1D-CHD-C4C	2.81	126.86	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	611	CLA	C1D-CHD-C4C	2.81	126.86	122.60
10	A	611	CLA	C4A-NA-C1A	2.81	110.00	106.36
10	D	611	CLA	CMB-C2B-C3B	2.81	130.59	125.09
10	B	604	CLA	C1D-CHD-C4C	2.81	126.86	122.60
10	I	614	CLA	C1D-CHD-C4C	2.82	126.86	122.60
10	E	602	CLA	C4-C3-C5	2.82	119.71	115.41
4	E	4621	LUT	C18-C5-C6	2.82	127.37	124.61
10	D	603	CLA	C6-C5-C3	2.82	118.66	112.48
10	D	612	CLA	C4A-NA-C1A	2.82	110.00	106.36
2	H	7633	BNG	C1'-O1-C1	2.82	118.87	113.94
10	E	614	CLA	C4A-NA-C1A	2.82	110.01	106.36
10	F	614	CLA	CAA-CBA-CGA	2.82	121.58	113.32
10	H	610	CLA	C14-C13-C15	2.82	121.93	111.08
10	C	614	CLA	O2A-CGA-CBA	2.83	120.51	111.90
10	E	613	CLA	C5-C3-C2	2.83	126.41	121.05
10	E	602	CLA	CMC-C2C-C1C	2.83	129.39	125.02
10	B	602	CLA	C1D-CHD-C4C	2.83	126.88	122.60
9	G	609	CHL	C16-C15-C13	2.83	124.87	115.49
7	G	6630	LHG	C27-C26-C25	2.83	129.14	114.53
10	G	603	CLA	C16-C15-C13	2.83	124.87	115.49
2	F	5633	BNG	C1'-O1-C1	2.83	118.89	113.94
10	I	603	CLA	C4A-NA-C1A	2.83	110.02	106.36
10	J	602	CLA	CED-O2D-CGD	2.83	122.63	115.99
10	H	604	CLA	CAA-CBA-CGA	2.83	121.61	113.32
10	D	612	CLA	C11-C10-C8	2.83	124.89	115.49
10	G	614	CLA	C4A-NA-C1A	2.83	110.02	106.36
10	G	603	CLA	C4A-NA-C1A	2.83	110.02	106.36
10	H	612	CLA	C1D-CHD-C4C	2.83	126.89	122.60
4	D	3620	LUT	C2-C3-C4	2.84	115.34	110.32
10	F	603	CLA	O2A-CGA-CBA	2.84	120.55	111.90
10	D	604	CLA	C4A-NA-C1A	2.84	110.03	106.36
10	H	611	CLA	CAA-C2A-C1A	2.84	122.48	112.47
10	B	602	CLA	O2A-CGA-CBA	2.84	120.56	111.90
10	E	612	CLA	C1D-CHD-C4C	2.84	126.90	122.60
9	H	608	CHL	CMB-C2B-C3B	2.84	130.65	125.09
10	H	612	CLA	C4-C3-C2	2.85	129.09	123.50
10	F	602	CLA	C1D-CHD-C4C	2.85	126.91	122.60
9	A	608	CHL	O2D-CGD-CBD	2.85	115.20	111.30
9	H	609	CHL	CMB-C2B-C3B	2.85	130.66	125.09
10	G	604	CLA	CED-O2D-CGD	2.85	122.67	115.99
10	B	602	CLA	C4A-NA-C1A	2.85	110.04	106.36
10	G	611	CLA	C4A-NA-C1A	2.86	110.05	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	2630	LHG	O7-C7-C8	2.86	117.73	111.53
9	J	607	CHL	C5-C3-C2	2.86	126.47	121.05
7	G	6630	LHG	O7-C7-C8	2.86	117.74	111.53
4	E	4621	LUT	C1-C2-C3	2.86	120.12	113.41
9	B	608	CHL	CMB-C2B-C3B	2.86	130.68	125.09
10	B	604	CLA	C4A-NA-C1A	2.86	110.06	106.36
10	G	602	CLA	O2A-CGA-CBA	2.86	120.61	111.90
10	J	613	CLA	C4A-NA-C1A	2.86	110.06	106.36
10	E	603	CLA	CED-O2D-CGD	2.86	122.70	115.99
9	I	609	CHL	C4B-CHC-C1C	2.86	126.93	122.60
7	C	2630	LHG	C27-C26-C25	2.86	129.32	114.53
2	B	1633	BNG	C1'-O1-C1	2.87	118.95	113.94
10	J	614	CLA	CMB-C2B-C3B	2.87	130.69	125.09
8	B	1632	DGD	O3G-C1D-C2D	2.87	111.66	108.04
10	E	611	CLA	CAA-C2A-C1A	2.87	122.58	112.47
10	D	611	CLA	C1D-CHD-C4C	2.87	126.94	122.60
10	I	602	CLA	O2A-CGA-CBA	2.87	120.65	111.90
9	A	608	CHL	O2A-CGA-CBA	2.87	120.65	111.90
10	A	610	CLA	C1D-CHD-C4C	2.87	126.95	122.60
8	G	9632	DGD	C3G-O3G-C1D	2.87	119.85	113.82
8	B	2632	DGD	C3D-C4D-C5D	2.87	115.21	110.20
10	J	612	CLA	O2A-CGA-CBA	2.88	120.66	111.90
10	B	614	CLA	CMB-C2B-C3B	2.88	130.71	125.09
9	A	606	CHL	O2D-CGD-CBD	2.88	115.24	111.30
10	I	610	CLA	C14-C13-C15	2.88	122.13	111.08
4	I	8621	LUT	C1-C2-C3	2.88	120.16	113.41
10	J	602	CLA	C4A-NA-C1A	2.88	110.08	106.36
9	J	609	CHL	C16-C15-C13	2.88	125.04	115.49
4	C	2620	LUT	C3-C4-C5	2.88	117.79	111.86
4	A	621	LUT	C2-C3-C4	2.88	115.42	110.32
10	H	604	CLA	C6-C7-C8	2.88	125.05	115.49
10	E	610	CLA	C4A-NA-C1A	2.88	110.09	106.36
10	H	604	CLA	C4A-NA-C1A	2.89	110.09	106.36
9	J	609	CHL	O2D-CGD-CBD	2.89	115.26	111.30
10	A	603	CLA	C4A-NA-C1A	2.89	110.09	106.36
10	I	602	CLA	C7-C6-C5	2.89	121.60	113.06
10	G	612	CLA	C1D-CHD-C4C	2.89	126.97	122.60
10	D	602	CLA	C4A-NA-C1A	2.89	110.09	106.36
9	I	609	CHL	C6-C5-C3	2.89	118.83	112.48
10	E	604	CLA	O2D-CGD-CBD	2.89	115.27	111.30
9	F	605	CHL	CED-O2D-CGD	2.89	122.77	115.99
9	A	601	CHL	CMB-C2B-C3B	2.90	130.75	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	6621	LUT	C1-C2-C3	2.90	120.21	113.41
10	C	611	CLA	C4A-NA-C1A	2.90	110.10	106.36
10	H	614	CLA	O2A-CGA-CBA	2.90	120.73	111.90
4	H	7620	LUT	C3-C4-C5	2.90	117.83	111.86
10	I	612	CLA	C1D-CHD-C4C	2.90	126.99	122.60
7	B	1630	LHG	O7-C7-C8	2.90	117.83	111.53
10	F	610	CLA	C4A-NA-C1A	2.90	110.11	106.36
9	F	609	CHL	CED-O2D-CGD	2.90	122.80	115.99
4	F	5620	LUT	C2-C3-C4	2.90	115.46	110.32
8	H	6632	DGD	C3G-O3G-C1D	2.91	119.92	113.82
10	G	614	CLA	O2A-CGA-CBA	2.91	120.75	111.90
5	F	6622	XAT	C1-C2-C3	2.91	119.93	115.02
10	C	614	CLA	C1D-CHD-C4C	2.91	127.00	122.60
10	H	610	CLA	C1D-CHD-C4C	2.91	127.01	122.60
10	A	612	CLA	O2A-CGA-CBA	2.91	120.78	111.90
8	H	6632	DGD	O2G-C1B-C2B	2.92	117.86	111.53
9	D	608	CHL	O2A-CGA-CBA	2.92	120.78	111.90
10	G	604	CLA	C4A-NA-C1A	2.92	110.13	106.36
10	C	602	CLA	C1D-CHD-C4C	2.92	127.02	122.60
4	A	621	LUT	C1-C2-C3	2.92	120.26	113.41
10	H	614	CLA	C1D-CHD-C4C	2.92	127.02	122.60
10	E	613	CLA	C6-C5-C3	2.92	118.90	112.48
2	C	2633	BNG	C1'-O1-C1	2.92	119.05	113.94
10	F	602	CLA	C14-C13-C15	2.93	122.33	111.08
10	H	611	CLA	O2D-CGD-CBD	2.93	115.32	111.30
9	B	605	CHL	CED-O2D-CGD	2.93	122.86	115.99
10	D	602	CLA	C14-C13-C15	2.93	122.34	111.08
10	B	612	CLA	C14-C13-C15	2.93	122.34	111.08
10	H	602	CLA	O2A-CGA-CBA	2.93	120.84	111.90
10	A	614	CLA	C1D-CHD-C4C	2.94	127.04	122.60
10	J	610	CLA	C14-C13-C15	2.94	122.36	111.08
9	E	609	CHL	CMB-C2B-C3B	2.94	130.83	125.09
10	J	611	CLA	C4A-NA-C1A	2.94	110.16	106.36
7	B	1630	LHG	C27-C26-C25	2.94	129.71	114.53
10	G	613	CLA	C6-C5-C3	2.94	118.94	112.48
8	I	8632	DGD	O3G-C1D-C2D	2.94	111.75	108.04
10	F	612	CLA	C1D-CHD-C4C	2.94	127.05	122.60
10	B	613	CLA	C4A-NA-C1A	2.94	110.16	106.36
10	E	604	CLA	C4A-NA-C1A	2.94	110.17	106.36
10	J	603	CLA	C4A-NA-C1A	2.95	110.17	106.36
10	A	610	CLA	CMB-C2B-C3B	2.95	130.85	125.09
10	A	610	CLA	C14-C13-C15	2.95	122.41	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	5621	LUT	C1-C2-C3	2.95	120.33	113.41
10	J	604	CLA	CAA-CBA-CGA	2.95	121.96	113.32
7	H	7630	LHG	O7-C7-C8	2.95	117.94	111.53
10	C	611	CLA	C1D-CHD-C4C	2.95	127.07	122.60
9	F	608	CHL	CBA-CAA-C2A	2.95	122.07	113.73
10	C	603	CLA	CMB-C2B-C3B	2.96	130.87	125.09
2	J	9633	BNG	C1'-O1-C1	2.96	119.11	113.94
9	H	601	CHL	C11-C12-C13	2.96	125.30	115.49
10	F	614	CLA	C1D-CHD-C4C	2.96	127.08	122.60
4	E	4620	LUT	C3-C4-C5	2.96	117.95	111.86
9	F	601	CHL	C6-C5-C3	2.96	118.99	112.48
10	J	610	CLA	C4A-NA-C1A	2.96	110.19	106.36
10	B	611	CLA	C1D-CHD-C4C	2.96	127.09	122.60
10	A	604	CLA	CED-O2D-CGD	2.97	122.94	115.99
10	E	611	CLA	C4A-NA-C1A	2.97	110.19	106.36
10	A	611	CLA	C1D-CHD-C4C	2.97	127.09	122.60
7	J	9630	LHG	O7-C7-C8	2.97	117.98	111.53
10	F	610	CLA	CED-O2D-CGD	2.97	122.96	115.99
10	F	610	CLA	CMC-C2C-C1C	2.97	129.62	125.02
9	E	605	CHL	CED-O2D-CGD	2.97	122.96	115.99
10	J	604	CLA	C4A-NA-C1A	2.97	110.20	106.36
9	H	609	CHL	C16-C15-C13	2.97	125.35	115.49
9	I	601	CHL	CMB-C2B-C3B	2.97	130.91	125.09
8	B	1632	DGD	C3D-C4D-C5D	2.98	115.38	110.20
10	G	610	CLA	C1D-CHD-C4C	2.98	127.10	122.60
4	C	2621	LUT	C2-C3-C4	2.98	115.59	110.32
10	I	610	CLA	CED-O2D-CGD	2.98	122.97	115.99
10	D	611	CLA	CED-O2D-CGD	2.98	122.98	115.99
10	H	610	CLA	C4A-NA-C1A	2.98	110.21	106.36
10	A	602	CLA	C1D-CHD-C4C	2.98	127.11	122.60
10	A	604	CLA	C4A-NA-C1A	2.98	110.22	106.36
10	H	602	CLA	CED-O2D-CGD	2.99	122.99	115.99
8	D	5632	DGD	O3G-C1D-C2D	2.99	111.82	108.04
9	J	601	CHL	OMC-CMC-C2C	2.99	133.27	125.58
9	E	609	CHL	C14-C13-C15	2.99	122.58	111.08
9	H	608	CHL	C4B-CHC-C1C	3.00	127.14	122.60
10	F	604	CLA	C4A-NA-C1A	3.00	110.23	106.36
10	I	602	CLA	CMC-C2C-C1C	3.00	129.66	125.02
10	H	614	CLA	CMB-C2B-C3B	3.00	130.95	125.09
10	I	610	CLA	C1D-CHD-C4C	3.00	127.14	122.60
10	D	611	CLA	CAA-C2A-C1A	3.00	123.06	112.47
10	J	603	CLA	CAA-CBA-CGA	3.00	122.11	113.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	610	CLA	C4A-NA-C1A	3.00	110.24	106.36
10	G	610	CLA	C4A-NA-C1A	3.00	110.24	106.36
9	E	609	CHL	CAA-CBA-CGA	3.00	122.11	113.32
10	J	614	CLA	C1D-CHD-C4C	3.00	127.15	122.60
9	D	609	CHL	CED-O2D-CGD	3.00	123.04	115.99
10	H	603	CLA	C4A-NA-C1A	3.01	110.25	106.36
10	A	614	CLA	CMB-C2B-C3B	3.01	130.97	125.09
9	I	607	CHL	C6-C5-C3	3.01	119.09	112.48
9	A	601	CHL	C14-C13-C15	3.01	122.65	111.08
4	D	3621	LUT	C1-C2-C3	3.02	120.49	113.41
9	B	607	CHL	CED-O2D-CGD	3.02	123.07	115.99
8	A	632	DGD	O2G-C1B-C2B	3.03	118.11	111.53
10	G	604	CLA	CBA-CAA-C2A	3.03	122.28	113.73
9	J	607	CHL	C6-C5-C3	3.03	119.14	112.48
9	C	601	CHL	C11-C12-C13	3.03	125.55	115.49
10	A	610	CLA	O2D-CGD-CBD	3.03	115.46	111.30
10	A	613	CLA	C4A-NA-C1A	3.03	110.28	106.36
10	A	602	CLA	C7-C6-C5	3.04	122.03	113.06
4	J	9620	LUT	C2-C1-C6	3.04	115.33	110.49
9	I	608	CHL	OMC-CMC-C2C	3.04	133.39	125.58
4	I	8620	LUT	C3-C4-C5	3.04	118.11	111.86
9	J	609	CHL	CMB-C2B-C3B	3.04	131.04	125.09
9	J	608	CHL	OMC-CMC-C2C	3.04	133.41	125.58
8	H	7632	DGD	C3D-C4D-C5D	3.05	115.51	110.20
10	C	603	CLA	CAA-CBA-CGA	3.05	122.24	113.32
9	E	606	CHL	CED-O2D-CGD	3.05	123.14	115.99
9	E	601	CHL	C11-C12-C13	3.05	125.61	115.49
10	H	611	CLA	C1D-CHD-C4C	3.05	127.22	122.60
9	I	608	CHL	O2A-CGA-CBA	3.05	121.20	111.90
10	C	612	CLA	C1D-CHD-C4C	3.06	127.23	122.60
10	F	603	CLA	CMB-C2B-C3B	3.06	131.07	125.09
9	C	608	CHL	O2A-CGA-CBA	3.06	121.22	111.90
9	D	606	CHL	CED-O2D-CGD	3.06	123.17	115.99
8	B	2632	DGD	O3G-C1D-C2D	3.06	111.91	108.04
9	D	608	CHL	CBA-CAA-C2A	3.06	122.37	113.73
9	E	609	CHL	C4B-CHC-C1C	3.06	127.24	122.60
10	G	611	CLA	CAA-C2A-C1A	3.06	123.28	112.47
4	I	8621	LUT	C2-C3-C4	3.07	115.75	110.32
10	C	610	CLA	C1D-CHD-C4C	3.07	127.24	122.60
10	A	611	CLA	CAA-CBA-CGA	3.07	122.31	113.32
9	E	607	CHL	C4B-CHC-C1C	3.07	127.25	122.60
10	B	603	CLA	O2A-CGA-CBA	3.08	121.27	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	607	CHL	C14-C13-C12	3.08	122.90	111.08
9	H	608	CHL	C16-C15-C13	3.08	125.70	115.49
4	F	5621	LUT	C2-C3-C4	3.08	115.78	110.32
10	E	613	CLA	O2A-CGA-CBA	3.08	121.29	111.90
10	E	611	CLA	CAA-CBA-CGA	3.08	122.35	113.32
10	H	604	CLA	CBA-CAA-C2A	3.09	122.44	113.73
7	E	4630	LHG	C27-C26-C25	3.09	130.48	114.53
9	H	605	CHL	OMC-CMC-C2C	3.09	133.53	125.58
9	D	609	CHL	CMB-C2B-C3B	3.09	131.14	125.09
9	F	609	CHL	CMB-C2B-C3B	3.10	131.14	125.09
9	F	609	CHL	C6-C5-C3	3.10	119.28	112.48
9	I	606	CHL	C1-C2-C3	3.10	131.78	126.71
8	H	6632	DGD	O3G-C1D-C2D	3.10	111.95	108.04
10	I	613	CLA	C4A-NA-C1A	3.10	110.37	106.36
7	I	8630	LHG	C27-C26-C25	3.10	130.55	114.53
10	C	602	CLA	CED-O2D-CGD	3.10	123.27	115.99
4	E	4621	LUT	C2-C3-C4	3.10	115.81	110.32
10	I	614	CLA	CBA-CAA-C2A	3.11	122.50	113.73
9	F	609	CHL	C4B-CHC-C1C	3.11	127.30	122.60
10	J	611	CLA	CAA-C2A-C1A	3.11	123.44	112.47
10	H	613	CLA	C4A-NA-C1A	3.11	110.38	106.36
2	D	3633	BNG	C1'-O1-C1	3.11	119.38	113.94
9	F	608	CHL	O2A-CGA-CBA	3.11	121.38	111.90
9	G	608	CHL	C4A-NA-C1A	3.11	109.71	106.04
4	C	2621	LUT	C1-C2-C3	3.12	120.73	113.41
10	B	602	CLA	C14-C13-C15	3.12	123.07	111.08
8	G	9632	DGD	O3G-C1D-C2D	3.13	111.99	108.04
10	A	611	CLA	CAA-C2A-C1A	3.13	123.50	112.47
8	G	9632	DGD	C3D-C4D-C5D	3.13	115.65	110.20
9	H	608	CHL	O2A-CGA-CBA	3.13	121.44	111.90
10	I	611	CLA	C1D-CHD-C4C	3.13	127.34	122.60
10	B	604	CLA	CBA-CAA-C2A	3.13	122.58	113.73
9	G	609	CHL	CED-O2D-CGD	3.14	123.35	115.99
10	G	611	CLA	C1D-CHD-C4C	3.14	127.35	122.60
10	D	613	CLA	C4A-NA-C1A	3.14	110.42	106.36
10	E	613	CLA	C4A-NA-C1A	3.14	110.42	106.36
10	B	611	CLA	CMB-C2B-C3B	3.14	131.24	125.09
10	C	613	CLA	CBA-CAA-C2A	3.14	122.60	113.73
10	G	613	CLA	C4A-NA-C1A	3.15	110.44	106.36
9	A	601	CHL	C16-C15-C13	3.15	125.95	115.49
10	I	604	CLA	C4A-NA-C1A	3.15	110.44	106.36
9	J	601	CHL	C11-C12-C13	3.16	125.96	115.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	7621	LUT	C1-C2-C3	3.16	120.82	113.41
4	B	1620	LUT	C3-C4-C5	3.16	118.36	111.86
9	J	609	CHL	C4A-NA-C1A	3.16	109.77	106.04
9	F	607	CHL	CMB-C2B-C3B	3.16	131.27	125.09
9	J	605	CHL	CED-O2D-CGD	3.16	123.40	115.99
9	D	601	CHL	C6-C5-C3	3.16	119.42	112.48
10	D	614	CLA	CBA-CAA-C2A	3.16	122.66	113.73
8	E	4632	DGD	O3G-C1D-C2D	3.17	112.04	108.04
9	H	608	CHL	C4A-NA-C1A	3.17	109.77	106.04
10	J	613	CLA	C5-C3-C2	3.17	127.06	121.05
10	J	614	CLA	CBA-CAA-C2A	3.17	122.67	113.73
10	C	603	CLA	CBA-CAA-C2A	3.17	122.68	113.73
10	G	614	CLA	C1D-CHD-C4C	3.17	127.41	122.60
9	F	609	CHL	C4A-NA-C1A	3.18	109.79	106.04
10	A	613	CLA	CMB-C2B-C3B	3.18	131.31	125.09
10	A	611	CLA	CED-O2D-CGD	3.18	123.45	115.99
10	H	613	CLA	C5-C3-C2	3.18	127.09	121.05
8	E	4632	DGD	O2G-C1B-C2B	3.18	118.45	111.53
10	J	603	CLA	CED-O2D-CGD	3.19	123.46	115.99
9	G	608	CHL	C16-C15-C13	3.19	126.07	115.49
8	E	4632	DGD	C3D-C4D-C5D	3.19	115.76	110.20
10	C	610	CLA	CED-O2D-CGD	3.19	123.48	115.99
10	D	602	CLA	O2A-CGA-CBA	3.20	121.64	111.90
10	B	602	CLA	CMC-C2C-C1C	3.20	129.97	125.02
10	F	603	CLA	CAA-CBA-CGA	3.20	122.69	113.32
10	C	613	CLA	C4A-NA-C1A	3.20	110.50	106.36
8	D	5632	DGD	C6D-O5D-C1E	3.20	120.54	113.82
9	G	605	CHL	C4B-CHC-C1C	3.20	127.45	122.60
9	B	607	CHL	C5-C3-C2	3.20	127.13	121.05
9	F	608	CHL	CED-O2D-CGD	3.21	123.51	115.99
10	G	613	CLA	O2A-CGA-CBA	3.21	121.67	111.90
8	H	6632	DGD	C3D-C4D-C5D	3.21	115.80	110.20
10	E	613	CLA	CBA-CAA-C2A	3.21	122.79	113.73
10	D	604	CLA	CED-O2D-CGD	3.22	123.53	115.99
10	F	613	CLA	C4A-NA-C1A	3.22	110.52	106.36
9	C	608	CHL	CBA-CAA-C2A	3.22	122.82	113.73
4	H	7621	LUT	C2-C3-C4	3.22	116.03	110.32
9	J	608	CHL	C4B-CHC-C1C	3.22	127.48	122.60
10	B	611	CLA	CAA-C2A-C1A	3.22	123.84	112.47
7	D	3630	LHG	O7-C7-C8	3.23	118.54	111.53
10	E	612	CLA	CED-O2D-CGD	3.23	123.56	115.99
9	J	609	CHL	C4B-CHC-C1C	3.23	127.49	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	612	CLA	CED-O2D-CGD	3.23	123.58	115.99
4	J	9621	LUT	C2-C3-C4	3.23	116.05	110.32
9	A	609	CHL	C4A-NA-C1A	3.24	109.86	106.04
10	E	602	CLA	CED-O2D-CGD	3.24	123.58	115.99
9	I	608	CHL	CED-O2D-CGD	3.24	123.59	115.99
8	I	8632	DGD	O2G-C1B-C2B	3.24	118.57	111.53
9	I	608	CHL	C4B-CHC-C1C	3.25	127.51	122.60
9	A	607	CHL	C4B-CHC-C1C	3.25	127.51	122.60
9	B	609	CHL	C4B-CHC-C1C	3.25	127.51	122.60
9	I	601	CHL	C11-C12-C13	3.25	126.26	115.49
10	C	602	CLA	O2A-CGA-CBA	3.25	121.79	111.90
8	H	7632	DGD	O3G-C1D-C2D	3.25	112.14	108.04
9	D	609	CHL	C4B-CHC-C1C	3.25	127.52	122.60
10	D	602	CLA	CED-O2D-CGD	3.25	123.61	115.99
10	D	602	CLA	CMC-C2C-C1C	3.25	130.05	125.02
9	G	606	CHL	C4B-CHC-C1C	3.26	127.54	122.60
9	E	607	CHL	O2A-CGA-CBA	3.26	121.84	111.90
9	I	607	CHL	C5-C3-C2	3.26	127.24	121.05
9	A	601	CHL	C6-C5-C3	3.26	119.65	112.48
9	D	609	CHL	C14-C13-C15	3.27	123.66	111.08
9	I	607	CHL	CBA-CAA-C2A	3.28	122.98	113.73
9	E	609	CHL	C4A-NA-C1A	3.28	109.90	106.04
9	C	609	CHL	C4A-NA-C1A	3.28	109.91	106.04
9	G	605	CHL	C4A-NA-C1A	3.28	109.91	106.04
10	F	611	CLA	O2A-CGA-CBA	3.28	121.91	111.90
9	G	608	CHL	CBA-CAA-C2A	3.28	123.00	113.73
10	F	604	CLA	C6-C5-C3	3.29	119.71	112.48
10	D	614	CLA	O2A-CGA-CBA	3.29	121.93	111.90
10	I	614	CLA	O2A-CGA-CBA	3.30	121.95	111.90
5	H	4622	XAT	C21-C22-C23	3.30	120.58	115.02
9	B	609	CHL	C14-C13-C15	3.30	123.76	111.08
10	B	612	CLA	C16-C15-C13	3.30	126.43	115.49
10	C	612	CLA	C16-C15-C13	3.30	126.44	115.49
5	B	1622	XAT	C21-C22-C23	3.30	120.59	115.02
9	B	609	CHL	C4A-NA-C1A	3.30	109.93	106.04
5	B	5622	XAT	C21-C22-C23	3.30	120.59	115.02
9	B	608	CHL	C4A-NA-C1A	3.31	109.94	106.04
9	G	607	CHL	C6-C5-C3	3.31	119.74	112.48
9	G	608	CHL	C4B-CHC-C1C	3.31	127.61	122.60
10	D	611	CLA	CAA-CBA-CGA	3.31	123.01	113.32
9	H	609	CHL	C4A-NA-C1A	3.32	109.95	106.04
9	D	601	CHL	C16-C15-C13	3.32	126.49	115.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	608	CHL	C4A-NA-C1A	3.32	109.95	106.04
10	J	614	CLA	CAA-CBA-CGA	3.32	123.04	113.32
10	D	610	CLA	C14-C13-C15	3.33	123.86	111.08
10	I	611	CLA	O2A-CGA-CBA	3.33	122.03	111.90
10	G	604	CLA	C6-C7-C8	3.33	126.52	115.49
10	I	612	CLA	C16-C15-C13	3.33	126.53	115.49
9	E	608	CHL	C16-C15-C13	3.33	126.53	115.49
5	E	2622	XAT	C21-C22-C23	3.34	120.65	115.02
9	G	608	CHL	O2A-CGA-CBA	3.34	122.09	111.90
9	G	606	CHL	CBA-CAA-C2A	3.35	123.18	113.73
9	I	607	CHL	C4B-CHC-C1C	3.35	127.67	122.60
10	A	604	CLA	CBA-CAA-C2A	3.35	123.18	113.73
9	B	608	CHL	OMC-CMC-C2C	3.35	134.20	125.58
10	I	613	CLA	C6-C5-C3	3.35	119.84	112.48
10	H	602	CLA	C14-C13-C15	3.35	123.97	111.08
10	I	602	CLA	C14-C13-C15	3.36	123.97	111.08
10	H	614	CLA	CBA-CAA-C2A	3.36	123.20	113.73
9	C	606	CHL	C4B-CHC-C1C	3.36	127.68	122.60
9	J	606	CHL	C4B-CHC-C1C	3.36	127.68	122.60
9	J	605	CHL	C4B-CHC-C1C	3.36	127.68	122.60
9	D	605	CHL	C4B-CHC-C1C	3.36	127.69	122.60
10	C	602	CLA	C14-C13-C15	3.36	123.99	111.08
9	J	608	CHL	C4A-NA-C1A	3.36	110.01	106.04
7	A	630	LHG	O7-C7-C8	3.36	118.84	111.53
10	F	613	CLA	C6-C5-C3	3.37	119.87	112.48
10	F	602	CLA	CMC-C2C-C1C	3.37	130.23	125.02
9	B	601	CHL	OMC-CMC-C2C	3.37	134.24	125.58
9	F	601	CHL	C4B-CHC-C1C	3.37	127.70	122.60
10	G	610	CLA	C14-C13-C15	3.37	124.02	111.08
10	A	612	CLA	C16-C15-C13	3.37	126.67	115.49
9	C	609	CHL	C4B-CHC-C1C	3.37	127.70	122.60
10	H	602	CLA	CMC-C2C-C1C	3.38	130.24	125.02
9	D	607	CHL	C4B-CHC-C1C	3.38	127.71	122.60
10	G	613	CLA	C5-C3-C2	3.38	127.46	121.05
10	F	604	CLA	CAA-CBA-CGA	3.38	123.20	113.32
9	E	605	CHL	C4B-CHC-C1C	3.38	127.71	122.60
9	B	605	CHL	C4B-CHC-C1C	3.38	127.72	122.60
9	F	608	CHL	C4B-CHC-C1C	3.38	127.72	122.60
10	E	602	CLA	O2A-CGA-CBA	3.39	122.22	111.90
9	B	607	CHL	CBA-CAA-C2A	3.39	123.30	113.73
5	D	8622	XAT	C21-C22-C23	3.39	120.74	115.02
4	A	620	LUT	C3-C4-C5	3.39	118.84	111.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	C	602	CLA	CMC-C2C-C1C	3.39	130.27	125.02
10	F	614	CLA	CBA-CAA-C2A	3.39	123.31	113.73
9	B	609	CHL	CED-O2D-CGD	3.39	123.95	115.99
9	E	607	CHL	CBA-CAA-C2A	3.40	123.32	113.73
9	A	608	CHL	C4B-CHC-C1C	3.40	127.75	122.60
10	C	614	CLA	CBA-CAA-C2A	3.40	123.33	113.73
9	I	609	CHL	C4A-NA-C1A	3.40	110.05	106.04
10	B	610	CLA	C14-C13-C15	3.40	124.16	111.08
10	E	604	CLA	CED-O2D-CGD	3.41	123.98	115.99
10	H	603	CLA	CED-O2D-CGD	3.41	123.99	115.99
10	G	611	CLA	CED-O2D-CGD	3.41	124.00	115.99
9	I	606	CHL	C4B-CHC-C1C	3.42	127.78	122.60
4	F	5620	LUT	C3-C4-C5	3.42	118.90	111.86
9	F	605	CHL	C4B-CHC-C1C	3.42	127.78	122.60
10	B	614	CLA	CAA-CBA-CGA	3.42	123.34	113.32
9	H	601	CHL	C6-C5-C3	3.43	120.00	112.48
10	H	612	CLA	C16-C15-C13	3.43	126.86	115.49
9	D	609	CHL	C6-C5-C3	3.43	120.01	112.48
9	C	607	CHL	C4B-CHC-C1C	3.43	127.79	122.60
9	H	609	CHL	C4B-CHC-C1C	3.43	127.79	122.60
9	D	608	CHL	C4B-CHC-C1C	3.43	127.79	122.60
9	H	605	CHL	C4A-NA-C1A	3.43	110.09	106.04
9	E	608	CHL	C4A-NA-C1A	3.44	110.09	106.04
9	C	608	CHL	C4B-CHC-C1C	3.44	127.80	122.60
9	G	609	CHL	C4A-NA-C1A	3.44	110.09	106.04
10	E	614	CLA	O2A-CGA-CBA	3.44	122.38	111.90
9	F	607	CHL	C4B-CHC-C1C	3.44	127.81	122.60
9	A	605	CHL	C4A-NA-C1A	3.44	110.09	106.04
9	C	609	CHL	CMB-C2B-C3B	3.44	131.82	125.09
9	C	608	CHL	C4A-NA-C1A	3.44	110.10	106.04
9	H	606	CHL	C4B-CHC-C1C	3.44	127.81	122.60
10	C	603	CLA	CED-O2D-CGD	3.46	124.09	115.99
9	E	609	CHL	CED-O2D-CGD	3.46	124.10	115.99
9	A	609	CHL	C4B-CHC-C1C	3.46	127.83	122.60
9	H	607	CHL	C4B-CHC-C1C	3.46	127.84	122.60
10	F	612	CLA	O2A-CGA-CBA	3.46	122.45	111.90
9	G	601	CHL	C4B-CHC-C1C	3.46	127.84	122.60
9	H	605	CHL	C4B-CHC-C1C	3.47	127.84	122.60
9	B	607	CHL	C4B-CHC-C1C	3.47	127.84	122.60
9	A	608	CHL	C4A-NA-C1A	3.47	110.13	106.04
9	J	605	CHL	C4A-NA-C1A	3.47	110.13	106.04
9	A	606	CHL	CED-O2D-CGD	3.47	124.12	115.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	4620	LUT	C2-C1-C6	3.47	116.03	110.49
10	J	610	CLA	CED-O2D-CGD	3.48	124.14	115.99
9	H	606	CHL	CED-O2D-CGD	3.48	124.15	115.99
9	F	608	CHL	C4A-NA-C1A	3.48	110.14	106.04
9	F	605	CHL	C4A-NA-C1A	3.48	110.14	106.04
9	A	605	CHL	C4B-CHC-C1C	3.48	127.87	122.60
9	G	609	CHL	C4B-CHC-C1C	3.48	127.87	122.60
10	B	602	CLA	CBA-CAA-C2A	3.48	123.56	113.73
9	D	607	CHL	O2A-CGA-CBA	3.49	122.52	111.90
9	F	606	CHL	C4B-CHC-C1C	3.49	127.88	122.60
9	J	607	CHL	CBA-CAA-C2A	3.49	123.58	113.73
9	C	605	CHL	C4A-NA-C1A	3.49	110.16	106.04
9	E	608	CHL	OMC-CMC-C2C	3.50	134.58	125.58
10	F	612	CLA	CED-O2D-CGD	3.50	124.20	115.99
9	C	605	CHL	C4B-CHC-C1C	3.50	127.90	122.60
10	A	614	CLA	CBA-CAA-C2A	3.50	123.62	113.73
9	B	608	CHL	C4B-CHC-C1C	3.51	127.91	122.60
10	J	604	CLA	CED-O2D-CGD	3.51	124.21	115.99
9	I	605	CHL	C4A-NA-C1A	3.51	110.17	106.04
9	C	601	CHL	OMC-CMC-C2C	3.51	134.61	125.58
10	A	602	CLA	CED-O2D-CGD	3.51	124.23	115.99
9	E	601	CHL	C4A-NA-C1A	3.51	110.18	106.04
9	G	605	CHL	O2A-CGA-CBA	3.51	122.61	111.90
9	D	608	CHL	C4A-NA-C1A	3.51	110.18	106.04
10	C	612	CLA	O2A-CGA-CBA	3.52	122.61	111.90
10	B	610	CLA	CED-O2D-CGD	3.52	124.24	115.99
8	B	2632	DGD	O2G-C1B-C2B	3.52	119.18	111.53
9	G	607	CHL	OMC-CMC-C2C	3.52	134.64	125.58
10	B	611	CLA	O2D-CGD-CBD	3.52	116.13	111.30
9	E	608	CHL	C4B-CHC-C1C	3.52	127.93	122.60
9	H	608	CHL	CED-O2D-CGD	3.52	124.25	115.99
9	J	601	CHL	C4A-NA-C1A	3.52	110.19	106.04
9	B	605	CHL	C4A-NA-C1A	3.53	110.20	106.04
9	C	605	CHL	OMC-CMC-C2C	3.53	134.66	125.58
9	D	605	CHL	C4A-NA-C1A	3.54	110.21	106.04
10	E	614	CLA	CBA-CAA-C2A	3.54	123.72	113.73
9	J	608	CHL	C16-C15-C13	3.55	127.25	115.49
9	E	605	CHL	C4A-NA-C1A	3.55	110.22	106.04
9	F	607	CHL	C6-C5-C3	3.55	120.27	112.48
4	F	5621	LUT	C18-C5-C6	3.55	128.09	124.61
10	C	610	CLA	CMC-C2C-C1C	3.55	130.52	125.02
9	C	609	CHL	CAA-CBA-CGA	3.55	123.72	113.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	601	CHL	OMC-CMC-C2C	3.56	134.73	125.58
10	B	603	CLA	C6-C5-C3	3.56	120.29	112.48
9	F	601	CHL	C4A-NA-C1A	3.57	110.24	106.04
9	C	601	CHL	C4B-CHC-C1C	3.57	128.00	122.60
8	B	1632	DGD	O2G-C1B-C2B	3.57	119.29	111.53
10	B	604	CLA	CAA-CBA-CGA	3.57	123.77	113.32
10	H	602	CLA	CBA-CAA-C2A	3.57	123.81	113.73
10	J	603	CLA	C5-C3-C2	3.58	127.83	121.05
9	H	607	CHL	CBA-CAA-C2A	3.58	123.83	113.73
10	B	612	CLA	O2A-CGA-CBA	3.58	122.81	111.90
9	D	609	CHL	C4A-NA-C1A	3.58	110.26	106.04
10	G	612	CLA	O2A-CGA-CBA	3.58	122.82	111.90
10	J	612	CLA	C16-C15-C13	3.58	127.38	115.49
10	C	602	CLA	CBA-CAA-C2A	3.59	123.86	113.73
9	C	606	CHL	C4A-NA-C1A	3.59	110.27	106.04
9	A	606	CHL	C4B-CHC-C1C	3.60	128.04	122.60
8	G	9632	DGD	O2G-C1B-C2B	3.60	119.34	111.53
9	E	605	CHL	O2A-CGA-CBA	3.60	122.87	111.90
9	J	607	CHL	O2A-CGA-CBA	3.60	122.87	111.90
9	B	601	CHL	C4A-NA-C1A	3.60	110.29	106.04
9	A	601	CHL	C4B-CHC-C1C	3.61	128.06	122.60
10	A	602	CLA	CBA-CAA-C2A	3.61	123.93	113.73
10	A	610	CLA	CED-O2D-CGD	3.62	124.48	115.99
9	J	608	CHL	CBA-CAA-C2A	3.62	123.96	113.73
9	J	601	CHL	C4B-CHC-C1C	3.63	128.09	122.60
10	D	603	CLA	CED-O2D-CGD	3.63	124.50	115.99
9	I	605	CHL	C4B-CHC-C1C	3.63	128.09	122.60
10	F	603	CLA	CBA-CAA-C2A	3.63	123.97	113.73
10	G	603	CLA	O2A-CGA-CBA	3.63	122.96	111.90
9	A	601	CHL	C4A-NA-C1A	3.63	110.32	106.04
9	B	601	CHL	CED-O2D-CGD	3.63	124.51	115.99
9	D	606	CHL	C4B-CHC-C1C	3.63	128.10	122.60
9	B	606	CHL	C4B-CHC-C1C	3.64	128.10	122.60
10	G	610	CLA	CED-O2D-CGD	3.64	124.52	115.99
9	H	601	CHL	C4A-NA-C1A	3.64	110.33	106.04
5	I	9622	XAT	C21-C22-C23	3.64	121.16	115.02
10	B	611	CLA	CED-O2D-CGD	3.64	124.52	115.99
9	F	607	CHL	CBA-CAA-C2A	3.64	124.00	113.73
9	B	607	CHL	O2A-CGA-CBA	3.64	122.99	111.90
9	A	606	CHL	CMB-C2B-C3B	3.64	132.22	125.09
9	G	601	CHL	C4A-NA-C1A	3.65	110.34	106.04
10	I	602	CLA	CBA-CAA-C2A	3.65	124.03	113.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	D	604	CLA	CBA-CAA-C2A	3.65	124.03	113.73
9	J	607	CHL	C4B-CHC-C1C	3.65	128.13	122.60
10	G	611	CLA	O2A-CGA-CBA	3.65	123.03	111.90
9	A	608	CHL	C16-C15-C13	3.66	127.62	115.49
9	B	606	CHL	C4A-NA-C1A	3.66	110.35	106.04
9	B	601	CHL	C4B-CHC-C1C	3.66	128.14	122.60
9	A	608	CHL	OMC-CMC-C2C	3.66	135.00	125.58
10	G	614	CLA	CBA-CAA-C2A	3.66	124.07	113.73
9	G	608	CHL	OMC-CMC-C2C	3.67	135.01	125.58
9	D	601	CHL	C4A-NA-C1A	3.67	110.36	106.04
10	I	610	CLA	O2A-CGA-CBA	3.67	123.08	111.90
9	E	601	CHL	C4B-CHC-C1C	3.67	128.16	122.60
9	C	601	CHL	C4A-NA-C1A	3.67	110.37	106.04
10	F	612	CLA	C16-C15-C13	3.68	127.68	115.49
10	C	610	CLA	O2A-CGA-CBA	3.68	123.11	111.90
10	A	613	CLA	CED-O2D-CGD	3.68	124.62	115.99
9	D	606	CHL	C4A-NA-C1A	3.68	110.38	106.04
10	H	602	CLA	C4-C3-C5	3.68	121.03	115.41
9	H	609	CHL	OMC-CMC-C2C	3.68	135.05	125.58
10	F	604	CLA	CBA-CAA-C2A	3.69	124.13	113.73
4	I	8620	LUT	C2-C1-C6	3.69	116.38	110.49
9	D	601	CHL	C4B-CHC-C1C	3.69	128.19	122.60
9	B	608	CHL	O2A-CGA-CBA	3.69	123.16	111.90
10	J	613	CLA	CMB-C2B-C3B	3.70	132.32	125.09
10	E	612	CLA	C16-C15-C13	3.70	127.75	115.49
4	H	7621	LUT	C18-C5-C6	3.70	128.24	124.61
9	G	605	CHL	OMC-CMC-C2C	3.70	135.10	125.58
9	B	605	CHL	O2A-CGA-CBA	3.70	123.18	111.90
9	C	606	CHL	O2D-CGD-CBD	3.70	116.38	111.30
9	I	609	CHL	CAA-CBA-CGA	3.71	124.17	113.32
5	A	622	XAT	C21-C22-C23	3.71	121.27	115.02
10	E	602	CLA	CBA-CAA-C2A	3.71	124.21	113.73
9	J	608	CHL	CED-O2D-CGD	3.72	124.70	115.99
9	F	607	CHL	C5-C3-C2	3.72	128.10	121.05
10	C	610	CLA	C14-C13-C15	3.72	125.36	111.08
4	D	3620	LUT	C3-C4-C5	3.72	119.51	111.86
10	H	611	CLA	CED-O2D-CGD	3.72	124.72	115.99
10	F	613	CLA	CBA-CAA-C2A	3.72	124.24	113.73
9	A	606	CHL	CAA-CBA-CGA	3.73	124.24	113.32
10	F	602	CLA	CBA-CAA-C2A	3.73	124.26	113.73
9	H	609	CHL	CED-O2D-CGD	3.73	124.75	115.99
10	C	613	CLA	C6-C5-C3	3.74	120.69	112.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	607	CHL	C4A-NA-C1A	3.74	110.45	106.04
9	I	601	CHL	C4A-NA-C1A	3.74	110.45	106.04
5	E	2622	XAT	C24-C23-C22	3.74	118.69	110.41
9	E	606	CHL	C4B-CHC-C1C	3.75	128.27	122.60
9	J	606	CHL	CMB-C2B-C3B	3.75	132.41	125.09
10	J	602	CLA	O2A-CGA-CBA	3.75	123.32	111.90
9	B	607	CHL	CMB-C2B-C3B	3.75	132.42	125.09
9	F	605	CHL	O2A-CGA-CBA	3.75	123.34	111.90
9	C	607	CHL	CMB-C2B-C3B	3.75	132.43	125.09
9	G	607	CHL	C4B-CHC-C1C	3.76	128.29	122.60
10	F	603	CLA	C6-C5-C3	3.76	120.73	112.48
9	E	601	CHL	C6-C5-C3	3.76	120.74	112.48
9	A	607	CHL	O2A-CGA-CBA	3.76	123.37	111.90
9	F	606	CHL	CMB-C2B-C3B	3.76	132.45	125.09
10	H	610	CLA	CED-O2D-CGD	3.77	124.82	115.99
9	E	606	CHL	C4A-NA-C1A	3.77	110.48	106.04
9	G	608	CHL	CED-O2D-CGD	3.77	124.82	115.99
10	J	604	CLA	CBA-CAA-C2A	3.77	124.36	113.73
10	D	602	CLA	C4-C3-C5	3.77	121.16	115.41
10	G	610	CLA	O2A-CGA-CBA	3.77	123.39	111.90
9	I	607	CHL	C4A-NA-C1A	3.77	110.49	106.04
9	J	606	CHL	C1-C2-C3	3.77	132.89	126.71
9	D	607	CHL	CMB-C2B-C3B	3.77	132.47	125.09
4	B	1620	LUT	C2-C1-C6	3.78	116.51	110.49
9	H	601	CHL	C4B-CHC-C1C	3.78	128.32	122.60
9	D	606	CHL	CAA-CBA-CGA	3.78	124.39	113.32
9	F	609	CHL	CAA-CBA-CGA	3.78	124.39	113.32
10	J	602	CLA	CBA-CAA-C2A	3.78	124.41	113.73
7	D	3630	LHG	O8-C23-C24	3.79	123.45	111.90
10	G	603	CLA	CBA-CAA-C2A	3.79	124.43	113.73
9	I	601	CHL	C4B-CHC-C1C	3.79	128.34	122.60
9	H	607	CHL	C4A-NA-C1A	3.79	110.51	106.04
9	G	606	CHL	CED-O2D-CGD	3.79	124.89	115.99
9	I	606	CHL	O2A-CGA-CBA	3.79	123.46	111.90
9	I	606	CHL	C4A-NA-C1A	3.80	110.52	106.04
10	J	613	CLA	CBA-CAA-C2A	3.80	124.47	113.73
4	A	621	LUT	C18-C5-C6	3.80	128.34	124.61
10	J	613	CLA	C6-C5-C3	3.81	120.84	112.48
9	D	605	CHL	CED-O2D-CGD	3.81	124.92	115.99
10	B	604	CLA	O2D-CGD-CBD	3.81	116.52	111.30
9	C	609	CHL	CED-O2D-CGD	3.81	124.92	115.99
9	G	606	CHL	C4A-NA-C1A	3.81	110.53	106.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	609	CHL	OMC-CMC-C2C	3.82	135.40	125.58
9	D	608	CHL	C16-C15-C13	3.82	128.15	115.49
9	A	606	CHL	C4A-NA-C1A	3.82	110.54	106.04
10	C	604	CLA	CED-O2D-CGD	3.82	124.95	115.99
10	G	603	CLA	CAA-CBA-CGA	3.82	124.51	113.32
7	F	5630	LHG	O7-C7-C8	3.83	119.85	111.53
9	J	608	CHL	O2A-CGA-CBA	3.83	123.58	111.90
10	H	612	CLA	O2A-CGA-CBA	3.83	123.58	111.90
9	H	606	CHL	C4A-NA-C1A	3.84	110.57	106.04
9	H	608	CHL	OMC-CMC-C2C	3.85	135.48	125.58
9	B	608	CHL	CBA-CAA-C2A	3.85	124.60	113.73
10	F	611	CLA	CAA-CBA-CGA	3.85	124.60	113.32
10	I	602	CLA	CED-O2D-CGD	3.86	125.03	115.99
10	C	610	CLA	CBA-CAA-C2A	3.86	124.62	113.73
9	J	606	CHL	CED-O2D-CGD	3.86	125.04	115.99
10	D	602	CLA	CBA-CAA-C2A	3.86	124.63	113.73
9	I	605	CHL	OMC-CMC-C2C	3.86	135.52	125.58
9	E	601	CHL	CED-O2D-CGD	3.87	125.06	115.99
9	D	607	CHL	C4A-NA-C1A	3.87	110.61	106.04
9	C	607	CHL	CBA-CAA-C2A	3.87	124.66	113.73
10	B	613	CLA	C6-C5-C3	3.87	120.98	112.48
4	I	8621	LUT	C18-C5-C6	3.87	128.41	124.61
10	G	602	CLA	CMC-C2C-C1C	3.88	131.02	125.02
9	H	606	CHL	CMB-C2B-C3B	3.88	132.68	125.09
9	J	607	CHL	C4A-NA-C1A	3.89	110.62	106.04
10	C	602	CLA	C4-C3-C5	3.91	121.37	115.41
9	J	606	CHL	C4A-NA-C1A	3.91	110.64	106.04
9	D	608	CHL	CED-O2D-CGD	3.91	125.16	115.99
10	A	613	CLA	C6-C5-C3	3.91	121.07	112.48
9	A	605	CHL	CED-O2D-CGD	3.91	125.17	115.99
9	E	608	CHL	O2A-CGA-CBA	3.92	123.83	111.90
9	D	605	CHL	O2A-CGA-CBA	3.92	123.83	111.90
10	J	611	CLA	O2A-CGA-CBA	3.92	123.85	111.90
10	I	603	CLA	CBA-CAA-C2A	3.93	124.81	113.73
10	D	610	CLA	CED-O2D-CGD	3.93	125.21	115.99
9	F	601	CHL	CED-O2D-CGD	3.93	125.22	115.99
9	E	601	CHL	OMC-CMC-C2C	3.94	135.71	125.58
7	I	8630	LHG	O8-C6-C5	3.94	119.29	108.69
10	F	610	CLA	O2A-CGA-CBA	3.94	123.90	111.90
5	J	3622	XAT	C21-C22-C23	3.94	121.67	115.02
9	E	606	CHL	CAA-CBA-CGA	3.94	124.86	113.32
9	C	607	CHL	C4A-NA-C1A	3.94	110.69	106.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	601	CHL	CED-O2D-CGD	3.95	125.26	115.99
9	B	601	CHL	C11-C12-C13	3.97	128.66	115.49
9	A	601	CHL	OMC-CMC-C2C	3.98	135.81	125.58
9	F	606	CHL	C4A-NA-C1A	3.98	110.74	106.04
8	D	5632	DGD	O2G-C1B-C2B	3.99	120.19	111.53
9	A	607	CHL	CBA-CAA-C2A	3.99	124.98	113.73
10	G	602	CLA	CBA-CAA-C2A	3.99	124.98	113.73
9	B	605	CHL	OMC-CMC-C2C	3.99	135.83	125.58
9	A	605	CHL	O2A-CGA-CBA	3.99	124.05	111.90
9	I	609	CHL	CED-O2D-CGD	3.99	125.36	115.99
9	B	607	CHL	C4A-NA-C1A	3.99	110.75	106.04
4	H	7621	LUT	C3-C4-C5	4.00	120.08	111.86
9	A	607	CHL	C4A-NA-C1A	4.00	110.75	106.04
9	D	607	CHL	C6-C5-C3	4.00	121.26	112.48
10	I	612	CLA	O2A-CGA-CBA	4.00	124.09	111.90
9	I	608	CHL	CBA-CAA-C2A	4.00	125.03	113.73
10	F	613	CLA	CED-O2D-CGD	4.00	125.38	115.99
4	A	620	LUT	C2-C1-C6	4.01	116.88	110.49
10	A	610	CLA	O2A-CGA-CBA	4.01	124.12	111.90
10	E	610	CLA	O2A-CGA-CBA	4.02	124.14	111.90
10	C	611	CLA	O2A-CGA-CBA	4.02	124.16	111.90
10	B	610	CLA	O2A-CGA-CBA	4.03	124.17	111.90
9	I	607	CHL	OMC-CMC-C2C	4.03	135.94	125.58
9	A	606	CHL	C1-C2-C3	4.04	133.33	126.71
10	G	613	CLA	CBA-CAA-C2A	4.04	125.13	113.73
9	C	606	CHL	CAA-CBA-CGA	4.04	125.16	113.32
10	E	603	CLA	C6-C5-C3	4.04	121.36	112.48
9	I	601	CHL	CED-O2D-CGD	4.05	125.48	115.99
10	D	611	CLA	O2A-CGA-CBA	4.05	124.24	111.90
9	B	606	CHL	C1-C2-C3	4.05	133.35	126.71
10	I	604	CLA	CAA-CBA-CGA	4.05	125.18	113.32
9	D	601	CHL	CED-O2D-CGD	4.05	125.49	115.99
9	F	607	CHL	C4A-NA-C1A	4.05	110.82	106.04
10	D	612	CLA	O2A-CGA-CBA	4.06	124.27	111.90
9	G	606	CHL	CMB-C2B-C3B	4.06	133.03	125.09
7	E	4630	LHG	O8-C6-C5	4.07	119.64	108.69
7	B	1630	LHG	O8-C6-C5	4.07	119.65	108.69
9	H	605	CHL	O2A-CGA-CBA	4.07	124.31	111.90
9	I	601	CHL	OMC-CMC-C2C	4.07	136.06	125.58
9	C	605	CHL	O2A-CGA-CBA	4.08	124.32	111.90
10	H	602	CLA	C6-C5-C3	4.08	121.44	112.48
10	J	602	CLA	CMC-C2C-C1C	4.09	131.35	125.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	606	CHL	CAA-CBA-CGA	4.10	125.31	113.32
9	I	607	CHL	O2A-CGA-CBA	4.10	124.39	111.90
9	G	607	CHL	C4A-NA-C1A	4.11	110.88	106.04
9	E	606	CHL	CMB-C2B-C3B	4.11	133.12	125.09
5	C	7622	XAT	C21-C22-C23	4.11	121.95	115.02
10	F	610	CLA	CBA-CAA-C2A	4.11	125.33	113.73
10	G	603	CLA	CED-O2D-CGD	4.11	125.64	115.99
10	B	602	CLA	C4-C3-C5	4.12	121.69	115.41
5	J	3622	XAT	C24-C23-C22	4.12	119.51	110.41
9	H	607	CHL	O2A-CGA-CBA	4.14	124.52	111.90
9	H	608	CHL	CBA-CAA-C2A	4.14	125.42	113.73
9	C	605	CHL	CED-O2D-CGD	4.14	125.71	115.99
10	I	610	CLA	CBA-CAA-C2A	4.15	125.43	113.73
9	B	608	CHL	CED-O2D-CGD	4.15	125.71	115.99
4	B	1621	LUT	C3-C4-C5	4.15	120.39	111.86
9	F	605	CHL	OMC-CMC-C2C	4.15	136.25	125.58
9	C	608	CHL	C16-C15-C13	4.15	129.25	115.49
10	C	603	CLA	C6-C5-C3	4.15	121.59	112.48
4	C	2621	LUT	C38-C25-C26	4.15	119.15	116.04
10	B	613	CLA	CBA-CAA-C2A	4.16	125.48	113.73
10	D	612	CLA	C16-C15-C13	4.17	129.33	115.49
10	I	603	CLA	C6-C5-C3	4.17	121.64	112.48
9	I	605	CHL	O2A-CGA-CBA	4.17	124.62	111.90
10	A	602	CLA	CMC-C2C-C1C	4.18	131.49	125.02
9	B	609	CHL	OMC-CMC-C2C	4.19	136.36	125.58
10	I	613	CLA	CED-O2D-CGD	4.19	125.82	115.99
10	H	611	CLA	O2A-CGA-CBA	4.19	124.68	111.90
9	J	605	CHL	OMC-CMC-C2C	4.20	136.38	125.58
9	E	606	CHL	O2A-CGA-CBA	4.20	124.71	111.90
10	E	613	CLA	CMB-C2B-C3B	4.21	133.31	125.09
10	J	603	CLA	CBA-CAA-C2A	4.21	125.61	113.73
10	A	611	CLA	O2A-CGA-CBA	4.22	124.77	111.90
10	D	613	CLA	C6-C5-C3	4.23	121.78	112.48
10	D	610	CLA	O2A-CGA-CBA	4.24	124.81	111.90
9	E	605	CHL	OMC-CMC-C2C	4.24	136.49	125.58
9	C	601	CHL	CBA-CAA-C2A	4.25	125.73	113.73
4	D	3621	LUT	C38-C25-C26	4.26	119.22	116.04
9	A	608	CHL	CBA-CAA-C2A	4.26	125.75	113.73
4	I	8621	LUT	C3-C4-C5	4.26	120.62	111.86
9	C	607	CHL	O2A-CGA-CBA	4.26	124.89	111.90
7	F	5630	LHG	O8-C23-C24	4.27	124.91	111.90
9	E	608	CHL	CBA-CAA-C2A	4.28	125.80	113.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	H	606	CHL	O2A-CGA-CBA	4.28	124.93	111.90
9	D	601	CHL	OMC-CMC-C2C	4.28	136.59	125.58
9	H	601	CHL	CED-O2D-CGD	4.28	126.03	115.99
10	D	611	CLA	O2D-CGD-CBD	4.29	117.18	111.30
10	B	612	CLA	O2D-CGD-CBD	4.31	117.21	111.30
9	F	608	CHL	C7-C6-C5	4.31	125.79	113.06
4	H	7621	LUT	C2-C1-C6	4.31	117.36	110.49
9	C	606	CHL	CMB-C2B-C3B	4.31	133.52	125.09
10	G	613	CLA	CED-O2D-CGD	4.32	126.11	115.99
5	A	622	XAT	C24-C23-C22	4.32	119.96	110.41
9	G	606	CHL	O2A-CGA-CBA	4.32	125.06	111.90
9	A	607	CHL	CMB-C2B-C3B	4.33	133.55	125.09
4	G	6620	LUT	C2-C1-C6	4.33	117.39	110.49
9	B	608	CHL	C7-C6-C5	4.33	125.85	113.06
9	F	608	CHL	C6-C5-C3	4.33	121.98	112.48
5	B	5622	XAT	C24-C23-C22	4.33	119.98	110.41
10	J	610	CLA	CBA-CAA-C2A	4.33	125.95	113.73
7	J	9630	LHG	O8-C6-C5	4.34	120.36	108.69
9	G	607	CHL	CBA-CAA-C2A	4.34	125.98	113.73
10	D	613	CLA	CED-O2D-CGD	4.35	126.18	115.99
9	G	606	CHL	CAA-CBA-CGA	4.36	126.07	113.32
9	E	601	CHL	CBA-CAA-C2A	4.36	126.03	113.73
10	E	613	CLA	CED-O2D-CGD	4.36	126.22	115.99
10	E	610	CLA	CBA-CAA-C2A	4.37	126.06	113.73
4	D	3621	LUT	C3-C4-C5	4.37	120.86	111.86
9	G	607	CHL	O2A-CGA-CBA	4.38	125.23	111.90
9	B	606	CHL	CMB-C2B-C3B	4.38	133.66	125.09
4	C	2620	LUT	C2-C1-C6	4.38	117.48	110.49
4	F	5620	LUT	C2-C1-C6	4.39	117.49	110.49
9	H	607	CHL	CMB-C2B-C3B	4.39	133.68	125.09
10	D	603	CLA	CBA-CAA-C2A	4.39	126.13	113.73
9	D	605	CHL	OMC-CMC-C2C	4.40	136.89	125.58
9	J	605	CHL	O2A-CGA-CBA	4.40	125.31	111.90
7	C	2630	LHG	O8-C6-C5	4.43	120.61	108.69
10	F	602	CLA	O2D-CGD-CBD	4.44	117.39	111.30
4	G	6621	LUT	C38-C25-C26	4.45	119.37	116.04
7	F	5630	LHG	O8-C6-C5	4.46	120.69	108.69
10	G	602	CLA	C6-C5-C3	4.46	122.27	112.48
10	E	611	CLA	O2A-CGA-CBA	4.47	125.51	111.90
7	D	3630	LHG	O8-C6-C5	4.47	120.73	108.69
4	H	7620	LUT	C2-C1-C6	4.48	117.63	110.49
9	J	607	CHL	OMC-CMC-C2C	4.48	137.11	125.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	9621	LUT	C18-C5-C6	4.49	129.01	124.61
10	D	610	CLA	CBA-CAA-C2A	4.49	126.40	113.73
4	J	9621	LUT	C2-C1-C6	4.50	117.66	110.49
5	F	6622	XAT	C24-C23-C22	4.50	120.35	110.41
5	I	9622	XAT	C24-C23-C22	4.50	120.36	110.41
7	H	7630	LHG	O8-C23-C24	4.51	125.63	111.90
9	G	609	CHL	OMC-CMC-C2C	4.51	137.18	125.58
9	B	608	CHL	C6-C5-C3	4.51	122.39	112.48
10	F	611	CLA	CBA-CAA-C2A	4.52	126.48	113.73
9	G	607	CHL	CMB-C2B-C3B	4.52	133.94	125.09
9	I	607	CHL	CMB-C2B-C3B	4.53	133.95	125.09
9	J	607	CHL	CMB-C2B-C3B	4.54	133.97	125.09
4	D	3620	LUT	C2-C1-C6	4.54	117.73	110.49
10	J	604	CLA	O2D-CGD-CBD	4.54	117.53	111.30
9	F	606	CHL	C1-C2-C3	4.55	134.16	126.71
9	E	606	CHL	C1-C2-C3	4.55	134.16	126.71
10	A	610	CLA	CBA-CAA-C2A	4.55	126.58	113.73
9	F	609	CHL	OMC-CMC-C2C	4.55	137.29	125.58
4	C	2621	LUT	C3-C4-C5	4.57	121.26	111.86
10	J	613	CLA	CED-O2D-CGD	4.57	126.71	115.99
9	A	606	CHL	O2A-CGA-CBA	4.57	125.83	111.90
9	G	601	CHL	CED-O2D-CGD	4.58	126.73	115.99
10	J	611	CLA	CBA-CAA-C2A	4.58	126.66	113.73
4	I	8621	LUT	C2-C1-C6	4.59	117.80	110.49
4	G	6621	LUT	C3-C4-C5	4.59	121.30	111.86
10	B	610	CLA	CBA-CAA-C2A	4.59	126.68	113.73
9	G	601	CHL	OMC-CMC-C2C	4.61	137.43	125.58
10	H	604	CLA	CMB-C2B-C3B	4.61	134.10	125.09
10	I	613	CLA	CBA-CAA-C2A	4.61	126.74	113.73
10	H	610	CLA	O2A-CGA-CBA	4.61	125.95	111.90
9	C	608	CHL	CED-O2D-CGD	4.61	126.81	115.99
4	F	5621	LUT	C3-C4-C5	4.62	121.36	111.86
5	D	8622	XAT	C24-C23-C22	4.62	120.63	110.41
9	C	606	CHL	O2A-CGA-CBA	4.63	126.00	111.90
10	H	612	CLA	O2D-CGD-CBD	4.65	117.68	111.30
10	J	610	CLA	O2A-CGA-CBA	4.65	126.08	111.90
10	I	602	CLA	C4-C3-C5	4.66	122.52	115.41
10	A	603	CLA	CBA-CAA-C2A	4.67	126.90	113.73
9	H	607	CHL	OMC-CMC-C2C	4.67	137.59	125.58
9	I	601	CHL	CBA-CAA-C2A	4.67	126.92	113.73
9	H	608	CHL	C7-C6-C5	4.68	126.90	113.06
10	A	603	CLA	C6-C5-C3	4.70	122.80	112.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	602	CLA	O2D-CGD-CBD	4.70	117.75	111.30
10	I	604	CLA	CED-O2D-CGD	4.71	127.03	115.99
9	D	606	CHL	C1-C2-C3	4.71	134.42	126.71
4	A	621	LUT	C3-C4-C5	4.71	121.56	111.86
10	B	611	CLA	O2A-CGA-CBA	4.73	126.30	111.90
9	F	607	CHL	O2A-CGA-CBA	4.73	126.31	111.90
10	D	602	CLA	C6-C5-C3	4.73	122.87	112.48
10	I	602	CLA	C6-C5-C3	4.73	122.87	112.48
10	H	603	CLA	CBA-CAA-C2A	4.74	127.09	113.73
10	G	602	CLA	C4-C3-C5	4.74	122.65	115.41
10	D	603	CLA	O2D-CGD-CBD	4.75	117.82	111.30
9	F	608	CHL	OMC-CMC-C2C	4.75	137.80	125.58
10	G	610	CLA	CBA-CAA-C2A	4.76	127.16	113.73
9	H	606	CHL	C1-C2-C3	4.76	134.51	126.71
9	D	606	CHL	CMB-C2B-C3B	4.76	134.40	125.09
4	B	1621	LUT	C2-C1-C6	4.76	118.09	110.49
9	B	601	CHL	CBA-CAA-C2A	4.77	127.18	113.73
9	F	601	CHL	CBA-CAA-C2A	4.77	127.18	113.73
9	D	608	CHL	OMC-CMC-C2C	4.79	137.89	125.58
10	F	612	CLA	O2D-CGD-CBD	4.79	117.87	111.30
10	A	604	CLA	O2D-CGD-CBD	4.79	117.88	111.30
10	E	612	CLA	O2D-CGD-CBD	4.80	117.88	111.30
9	E	607	CHL	CMB-C2B-C3B	4.80	134.48	125.09
9	J	609	CHL	OMC-CMC-C2C	4.80	137.94	125.58
10	E	603	CLA	CBA-CAA-C2A	4.80	127.29	113.73
9	H	608	CHL	C6-C5-C3	4.81	123.03	112.48
9	I	606	CHL	CAA-CBA-CGA	4.81	127.40	113.32
9	J	601	CHL	CED-O2D-CGD	4.81	127.27	115.99
7	J	9630	LHG	O8-C23-C24	4.82	126.59	111.90
9	D	607	CHL	OMC-CMC-C2C	4.82	137.99	125.58
10	B	603	CLA	CBA-CAA-C2A	4.82	127.34	113.73
10	C	604	CLA	O2D-CGD-CBD	4.82	117.92	111.30
10	A	612	CLA	O2D-CGD-CBD	4.83	117.93	111.30
9	D	609	CHL	OMC-CMC-C2C	4.85	138.04	125.58
9	J	606	CHL	CAA-CBA-CGA	4.85	127.53	113.32
10	J	602	CLA	C4-C3-C5	4.85	122.82	115.41
9	F	601	CHL	OMC-CMC-C2C	4.86	138.07	125.58
9	C	606	CHL	C1-C2-C3	4.86	134.68	126.71
10	C	613	CLA	CED-O2D-CGD	4.87	127.41	115.99
7	H	7630	LHG	O8-C6-C5	4.87	121.80	108.69
10	F	602	CLA	C6-C5-C3	4.87	123.18	112.48
9	C	601	CHL	CED-O2D-CGD	4.87	127.42	115.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	607	CHL	OMC-CMC-C2C	4.88	138.13	125.58
7	B	1630	LHG	O8-C23-C24	4.88	126.77	111.90
10	H	610	CLA	CBA-CAA-C2A	4.90	127.57	113.73
10	H	602	CLA	O2D-CGD-CBD	4.91	118.04	111.30
10	J	602	CLA	C6-C5-C3	4.92	123.28	112.48
4	J	9621	LUT	C3-C4-C5	4.92	121.99	111.86
7	C	2630	LHG	O8-C23-C24	4.92	126.90	111.90
4	E	4621	LUT	C38-C25-C26	4.93	119.73	116.04
10	F	604	CLA	O2D-CGD-CBD	4.94	118.07	111.30
7	G	6630	LHG	O8-C23-C24	4.94	126.95	111.90
4	F	5621	LUT	C2-C1-C6	4.94	118.37	110.49
9	I	606	CHL	CMB-C2B-C3B	4.95	134.77	125.09
4	E	4621	LUT	C2-C1-C6	4.96	118.40	110.49
10	H	613	CLA	CED-O2D-CGD	4.96	127.62	115.99
7	E	4630	LHG	O8-C23-C24	4.96	127.03	111.90
10	J	603	CLA	C6-C5-C3	4.96	123.38	112.48
10	G	604	CLA	O2D-CGD-CBD	4.97	118.12	111.30
9	H	601	CHL	CBA-CAA-C2A	4.99	127.81	113.73
9	D	606	CHL	O2A-CGA-CBA	4.99	127.11	111.90
10	A	604	CLA	O2A-CGA-CBA	5.00	127.13	111.90
7	G	6630	LHG	O8-C6-C5	5.00	122.15	108.69
9	G	606	CHL	C1-C2-C3	5.00	134.91	126.71
4	H	7620	LUT	C18-C5-C6	5.03	129.54	124.61
10	I	612	CLA	O2D-CGD-CBD	5.03	118.20	111.30
10	B	604	CLA	CED-O2D-CGD	5.03	127.79	115.99
10	D	602	CLA	O2D-CGD-CBD	5.03	118.21	111.30
4	C	2621	LUT	C2-C1-C6	5.04	118.52	110.49
9	F	606	CHL	O2A-CGA-CBA	5.04	127.25	111.90
7	A	630	LHG	O8-C6-C5	5.04	122.26	108.69
10	F	603	CLA	O2D-CGD-CBD	5.05	118.22	111.30
10	J	604	CLA	CMB-C2B-C3B	5.05	134.97	125.09
7	A	630	LHG	O8-C23-C24	5.06	127.30	111.90
10	B	602	CLA	CED-O2D-CGD	5.06	127.87	115.99
10	J	612	CLA	O2D-CGD-CBD	5.08	118.27	111.30
9	J	601	CHL	CBA-CAA-C2A	5.08	128.08	113.73
9	E	608	CHL	CED-O2D-CGD	5.09	127.92	115.99
9	A	601	CHL	CBA-CAA-C2A	5.09	128.09	113.73
10	I	604	CLA	O2D-CGD-CBD	5.09	118.29	111.30
4	E	4621	LUT	C3-C4-C5	5.10	122.35	111.86
5	C	7622	XAT	C24-C23-C22	5.10	121.69	110.41
4	D	3621	LUT	C2-C1-C6	5.11	118.64	110.49
10	H	613	CLA	CBA-CAA-C2A	5.12	128.19	113.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	621	LUT	C2-C1-C6	5.13	118.67	110.49
10	G	602	CLA	O2D-CGD-CBD	5.13	118.34	111.30
4	F	5620	LUT	C18-C5-C6	5.14	129.65	124.61
10	I	604	CLA	CMB-C2B-C3B	5.15	135.17	125.09
10	F	602	CLA	C4-C3-C5	5.17	123.30	115.41
10	C	602	CLA	C6-C5-C3	5.17	123.84	112.48
10	C	602	CLA	O2D-CGD-CBD	5.17	118.40	111.30
4	B	1620	LUT	C18-C5-C6	5.18	129.69	124.61
9	J	606	CHL	O2A-CGA-CBA	5.18	127.67	111.90
10	G	603	CLA	O2D-CGD-CBD	5.19	118.41	111.30
10	G	604	CLA	O2A-CGA-CBA	5.19	127.70	111.90
5	H	4622	XAT	C24-C23-C22	5.19	121.89	110.41
10	A	613	CLA	CBA-CAA-C2A	5.20	128.39	113.73
10	G	604	CLA	CMB-C2B-C3B	5.21	135.27	125.09
9	I	609	CHL	OMC-CMC-C2C	5.22	139.01	125.58
9	A	608	CHL	CED-O2D-CGD	5.23	128.26	115.99
4	G	6620	LUT	C18-C5-C6	5.23	129.74	124.61
10	F	613	CLA	CMB-C2B-C3B	5.29	135.44	125.09
10	B	604	CLA	CMB-C2B-C3B	5.30	135.45	125.09
10	D	612	CLA	O2D-CGD-CBD	5.31	118.59	111.30
9	E	607	CHL	OMC-CMC-C2C	5.33	139.30	125.58
10	H	603	CLA	O2D-CGD-CBD	5.36	118.65	111.30
4	G	6621	LUT	C2-C1-C6	5.37	119.05	110.49
10	E	604	CLA	CMB-C2B-C3B	5.37	135.59	125.09
9	E	609	CHL	OMC-CMC-C2C	5.38	139.42	125.58
9	B	607	CHL	OMC-CMC-C2C	5.39	139.45	125.58
5	B	1622	XAT	C24-C23-C22	5.40	122.34	110.41
10	J	602	CLA	O2D-CGD-CBD	5.41	118.72	111.30
10	B	611	CLA	CBA-CAA-C2A	5.41	129.00	113.73
10	E	603	CLA	O2D-CGD-CBD	5.42	118.73	111.30
10	E	602	CLA	C6-C5-C3	5.42	124.39	112.48
10	I	611	CLA	CAA-CBA-CGA	5.43	129.21	113.32
9	D	601	CHL	CBA-CAA-C2A	5.44	129.07	113.73
10	F	604	CLA	CMB-C2B-C3B	5.45	135.74	125.09
4	C	2620	LUT	C18-C5-C6	5.45	129.96	124.61
10	B	602	CLA	O2D-CGD-CBD	5.46	118.80	111.30
10	I	604	CLA	O2A-CGA-CBA	5.47	128.57	111.90
4	D	3620	LUT	C18-C5-C6	5.49	130.00	124.61
10	A	602	CLA	C6-C5-C3	5.51	124.57	112.48
10	B	613	CLA	CED-O2D-CGD	5.52	128.93	115.99
9	B	606	CHL	O2A-CGA-CBA	5.52	128.72	111.90
10	B	613	CLA	CMB-C2B-C3B	5.53	135.90	125.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	H	613	CLA	CMB-C2B-C3B	5.54	135.92	125.09
10	I	603	CLA	O2D-CGD-CBD	5.54	118.91	111.30
4	A	620	LUT	C18-C5-C6	5.56	130.06	124.61
4	I	8620	LUT	C18-C5-C6	5.57	130.07	124.61
10	D	604	CLA	O2D-CGD-CBD	5.58	118.95	111.30
10	C	613	CLA	CMB-C2B-C3B	5.58	136.00	125.09
10	H	604	CLA	O2A-CGA-CBA	5.59	128.93	111.90
10	A	604	CLA	CMB-C2B-C3B	5.59	136.03	125.09
4	C	2620	LUT	C38-C25-C26	5.59	120.22	116.04
4	A	621	LUT	C38-C25-C26	5.59	120.22	116.04
10	E	602	CLA	O2D-CGD-CBD	5.59	118.97	111.30
10	B	602	CLA	C6-C5-C3	5.60	124.78	112.48
9	C	608	CHL	OMC-CMC-C2C	5.62	140.03	125.58
9	A	609	CHL	OMC-CMC-C2C	5.63	140.05	125.58
10	D	604	CLA	CMB-C2B-C3B	5.63	136.11	125.09
7	I	8630	LHG	O8-C23-C24	5.65	129.13	111.90
10	G	603	CLA	C6-C5-C3	5.68	124.95	112.48
10	F	604	CLA	O2A-CGA-CBA	5.69	129.22	111.90
9	A	607	CHL	OMC-CMC-C2C	5.69	140.22	125.58
10	D	613	CLA	CMB-C2B-C3B	5.70	136.24	125.09
10	C	604	CLA	CMB-C2B-C3B	5.71	136.26	125.09
4	J	9620	LUT	C18-C5-C6	5.71	130.22	124.61
10	C	612	CLA	O2D-CGD-CBD	5.72	119.15	111.30
9	H	606	CHL	CAA-CBA-CGA	5.72	130.08	113.32
10	I	613	CLA	CMB-C2B-C3B	5.77	136.38	125.09
10	J	604	CLA	O2A-CGA-CBA	5.79	129.56	111.90
10	J	603	CLA	O2D-CGD-CBD	5.82	119.28	111.30
10	G	613	CLA	CMB-C2B-C3B	5.82	136.47	125.09
9	C	607	CHL	OMC-CMC-C2C	5.85	140.62	125.58
9	G	601	CHL	CBA-CAA-C2A	5.85	130.25	113.73
10	E	604	CLA	O2A-CGA-CBA	5.91	129.91	111.90
10	D	613	CLA	CBA-CAA-C2A	6.04	130.78	113.73
10	B	603	CLA	O2D-CGD-CBD	6.05	119.60	111.30
10	H	611	CLA	CBA-CAA-C2A	6.13	131.02	113.73
10	H	604	CLA	O2D-CGD-CBD	6.17	119.77	111.30
10	C	611	CLA	CBA-CAA-C2A	6.20	131.22	113.73
10	A	611	CLA	CBA-CAA-C2A	6.23	131.31	113.73
10	A	603	CLA	O2D-CGD-CBD	6.25	119.88	111.30
10	E	611	CLA	CBA-CAA-C2A	6.28	131.45	113.73
10	D	611	CLA	CBA-CAA-C2A	6.31	131.54	113.73
10	G	612	CLA	O2D-CGD-CBD	6.34	120.00	111.30
4	F	5620	LUT	C38-C25-C26	6.39	120.82	116.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1620	LUT	C38-C25-C26	6.39	120.82	116.04
10	I	602	CLA	O2D-CGD-CBD	6.48	120.19	111.30
4	J	9621	LUT	C38-C25-C26	6.51	120.91	116.04
4	H	7621	LUT	C38-C25-C26	6.57	120.95	116.04
10	B	604	CLA	O2A-CGA-CBA	6.64	132.13	111.90
10	D	604	CLA	O2A-CGA-CBA	6.64	132.14	111.90
10	C	604	CLA	O2A-CGA-CBA	6.65	132.17	111.90
10	G	611	CLA	CBA-CAA-C2A	6.67	132.55	113.73
10	C	603	CLA	O2D-CGD-CBD	6.75	120.56	111.30
4	E	4620	LUT	C18-C5-C6	6.80	131.28	124.61
4	E	4620	LUT	C38-C25-C26	7.00	121.28	116.04
4	F	5621	LUT	C38-C25-C26	7.03	121.30	116.04
4	I	8621	LUT	C38-C25-C26	7.08	121.33	116.04
4	D	3620	LUT	C38-C25-C26	7.21	121.43	116.04
4	G	6620	LUT	C38-C25-C26	7.22	121.44	116.04
4	A	620	LUT	C38-C25-C26	7.49	121.64	116.04
4	B	1621	LUT	C38-C25-C26	7.60	121.73	116.04
10	J	614	CLA	O2D-CGD-CBD	7.72	121.89	111.30
4	I	8620	LUT	C38-C25-C26	7.87	121.93	116.04
10	G	614	CLA	O2D-CGD-CBD	7.88	122.11	111.30
10	F	614	CLA	O2D-CGD-CBD	7.98	122.25	111.30
10	D	614	CLA	O2D-CGD-CBD	8.49	122.95	111.30
10	I	614	CLA	O2D-CGD-CBD	8.89	123.49	111.30
4	J	9620	LUT	C38-C25-C26	8.92	122.72	116.04
10	A	614	CLA	O2D-CGD-CBD	8.99	123.63	111.30
10	H	614	CLA	O2D-CGD-CBD	9.01	123.66	111.30
10	E	614	CLA	O2D-CGD-CBD	9.11	123.80	111.30
10	B	614	CLA	O2D-CGD-CBD	9.50	124.34	111.30
4	H	7620	LUT	C38-C25-C26	9.54	123.18	116.04
10	C	614	CLA	O2D-CGD-CBD	9.65	124.54	111.30

All (303) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	611	CLA	NC
10	B	611	CLA	ND
10	B	611	CLA	NA
10	F	611	CLA	NC
10	F	611	CLA	ND
10	F	611	CLA	NA
9	D	609	CHL	C13
9	H	607	CHL	C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	A	610	CLA	NC
10	A	610	CLA	NA
10	A	610	CLA	ND
10	G	613	CLA	NC
10	G	613	CLA	ND
10	G	613	CLA	NA
10	F	610	CLA	NC
10	F	610	CLA	ND
10	F	610	CLA	NA
10	A	602	CLA	C8
10	A	602	CLA	NC
10	A	602	CLA	ND
10	A	602	CLA	NA
10	G	610	CLA	NC
10	G	610	CLA	NA
10	G	610	CLA	ND
9	F	609	CHL	C13
10	B	603	CLA	C8
10	B	603	CLA	NC
10	B	603	CLA	ND
10	B	603	CLA	NA
10	I	604	CLA	NC
10	I	604	CLA	ND
10	I	604	CLA	NA
10	C	610	CLA	NC
10	C	610	CLA	NA
10	C	610	CLA	ND
8	I	8632	DGD	C2D
8	I	8632	DGD	C5D
10	D	611	CLA	NC
10	D	611	CLA	ND
10	D	611	CLA	NA
10	F	602	CLA	C8
10	F	602	CLA	NC
10	F	602	CLA	ND
10	F	602	CLA	NA
10	H	611	CLA	NC
10	H	611	CLA	NA
10	H	611	CLA	ND
10	C	611	CLA	NC
10	C	611	CLA	ND
10	C	611	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	J	612	CLA	NC
10	J	612	CLA	ND
10	J	612	CLA	NA
10	G	602	CLA	C8
10	G	602	CLA	NC
10	G	602	CLA	ND
10	G	602	CLA	NA
10	B	614	CLA	NC
10	B	614	CLA	ND
10	B	614	CLA	NA
10	J	604	CLA	NC
10	J	604	CLA	ND
10	J	604	CLA	NA
10	H	614	CLA	NC
10	H	614	CLA	ND
10	H	614	CLA	NA
8	D	5632	DGD	C2D
8	D	5632	DGD	C5D
10	E	604	CLA	NC
10	E	604	CLA	ND
10	E	604	CLA	NA
8	A	632	DGD	C2D
8	A	632	DGD	C5D
8	E	4632	DGD	C2D
8	E	4632	DGD	C5D
10	F	603	CLA	C8
10	F	603	CLA	NC
10	F	603	CLA	ND
10	F	603	CLA	NA
9	A	607	CHL	C8
10	I	602	CLA	C8
10	I	602	CLA	NC
10	I	602	CLA	ND
10	I	602	CLA	NA
10	I	614	CLA	NC
10	I	614	CLA	ND
10	I	614	CLA	NA
10	B	602	CLA	C8
10	B	602	CLA	NC
10	B	602	CLA	ND
10	B	602	CLA	NA
9	C	609	CHL	C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	C	612	CLA	NC
10	C	612	CLA	ND
10	C	612	CLA	NA
10	A	612	CLA	NC
10	A	612	CLA	ND
10	A	612	CLA	NA
10	C	604	CLA	NC
10	C	604	CLA	ND
10	C	604	CLA	NA
10	D	604	CLA	NC
10	D	604	CLA	ND
10	D	604	CLA	NA
10	J	602	CLA	C8
10	J	602	CLA	NC
10	J	602	CLA	ND
10	J	602	CLA	NA
10	G	614	CLA	NC
10	G	614	CLA	NA
10	G	614	CLA	ND
8	G	9632	DGD	C2D
8	G	9632	DGD	C5D
10	H	610	CLA	C13
10	H	610	CLA	NC
10	H	610	CLA	NA
10	H	610	CLA	ND
9	A	609	CHL	C13
10	I	613	CLA	NC
10	I	613	CLA	ND
10	I	613	CLA	NA
10	F	613	CLA	NC
10	F	613	CLA	ND
10	F	613	CLA	NA
10	E	602	CLA	C8
10	E	602	CLA	NC
10	E	602	CLA	ND
10	E	602	CLA	NA
9	G	609	CHL	C13
10	E	603	CLA	C8
10	E	603	CLA	NC
10	E	603	CLA	ND
10	E	603	CLA	NA
10	D	610	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	D	610	CLA	ND
10	D	610	CLA	NA
10	J	610	CLA	NC
10	J	610	CLA	NA
10	J	610	CLA	ND
10	B	604	CLA	NC
10	B	604	CLA	ND
10	B	604	CLA	NA
10	G	604	CLA	NC
10	G	604	CLA	ND
10	G	604	CLA	NA
10	A	604	CLA	NC
10	A	604	CLA	ND
10	A	604	CLA	NA
10	B	613	CLA	NC
10	B	613	CLA	ND
10	B	613	CLA	NA
10	D	613	CLA	NC
10	D	613	CLA	ND
10	D	613	CLA	NA
10	I	610	CLA	C13
10	I	610	CLA	NC
10	I	610	CLA	NA
10	I	610	CLA	ND
9	G	607	CHL	C8
10	J	614	CLA	NC
10	J	614	CLA	ND
10	J	614	CLA	NA
9	F	607	CHL	C8
10	I	603	CLA	C8
10	I	603	CLA	NC
10	I	603	CLA	ND
10	I	603	CLA	NA
10	J	611	CLA	NC
10	J	611	CLA	ND
10	J	611	CLA	NA
10	A	611	CLA	NC
10	A	611	CLA	NA
10	A	611	CLA	ND
10	J	613	CLA	NC
10	J	613	CLA	ND
10	J	613	CLA	NA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	C	602	CLA	C8
10	C	602	CLA	NC
10	C	602	CLA	ND
10	C	602	CLA	NA
10	G	612	CLA	NC
10	G	612	CLA	ND
10	G	612	CLA	NA
9	I	609	CHL	C13
10	H	612	CLA	NC
10	H	612	CLA	ND
10	H	612	CLA	NA
10	D	603	CLA	C8
10	D	603	CLA	NC
10	D	603	CLA	ND
10	D	603	CLA	NA
10	I	611	CLA	NC
10	I	611	CLA	NA
10	I	611	CLA	ND
9	E	607	CHL	C8
10	G	603	CLA	C8
10	G	603	CLA	NC
10	G	603	CLA	ND
10	G	603	CLA	NA
10	B	610	CLA	NC
10	B	610	CLA	NA
10	B	610	CLA	ND
10	D	612	CLA	NC
10	D	612	CLA	ND
10	D	612	CLA	NA
9	C	607	CHL	C8
10	C	614	CLA	NC
10	C	614	CLA	ND
10	C	614	CLA	NA
9	E	609	CHL	C13
9	A	601	CHL	C13
10	H	602	CLA	C8
10	H	602	CLA	NC
10	H	602	CLA	ND
10	H	602	CLA	NA
8	H	7632	DGD	C2D
8	H	7632	DGD	C5D
10	E	610	CLA	NC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	E	610	CLA	NA
10	E	610	CLA	ND
9	H	609	CHL	C13
10	A	613	CLA	NC
10	A	613	CLA	ND
10	A	613	CLA	NA
10	C	603	CLA	C8
10	C	603	CLA	NC
10	C	603	CLA	ND
10	C	603	CLA	NA
10	J	603	CLA	C8
10	J	603	CLA	NC
10	J	603	CLA	ND
10	J	603	CLA	NA
9	J	609	CHL	C13
10	I	612	CLA	NC
10	I	612	CLA	ND
10	I	612	CLA	NA
10	H	604	CLA	NC
10	H	604	CLA	ND
10	H	604	CLA	NA
8	B	2632	DGD	C2D
8	B	2632	DGD	C5D
10	E	611	CLA	NC
10	E	611	CLA	ND
10	E	611	CLA	NA
9	J	607	CHL	C8
8	B	1632	DGD	C2D
8	B	1632	DGD	C5D
10	F	614	CLA	NC
10	F	614	CLA	NA
10	F	614	CLA	ND
9	I	607	CHL	C8
10	F	612	CLA	NC
10	F	612	CLA	ND
10	F	612	CLA	NA
10	E	612	CLA	NC
10	E	612	CLA	ND
10	E	612	CLA	NA
10	D	602	CLA	C8
10	D	602	CLA	NC
10	D	602	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
10	D	602	CLA	NA
10	F	604	CLA	NC
10	F	604	CLA	ND
10	F	604	CLA	NA
10	B	612	CLA	NC
10	B	612	CLA	ND
10	B	612	CLA	NA
10	A	614	CLA	NC
10	A	614	CLA	ND
10	A	614	CLA	NA
10	H	603	CLA	C8
10	H	603	CLA	NC
10	H	603	CLA	ND
10	H	603	CLA	NA
10	D	614	CLA	NC
10	D	614	CLA	ND
10	D	614	CLA	NA
10	G	611	CLA	NC
10	G	611	CLA	NA
10	G	611	CLA	ND
8	H	6632	DGD	C2D
8	H	6632	DGD	C5D
10	H	613	CLA	NC
10	H	613	CLA	ND
10	H	613	CLA	NA
8	D	3632	DGD	C2D
8	D	3632	DGD	C5D
10	C	613	CLA	NC
10	C	613	CLA	ND
10	C	613	CLA	NA
10	E	613	CLA	NC
10	E	613	CLA	ND
10	E	613	CLA	NA
10	A	603	CLA	C8
10	A	603	CLA	NC
10	A	603	CLA	ND
10	A	603	CLA	NA
9	D	607	CHL	C8
10	E	614	CLA	NC
10	E	614	CLA	ND
10	E	614	CLA	NA
9	B	609	CHL	C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
9	B	607	CHL	C8

There are no torsion outliers.

There are no ring outliers.

139 monomers are involved in 193 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	601	CHL	2	0
10	A	602	CLA	3	0
10	A	603	CLA	3	0
10	A	604	CLA	1	0
9	A	605	CHL	1	0
9	A	608	CHL	1	0
10	A	610	CLA	2	0
10	A	611	CLA	3	0
10	A	612	CLA	2	0
4	A	620	LUT	2	0
4	A	621	LUT	1	0
7	A	630	LHG	2	0
8	A	632	DGD	1	0
4	B	1620	LUT	2	0
4	B	1621	LUT	2	0
5	B	1622	XAT	1	0
7	B	1630	LHG	3	0
9	B	601	CHL	3	0
10	B	602	CLA	2	0
10	B	603	CLA	4	0
10	B	604	CLA	1	0
9	B	605	CHL	2	0
9	B	606	CHL	1	0
9	B	608	CHL	1	0
9	B	609	CHL	1	0
10	B	610	CLA	2	0
10	B	611	CLA	3	0
10	B	612	CLA	2	0
10	B	613	CLA	1	0
4	C	2621	LUT	2	0
7	C	2630	LHG	1	0
9	C	601	CHL	1	0
10	C	602	CLA	3	0
10	C	603	CLA	4	0
10	C	604	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	608	CHL	2	0
9	C	609	CHL	2	0
10	C	610	CLA	1	0
10	C	611	CLA	3	0
10	C	612	CLA	2	0
10	C	613	CLA	1	0
10	C	614	CLA	1	0
4	D	3621	LUT	1	0
7	D	3630	LHG	1	0
2	D	3633	BNG	1	0
8	D	5632	DGD	1	0
9	D	601	CHL	1	0
10	D	602	CLA	2	0
10	D	603	CLA	1	0
10	D	604	CLA	2	0
9	D	609	CHL	1	0
10	D	610	CLA	1	0
10	D	611	CLA	2	0
10	D	612	CLA	2	0
10	D	613	CLA	1	0
5	E	2622	XAT	2	0
4	E	4620	LUT	2	0
4	E	4621	LUT	1	0
7	E	4630	LHG	1	0
9	E	601	CHL	1	0
10	E	602	CLA	2	0
10	E	603	CLA	4	0
10	E	604	CLA	1	0
9	E	605	CHL	1	0
9	E	609	CHL	1	0
10	E	610	CLA	1	0
10	E	611	CLA	1	0
10	E	612	CLA	2	0
10	E	613	CLA	1	0
10	E	614	CLA	1	0
4	F	5620	LUT	1	0
4	F	5621	LUT	1	0
7	F	5630	LHG	3	0
9	F	601	CHL	3	0
10	F	602	CLA	3	0
10	F	603	CLA	3	0
10	F	604	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	608	CHL	1	0
9	F	609	CHL	1	0
10	F	610	CLA	1	0
10	F	611	CLA	1	0
10	F	613	CLA	2	0
5	F	6622	XAT	1	0
9	G	601	CHL	3	0
10	G	602	CLA	2	0
10	G	603	CLA	3	0
10	G	604	CLA	1	0
9	G	606	CHL	1	0
9	G	607	CHL	1	0
9	G	608	CHL	2	0
9	G	609	CHL	2	0
10	G	610	CLA	1	0
10	G	611	CLA	4	0
10	G	612	CLA	2	0
10	G	613	CLA	1	0
4	G	6621	LUT	1	0
6	G	6623	NEX	1	0
7	G	6630	LHG	2	0
5	H	4622	XAT	1	0
9	H	601	CHL	1	0
10	H	602	CLA	3	0
10	H	603	CLA	4	0
9	H	605	CHL	1	0
9	H	608	CHL	1	0
9	H	609	CHL	2	0
10	H	610	CLA	2	0
10	H	611	CLA	3	0
10	H	612	CLA	2	0
10	H	613	CLA	1	0
8	H	6632	DGD	1	0
4	H	7621	LUT	2	0
7	H	7630	LHG	2	0
9	I	601	CHL	2	0
10	I	602	CLA	2	0
10	I	603	CLA	3	0
10	I	604	CLA	1	0
9	I	605	CHL	1	0
9	I	606	CHL	1	0
9	I	609	CHL	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	610	CLA	2	0
10	I	611	CLA	2	0
10	I	612	CLA	1	0
10	I	613	CLA	1	0
4	I	8620	LUT	2	0
4	I	8621	LUT	1	0
7	I	8630	LHG	3	0
8	I	8632	DGD	1	0
5	I	9622	XAT	1	0
5	J	3622	XAT	1	0
10	J	602	CLA	2	0
10	J	603	CLA	3	0
10	J	604	CLA	1	0
9	J	605	CHL	2	0
10	J	610	CLA	1	0
10	J	611	CLA	3	0
10	J	612	CLA	2	0
10	J	613	CLA	1	0
10	J	614	CLA	1	0
4	J	9621	LUT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	218/232 (93%)	-0.43	5 (2%)	64	64	18, 31, 53, 67	0
1	B	218/232 (93%)	-0.55	4 (1%)	71	72	15, 23, 42, 50	0
1	C	218/232 (93%)	-0.51	7 (3%)	51	52	14, 23, 40, 53	0
1	D	218/232 (93%)	-0.55	4 (1%)	71	72	16, 26, 44, 60	0
1	E	218/232 (93%)	-0.54	5 (2%)	64	64	14, 25, 41, 54	0
1	F	219/232 (94%)	-0.50	6 (2%)	58	58	14, 24, 42, 69	0
1	G	218/232 (93%)	-0.51	9 (4%)	41	41	16, 27, 47, 59	0
1	H	218/232 (93%)	-0.47	7 (3%)	51	52	18, 27, 49, 58	0
1	I	218/232 (93%)	-0.47	8 (3%)	45	46	17, 26, 45, 61	0
1	J	218/232 (93%)	-0.56	5 (2%)	64	64	15, 24, 42, 52	0
All	All	2181/2320 (94%)	-0.51	60 (2%)	56	57	14, 26, 46, 69	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	232	LYS	6.3
1	E	231	GLY	5.4
1	A	231	GLY	5.1
1	G	231	GLY	4.1
1	I	231	GLY	4.0
1	D	231	GLY	3.7
1	H	152	VAL	3.5
1	H	107	GLU	3.4
1	A	152	VAL	3.2
1	J	231	GLY	3.2
1	C	107	GLU	3.0
1	H	89	GLY	2.9
1	I	152	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	91	LYS	2.9
1	I	89	GLY	2.8
1	B	107	GLU	2.8
1	G	89	GLY	2.8
1	C	152	VAL	2.8
1	F	14	SER	2.7
1	J	168	ASP	2.7
1	A	168	ASP	2.7
1	C	89	GLY	2.7
1	D	107	GLU	2.7
1	D	89	GLY	2.6
1	H	231	GLY	2.6
1	A	107	GLU	2.6
1	G	88	ASN	2.6
1	E	168	ASP	2.6
1	E	89	GLY	2.5
1	H	91	LYS	2.5
1	E	88	ASN	2.5
1	F	88	ASN	2.5
1	J	152	VAL	2.5
1	B	20	ASP	2.5
1	J	88	ASN	2.4
1	F	168	ASP	2.3
1	E	107	GLU	2.3
1	G	31	GLU	2.3
1	G	107	GLU	2.3
1	I	20	ASP	2.3
1	C	168	ASP	2.3
1	H	31	GLU	2.3
1	A	20	ASP	2.3
1	J	107	GLU	2.3
1	F	107	GLU	2.3
1	B	88	ASN	2.3
1	I	31	GLU	2.2
1	I	165	GLY	2.2
1	G	19	PRO	2.2
1	F	89	GLY	2.2
1	G	170	PRO	2.2
1	C	231	GLY	2.2
1	I	91	LYS	2.1
1	C	91	LYS	2.1
1	B	89	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	88	ASN	2.0
1	D	171	GLU	2.0
1	I	88	ASN	2.0
1	G	169	ASP	2.0
1	H	168	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NEX	G	6623	44/44	0.76	0.28	5.31	30,42,80,82	0
8	DGD	I	8632	66/66	0.89	0.24	5.28	24,49,85,86	0
8	DGD	D	5632	66/66	0.89	0.23	5.07	23,43,89,91	0
10	CLA	E	614	49/65	0.96	0.12	4.89	15,23,57,68	0
8	DGD	E	4632	66/66	0.89	0.22	4.83	27,41,87,89	0
7	LHG	A	630	49/49	0.91	0.22	4.72	39,47,61,63	0
6	NEX	E	4623	44/44	0.80	0.25	4.36	16,30,74,76	0
6	NEX	C	2623	44/44	0.83	0.25	4.35	17,35,85,87	0
6	NEX	J	9623	44/44	0.77	0.29	4.17	22,40,85,86	0
6	NEX	F	5623	44/44	0.85	0.23	3.99	21,33,78,81	0
8	DGD	A	632	66/66	0.88	0.22	3.98	26,46,79,80	0
6	NEX	D	3623	44/44	0.79	0.25	3.94	22,34,76,79	0
8	DGD	H	7632	66/66	0.88	0.22	3.92	30,50,82,83	0
8	DGD	G	9632	66/66	0.88	0.22	3.83	23,48,83,86	0
4	LUT	G	6621	42/42	0.97	0.15	3.77	16,21,23,25	0
8	DGD	B	2632	66/66	0.89	0.22	3.75	21,44,77,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	NEX	B	1623	44/44	0.81	0.24	3.68	19,36,75,78	0
6	NEX	H	7623	44/44	0.75	0.29	3.59	28,46,82,84	0
8	DGD	B	1632	66/66	0.89	0.22	3.55	20,45,80,82	0
4	LUT	H	7621	42/42	0.97	0.15	3.46	13,20,24,25	0
8	DGD	D	3632	66/66	0.90	0.21	3.42	20,47,77,79	0
6	NEX	I	8623	44/44	0.78	0.27	3.27	27,36,77,80	0
7	LHG	B	1630	49/49	0.91	0.21	3.25	32,40,55,60	0
7	LHG	D	3630	49/49	0.92	0.18	3.25	30,36,55,60	0
7	LHG	E	4630	49/49	0.92	0.21	3.21	28,37,52,55	0
4	LUT	D	3621	42/42	0.96	0.17	3.20	11,19,23,23	0
4	LUT	J	9621	42/42	0.97	0.14	2.98	14,19,21,24	0
6	NEX	A	623	44/44	0.80	0.25	2.90	27,53,90,91	0
10	CLA	A	611	65/65	0.90	0.19	2.78	40,48,78,78	0
7	LHG	J	9630	49/49	0.93	0.20	2.68	26,35,54,59	0
8	DGD	H	6632	66/66	0.89	0.22	2.66	24,49,83,84	0
9	CHL	J	606	51/66	0.93	0.16	2.62	16,22,60,62	0
10	CLA	F	604	62/65	0.94	0.16	2.57	17,21,76,81	0
10	CLA	G	603	65/65	0.95	0.12	2.40	17,22,69,71	0
10	CLA	D	611	65/65	0.91	0.18	2.39	25,34,65,66	0
4	LUT	B	1621	42/42	0.96	0.14	2.37	8,14,23,25	0
10	CLA	B	604	62/65	0.93	0.17	2.34	19,22,75,78	0
10	CLA	B	611	65/65	0.91	0.17	2.27	24,31,69,69	0
10	CLA	A	604	62/65	0.94	0.16	2.22	18,25,74,79	0
4	LUT	A	621	42/42	0.97	0.15	2.20	17,20,25,26	0
10	CLA	C	611	65/65	0.92	0.19	2.19	28,33,76,77	0
9	CHL	A	606	51/66	0.93	0.15	2.03	19,24,66,67	0
4	LUT	I	8621	42/42	0.97	0.14	2.01	12,20,22,24	0
4	LUT	E	4621	42/42	0.98	0.14	1.96	11,16,22,24	0
10	CLA	A	612	65/65	0.94	0.16	1.93	33,38,86,88	0
10	CLA	I	614	49/65	0.95	0.14	1.92	20,23,58,67	0
10	CLA	H	602	65/65	0.96	0.16	1.89	20,23,47,48	0
10	CLA	J	604	62/65	0.93	0.16	1.88	15,22,72,76	0
10	CLA	C	614	49/65	0.96	0.11	1.88	14,18,54,65	0
10	CLA	G	602	65/65	0.96	0.14	1.86	17,21,44,46	0
10	CLA	D	612	65/65	0.94	0.14	1.85	22,30,83,85	0
5	XAT	A	622	44/44	0.90	0.17	1.85	16,26,34,38	0
9	CHL	D	606	51/66	0.94	0.16	1.83	16,22,60,61	0
10	CLA	J	614	49/65	0.95	0.13	1.82	14,22,57,67	0
10	CLA	H	604	62/65	0.94	0.16	1.80	18,25,69,74	0
7	LHG	H	7630	49/49	0.93	0.20	1.78	30,37,57,62	0
10	CLA	H	612	65/65	0.94	0.17	1.70	24,34,86,87	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	CLA	I	604	62/65	0.94	0.17	1.69	20,25,77,81	0
10	CLA	A	602	65/65	0.96	0.15	1.69	20,30,52,54	0
10	CLA	B	602	65/65	0.97	0.14	1.68	16,21,51,54	0
4	LUT	F	5621	42/42	0.97	0.14	1.66	11,19,22,24	0
10	CLA	E	602	65/65	0.96	0.15	1.61	13,20,48,49	0
10	CLA	J	602	65/65	0.96	0.16	1.60	12,17,47,48	0
10	CLA	D	602	65/65	0.97	0.14	1.57	13,20,45,46	0
10	CLA	E	604	62/65	0.94	0.16	1.57	18,23,75,79	0
9	CHL	F	606	51/66	0.93	0.15	1.57	13,21,61,62	0
10	CLA	J	612	65/65	0.96	0.14	1.54	18,25,79,82	0
10	CLA	G	604	62/65	0.94	0.15	1.54	17,24,75,79	0
7	LHG	G	6630	49/49	0.92	0.20	1.53	31,38,57,61	0
10	CLA	B	614	49/65	0.95	0.11	1.49	10,22,59,69	0
4	LUT	C	2621	42/42	0.97	0.14	1.48	13,18,21,22	0
10	CLA	E	611	65/65	0.92	0.17	1.48	26,32,70,72	0
10	CLA	D	604	62/65	0.95	0.16	1.46	20,25,66,70	0
9	CHL	H	606	51/66	0.94	0.14	1.38	17,22,67,69	0
9	CHL	A	601	66/66	0.93	0.16	1.36	31,36,39,43	0
9	CHL	C	606	51/66	0.94	0.15	1.35	16,22,63,64	0
9	CHL	I	601	66/66	0.95	0.14	1.33	22,26,34,35	0
10	CLA	C	602	65/65	0.97	0.15	1.31	10,19,38,39	0
9	CHL	B	605	48/66	0.94	0.16	1.30	23,26,58,74	0
10	CLA	J	611	65/65	0.93	0.15	1.27	20,26,68,69	0
10	CLA	B	612	65/65	0.95	0.13	1.25	18,27,88,89	0
9	CHL	G	606	51/66	0.95	0.14	1.24	15,23,59,60	0
9	CHL	E	606	51/66	0.94	0.15	1.23	18,21,60,62	0
10	CLA	G	612	65/65	0.94	0.16	1.22	22,33,89,91	0
10	CLA	G	614	49/65	0.96	0.12	1.21	12,22,58,67	0
10	CLA	G	611	65/65	0.91	0.18	1.18	33,39,75,77	0
10	CLA	F	614	49/65	0.96	0.11	1.18	12,20,57,68	0
9	CHL	B	606	51/66	0.95	0.14	1.18	11,20,60,62	0
10	CLA	I	602	65/65	0.96	0.15	1.17	17,21,52,57	0
5	XAT	E	2622	44/44	0.90	0.16	1.15	16,22,27,30	0
10	CLA	C	604	62/65	0.94	0.15	1.13	15,21,70,75	0
10	CLA	D	614	49/65	0.96	0.12	1.13	10,21,54,64	0
10	CLA	H	610	65/65	0.94	0.15	1.12	24,32,69,74	0
7	LHG	F	5630	49/49	0.93	0.19	1.12	25,33,48,52	0
9	CHL	D	605	48/66	0.95	0.16	1.10	23,29,57,71	0
9	CHL	G	605	48/66	0.93	0.16	1.10	24,27,59,75	0
10	CLA	H	614	49/65	0.94	0.12	1.10	16,26,60,68	0
9	CHL	A	605	48/66	0.95	0.15	1.08	19,25,57,71	0
5	XAT	F	6622	44/44	0.92	0.15	1.07	15,22,29,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	CHL	C	605	48/66	0.94	0.16	1.07	25,29,58,72	0
10	CLA	F	612	65/65	0.94	0.15	1.05	22,28,79,81	0
5	XAT	B	5622	44/44	0.91	0.17	1.05	12,22,27,31	0
9	CHL	I	606	51/66	0.94	0.14	1.03	15,19,62,64	0
7	LHG	C	2630	49/49	0.93	0.18	1.02	24,30,48,50	0
10	CLA	I	612	65/65	0.94	0.15	1.00	23,30,87,90	0
7	LHG	I	8630	49/49	0.92	0.19	1.00	29,34,55,57	0
10	CLA	E	613	65/65	0.97	0.12	0.91	15,18,54,57	0
10	CLA	H	611	65/65	0.91	0.17	0.90	33,39,71,72	0
5	XAT	D	8622	44/44	0.92	0.15	0.85	18,23,30,33	0
9	CHL	B	601	66/66	0.95	0.14	0.83	22,26,37,38	0
9	CHL	J	601	66/66	0.96	0.14	0.81	19,23,29,33	0
5	XAT	I	9622	44/44	0.92	0.15	0.79	15,22,29,32	0
9	CHL	G	601	66/66	0.95	0.14	0.79	27,32,36,40	0
9	CHL	H	605	48/66	0.94	0.14	0.78	24,30,60,73	0
5	XAT	B	1622	44/44	0.93	0.14	0.77	17,23,28,30	0
10	CLA	J	603	65/65	0.96	0.11	0.76	13,20,71,72	0
10	CLA	G	613	65/65	0.96	0.13	0.76	14,17,55,56	0
10	CLA	F	602	65/65	0.97	0.14	0.75	9,17,42,48	0
9	CHL	G	609	66/66	0.97	0.12	0.72	18,25,42,46	0
9	CHL	E	605	48/66	0.95	0.15	0.70	20,25,58,71	0
5	XAT	H	4622	44/44	0.92	0.15	0.70	20,24,30,34	0
5	XAT	J	3622	44/44	0.93	0.14	0.70	17,24,29,31	0
10	CLA	J	613	65/65	0.97	0.12	0.69	11,17,56,59	0
10	CLA	B	613	65/65	0.97	0.13	0.68	13,17,52,56	0
10	CLA	F	613	65/65	0.97	0.12	0.68	14,17,45,48	0
5	XAT	C	7622	44/44	0.92	0.15	0.66	17,23,31,34	0
10	CLA	I	611	65/65	0.91	0.16	0.65	27,33,71,72	0
9	CHL	I	605	48/66	0.94	0.15	0.65	29,32,60,73	0
10	CLA	G	610	65/65	0.95	0.14	0.63	24,31,73,79	0
9	CHL	E	601	66/66	0.95	0.14	0.63	23,28,31,33	0
10	CLA	C	612	65/65	0.94	0.15	0.63	20,31,82,85	0
9	CHL	F	601	66/66	0.96	0.14	0.62	22,24,32,33	0
10	CLA	A	614	49/65	0.95	0.13	0.61	20,27,59,66	0
9	CHL	D	601	66/66	0.96	0.13	0.60	22,27,30,32	0
9	CHL	H	601	66/66	0.95	0.14	0.60	28,31,32,36	0
10	CLA	E	610	65/65	0.95	0.13	0.56	17,25,59,66	0
10	CLA	I	603	65/65	0.96	0.11	0.51	16,20,64,65	0
10	CLA	C	603	65/65	0.97	0.11	0.50	12,18,76,78	0
9	CHL	J	607	66/66	0.96	0.12	0.49	12,17,45,47	0
10	CLA	D	613	65/65	0.97	0.12	0.46	15,18,50,52	0
10	CLA	F	611	65/65	0.93	0.15	0.45	20,26,73,75	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	CHL	C	601	66/66	0.96	0.13	0.44	17,22,32,33	0
9	CHL	H	609	66/66	0.97	0.11	0.43	21,26,45,51	0
9	CHL	J	605	48/66	0.95	0.13	0.41	20,26,59,71	0
9	CHL	J	609	66/66	0.97	0.11	0.40	13,19,39,43	0
10	CLA	E	612	65/65	0.95	0.12	0.40	19,25,80,82	0
10	CLA	I	613	65/65	0.97	0.12	0.40	15,19,49,51	0
10	CLA	A	603	65/65	0.95	0.11	0.37	20,26,77,78	0
10	CLA	A	613	65/65	0.97	0.13	0.37	15,19,46,49	0
10	CLA	I	610	65/65	0.94	0.14	0.36	21,26,62,68	0
9	CHL	A	609	66/66	0.96	0.12	0.31	23,27,50,54	0
10	CLA	B	603	65/65	0.96	0.12	0.28	10,19,74,76	0
10	CLA	D	603	65/65	0.96	0.10	0.28	14,21,74,75	0
10	CLA	A	610	65/65	0.93	0.14	0.27	27,36,73,78	0
10	CLA	H	603	65/65	0.96	0.11	0.25	15,19,78,79	0
9	CHL	G	608	66/66	0.94	0.14	0.25	27,31,67,68	0
9	CHL	I	609	66/66	0.97	0.12	0.25	17,20,45,50	0
9	CHL	H	608	66/66	0.95	0.15	0.24	28,31,69,72	0
10	CLA	D	610	65/65	0.96	0.12	0.24	21,26,64,69	0
9	CHL	F	608	66/66	0.95	0.14	0.22	22,28,63,65	0
10	CLA	B	610	65/65	0.96	0.12	0.21	19,25,62,68	0
9	CHL	E	607	66/66	0.96	0.13	0.21	16,20,51,51	0
10	CLA	F	603	65/65	0.96	0.11	0.19	14,22,74,77	0
9	CHL	A	607	66/66	0.95	0.13	0.17	17,20,48,49	0
9	CHL	F	605	48/66	0.94	0.13	0.17	26,29,59,72	0
4	LUT	G	6620	42/42	0.95	0.14	0.17	16,25,36,37	0
10	CLA	J	610	65/65	0.95	0.12	0.15	18,24,64,67	0
9	CHL	E	609	66/66	0.97	0.11	0.14	16,19,40,43	0
9	CHL	F	609	66/66	0.97	0.11	0.14	14,22,43,47	0
10	CLA	C	610	65/65	0.95	0.13	0.13	15,21,65,70	0
9	CHL	G	607	66/66	0.97	0.13	0.12	15,17,49,51	0
4	LUT	C	2620	42/42	0.96	0.14	0.10	18,23,28,29	0
10	CLA	C	613	65/65	0.97	0.11	0.09	13,15,43,47	0
9	CHL	H	607	66/66	0.97	0.12	0.08	12,18,49,50	0
9	CHL	D	609	66/66	0.97	0.10	0.07	18,23,42,46	0
9	CHL	D	607	66/66	0.97	0.12	0.05	11,14,52,57	0
4	LUT	F	5620	42/42	0.97	0.12	0.05	15,22,26,26	0
9	CHL	D	608	66/66	0.95	0.14	0.03	24,29,65,67	0
9	CHL	B	609	66/66	0.97	0.11	0.02	14,20,43,47	0
10	CLA	H	613	65/65	0.97	0.12	0.01	10,17,55,57	0
9	CHL	C	609	66/66	0.97	0.10	-0.03	15,22,41,42	0
9	CHL	C	607	66/66	0.97	0.12	-0.04	15,18,46,49	0
4	LUT	D	3620	42/42	0.96	0.13	-0.04	18,24,35,36	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
10	CLA	F	610	65/65	0.95	0.12	-0.05	15,20,63,68	0
9	CHL	J	608	66/66	0.95	0.14	-0.06	19,26,67,68	0
9	CHL	F	607	66/66	0.96	0.11	-0.07	13,19,41,43	0
4	LUT	H	7620	42/42	0.96	0.12	-0.08	16,22,35,36	0
4	LUT	I	8620	42/42	0.96	0.13	-0.09	15,23,35,36	0
10	CLA	E	603	65/65	0.96	0.11	-0.12	11,20,73,74	0
9	CHL	E	608	66/66	0.96	0.12	-0.17	14,19,67,69	0
4	LUT	B	1620	42/42	0.97	0.11	-0.19	13,19,30,30	0
9	CHL	B	607	66/66	0.97	0.12	-0.19	13,16,44,45	0
4	LUT	E	4620	42/42	0.97	0.10	-0.21	16,21,29,30	0
9	CHL	I	608	66/66	0.95	0.13	-0.23	21,26,66,67	0
9	CHL	B	608	66/66	0.95	0.12	-0.27	16,22,63,63	0
9	CHL	C	608	66/66	0.95	0.13	-0.28	23,28,60,61	0
4	LUT	A	620	42/42	0.96	0.12	-0.30	19,26,38,39	0
4	LUT	J	9620	42/42	0.97	0.10	-0.35	11,18,34,35	0
9	CHL	A	608	66/66	0.95	0.12	-0.37	30,35,67,68	0
9	CHL	I	607	66/66	0.97	0.11	-0.39	11,17,53,56	0
3	NA	A	634	1/1	0.92	0.34	-	1,1,1,1	1
2	BNG	C	2633	21/21	0.62	0.36	-	59,85,92,93	0
2	BNG	I	8633	21/21	0.70	0.35	-	67,86,93,93	0
2	BNG	E	4633	21/21	0.64	0.33	-	65,89,96,97	0
2	BNG	B	1633	21/21	0.66	0.36	-	63,86,92,93	0
2	BNG	A	633	21/21	0.63	0.34	-	72,92,95,96	0
2	BNG	H	7633	21/21	0.64	0.38	-	71,90,97,99	0
2	BNG	F	5633	21/21	0.68	0.35	-	55,83,91,91	0
2	BNG	G	6633	21/21	0.61	0.43	-	75,96,102,104	0
2	BNG	J	9633	21/21	0.64	0.36	-	63,83,92,93	0
2	BNG	D	3633	21/21	0.62	0.41	-	61,86,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.