wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary 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:

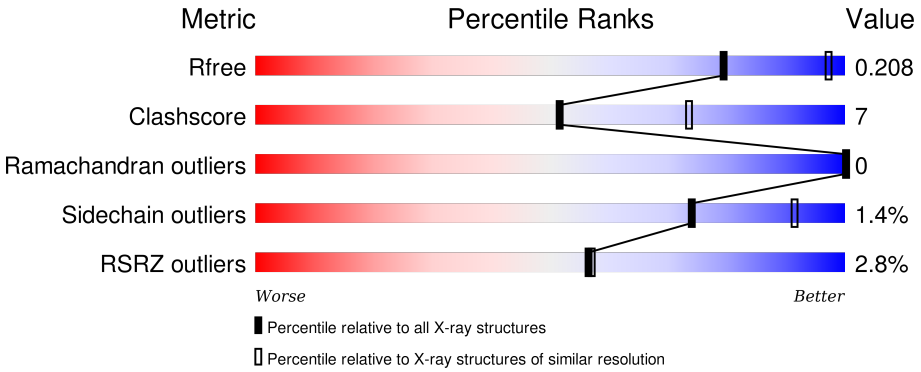
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

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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	-	-	-

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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	-	-	-

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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

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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 (i)

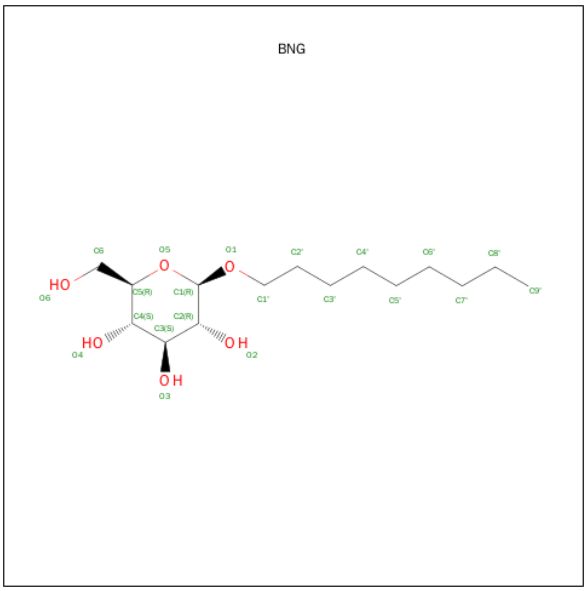
There are 11 unique types of molecules in this entry. The entry contains 29039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: $C_{15}H_{30}O_6$).



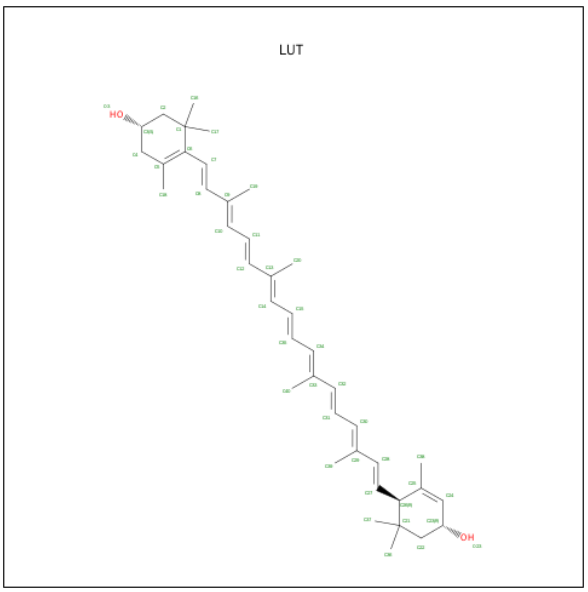
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 21 15 6	0	0
2	B	1	Total C O 21 15 6	0	0
2	C	1	Total C O 21 15 6	0	0
2	D	1	Total C O 21 15 6	0	0
2	E	1	Total C O 21 15 6	0	0
2	F	1	Total C O 21 15 6	0	0
2	G	1	Total C O 21 15 6	0	0
2	H	1	Total C O 21 15 6	0	0
2	I	1	Total C O 21 15 6	0	0
2	J	1	Total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

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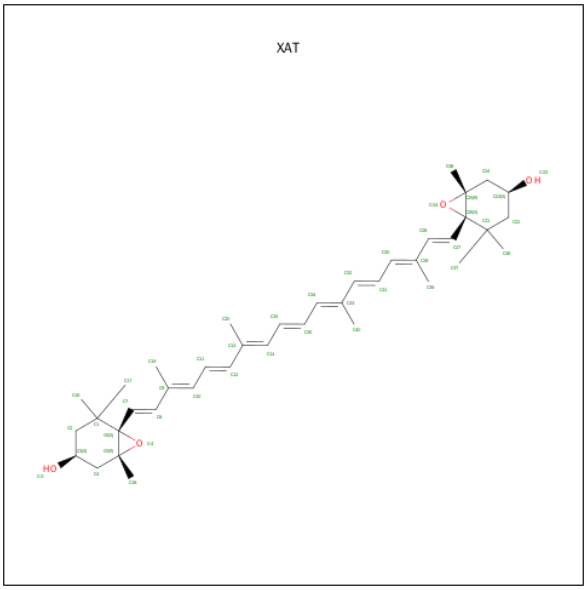
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total C O 42 40 2	0	0
4	H	1	Total C O 42 40 2	0	0
4	H	1	Total C O 42 40 2	0	0
4	I	1	Total C O 42 40 2	0	0
4	I	1	Total C O 42 40 2	0	0
4	J	1	Total C O 42 40 2	0	0
4	J	1	Total C O 42 40 2	0	0

- 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

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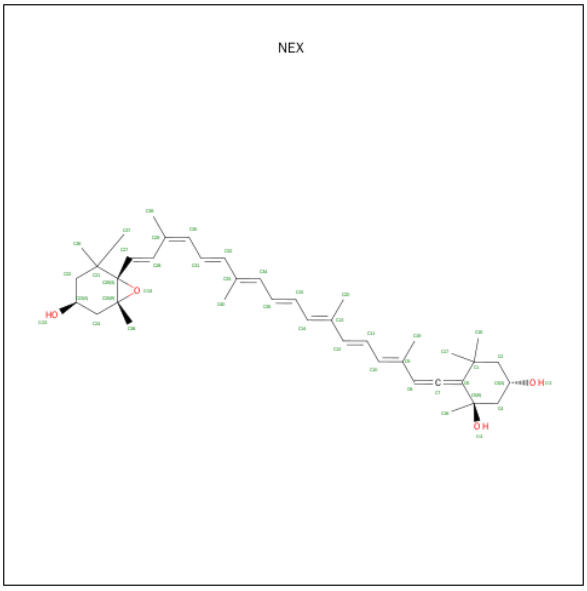
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 44 40 4	0	0
5	B	1	Total C O 44 40 4	0	0
5	F	1	Total C O 44 40 4	0	0
5	C	1	Total C O 44 40 4	0	0
5	D	1	Total C O 44 40 4	0	0
5	I	1	Total C O 44 40 4	0	0

- 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

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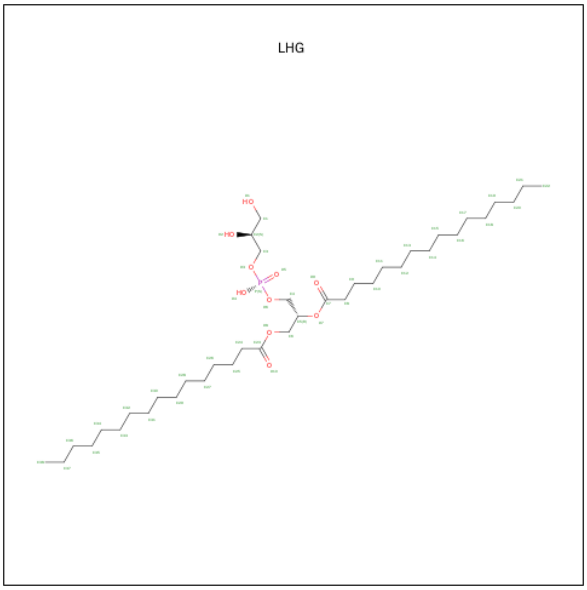
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 44 40 4	0	0
6	F	1	Total C O 44 40 4	0	0
6	G	1	Total C O 44 40 4	0	0
6	H	1	Total C O 44 40 4	0	0
6	I	1	Total C O 44 40 4	0	0
6	J	1	Total C O 44 40 4	0	0

- 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

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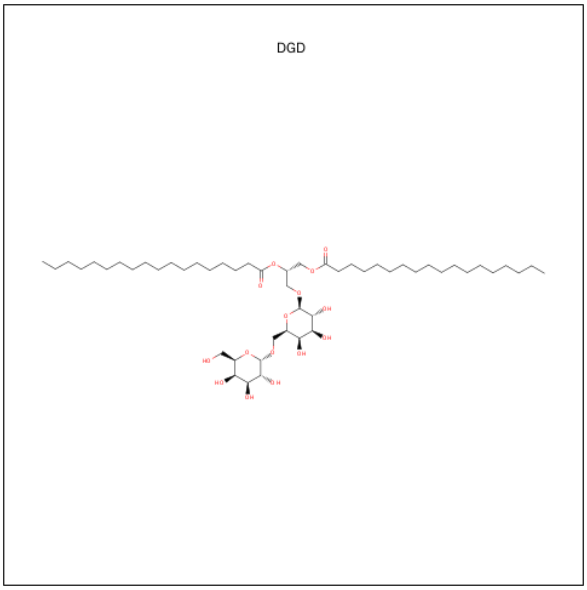
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	O	P	0	0
			49	38	10	1		
7	G	1	Total	C	O	P	0	0
			49	38	10	1		
7	H	1	Total	C	O	P	0	0
			49	38	10	1		
7	I	1	Total	C	O	P	0	0
			49	38	10	1		
7	J	1	Total	C	O	P	0	0
			49	38	10	1		

- 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		

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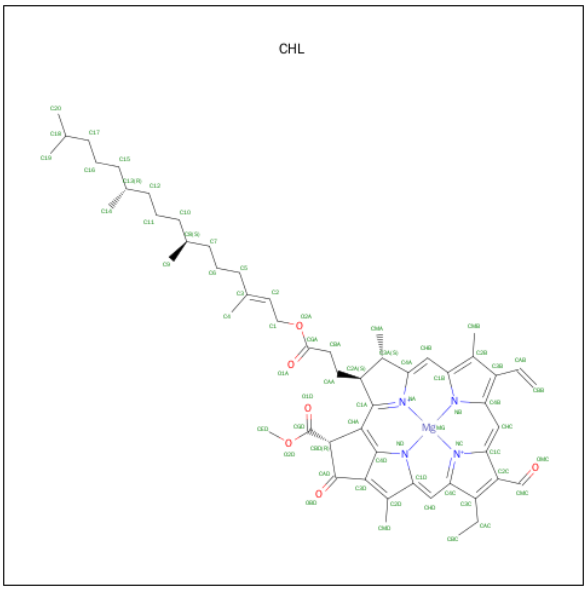
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total C O 66 51 15	0	0
8	H	1	Total C O 66 51 15	0	0
8	I	1	Total C O 66 51 15	0	0
8	G	1	Total C O 66 51 15	0	0

- 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

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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		

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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		

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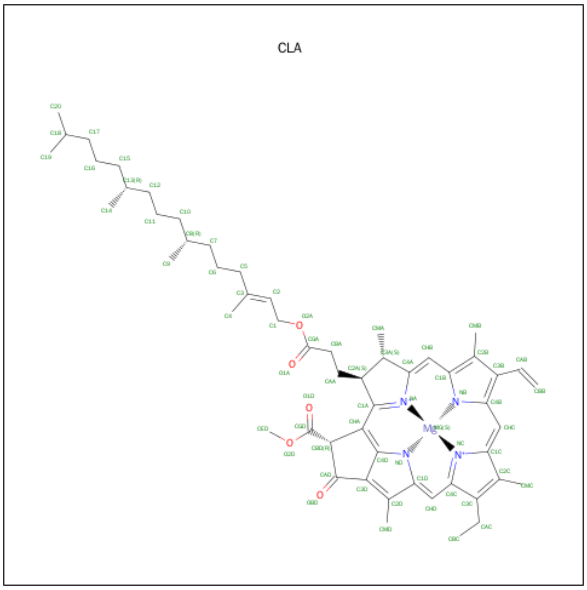
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	I	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	I	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	J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

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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		

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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		

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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		

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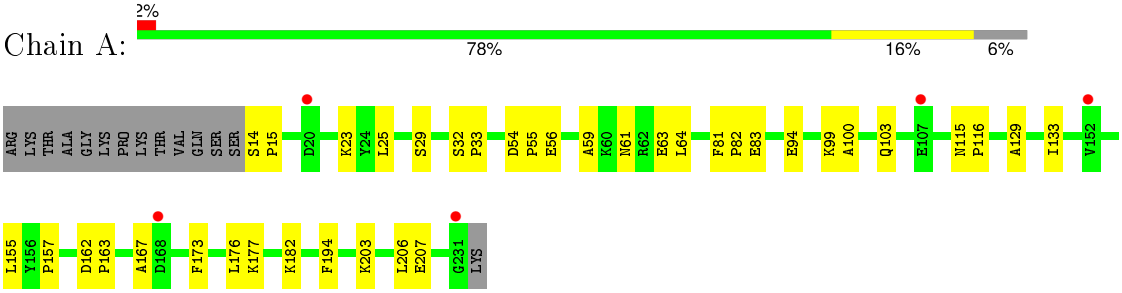
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	77	Total O 77 77	0	0
11	E	67	Total O 67 67	0	0
11	F	73	Total O 73 73	0	0
11	G	71	Total O 71 71	0	0
11	H	70	Total O 70 70	0	0
11	I	68	Total O 68 68	0	0
11	J	66	Total O 66 66	0	0

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.

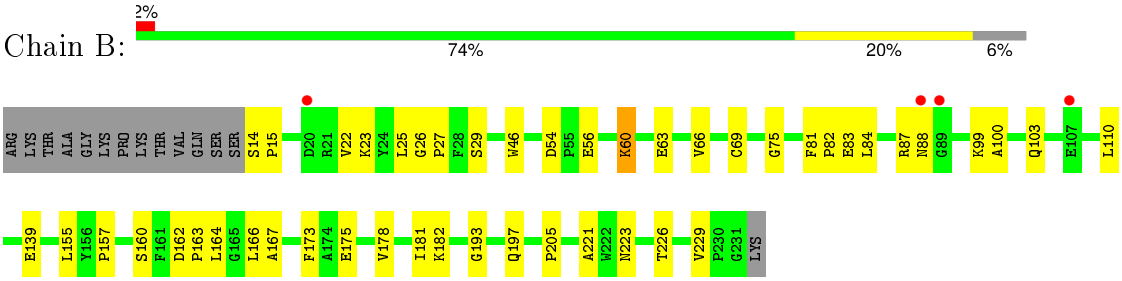
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain A:



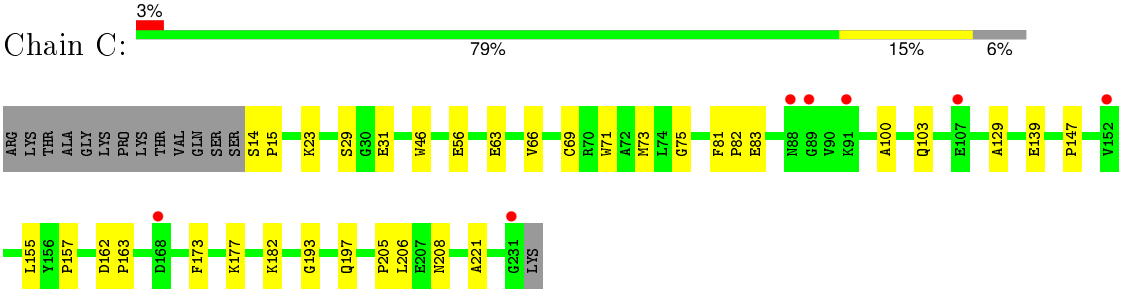
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain B:



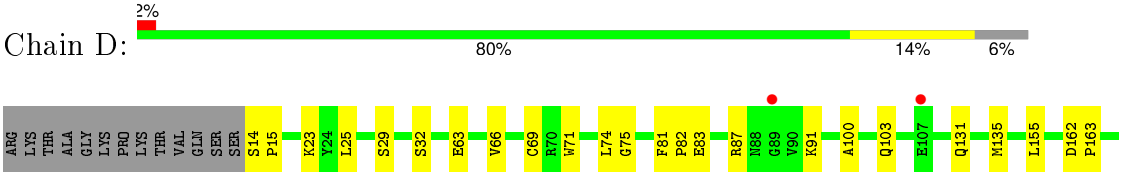
- Molecule 1: Chlorophyll A-B binding protein, chloroplast

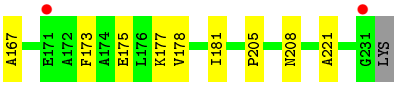
Chain C:



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

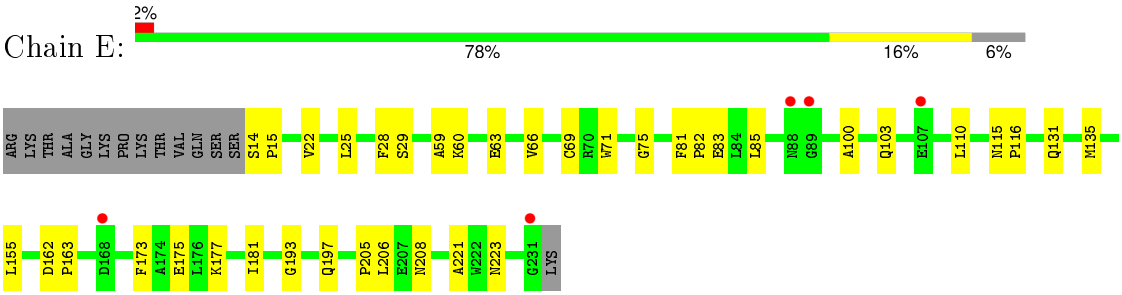
Chain D:





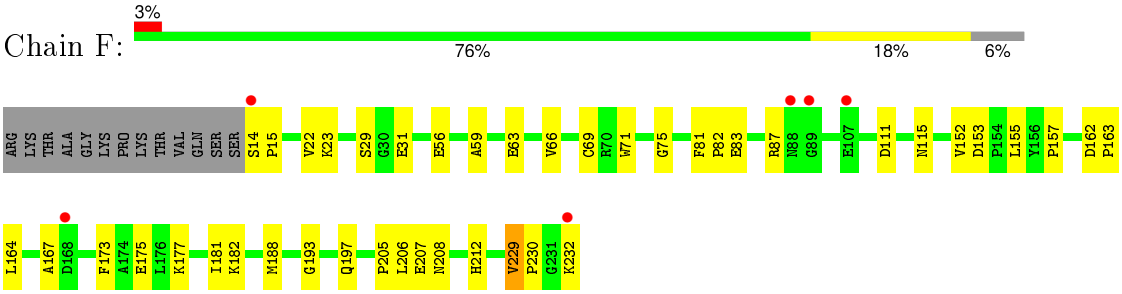
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain E:



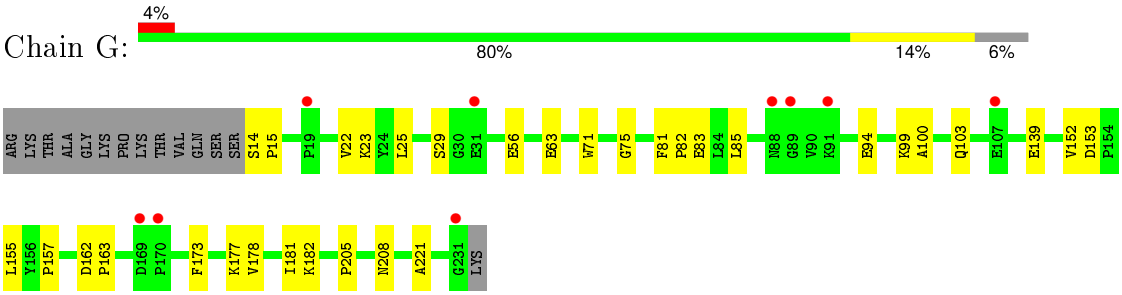
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain F:



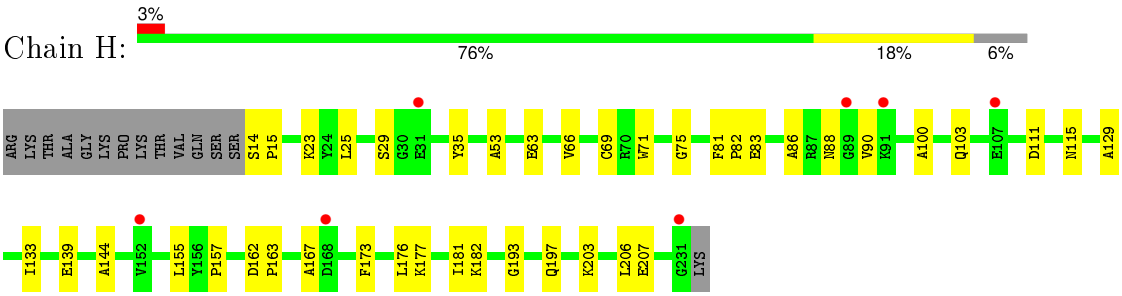
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain G:



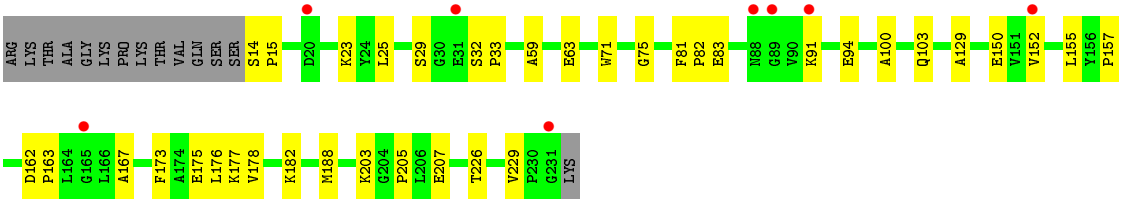
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

Chain H:

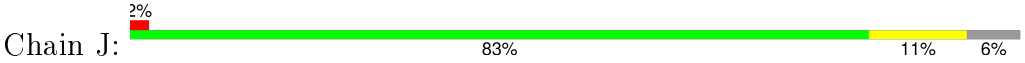


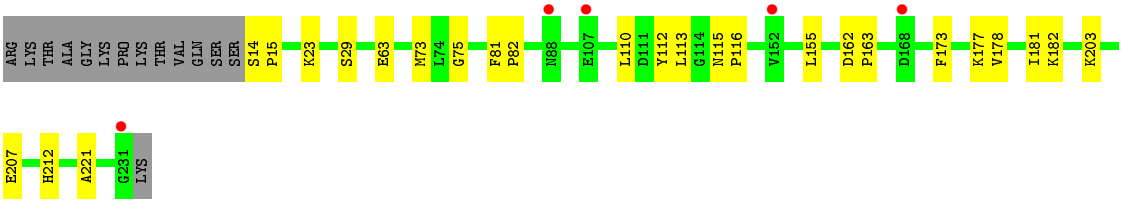
• Molecule 1: Chlorophyll A-B binding protein, chloroplast

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

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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

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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

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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.

The worst 5 of 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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	181	ILE
1	F	31	GLU
1	I	175	GLU
1	E	223	ASN
1	F	56	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	223	ASN
1	F	88	ASN
1	I	88	ASN
1	E	88	ASN
1	H	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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CHL	B	606	11	42,59,74	1.68	7 (16%)	39,96,114	2.12	12 (30%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	DGD	D	5632	-	67,67,67	0.91	1 (1%)	81,81,81	1.10	9 (11%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CLA	E	613	1	55,73,73	1.27	6 (10%)	61,113,113	1.83	13 (21%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	CLA	G	614	1	39,57,73	1.39	6 (15%)	43,93,113	2.32	13 (30%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	CHL	I	607	11	57,74,74	1.51	7 (12%)	56,114,114	1.99	16 (28%)
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

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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

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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

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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

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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

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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

The worst 5 of 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

The worst 5 of 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

5 of 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

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	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

The worst 5 of 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

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

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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
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.