



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 13, 2017 – 09:09 AM EDT

PDB ID : 5XNO
EMDB ID: : EMD-6744
Title : Structure of M-LHCII and CP24 complexes in the unstacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : unknown
Resolution : 3.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

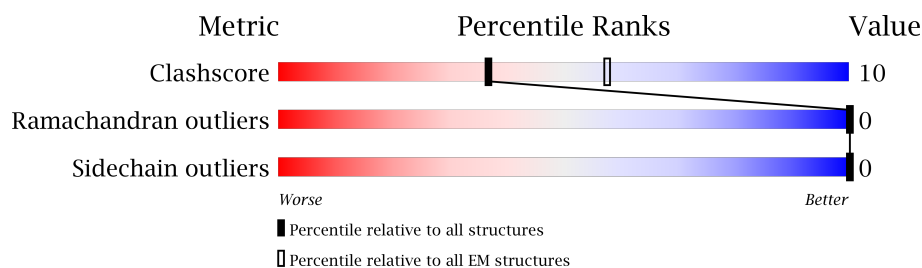
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	232	78% 16% 6%
1	2	232	77% 17% 6%
2	3	243	75% 16% 9%
3	4	210	78% 16% 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
5	CLA	1	602	X	-	-	-
5	CLA	1	603	X	-	-	-
5	CLA	1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLA	1	610	X	-	-	-
5	CLA	1	611	X	-	-	-
5	CLA	1	612	X	-	-	-
5	CLA	1	613	X	-	-	-
5	CLA	1	614	X	-	-	-
5	CLA	2	602	X	-	-	-
5	CLA	2	603	X	-	-	-
5	CLA	2	604	X	-	-	-
5	CLA	2	610	X	-	-	-
5	CLA	2	611	X	-	-	-
5	CLA	2	612	X	-	-	-
5	CLA	2	613	X	-	-	-
5	CLA	2	614	X	-	-	-
5	CLA	3	602	X	-	-	-
5	CLA	3	603	X	-	-	-
5	CLA	3	604	X	-	-	-
5	CLA	3	610	X	-	-	-
5	CLA	3	611	X	-	-	-
5	CLA	3	612	X	-	-	-
5	CLA	3	613	X	-	-	-
5	CLA	3	614	X	-	-	-
5	CLA	4	602	X	-	-	-
5	CLA	4	603	X	-	-	-
5	CLA	4	604	X	-	-	-
5	CLA	4	610	X	-	-	-
5	CLA	4	611	X	-	-	-
5	CLA	4	612	X	-	-	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 10020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		

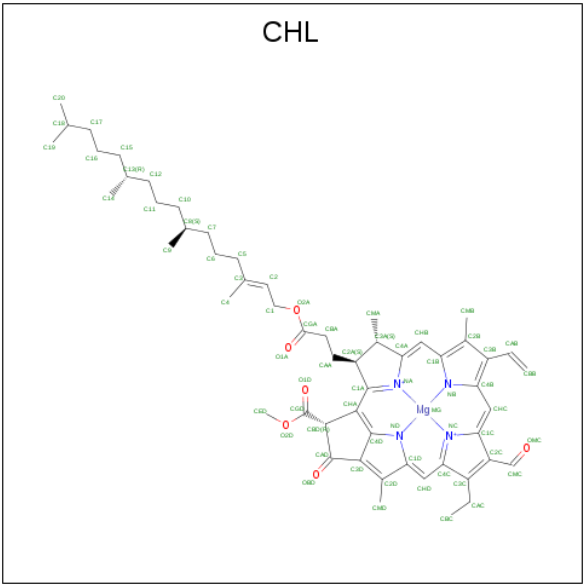
- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

- Molecule 4 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



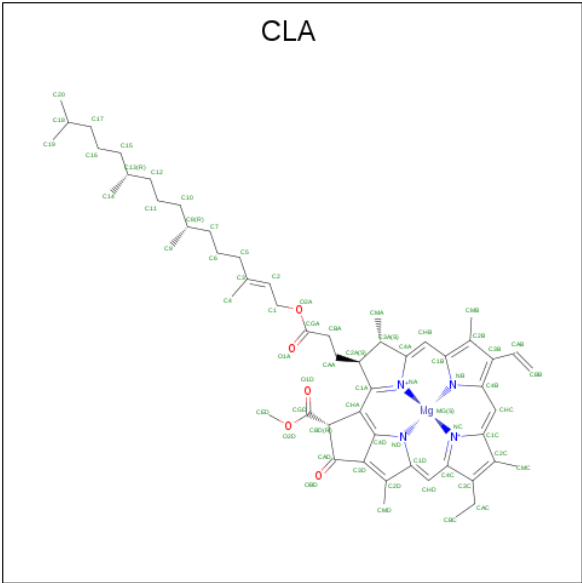
Mol	Chain	Residues	Atoms					AltConf
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	

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Mol	Chain	Residues	Atoms					AltConf
4	4	1	Total	C	Mg	N	O	0
			229	174	5	20	30	

- Molecule 5 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



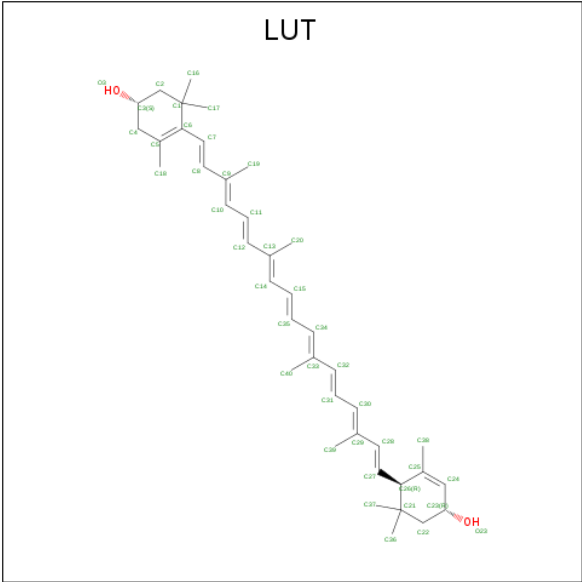
Mol	Chain	Residues	Atoms					AltConf
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	

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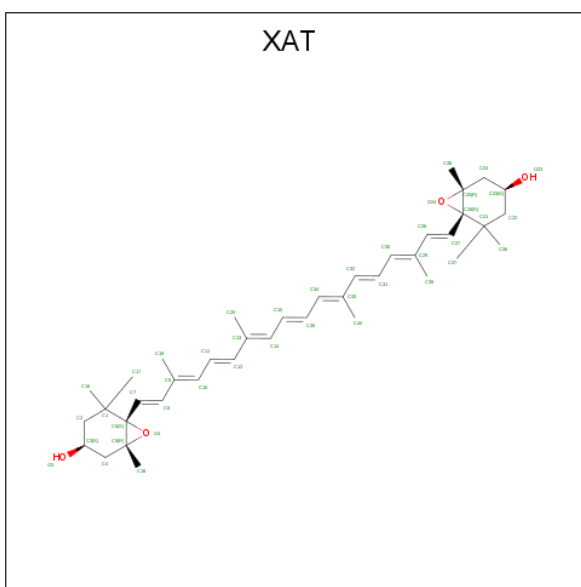
Mol	Chain	Residues	Atoms					AltConf
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	3	1	Total	C	Mg	N	O	0
			426	346	8	32	40	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
5	4	1	Total	C	Mg	N	O	0
			270	210	6	24	30	

- Molecule 6 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3, 3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



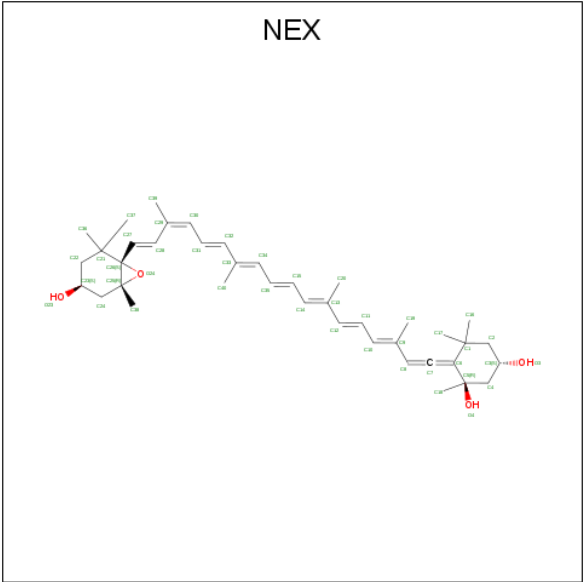
Mol	Chain	Residues	Atoms			AltConf
6	1	1	Total	C	O	0
			84	80	4	
6	1	1	Total	C	O	0
			84	80	4	
6	2	1	Total	C	O	0
			84	80	4	
6	2	1	Total	C	O	0
			84	80	4	
6	3	1	Total	C	O	0
			84	80	4	
6	3	1	Total	C	O	0
			84	80	4	
6	4	1	Total	C	O	0
			42	40	2	

- Molecule 7 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: C₄₀H₅₆O₄).



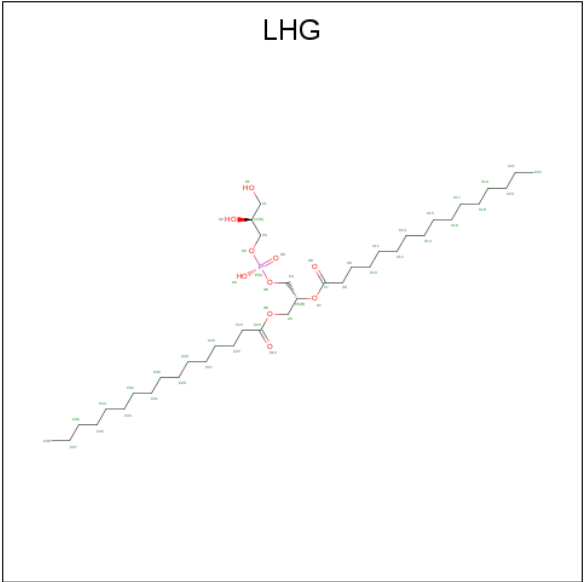
Mol	Chain	Residues	Atoms			AltConf
7	1	1	Total	C	O	0
			44	40	4	
7	2	1	Total	C	O	0
			44	40	4	
7	3	1	Total	C	O	0
			44	40	4	
7	4	1	Total	C	O	0
			44	40	4	

- Molecule 8 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



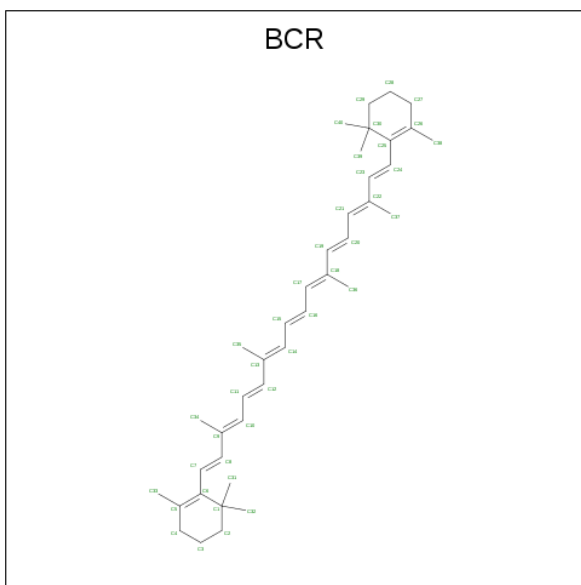
Mol	Chain	Residues	Atoms			AltConf
8	1	1	Total	C	O	0
			44	40	4	
8	2	1	Total	C	O	0
			44	40	4	
8	3	1	Total	C	O	0
			44	40	4	

- Molecule 9 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
9	1	1	Total	C	O	P	0
			41	30	10	1	
9	2	1	Total	C	O	P	0
			37	26	10	1	
9	3	1	Total	C	O	P	0
			47	36	10	1	
9	4	1	Total	C	O	P	0
			21	10	10	1	

- Molecule 10 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).

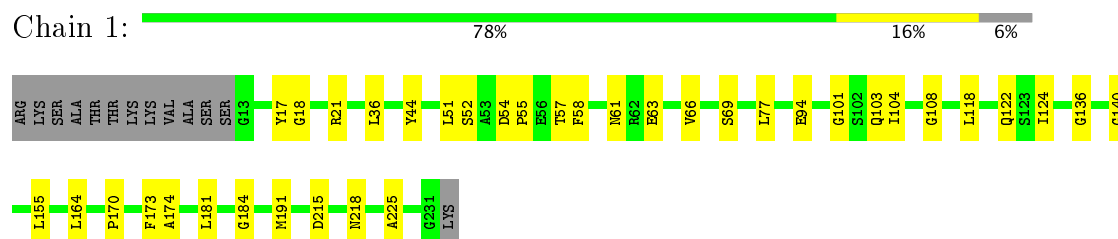


Mol	Chain	Residues	Atoms		AltConf
10	4	1	Total	C	0
			40	40	

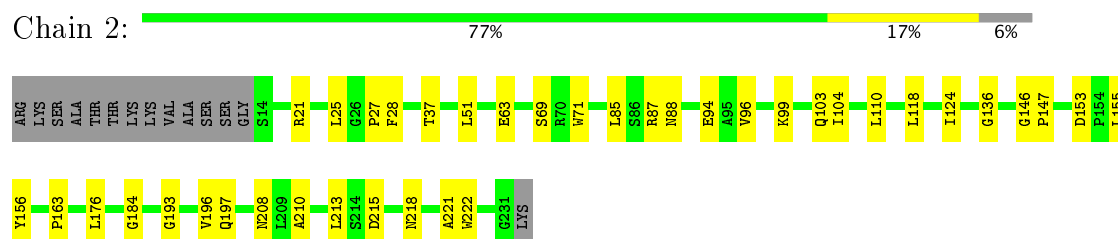
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

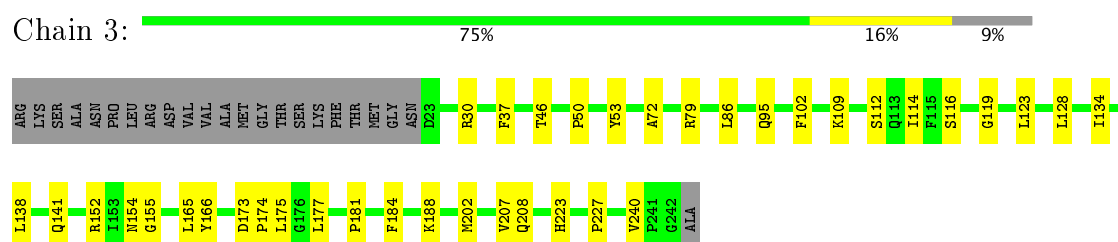
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



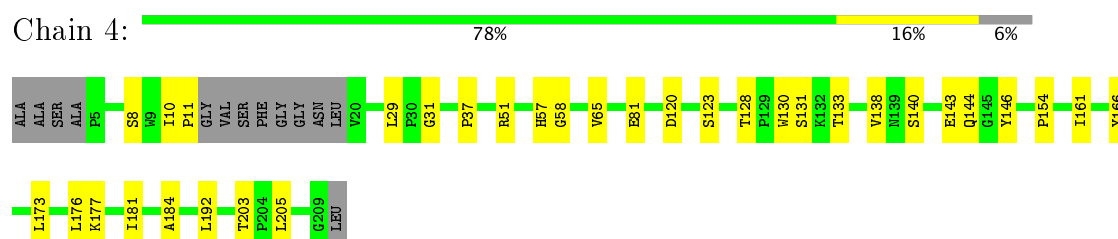
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50237	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	1	0.48	0/1720	0.55	0/2342
1	2	0.43	0/1716	0.54	0/2337
2	3	0.49	0/1759	0.59	1/2396 (0.0%)
3	4	0.42	0/1586	0.59	0/2158
All	All	0.46	0/6781	0.57	1/9233 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	123	LEU	CA-CB-CG	6.24	129.65	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1668	0	1596	26	0
1	2	1664	0	1593	29	0
2	3	1707	0	1659	31	0
3	4	1534	0	1486	23	0
4	1	309	0	244	10	0
4	2	306	0	238	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3	316	0	254	18	0
4	4	229	0	152	4	0
5	1	412	0	348	14	0
5	2	391	0	314	15	0
5	3	426	0	373	20	0
5	4	270	0	198	4	0
6	1	84	0	112	9	0
6	2	84	0	112	7	0
6	3	84	0	112	11	0
6	4	42	0	56	4	0
7	1	44	0	56	4	0
7	2	44	0	56	6	0
7	3	44	0	56	5	0
7	4	44	0	56	3	0
8	1	44	0	56	2	0
8	2	44	0	56	1	0
8	3	44	0	56	3	0
9	1	41	0	55	0	0
9	2	37	0	44	2	0
9	3	47	0	67	5	0
9	4	21	0	12	1	0
10	4	40	0	56	3	0
All	All	10020	0	9473	186	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 10.

The worst 5 of 186 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:606:CHL:HBB2	4:3:607:CHL:HBB1	1.57	0.86
5:1:602:CLA:HAB	6:1:1621:LUT:H32	1.66	0.77
5:2:610:CLA:H2	6:2:1620:LUT:H28	1.72	0.72
2:3:95:GLN:HE22	2:3:102:PHE:H	1.39	0.70
2:3:208:GLN:HE22	6:3:1620:LUT:H41	1.63	0.64

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 PDB entries followed by that with respect to all EM entries.

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	1	217/232 (94%)	211 (97%)	6 (3%)	0	100	100
1	2	216/232 (93%)	211 (98%)	5 (2%)	0	100	100
2	3	218/243 (90%)	208 (95%)	10 (5%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
All	All	844/917 (92%)	809 (96%)	35 (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 PDB entries followed by that with respect to all EM entries.

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	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
2	3	175/193 (91%)	175 (100%)	0	100	100
3	4	154/162 (95%)	154 (100%)	0	100	100
All	All	671/719 (93%)	671 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	3	95	GLN
3	4	122	GLN
2	3	219	ASN
1	2	61	ASN
3	4	72	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

72 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	LUT	1	1620	-	41,43,43	0.91	2 (4%)	50,60,60	2.03	15 (30%)
6	LUT	1	1621	-	41,43,43	1.02	3 (7%)	50,60,60	1.96	17 (34%)
7	XAT	1	1622	-	39,47,47	0.93	1 (2%)	54,74,74	2.89	21 (38%)
8	NEX	1	1623	-	38,46,46	1.11	4 (10%)	49,70,70	2.65	18 (36%)
9	LHG	1	2630	5	40,40,48	0.73	1 (2%)	41,46,54	1.36	6 (14%)
4	CHL	1	601	1	41,54,74	5.23	27 (65%)	24,90,114	3.44	14 (58%)
5	CLA	1	602	1	52,69,73	1.21	7 (13%)	60,108,113	1.39	9 (15%)
5	CLA	1	603	1	46,63,73	1.34	8 (17%)	53,101,113	1.52	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CLA	1	604	-	41,58,73	1.38	8 (19%)	47,95,113	1.53	9 (19%)
4	CHL	1	605	1	41,54,74	5.12	24 (58%)	24,90,114	3.45	15 (62%)
4	CHL	1	606	-	41,54,74	5.20	27 (65%)	24,90,114	3.37	14 (58%)
4	CHL	1	607	-	61,71,74	4.29	27 (44%)	46,110,114	2.69	16 (34%)
4	CHL	1	608	-	41,54,74	5.25	27 (65%)	24,90,114	3.41	14 (58%)
4	CHL	1	609	1	60,70,74	4.43	28 (46%)	46,109,114	2.76	17 (36%)
5	CLA	1	610	1	47,64,73	1.22	6 (12%)	54,102,113	1.47	8 (14%)
5	CLA	1	611	9	33,53,73	1.39	7 (21%)	37,89,113	1.52	7 (18%)
5	CLA	1	612	1	33,53,73	1.42	7 (21%)	37,89,113	1.67	10 (27%)
5	CLA	1	613	1	46,63,73	1.22	8 (17%)	53,101,113	1.40	7 (13%)
5	CLA	1	614	1	33,53,73	1.37	6 (18%)	37,89,113	1.50	5 (13%)
6	LUT	2	1620	-	41,43,43	0.79	0	50,60,60	1.84	16 (32%)
6	LUT	2	1621	-	41,43,43	0.85	1 (2%)	50,60,60	1.83	16 (32%)
7	XAT	2	1622	-	39,47,47	1.00	0	54,74,74	3.01	22 (40%)
8	NEX	2	1623	-	38,46,46	0.96	1 (2%)	49,70,70	2.45	13 (26%)
9	LHG	2	2630	5	36,36,48	0.72	1 (2%)	37,42,54	1.30	5 (13%)
4	CHL	2	601	1	41,54,74	5.10	26 (63%)	24,90,114	3.52	12 (50%)
5	CLA	2	602	1	52,69,73	1.16	5 (9%)	60,108,113	1.42	10 (16%)
5	CLA	2	603	1	46,63,73	1.23	7 (15%)	53,101,113	1.49	10 (18%)
5	CLA	2	604	-	33,53,73	1.35	8 (24%)	37,89,113	1.70	6 (16%)
4	CHL	2	605	1	41,54,74	4.99	24 (58%)	24,90,114	3.58	17 (70%)
4	CHL	2	606	-	41,54,74	5.16	25 (60%)	24,90,114	3.47	14 (58%)
4	CHL	2	607	-	59,69,74	4.31	26 (44%)	45,108,114	2.76	18 (40%)
4	CHL	2	608	-	41,54,74	5.09	27 (65%)	24,90,114	3.31	12 (50%)
4	CHL	2	609	1	59,69,74	4.31	27 (45%)	45,108,114	2.82	20 (44%)
5	CLA	2	610	1	41,58,73	1.33	7 (17%)	47,95,113	1.32	7 (14%)
5	CLA	2	611	9	33,53,73	1.33	6 (18%)	37,89,113	1.61	8 (21%)
5	CLA	2	612	1	33,53,73	1.41	5 (15%)	37,89,113	1.68	10 (27%)
5	CLA	2	613	1	33,53,73	1.39	7 (21%)	37,89,113	1.51	6 (16%)
5	CLA	2	614	1	33,53,73	1.35	6 (18%)	37,89,113	1.55	6 (16%)
6	LUT	3	1620	-	41,43,43	0.97	3 (7%)	50,60,60	2.02	18 (36%)
6	LUT	3	1621	-	41,43,43	0.92	1 (2%)	50,60,60	1.68	12 (24%)
7	XAT	3	1622	-	39,47,47	1.16	4 (10%)	54,74,74	3.07	27 (50%)
8	NEX	3	1623	-	38,46,46	0.93	2 (5%)	49,70,70	2.51	16 (32%)
9	LHG	3	2630	5	46,46,48	0.77	1 (2%)	47,52,54	1.33	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CHL	3	601	2	62,72,74	4.36	27 (43%)	48,111,114	2.71	19 (39%)
5	CLA	3	602	2	51,68,73	1.18	7 (13%)	59,107,113	1.41	7 (11%)
5	CLA	3	603	2	46,63,73	1.26	9 (19%)	53,101,113	1.50	11 (20%)
5	CLA	3	604	-	33,53,73	1.43	7 (21%)	37,89,113	1.46	7 (18%)
4	CHL	3	605	2	41,54,74	5.04	25 (60%)	24,90,114	3.52	16 (66%)
4	CHL	3	606	-	41,54,74	5.22	26 (63%)	24,90,114	3.68	15 (62%)
4	CHL	3	607	-	51,61,74	4.57	27 (52%)	35,98,114	2.93	16 (45%)
4	CHL	3	608	-	41,54,74	5.19	27 (65%)	24,90,114	3.40	13 (54%)
4	CHL	3	609	2	59,69,74	4.31	27 (45%)	45,108,114	2.78	19 (42%)
5	CLA	3	610	2	51,68,73	1.21	7 (13%)	59,107,113	1.32	8 (13%)
5	CLA	3	611	9	46,63,73	1.38	6 (13%)	53,101,113	1.42	11 (20%)
5	CLA	3	612	2	33,53,73	1.48	8 (24%)	37,89,113	1.77	10 (27%)
5	CLA	3	613	2	49,66,73	1.22	7 (14%)	56,104,113	1.34	7 (12%)
5	CLA	3	614	2	39,56,73	1.25	5 (12%)	45,92,113	1.40	7 (15%)
9	LHG	4	2630	5	20,20,48	0.85	0	21,26,54	1.35	1 (4%)
4	CHL	4	601	3	36,53,74	5.08	21 (58%)	19,89,114	3.73	14 (73%)
5	CLA	4	602	3	33,53,73	1.31	6 (18%)	37,89,113	1.78	7 (18%)
5	CLA	4	603	3	33,53,73	1.39	6 (18%)	37,89,113	1.58	8 (21%)
5	CLA	4	604	-	33,53,73	1.44	7 (21%)	37,89,113	1.55	6 (16%)
4	CHL	4	606	-	41,54,74	5.06	26 (63%)	24,90,114	3.37	14 (58%)
4	CHL	4	607	-	41,54,74	5.02	25 (60%)	24,90,114	3.45	15 (62%)
4	CHL	4	608	-	41,54,74	5.10	25 (60%)	24,90,114	3.50	16 (66%)
4	CHL	4	609	3	41,54,74	5.11	25 (60%)	24,90,114	3.46	15 (62%)
5	CLA	4	610	3	33,53,73	1.43	7 (21%)	37,89,113	1.52	5 (13%)
5	CLA	4	611	9	33,53,73	1.41	6 (18%)	37,89,113	1.38	6 (16%)
5	CLA	4	612	3	33,53,73	1.32	5 (15%)	37,89,113	1.70	8 (21%)
6	LUT	4	620	-	41,43,43	0.95	3 (7%)	50,60,60	2.23	15 (30%)
7	XAT	4	622	-	39,47,47	0.95	1 (2%)	54,74,74	2.70	20 (37%)
10	BCR	4	623	-	41,41,41	0.76	0	56,56,56	2.18	14 (25%)

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
6	LUT	1	1620	-	-	0/29/67/67	0/2/2/2
6	LUT	1	1621	-	-	0/29/67/67	0/2/2/2
7	XAT	1	1622	-	-	0/31/93/93	0/2/4/4
8	NEX	1	1623	-	-	0/27/83/83	0/2/3/3
9	LHG	1	2630	5	-	0/45/45/53	0/0/0/0
4	CHL	1	601	1	-	0/15/153/177	0/0/9/9
5	CLA	1	602	1	3/3/19/25	0/33/131/135	0/0/9/9
5	CLA	1	603	1	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	1	604	-	3/3/17/25	0/19/117/135	0/0/9/9
4	CHL	1	605	1	-	0/15/153/177	0/0/9/9
4	CHL	1	606	-	-	0/15/153/177	0/0/9/9
4	CHL	1	607	-	-	0/38/174/177	0/0/9/9
4	CHL	1	608	-	-	0/15/153/177	0/0/9/9
4	CHL	1	609	1	-	0/37/173/177	0/0/9/9
5	CLA	1	610	1	3/3/18/25	0/27/125/135	0/0/9/9
5	CLA	1	611	9	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	1	612	1	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	1	613	1	2/2/18/25	0/25/123/135	0/0/9/9
5	CLA	1	614	1	3/3/16/25	0/11/111/135	0/0/9/9
6	LUT	2	1620	-	-	0/29/67/67	0/2/2/2
6	LUT	2	1621	-	-	0/29/67/67	0/2/2/2
7	XAT	2	1622	-	-	0/31/93/93	0/2/4/4
8	NEX	2	1623	-	-	0/27/83/83	0/2/3/3
9	LHG	2	2630	5	-	0/41/41/53	0/0/0/0
4	CHL	2	601	1	-	0/15/153/177	0/0/9/9
5	CLA	2	602	1	3/3/19/25	0/33/131/135	0/0/9/9
5	CLA	2	603	1	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	2	604	-	2/2/16/25	0/11/111/135	0/0/9/9
4	CHL	2	605	1	-	0/15/153/177	0/0/9/9
4	CHL	2	606	-	-	0/15/153/177	0/0/9/9
4	CHL	2	607	-	-	0/35/171/177	0/0/9/9
4	CHL	2	608	-	-	0/15/153/177	0/0/9/9
4	CHL	2	609	1	-	0/35/171/177	0/0/9/9
5	CLA	2	610	1	3/3/17/25	0/19/117/135	0/0/9/9
5	CLA	2	611	9	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	2	612	1	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	2	613	1	2/2/16/25	0/11/111/135	0/0/9/9
5	CLA	2	614	1	2/2/16/25	0/11/111/135	0/0/9/9
6	LUT	3	1620	-	-	0/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
7	XAT	3	1622	-	-	0/31/93/93	0/2/4/4
8	NEX	3	1623	-	-	0/27/83/83	0/2/3/3
9	LHG	3	2630	5	-	0/51/51/53	0/0/0/0
4	CHL	3	601	2	-	0/39/175/177	0/0/9/9
5	CLA	3	602	2	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	3	603	2	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	3	604	-	3/3/16/25	0/11/111/135	0/0/9/9
4	CHL	3	605	2	-	0/15/153/177	0/0/9/9
4	CHL	3	606	-	-	0/15/153/177	0/0/9/9
4	CHL	3	607	-	-	0/26/162/177	0/0/9/9
4	CHL	3	608	-	-	0/15/153/177	0/0/9/9
4	CHL	3	609	2	-	0/35/171/177	0/0/9/9
5	CLA	3	610	2	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	3	611	9	3/3/18/25	0/25/123/135	0/0/9/9
5	CLA	3	612	2	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	3	613	2	3/3/18/25	0/29/127/135	0/0/9/9
5	CLA	3	614	2	3/3/16/25	0/17/115/135	0/0/9/9
9	LHG	4	2630	5	-	0/23/23/53	0/0/0/0
4	CHL	4	601	3	-	0/9/151/177	0/0/9/9
5	CLA	4	602	3	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	603	3	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	604	-	2/2/16/25	0/11/111/135	0/0/9/9
4	CHL	4	606	-	-	0/15/153/177	0/0/9/9
4	CHL	4	607	-	-	0/15/153/177	0/0/9/9
4	CHL	4	608	-	-	0/15/153/177	0/0/9/9
4	CHL	4	609	3	-	0/15/153/177	0/0/9/9
5	CLA	4	610	3	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	611	9	3/3/16/25	0/11/111/135	0/0/9/9
5	CLA	4	612	3	3/3/16/25	0/11/111/135	0/0/9/9
6	LUT	4	620	-	-	0/29/67/67	0/2/2/2
7	XAT	4	622	-	-	0/31/93/93	0/2/4/4
10	BCR	4	623	-	-	0/29/63/63	0/2/2/2

The worst 5 of 826 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	606	CHL	C3D-C4D	-20.50	1.31	1.54
4	3	601	CHL	C3D-C4D	-20.47	1.31	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	1	601	CHL	C3D-C4D	-20.41	1.31	1.54
4	1	608	CHL	C3D-C4D	-20.35	1.31	1.54
4	1	609	CHL	C3D-C4D	-20.26	1.31	1.54

The worst 5 of 868 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	623	BCR	C24-C23-C22	-7.63	114.74	126.21
4	3	601	CHL	C1C-C2C-C3C	-7.30	104.24	111.52
4	2	601	CHL	C1C-C2C-C3C	-7.27	104.27	111.52
4	1	601	CHL	C1C-C2C-C3C	-7.06	104.48	111.52
6	4	620	LUT	C23-C24-C25	-7.04	118.63	125.22

5 of 85 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	4	612	CLA	NC
5	4	612	CLA	ND
5	4	612	CLA	NA
5	3	614	CLA	NC
5	3	614	CLA	ND

There are no torsion outliers.

There are no ring outliers.

64 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	1620	LUT	5	0
6	1	1621	LUT	4	0
7	1	1622	XAT	4	0
8	1	1623	NEX	2	0
4	1	601	CHL	1	0
5	1	602	CLA	5	0
5	1	603	CLA	3	0
5	1	604	CLA	1	0
4	1	606	CHL	1	0
4	1	607	CHL	4	0
4	1	608	CHL	1	0
4	1	609	CHL	3	0
5	1	610	CLA	2	0
5	1	612	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	613	CLA	2	0
5	1	614	CLA	1	0
6	2	1620	LUT	4	0
6	2	1621	LUT	3	0
7	2	1622	XAT	6	0
8	2	1623	NEX	1	0
9	2	2630	LHG	2	0
4	2	601	CHL	1	0
5	2	602	CLA	3	0
5	2	603	CLA	3	0
5	2	604	CLA	1	0
4	2	605	CHL	1	0
4	2	606	CHL	3	0
4	2	607	CHL	2	0
4	2	608	CHL	2	0
4	2	609	CHL	5	0
5	2	610	CLA	3	0
5	2	612	CLA	2	0
5	2	613	CLA	3	0
5	2	614	CLA	1	0
6	3	1620	LUT	8	0
6	3	1621	LUT	3	0
7	3	1622	XAT	5	0
8	3	1623	NEX	3	0
9	3	2630	LHG	5	0
4	3	601	CHL	2	0
5	3	602	CLA	5	0
5	3	603	CLA	2	0
5	3	604	CLA	1	0
4	3	605	CHL	1	0
4	3	606	CHL	4	0
4	3	607	CHL	6	0
4	3	608	CHL	3	0
4	3	609	CHL	5	0
5	3	610	CLA	2	0
5	3	611	CLA	5	0
5	3	613	CLA	4	0
5	3	614	CLA	1	0
9	4	2630	LHG	1	0
4	4	601	CHL	1	0
5	4	603	CLA	1	0
4	4	606	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	4	607	CHL	1	0
4	4	608	CHL	1	0
5	4	610	CLA	1	0
5	4	611	CLA	1	0
5	4	612	CLA	2	0
6	4	620	LUT	4	0
7	4	622	XAT	3	0
10	4	623	BCR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.