wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BHW
Title	:	PEA LIGHT-HARVESTING COMPLEX II AT 2.5 ANGSTROM RESOLUTION
Authors	:	Standfuss, J.; Terwisscha Van Scheltinga, A.C.; Lamborghini, M.; Kuehlbrandt, W.
Deposited on	:	2005-01-19
Resolution	:	2.50 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:

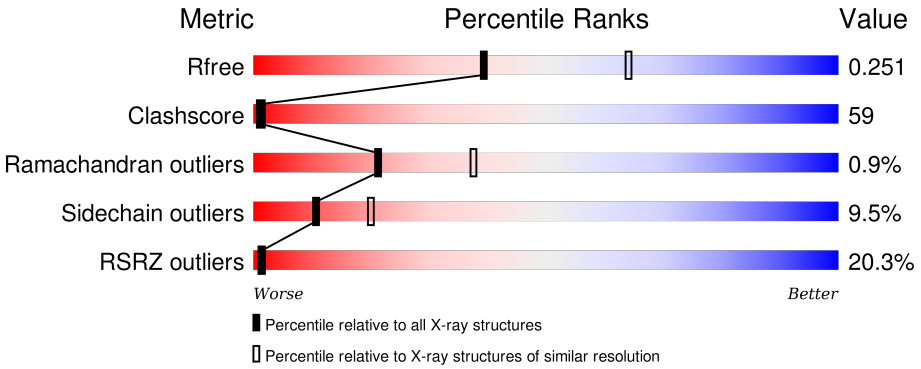
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	22% 55% 38%
1	B	232	18% 52% 40% 5%
1	C	232	19% 54% 38%

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
2	LUX	A	501	X	-	X	-
2	LUX	A	502	X	-	X	-
2	LUX	B	501	X	-	X	-
2	LUX	B	502	X	-	-	X
2	LUX	C	501	X	-	X	-
2	LUX	C	502	X	-	-	X
3	NEX	A	503	-	-	-	X
3	NEX	B	503	-	-	-	X
3	NEX	C	503	-	-	-	X
4	XAT	A	504	X	-	-	-
4	XAT	B	504	X	-	-	-
4	XAT	C	504	X	-	-	-
5	CLA	A	601	X	-	X	-
5	CLA	A	602	X	-	-	-
5	CLA	A	603	X	-	-	-
5	CLA	A	604	X	-	X	-
5	CLA	A	605	X	-	X	X
5	CLA	A	606	X	-	-	-
5	CLA	A	607	X	-	-	-
5	CLA	A	608	X	-	-	-
5	CLA	B	601	X	-	X	-
5	CLA	B	602	X	-	-	-
5	CLA	B	603	X	-	X	-
5	CLA	B	604	X	-	X	-
5	CLA	B	605	X	-	X	X
5	CLA	B	606	X	-	-	-
5	CLA	B	607	X	-	-	-
5	CLA	B	608	X	-	X	-
5	CLA	C	601	X	-	X	-
5	CLA	C	602	X	-	-	-
5	CLA	C	603	X	-	-	-
5	CLA	C	604	X	-	-	X
5	CLA	C	605	X	-	X	X
5	CLA	C	606	X	-	-	-
5	CLA	C	607	X	-	-	-
5	CLA	C	608	X	-	-	-
6	CHL	A	609	-	-	X	-
6	CHL	A	610	-	-	X	-
6	CHL	A	611	-	-	X	-
6	CHL	A	612	X	-	-	X
6	CHL	A	614	-	-	-	X
6	CHL	B	609	-	-	X	-
6	CHL	B	610	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CHL	B	611	-	-	X	-
6	CHL	B	612	X	-	X	-
6	CHL	B	614	-	-	-	X
6	CHL	C	609	-	-	X	-
6	CHL	C	610	-	-	X	-
6	CHL	C	611	-	-	X	-
6	CHL	C	612	X	-	X	-
6	CHL	C	614	-	-	-	X
8	DGD	A	802	X	-	-	X
8	DGD	B	802	X	-	-	X
8	DGD	C	802	X	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8373 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.

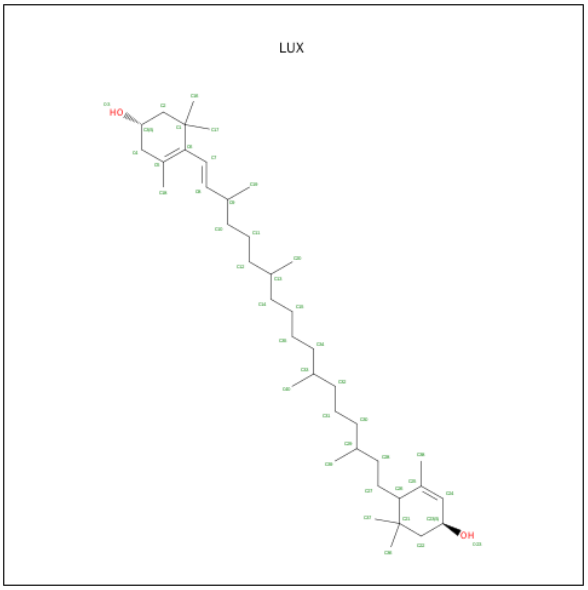
- Molecule 1 is a protein called CHLOROPHYLL A-B BINDING PROTEIN AB80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	B	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			
1	C	223	Total	C	N	O	S	0	0	0
			1683	1090	274	315	4			

There are 3 discrepancies between the modelled and reference sequences:

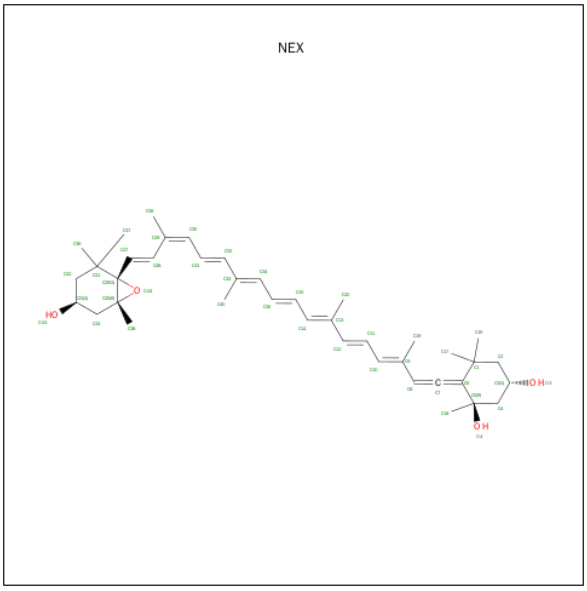
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	SER	CYS	CONFLICT	UNP P07371
B	79	SER	CYS	CONFLICT	UNP P07371
C	79	SER	CYS	CONFLICT	UNP P07371

- Molecule 2 is (3R,3'R,6'S,9R,9'R,13R,13'S)-4',5'-DIDEHYDRO-5',6',7',8',9,9',10,10',11,11',12,12',13,13',14,14',15,15'-OCTADECAHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUX) (formula: $C_{40}H_{72}O_2$).



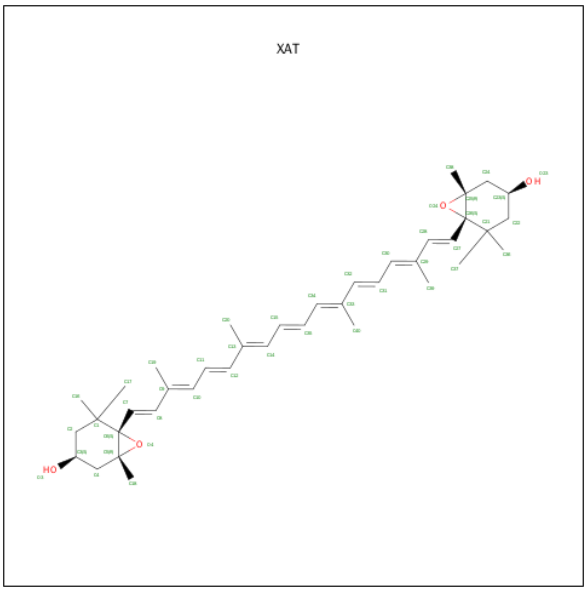
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 42 40 2	0	0
2	A	1	Total C O 42 40 2	0	0
2	B	1	Total C O 42 40 2	0	0
2	B	1	Total C O 42 40 2	0	0
2	C	1	Total C O 42 40 2	0	0
2	C	1	Total C O 42 40 2	0	0

- Molecule 3 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: $C_{40}H_{56}O_4$).



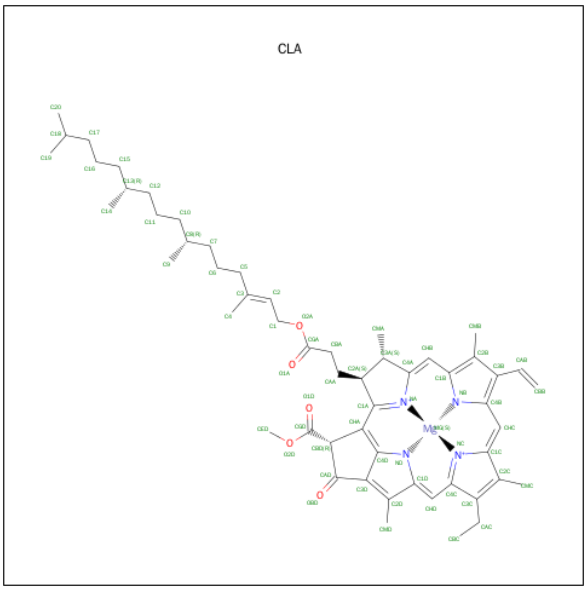
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 44 40 4	0	0
3	B	1	Total C O 44 40 4	0	0
3	C	1	Total C O 44 40 4	0	0

- Molecule 4 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
4	A	1	Total C O 44 40 4	0	0
4	B	1	Total C O 44 40 4	0	0
4	C	1	Total C O 44 40 4	0	0

- Molecule 5 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	A	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	B	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			57	47	1	4	5		

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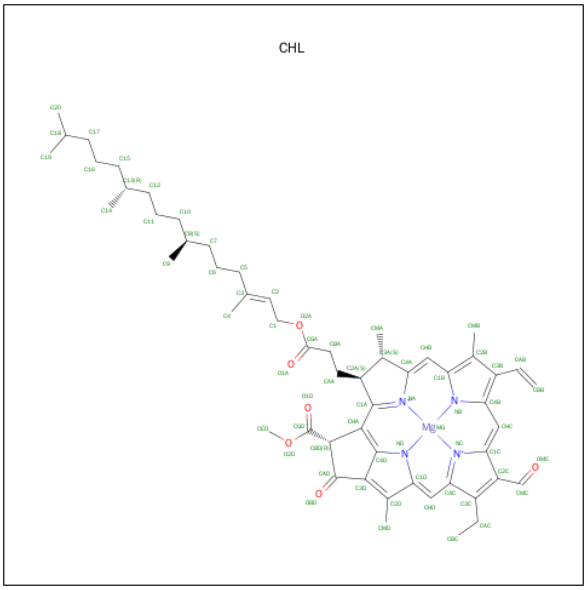
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
5	C	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		

- Molecule 6 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	A	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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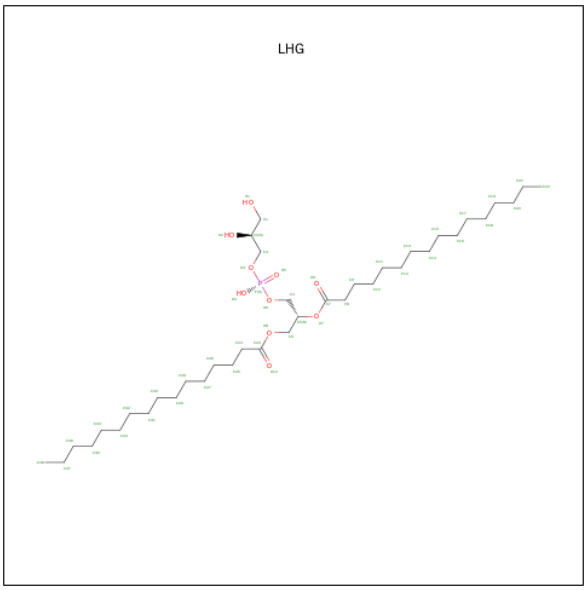
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	B	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
6	C	1	Total	C	Mg	N	O	0	0
			42	33	1	4	4		

- 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	0	0
			49	38	10	1		
7	B	1	Total	C	O	P	0	0
			49	38	10	1		

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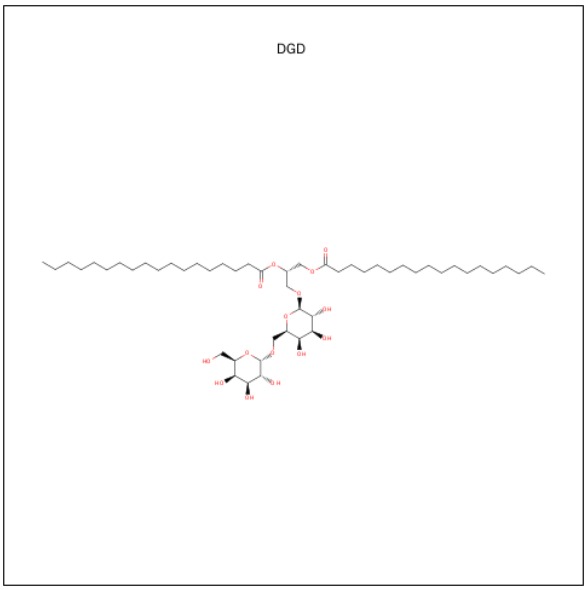
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	O	P	0	0
			49	38	10	1		

- 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
			38	25	13		
8	B	1	Total	C	O	0	0
			38	25	13		
8	C	1	Total	C	O	0	0
			38	25	13		

- Molecule 9 is water.

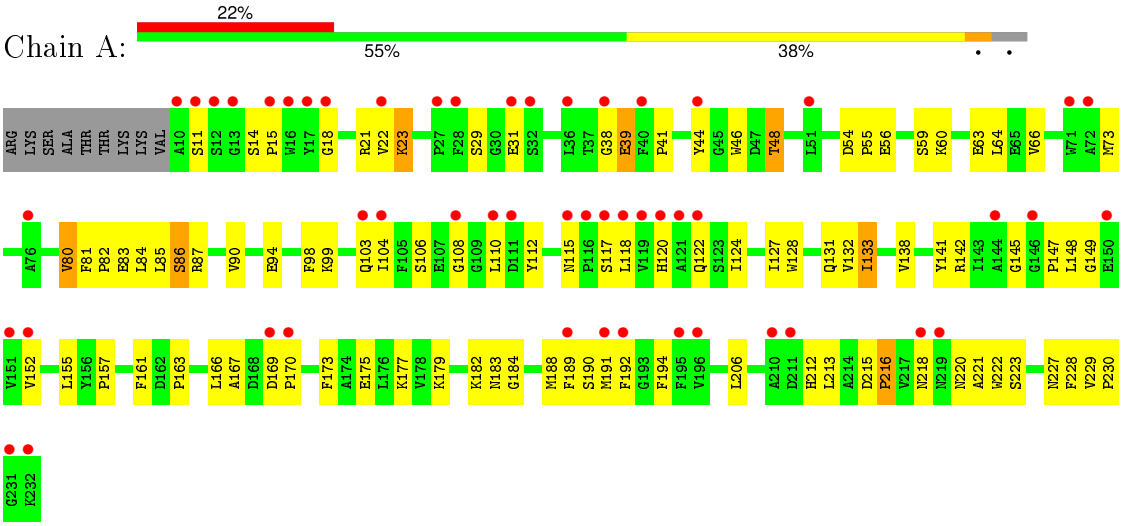
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total	O	0	0
			9	9		
9	B	7	Total	O	0	0
			7	7		
9	C	5	Total	O	0	0
			5	5		

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.

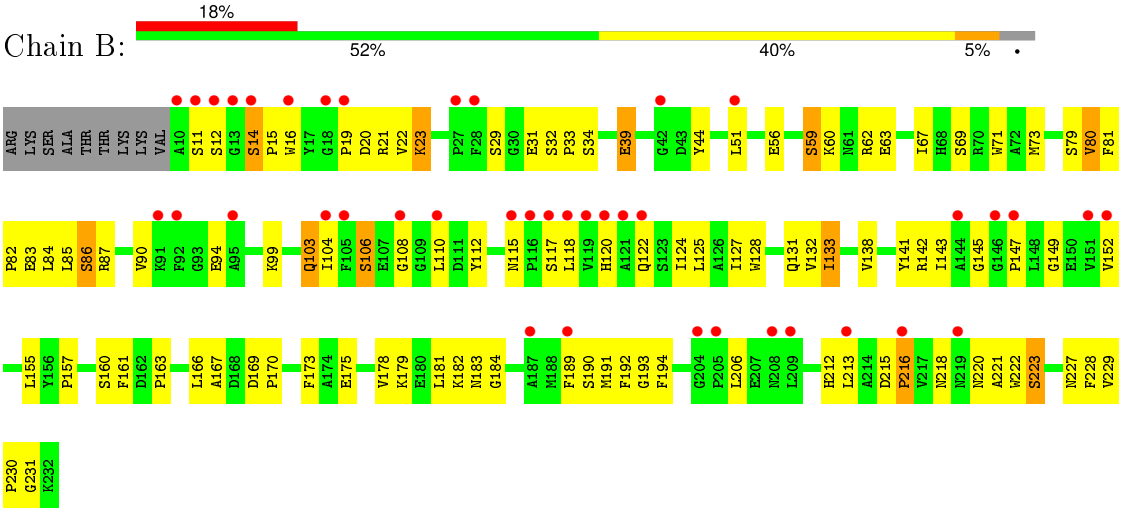
- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain A:



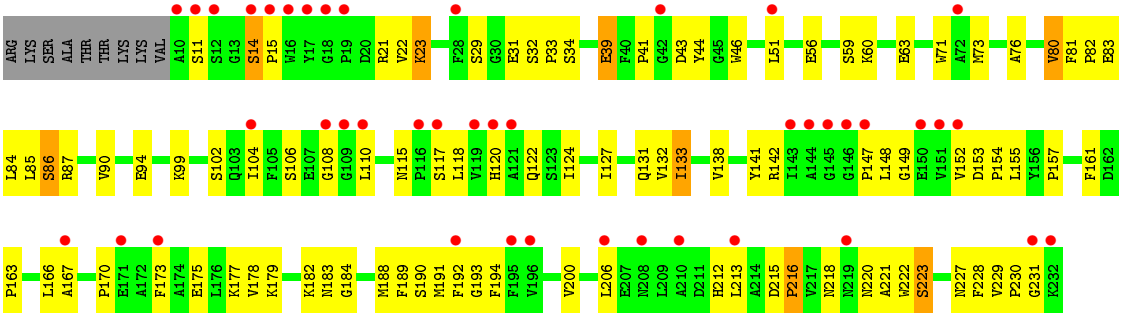
- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain B:



- Molecule 1: CHLOROPHYLL A-B BINDING PROTEIN AB80

Chain C:


ARG LYS SER ALA THR THR LYS LYS VAL A10 S11 S12 G13 S14 P15 W16 Y17 G18 P19 D20 R21 V22 K23 F28 S29 G30 E31 S32 P33 S34 E39 F40 P41 G42 D43 Y44 G45 W46 L51 E56 S59 K60 E63 W71 A72 M73 A76 W80 F81 P82 E83
L84 L85 S86 R87 V90 E94 K99 S102 Q103 I104 F105 S106 E107 G108 G109 L110 N115 P116 S117 L118 V119 H120 A121 Q122 S123 I124 I127 Q131 V132 I133 V138 Y141 R142 I143 A144 G145 G146 P147 L148 G149 E150 V151 V152 D153 P154 L155 Y156 P157 F161 D162
P163 L166 A167 P170 E171 A172 F173 A174 E175 L176 K177 V178 K179 K182 N183 G184 M188 F189 S190 M191 F192 G193 F194 F195 V196 V200 L206 E207 N208 L209 A210 D211 H212 L213 A214 D215 P216 V217 N218 N219 N220 A221 W222 S223 N227 F228 V229 P230 G231 K232

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	211.40Å 128.00Å 62.00Å 90.00° 101.80° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 85.7 (48.22-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 2.51Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.220 , 0.241 0.232 , 0.251	Depositor DCC
R_{free} test set	990 reflections (2.11%)	DCC
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 103.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 47843 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8373	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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, DGD, LUX, XAT, CHL, CLA, NEX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/1735	0.66	0/2363
1	B	0.53	0/1735	0.69	0/2363
1	C	0.52	0/1735	0.66	0/2363
All	All	0.51	0/5205	0.67	0/7089

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	1683	0	1601	127	0
1	B	1683	0	1601	138	0
1	C	1683	0	1601	135	0
2	A	84	0	134	50	0
2	B	84	0	134	49	0
2	C	84	0	134	50	0
3	A	44	0	56	4	0
3	B	44	0	56	4	0
3	C	44	0	56	4	0
4	A	44	0	56	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	56	16	0
4	C	44	0	56	16	0
5	A	490	0	508	133	0
5	B	490	0	508	141	0
5	C	490	0	508	131	0
6	A	352	0	338	114	0
6	B	352	0	338	112	0
6	C	352	0	338	114	0
7	A	49	0	74	12	0
7	B	49	0	74	13	0
7	C	49	0	74	13	0
8	A	38	0	40	4	0
8	B	38	0	40	2	0
8	C	38	0	40	4	0
9	A	9	0	0	1	0
9	B	7	0	0	1	0
9	C	5	0	0	1	0
All	All	8373	0	8421	982	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 59.

The worst 5 of 982 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)
5:A:604:CLA:HMB1	5:A:604:CLA:HBB1	1.22	1.18
5:B:601:CLA:HMB1	5:B:601:CLA:HBB1	1.21	1.18
5:B:604:CLA:HMB1	5:B:604:CLA:HBB1	1.22	1.16
6:B:613:CHL:HBB1	6:B:613:CHL:HMB1	1.27	1.16
6:C:613:CHL:HBB1	6:C:613:CHL:HMB1	1.28	1.16

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	221/232 (95%)	210 (95%)	10 (4%)	1 (0%)	34 55
1	B	221/232 (95%)	210 (95%)	9 (4%)	2 (1%)	21 37
1	C	221/232 (95%)	208 (94%)	10 (4%)	3 (1%)	14 24
All	All	663/696 (95%)	628 (95%)	29 (4%)	6 (1%)	21 37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	SER
1	C	14	SER
1	A	216	PRO
1	B	216	PRO
1	C	216	PRO

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	169/181 (93%)	154 (91%)	15 (9%)	12 23
1	B	169/181 (93%)	150 (89%)	19 (11%)	7 14
1	C	169/181 (93%)	155 (92%)	14 (8%)	14 26
All	All	507/543 (93%)	459 (90%)	48 (10%)	11 20

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	59	SER
1	B	103	GLN
1	C	133	ILE
1	B	62	ARG
1	B	80	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	GLN
1	B	197	GLN
1	C	122	GLN
1	B	122	GLN
1	B	218	ASN

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)

60 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	$\#\|Z\| > 2$
2	LUX	A	501	-	42,43,43	4.31	26 (61%)	55,60,60	3.58	30 (54%)
2	LUX	A	502	-	42,43,43	4.28	24 (57%)	55,60,60	3.57	31 (56%)
3	NEX	A	503	-	39,46,46	2.55	12 (30%)	48,70,70	2.02	11 (22%)
4	XAT	A	504	-	41,47,47	2.45	14 (34%)	48,74,74	2.75	19 (39%)
5	CLA	A	601	1	55,73,73	1.21	6 (10%)	61,113,113	1.75	14 (22%)
5	CLA	A	602	1	50,68,73	1.36	6 (12%)	55,107,113	1.49	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CLA	A	603	1	55,73,73	1.10	5 (9%)	61,113,113	1.54	11 (18%)
5	CLA	A	604	1	55,73,73	1.08	4 (7%)	61,113,113	1.56	11 (18%)
5	CLA	A	605	1	55,73,73	1.26	7 (12%)	61,113,113	1.69	10 (16%)
5	CLA	A	606	-	47,65,73	1.21	6 (12%)	50,103,113	1.64	9 (18%)
5	CLA	A	607	7	55,73,73	1.20	7 (12%)	61,113,113	1.64	10 (16%)
5	CLA	A	608	1	38,56,73	1.58	6 (15%)	42,92,113	1.90	11 (26%)
6	CHL	A	609	1	57,74,74	1.43	8 (14%)	56,114,114	1.54	9 (16%)
6	CHL	A	610	9	57,74,74	1.64	10 (17%)	56,114,114	1.51	11 (19%)
6	CHL	A	611	9	57,74,74	1.44	9 (15%)	56,114,114	1.63	11 (19%)
6	CHL	A	612	1	57,74,74	1.53	9 (15%)	56,114,114	1.58	8 (14%)
6	CHL	A	613	-	34,54,74	1.91	4 (11%)	32,90,114	1.75	9 (28%)
6	CHL	A	614	1	32,50,74	1.80	6 (18%)	31,85,114	1.98	10 (32%)
7	LHG	A	801	5	48,48,48	1.62	6 (12%)	49,54,54	1.33	4 (8%)
8	DGD	A	802	-	39,39,67	1.28	3 (7%)	51,51,81	1.99	10 (19%)
2	LUX	B	501	-	42,43,43	4.34	24 (57%)	55,60,60	3.82	31 (56%)
2	LUX	B	502	-	42,43,43	4.38	24 (57%)	55,60,60	3.59	30 (54%)
3	NEX	B	503	-	39,46,46	2.54	11 (28%)	48,70,70	2.08	10 (20%)
4	XAT	B	504	-	41,47,47	2.44	14 (34%)	48,74,74	2.73	18 (37%)
5	CLA	B	601	1	55,73,73	1.18	7 (12%)	61,113,113	1.60	11 (18%)
5	CLA	B	602	1	50,68,73	1.31	7 (14%)	55,107,113	1.55	9 (16%)
5	CLA	B	603	1	55,73,73	1.10	5 (9%)	61,113,113	1.62	11 (18%)
5	CLA	B	604	1	55,73,73	1.19	4 (7%)	61,113,113	1.57	11 (18%)
5	CLA	B	605	1	55,73,73	1.31	7 (12%)	61,113,113	1.63	11 (18%)
5	CLA	B	606	-	47,65,73	1.23	6 (12%)	50,103,113	1.63	9 (18%)
5	CLA	B	607	7	55,73,73	1.22	7 (12%)	61,113,113	1.66	11 (18%)
5	CLA	B	608	1	38,56,73	1.45	5 (13%)	42,92,113	1.78	10 (23%)
6	CHL	B	609	1	57,74,74	1.49	7 (12%)	56,114,114	1.59	9 (16%)
6	CHL	B	610	9	57,74,74	1.64	9 (15%)	56,114,114	1.54	11 (19%)
6	CHL	B	611	9	57,74,74	1.45	8 (14%)	56,114,114	1.60	12 (21%)
6	CHL	B	612	1	57,74,74	1.58	8 (14%)	56,114,114	1.57	9 (16%)
6	CHL	B	613	-	34,54,74	1.80	4 (11%)	32,90,114	1.76	8 (25%)
6	CHL	B	614	1	32,50,74	1.74	6 (18%)	31,85,114	1.98	9 (29%)
7	LHG	B	801	5	48,48,48	1.58	6 (12%)	49,54,54	1.35	5 (10%)
8	DGD	B	802	-	39,39,67	1.28	4 (10%)	51,51,81	1.96	11 (21%)
2	LUX	C	501	-	42,43,43	4.35	24 (57%)	55,60,60	3.66	30 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LUX	C	502	-	42,43,43	4.30	25 (59%)	55,60,60	3.69	32 (58%)
3	NEX	C	503	-	39,46,46	2.43	9 (23%)	48,70,70	2.14	12 (25%)
4	XAT	C	504	-	41,47,47	2.41	14 (34%)	48,74,74	2.41	15 (31%)
5	CLA	C	601	1	55,73,73	1.28	7 (12%)	61,113,113	1.71	13 (21%)
5	CLA	C	602	1	50,68,73	1.32	6 (12%)	55,107,113	1.49	10 (18%)
5	CLA	C	603	1	55,73,73	1.14	5 (9%)	61,113,113	1.59	10 (16%)
5	CLA	C	604	1	55,73,73	1.01	4 (7%)	61,113,113	1.61	10 (16%)
5	CLA	C	605	1	55,73,73	1.22	6 (10%)	61,113,113	1.61	9 (14%)
5	CLA	C	606	-	47,65,73	1.23	5 (10%)	50,103,113	1.60	10 (20%)
5	CLA	C	607	7	55,73,73	1.18	7 (12%)	61,113,113	1.64	11 (18%)
5	CLA	C	608	1	38,56,73	1.40	6 (15%)	42,92,113	1.81	13 (30%)
6	CHL	C	609	1	57,74,74	1.56	7 (12%)	56,114,114	1.55	11 (19%)
6	CHL	C	610	9	57,74,74	1.58	8 (14%)	56,114,114	1.50	11 (19%)
6	CHL	C	611	9	57,74,74	1.50	9 (15%)	56,114,114	1.61	10 (17%)
6	CHL	C	612	1	57,74,74	1.56	9 (15%)	56,114,114	1.57	10 (17%)
6	CHL	C	613	-	34,54,74	1.78	4 (11%)	32,90,114	1.79	9 (28%)
6	CHL	C	614	1	32,50,74	1.79	6 (18%)	31,85,114	1.98	9 (29%)
7	LHG	C	801	5	48,48,48	1.59	6 (12%)	49,54,54	1.31	4 (8%)
8	DGD	C	802	-	39,39,67	1.36	5 (12%)	51,51,81	2.01	10 (19%)

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
2	LUX	A	501	-	5/5/12/15	0/29/67/67	0/2/2/2
2	LUX	A	502	-	5/5/12/15	0/29/67/67	0/2/2/2
3	NEX	A	503	-	-	0/27/83/83	0/2/3/3
4	XAT	A	504	-	2/2/12/26	0/31/93/93	0/2/4/4
5	CLA	A	601	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	602	1	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	A	603	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	604	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	605	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	A	606	-	4/4/18/25	0/28/126/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CLA	A	607	7	3/3/20/25	0/37/135/135	0/0/9/9
5	CLA	A	608	1	3/3/16/25	0/17/115/135	0/0/9/9
6	CHL	A	609	1	-	0/39/137/137	0/0/9/9
6	CHL	A	610	9	-	0/39/137/137	0/0/9/9
6	CHL	A	611	9	-	0/39/137/137	0/0/9/9
6	CHL	A	612	1	1/1/20/26	0/39/137/137	0/0/9/9
6	CHL	A	613	-	-	0/13/113/137	0/0/9/9
6	CHL	A	614	1	-	0/10/108/137	0/0/9/9
7	LHG	A	801	5	-	0/53/53/53	0/0/0/0
8	DGD	A	802	-	1/1/11/13	0/24/64/95	0/2/2/2
2	LUX	B	501	-	5/5/12/15	0/29/67/67	0/2/2/2
2	LUX	B	502	-	5/5/12/15	0/29/67/67	0/2/2/2
3	NEX	B	503	-	-	0/27/83/83	0/2/3/3
4	XAT	B	504	-	2/2/12/26	0/31/93/93	0/2/4/4
5	CLA	B	601	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	602	1	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	B	603	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	604	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	605	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	B	606	-	4/4/18/25	0/28/126/135	0/0/9/9
5	CLA	B	607	7	3/3/20/25	0/37/135/135	0/0/9/9
5	CLA	B	608	1	3/3/16/25	0/17/115/135	0/0/9/9
6	CHL	B	609	1	-	0/39/137/137	0/0/9/9
6	CHL	B	610	9	-	0/39/137/137	0/0/9/9
6	CHL	B	611	9	-	0/39/137/137	0/0/9/9
6	CHL	B	612	1	1/1/20/26	0/39/137/137	0/0/9/9
6	CHL	B	613	-	-	0/13/113/137	0/0/9/9
6	CHL	B	614	1	-	0/10/108/137	0/0/9/9
7	LHG	B	801	5	-	0/53/53/53	0/0/0/0
8	DGD	B	802	-	1/1/11/13	0/24/64/95	0/2/2/2
2	LUX	C	501	-	5/5/12/15	0/29/67/67	0/2/2/2
2	LUX	C	502	-	5/5/12/15	0/29/67/67	0/2/2/2
3	NEX	C	503	-	-	0/27/83/83	0/2/3/3
4	XAT	C	504	-	2/2/12/26	0/31/93/93	0/2/4/4
5	CLA	C	601	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	C	602	1	3/3/19/25	0/31/129/135	0/0/9/9
5	CLA	C	603	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	C	604	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
5	CLA	C	605	1	4/4/20/25	0/37/135/135	0/0/9/9
5	CLA	C	606	-	4/4/18/25	0/28/126/135	0/0/9/9
5	CLA	C	607	7	3/3/20/25	0/37/135/135	0/0/9/9
5	CLA	C	608	1	3/3/16/25	0/17/115/135	0/0/9/9
6	CHL	C	609	1	-	0/39/137/137	0/0/9/9
6	CHL	C	610	9	-	0/39/137/137	0/0/9/9
6	CHL	C	611	9	-	0/39/137/137	0/0/9/9
6	CHL	C	612	1	1/1/20/26	0/39/137/137	0/0/9/9
6	CHL	C	613	-	-	0/13/113/137	0/0/9/9
6	CHL	C	614	1	-	0/10/108/137	0/0/9/9
7	LHG	C	801	5	-	0/53/53/53	0/0/0/0
8	DGD	C	802	-	1/1/11/13	0/24/64/95	0/2/2/2

The worst 5 of 523 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	LUX	C26-C25	-10.98	1.34	1.52
2	B	502	LUX	C26-C25	-10.63	1.34	1.52
2	C	502	LUX	C26-C25	-10.59	1.34	1.52
2	A	501	LUX	C26-C25	-10.33	1.35	1.52
2	A	502	LUX	C26-C25	-9.95	1.35	1.52

The worst 5 of 743 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	LUX	C23-C24-C25	-16.95	109.38	125.22
2	A	501	LUX	C23-C24-C25	-15.25	110.96	125.22
2	C	501	LUX	C23-C24-C25	-14.86	111.33	125.22
2	A	502	LUX	C23-C24-C25	-12.43	113.60	125.22
2	C	502	LUX	C23-C24-C25	-11.87	114.12	125.22

5 of 129 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	C	802	DGD	C5E
6	C	612	CHL	C8
2	A	502	LUX	C13
2	A	502	LUX	C33
2	A	502	LUX	C29

There are no torsion outliers.

There are no ring outliers.

60 monomers are involved in 801 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	LUX	29	0
2	A	502	LUX	21	0
3	A	503	NEX	4	0
4	A	504	XAT	18	0
5	A	601	CLA	21	0
5	A	602	CLA	13	0
5	A	603	CLA	18	0
5	A	604	CLA	22	0
5	A	605	CLA	21	0
5	A	606	CLA	18	0
5	A	607	CLA	17	0
5	A	608	CLA	16	0
6	A	609	CHL	31	0
6	A	610	CHL	31	0
6	A	611	CHL	22	0
6	A	612	CHL	18	0
6	A	613	CHL	6	0
6	A	614	CHL	15	0
7	A	801	LHG	12	0
8	A	802	DGD	4	0
2	B	501	LUX	31	0
2	B	502	LUX	18	0
3	B	503	NEX	4	0
4	B	504	XAT	16	0
5	B	601	CLA	23	0
5	B	602	CLA	11	0
5	B	603	CLA	24	0
5	B	604	CLA	24	0
5	B	605	CLA	23	0
5	B	606	CLA	17	0
5	B	607	CLA	17	0
5	B	608	CLA	21	0
6	B	609	CHL	27	0
6	B	610	CHL	28	0
6	B	611	CHL	22	0
6	B	612	CHL	22	0
6	B	613	CHL	9	0
6	B	614	CHL	16	0
7	B	801	LHG	13	0
8	B	802	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	LUX	31	0
2	C	502	LUX	19	0
3	C	503	NEX	4	0
4	C	504	XAT	16	0
5	C	601	CLA	23	0
5	C	602	CLA	11	0
5	C	603	CLA	17	0
5	C	604	CLA	20	0
5	C	605	CLA	21	0
5	C	606	CLA	17	0
5	C	607	CLA	19	0
5	C	608	CLA	16	0
6	C	609	CHL	30	0
6	C	610	CHL	31	0
6	C	611	CHL	23	0
6	C	612	CHL	21	0
6	C	613	CHL	5	0
6	C	614	CHL	14	0
7	C	801	LHG	13	0
8	C	802	DGD	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	223/232 (96%)	1.25	52 (23%)	1	1	72, 91, 109, 128	0
1	B	223/232 (96%)	1.10	41 (18%)	2	2	70, 89, 107, 126	0
1	C	223/232 (96%)	1.14	43 (19%)	2	1	73, 91, 109, 129	0
All	All	669/696 (96%)	1.16	136 (20%)	1	1	70, 90, 109, 129	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	SER	10.0
1	B	12	SER	9.6
1	B	10	ALA	8.2
1	C	10	ALA	7.6
1	A	10	ALA	7.0

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

There are no carbohydrates in this entry.

6.4 Ligands

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
5	CLA	B	605	65/65	0.93	0.45	6.92	75,84,105,108	0
8	DGD	A	802	38/66	0.49	0.46	5.42	106,119,140,140	0
5	CLA	A	605	65/65	0.91	0.49	5.41	77,86,107,110	0
8	DGD	B	802	38/66	0.41	0.50	3.93	104,118,139,140	0
5	CLA	C	605	65/65	0.92	0.41	3.57	77,86,108,110	0
2	LUX	C	502	42/42	0.88	0.35	3.07	58,79,115,128	0
3	NEX	C	503	44/44	0.65	0.40	3.02	67,98,128,133	0
2	LUX	B	502	42/42	0.84	0.35	2.91	53,76,113,126	0
6	CHL	A	612	66/66	0.83	0.36	2.82	76,85,102,104	0
3	NEX	B	503	44/44	0.81	0.35	2.78	64,96,126,131	0
3	NEX	A	503	44/44	0.80	0.30	2.52	66,97,128,132	0
5	CLA	C	604	65/65	0.85	0.30	2.08	60,72,97,102	0
6	CHL	A	610	66/66	0.92	0.29	1.72	65,80,108,110	0
2	LUX	A	502	42/42	0.89	0.32	1.72	57,78,115,128	0
5	CLA	B	604	65/65	0.87	0.30	1.62	56,69,95,100	0
6	CHL	B	612	66/66	0.91	0.27	1.59	74,83,100,102	0
6	CHL	C	614	42/66	0.83	0.41	1.55	99,107,113,137	0
8	DGD	C	802	38/66	0.58	0.43	1.48	106,119,141,141	0
4	XAT	B	504	44/44	0.88	0.21	1.42	63,89,115,147	0
2	LUX	A	501	42/42	0.92	0.27	1.32	61,87,120,136	0
7	LHG	B	801	49/49	0.85	0.28	1.29	72,88,109,115	0
4	XAT	C	504	44/44	0.87	0.20	1.26	65,91,117,149	0
6	CHL	C	612	66/66	0.83	0.31	1.22	77,85,102,104	0
5	CLA	B	601	65/65	0.86	0.23	1.18	68,77,111,113	0
6	CHL	B	614	42/66	0.86	0.42	1.08	97,105,111,134	0
5	CLA	B	607	65/65	0.84	0.24	1.05	75,88,101,104	0
5	CLA	A	602	60/65	0.91	0.24	1.03	79,87,115,116	0
6	CHL	C	610	66/66	0.90	0.24	1.01	67,81,108,110	0
6	CHL	A	614	42/66	0.88	0.43	0.89	99,106,113,136	0
6	CHL	C	609	66/66	0.87	0.24	0.87	77,85,98,101	0
2	LUX	B	501	42/42	0.90	0.26	0.78	59,86,118,134	0
5	CLA	A	601	65/65	0.88	0.23	0.76	69,79,112,115	0
6	CHL	B	610	66/66	0.92	0.23	0.73	65,79,106,108	0
6	CHL	B	611	66/66	0.91	0.26	0.63	68,82,115,121	0
6	CHL	C	611	66/66	0.89	0.28	0.60	69,85,118,124	0
2	LUX	C	501	42/42	0.88	0.26	0.56	62,88,120,136	0
4	XAT	A	504	44/44	0.91	0.18	0.55	65,91,117,148	0
5	CLA	C	606	57/65	0.91	0.25	0.50	80,91,107,111	0
5	CLA	C	601	65/65	0.88	0.24	0.49	70,79,113,115	0
5	CLA	C	602	60/65	0.91	0.21	0.40	80,87,116,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CLA	A	604	65/65	0.85	0.27	0.37	59,71,96,101	0
5	CLA	B	606	57/65	0.89	0.28	0.37	78,89,105,109	0
6	CHL	A	611	66/66	0.89	0.24	0.30	70,85,117,123	0
6	CHL	B	609	66/66	0.88	0.22	0.26	75,83,95,99	0
6	CHL	A	609	66/66	0.87	0.22	0.04	75,85,97,100	0
5	CLA	C	607	65/65	0.83	0.22	0.00	77,91,104,106	0
5	CLA	A	606	57/65	0.90	0.26	-0.04	79,90,107,110	0
5	CLA	B	602	60/65	0.92	0.19	-0.06	77,85,114,114	0
7	LHG	C	801	49/49	0.90	0.24	-0.07	74,90,111,117	0
5	CLA	C	608	48/65	0.90	0.21	-0.08	90,99,117,119	0
5	CLA	A	603	65/65	0.91	0.21	-0.11	75,85,102,105	0
5	CLA	A	607	65/65	0.83	0.23	-0.20	77,90,103,106	0
5	CLA	C	603	65/65	0.92	0.22	-0.20	75,85,102,105	0
5	CLA	B	608	48/65	0.89	0.22	-0.21	88,97,115,117	0
6	CHL	B	613	46/66	0.91	0.20	-0.25	71,80,106,119	0
5	CLA	A	608	48/65	0.90	0.16	-0.33	90,99,116,118	0
6	CHL	A	613	46/66	0.92	0.20	-0.47	73,81,107,120	0
7	LHG	A	801	49/49	0.89	0.25	-0.59	74,90,110,116	0
6	CHL	C	613	46/66	0.91	0.17	-0.60	73,82,107,121	0
5	CLA	B	603	65/65	0.90	0.20	-0.64	74,83,100,103	0

6.5 Other polymers (i)

There are no such residues in this entry.