



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 08:24 am GMT

PDB ID : 2FKW
Title : Structure of LH2 from Rps. acidophila crystallized in lipidic mesophases
Authors : Papiz, M.Z.; Cherezov, V.; Clogston, J.; Caffrey, M.
Deposited on : 2006-01-05
Resolution : 2.45 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

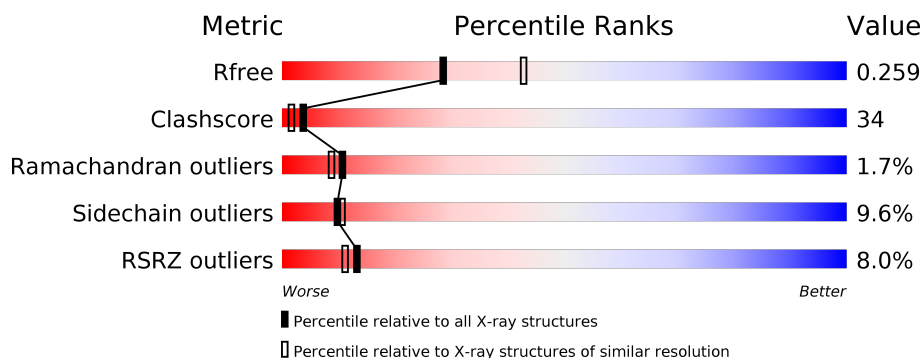
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	53	<div> <div>11%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>9%</div> </div> </div>
1	C	53	<div> <div>13%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>6%</div> <div>.</div> </div> </div>
1	E	53	<div> <div>13%</div> <div> <div></div> <div>66%</div> <div>23%</div> <div>9%</div> <div>.</div> </div> </div>
1	G	53	<div> <div>11%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>8%</div> </div> </div>
1	I	53	<div> <div>11%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>.</div> <div>.</div> </div> </div>
1	K	53	<div> <div>11%</div> <div> <div></div> <div>68%</div> <div>28%</div> <div>.</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	M	53	
1	O	53	
1	R	53	
2	B	41	
2	D	41	
2	F	41	
2	H	41	
2	J	41	
2	L	41	
2	N	41	
2	P	41	
2	S	41	

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
3	RG1	D	1402	X	-	-	-
3	RG1	F	1403	X	-	-	-
3	RG1	H	1404	X	-	-	-
3	RG1	J	1405	X	-	-	-
3	RG1	L	1406	X	-	-	-
3	RG1	N	1407	X	-	-	-
3	RG1	P	1408	X	-	-	-
3	RG1	R	1401	X	-	-	-
3	RG1	S	1409	X	-	-	-
4	BCL	A	1501	X	-	-	-
4	BCL	A	1701	X	-	-	-
4	BCL	B	1601	X	-	-	-
4	BCL	C	1502	X	-	-	-
4	BCL	C	1702	X	-	-	-
4	BCL	G	1704	X	-	X	-
4	BCL	H	1604	X	-	-	-
4	BCL	I	1705	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BCL	J	1605	X	-	-	-
4	BCL	K	1506	X	-	-	-
4	BCL	K	1706	X	-	-	-
4	BCL	L	1606	X	-	X	-
4	BCL	M	1707	X	-	X	-
4	BCL	N	1607	X	-	-	-
4	BCL	O	1508	X	-	-	-
4	BCL	O	1708	X	-	-	-
4	BCL	P	1608	X	-	-	-
4	BCL	R	1509	X	-	-	-
4	BCL	R	1709	X	-	X	X
4	BCL	S	1609	X	-	-	-
5	LDA	A	1816	-	-	-	X
5	LDA	A	1817	-	-	-	X
5	LDA	B	1801	-	-	-	X
5	LDA	C	1815	-	-	-	X
5	LDA	C	1821	-	-	-	X
5	LDA	D	1802	-	-	-	X
5	LDA	E	1822	-	-	-	X
5	LDA	E	1823	-	-	-	X
5	LDA	F	1803	-	-	-	X
5	LDA	G	1814	-	-	-	X
5	LDA	G	1824	-	-	X	X
5	LDA	H	1804	-	-	-	X
5	LDA	I	1812	-	-	-	X
5	LDA	I	1825	-	-	-	X
5	LDA	K	1810	-	-	-	X
5	LDA	K	1826	-	-	-	X
5	LDA	L	1806	-	-	-	X
5	LDA	M	1811	-	-	-	X
5	LDA	M	1827	-	-	-	X
5	LDA	N	1807	-	-	-	X
5	LDA	O	1820	-	-	-	X
5	LDA	P	1808	-	-	-	X
5	LDA	R	1809	-	-	-	X
5	LDA	R	1818	-	-	X	X
5	LDA	R	1819	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9829 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 Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	C	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	E	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	G	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	I	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	K	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	M	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	O	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			
1	R	53	Total	C	N	O	S	0	0	0
			403	269	67	66	1			

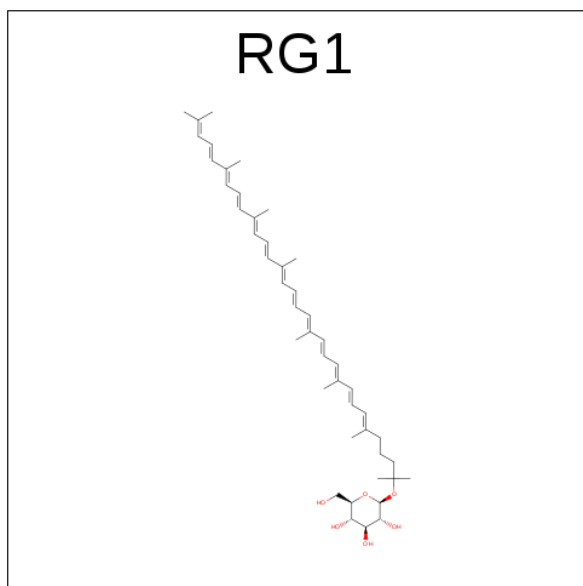
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
C	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
E	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
G	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
I	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
K	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
M	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
O	1	CXM	MET	MODIFIED RESIDUE	UNP P26789
R	1	CXM	MET	MODIFIED RESIDUE	UNP P26789

- Molecule 2 is a protein called Light-harvesting protein B-800/850, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	D	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	F	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	H	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	J	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	L	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	N	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	P	41	Total	C	N	O	0	0	0
			323	213	53	57			
2	S	41	Total	C	N	O	0	0	0
			323	213	53	57			

- Molecule 3 is SUGAR (RHODOPIN B-D-GLUCOSIDE) (three-letter code: RG1) (formula: $C_{46}H_{66}O_6$).



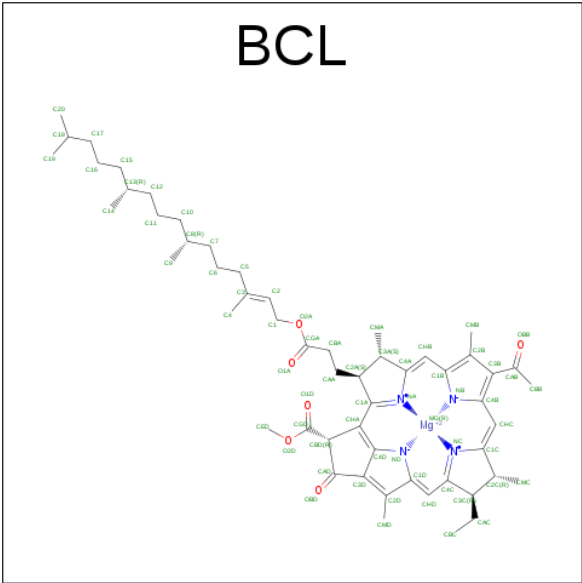
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	R	1	Total	C	O	0	0
			52	46	6		
3	D	1	Total	C	O	0	0
			52	46	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			52	46	6		
3	H	1	Total	C	O	0	0
			52	46	6		
3	J	1	Total	C	O	0	0
			52	46	6		
3	L	1	Total	C	O	0	0
			52	46	6		
3	N	1	Total	C	O	0	0
			52	46	6		
3	P	1	Total	C	O	0	0
			52	46	6		
3	S	1	Total	C	O	0	0
			52	46	6		

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

Continued on next page...

Continued from previous page...

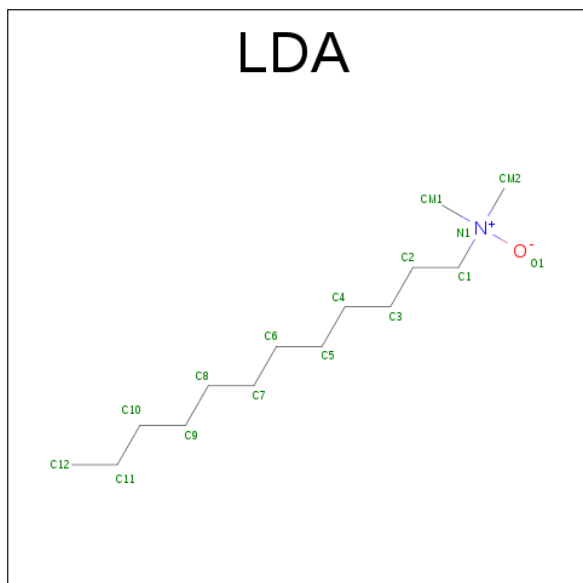
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	C	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	F	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	E	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	H	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	G	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	J	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	I	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	K	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	N	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	P	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	O	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			16	14	1	1		
5	D	1	Total	C	N	O	0	0
			16	14	1	1		
5	F	1	Total	C	N	O	0	0
			16	14	1	1		
5	H	1	Total	C	N	O	0	0
			16	14	1	1		
5	J	1	Total	C	N	O	0	0
			16	14	1	1		
5	L	1	Total	C	N	O	0	0
			16	14	1	1		
5	N	1	Total	C	N	O	0	0
			16	14	1	1		
5	P	1	Total	C	N	O	0	0
			16	14	1	1		
5	R	1	Total	C	N	O	0	0
			16	14	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	K	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	I	1	Total	C	N	O	0	0
			16	14	1	1		
5	I	1	Total	C	N	O	0	0
			16	14	1	1		
5	G	1	Total	C	N	O	0	0
			16	14	1	1		
5	C	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	A	1	Total	C	N	O	0	0
			16	14	1	1		
5	R	1	Total	C	N	O	0	0
			16	14	1	1		
5	R	1	Total	C	N	O	0	0
			16	14	1	1		
5	O	1	Total	C	N	O	0	0
			16	14	1	1		
5	C	1	Total	C	N	O	0	0
			16	14	1	1		
5	E	1	Total	C	N	O	0	0
			16	14	1	1		
5	E	1	Total	C	N	O	0	0
			16	14	1	1		
5	G	1	Total	C	N	O	0	0
			16	14	1	1		
5	I	1	Total	C	N	O	0	0
			16	14	1	1		
5	K	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	33	Total	O	0	0
			33	33		

Continued on next page...

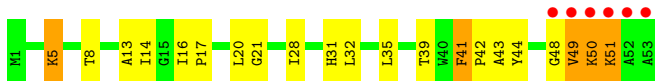
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	26	Total 26	O 26	0	0
6	C	24	Total 24	O 24	0	0
6	D	27	Total 27	O 27	0	0
6	E	40	Total 40	O 40	0	0
6	F	28	Total 28	O 28	0	0
6	G	41	Total 41	O 41	0	0
6	H	37	Total 37	O 37	2	0
6	I	38	Total 38	O 38	0	0
6	J	39	Total 39	O 39	1	0
6	K	47	Total 47	O 47	0	0
6	L	29	Total 29	O 29	0	0
6	M	36	Total 36	O 36	0	0
6	N	30	Total 30	O 30	0	0
6	O	33	Total 33	O 33	1	0
6	P	32	Total 32	O 32	0	0
6	R	39	Total 39	O 39	0	0
6	S	34	Total 34	O 34	0	0

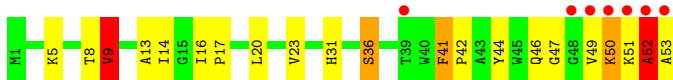
3 Residue-property plots [i](#)

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

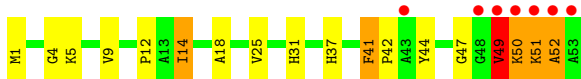
- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



- Molecule 1: Light-harvesting protein B-800/850, alpha chain



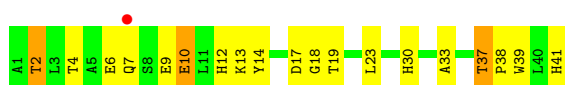
- Molecule 2: Light-harvesting protein B-800/850, beta chain



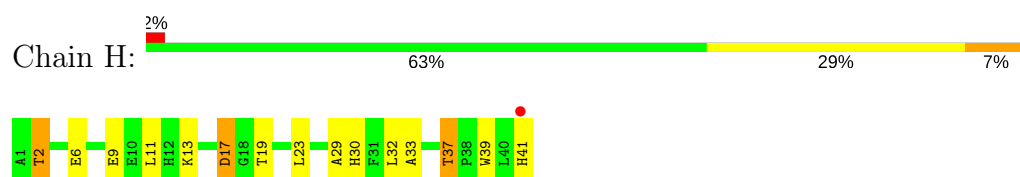
- Molecule 2: Light-harvesting protein B-800/850, beta chain



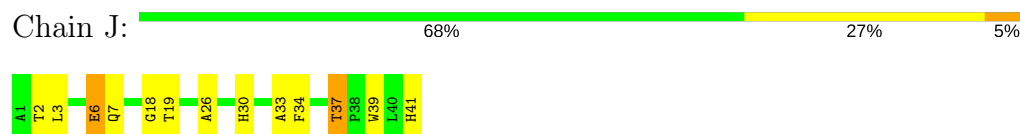
- Molecule 2: Light-harvesting protein B-800/850, beta chain



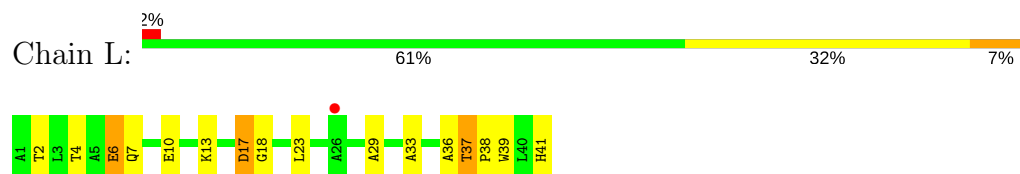
- Molecule 2: Light-harvesting protein B-800/850, beta chain



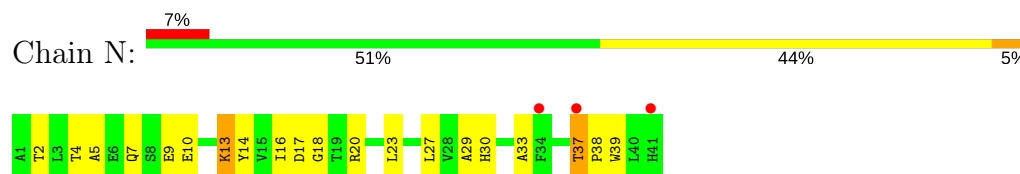
- Molecule 2: Light-harvesting protein B-800/850, beta chain



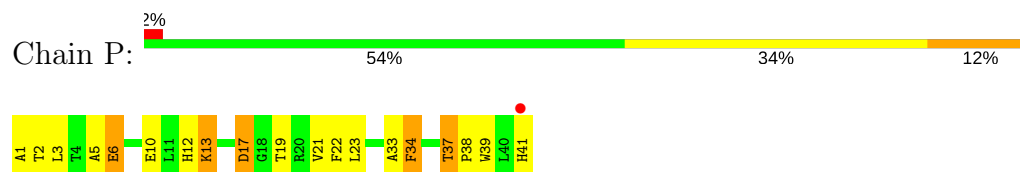
- Molecule 2: Light-harvesting protein B-800/850, beta chain



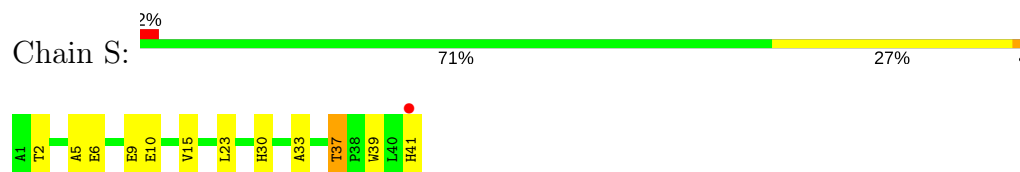
- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain



- Molecule 2: Light-harvesting protein B-800/850, beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.44Å 126.38Å 129.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 38.85 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (10.00-2.45) 99.7 (38.85-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.254 0.204 , 0.259	Depositor DCC
R_{free} test set	2526 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9829	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, RG1, LDA, CXM

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	1.27	1/404 (0.2%)	0.51	0/556
1	C	1.51	4/404 (1.0%)	0.51	0/556
1	E	1.35	1/404 (0.2%)	0.53	0/556
1	G	1.34	2/404 (0.5%)	0.50	0/556
1	I	1.38	1/404 (0.2%)	0.53	0/556
1	K	1.47	2/404 (0.5%)	0.55	0/556
1	M	1.35	1/404 (0.2%)	0.57	0/556
1	O	1.36	2/404 (0.5%)	0.51	0/556
1	R	1.35	3/404 (0.7%)	0.53	0/556
2	B	1.40	1/332 (0.3%)	0.49	0/453
2	D	1.25	1/332 (0.3%)	0.45	0/453
2	F	1.48	2/332 (0.6%)	0.42	0/453
2	H	1.40	2/332 (0.6%)	0.45	0/453
2	J	1.29	2/332 (0.6%)	0.44	0/453
2	L	1.62	5/332 (1.5%)	0.47	0/453
2	N	1.38	2/332 (0.6%)	0.44	0/453
2	P	1.60	3/332 (0.9%)	0.49	0/453
2	S	1.21	1/332 (0.3%)	0.45	0/453
All	All	1.39	36/6624 (0.5%)	0.50	0/9081

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	2	1
1	E	1	0
1	G	1	0
1	I	2	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	1	1
1	M	3	1
1	O	0	1
1	R	2	0
All	All	12	7

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	6	GLU	CG-CD	11.70	1.69	1.51
2	L	10	GLU	CG-CD	11.28	1.68	1.51
2	F	10	GLU	CG-CD	9.26	1.65	1.51
2	L	17	ASP	CB-CG	7.49	1.67	1.51
1	A	49	VAL	CA-CB	7.42	1.70	1.54

There are no bond angle outliers.

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	52	ALA	CA
1	C	53	ALA	CA
1	E	51	LYS	CA
1	G	50	LYS	CA
1	I	49	VAL	CA

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	50	LYS	Peptide
1	A	51	LYS	Peptide
1	C	52	ALA	Peptide
1	I	51	LYS	Peptide
1	K	50	LYS	Peptide

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	403	0	422	25	0
1	C	403	0	422	27	0
1	E	403	0	422	27	0
1	G	403	0	422	21	0
1	I	403	0	422	21	0
1	K	403	0	422	27	0
1	M	403	0	422	32	0
1	O	403	0	422	17	0
1	R	403	0	422	22	0
2	B	323	0	321	25	0
2	D	323	0	321	22	0
2	F	323	0	321	24	0
2	H	323	0	321	19	0
2	J	323	0	321	23	0
2	L	323	0	321	22	0
2	N	323	0	321	29	0
2	P	323	0	321	30	0
2	S	323	0	321	11	0
3	D	52	0	66	5	0
3	F	52	0	66	5	0
3	H	52	0	66	5	0
3	J	52	0	66	1	0
3	L	52	0	66	4	0
3	N	52	0	66	4	0
3	P	52	0	66	4	0
3	R	52	0	66	4	0
3	S	52	0	66	5	0
4	A	132	0	146	25	0
4	B	66	0	74	11	0
4	C	132	0	148	15	0
4	D	66	0	74	8	0
4	E	132	0	147	12	0
4	F	66	0	74	12	0
4	G	132	0	147	27	0
4	H	66	0	73	12	0
4	I	132	0	148	33	0
4	J	66	0	73	17	0
4	K	132	0	146	14	0
4	L	66	0	74	25	0
4	M	132	0	147	28	0
4	N	66	0	74	16	0
4	O	132	0	147	21	0
4	P	66	0	73	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	132	0	147	28	0
4	S	66	0	74	13	0
5	A	32	0	62	11	0
5	B	16	0	31	2	0
5	C	32	0	62	6	0
5	D	16	0	31	3	0
5	E	32	0	62	14	0
5	F	16	0	31	7	0
5	G	32	0	62	17	0
5	H	16	0	31	3	0
5	I	48	0	93	15	0
5	J	16	0	31	1	0
5	K	32	0	62	12	0
5	L	16	0	31	5	0
5	M	32	0	62	6	0
5	N	16	0	31	2	0
5	O	16	0	31	7	0
5	P	16	0	31	3	0
5	R	48	0	93	12	0
6	A	33	0	0	9	0
6	B	26	0	0	6	0
6	C	24	0	0	3	0
6	D	27	0	0	8	0
6	E	40	0	0	20	0
6	F	28	0	0	7	0
6	G	41	0	0	22	0
6	H	37	0	0	5	0
6	I	38	0	0	11	0
6	J	39	0	0	14	0
6	K	47	0	0	28	0
6	L	29	0	0	2	0
6	M	36	0	0	10	0
6	N	30	0	0	8	0
6	O	33	0	0	11	0
6	P	32	0	0	8	0
6	R	39	0	0	24	0
6	S	34	0	0	4	0
All	All	9829	0	10104	659	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 34.

The worst 5 of 659 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:M:1:CXM:CE	1:M:1:CXM:SD	2.21	1.28
1:G:48:GLY:HA2	6:G:1839:HOH:O	1.32	1.24
5:I:1825:LDA:HM22	6:I:1845:HOH:O	1.06	1.24
5:H:1804:LDA:H92	6:H:1825:HOH:O	1.38	1.22
1:E:49:VAL:HG11	6:E:1850:HOH:O	1.45	1.15

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
1	C	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	2	0
1	E	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	2	0
1	G	51/53 (96%)	51 (100%)	0	0	100	100
1	I	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
1	K	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	9	6
1	M	51/53 (96%)	47 (92%)	1 (2%)	3 (6%)	2	0
1	O	51/53 (96%)	47 (92%)	3 (6%)	1 (2%)	9	6
1	R	51/53 (96%)	46 (90%)	2 (4%)	3 (6%)	2	0
2	B	39/41 (95%)	39 (100%)	0	0	100	100
2	D	39/41 (95%)	39 (100%)	0	0	100	100
2	F	39/41 (95%)	39 (100%)	0	0	100	100
2	H	39/41 (95%)	39 (100%)	0	0	100	100
2	J	39/41 (95%)	39 (100%)	0	0	100	100
2	L	39/41 (95%)	39 (100%)	0	0	100	100
2	N	39/41 (95%)	39 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
2	S	39/41 (95%)	39 (100%)	0	0	100	100
All	All	810/846 (96%)	775 (96%)	21 (3%)	14 (2%)	11	9

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	LYS
1	E	51	LYS
1	E	52	ALA
1	K	50	LYS
1	M	50	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	40/40 (100%)	37 (92%)	3 (8%)	16	20
1	C	40/40 (100%)	37 (92%)	3 (8%)	16	20
1	E	40/40 (100%)	34 (85%)	6 (15%)	3	2
1	G	40/40 (100%)	36 (90%)	4 (10%)	9	9
1	I	40/40 (100%)	35 (88%)	5 (12%)	5	4
1	K	40/40 (100%)	39 (98%)	1 (2%)	53	67
1	M	40/40 (100%)	38 (95%)	2 (5%)	28	38
1	O	40/40 (100%)	38 (95%)	2 (5%)	28	38
1	R	40/40 (100%)	36 (90%)	4 (10%)	9	9
2	B	33/33 (100%)	30 (91%)	3 (9%)	11	12
2	D	33/33 (100%)	30 (91%)	3 (9%)	11	12
2	F	33/33 (100%)	29 (88%)	4 (12%)	6	5
2	H	33/33 (100%)	29 (88%)	4 (12%)	6	5
2	J	33/33 (100%)	31 (94%)	2 (6%)	22	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	N	33/33 (100%)	30 (91%)	3 (9%)	11	12
2	P	33/33 (100%)	28 (85%)	5 (15%)	3	2
2	S	33/33 (100%)	29 (88%)	4 (12%)	6	5
All	All	657/657 (100%)	594 (90%)	63 (10%)	10	10

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	17	ASP
2	J	2	THR
1	R	50	LYS
2	H	37	THR
1	I	36	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	37	HIS
1	K	37	HIS
2	N	7	GLN
2	H	7	GLN
2	L	7	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CXM	A	1	1,4	7,10,11	1.52	1 (14%)	5,11,13	1.27	1 (20%)
1	CXM	C	1	1,4	7,10,11	1.67	1 (14%)	5,11,13	1.10	0
1	CXM	E	1	1,4	7,10,11	1.56	2 (28%)	5,11,13	1.46	2 (40%)
1	CXM	G	1	1,4	7,10,11	1.49	1 (14%)	5,11,13	1.38	1 (20%)
1	CXM	I	1	1,4	7,10,11	1.27	1 (14%)	5,11,13	1.02	0
1	CXM	K	1	1,4	7,10,11	1.46	2 (28%)	5,11,13	1.56	1 (20%)
1	CXM	M	1	1,4	7,10,11	2.79	1 (14%)	5,11,13	1.17	0
1	CXM	O	1	1,4	7,10,11	1.22	1 (14%)	5,11,13	1.05	0
1	CXM	R	1	1,4	7,10,11	1.23	0	5,11,13	1.11	0

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
1	CXM	A	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	C	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	E	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	G	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	I	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	K	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	M	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	O	1	1,4	-	0/6/10/12	0/0/0/0
1	CXM	R	1	1,4	-	0/6/10/12	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	1	CXM	CB-CA	-2.62	1.48	1.53
1	K	1	CXM	CB-CA	-2.24	1.49	1.53
1	I	1	CXM	CA-N	2.16	1.49	1.46
1	K	1	CXM	CA-N	2.21	1.49	1.46
1	E	1	CXM	CE-SD	2.35	1.93	1.78

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	1	CXM	CB-CA-C	-2.59	107.38	111.65
1	G	1	CXM	O-C-CA	-2.53	119.26	125.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1	CXM	O-C-CA	-2.36	119.65	125.15
1	A	1	CXM	O-C-CA	-2.31	119.76	125.15
1	E	1	CXM	CB-CA-C	-2.02	108.31	111.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	1	CXM	2	0
1	K	1	CXM	2	0
1	M	1	CXM	4	0
1	O	1	CXM	1	0
1	R	1	CXM	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

63 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
4	BCL	A	1501	1	55,74,74	2.74	15 (27%)	65,115,115	1.98	21 (32%)
4	BCL	A	1701	1	55,74,74	2.95	19 (34%)	65,115,115	2.06	20 (30%)
5	LDA	A	1816	-	13,15,15	2.29	1 (7%)	14,17,17	0.51	0
5	LDA	A	1817	-	13,15,15	2.31	1 (7%)	14,17,17	0.50	0
4	BCL	B	1601	2	55,74,74	2.32	13 (23%)	65,115,115	1.99	18 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LDA	B	1801	-	13,15,15	2.35	1 (7%)	14,17,17	0.69	1 (7%)
4	BCL	C	1502	1	55,74,74	2.69	13 (23%)	65,115,115	1.99	19 (29%)
4	BCL	C	1702	1	55,74,74	2.79	12 (21%)	65,115,115	1.94	17 (26%)
5	LDA	C	1815	-	13,15,15	2.37	1 (7%)	14,17,17	0.48	0
5	LDA	C	1821	-	13,15,15	2.18	1 (7%)	14,17,17	0.50	0
3	RG1	D	1402	-	52,52,52	1.31	7 (13%)	63,67,67	1.60	15 (23%)
4	BCL	D	1602	2	55,74,74	2.67	15 (27%)	65,115,115	1.96	18 (27%)
5	LDA	D	1802	-	13,15,15	2.43	2 (15%)	14,17,17	0.67	0
4	BCL	E	1503	1	55,74,74	2.30	10 (18%)	65,115,115	1.94	18 (27%)
4	BCL	E	1703	1	55,74,74	2.28	8 (14%)	65,115,115	1.84	19 (29%)
5	LDA	E	1822	-	13,15,15	2.17	1 (7%)	14,17,17	0.59	0
5	LDA	E	1823	-	13,15,15	2.12	1 (7%)	14,17,17	0.49	0
3	RG1	F	1403	-	52,52,52	1.33	5 (9%)	63,67,67	1.62	16 (25%)
4	BCL	F	1603	2	55,74,74	2.44	13 (23%)	65,115,115	1.91	18 (27%)
5	LDA	F	1803	-	13,15,15	2.50	1 (7%)	14,17,17	0.77	1 (7%)
4	BCL	G	1504	1	55,74,74	2.65	10 (18%)	65,115,115	1.90	22 (33%)
4	BCL	G	1704	1	55,74,74	2.53	13 (23%)	65,115,115	2.01	20 (30%)
5	LDA	G	1814	-	13,15,15	2.32	1 (7%)	14,17,17	0.61	0
5	LDA	G	1824	-	13,15,15	2.36	1 (7%)	14,17,17	0.39	0
3	RG1	H	1404	-	52,52,52	1.38	4 (7%)	63,67,67	1.65	13 (20%)
4	BCL	H	1604	2	55,74,74	2.65	17 (30%)	65,115,115	2.19	27 (41%)
5	LDA	H	1804	-	13,15,15	2.29	2 (15%)	14,17,17	0.57	0
4	BCL	I	1505	1	55,74,74	2.45	14 (25%)	65,115,115	1.85	17 (26%)
4	BCL	I	1705	1	55,74,74	2.32	15 (27%)	65,115,115	1.93	13 (20%)
5	LDA	I	1812	-	13,15,15	2.69	1 (7%)	14,17,17	0.53	0
5	LDA	I	1813	-	13,15,15	2.32	1 (7%)	14,17,17	0.52	0
5	LDA	I	1825	-	13,15,15	2.33	1 (7%)	14,17,17	0.55	0
3	RG1	J	1405	-	52,52,52	1.28	7 (13%)	63,67,67	1.60	14 (22%)
4	BCL	J	1605	2	55,74,74	2.62	17 (30%)	65,115,115	1.88	18 (27%)
5	LDA	J	1805	-	13,15,15	2.09	1 (7%)	14,17,17	0.31	0
4	BCL	K	1506	1	55,74,74	2.87	15 (27%)	65,115,115	2.15	23 (35%)
4	BCL	K	1706	1	55,74,74	2.46	12 (21%)	65,115,115	1.94	16 (24%)
5	LDA	K	1810	-	13,15,15	2.43	1 (7%)	14,17,17	0.59	0
5	LDA	K	1826	-	13,15,15	2.18	1 (7%)	14,17,17	0.62	0
3	RG1	L	1406	-	52,52,52	1.37	6 (11%)	63,67,67	1.49	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BCL	L	1606	2	55,74,74	2.87	17 (30%)	65,115,115	2.23	22 (33%)
5	LDA	L	1806	-	13,15,15	2.35	1 (7%)	14,17,17	0.76	0
4	BCL	M	1507	1	55,74,74	2.54	12 (21%)	65,115,115	1.94	19 (29%)
4	BCL	M	1707	1	55,74,74	2.72	12 (21%)	65,115,115	1.81	14 (21%)
5	LDA	M	1811	-	13,15,15	2.17	1 (7%)	14,17,17	0.60	0
5	LDA	M	1827	-	13,15,15	2.27	1 (7%)	14,17,17	0.56	0
3	RG1	N	1407	-	52,52,52	1.20	4 (7%)	63,67,67	1.55	13 (20%)
4	BCL	N	1607	2	55,74,74	2.44	12 (21%)	65,115,115	2.03	18 (27%)
5	LDA	N	1807	-	13,15,15	2.11	1 (7%)	14,17,17	0.62	0
4	BCL	O	1508	1	55,74,74	2.39	11 (20%)	65,115,115	1.99	22 (33%)
4	BCL	O	1708	1	55,74,74	2.76	13 (23%)	65,115,115	1.94	16 (24%)
5	LDA	O	1820	-	13,15,15	2.41	1 (7%)	14,17,17	0.45	0
3	RG1	P	1408	-	52,52,52	1.37	9 (17%)	63,67,67	1.61	12 (19%)
4	BCL	P	1608	2	55,74,74	2.82	16 (29%)	65,115,115	1.93	18 (27%)
5	LDA	P	1808	-	13,15,15	2.19	1 (7%)	14,17,17	0.73	0
3	RG1	R	1401	-	52,52,52	1.25	6 (11%)	63,67,67	1.61	12 (19%)
4	BCL	R	1509	1	55,74,74	2.88	14 (25%)	65,115,115	2.12	22 (33%)
4	BCL	R	1709	1	55,74,74	2.71	18 (32%)	65,115,115	2.02	19 (29%)
5	LDA	R	1809	-	13,15,15	2.20	1 (7%)	14,17,17	0.63	0
5	LDA	R	1818	-	13,15,15	2.24	1 (7%)	14,17,17	0.65	0
5	LDA	R	1819	-	13,15,15	2.24	1 (7%)	14,17,17	0.47	0
3	RG1	S	1409	-	52,52,52	1.42	8 (15%)	63,67,67	1.58	16 (25%)
4	BCL	S	1609	2	55,74,74	2.32	11 (20%)	65,115,115	1.96	20 (30%)

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
4	BCL	A	1501	1	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	A	1701	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	A	1816	-	-	0/13/13/13	0/0/0/0
5	LDA	A	1817	-	-	0/13/13/13	0/0/0/0
4	BCL	B	1601	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	B	1801	-	-	0/13/13/13	0/0/0/0
4	BCL	C	1502	1	1/1/21/25	0/37/137/137	0/0/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	C	1702	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	C	1815	-	-	0/13/13/13	0/0/0/0
5	LDA	C	1821	-	-	0/13/13/13	0/0/0/0
3	RG1	D	1402	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	D	1602	2	-	0/37/137/137	0/0/9/9
5	LDA	D	1802	-	-	0/13/13/13	0/0/0/0
4	BCL	E	1503	1	-	0/37/137/137	0/0/9/9
4	BCL	E	1703	1	-	0/37/137/137	0/0/9/9
5	LDA	E	1822	-	-	0/13/13/13	0/0/0/0
5	LDA	E	1823	-	-	0/13/13/13	0/0/0/0
3	RG1	F	1403	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	F	1603	2	-	0/37/137/137	0/0/9/9
5	LDA	F	1803	-	-	0/13/13/13	0/0/0/0
4	BCL	G	1504	1	-	0/37/137/137	0/0/9/9
4	BCL	G	1704	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	G	1814	-	-	0/13/13/13	0/0/0/0
5	LDA	G	1824	-	-	0/13/13/13	0/0/0/0
3	RG1	H	1404	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	H	1604	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	H	1804	-	-	0/13/13/13	0/0/0/0
4	BCL	I	1505	1	-	0/37/137/137	0/0/9/9
4	BCL	I	1705	1	-	0/37/137/137	0/0/9/9
5	LDA	I	1812	-	-	0/13/13/13	0/0/0/0
5	LDA	I	1813	-	-	0/13/13/13	0/0/0/0
5	LDA	I	1825	-	-	0/13/13/13	0/0/0/0
3	RG1	J	1405	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	J	1605	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	J	1805	-	-	0/13/13/13	0/0/0/0
4	BCL	K	1506	1	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	K	1706	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	K	1810	-	-	0/13/13/13	0/0/0/0
5	LDA	K	1826	-	-	0/13/13/13	0/0/0/0
3	RG1	L	1406	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	L	1606	2	3/3/21/25	0/37/137/137	0/0/9/9
5	LDA	L	1806	-	-	0/13/13/13	0/0/0/0
4	BCL	M	1507	1	-	0/37/137/137	0/0/9/9
4	BCL	M	1707	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	M	1811	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1827	-	-	0/13/13/13	0/0/0/0
3	RG1	N	1407	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	N	1607	2	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	N	1807	-	-	0/13/13/13	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BCL	O	1508	1	2/2/21/25	0/37/137/137	0/0/9/9
4	BCL	O	1708	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	O	1820	-	-	0/13/13/13	0/0/0/0
3	RG1	P	1408	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	P	1608	2	2/2/21/25	0/37/137/137	0/0/9/9
5	LDA	P	1808	-	-	0/13/13/13	0/0/0/0
3	RG1	R	1401	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	R	1509	1	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	R	1709	1	1/1/21/25	0/37/137/137	0/0/9/9
5	LDA	R	1809	-	-	0/13/13/13	0/0/0/0
5	LDA	R	1818	-	-	0/13/13/13	0/0/0/0
5	LDA	R	1819	-	-	0/13/13/13	0/0/0/0
3	RG1	S	1409	-	1/1/13/32	0/51/71/71	0/1/1/1
4	BCL	S	1609	2	1/1/21/25	0/37/137/137	0/0/9/9

The worst 5 of 452 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	1812	LDA	O1-N1	-9.25	1.23	1.42
5	F	1803	LDA	O1-N1	-8.48	1.25	1.42
5	K	1810	LDA	O1-N1	-8.42	1.25	1.42
5	O	1820	LDA	O1-N1	-8.42	1.25	1.42
5	D	1802	LDA	O1-N1	-8.41	1.25	1.42

The worst 5 of 640 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1704	BCL	C1-C2-C3	-7.15	112.78	125.96
4	K	1706	BCL	C1-C2-C3	-6.87	113.31	125.96
4	M	1707	BCL	C1-C2-C3	-6.72	113.58	125.96
4	K	1506	BCL	C1-C2-C3	-6.66	113.69	125.96
4	I	1705	BCL	C1-C2-C3	-6.63	113.75	125.96

5 of 32 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	N	1407	RG1	C1'
4	A	1501	BCL	CBD
4	R	1709	BCL	C13
4	C	1502	BCL	C13
4	N	1607	BCL	C2C

There are no torsion outliers.

There are no ring outliers.

60 monomers are involved in 432 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1501	BCL	17	0
4	A	1701	BCL	8	0
5	A	1816	LDA	8	0
5	A	1817	LDA	3	0
4	B	1601	BCL	11	0
5	B	1801	LDA	2	0
4	C	1502	BCL	7	0
4	C	1702	BCL	8	0
5	C	1815	LDA	6	0
3	D	1402	RG1	5	0
4	D	1602	BCL	8	0
5	D	1802	LDA	3	0
4	E	1503	BCL	5	0
4	E	1703	BCL	7	0
5	E	1822	LDA	8	0
5	E	1823	LDA	6	0
3	F	1403	RG1	5	0
4	F	1603	BCL	12	0
5	F	1803	LDA	7	0
4	G	1504	BCL	6	0
4	G	1704	BCL	21	0
5	G	1814	LDA	3	0
5	G	1824	LDA	14	0
3	H	1404	RG1	5	0
4	H	1604	BCL	12	0
5	H	1804	LDA	3	0
4	I	1505	BCL	12	0
4	I	1705	BCL	21	0
5	I	1812	LDA	7	0
5	I	1813	LDA	2	0
5	I	1825	LDA	6	0
3	J	1405	RG1	1	0
4	J	1605	BCL	17	0
5	J	1805	LDA	1	0
4	K	1506	BCL	9	0
4	K	1706	BCL	5	0
5	K	1810	LDA	8	0
5	K	1826	LDA	4	0
3	L	1406	RG1	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1606	BCL	25	0
5	L	1806	LDA	5	0
4	M	1507	BCL	7	0
4	M	1707	BCL	21	0
5	M	1811	LDA	4	0
5	M	1827	LDA	2	0
3	N	1407	RG1	4	0
4	N	1607	BCL	16	0
5	N	1807	LDA	2	0
4	O	1508	BCL	11	0
4	O	1708	BCL	10	0
5	O	1820	LDA	7	0
3	P	1408	RG1	4	0
4	P	1608	BCL	10	0
5	P	1808	LDA	3	0
3	R	1401	RG1	4	0
4	R	1509	BCL	7	0
4	R	1709	BCL	21	0
5	R	1818	LDA	12	0
3	S	1409	RG1	5	0
4	S	1609	BCL	13	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	52/53 (98%)	0.42	6 (11%) 5 4	35, 41, 88, 98	0
1	C	52/53 (98%)	0.99	7 (13%) 3 2	34, 41, 88, 102	0
1	E	52/53 (98%)	1.41	7 (13%) 3 2	35, 40, 88, 101	0
1	G	52/53 (98%)	0.77	6 (11%) 5 4	33, 40, 87, 99	0
1	I	52/53 (98%)	0.96	6 (11%) 5 4	34, 39, 88, 100	0
1	K	52/53 (98%)	0.68	6 (11%) 5 4	33, 40, 88, 100	0
1	M	52/53 (98%)	0.60	6 (11%) 5 4	35, 40, 88, 101	0
1	O	52/53 (98%)	0.90	6 (11%) 5 4	34, 41, 87, 100	0
1	R	52/53 (98%)	0.74	6 (11%) 5 4	35, 41, 87, 97	0
2	B	41/41 (100%)	-0.23	1 (2%) 59 55	42, 46, 54, 67	0
2	D	41/41 (100%)	0.02	2 (4%) 30 28	41, 46, 55, 64	0
2	F	41/41 (100%)	0.01	1 (2%) 59 55	38, 45, 52, 65	0
2	H	41/41 (100%)	-0.21	1 (2%) 59 55	37, 45, 52, 64	0
2	J	41/41 (100%)	-0.24	0 100 100	40, 45, 53, 65	0
2	L	41/41 (100%)	0.44	1 (2%) 59 55	39, 43, 52, 65	0
2	N	41/41 (100%)	0.21	3 (7%) 16 14	41, 45, 52, 69	0
2	P	41/41 (100%)	-0.02	1 (2%) 59 55	40, 46, 53, 68	0
2	S	41/41 (100%)	-0.35	1 (2%) 59 55	41, 46, 54, 67	0
All	All	837/846 (98%)	0.45	67 (8%) 13 11	33, 43, 79, 102	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	ALA	23.9
1	E	52	ALA	20.1
1	E	49	VAL	17.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	49	VAL	16.6
1	C	52	ALA	16.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CXM	M	1	11/12	0.96	0.13	-	40,45,51,52	0
1	CXM	I	1	11/12	0.95	0.15	-	38,45,51,52	0
1	CXM	O	1	11/12	0.96	0.14	-	45,47,54,58	0
1	CXM	E	1	11/12	0.95	0.15	-	41,46,48,50	0
1	CXM	K	1	11/12	0.94	0.12	-	40,46,54,54	0
1	CXM	A	1	11/12	0.95	0.12	-	45,48,60,62	0
1	CXM	G	1	11/12	0.96	0.16	-	45,46,52,58	0
1	CXM	R	1	11/12	0.95	0.21	-	45,48,54,59	0
1	CXM	C	1	11/12	0.95	0.28	-	45,47,55,58	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	LDA	K	1810	16/16	0.56	0.56	27.48	107,110,116,116	0
5	LDA	I	1812	16/16	0.57	0.46	19.56	87,106,111,111	0
5	LDA	R	1818	16/16	0.58	0.41	18.04	85,90,95,96	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	LDA	E	1823	16/16	0.18	0.65	17.99	89,99,122,123	0
5	LDA	C	1821	16/16	0.63	0.34	15.39	82,90,101,103	0
5	LDA	R	1819	16/16	0.76	0.33	14.59	80,83,85,87	0
5	LDA	M	1811	16/16	0.60	0.36	12.69	75,77,84,84	0
5	LDA	C	1815	16/16	0.46	0.53	11.07	79,96,103,103	0
5	LDA	M	1827	16/16	0.48	0.40	9.68	96,101,105,107	0
5	LDA	I	1825	16/16	0.65	0.40	9.13	95,101,108,108	0
5	LDA	A	1816	16/16	0.61	0.42	8.86	86,87,91,93	0
5	LDA	G	1824	16/16	0.61	0.37	8.58	89,105,120,121	0
5	LDA	H	1804	16/16	0.84	0.26	8.19	49,57,66,67	0
5	LDA	P	1808	16/16	0.64	0.38	7.37	53,61,84,86	0
5	LDA	A	1817	16/16	0.82	0.21	6.04	67,69,87,87	0
5	LDA	O	1820	16/16	0.71	0.29	5.92	71,80,92,95	0
5	LDA	E	1822	16/16	0.57	0.34	5.41	69,91,107,108	0
5	LDA	G	1814	16/16	0.63	0.29	5.40	70,74,83,84	0
5	LDA	D	1802	16/16	0.71	0.34	4.81	53,57,75,77	0
5	LDA	B	1801	16/16	0.70	0.29	4.09	49,62,76,78	0
5	LDA	R	1809	16/16	0.71	0.26	4.06	57,63,71,73	0
5	LDA	F	1803	16/16	0.73	0.24	3.83	50,56,67,67	0
5	LDA	L	1806	16/16	0.70	0.30	3.26	44,52,74,75	0
4	BCL	R	1709	66/66	0.89	0.19	3.16	43,53,78,82	0
5	LDA	K	1826	16/16	0.80	0.24	2.87	83,88,103,104	0
5	LDA	N	1807	16/16	0.52	0.32	2.39	61,66,76,78	0
3	RG1	J	1405	52/52	0.81	0.24	1.87	28,37,76,80	0
4	BCL	A	1701	66/66	0.91	0.17	1.87	42,49,80,83	0
3	RG1	F	1403	52/52	0.77	0.25	1.85	28,38,77,82	0
3	RG1	R	1401	52/52	0.87	0.23	1.84	30,40,74,77	0
3	RG1	P	1408	52/52	0.88	0.22	1.77	32,42,75,78	0
4	BCL	G	1704	66/66	0.90	0.20	1.55	32,45,73,76	0
3	RG1	H	1404	52/52	0.89	0.21	1.46	27,37,78,80	0
4	BCL	C	1702	66/66	0.88	0.19	1.45	41,48,78,80	0
3	RG1	S	1409	52/52	0.85	0.20	1.42	29,40,77,78	0
5	LDA	J	1805	16/16	0.75	0.21	1.35	44,54,67,68	0
5	LDA	I	1813	16/16	0.76	0.19	1.29	50,54,76,76	0
4	BCL	A	1501	66/66	0.92	0.17	1.29	33,42,51,65	0
3	RG1	N	1407	52/52	0.85	0.20	1.29	29,37,69,73	0
3	RG1	D	1402	52/52	0.83	0.19	1.02	30,44,77,81	0
4	BCL	B	1601	66/66	0.95	0.15	0.96	33,42,67,68	0
4	BCL	R	1509	66/66	0.93	0.17	0.75	31,38,49,57	0
4	BCL	O	1708	66/66	0.92	0.16	0.72	42,50,79,81	0
4	BCL	P	1608	66/66	0.94	0.16	0.72	34,42,66,68	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BCL	M	1707	66/66	0.92	0.17	0.57	29,44,74,76	0
4	BCL	F	1603	66/66	0.94	0.17	0.56	26,35,62,64	0
4	BCL	S	1609	66/66	0.93	0.15	0.54	31,41,69,72	0
4	BCL	I	1705	66/66	0.92	0.17	0.44	34,41,73,75	0
4	BCL	H	1604	66/66	0.94	0.15	0.42	29,39,63,64	0
3	RG1	L	1406	52/52	0.91	0.18	0.39	26,35,74,77	0
4	BCL	J	1605	66/66	0.90	0.16	0.33	31,39,64,66	0
4	BCL	I	1505	66/66	0.93	0.15	0.12	28,36,42,48	0
4	BCL	K	1506	66/66	0.94	0.18	0.10	28,35,47,51	0
4	BCL	N	1607	66/66	0.89	0.15	0.08	31,41,63,65	0
4	BCL	D	1602	66/66	0.95	0.13	0.04	30,37,64,67	0
4	BCL	E	1703	66/66	0.93	0.17	0.03	29,37,69,72	0
4	BCL	G	1504	66/66	0.95	0.15	0.01	26,34,44,49	0
4	BCL	L	1606	66/66	0.94	0.16	-0.14	27,36,66,69	0
4	BCL	O	1508	66/66	0.93	0.14	-0.18	30,37,46,54	0
4	BCL	C	1502	66/66	0.96	0.12	-0.21	33,38,50,57	0
4	BCL	K	1706	66/66	0.94	0.15	-0.47	27,36,78,82	0
4	BCL	M	1507	66/66	0.96	0.12	-0.50	27,35,41,48	0
4	BCL	E	1503	66/66	0.97	0.11	-0.70	28,35,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.