



wwPDB X-ray Structure Validation Summary Report i

Mar 11, 2014 – 06:50 PM GMT

PDB ID : 1PYH
Title : Crystal structure of RC-LH1 core complex from Rhodopseudomonas palustris
Authors : Roszak, A.W.; Howard, T.D.; Southall, J.; Gardiner, A.T.; Law, C.J.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2003-07-08
Resolution : 4.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

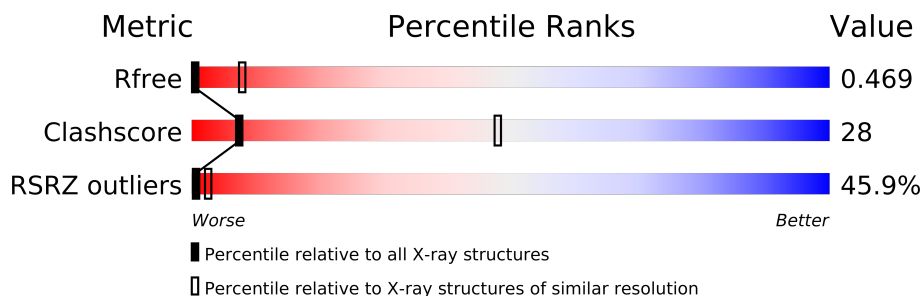
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22699
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22699

1 Overall quality at a glance









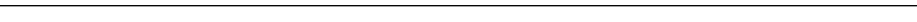


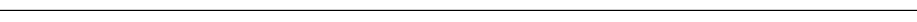





The reported resolution of this entry is 4.80 Å.

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.











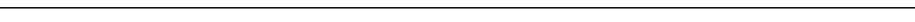








Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1046 (6.00-3.50)
Clashscore	79885	1320 (6.00-3.50)
RSRZ outliers	66119	1045 (6.00-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	281	
2	B	302	
3	C	241	
4	1	26	
4	3	26	
4	5	26	
4	7	26	
4	D	26	
4	F	26	
4	H	26	
4	J	26	
4	L	26	
4	N	26	
4	P	26	
4	R	26	
4	T	26	
4	V	26	

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Mol	Chain	Length	Quality of chain
4	X	26	
4	Z	26	
5	2	30	
5	4	30	
5	6	30	
5	8	30	
5	E	30	
5	G	30	
5	I	30	
5	K	30	
5	M	30	
5	O	30	
5	Q	30	
5	S	30	
5	U	30	
5	W	30	
5	Y	30	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10100 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	0	0	0
			1373	811	281	281			

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	0	0	0
			1474	870	302	302			

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	0	0	0
			1182	700	241	241			

- Molecule 4 is a protein called Light-harvesting protein B-800/850, alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	F	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	H	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	J	26	Total	C	N	O	0	0	0
			127	75	26	26			
4	L	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	N	26	Total	C	N	O	0	0	0
			128	76	26	26			
4	P	26	Total	C	N	O	0	0	0
			128	76	26	26			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	R	26	Total 128	C 76	N 26	O 26	0	0	0
4	T	26	Total 128	C 76	N 26	O 26	0	0	0
4	V	26	Total 128	C 76	N 26	O 26	0	0	0
4	X	26	Total 127	C 75	N 26	O 26	0	0	0
4	Z	26	Total 128	C 76	N 26	O 26	0	0	0
4	1	26	Total 128	C 76	N 26	O 26	0	0	0
4	3	26	Total 128	C 76	N 26	O 26	0	0	0
4	5	26	Total 128	C 76	N 26	O 26	0	0	0
4	7	26	Total 128	C 76	N 26	O 26	0	0	0

- Molecule 5 is a protein called Light-harvesting protein B-800/850, beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	30	Total 148	C 88	N 30	O 30	0	0	0
5	G	30	Total 148	C 88	N 30	O 30	0	0	0
5	I	30	Total 148	C 88	N 30	O 30	0	0	0
5	K	30	Total 148	C 88	N 30	O 30	0	0	0
5	M	30	Total 148	C 88	N 30	O 30	0	0	0
5	O	30	Total 148	C 88	N 30	O 30	0	0	0
5	Q	30	Total 148	C 88	N 30	O 30	0	0	0
5	S	30	Total 148	C 88	N 30	O 30	0	0	0
5	U	30	Total 148	C 88	N 30	O 30	0	0	0
5	W	30	Total 148	C 88	N 30	O 30	0	0	0

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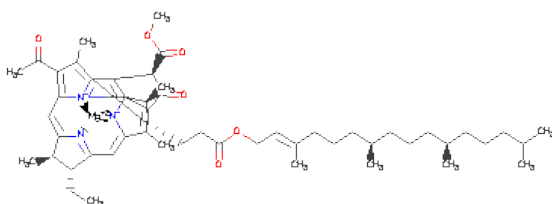
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	2	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	4	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	6	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	8	30	Total	C	N	O	0	0	0
			148	88	30	30			

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe	0	0
			1	1		

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

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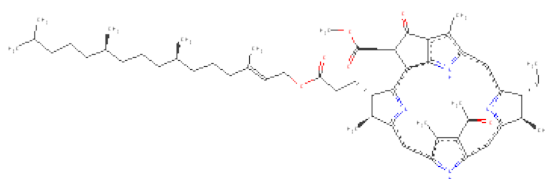
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
7	E	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	D	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	G	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	F	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	I	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	H	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	K	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	J	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	M	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	L	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	N	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	P	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	S	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	R	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	U	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	T	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	V	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	W	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	3	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	6	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	5	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	8	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	7	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			65	55	4	6		

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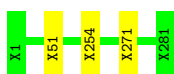
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			65	55	4	6		

3 Residue-property plots

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.

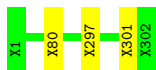
- Molecule 1: Reaction center protein L chain

Chain A: 



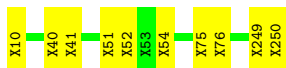
- Molecule 2: Reaction center protein M chain

Chain B: 



- Molecule 3: Reaction center protein H chain

Chain C: 



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain D: 

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain F: 



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain H: 

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain J: 



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain L:



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain N:

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain P:

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain R:



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain T:



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain V:



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain X:

There are no outlier residues recorded for this chain.

- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain Z:



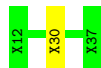
- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 1:



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 3:



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 5:



- Molecule 4: Light-harvesting protein B-800/850, alpha chain

Chain 7:



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain E:



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain G:



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain I:

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain K:



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain M:



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain O: 

There are no outlier residues recorded for this chain.

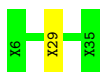
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain Q: 



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain S: 



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain U: 

There are no outlier residues recorded for this chain.

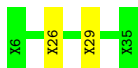
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain W: 



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain Y: 



- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 2: 

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 4: 

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 6: 

There are no outlier residues recorded for this chain.

- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain 8: 

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.04Å 119.02Å 130.43Å 69.32° 72.69° 66.52°	Depositor
Resolution (Å)	60.00 – 4.80 59.99 – 4.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (60.00-4.80) 97.3 (59.99-4.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 4.86Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.467 , 0.491 0.442 , 0.469	Depositor DCC
R_{free} test set	942 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	202.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 18334 reflections	Xtriage
F_o, F_c correlation	0.77	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, FE

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1373	0	257	10	0
2	B	1474	0	274	2	0
3	C	1182	0	230	13	0
4	1	128	0	26	2	0
4	3	128	0	26	1	0
4	5	128	0	26	1	0
4	7	128	0	26	2	0
4	D	128	0	26	0	0
4	F	128	0	26	7	0
4	H	128	0	26	0	0
4	J	127	0	25	7	0
4	L	128	0	26	3	0
4	N	128	0	26	0	0
4	P	128	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	R	128	0	26	1	0
4	T	128	0	26	1	0
4	V	128	0	26	5	0
4	X	127	0	25	0	0
4	Z	128	0	26	4	0
5	2	148	0	30	0	0
5	4	148	0	30	0	0
5	6	148	0	30	0	0
5	8	148	0	30	0	0
5	E	148	0	30	11	0
5	G	148	0	30	3	0
5	I	148	0	30	0	0
5	K	148	0	30	4	0
5	M	148	0	30	1	0
5	O	148	0	30	0	0
5	Q	148	0	30	5	0
5	S	148	0	30	1	0
5	U	148	0	30	0	0
5	W	148	0	30	2	0
5	Y	148	0	30	4	0
6	B	1	0	0	0	0
7	1	47	0	34	18	0
7	2	47	0	34	10	0
7	3	94	0	68	15	0
7	5	47	0	33	12	0
7	6	47	0	34	3	0
7	7	47	0	34	8	0
7	8	47	0	34	5	0
7	A	132	0	148	9	0
7	B	132	0	148	6	0
7	D	47	0	34	14	0
7	E	47	0	34	14	0
7	F	47	0	34	7	0
7	G	47	0	34	11	0
7	H	47	0	33	11	0
7	I	47	0	34	6	0
7	J	47	0	33	32	0
7	K	47	0	34	18	0
7	L	47	0	34	25	0
7	M	47	0	34	13	0
7	N	94	0	68	39	0
7	P	94	0	68	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	47	0	34	16	0
7	S	47	0	34	10	0
7	T	47	0	34	10	0
7	U	47	0	34	8	0
7	V	47	0	34	8	0
7	W	47	0	34	6	0
7	Y	94	0	68	23	0
8	A	65	0	76	5	0
8	B	65	0	76	0	0
All	All	10100	0	3090	367	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 367 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:N:38:BCL:HMC3	7:P:38:BCL:CBB	1.44	1.47
7:H:6:BCL:C1	7:H:6:BCL:O2A	1.63	1.46
7:R:38:BCL:O2A	7:R:38:BCL:C1	1.63	1.42
7:P:38:BCL:CBC	7:P:39:BCL:HMD2	1.56	1.33
7:L:10:BCL:CMB	7:N:11:BCL:HMA1	1.64	1.26

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	BCL	1	38	-	54,55,74	3.20	34 (62%)	74,92,115	3.33	32 (43%)
7	BCL	2	36	-	54,55,74	3.54	24 (44%)	74,92,115	3.26	31 (41%)
7	BCL	3	38	-	54,55,74	3.53	25 (46%)	74,92,115	3.19	30 (40%)
7	BCL	3	39	-	54,55,74	3.18	33 (61%)	74,92,115	3.31	30 (40%)
7	BCL	5	38	-	54,55,74	3.11	33 (61%)	74,92,115	3.29	28 (37%)
7	BCL	6	36	-	54,55,74	3.50	24 (44%)	74,92,115	3.21	30 (40%)
7	BCL	7	38	-	54,55,74	3.13	32 (59%)	74,92,115	3.27	30 (40%)
7	BCL	8	36	-	54,55,74	3.51	23 (42%)	74,92,115	3.31	32 (43%)
7	BCL	A	301	-	74,74,74	1.46	9 (12%)	98,115,115	1.83	25 (25%)
7	BCL	A	302	-	74,74,74	1.36	9 (12%)	98,115,115	1.59	25 (25%)
8	BPH	A	401	-	70,70,70	1.27	9 (12%)	94,101,101	1.36	10 (10%)
7	BCL	B	303	-	74,74,74	1.51	11 (14%)	98,115,115	1.57	18 (18%)
7	BCL	B	304	-	74,74,74	1.49	12 (16%)	98,115,115	1.56	17 (17%)
8	BPH	B	402	-	70,70,70	1.15	7 (10%)	94,101,101	1.17	7 (7%)
7	BCL	D	2	-	54,55,74	3.24	34 (62%)	74,92,115	3.26	30 (40%)
7	BCL	E	1	-	54,55,74	3.67	24 (44%)	74,92,115	3.26	32 (43%)
7	BCL	F	4	-	54,55,74	3.25	35 (64%)	74,92,115	3.26	29 (39%)
7	BCL	G	3	-	54,55,74	3.57	23 (42%)	74,92,115	3.26	31 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BCL	H	6	-	54,55,74	3.29	35 (64%)	74,92,115	3.26	31 (41%)
7	BCL	I	5	-	54,55,74	3.64	24 (44%)	74,92,115	3.35	32 (43%)
7	BCL	J	8	-	54,55,74	3.24	33 (61%)	74,92,115	3.26	28 (37%)
7	BCL	K	36	-	54,55,74	3.65	24 (44%)	74,92,115	3.23	29 (39%)
7	BCL	L	10	-	54,55,74	3.24	33 (61%)	74,92,115	3.29	31 (41%)
7	BCL	M	36	-	54,55,74	3.63	25 (46%)	74,92,115	3.30	32 (43%)
7	BCL	N	11	-	54,55,74	3.50	23 (42%)	74,92,115	3.44	33 (44%)
7	BCL	N	38	-	54,55,74	3.18	34 (62%)	74,92,115	3.28	31 (41%)
7	BCL	P	38	-	54,55,74	3.56	24 (44%)	74,92,115	3.26	32 (43%)
7	BCL	P	39	-	54,55,74	3.18	34 (62%)	74,92,115	3.28	30 (40%)
7	BCL	R	38	-	54,55,74	3.20	33 (61%)	74,92,115	3.29	31 (41%)
7	BCL	S	36	-	54,55,74	3.66	25 (46%)	74,92,115	3.24	31 (41%)
7	BCL	T	38	-	54,55,74	3.23	35 (64%)	74,92,115	3.26	30 (40%)
7	BCL	U	36	-	54,55,74	3.62	24 (44%)	74,92,115	3.21	30 (40%)
7	BCL	V	38	-	54,55,74	3.55	24 (44%)	74,92,115	3.40	32 (43%)
7	BCL	W	36	-	54,55,74	3.21	35 (64%)	74,92,115	3.29	29 (39%)
7	BCL	Y	36	-	54,55,74	3.54	25 (46%)	74,92,115	3.19	28 (37%)
7	BCL	Y	37	-	54,55,74	3.22	34 (62%)	74,92,115	3.31	31 (41%)

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
7	BCL	1	38	-	-	0/19/115/137	0/0/9/9
7	BCL	2	36	-	-	0/19/115/137	0/0/9/9
7	BCL	3	38	-	-	0/19/115/137	0/0/9/9
7	BCL	3	39	-	-	0/19/115/137	0/0/9/9
7	BCL	5	38	-	-	0/19/115/137	0/0/9/9
7	BCL	6	36	-	-	0/19/115/137	0/0/9/9
7	BCL	7	38	-	-	0/19/115/137	0/0/9/9
7	BCL	8	36	-	-	0/19/115/137	0/0/9/9
7	BCL	A	301	-	-	0/41/137/137	0/0/9/9
7	BCL	A	302	-	-	0/41/137/137	0/0/9/9
8	BPH	A	401	-	2/2/18/22	0/51/105/105	0/1/6/6
7	BCL	B	303	-	-	0/41/137/137	0/0/9/9
7	BCL	B	304	-	-	0/41/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BPH	B	402	-	2/2/18/22	0/51/105/105	0/1/6/6
7	BCL	D	2	-	-	0/19/115/137	0/0/9/9
7	BCL	E	1	-	-	0/19/115/137	0/0/9/9
7	BCL	F	4	-	-	0/19/115/137	0/0/9/9
7	BCL	G	3	-	-	0/19/115/137	0/0/9/9
7	BCL	H	6	-	-	0/19/115/137	0/0/9/9
7	BCL	I	5	-	-	0/19/115/137	0/0/9/9
7	BCL	J	8	-	-	0/19/115/137	0/0/9/9
7	BCL	K	36	-	-	0/19/115/137	0/0/9/9
7	BCL	L	10	-	-	0/19/115/137	0/0/9/9
7	BCL	M	36	-	-	0/19/115/137	0/0/9/9
7	BCL	N	11	-	-	0/19/115/137	0/0/9/9
7	BCL	N	38	-	-	0/19/115/137	0/0/9/9
7	BCL	P	38	-	-	0/19/115/137	0/0/9/9
7	BCL	P	39	-	-	0/19/115/137	0/0/9/9
7	BCL	R	38	-	-	0/19/115/137	0/0/9/9
7	BCL	S	36	-	-	0/19/115/137	0/0/9/9
7	BCL	T	38	-	-	0/19/115/137	0/0/9/9
7	BCL	U	36	-	-	0/19/115/137	0/0/9/9
7	BCL	V	38	-	-	0/19/115/137	0/0/9/9
7	BCL	W	36	-	-	0/19/115/137	0/0/9/9
7	BCL	Y	36	-	-	1/19/115/137	0/0/9/9
7	BCL	Y	37	-	-	0/19/115/137	0/0/9/9

The worst 5 of 925 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	3	BCL	C1B-NB	10.10	1.50	1.34
7	I	5	BCL	C1B-NB	9.85	1.50	1.34
7	S	36	BCL	C1B-NB	9.82	1.50	1.34
7	E	1	BCL	C1B-NB	9.75	1.50	1.34
7	V	38	BCL	C1B-NB	9.73	1.50	1.34

The worst 5 of 1018 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1	38	BCL	C4D-C3D-CAD	-12.64	92.52	108.05
7	5	38	BCL	C4D-C3D-CAD	-12.44	92.76	108.05
7	Y	37	BCL	C4D-C3D-CAD	-12.38	92.83	108.05
7	3	39	BCL	C4D-C3D-CAD	-12.38	92.83	108.05
7	W	36	BCL	C4D-C3D-CAD	-12.26	92.98	108.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	B	402	BPH	C8
8	B	402	BPH	C13
8	A	401	BPH	C8
8	A	401	BPH	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	Y	36	BCL	CED-O2D-CGD-CBD

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	0/281	-	-	-	-
2	B	0/302	-	-	-	-
3	C	0/241	-	-	-	-
4	1	0/26	-	-	-	-
4	3	0/26	-	-	-	-
4	5	0/26	-	-	-	-
4	7	0/26	-	-	-	-
4	D	0/26	-	-	-	-
4	F	0/26	-	-	-	-
4	H	0/26	-	-	-	-
4	J	0/26	-	-	-	-
4	L	0/26	-	-	-	-
4	N	0/26	-	-	-	-
4	P	0/26	-	-	-	-
4	R	0/26	-	-	-	-
4	T	0/26	-	-	-	-
4	V	0/26	-	-	-	-
4	X	0/26	-	-	-	-
4	Z	0/26	-	-	-	-
5	2	0/30	-	-	-	-
5	4	0/30	-	-	-	-
5	6	0/30	-	-	-	-
5	8	0/30	-	-	-	-
5	E	0/30	-	-	-	-
5	G	0/30	-	-	-	-
5	I	0/30	-	-	-	-
5	K	0/30	-	-	-	-
5	M	0/30	-	-	-	-
5	O	0/30	-	-	-	-
5	Q	0/30	-	-	-	-
5	S	0/30	-	-	-	-
5	U	0/30	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	W	0/30	-	-	-	-
5	Y	0/30	-	-	-	-
All	All	0/1690	-	-	-	-

There are no RSRZ outliers to report.

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	BCL	L	10	47/66	0.26	-	198,198,198,198	0
6	FE	B	500	1/1	0.45	-	198,198,198,198	0
7	BCL	B	303	66/66	0.57	-	198,198,198,198	0
7	BCL	P	39	47/66	0.25	-	198,198,198,198	0
7	BCL	H	6	47/66	0.24	-	198,198,198,198	0
7	BCL	S	36	47/66	0.35	-	198,198,198,198	0
7	BCL	U	36	47/66	0.35	-	198,198,198,198	0
7	BCL	F	4	47/66	0.32	-	198,198,198,198	0
7	BCL	V	38	47/66	0.27	-	198,198,198,198	0
7	BCL	5	38	47/66	0.35	-	198,198,198,198	0
7	BCL	D	2	47/66	0.23	-	198,198,198,198	0
7	BCL	Y	37	47/66	0.43	-	198,198,198,198	0
7	BCL	A	301	66/66	0.46	-	198,198,198,198	0
7	BCL	N	11	47/66	0.23	-	198,198,198,198	0
8	BPH	B	402	65/65	0.47	-	198,198,198,198	0
7	BCL	A	302	66/66	0.52	-	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	BCL	N	38	47/66	0.17	-	198,198,198,198	0
7	BCL	3	39	47/66	0.24	-	198,198,198,198	0
7	BCL	7	38	47/66	0.33	-	198,198,198,198	0
7	BCL	3	38	47/66	0.24	-	198,198,198,198	0
7	BCL	R	38	47/66	0.29	-	198,198,198,198	0
7	BCL	E	1	47/66	0.28	-	198,198,198,198	0
7	BCL	2	36	47/66	0.21	-	198,198,198,198	0
7	BCL	Y	36	47/66	0.19	-	198,198,198,198	0
7	BCL	I	5	47/66	0.25	-	198,198,198,198	0
7	BCL	G	3	47/66	0.21	-	198,198,198,198	0
7	BCL	W	36	47/66	0.53	-	198,198,198,198	0
7	BCL	K	36	47/66	0.23	-	198,198,198,198	0
7	BCL	T	38	47/66	0.27	-	198,198,198,198	0
7	BCL	M	36	47/66	0.27	-	198,198,198,198	0
7	BCL	J	8	47/66	0.20	-	198,198,198,198	0
8	BPH	A	401	65/65	0.66	-	198,198,198,198	0
7	BCL	6	36	47/66	0.34	-	198,198,198,198	0
7	BCL	8	36	47/66	0.35	-	198,198,198,198	0
7	BCL	B	304	66/66	0.48	-	198,198,198,198	0
7	BCL	1	38	47/66	0.34	-	198,198,198,198	0
7	BCL	P	38	47/66	0.21	-	198,198,198,198	0

6.5 Other polymers ⓘ

There are no such residues in this entry.