



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:42 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 X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

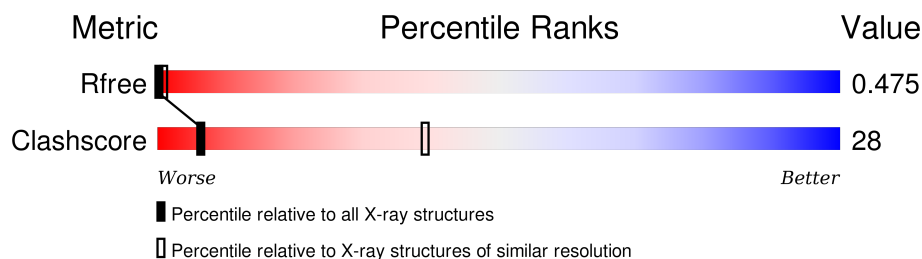
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

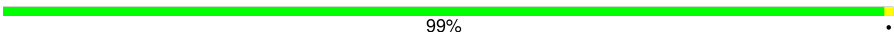
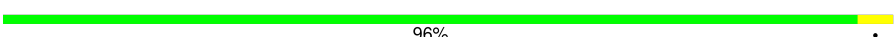
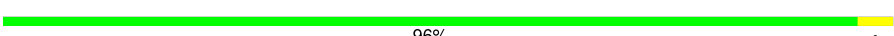

The reported resolution of this entry is 4.80 Å.

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))
$R_{free}$	91344	1117 (6.00-3.60)
Clashscore	102246	1017 (5.96-3.64)

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  $\geq 3$ , 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	281	 99% .
2	B	302	 99% .
3	C	241	 96% .
4	1	26	 96% .
4	3	26	 96% .
4	5	26	 96% .
4	7	26	 96% .
4	D	26	 100%
4	F	26	 92% 8%

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Mol	Chain	Length	Quality of chain
4	H	26	100%
4	J	26	88% 12%
4	L	26	92% 8%
4	N	26	100%
4	P	26	100%
4	R	26	96% .
4	T	26	96% .
4	V	26	85% 15%
4	X	26	100%
4	Z	26	92% 8%
5	2	30	100%
5	4	30	100%
5	6	30	100%
5	8	30	100%
5	E	30	87% 13%
5	G	30	97% .
5	I	30	100%
5	K	30	97% .
5	M	30	97% .
5	O	30	100%
5	Q	30	97% .
5	S	30	97% .
5	U	30	100%
5	W	30	97% .
5	Y	30	93% 7%

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
7	BCL	J	8	-	-	X	-
7	BCL	L	10	-	-	X	-
7	BCL	N	38	-	-	X	-
7	BCL	P	38	-	-	X	-
7	BCL	P	39	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 10100 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 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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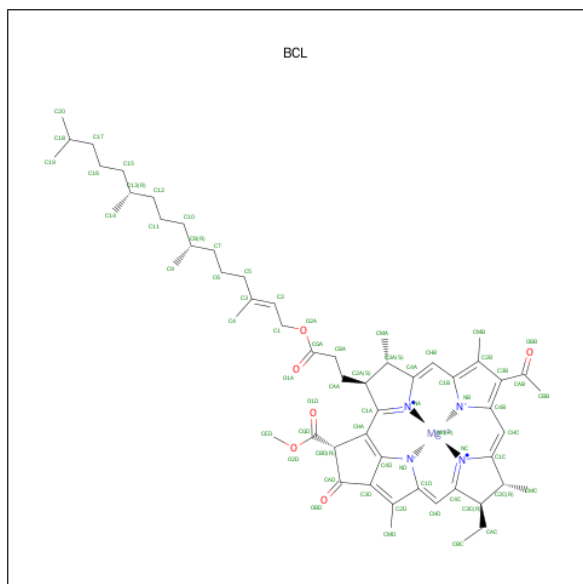
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Y	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	2	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	4	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	6	30	Total	C	N	O	0	0	0
			148	88	30	30			
5	8	30	Total	C	N	O	0	0	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: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

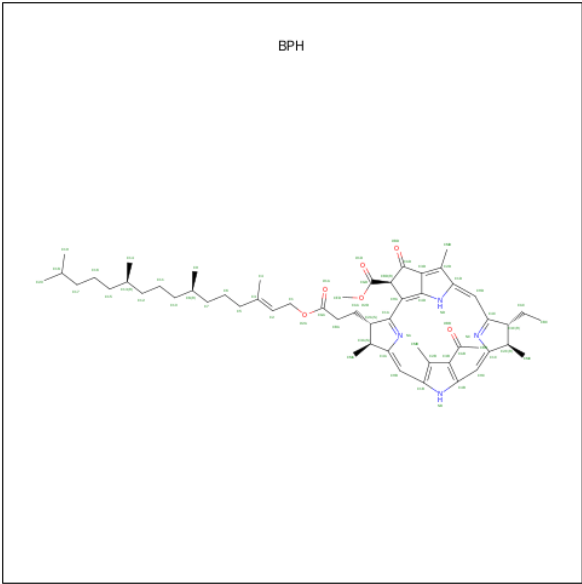
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	Y	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	2	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
7	3	1	Total	C	Mg	N	O	0	0
			47	36	1	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<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



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

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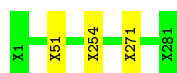
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	65	55	4	6	0	0

### 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:  99% .



- Molecule 2: Reaction center protein M chain

Chain B:  99% .



- Molecule 3: Reaction center protein H chain

Chain C:  96% .



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

Chain D:  100%

There are no outlier residues recorded for this chain.

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

Chain F:  92% 8%




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

Chain H:  100%

There are no outlier residues recorded for this chain.

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

Chain J:  88% 12%



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

Chain L:  92% 8%



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

Chain N:  100%

There are no outlier residues recorded for this chain.

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

Chain P:  100%

There are no outlier residues recorded for this chain.

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

Chain R:  96% .




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

Chain T:  96% .



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

Chain V:  85% 15%



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

Chain X:  100%

There are no outlier residues recorded for this chain.

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

Chain Z:  92% 8%



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

Chain 1:  96% .



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

Chain 3:  96% .



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

Chain 5:  96% .




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

Chain 7:  96% .



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

Chain E:  87% 13%



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

Chain G:  97% .



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

Chain I:  100%

There are no outlier residues recorded for this chain.

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

Chain K:  97%



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

Chain M:  97%



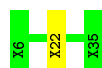
- Molecule 5: Light-harvesting protein B-800/850, beta chain

Chain O:  100%

There are no outlier residues recorded for this chain.

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

Chain Q:  97%



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

Chain S:  97%



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

Chain U:  100%

There are no outlier residues recorded for this chain.

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

Chain W:  97%



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

Chain Y:  93% 7%



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

Chain 2:  100%

There are no outlier residues recorded for this chain.

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

Chain 4:  100%

There are no outlier residues recorded for this chain.

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

Chain 6:  100%

There are no outlier residues recorded for this chain.

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

Chain 8:  100%

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, $\alpha$ , $\beta$ , $\gamma$	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) 88.6 (59.99-4.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 4.86Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, $R_{free}$	0.467 , 0.491 0.453 , 0.475	Depositor DCC
$R_{free}$ test set	944 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	202.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.03 , 289.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 18334 reflections	Xtriage
$F_o, F_c$ correlation	0.76	EDS
Total number of atoms	10100	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
4	R	128	0	26	1	0
4	T	128	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
7	R	47	0	34	16	0
7	S	47	0	34	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 28.

The worst 5 of 367 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)
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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

### 5.3.2 Protein sidechains [i](#)

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	-	34,55,74	2.99	21 (61%)	37,92,115	3.22	15 (40%)
7	BCL	2	36	-	34,55,74	2.91	12 (35%)	37,92,115	2.72	16 (43%)
7	BCL	3	38	-	34,55,74	2.91	13 (38%)	37,92,115	2.71	15 (40%)
7	BCL	3	39	-	34,55,74	2.91	20 (58%)	37,92,115	3.20	15 (40%)
7	BCL	5	38	-	34,55,74	2.95	19 (55%)	37,92,115	3.21	15 (40%)
7	BCL	6	36	-	34,55,74	2.88	11 (32%)	37,92,115	2.69	15 (40%)
7	BCL	7	38	-	34,55,74	2.91	18 (52%)	37,92,115	3.17	13 (35%)
7	BCL	8	36	-	34,55,74	2.89	12 (35%)	37,92,115	2.79	15 (40%)
7	BCL	A	301	-	53,74,74	0.79	1 (1%)	57,115,115	1.81	14 (24%)
7	BCL	A	302	-	53,74,74	0.79	1 (1%)	57,115,115	1.57	15 (26%)
8	BPH	A	401	-	64,70,70	0.83	1 (1%)	73,101,101	1.42	11 (15%)
7	BCL	B	303	-	53,74,74	0.83	0	57,115,115	1.33	9 (15%)
7	BCL	B	304	-	53,74,74	0.91	4 (7%)	57,115,115	1.48	10 (17%)
8	BPH	B	402	-	64,70,70	0.82	1 (1%)	73,101,101	1.38	10 (13%)
7	BCL	D	2	-	34,55,74	2.99	20 (58%)	37,92,115	3.14	13 (35%)
7	BCL	E	1	-	34,55,74	3.13	14 (41%)	37,92,115	2.72	15 (40%)
7	BCL	F	4	-	34,55,74	2.93	21 (61%)	37,92,115	3.15	13 (35%)
7	BCL	G	3	-	34,55,74	2.93	13 (38%)	37,92,115	2.75	16 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	BCL	H	6	-	34,55,74	3.33	22 (64%)	37,92,115	3.19	14 (37%)
7	BCL	I	5	-	34,55,74	3.07	15 (44%)	37,92,115	2.87	17 (45%)
7	BCL	J	8	-	34,55,74	3.01	19 (55%)	37,92,115	3.18	13 (35%)
7	BCL	K	36	-	34,55,74	2.97	12 (35%)	37,92,115	2.73	15 (40%)
7	BCL	L	10	-	34,55,74	2.98	20 (58%)	37,92,115	3.20	14 (37%)
7	BCL	M	36	-	34,55,74	2.99	14 (41%)	37,92,115	2.84	17 (45%)
7	BCL	N	11	-	34,55,74	2.92	11 (32%)	37,92,115	3.09	17 (45%)
7	BCL	N	38	-	34,55,74	2.94	20 (58%)	37,92,115	3.20	14 (37%)
7	BCL	P	38	-	34,55,74	3.00	14 (41%)	37,92,115	2.82	15 (40%)
7	BCL	P	39	-	34,55,74	3.16	21 (61%)	37,92,115	3.19	15 (40%)
7	BCL	R	38	-	34,55,74	3.18	20 (58%)	37,92,115	3.19	15 (40%)
7	BCL	S	36	-	34,55,74	3.11	14 (41%)	37,92,115	2.75	15 (40%)
7	BCL	T	38	-	34,55,74	3.18	21 (61%)	37,92,115	3.15	13 (35%)
7	BCL	U	36	-	34,55,74	3.02	14 (41%)	37,92,115	2.67	14 (37%)
7	BCL	V	38	-	34,55,74	2.98	14 (41%)	37,92,115	2.94	18 (48%)
7	BCL	W	36	-	34,55,74	2.90	20 (58%)	37,92,115	3.17	13 (35%)
7	BCL	Y	36	-	34,55,74	2.95	13 (38%)	37,92,115	2.66	14 (37%)
7	BCL	Y	37	-	34,55,74	2.95	20 (58%)	37,92,115	3.18	13 (35%)

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	-	-	0/15/115/137	0/0/9/9
7	BCL	2	36	-	-	0/15/115/137	0/0/9/9
7	BCL	3	38	-	-	0/15/115/137	0/0/9/9
7	BCL	3	39	-	-	0/15/115/137	0/0/9/9
7	BCL	5	38	-	-	0/15/115/137	0/0/9/9
7	BCL	6	36	-	-	0/15/115/137	0/0/9/9
7	BCL	7	38	-	-	0/15/115/137	0/0/9/9
7	BCL	8	36	-	-	0/15/115/137	0/0/9/9
7	BCL	A	301	-	-	0/37/137/137	0/0/9/9
7	BCL	A	302	-	-	0/37/137/137	0/0/9/9
8	BPH	A	401	-	-	0/54/105/105	0/1/6/6
7	BCL	B	303	-	-	0/37/137/137	0/0/9/9
7	BCL	B	304	-	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BPH	B	402	-	-	0/54/105/105	0/1/6/6
7	BCL	D	2	-	-	0/15/115/137	0/0/9/9
7	BCL	E	1	-	-	0/15/115/137	0/0/9/9
7	BCL	F	4	-	-	0/15/115/137	0/0/9/9
7	BCL	G	3	-	-	0/15/115/137	0/0/9/9
7	BCL	H	6	-	-	0/15/115/137	0/0/9/9
7	BCL	I	5	-	-	0/15/115/137	0/0/9/9
7	BCL	J	8	-	-	0/15/115/137	0/0/9/9
7	BCL	K	36	-	-	0/15/115/137	0/0/9/9
7	BCL	L	10	-	-	0/15/115/137	0/0/9/9
7	BCL	M	36	-	-	0/15/115/137	0/0/9/9
7	BCL	N	11	-	-	0/15/115/137	0/0/9/9
7	BCL	N	38	-	-	0/15/115/137	0/0/9/9
7	BCL	P	38	-	-	0/15/115/137	0/0/9/9
7	BCL	P	39	-	-	0/15/115/137	0/0/9/9
7	BCL	R	38	-	-	0/15/115/137	0/0/9/9
7	BCL	S	36	-	-	0/15/115/137	0/0/9/9
7	BCL	T	38	-	-	0/15/115/137	0/0/9/9
7	BCL	U	36	-	-	0/15/115/137	0/0/9/9
7	BCL	V	38	-	-	0/15/115/137	0/0/9/9
7	BCL	W	36	-	-	0/15/115/137	0/0/9/9
7	BCL	Y	36	-	-	1/15/115/137	0/0/9/9
7	BCL	Y	37	-	-	0/15/115/137	0/0/9/9

The worst 5 of 506 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	8	36	BCL	CBB-CAB	-7.57	1.26	1.49
7	3	38	BCL	CBB-CAB	-7.49	1.26	1.49
7	Y	36	BCL	CBB-CAB	-7.48	1.26	1.49
7	G	3	BCL	CBB-CAB	-7.46	1.26	1.49
7	6	36	BCL	CBB-CAB	-7.45	1.26	1.49

The worst 5 of 511 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	J	8	BCL	CMB-C2B-C1B	-6.31	117.93	128.36
7	N	38	BCL	CMB-C2B-C1B	-6.23	118.06	128.36
7	1	38	BCL	CMB-C2B-C1B	-6.23	118.06	128.36
7	3	39	BCL	CMB-C2B-C1B	-6.22	118.07	128.36
7	L	10	BCL	CMB-C2B-C1B	-6.19	118.12	128.36

There are no chirality outliers.

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.

35 monomers are involved in 341 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	1	38	BCL	18	0
7	2	36	BCL	10	0
7	3	38	BCL	8	0
7	3	39	BCL	7	0
7	5	38	BCL	12	0
7	6	36	BCL	3	0
7	7	38	BCL	8	0
7	8	36	BCL	5	0
7	A	301	BCL	7	0
7	A	302	BCL	2	0
8	A	401	BPH	5	0
7	B	303	BCL	4	0
7	B	304	BCL	2	0
7	D	2	BCL	14	0
7	E	1	BCL	14	0
7	F	4	BCL	7	0
7	G	3	BCL	11	0
7	H	6	BCL	11	0
7	I	5	BCL	6	0
7	J	8	BCL	32	0
7	K	36	BCL	18	0
7	L	10	BCL	25	0
7	M	36	BCL	13	0
7	N	11	BCL	17	0
7	N	38	BCL	27	0
7	P	38	BCL	41	0
7	P	39	BCL	27	0
7	R	38	BCL	16	0
7	S	36	BCL	10	0
7	T	38	BCL	10	0
7	U	36	BCL	8	0
7	V	38	BCL	8	0
7	W	36	BCL	6	0
7	Y	36	BCL	17	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Y	37	BCL	9	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<sup>th</sup> 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 <sup>2</sup> )	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 <sup>2</sup> )	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 [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	BCL	L	10	47/66	0.73	0.27	-	198,198,198,198	0
6	FE	B	500	1/1	0.94	0.53	-	198,198,198,198	0
7	BCL	B	303	66/66	0.70	0.50	-	198,198,198,198	0
7	BCL	P	39	47/66	0.65	0.30	-	198,198,198,198	0
7	BCL	H	6	47/66	0.77	0.24	-	198,198,198,198	0
7	BCL	S	36	47/66	0.60	0.44	-	198,198,198,198	0
7	BCL	U	36	47/66	0.60	0.37	-	198,198,198,198	0
7	BCL	F	4	47/66	0.67	0.51	-	198,198,198,198	0
7	BCL	V	38	47/66	0.65	0.41	-	198,198,198,198	0
7	BCL	5	38	47/66	0.58	0.57	-	198,198,198,198	0
7	BCL	D	2	47/66	0.68	0.31	-	198,198,198,198	0
7	BCL	Y	37	47/66	0.67	0.47	-	198,198,198,198	0
7	BCL	A	301	66/66	0.71	0.50	-	198,198,198,198	0
7	BCL	N	11	47/66	0.79	0.20	-	198,198,198,198	0
8	BPH	B	402	65/65	0.63	0.55	-	198,198,198,198	0
7	BCL	A	302	66/66	0.69	0.56	-	198,198,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	BCL	N	38	47/66	0.81	0.19	-	198,198,198,198	0
7	BCL	3	39	47/66	0.73	0.30	-	198,198,198,198	0
7	BCL	7	38	47/66	0.68	0.35	-	198,198,198,198	0
7	BCL	3	38	47/66	0.82	0.19	-	198,198,198,198	0
7	BCL	R	38	47/66	0.67	0.33	-	198,198,198,198	0
7	BCL	E	1	47/66	0.70	0.34	-	198,198,198,198	0
7	BCL	2	36	47/66	0.82	0.32	-	198,198,198,198	0
7	BCL	Y	36	47/66	0.83	0.30	-	198,198,198,198	0
7	BCL	I	5	47/66	0.79	0.31	-	198,198,198,198	0
7	BCL	G	3	47/66	0.79	0.28	-	198,198,198,198	0
7	BCL	W	36	47/66	0.79	0.81	-	198,198,198,198	0
7	BCL	K	36	47/66	0.72	0.29	-	198,198,198,198	0
7	BCL	T	38	47/66	0.67	0.28	-	198,198,198,198	0
7	BCL	M	36	47/66	0.72	0.27	-	198,198,198,198	0
7	BCL	J	8	47/66	0.67	0.27	-	198,198,198,198	0
8	BPH	A	401	65/65	0.52	0.71	-	198,198,198,198	0
7	BCL	6	36	47/66	0.74	0.40	-	198,198,198,198	0
7	BCL	8	36	47/66	0.65	0.59	-	198,198,198,198	0
7	BCL	B	304	66/66	0.70	0.57	-	198,198,198,198	0
7	BCL	1	38	47/66	0.74	0.26	-	198,198,198,198	0
7	BCL	P	38	47/66	0.73	0.24	-	198,198,198,198	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.