



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:08 PM GMT

PDB ID : 4HBH  
Title : Bacterial Photosynthetic Reaction Center from Rhodobacter sphaeroides with ILE M265 replaced with ASN  
Authors : Mattis, A.J.; Wraight, C.A.  
Deposited on : 2012-09-28  
Resolution : 2.93 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

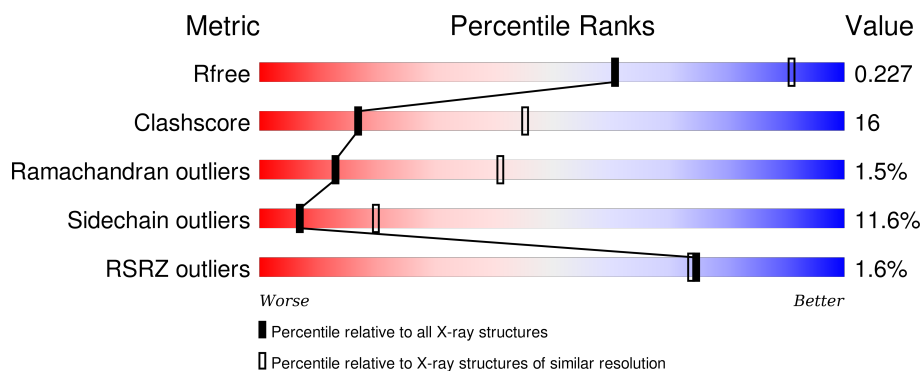
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	L	281	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>..</div> </div> </div>
2	M	313	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>...</div> </div> </div>
3	H	260	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>5%</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BPH	L	303	X	-	-	-
6	U10	L	304	-	-	X	X
6	U10	L	305	-	-	X	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6919 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	L	281	Total	C	N	O	S	0	0	0
			2209	1490	350	361	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2390	1594	391	395	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	265	ASN	ILE	ENGINEERED MUTATION	UNP P0C0Y9
M	303	MET	-	EXPRESSION TAG	UNP P0C0Y9
M	304	ALA	-	EXPRESSION TAG	UNP P0C0Y9
M	305	PRO	-	EXPRESSION TAG	UNP P0C0Y9
M	306	LEU	-	EXPRESSION TAG	UNP P0C0Y9
M	307	ASN	-	EXPRESSION TAG	UNP P0C0Y9
M	308	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	309	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	310	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	311	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	312	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	313	HIS	-	EXPRESSION TAG	UNP P0C0Y9

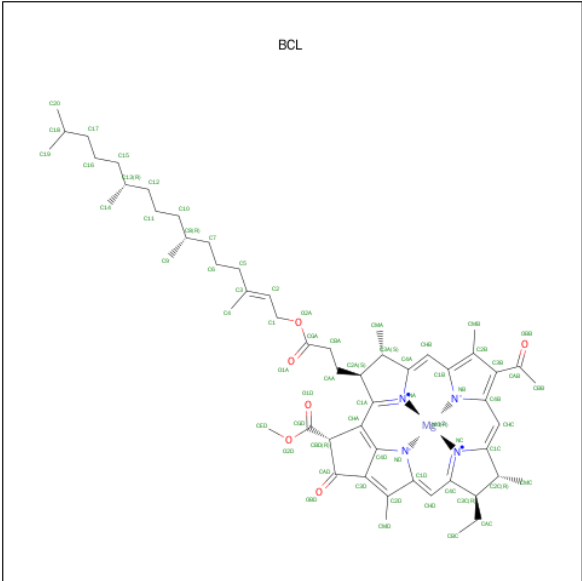
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1792	1146	305	332	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	MET	-	EXPRESSION TAG	UNP P0C0Y7
H	2	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	3	GLY	-	EXPRESSION TAG	UNP P0C0Y7
H	4	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	5	THR	-	EXPRESSION TAG	UNP P0C0Y7
H	6	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	7	PHE	-	EXPRESSION TAG	UNP P0C0Y7
H	8	GLY	-	EXPRESSION TAG	UNP P0C0Y7
H	9	ASN	-	EXPRESSION TAG	UNP P0C0Y7
H	10	PHE	-	EXPRESSION TAG	UNP P0C0Y7
H	251	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	252	VAL	-	EXPRESSION TAG	UNP P0C0Y7
H	253	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	254	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	255	MET	-	EXPRESSION TAG	UNP P0C0Y7
H	256	LEU	-	EXPRESSION TAG	UNP P0C0Y7
H	257	ALA	-	EXPRESSION TAG	UNP P0C0Y7
H	258	GLU	-	EXPRESSION TAG	UNP P0C0Y7
H	259	TYR	-	EXPRESSION TAG	UNP P0C0Y7
H	260	ALA	-	EXPRESSION TAG	UNP P0C0Y7

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



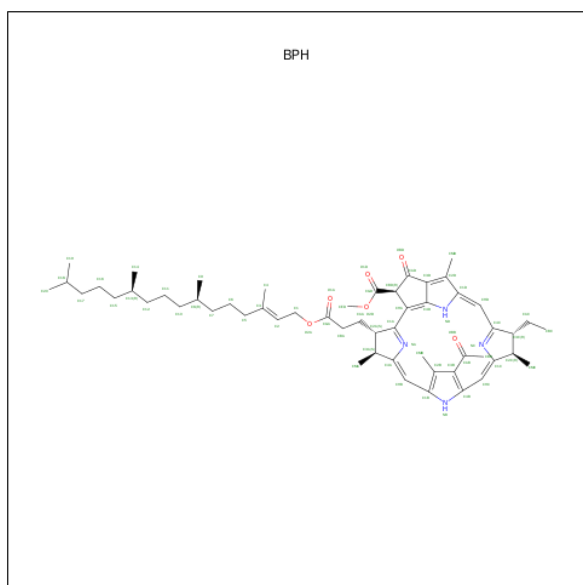
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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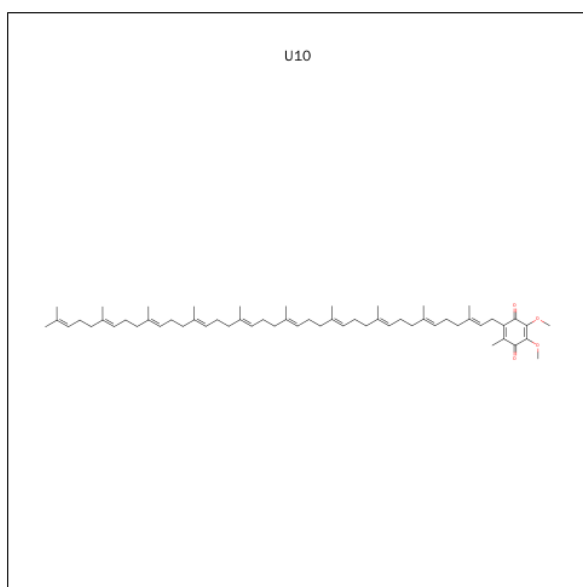
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	Mg	N	O	0	0
			55	44	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			53	43	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).

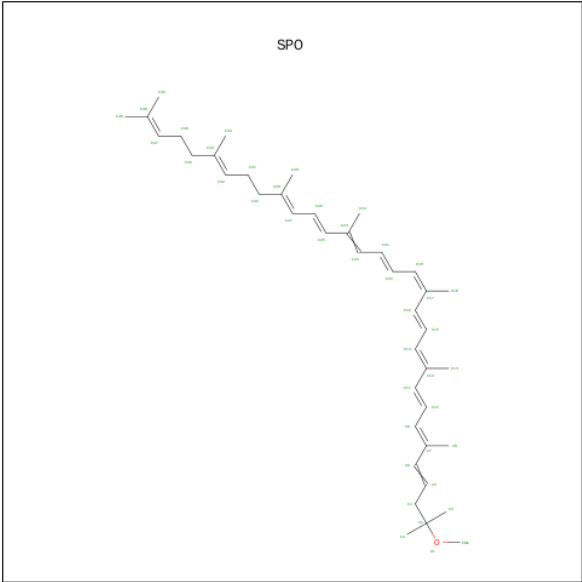


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			26	22	4		
6	L	1	Total	C	O	0	0
			26	22	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is SPHEROIDENE (three-letter code: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			35	34	1		

- Molecule 9 is water.

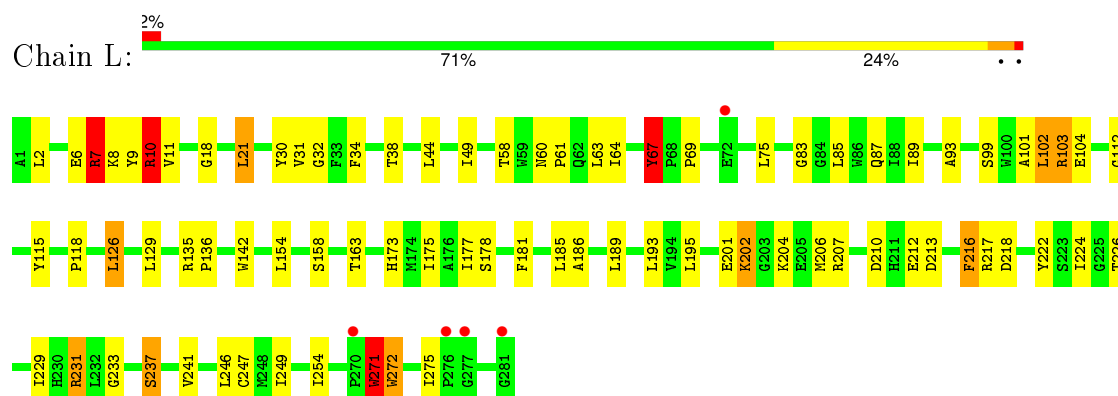
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	8	Total	O	0	0
			8	8		
9	M	11	Total	O	0	0
			11	11		
9	H	2	Total	O	0	0
			2	2		



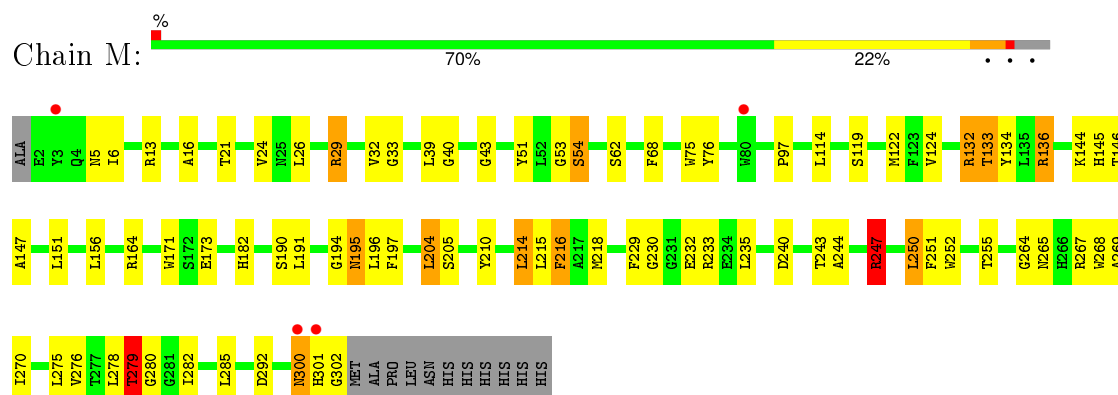
### 3 Residue-property plots [i](#)

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

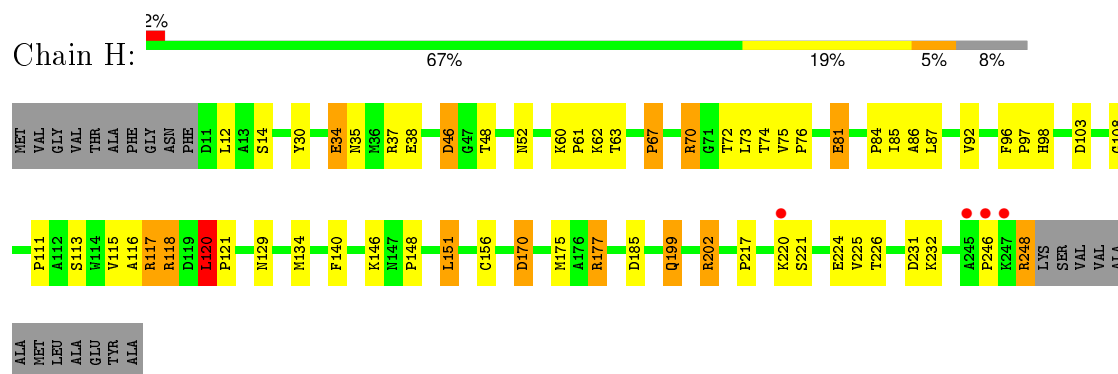
#### • Molecule 1: Reaction center protein L chain



#### • Molecule 2: Reaction center protein M chain



#### • Molecule 3: Reaction center protein H chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.72Å 139.72Å 183.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	121.00 – 2.93 19.84 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.6 (121.00-2.93) 100.0 (19.84-2.93)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.03 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.185 , 0.226 0.187 , 0.227	Depositor DCC
$R_{free}$ test set	2250 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.3	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 44997 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6919	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, U10, FE, SPO

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	L	1.02	1/2295 (0.0%)	0.97	9/3144 (0.3%)
2	M	0.98	0/2480	0.94	4/3386 (0.1%)
3	H	0.99	0/1840	1.02	5/2511 (0.2%)
All	All	1.00	1/6615 (0.0%)	0.97	18/9041 (0.2%)

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	L	0	1
2	M	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	67	TYR	CD2-CE2	5.75	1.48	1.39

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	247	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	L	231	ARG	NE-CZ-NH1	7.26	123.93	120.30
3	H	120	LEU	CA-CB-CG	6.83	131.01	115.30
2	M	21	THR	C-N-CA	-6.45	105.58	121.70
2	M	132	ARG	NE-CZ-NH1	-6.30	117.15	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide
2	M	278	LEU	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	L	2209	0	2144	76	0
2	M	2390	0	2281	63	0
3	H	1792	0	1760	44	0
4	L	132	0	148	7	0
4	M	121	0	124	19	0
5	L	65	0	76	9	0
5	M	53	0	49	7	0
6	L	52	0	56	47	0
6	M	48	0	63	6	0
7	M	1	0	0	0	0
8	M	35	0	46	6	0
9	H	2	0	0	0	0
9	L	8	0	0	2	0
9	M	11	0	0	0	0
All	All	6919	0	6747	224	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 16.

The worst 5 of 224 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)
6:L:304:U10:C3M	6:L:305:U10:H1M1	1.29	1.60
6:L:304:U10:C3M	6:L:305:U10:C1M	2.23	1.15
3:H:117:ARG:HG2	3:H:117:ARG:HH11	1.07	1.09
6:L:304:U10:H3M1	6:L:305:U10:C1M	1.84	1.06
6:L:304:U10:H3M3	6:L:305:U10:H1M1	1.34	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/281 (99%)	253 (91%)	22 (8%)	4 (1%)	14	43
2	M	299/313 (96%)	276 (92%)	19 (6%)	4 (1%)	15	45
3	H	236/260 (91%)	218 (92%)	14 (6%)	4 (2%)	11	37
All	All	814/854 (95%)	747 (92%)	55 (7%)	12 (2%)	13	41

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	279	THR
2	M	301	HIS
3	H	86	ALA
3	H	185	ASP

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	215/220 (98%)	192 (89%)	23 (11%)	8	24
2	M	231/246 (94%)	205 (89%)	26 (11%)	7	21
3	H	186/208 (89%)	162 (87%)	24 (13%)	5	15
All	All	632/674 (94%)	559 (88%)	73 (12%)	7	20

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	156	LEU
2	M	216	PHE
3	H	220	LYS
2	M	204	LEU
2	M	247	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	60	ASN
3	H	52	ASN
3	H	98	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z  > 2$
4	BCL	L	301	-	53,74,74	0.66	0	57,115,115	1.33	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BCL	L	302	-	53,74,74	0.80	1 (1%)	57,115,115	2.44	16 (28%)
5	BPH	L	303	-	64,70,70	1.48	10 (15%)	73,101,101	1.86	16 (21%)
6	U10	L	304	-	26,26,63	2.98	9 (34%)	31,34,79	2.32	9 (29%)
6	U10	L	305	-	26,26,63	3.38	13 (50%)	31,34,79	2.41	13 (41%)
4	BCL	M	401	-	42,63,74	0.90	2 (4%)	43,101,115	2.25	12 (27%)
4	BCL	M	403	-	53,74,74	0.68	0	57,115,115	1.74	12 (21%)
5	BPH	M	404	-	52,58,70	1.72	10 (19%)	58,86,101	2.21	22 (37%)
6	U10	M	405	-	48,48,63	3.22	12 (25%)	58,61,79	1.84	18 (31%)
8	SPO	M	406	-	33,34,41	1.26	3 (9%)	36,41,50	2.28	10 (27%)

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	L	301	-	-	0/37/137/137	0/0/9/9
4	BCL	L	302	-	-	0/37/137/137	0/0/9/9
5	BPH	L	303	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	304	-	-	0/19/43/87	0/1/1/1
6	U10	L	305	-	-	0/19/43/87	0/1/1/1
4	BCL	M	401	-	-	0/24/124/137	0/0/9/9
4	BCL	M	403	-	-	0/37/137/137	0/0/9/9
5	BPH	M	404	-	-	0/40/91/105	0/1/6/6
6	U10	M	405	-	-	0/45/69/87	0/1/1/1
8	SPO	M	406	-	-	0/39/39/47	0/0/0/0

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	304	U10	O4-C4	-4.94	1.24	1.37
6	L	304	U10	O3-C3	-4.51	1.25	1.37
6	L	305	U10	O4-C4	-4.29	1.25	1.37
6	M	405	U10	O4-C4	-4.23	1.25	1.37
5	M	404	BPH	C1B-C2B	-3.71	1.37	1.45

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	302	BCL	O1D-CGD-CBD	-9.90	110.44	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	U10	C7-C6-C5	-7.70	109.51	118.56
4	M	401	BCL	C4-C3-C2	-6.64	110.45	123.50
6	L	305	U10	C1-C6-C5	-6.12	113.14	120.12
8	M	406	SPO	C4-C5-C6	-5.51	116.83	124.67

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	303	BPH	C8
5	L	303	BPH	C13

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	BCL	4	0
4	L	302	BCL	4	0
5	L	303	BPH	9	0
6	L	304	U10	34	0
6	L	305	U10	39	0
4	M	401	BCL	6	0
4	M	403	BCL	14	0
5	M	404	BPH	7	0
6	M	405	U10	6	0
8	M	406	SPO	6	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	L	281/281 (100%)	-0.65	5 (1%) 71 70	30, 44, 77, 91	0
2	M	301/313 (96%)	-0.73	4 (1%) 79 79	29, 47, 75, 82	0
3	H	238/260 (91%)	-0.54	4 (1%) 73 72	34, 46, 61, 94	0
All	All	820/854 (96%)	-0.65	13 (1%) 74 74	29, 46, 74, 94	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	246	PRO	4.4
1	L	281	GLY	4.0
1	L	270	PRO	3.4
2	M	301	HIS	2.9
1	L	72	GLU	2.6

### 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( $\text{\AA}^2$ )	Q<0.9
6	U10	L	305	26/63	0.70	0.40	27.97	46,55,66,67	26
6	U10	L	304	26/63	0.81	0.37	13.74	67,90,94,99	26
8	SPO	M	406	35/42	0.90	0.21	1.98	54,68,86,87	0
6	U10	M	405	48/63	0.91	0.17	1.49	41,52,83,85	0
4	BCL	M	401	55/66	0.94	0.15	1.22	33,39,69,71	0
4	BCL	M	403	66/66	0.97	0.15	1.07	32,41,55,70	0
4	BCL	L	301	66/66	0.97	0.15	0.70	29,39,43,55	0
5	BPH	M	404	53/65	0.97	0.12	0.16	33,46,59,64	0
5	BPH	L	303	65/65	0.98	0.12	0.15	26,35,40,46	0
4	BCL	L	302	66/66	0.98	0.09	-0.69	27,33,48,55	0
7	FE	M	402	1/1	0.99	0.07	-1.53	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.