



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:06 am GMT

PDB ID : 3V3Z  
Title : I(L177)H mutant structure of photosynthetic reaction center from Rhodobacter sphaeroides  
Authors : Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Shuvalov, V.A.  
Deposited on : 2011-12-14  
Resolution : 2.90 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	:	1.7.2 (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

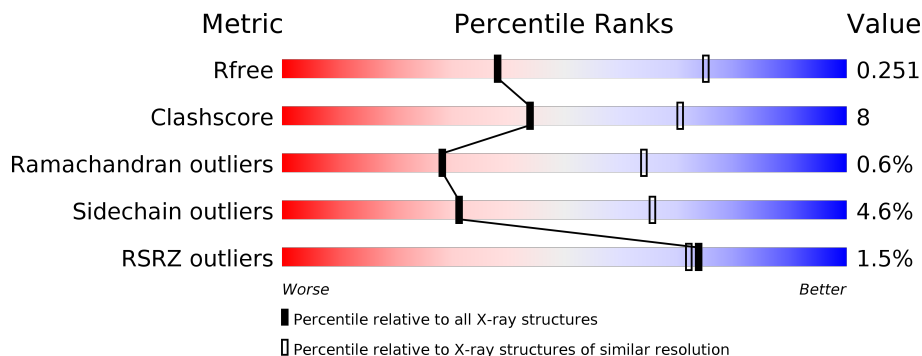
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	H	241	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
2	L	281	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div>.</div> </div> </div>
3	M	302	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</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
10	BPH	L	402	X	-	-	-
10	BPH	M	401	X	-	-	-
11	U10	L	502	-	-	-	X
13	SPN	M	600	-	-	-	X
4	LDA	H	704	-	-	-	X
4	LDA	M	701	-	-	-	X
4	LDA	M	702	-	-	-	X
4	LDA	M	703	-	-	-	X
4	LDA	M	705	-	-	-	X
6	HTO	H	2	-	-	-	X
6	HTO	L	282	-	-	-	X
7	DIO	H	251	-	-	X	-
9	BCL	L	301	-	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7216 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 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	0
			1840	1178	315	338	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2235	1508	357	362	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	177	HIS	ILE	ENGINEERED MUTATION	UNP P0C0Y8
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

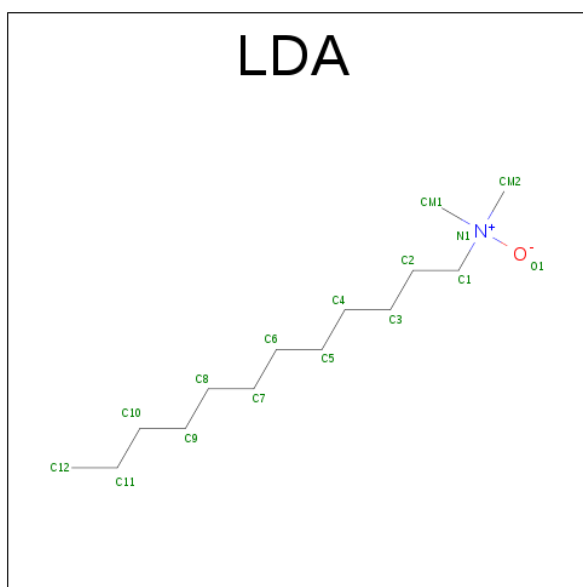
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There is a discrepancy between the modelled and reference sequences:

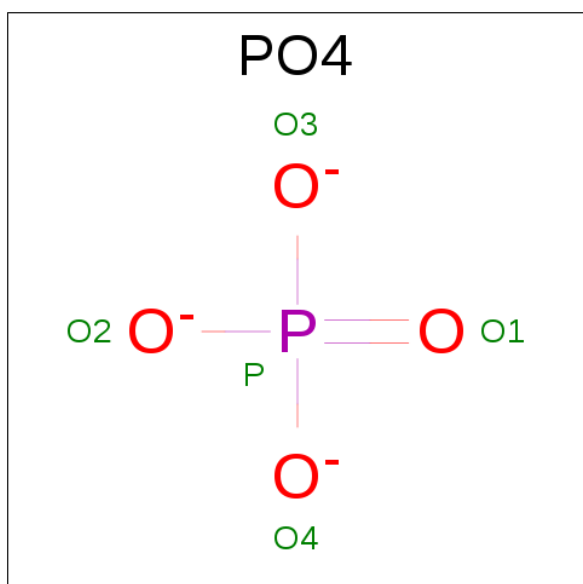
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



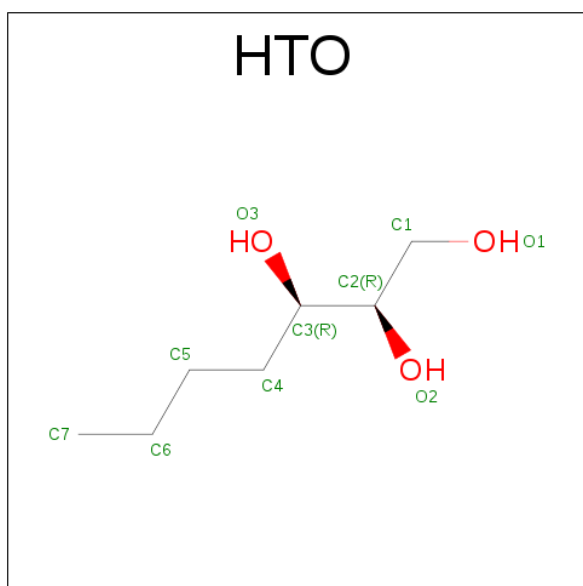
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



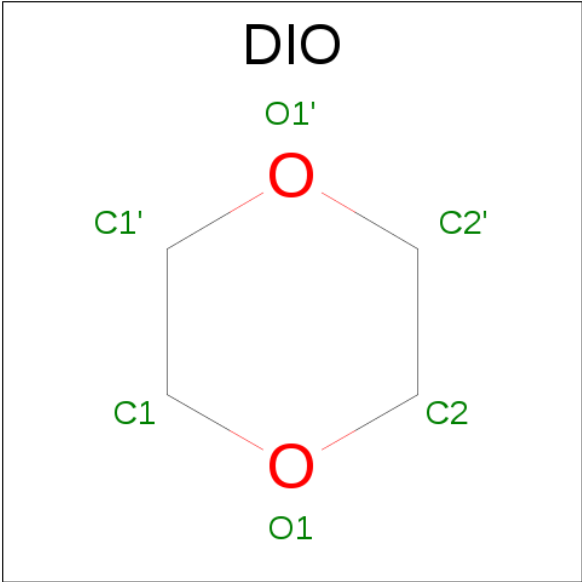
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0

- Molecule 6 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 10 7 3	0	0
6	H	1	Total C O 10 7 3	0	0
6	L	1	Total C O 10 7 3	0	0

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula:  $C_4H_8O_2$ ).

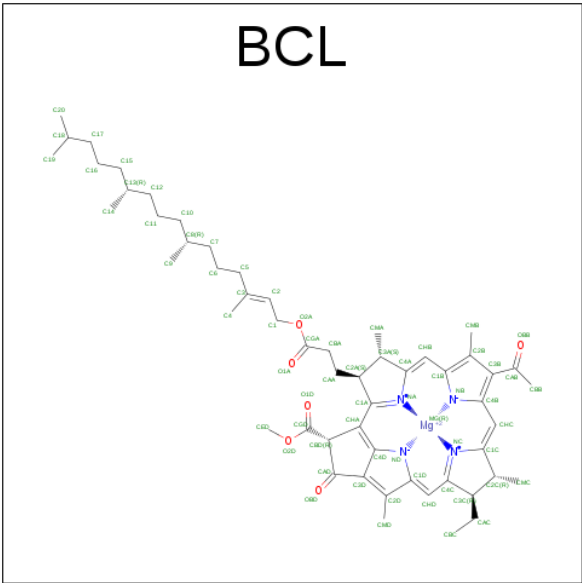


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			6	4	2		
7	L	1	Total	C	O	0	0
			6	4	2		

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

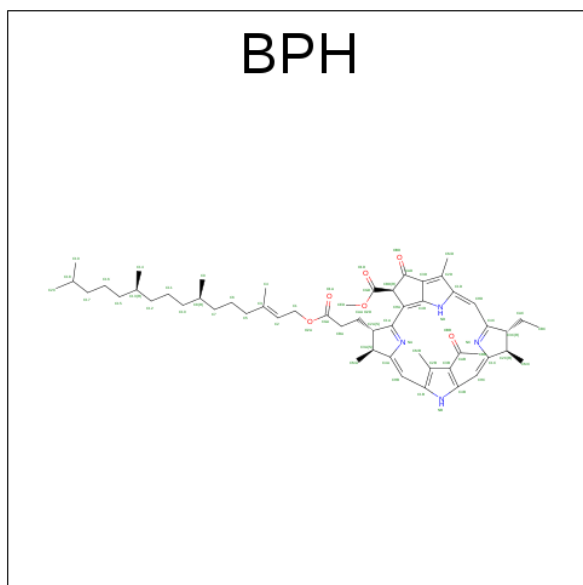
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	K	0	0
			1	1		

- Molecule 9 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
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).

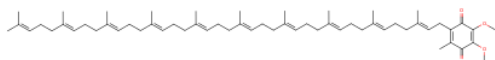


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	L	1	Total	C	N	O	0	0
			65	55	4	6		
10	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



# U10



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

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 13 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).

# SPN



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			43	41	2		

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	M	1	Total	Cl	0	0
			1	1		

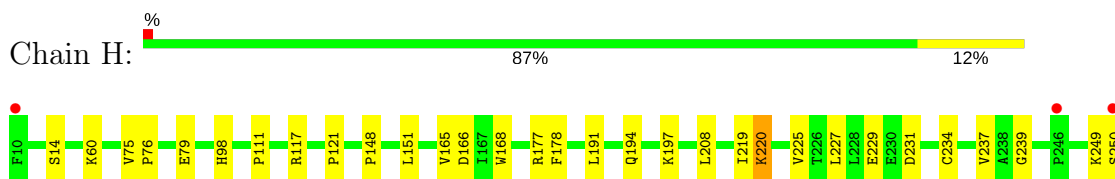
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	13	Total	O	0	0
			13	13		
15	L	19	Total	O	0	0
			19	19		
15	M	17	Total	O	0	0
			17	17		

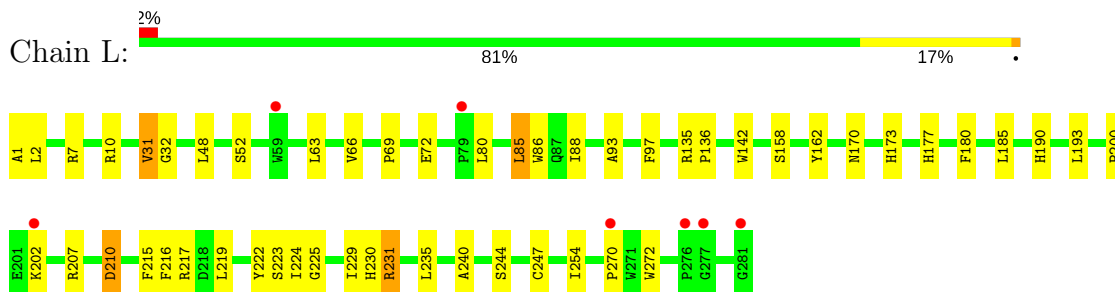
### 3 Residue-property plots [i](#)

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.

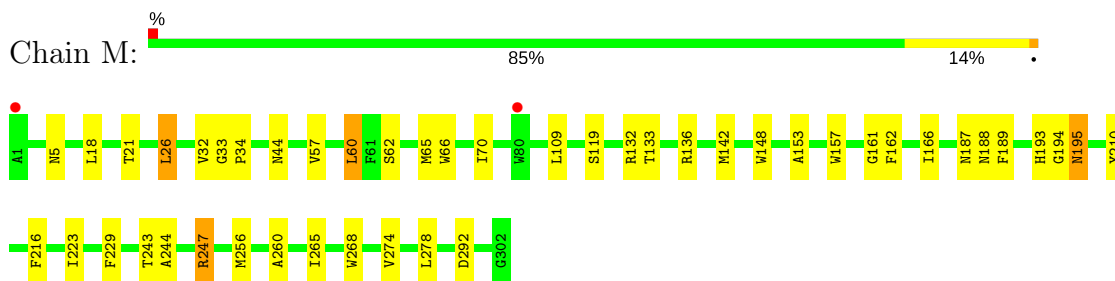
- Molecule 1: Reaction center protein H chain



- Molecule 2: Reaction center protein L chain



- Molecule 3: Reaction center protein M chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.13Å 140.13Å 186.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.90 – 2.90 28.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.90-2.90) 96.6 (28.90-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.204 , 0.251 0.204 , 0.251	Depositor DCC
$R_{free}$ test set	2286 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7216	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, LDA, DIO, CL, HTO, BPH, K, FE, SPN, U10, PO4

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	H	0.53	0/1889	0.62	0/2569
2	L	0.56	0/2324	0.59	0/3181
3	M	0.52	0/2501	0.60	1/3415 (0.0%)
All	All	0.54	0/6714	0.60	1/9165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	26	LEU	CA-CB-CG	5.02	126.85	115.30

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	H	1840	0	1845	20	0
2	L	2235	0	2185	48	0
3	M	2409	0	2323	32	0
4	H	16	0	31	0	0
4	M	64	0	124	1	0
5	H	10	0	0	0	0
5	M	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	20	0	32	0	0
6	L	10	0	16	0	0
7	H	6	0	8	5	0
7	L	6	0	8	0	0
8	H	1	0	0	0	0
9	L	198	0	222	20	0
9	M	66	0	74	5	0
10	L	65	0	76	7	0
10	M	65	0	76	5	0
11	L	48	0	63	9	0
11	M	48	0	63	2	0
12	M	1	0	0	0	0
13	M	43	0	70	6	0
14	M	1	0	0	0	0
15	H	13	0	0	1	0
15	L	19	0	0	2	0
15	M	17	0	0	0	0
All	All	7216	0	7216	109	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 8.

The worst 5 of 109 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)
2:L:177:HIS:CD2	9:L:302:BCL:HMB3	1.62	1.34
2:L:177:HIS:NE2	9:L:302:BCL:CMB	1.92	1.33
2:L:177:HIS:NE2	9:L:302:BCL:HMB3	1.52	1.16
2:L:177:HIS:NE2	9:L:302:BCL:HMB1	1.81	0.95
2:L:177:HIS:CD2	9:L:302:BCL:CMB	2.42	0.93

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	H	239/241 (99%)	222 (93%)	17 (7%)	0	100	100
2	L	279/281 (99%)	251 (90%)	25 (9%)	3 (1%)	17	48
3	M	300/302 (99%)	277 (92%)	21 (7%)	2 (1%)	25	60
All	All	818/824 (99%)	750 (92%)	63 (8%)	5 (1%)	28	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	80	LEU
3	M	34	PRO
3	M	195	ASN
2	L	270	PRO
2	L	31	VAL

### 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	H	196/196 (100%)	190 (97%)	6 (3%)	45	79
2	L	220/220 (100%)	206 (94%)	14 (6%)	20	50
3	M	236/236 (100%)	226 (96%)	10 (4%)	34	69
All	All	652/652 (100%)	622 (95%)	30 (5%)	31	65

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	210	ASP
2	L	235	LEU
3	M	274	VAL
2	L	231	ARG
2	L	247	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	206	ASN
2	L	183	ASN
3	M	187	ASN
3	M	193	HIS

### 5.3.3 RNA ⓘ

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 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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	$\# Z  > 2$
6	HTO	H	2	-	9,9,9	0.31	0	9,10,10	0.61	0
7	DIO	H	251	-	6,6,6	0.45	0	6,6,6	1.03	0
6	HTO	H	3	-	9,9,9	0.46	0	9,10,10	0.56	0
4	LDA	H	704	-	13,15,15	2.38	1 (7%)	14,17,17	0.61	0
5	PO4	H	803	-	4,4,4	0.69	0	6,6,6	0.49	0
5	PO4	H	804	-	4,4,4	0.80	0	6,6,6	0.37	0
6	HTO	L	282	-	9,9,9	0.48	0	9,10,10	0.55	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	DIO	L	283	-	6,6,6	0.62	0	6,6,6	0.73	0
9	BCL	L	301	-	55,74,74	0.70	0	65,115,115	1.40	10 (15%)
9	BCL	L	302	-	55,74,74	0.69	2 (3%)	65,115,115	1.58	14 (21%)
9	BCL	L	304	-	55,74,74	0.73	2 (3%)	65,115,115	1.51	11 (16%)
10	BPH	L	402	-	65,70,70	1.37	7 (10%)	75,101,101	1.50	11 (14%)
11	U10	L	502	-	48,48,63	2.75	14 (29%)	58,61,79	1.68	15 (25%)
9	BCL	M	303	-	55,74,74	0.72	2 (3%)	65,115,115	1.46	12 (18%)
10	BPH	M	401	-	65,70,70	1.39	7 (10%)	75,101,101	1.67	13 (17%)
11	U10	M	501	-	48,48,63	2.65	12 (25%)	58,61,79	1.51	11 (18%)
13	SPN	M	600	-	40,42,42	0.57	0	48,52,52	1.49	7 (14%)
4	LDA	M	701	-	13,15,15	2.35	1 (7%)	14,17,17	0.83	1 (7%)
4	LDA	M	702	-	13,15,15	2.27	1 (7%)	14,17,17	0.81	1 (7%)
4	LDA	M	703	-	13,15,15	2.38	1 (7%)	14,17,17	0.65	0
4	LDA	M	705	-	13,15,15	2.41	1 (7%)	14,17,17	0.44	0
5	PO4	M	800	-	4,4,4	0.89	0	6,6,6	0.47	0
5	PO4	M	801	-	4,4,4	0.78	0	6,6,6	0.35	0
5	PO4	M	802	-	4,4,4	0.76	0	6,6,6	0.30	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
6	HTO	H	2	-	-	0/10/10/10	0/0/0/0
7	DIO	H	251	-	-	0/0/6/6	0/1/1/1
6	HTO	H	3	-	-	0/10/10/10	0/0/0/0
4	LDA	H	704	-	-	0/13/13/13	0/0/0/0
5	PO4	H	803	-	-	0/0/0/0	0/0/0/0
5	PO4	H	804	-	-	0/0/0/0	0/0/0/0
6	HTO	L	282	-	-	0/10/10/10	0/0/0/0
7	DIO	L	283	-	-	0/0/6/6	0/1/1/1
9	BCL	L	301	-	-	0/37/137/137	0/0/9/9
9	BCL	L	302	-	-	0/37/137/137	0/0/9/9
9	BCL	L	304	-	-	0/37/137/137	0/0/9/9
10	BPH	L	402	-	2/2/18/22	0/54/105/105	0/1/6/6
11	U10	L	502	-	-	0/45/69/87	0/1/1/1
9	BCL	M	303	-	-	0/37/137/137	0/0/9/9
10	BPH	M	401	-	2/2/18/22	0/54/105/105	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	U10	M	501	-	-	0/45/69/87	0/1/1/1
13	SPN	M	600	-	-	0/50/51/51	0/0/0/0
4	LDA	M	701	-	-	0/13/13/13	0/0/0/0
4	LDA	M	702	-	-	0/13/13/13	0/0/0/0
4	LDA	M	703	-	-	0/13/13/13	0/0/0/0
4	LDA	M	705	-	-	0/13/13/13	0/0/0/0
5	PO4	M	800	-	-	0/0/0/0	0/0/0/0
5	PO4	M	801	-	-	0/0/0/0	0/0/0/0
5	PO4	M	802	-	-	0/0/0/0	0/0/0/0

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	705	LDA	O1-N1	-8.45	1.25	1.42
4	M	703	LDA	O1-N1	-8.35	1.25	1.42
4	H	704	LDA	O1-N1	-8.33	1.25	1.42
4	M	701	LDA	O1-N1	-8.22	1.26	1.42
4	M	702	LDA	O1-N1	-7.92	1.26	1.42

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	401	BPH	C4D-C3D-CAD	-4.98	104.93	107.78
10	L	402	BPH	C4D-CHA-C1A	-4.32	119.22	130.23
11	L	502	U10	O5-C5-C4	-4.26	111.90	120.95
10	M	401	BPH	C4D-CHA-C1A	-4.03	119.96	130.23
11	L	502	U10	C7-C6-C1	-3.70	116.19	123.47

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	M	401	BPH	C8
10	M	401	BPH	C13
10	L	402	BPH	C8
10	L	402	BPH	C13

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	251	DIO	5	0
9	L	301	BCL	5	0
9	L	302	BCL	13	0
9	L	304	BCL	2	0
10	L	402	BPH	7	0
11	L	502	U10	9	0
9	M	303	BCL	5	0
10	M	401	BPH	5	0
11	M	501	U10	2	0
13	M	600	SPN	6	0
4	M	703	LDA	1	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	H	241/241 (100%)	-0.38	3 (1%) 79 77	51, 65, 76, 101	0
2	L	281/281 (100%)	-0.43	7 (2%) 58 53	49, 65, 100, 106	0
3	M	302/302 (100%)	-0.45	2 (0%) 87 86	44, 67, 98, 101	0
All	All	824/824 (100%)	-0.43	12 (1%) 74 72	44, 66, 97, 106	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	5.0
1	H	10	PHE	4.4
2	L	59	TRP	3.4
3	M	80	TRP	3.3
3	M	1	ALA	3.2

### 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
11	U10	L	502	48/63	0.69	0.51	14.41	128,135,140,140	0
4	LDA	H	704	16/16	0.67	0.52	6.98	109,114,120,120	0
4	LDA	M	703	16/16	0.69	0.53	6.34	98,102,107,108	0
4	LDA	M	702	16/16	0.78	0.40	4.68	96,109,120,121	0
6	HTO	L	282	10/10	0.86	0.33	4.50	97,98,99,100	0
4	LDA	M	705	16/16	0.90	0.45	4.15	83,90,100,101	0
4	LDA	M	701	16/16	0.87	0.23	3.55	77,85,88,88	0
6	HTO	H	2	10/10	0.83	0.32	3.23	134,136,136,136	0
9	BCL	L	301	66/66	0.95	0.21	3.09	62,71,111,113	0
13	SPN	M	600	43/43	0.89	0.23	2.04	65,76,86,87	0
10	BPH	M	401	65/65	0.89	0.22	1.97	63,73,107,107	0
11	U10	M	501	48/63	0.93	0.20	1.17	53,60,89,89	0
7	DIO	H	251	6/6	0.95	0.23	0.80	84,84,85,86	0
10	BPH	L	402	65/65	0.97	0.16	0.71	48,56,66,66	0
5	PO4	M	801	5/5	0.86	0.28	0.51	140,140,140,140	0
9	BCL	L	302	66/66	0.97	0.17	0.33	45,61,64,65	0
9	BCL	M	303	66/66	0.98	0.15	-0.05	57,60,71,76	0
9	BCL	L	304	66/66	0.98	0.12	-0.78	37,42,64,66	0
5	PO4	M	802	5/5	0.90	0.15	-1.48	110,110,111,111	0
12	FE	M	500	1/1	0.99	0.11	-1.67	55,55,55,55	0
8	K	H	1	1/1	0.95	0.07	-1.83	64,64,64,64	0
6	HTO	H	3	10/10	0.72	0.35	-	113,114,114,115	0
14	CL	M	304	1/1	0.94	0.06	-	83,83,83,83	0
5	PO4	H	803	5/5	0.87	0.19	-	124,124,124,124	0
7	DIO	L	283	6/6	0.63	0.33	-	131,131,131,132	0
5	PO4	H	804	5/5	0.82	0.24	-	123,123,123,123	0
5	PO4	M	800	5/5	0.98	0.08	-	67,67,68,69	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.