



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:58 PM GMT

PDB ID : 1RG5  
Title : Structure of the photosynthetic reaction centre from Rhodobacter sphaeroides carotenoidless strain R-26.1  
Authors : Roszak, A.W.; Hashimoto, H.; Gardiner, A.T.; Cogdell, R.J.; Isaacs, N.W.  
Deposited on : 2003-11-11  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

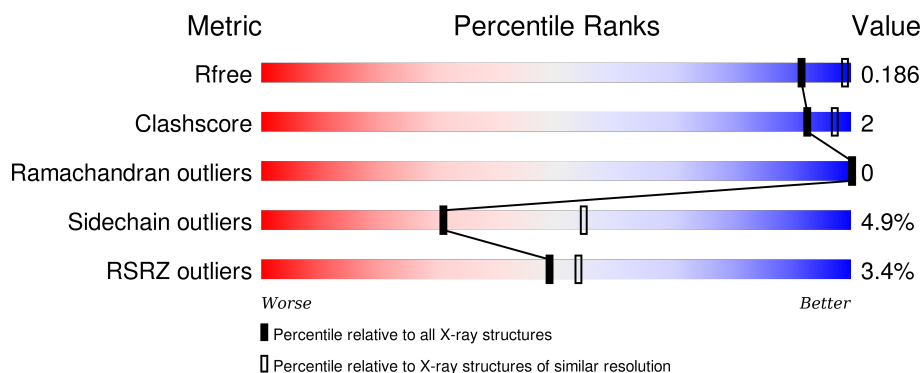
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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>92%</div> <div>6% •</div> </div>
2	M	307	<div> <div>3%</div> <div>92%</div> <div>5% ••</div> </div>
3	H	260	<div> <div>5%</div> <div>85%</div> <div>6% • 7%</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	LDA	M	902	-	-	-	X
10	LDA	M	905	-	-	-	X
10	LDA	M	907	-	-	-	X
10	LDA	M	920	-	-	-	X
7	U10	L	502	-	-	-	X
8	HTO	L	707	-	-	-	X
8	HTO	M	706	X	-	-	X
9	CDL	M	800	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7451 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	3	0
			2237	1509	355	365	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	6	0
			2440	1633	394	403	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	241	Total	C	N	O	S	0	2	0
			1843	1176	319	339	9			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

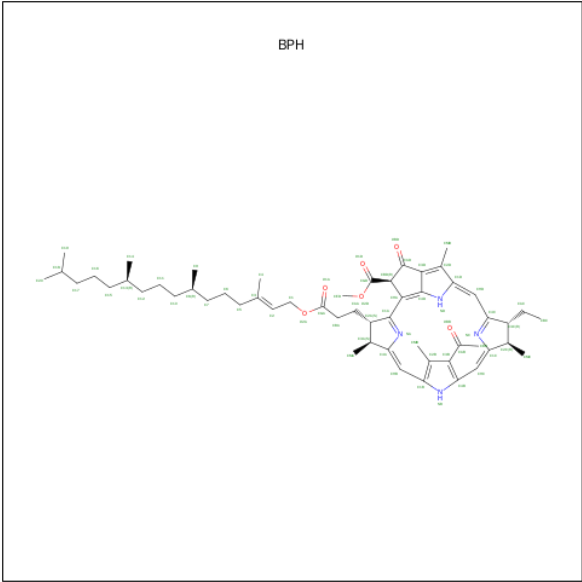
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



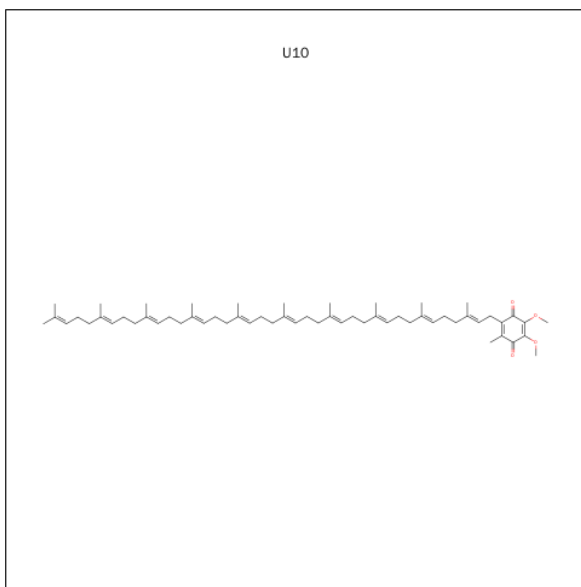
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



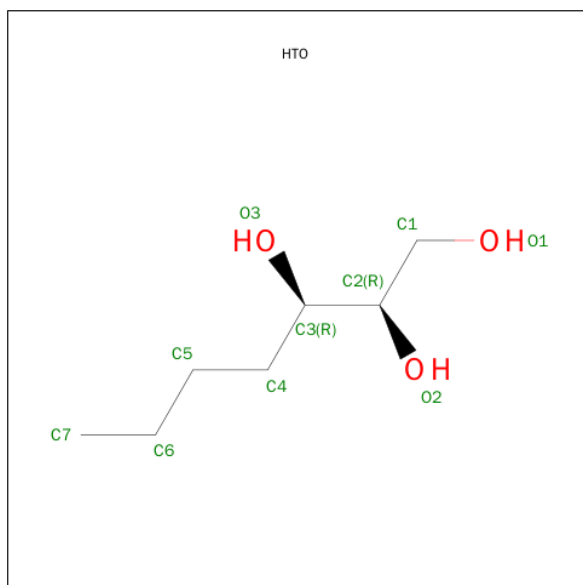
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total	C	N	O	0	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



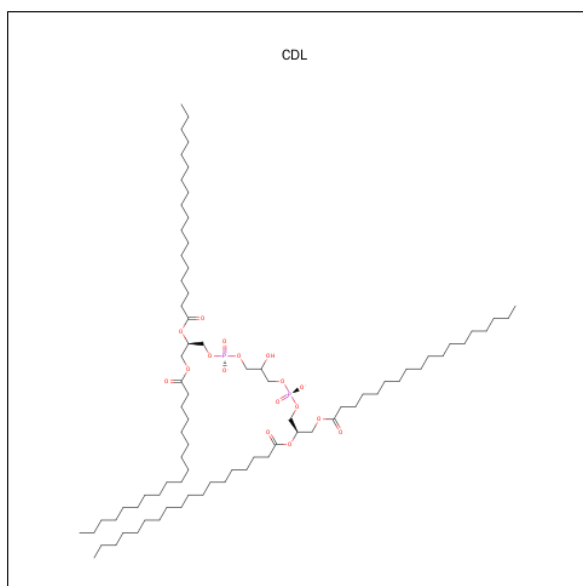
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		
7	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			10	7	3		
8	L	1	Total	C	O	0	0
			10	7	3		

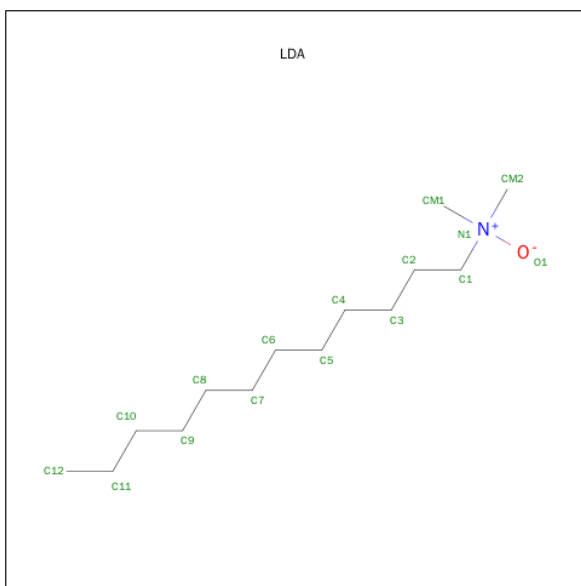
- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 10 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
10	H	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 11 is water.

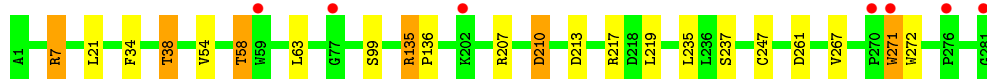
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	115	Total	O	0	0
			115	115		
11	L	54	Total	O	0	0
			54	54		
11	M	74	Total	O	0	0
			74	74		



### 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.

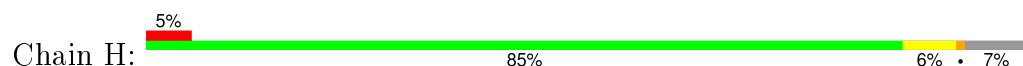
- Molecule 1: Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	144.03Å 144.03Å 190.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.34 – 2.50 23.34 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.1 (23.34-2.50) 99.3 (23.34-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, $R_{free}$	0.155 , 0.182 0.159 , 0.186	Depositor DCC
$R_{free}$ test set	3913 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 95.0	EDS
Estimated twinning fraction	0.012 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 78682 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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, LDA, CDL, BPH, HTO, FE, U10

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	0.79	0/2342	0.92	10/3205 (0.3%)
2	M	0.77	0/2570	0.77	4/3507 (0.1%)
3	H	0.84	2/1901 (0.1%)	0.95	9/2585 (0.3%)
All	All	0.80	2/6813 (0.0%)	0.87	23/9297 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CD-OE1	6.07	1.32	1.25
3	H	94	GLU	CG-CD	5.39	1.60	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	217	ARG	NE-CZ-NH1	11.61	126.10	120.30
1	L	135	ARG	NE-CZ-NH1	11.45	126.03	120.30
1	L	7	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	L	135	ARG	NE-CZ-NH2	-9.73	115.44	120.30
3	H	70	ARG	NE-CZ-NH1	8.83	124.71	120.30
3	H	70	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	L	210	ASP	CB-CG-OD1	7.25	124.82	118.30
1	L	217	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	L	213	ASP	CB-CG-OD2	6.27	123.94	118.30
2	M	88	ASP	CB-CG-OD2	6.14	123.83	118.30
3	H	225	VAL	CB-CA-C	-6.14	99.73	111.40
3	H	103	ASP	CB-CG-OD1	6.14	123.83	118.30
3	H	157	ASP	CB-CG-OD2	6.01	123.71	118.30
3	H	83	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	L	7	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	L	207	ARG	NE-CZ-NH2	-5.49	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	136	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	L	261	ASP	CB-CG-OD2	5.34	123.11	118.30
3	H	124	ASP	CB-CG-OD1	5.33	123.10	118.30
3	H	231	ASP	CB-CG-OD2	5.26	123.03	118.30
2	M	253	ARG	NE-CZ-NH2	5.19	122.89	120.30
3	H	82	ASP	CB-CG-OD2	5.16	122.94	118.30
2	M	204	LEU	CB-CG-CD1	5.07	119.61	111.00

There are no chirality outliers.

There are no planarity outliers.

## 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	2237	0	2193	7	0
2	M	2440	0	2349	9	0
3	H	1843	0	1849	1	0
4	M	1	0	0	0	0
5	L	132	0	148	3	0
5	M	132	0	148	5	0
6	L	65	0	75	0	0
6	M	65	0	76	2	0
7	L	48	0	63	2	0
7	M	48	0	63	1	0
8	L	10	0	16	0	0
8	M	10	0	16	0	0
9	M	81	0	106	0	0
10	H	16	0	31	0	0
10	M	80	0	155	1	0
11	H	115	0	0	0	0
11	L	54	0	0	0	0
11	M	74	0	0	1	0
All	All	7451	0	7288	29	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 2.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:THR:HG21	1:L:63:LEU:HD12	1.66	0.78
7:L:502:U10:H252	7:L:502:U10:H211	1.73	0.69
5:L:304:BCL:HMB1	5:L:304:BCL:HBB2	1.78	0.64
5:L:302:BCL:CBB	5:L:302:BCL:HMB1	2.31	0.60
2:M:162:PHE:O	2:M:166:ILE:HG12	2.02	0.60
5:L:302:BCL:HBB3	5:L:302:BCL:HMB1	1.84	0.60
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.02	0.59
2:M:199:ASN:HD22	2:M:199:ASN:C	2.07	0.58
5:M:501:BCL:HMB1	5:M:501:BCL:CBB	2.34	0.58
7:L:502:U10:C25	7:L:502:U10:H211	2.35	0.57
5:M:501:BCL:H72	5:M:501:BCL:H41	1.89	0.54
1:L:34:PHE:O	1:L:38:THR:HG23	2.07	0.54
5:M:502:BCL:CBB	5:M:502:BCL:HMB1	2.42	0.50
1:L:271:TRP:CD1	1:L:271:TRP:N	2.78	0.49
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.49
5:M:501:BCL:HBB2	5:M:501:BCL:HMB1	1.97	0.47
2:M:175:VAL:HB	10:M:920:LDA:C11	2.46	0.46
1:L:58:THR:HG21	1:L:63:LEU:CD1	2.41	0.46
2:M:25:ASN:ND2	11:M:983:HOH:O	2.49	0.45
6:M:401:BPH:HBC3	6:M:401:BPH:HHD	1.99	0.44
6:M:401:BPH:H4C1	6:M:401:BPH:H6C1	1.64	0.44
1:L:38:THR:HG22	1:L:99:SER:HB3	2.00	0.43
1:L:219:LEU:O	2:M:132:ARG:NH1	2.51	0.43
2:M:21:THR:HG23	2:M:26:LEU:HD21	2.00	0.42
2:M:136:ARG:NE	2:M:136:ARG:HA	2.35	0.41
2:M:51:TYR:O	2:M:132:ARG:NH2	2.54	0.41
7:M:503:U10:C4M	7:M:503:U10:O3	2.68	0.41
5:M:502:BCL:HMB1	5:M:502:BCL:HBB3	2.01	0.41
2:M:199:ASN:HD22	2:M:200:PRO:N	2.19	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	282/281 (100%)	275 (98%)	7 (2%)	0	100	100
2	M	307/307 (100%)	300 (98%)	7 (2%)	0	100	100
3	H	241/260 (93%)	237 (98%)	4 (2%)	0	100	100
All	All	830/848 (98%)	812 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	L	223/220 (101%)	210 (94%)	13 (6%)	25	45
2	M	243/240 (101%)	232 (96%)	11 (4%)	34	59
3	H	197/208 (95%)	186 (94%)	11 (6%)	26	47
All	All	663/668 (99%)	628 (95%)	35 (5%)	31	50

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	21	LEU
1	L	38	THR
1	L	54	VAL
1	L	58	THR
1	L	210	ASP
1	L	235	LEU
1	L	237[A]	SER
1	L	237[B]	SER
1	L	247	CYS
1	L	267	VAL
1	L	271	TRP
1	L	272	TRP

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Mol	Chain	Res	Type
2	M	12	VAL
2	M	60[A]	LEU
2	M	60[B]	LEU
2	M	67[A]	PHE
2	M	67[B]	PHE
2	M	124	VAL
2	M	132	ARG
2	M	182	HIS
2	M	199	ASN
2	M	204	LEU
2	M	216	PHE
3	H	11	ASP
3	H	14	SER
3	H	15	LEU
3	H	60	LYS
3	H	200	SER
3	H	202	ARG
3	H	220	LYS
3	H	221	SER
3	H	225	VAL
3	H	231	ASP
3	H	247	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	183	ASN
2	M	25	ASN
2	M	28	ASN
2	M	199	ASN

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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$
10	LDA	H	901	-	15,15,15	3.53	2 (13%)	16,17,17	1.18	1 (6%)
5	BCL	L	302	1	53,74,74	0.67	0	57,115,115	1.32	11 (19%)
5	BCL	L	304	1	53,74,74	0.77	0	57,115,115	1.49	8 (14%)
6	BPH	L	402	-	64,70,70	0.74	0	73,101,101	1.33	9 (12%)
7	U10	L	502	-	48,48,63	1.04	2 (4%)	58,61,79	1.64	13 (22%)
8	HTO	L	707	-	9,9,9	0.56	0	8,10,10	1.70	2 (25%)
6	BPH	M	401	-	64,70,70	0.67	1 (1%)	73,101,101	1.34	9 (12%)
5	BCL	M	501	2	53,74,74	0.70	1 (1%)	57,115,115	1.60	12 (21%)
5	BCL	M	502	2	53,74,74	0.64	0	57,115,115	1.41	8 (14%)
7	U10	M	503	-	48,48,63	1.08	3 (6%)	58,61,79	1.43	9 (15%)
8	HTO	M	706	-	9,9,9	0.43	0	8,10,10	1.52	2 (25%)
9	CDL	M	800	-	80,80,99	1.10	4 (5%)	82,92,111	1.26	7 (8%)
10	LDA	M	902	-	15,15,15	3.86	1 (6%)	16,17,17	1.47	1 (6%)
10	LDA	M	903	-	15,15,15	3.66	2 (13%)	16,17,17	0.70	0
10	LDA	M	905	-	15,15,15	3.56	1 (6%)	16,17,17	0.99	1 (6%)
10	LDA	M	907	-	15,15,15	3.80	1 (6%)	16,17,17	0.89	1 (6%)
10	LDA	M	920	-	15,15,15	3.29	1 (6%)	16,17,17	0.95	1 (6%)

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
10	LDA	H	901	-	-	0/13/13/13	0/0/0/0
5	BCL	L	302	1	-	0/37/137/137	0/0/9/9
5	BCL	L	304	1	-	0/37/137/137	0/0/9/9
6	BPH	L	402	-	-	0/54/105/105	0/1/6/6
7	U10	L	502	-	-	0/45/69/87	0/1/1/1
8	HTO	L	707	-	-	0/10/10/10	0/0/0/0
6	BPH	M	401	-	-	0/54/105/105	0/1/6/6
5	BCL	M	501	2	-	0/37/137/137	0/0/9/9
5	BCL	M	502	2	-	0/37/137/137	0/0/9/9
7	U10	M	503	-	-	0/45/69/87	0/1/1/1
8	HTO	M	706	-	1/1/2/2	0/10/10/10	0/0/0/0
9	CDL	M	800	-	-	0/91/91/110	0/0/0/0
10	LDA	M	902	-	-	0/13/13/13	0/0/0/0
10	LDA	M	903	-	-	0/13/13/13	0/0/0/0
10	LDA	M	905	-	-	0/13/13/13	0/0/0/0
10	LDA	M	907	-	-	0/13/13/13	0/0/0/0
10	LDA	M	920	-	-	0/13/13/13	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	902	LDA	O1-N1	-14.74	1.25	1.39
10	M	907	LDA	O1-N1	-14.49	1.25	1.39
10	M	903	LDA	O1-N1	-13.94	1.26	1.39
10	M	905	LDA	O1-N1	-13.59	1.26	1.39
10	H	901	LDA	O1-N1	-13.48	1.26	1.39
10	M	920	LDA	O1-N1	-12.61	1.27	1.39
10	M	903	LDA	C1-N1	-2.23	1.47	1.51
7	M	503	U10	O3-C3M	-2.11	1.40	1.45
10	H	901	LDA	C1-N1	-2.03	1.47	1.51
5	M	501	BCL	OBD-CAD	2.08	1.25	1.22
6	M	401	BPH	CHC-C1C	3.12	1.42	1.36
7	M	503	U10	O4-C4	3.20	1.45	1.37
7	L	502	U10	O4-C4	3.37	1.45	1.37
7	M	503	U10	O3-C3	3.42	1.46	1.37
9	M	800	CDL	OA6-CA5	3.98	1.46	1.34
7	L	502	U10	O3-C3	4.17	1.48	1.37
9	M	800	CDL	OB8-CB7	4.35	1.46	1.33
9	M	800	CDL	OA8-CA7	4.36	1.46	1.33
9	M	800	CDL	OB6-CB5	4.80	1.48	1.34

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	501	BCL	C4-C3-C2	-5.35	113.00	123.50
10	M	902	LDA	O1-N1-CM1	-5.28	102.00	109.05
5	M	502	BCL	CMB-C2B-C1B	-4.43	121.03	128.36
5	M	501	BCL	CMB-C2B-C1B	-4.00	121.75	128.36
5	L	304	BCL	CAC-C3C-C2C	-3.90	104.32	114.13
7	M	503	U10	C32-C33-C34	-3.30	120.58	127.76
6	M	401	BPH	C2B-C1B-NB	-3.24	104.86	109.73
7	L	502	U10	C35-C34-C33	-3.20	117.21	123.50
7	L	502	U10	C7-C8-C9	-3.15	121.36	126.70
7	M	503	U10	C26-C27-C28	-3.14	103.47	111.69
7	L	502	U10	O5-C5-C6	-3.06	115.93	121.68
5	L	304	BCL	CMB-C2B-C1B	-3.04	123.34	128.36
7	M	503	U10	C17-C18-C19	-2.99	121.25	127.76
5	M	502	BCL	CHA-C1A-NA	-2.99	118.71	126.06
5	L	302	BCL	CMB-C2B-C1B	-2.94	123.50	128.36
5	L	302	BCL	CAA-C2A-C3A	-2.90	104.86	113.22
9	M	800	CDL	OB2-PB2-OB3	-2.89	98.41	109.62
5	M	502	BCL	CAC-C3C-C4C	-2.81	106.34	112.58
10	M	905	LDA	O1-N1-CM2	-2.76	105.36	109.05
5	M	502	BCL	O2D-CGD-O1D	-2.76	118.10	123.79
7	L	502	U10	O2-C2-C3	-2.73	114.88	120.79
8	M	706	HTO	O1-C1-C2	-2.73	105.16	111.10
8	L	707	HTO	O2-C2-C1	-2.67	102.98	109.22
10	M	920	LDA	CM2-N1-CM1	-2.64	105.85	108.83
7	L	502	U10	C12-C13-C14	-2.64	122.03	127.76
8	L	707	HTO	C5-C4-C3	-2.63	109.49	114.20
5	M	501	BCL	CAA-C2A-C3A	-2.54	105.92	113.22
5	M	501	BCL	CHA-C1A-NA	-2.53	119.83	126.06
7	L	502	U10	C7-C6-C5	-2.53	115.58	118.56
6	L	402	BPH	C2B-C1B-NB	-2.53	105.93	109.73
6	M	401	BPH	C3B-C4B-NB	-2.52	104.62	109.98
5	L	302	BCL	OBB-CAB-CBB	-2.48	114.18	120.13
5	L	304	BCL	CAA-C2A-C3A	-2.48	106.08	113.22
6	M	401	BPH	C2D-C1D-ND	-2.44	106.29	110.29
5	L	302	BCL	CHA-C1A-NA	-2.43	120.08	126.06
6	L	402	BPH	O2A-CGA-O1A	-2.41	117.26	123.49
5	M	501	BCL	OBB-CAB-CBB	-2.41	114.36	120.13
10	H	901	LDA	CM1-N1-C1	-2.41	102.01	109.77
5	L	302	BCL	CMA-C3A-C2A	-2.39	103.76	114.35
5	M	502	BCL	OBB-CAB-CBB	-2.35	114.49	120.13
6	M	401	BPH	O1D-CGD-CBD	-2.34	121.27	124.62
7	M	503	U10	C7-C6-C5	-2.33	115.81	118.56
5	L	304	BCL	OBB-CAB-CBB	-2.33	114.55	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	706	HTO	O3-C3-C2	-2.31	105.08	109.79
7	L	502	U10	C1M-C1-C6	-2.30	119.18	124.10
7	L	502	U10	C17-C18-C19	-2.27	122.82	127.76
5	M	502	BCL	OBD-CAD-CBD	-2.26	122.53	125.94
5	L	302	BCL	CAC-C3C-C4C	-2.24	107.62	112.58
7	M	503	U10	C31-C29-C28	-2.21	116.87	121.05
5	L	302	BCL	O2A-CGA-O1A	-2.20	117.81	123.49
7	M	503	U10	C22-C23-C24	-2.15	123.08	127.76
5	L	302	BCL	C17-C16-C15	-2.15	102.32	112.99
5	M	501	BCL	CMA-C3A-C2A	-2.08	105.14	114.35
6	L	402	BPH	CMA-C3A-C4A	-2.07	106.27	113.01
9	M	800	CDL	CB2-C1-CA2	-2.04	106.33	112.92
10	M	907	LDA	CM2-N1-CM1	-2.03	106.54	108.83
6	L	402	BPH	C4-C3-C5	-2.01	112.34	115.41
5	L	304	BCL	CAA-CBA-CGA	2.04	119.28	113.32
7	L	502	U10	C21-C22-C23	2.05	117.07	111.69
5	L	302	BCL	C4-C3-C5	2.08	118.59	115.41
5	M	501	BCL	C2C-C3C-C4C	2.09	105.05	101.50
6	M	401	BPH	OBB-CAB-C3B	2.13	124.42	120.31
5	M	502	BCL	CMB-C2B-C3B	2.17	129.34	125.09
5	M	501	BCL	CMB-C2B-C3B	2.23	129.45	125.09
6	M	401	BPH	CAC-C3C-C4C	2.28	118.53	112.67
5	M	501	BCL	C5-C3-C2	2.29	125.40	121.05
5	M	502	BCL	O2D-CGD-CBD	2.37	114.56	111.30
9	M	800	CDL	OB8-CB7-C71	2.42	119.28	111.90
5	L	302	BCL	OBB-CAB-C3B	2.43	123.84	120.00
7	M	503	U10	C4M-O4-C4	2.43	125.26	116.61
6	M	401	BPH	C3C-C4C-NC	2.48	110.41	107.93
5	L	302	BCL	CBA-CAA-C2A	2.56	120.96	113.73
6	L	402	BPH	C1B-NB-C4B	2.67	111.80	106.51
5	L	304	BCL	CED-O2D-CGD	2.79	122.53	115.99
9	M	800	CDL	OA8-CA7-C31	2.83	120.53	111.90
6	L	402	BPH	CAC-C3C-C2C	3.00	121.67	114.13
5	M	501	BCL	CAA-CBA-CGA	3.07	122.31	113.32
7	L	502	U10	C35-C34-C36	3.15	120.21	115.41
6	L	402	BPH	C3C-C4C-NC	3.16	111.09	107.93
7	L	502	U10	C30-C29-C31	3.16	120.23	115.41
5	M	501	BCL	OBB-CAB-C3B	3.16	125.02	120.00
7	L	502	U10	C3M-O3-C3	3.17	127.87	116.61
7	L	502	U10	C15-C14-C16	3.18	120.27	115.41
9	M	800	CDL	CB6-OB8-CB7	3.28	126.03	116.85
5	L	304	BCL	OBB-CAB-C3B	3.33	125.28	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	503	U10	C3M-O3-C3	3.41	128.75	116.61
6	L	402	BPH	CAC-C3C-C4C	3.44	121.50	112.67
6	L	402	BPH	O2D-CGD-CBD	3.44	116.01	111.30
6	M	401	BPH	C1B-NB-C4B	3.45	113.33	106.51
9	M	800	CDL	OA6-CA5-C11	3.55	119.24	111.53
7	M	503	U10	C30-C29-C31	3.88	121.33	115.41
5	L	304	BCL	O2D-CGD-CBD	3.92	116.68	111.30
6	M	401	BPH	O2D-CGD-CBD	3.97	116.75	111.30
5	M	501	BCL	C4-C3-C5	4.04	121.58	115.41
9	M	800	CDL	OB6-CB5-C51	4.89	122.16	111.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	M	706	HTO	C2

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	302	BCL	2	0
5	L	304	BCL	1	0
7	L	502	U10	2	0
6	M	401	BPH	2	0
5	M	501	BCL	3	0
5	M	502	BCL	2	0
7	M	503	U10	1	0
10	M	920	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 ⓘ

### 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	L	281/281 (100%)	-0.41	7 (2%) 61 65	41, 52, 67, 75	0
2	M	302/307 (98%)	-0.42	9 (2%) 54 59	46, 52, 65, 85	0
3	H	241/260 (92%)	-0.31	12 (4%) 32 37	46, 52, 67, 101	0
All	All	824/848 (97%)	-0.38	28 (3%) 49 54	41, 52, 66, 101	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	9.0
3	H	250	SER	8.1
2	M	302	GLY	4.9
3	H	10	PHE	4.8
3	H	245	ALA	4.7
1	L	202	LYS	4.6
3	H	249	LYS	4.6
3	H	246	PRO	4.4
2	M	2[A]	GLU	4.0
1	L	270[A]	PRO	3.7
1	L	271	TRP	3.6
1	L	59	TRP	3.6
2	M	80	TRP	3.5
1	L	281	GLY	3.5
3	H	18	TYR	3.4
3	H	247	LYS	3.3
1	L	276	PRO	2.7
2	M	105	PHE	2.7
2	M	301	HIS	2.6
3	H	52	ASN	2.6
1	L	77	GLY	2.5
3	H	60	LYS	2.3
3	H	190	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	H	208	LEU	2.3
2	M	101	TYR	2.2
2	M	100	GLU	2.0
3	H	51	ALA	2.0
2	M	68[A]	PHE	2.0

## 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
10	LDA	M	920	16/16	0.71	0.44	9.44	84,86,102,103	0
8	HTO	M	706	10/10	0.51	0.44	7.60	48,53,56,57	10
7	U10	L	502	48/63	0.71	0.40	6.86	83,104,112,112	0
9	CDL	M	800	81/100	0.71	0.36	6.44	48,60,72,73	81
8	HTO	L	707	10/10	0.91	0.25	5.91	56,60,62,63	10
10	LDA	M	905	16/16	0.65	0.29	5.55	72,73,81,82	16
10	LDA	M	907	16/16	0.83	0.31	4.73	91,96,99,99	0
10	LDA	M	902	16/16	0.81	0.22	4.26	69,74,79,80	16
6	BPH	M	401	65/65	0.87	0.17	1.82	50,54,112,113	0
5	BCL	M	501	66/66	0.93	0.14	1.30	49,54,106,107	0
10	LDA	H	901	16/16	0.94	0.14	1.27	65,68,79,80	16
7	U10	M	503	48/63	0.91	0.15	0.90	51,64,91,93	0
5	BCL	L	302	66/66	0.96	0.13	0.30	43,48,67,76	0
5	BCL	M	502	66/66	0.97	0.13	0.19	43,48,73,77	0
6	BPH	L	402	65/65	0.96	0.12	-0.14	47,52,59,61	0
5	BCL	L	304	66/66	0.97	0.09	-0.84	45,49,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	FE	M	500	1/1	1.00	0.08	-1.12	49,49,49,49	0
10	LDA	M	903	16/16	0.53	0.31	-	68,72,74,74	16

## 6.5 Other polymers [i](#)

There are no such residues in this entry.