



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 03:37 AM GMT

PDB ID : 2UXM  
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC  
REACTION CENTER FROM RB. SPHAEROIDES AT PH 10 IN THE  
CHARGE-SEPARATED STATE, 2ND DATASET  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-28  
Resolution : 2.70 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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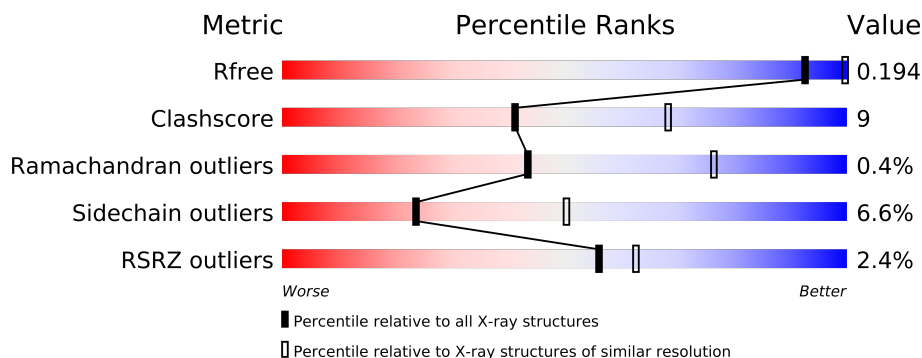
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	H	260	
2	L	281	
3	M	307	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
10	GOL	L	1290	-	X
10	GOL	M	1317	-	X
5	LDA	L	1284	-	X
5	LDA	M	1305	-	X
5	LDA	M	1306	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	LDA	M	1308	-	X
5	LDA	M	1309	-	X
5	LDA	M	1310	-	X
5	LDA	M	1311	-	X
5	LDA	M	1312	-	X
6	BPH	M	1314	-	X
7	UQ2	L	1286[A]	-	X
7	UQ2	L	1286[B]	-	X
8	PO4	L	1287	-	X
9	HTO	L	1288	-	X

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7442 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	3	1
			1846	1181	319	337	9			

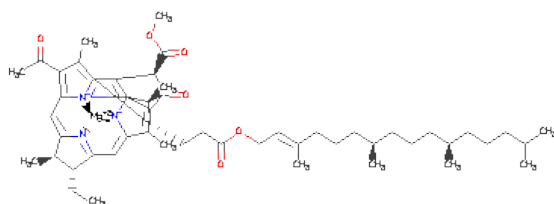
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

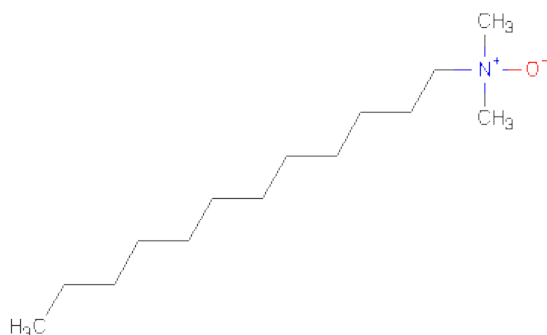
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



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		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



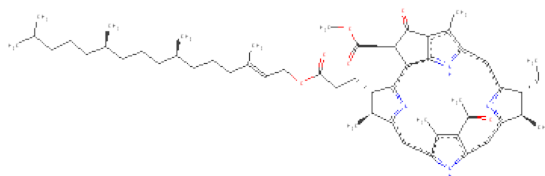
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		

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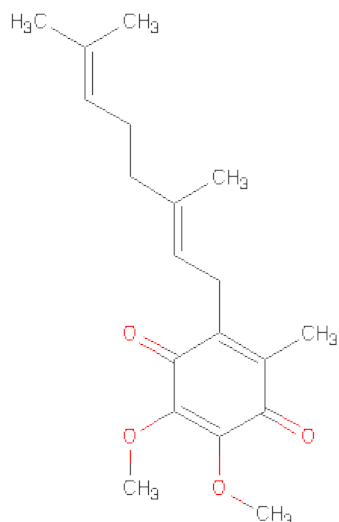
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			16	14	1	1		
5	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



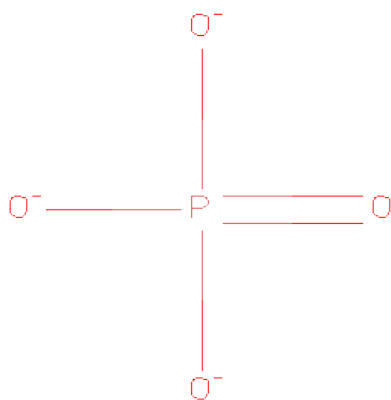
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-2 (three-letter code: UQ2) (formula:  $C_{19}H_{26}O_4$ ).



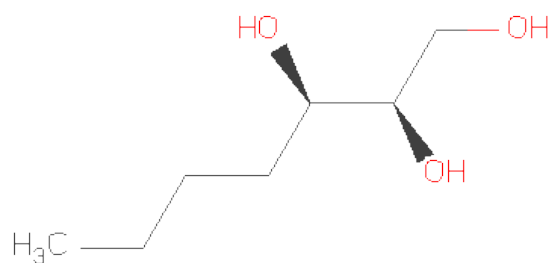
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



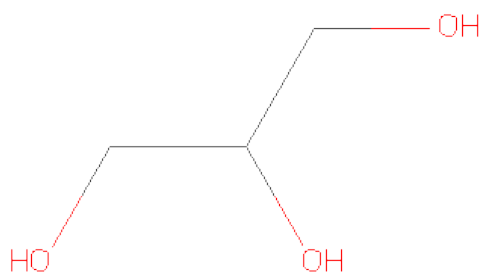
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula:  $C_7H_{16}O_3$ ).



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

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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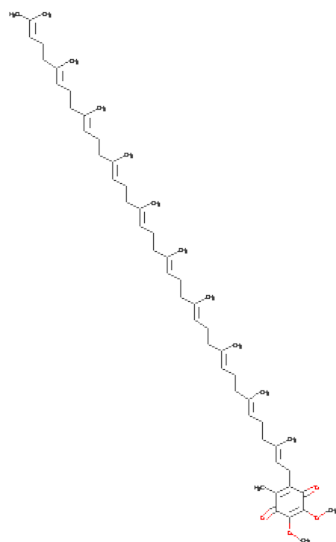
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	X	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

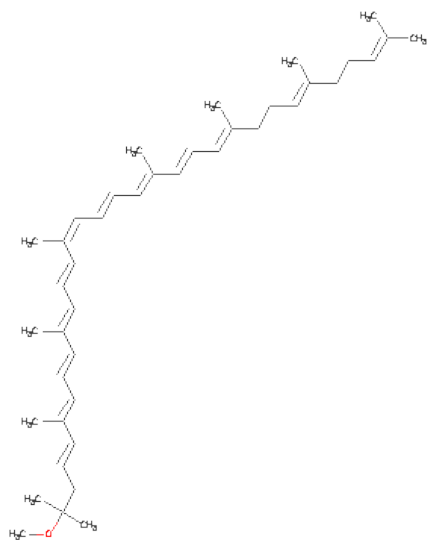
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	1	Total	Fe	0	0
			1	1		

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



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

- Molecule 13 is SPHEROIDENE (three-letter code: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	M	1	Total	C O	0	0
			42	41 1		

- Molecule 14 is water.

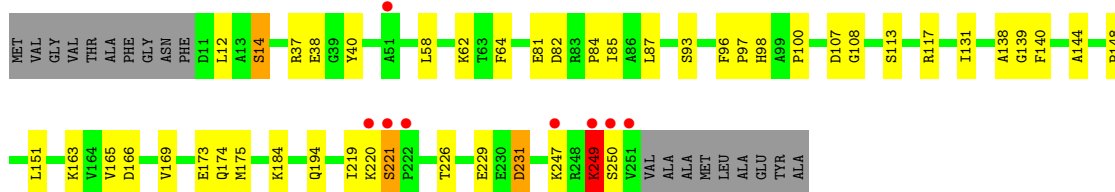
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	H	81	Total	O	0	0
			81	81		
14	L	87	Total	O	0	0
			87	87		
14	M	73	Total	O	0	0
			73	73		

### 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.

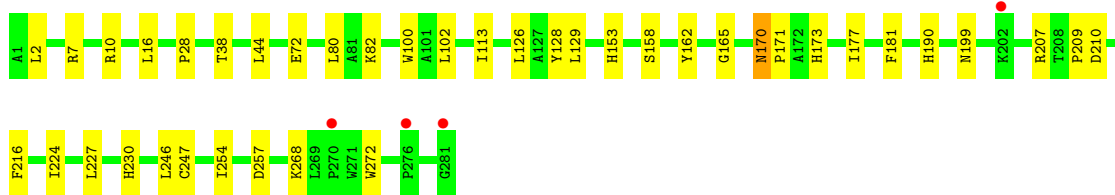
- Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H: 



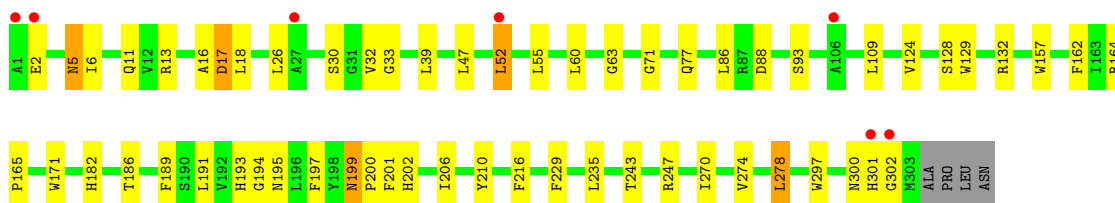
- Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L: 



- Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.45Å 139.45Å 185.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.70 29.89 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.4 (119.52-2.70) 85.5 (29.89-2.52)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.186 , 0.221 0.192 , 0.194	Depositor DCC
$R_{free}$ test set	3025 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.3	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 66734 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, HTO, BPH, PO4, FE, SPO, U10, UQ2

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	0.70	0/1906	0.81	5/2591 (0.2%)
2	L	0.73	0/2320	0.72	1/3175 (0.0%)
3	M	0.68	0/2501	0.75	3/3415 (0.1%)
All	All	0.70	0/6727	0.76	9/9181 (0.1%)

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	231	ASP	CB-CG-OD2	5.91	123.62	118.30
1	H	82	ASP	CB-CG-OD2	5.32	123.09	118.30
2	L	257	ASP	CB-CG-OD2	5.32	123.08	118.30
1	H	107	ASP	CB-CG-OD2	5.24	123.02	118.30
3	M	17	ASP	CB-CG-OD2	5.19	122.97	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1846	0	1861	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	2232	0	2187	26	0
3	M	2409	0	2321	47	0
4	L	132	0	148	9	0
4	M	132	0	148	20	0
5	L	16	0	31	1	0
5	M	128	0	248	18	0
6	L	65	0	76	8	0
6	M	65	0	76	6	0
7	L	46	0	52	13	0
8	L	5	0	0	0	0
9	L	10	0	16	0	0
10	L	12	0	16	1	0
10	M	6	0	8	1	0
10	X	6	0	8	0	0
11	M	1	0	0	0	0
12	M	48	0	63	4	0
13	M	42	0	60	6	0
14	H	81	0	0	1	1
14	L	87	0	0	1	0
14	M	73	0	0	1	0
All	All	7442	0	7319	134	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 134 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:L:1286[A]:UQ2:H152	5:M:1309:LDA:H111	1.47	0.97
4:M:1304:BCL:HHC	4:M:1304:BCL:HBB3	1.50	0.91
7:L:1286[B]:UQ2:H162	5:M:1312:LDA:H121	1.56	0.87
2:L:72:GLU:HB3	14:L:2026:HOH:O	1.74	0.87
1:H:249:LYS:HE3	1:H:249:LYS:HA	1.59	0.84

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:H:2030:HOH:O	14:H:2030:HOH:O[4_555]	1.99	0.21

## 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	H	242/260 (93%)	233 (96%)	8 (3%)	1 (0%)	43	76
2	L	279/281 (99%)	266 (95%)	13 (5%)	0	100	100
3	M	301/307 (98%)	282 (94%)	17 (6%)	2 (1%)	30	62
All	All	822/848 (97%)	781 (95%)	38 (5%)	3 (0%)	43	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	249	LYS
3	M	52	LEU
3	M	301	HIS

### 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	198/208 (95%)	187 (94%)	11 (6%)	30	59
2	L	220/220 (100%)	203 (92%)	17 (8%)	18	40
3	M	236/240 (98%)	220 (93%)	16 (7%)	22	48
All	All	654/668 (98%)	610 (93%)	44 (7%)	24	49

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	170	ASN
2	L	247	CYS
3	M	191	LEU

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Mol	Chain	Res	Type
2	L	207	ARG
2	L	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	5	ASN
3	M	199	ASN
3	M	187	ASN
2	L	170	ASN
3	M	77	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 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	1282	2	74,74,74	2.08	10 (13%)	97,115,115	1.98	22 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BCL	L	1283	2	74,74,74	2.12	11 (14%)	97,115,115	2.26	30 (30%)
5	LDA	L	1284	-	15,15,15	3.62	1 (6%)	17,17,17	0.92	1 (5%)
6	BPH	L	1285	-	70,70,70	3.05	14 (20%)	94,101,101	1.80	17 (18%)
7	UQ2	L	1286[A]	-	23,23,23	2.79	7 (30%)	31,31,31	1.15	2 (6%)
7	UQ2	L	1286[B]	-	23,23,23	2.71	8 (34%)	31,31,31	1.50	4 (12%)
8	PO4	L	1287	-	4,4,4	0.25	0	6,6,6	0.31	0
9	HTO	L	1288	-	9,9,9	0.59	0	10,10,10	0.66	0
10	GOL	L	1289	-	5,5,5	0.29	0	5,5,5	0.64	0
10	GOL	L	1290	-	5,5,5	0.25	0	5,5,5	0.44	0
4	BCL	M	1303	3	74,74,74	2.18	11 (14%)	97,115,115	2.09	25 (25%)
4	BCL	M	1304	3	74,74,74	2.11	11 (14%)	97,115,115	2.18	27 (27%)
5	LDA	M	1305	-	15,15,15	3.56	1 (6%)	17,17,17	2.09	4 (23%)
5	LDA	M	1306	-	15,15,15	3.77	1 (6%)	17,17,17	0.61	0
5	LDA	M	1307	-	15,15,15	3.76	2 (13%)	17,17,17	0.97	1 (5%)
5	LDA	M	1308	-	15,15,15	3.84	1 (6%)	17,17,17	0.85	1 (5%)
5	LDA	M	1309	-	15,15,15	3.87	1 (6%)	17,17,17	0.66	0
5	LDA	M	1310	-	15,15,15	3.64	1 (6%)	17,17,17	0.68	0
5	LDA	M	1311	-	15,15,15	3.73	1 (6%)	17,17,17	0.98	1 (5%)
5	LDA	M	1312	-	15,15,15	3.93	2 (13%)	17,17,17	1.00	1 (5%)
6	BPH	M	1314	-	70,70,70	2.85	16 (22%)	94,101,101	1.88	19 (20%)
12	U10	M	1315	-	48,48,63	3.15	13 (27%)	59,61,79	1.74	11 (18%)
13	SPO	M	1316	-	41,41,41	4.20	12 (29%)	50,50,50	2.02	13 (26%)
10	GOL	M	1317	-	5,5,5	0.29	0	5,5,5	0.51	0
10	GOL	X	1007	-	5,5,5	0.33	0	5,5,5	0.40	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
4	BCL	L	1282	2	2/2/21/25	0/41/137/137	0/0/9/9
4	BCL	L	1283	2	2/2/21/25	0/41/137/137	0/0/9/9
5	LDA	L	1284	-	-	0/13/13/13	0/0/0/0
6	BPH	L	1285	-	2/2/18/22	0/49/105/105	0/0/6/6
7	UQ2	L	1286[A]	-	-	0/15/39/39	0/1/1/1
7	UQ2	L	1286[B]	-	-	0/15/39/39	0/1/1/1
8	PO4	L	1287	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTO	L	1288	-	-	0/10/10/10	0/0/0/0
10	GOL	L	1289	-	-	0/4/4/4	0/0/0/0
10	GOL	L	1290	-	-	0/4/4/4	0/0/0/0
4	BCL	M	1303	3	2/2/21/25	0/41/137/137	0/0/9/9
4	BCL	M	1304	3	2/2/21/25	0/41/137/137	0/0/9/9
5	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1308	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1309	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1310	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1311	-	-	0/13/13/13	0/0/0/0
5	LDA	M	1312	-	-	0/13/13/13	0/0/0/0
6	BPH	M	1314	-	2/2/18/22	0/49/105/105	0/0/6/6
12	U10	M	1315	-	-	0/45/69/87	0/1/1/1
13	SPO	M	1316	-	-	0/47/47/47	0/0/0/0
10	GOL	M	1317	-	-	0/4/4/4	0/0/0/0
10	GOL	X	1007	-	-	0/4/4/4	0/0/0/0

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1312	LDA	O1-N1	-14.99	1.25	1.39
5	M	1309	LDA	O1-N1	-14.81	1.25	1.39
5	M	1308	LDA	O1-N1	-14.64	1.25	1.39
6	L	1285	BPH	C1D-CHD	14.63	1.51	1.35
5	M	1306	LDA	O1-N1	-14.39	1.25	1.39

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1283	BCL	CMB-C2B-C1B	-8.08	116.19	128.62
4	M	1304	BCL	CMB-C2B-C1B	-8.04	116.26	128.62
4	L	1282	BCL	C2D-C1D-ND	-7.92	103.43	109.41
6	M	1314	BPH	C3B-C2B-C1B	-7.76	102.37	107.01
4	M	1303	BCL	CMB-C2B-C1B	-7.10	117.70	128.62

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	1303	BCL	C8

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Mol	Chain	Res	Type	Atom
4	M	1303	BCL	C13
4	L	1283	BCL	C8
4	L	1283	BCL	C13
6	L	1285	BPH	C8

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	241/260 (92%)	-0.46	8 (3%)	44	49	38, 50, 63, 105	0
2	L	281/281 (100%)	-0.75	4 (1%)	72	77	32, 43, 69, 77	0
3	M	303/307 (98%)	-0.56	7 (2%)	57	64	31, 50, 75, 96	0
All	All	825/848 (97%)	-0.60	19 (2%)	56	64	31, 48, 71, 105	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	1	ALA	7.4
1	H	250	SER	7.1
1	H	251	VAL	7.0
1	H	249	LYS	3.9
3	M	302	GLY	3.8

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	LDA	M	1312	16/16	0.37	31.58	101,109,116,116	0
5	LDA	L	1284	16/16	0.46	27.00	61,96,114,115	0
5	LDA	M	1311	16/16	0.48	25.77	87,101,112,113	0
5	LDA	M	1308	16/16	0.43	15.99	91,99,110,110	0
7	UQ2	L	1286[A]	23/23	0.31	13.16	51,53,54,55	23
5	LDA	M	1309	16/16	0.45	11.32	111,117,128,129	0
7	UQ2	L	1286[B]	23/23	0.31	10.53	43,49,55,55	23
9	HTO	L	1288	10/10	0.30	6.90	77,81,82,82	0
5	LDA	M	1305	16/16	0.25	6.80	45,71,82,82	0
8	PO4	L	1287	5/5	0.61	6.78	156,156,157,157	0
10	GOL	M	1317	6/6	0.25	5.17	98,101,101,103	0
5	LDA	M	1310	16/16	0.61	5.09	100,116,126,126	0
5	LDA	M	1306	16/16	0.32	4.44	76,79,86,86	0
10	GOL	L	1290	6/6	0.24	2.45	81,81,82,82	0
6	BPH	M	1314	65/65	0.18	2.14	42,50,111,113	0
12	U10	M	1315	48/63	0.17	1.70	37,48,78,80	0
13	SPO	M	1316	42/42	0.18	1.67	44,60,78,81	0
10	GOL	L	1289	6/6	0.29	1.63	71,74,74,76	0
5	LDA	M	1307	16/16	0.19	1.40	65,67,78,79	0
4	BCL	M	1304	66/66	0.14	0.69	29,39,60,70	0
6	BPH	L	1285	65/65	0.12	0.68	26,32,41,43	0
4	BCL	M	1303	66/66	0.12	0.65	30,34,81,82	0
4	BCL	L	1282	66/66	0.12	0.45	30,36,47,52	0
4	BCL	L	1283	66/66	0.11	-0.36	30,37,58,62	0
11	FE	M	1313	1/1	0.04	-3.81	37,37,37,37	0
10	GOL	X	1007	6/6	0.33	-	96,97,98,98	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.