



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 03:40 AM GMT

PDB ID : 2UXL  
Title : X-RAY HIGH RESOLUTION STRUCTURE OF THE PHOTOSYNTHETIC  
REACTION CENTER FROM RB. SPHAEROIDES AT PH 10 IN THE NEU-  
TRAL STATE, 2ND DATASET  
Authors : Koepke, J.; Diehm, R.; Fritzsche, G.  
Deposited on : 2007-03-28  
Resolution : 2.88 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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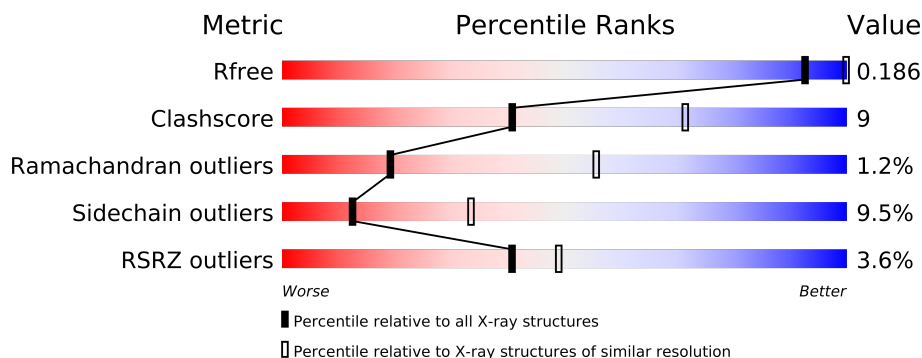
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.88 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	1360 (2.90-2.86)
Clashscore	79885	1696 (2.90-2.86)
Ramachandran outliers	78287	1647 (2.90-2.86)
Sidechain outliers	78261	1650 (2.90-2.86)
RSRZ outliers	66119	1362 (2.90-2.86)

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
11	U10	M	1310	-	X
12	SPO	M	1311	-	X
4	GOL	H	1251	-	X
4	GOL	H	1252	-	X
4	GOL	L	1287	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	BPH	M	1309	-	X
7	UQ2	L	1284[A]	-	X
7	UQ2	L	1284[B]	-	X
8	HTO	L	1286	-	X
9	LDA	M	1305	-	X
9	LDA	M	1306	-	X
9	LDA	M	1307	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7302 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			

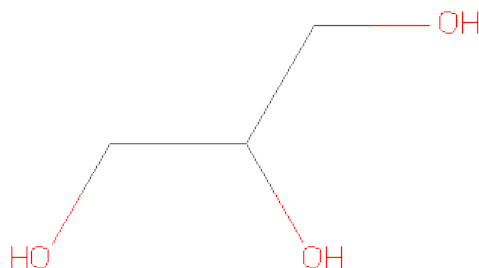
- Molecule 2 is a protein called REACTION CENTER PROTEIN L CHAIN.

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.

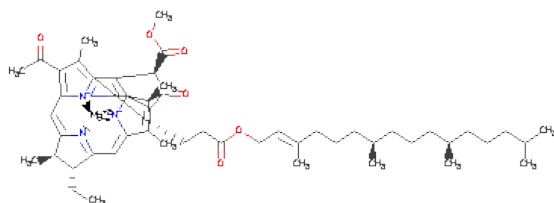
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2409	1607	395	397	10			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



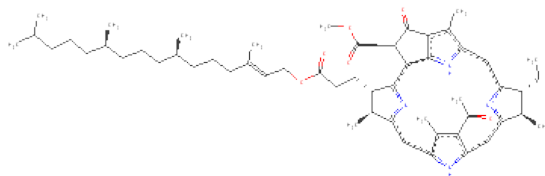
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



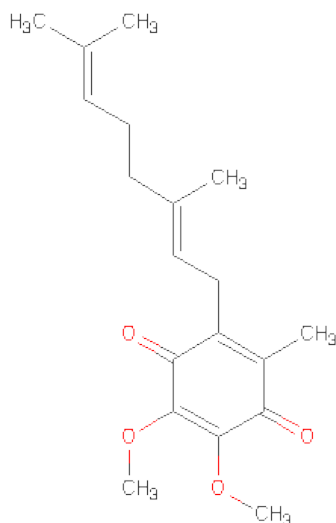
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



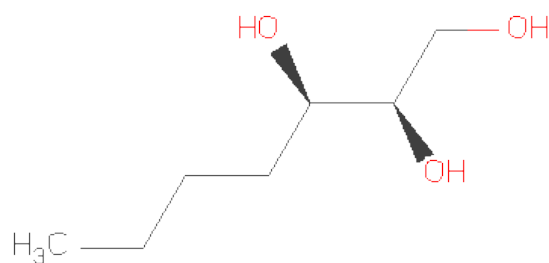
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



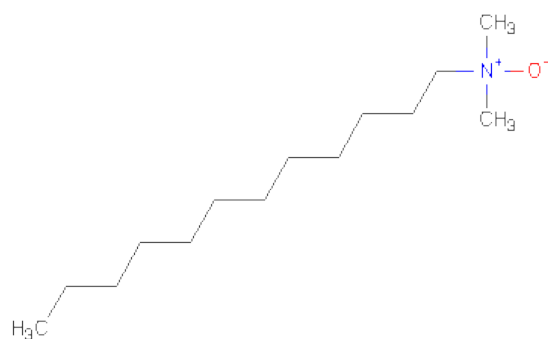
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	1
			46	38	8		

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



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

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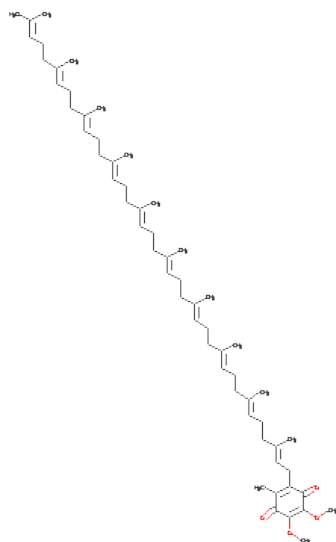
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 10 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

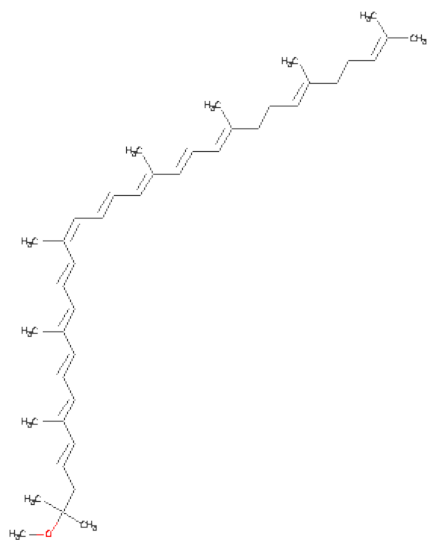
- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



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

- Molecule 12 is SPHEROIDENE (three-letter code: SPO) (formula: C<sub>41</sub>H<sub>60</sub>O).





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

- Molecule 13 is water.

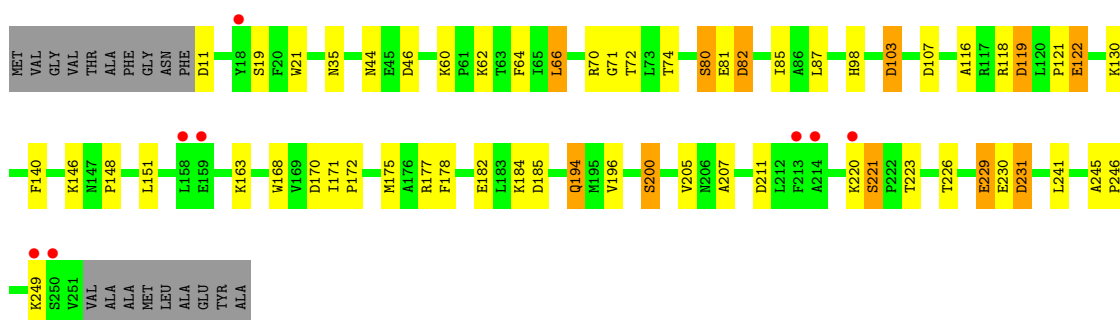
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	76	Total	O	0	0
			76	76		
13	L	68	Total	O	0	0
			68	68		
13	M	58	Total	O	0	0
			58	58		

### 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.

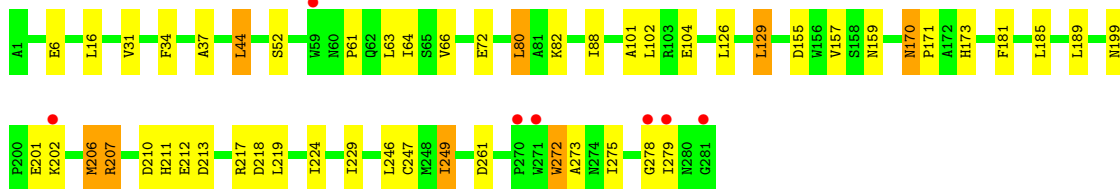
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H: 



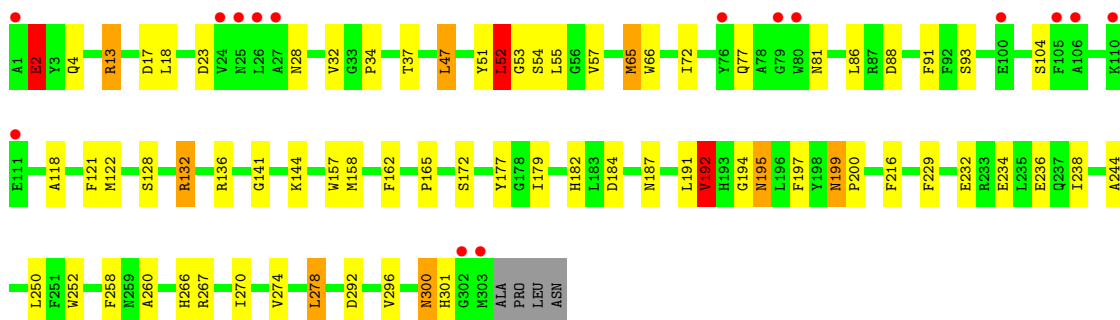
#### • Molecule 2: REACTION CENTER PROTEIN L CHAIN

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, $\alpha$ , $\beta$ , $\gamma$	139.00Å 139.00Å 183.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 2.88 42.91 – 2.88	Depositor EDS
% Data completeness (in resolution range)	81.2 (119.52-2.88) 77.9 (42.91-2.88)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.176 , 0.220 0.180 , 0.186	Depositor DCC
$R_{free}$ test set	1821 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 52.6	EDS
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 38278 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7302	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 2.68% 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, 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	0.83	2/1906 (0.1%)	0.92	7/2591 (0.3%)
2	L	0.80	0/2320	0.82	4/3175 (0.1%)
3	M	0.78	0/2501	0.81	5/3415 (0.1%)
All	All	0.80	2/6727 (0.0%)	0.85	16/9181 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	122	GLU	CG-CD	5.70	1.60	1.51
1	H	194	GLN	CG-CD	5.07	1.62	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	52	LEU	CA-CB-CG	8.47	134.77	115.30
2	L	261	ASP	CB-CG-OD2	7.19	124.77	118.30
1	H	107	ASP	CB-CG-OD2	5.88	123.59	118.30
3	M	23	ASP	CB-CG-OD2	5.83	123.55	118.30
1	H	103	ASP	CB-CG-OD2	5.79	123.51	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	32	0
2	L	2232	0	2187	35	0
3	M	2409	0	2321	41	0
4	H	18	0	24	3	0
4	L	6	0	8	2	0
5	L	132	0	148	3	0
5	M	132	0	148	13	0
6	L	65	0	76	8	0
6	M	65	0	76	11	0
7	L	46	0	52	14	0
8	L	10	0	16	0	0
9	M	48	0	93	3	0
10	M	1	0	0	0	0
11	M	48	0	63	1	0
12	M	42	0	60	1	0
13	H	76	0	0	3	0
13	L	68	0	0	1	0
13	M	58	0	0	2	0
All	All	7302	0	7133	133	0

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 133 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:L:1283:BPH:HHC	6:L:1283:BPH:CBB	1.94	0.97
6:M:1309:BPH:CBB	6:M:1309:BPH:HHC	1.94	0.95
5:M:1303:BCL:H151	5:M:1303:BCL:H91	1.53	0.89
7:L:1284[B]:UQ2:H5M1	7:L:1284[B]:UQ2:C8	2.02	0.88
3:M:197:PHE:HZ	5:M:1304:BCL:HBB2	1.39	0.86

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	H	242/260 (93%)	226 (93%)	14 (6%)	2 (1%)	27	67
2	L	279/281 (99%)	265 (95%)	11 (4%)	3 (1%)	21	58
3	M	301/307 (98%)	277 (92%)	19 (6%)	5 (2%)	14	44
All	All	822/848 (97%)	768 (93%)	44 (5%)	10 (1%)	19	55

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	2	GLU
3	M	52	LEU
1	H	116	ALA
2	L	273	ALA
1	H	245	ALA

### 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%)	182 (92%)	16 (8%)	17	43
2	L	220/220 (100%)	200 (91%)	20 (9%)	14	36
3	M	236/240 (98%)	210 (89%)	26 (11%)	9	24
All	All	654/668 (98%)	592 (90%)	62 (10%)	12	33

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	185	LEU
2	L	249	ILE
3	M	258	PHE
2	L	207	ARG
3	M	2	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	264	GLN
3	M	4	GLN
3	M	193	HIS
2	L	170	ASN
3	M	187	ASN

### 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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	GOL	H	1251	-	5,5,5	0.51	0	5,5,5	0.74	0
4	GOL	H	1252	-	5,5,5	0.21	0	5,5,5	0.59	0
4	GOL	H	1253	-	5,5,5	0.33	0	5,5,5	0.48	0
5	BCL	L	1282	2	74,74,74	2.20	11 (14%)	97,115,115	2.17	27 (27%)
6	BPH	L	1283	-	70,70,70	3.08	14 (20%)	94,101,101	1.96	20 (21%)
7	UQ2	L	1284[A]	-	23,23,23	2.83	7 (30%)	31,31,31	1.33	4 (12%)
7	UQ2	L	1284[B]	-	23,23,23	2.65	7 (30%)	31,31,31	1.40	5 (16%)
5	BCL	L	1285	2	74,74,74	2.03	12 (16%)	97,115,115	2.35	30 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	HTO	L	1286	-	9,9,9	0.95	1 (11%)	10,10,10	1.29	2 (20%)
4	GOL	L	1287	-	5,5,5	0.36	0	5,5,5	0.47	0
5	BCL	M	1303	3	74,74,74	2.19	11 (14%)	97,115,115	2.08	26 (26%)
5	BCL	M	1304	3	74,74,74	2.11	11 (14%)	97,115,115	2.09	25 (25%)
9	LDA	M	1305	-	15,15,15	3.72	1 (6%)	17,17,17	1.41	3 (17%)
9	LDA	M	1306	-	15,15,15	3.51	2 (13%)	17,17,17	0.83	1 (5%)
9	LDA	M	1307	-	15,15,15	3.82	1 (6%)	17,17,17	0.66	0
6	BPH	M	1309	-	70,70,70	2.98	13 (18%)	94,101,101	2.09	21 (22%)
11	U10	M	1310	-	48,48,63	3.19	14 (29%)	59,61,79	1.85	12 (20%)
12	SPO	M	1311	-	41,41,41	4.21	12 (29%)	50,50,50	2.01	12 (24%)

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	GOL	H	1251	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1252	-	-	0/4/4/4	0/0/0/0
4	GOL	H	1253	-	-	0/4/4/4	0/0/0/0
5	BCL	L	1282	2	2/2/21/25	0/41/137/137	0/0/9/9
6	BPH	L	1283	-	2/2/18/22	0/49/105/105	0/0/6/6
7	UQ2	L	1284[A]	-	-	0/15/39/39	0/1/1/1
7	UQ2	L	1284[B]	-	-	0/15/39/39	0/1/1/1
5	BCL	L	1285	2	2/2/21/25	0/41/137/137	0/0/9/9
8	HTO	L	1286	-	-	0/10/10/10	0/0/0/0
4	GOL	L	1287	-	-	0/4/4/4	0/0/0/0
5	BCL	M	1303	3	2/2/21/25	0/41/137/137	0/0/9/9
5	BCL	M	1304	3	2/2/21/25	0/41/137/137	0/0/9/9
9	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
6	BPH	M	1309	-	2/2/18/22	0/49/105/105	0/0/6/6
11	U10	M	1310	-	-	0/45/69/87	0/1/1/1
12	SPO	M	1311	-	-	0/47/47/47	0/0/0/0

The worst 5 of 117 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1307	LDA	O1-N1	-14.60	1.25	1.39
6	M	1309	BPH	C1D-CHD	14.30	1.51	1.35
9	M	1305	LDA	O1-N1	-14.18	1.26	1.39
6	L	1283	BPH	C1D-CHD	13.90	1.51	1.35
5	L	1282	BCL	OBD-CAD	13.81	1.42	1.22

The worst 5 of 188 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1285	BCL	C2D-C1D-ND	-9.06	102.57	109.41
6	M	1309	BPH	OBD-CAD-CBD	-8.26	113.48	125.94
6	L	1283	BPH	C3B-C2B-C1B	-7.80	102.35	107.01
6	M	1309	BPH	C3B-C2B-C1B	-7.26	102.67	107.01
5	M	1304	BCL	C2D-C1D-ND	-7.09	104.06	109.41

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	1304	BCL	C8
5	M	1304	BCL	C13
5	L	1282	BCL	C8
5	L	1282	BCL	C13
5	M	1303	BCL	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%)	-0.25	8 (3%)	44 54	36, 51, 66, 102	0
2	L	281/281 (100%)	-0.48	7 (2%)	54 65	32, 44, 69, 84	0
3	M	303/307 (98%)	-0.29	15 (4%)	28 34	34, 51, 76, 104	0
All	All	825/848 (97%)	-0.34	30 (3%)	41 49	32, 49, 72, 104	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	249	LYS	3.9
2	L	279	ILE	3.9
1	H	250	SER	3.7
1	H	220[A]	LYS	3.5
2	L	281	GLY	3.5

### 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( $\text{\AA}^2$ )	Q<0.9
8	HTO	L	1286	10/10	0.57	14.44	71,83,83,84	0
4	GOL	H	1251	6/6	0.35	12.07	69,77,81,82	0
7	UQ2	L	1284[B]	23/23	0.34	9.43	31,35,43,45	23
7	UQ2	L	1284[A]	23/23	0.34	9.41	51,59,74,74	23
9	LDA	M	1307	16/16	0.42	8.25	98,102,114,115	0
4	GOL	L	1287	6/6	0.46	6.82	85,86,86,87	0
9	LDA	M	1306	16/16	0.30	6.09	49,62,72,72	0
9	LDA	M	1305	16/16	0.28	5.25	74,83,86,87	0
12	SPO	M	1311	42/42	0.36	3.38	47,59,82,85	0
4	GOL	H	1252	6/6	0.38	2.83	81,84,85,87	0
6	BPH	M	1309	65/65	0.22	2.25	39,48,109,110	0
11	U10	M	1310	48/63	0.24	2.23	42,52,81,82	0
6	BPH	L	1283	65/65	0.16	0.76	25,35,53,55	0
5	BCL	M	1304	66/66	0.15	0.58	32,40,59,68	0
5	BCL	L	1285	66/66	0.14	0.45	30,37,55,60	0
5	BCL	M	1303	66/66	0.15	0.05	29,41,93,96	0
5	BCL	L	1282	66/66	0.13	-0.21	31,40,64,75	0
10	FE	M	1308	1/1	0.07	-3.23	41,41,41,41	0
4	GOL	H	1253	6/6	0.32	-	113,114,115,116	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.