



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:15 PM GMT

PDB ID : 2HHK  
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with dibrominated phosphatidylglycerol  
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.  
Deposited on : 2006-06-28  
Resolution : 2.50 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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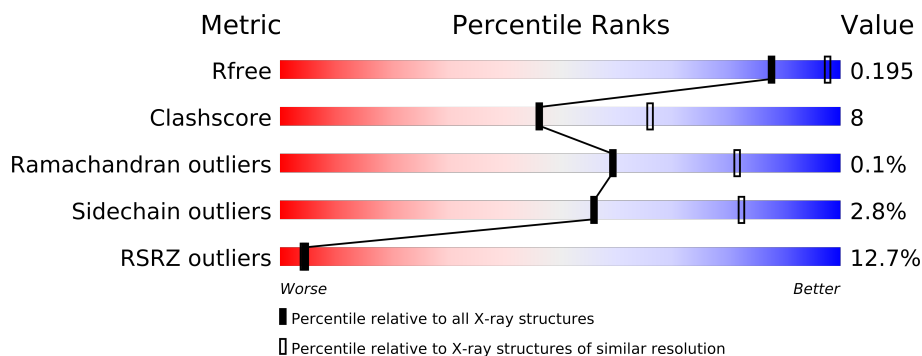
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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. 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	L	281	
2	M	307	
3	H	260	

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	U10	L	502	-	X
11	CDL	M	800	-	X
12	PGT	H	801[A]	-	X
12	PGT	H	801[B]	-	X
13	PGK	M	802	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
14	LDA	H	901	-	X
14	LDA	H	903	-	X
14	LDA	H	904	-	X
14	LDA	M	902	-	X
14	LDA	M	907	-	X
14	LDA	M	920	-	X
15	GOL	H	706	-	X
15	GOL	L	707	-	X
15	GOL	L	708	-	X
15	GOL	L	709	-	X
7	PO4	M	705	-	X

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7824 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 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	1	0
			2235	1510	356	361	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	10	0
			2448	1633	402	402	11			

- 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	8	0
			1862	1189	323	339	11			

- 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		

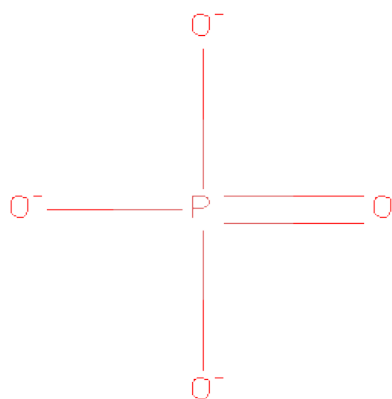
- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

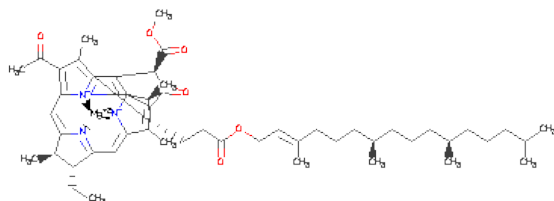
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Cl	0	0
			1	1		

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



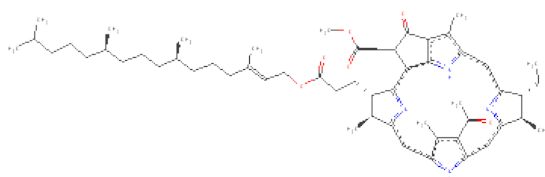
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	O	P	0	0
			5	4	1		
7	M	1	Total	O	P	0	0
			5	4	1		
7	H	1	Total	O	P	0	0
			5	4	1		
7	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



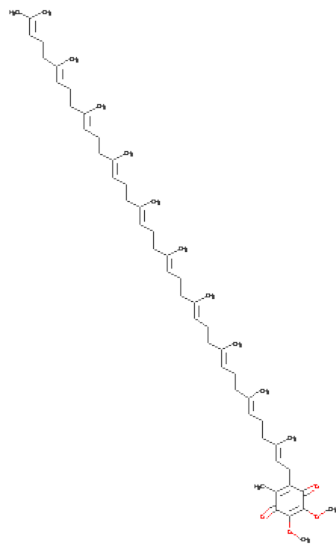
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 9 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



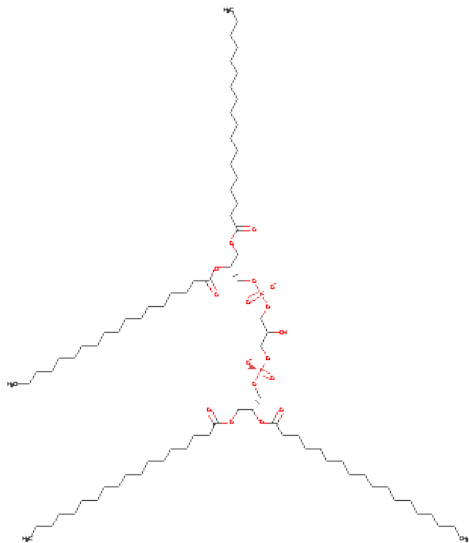
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



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

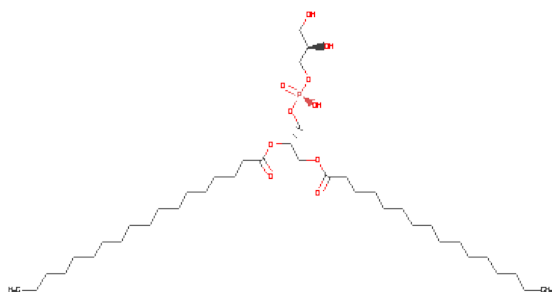
- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

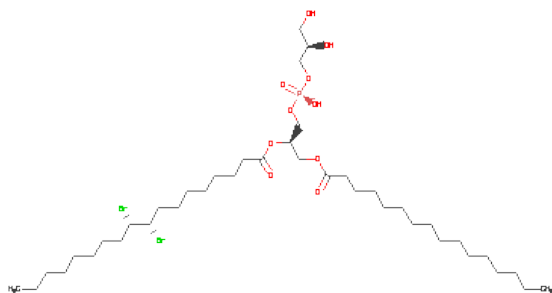
- Molecule 12 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSP

HORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYLSTEARATE (three-letter code: PGT) (formula:  $C_{40}H_{79}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
12	H	1	102	80	20	2	0	1

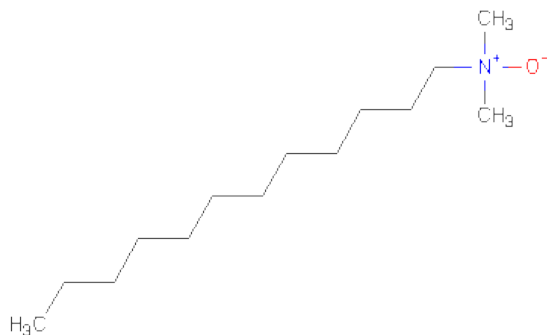
- Molecule 13 is (1R)-2-{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL(9S,10S)-9,10-DIBROMOOCTADECANOATE (three-letter code: PGK) (formula:  $C_{40}H_{77}Br_2O_{10}P$ ).





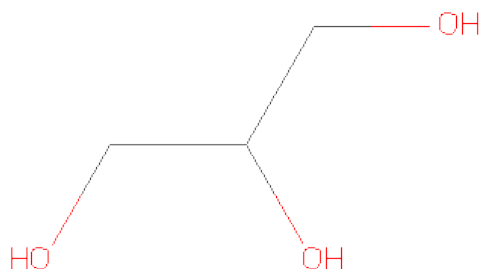
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	M	1	Total	Br	C	O	P	0	0
			53	2	40	10	1		

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



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

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

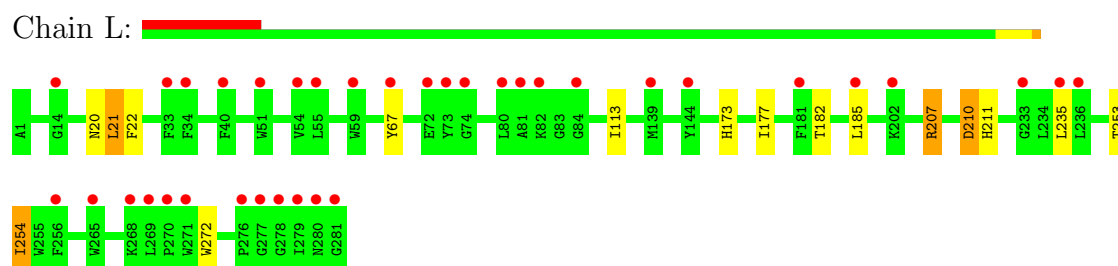
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	199	Total	O	0	0
			199	199		
16	L	92	Total	O	0	0
			92	92		
16	M	119	Total	O	0	0
			119	119		

### 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

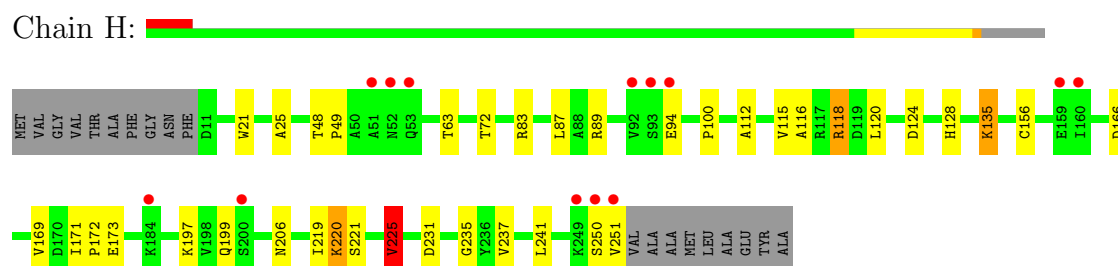
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.42Å 139.42Å 183.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.50 45.63 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.00-2.50) 99.5 (45.63-2.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.197 0.173 , 0.195	Depositor DCC
$R_{free}$ test set	3546 reflections (4.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 67.4	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 71469 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7824	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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, CL, CDL, BPH, K, PGK, PGT, FE, 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	L	0.88	0/2328	0.73	1/3186 (0.0%)
2	M	0.87	0/2592	0.78	1/3536 (0.0%)
3	H	0.93	5/1953 (0.3%)	0.82	4/2652 (0.2%)
All	All	0.89	5/6873 (0.1%)	0.78	6/9374 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	173	GLU	CD-OE2	5.32	1.31	1.25
3	H	237	VAL	CB-CG2	5.12	1.63	1.52
3	H	221[A]	SER	CB-OG	5.07	1.48	1.42
3	H	221[B]	SER	CB-OG	5.07	1.48	1.42
3	H	94	GLU	CG-CD	5.05	1.59	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	210	ASP	CB-CG-OD1	6.50	124.15	118.30
3	H	124	ASP	CB-CG-OD1	6.31	123.98	118.30
3	H	225	VAL	CB-CA-C	-5.53	100.90	111.40
3	H	89	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	M	240	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	1	ALA	Peptide

## 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	L	2235	0	2196	10	0
2	M	2448	0	2367	26	0
3	H	1862	0	1883	25	0
4	M	1	0	0	0	0
5	H	1	0	0	0	0
6	M	1	0	0	0	0
7	H	5	0	0	0	0
7	M	15	0	0	1	0
8	L	132	0	148	6	0
8	M	132	0	148	20	0
9	L	65	0	75	0	0
9	M	65	0	76	4	0
10	L	48	0	63	4	0
10	M	48	0	63	1	0
11	M	81	0	106	3	0
12	H	102	0	156	20	0
13	M	53	0	74	11	0
14	H	48	0	93	25	0
14	M	48	0	93	12	0
15	H	6	0	8	0	0
15	L	18	0	24	5	0
16	H	199	0	0	4	0
16	L	92	0	0	2	0
16	M	119	0	0	2	0
All	All	7824	0	7573	123	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 8.

The worst 5 of 123 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:301[A]:HIS:HE1	16:M:1031:HOH:O	1.41	1.03
8:M:311:BCL:C9	8:M:311:BCL:H41	1.91	0.99
8:M:311:BCL:C7	8:M:311:BCL:H41	1.92	0.98
14:M:902:LDA:C12	14:H:903:LDA:C12	2.43	0.96
14:M:902:LDA:C12	14:H:903:LDA:H123	1.96	0.95

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	280/281 (100%)	274 (98%)	6 (2%)	0	100	100
2	M	310/307 (101%)	298 (96%)	11 (4%)	1 (0%)	50	73
3	H	247/260 (95%)	242 (98%)	5 (2%)	0	100	100
All	All	837/848 (99%)	814 (97%)	22 (3%)	1 (0%)	59	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

### 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	221/220 (100%)	214 (97%)	7 (3%)	51	77
2	M	246/240 (102%)	240 (98%)	6 (2%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	H	204/208 (98%)	197 (97%)	7 (3%)	49	75
All	All	671/668 (100%)	651 (97%)	20 (3%)	56	80

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	86	LEU
2	M	114	LEU
3	H	220[A]	LYS
2	M	2	GLU
2	M	52	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	28	ASN
3	H	199	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 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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$
7	PO4	H	704	-	4,4,4	0.30	0	6,6,6	0.31	0
15	GOL	H	706	-	5,5,5	0.23	0	5,5,5	0.82	0
12	PGT	H	801[A]	-	50,50,50	0.70	0	56,56,56	0.94	3 (5%)
12	PGT	H	801[B]	-	50,50,50	0.84	1 (2%)	56,56,56	1.07	5 (8%)
14	LDA	H	901	-	15,15,15	3.28	2 (13%)	17,17,17	1.07	1 (5%)
14	LDA	H	903	-	15,15,15	3.51	2 (13%)	17,17,17	0.95	2 (11%)
14	LDA	H	904	-	15,15,15	3.77	2 (13%)	17,17,17	0.88	2 (11%)
8	BCL	L	312	1	74,74,74	1.43	10 (13%)	97,115,115	1.53	16 (16%)
8	BCL	L	314	1	74,74,74	1.42	12 (16%)	97,115,115	1.52	18 (18%)
9	BPH	L	402	-	70,70,70	1.34	8 (11%)	94,101,101	1.22	13 (13%)
10	U10	L	502	-	48,48,63	1.17	5 (10%)	59,61,79	1.76	11 (18%)
15	GOL	L	707	-	5,5,5	0.30	0	5,5,5	0.52	0
15	GOL	L	708	-	5,5,5	0.45	0	5,5,5	0.64	0
15	GOL	L	709	-	5,5,5	0.55	0	5,5,5	0.75	0
8	BCL	M	311	2	74,74,74	1.33	9 (12%)	97,115,115	1.85	25 (25%)
8	BCL	M	313	2	74,74,74	1.36	10 (13%)	97,115,115	1.87	26 (26%)
9	BPH	M	401	-	70,70,70	1.36	6 (8%)	94,101,101	1.45	13 (13%)
10	U10	M	501	-	48,48,63	1.18	5 (10%)	59,61,79	1.60	9 (15%)
7	PO4	M	702	-	4,4,4	0.27	0	6,6,6	0.31	0
7	PO4	M	703	-	4,4,4	0.33	0	6,6,6	0.37	0
7	PO4	M	705	-	4,4,4	0.27	0	6,6,6	0.33	0
11	CDL	M	800	-	80,80,99	1.51	8 (10%)	92,92,111	1.48	14 (15%)
13	PGK	M	802	-	52,52,52	0.83	2 (3%)	60,60,60	1.41	6 (10%)
14	LDA	M	902	-	15,15,15	3.53	1 (6%)	17,17,17	0.81	0
14	LDA	M	907	-	15,15,15	3.76	1 (6%)	17,17,17	1.05	2 (11%)
14	LDA	M	920	-	15,15,15	3.41	2 (13%)	17,17,17	1.52	2 (11%)

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
7	PO4	H	704	-	-	0/0/0/0	0/0/0/0
15	GOL	H	706	-	-	0/4/4/4	0/0/0/0
12	PGT	H	801[A]	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PGT	H	801[B]	-	-	0/55/55/55	0/0/0/0
14	LDA	H	901	-	-	0/13/13/13	0/0/0/0
14	LDA	H	903	-	-	0/13/13/13	0/0/0/0
14	LDA	H	904	-	-	0/13/13/13	0/0/0/0
8	BCL	L	312	1	-	0/41/137/137	0/0/9/9
8	BCL	L	314	1	-	0/41/137/137	0/0/9/9
9	BPH	L	402	-	2/2/18/22	0/49/105/105	0/0/6/6
10	U10	L	502	-	-	0/45/69/87	0/1/1/1
15	GOL	L	707	-	-	0/4/4/4	0/0/0/0
15	GOL	L	708	-	-	0/4/4/4	0/0/0/0
15	GOL	L	709	-	-	0/4/4/4	0/0/0/0
8	BCL	M	311	2	-	0/41/137/137	0/0/9/9
8	BCL	M	313	2	-	0/41/137/137	0/0/9/9
9	BPH	M	401	-	2/2/18/22	0/49/105/105	0/0/6/6
10	U10	M	501	-	-	0/45/69/87	0/1/1/1
7	PO4	M	702	-	-	0/0/0/0	0/0/0/0
7	PO4	M	703	-	-	0/0/0/0	0/0/0/0
7	PO4	M	705	-	-	0/0/0/0	0/0/0/0
11	CDL	M	800	-	1/1/9/9	0/91/91/110	0/0/0/0
13	PGK	M	802	-	-	0/60/60/60	0/0/0/0
14	LDA	M	902	-	-	0/13/13/13	0/0/0/0
14	LDA	M	907	-	-	0/13/13/13	0/0/0/0
14	LDA	M	920	-	-	0/13/13/13	0/0/0/0

The worst 5 of 86 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	907	LDA	O1-N1	-14.36	1.25	1.39
14	H	904	LDA	O1-N1	-14.22	1.26	1.39
14	M	902	LDA	O1-N1	-13.48	1.26	1.39
14	H	903	LDA	O1-N1	-13.33	1.26	1.39
14	M	920	LDA	O1-N1	-12.89	1.27	1.39

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	313	BCL	CMB-C2B-C1B	-6.01	119.38	128.62
11	M	800	CDL	OB6-CB5-C51	5.26	123.09	111.56
8	M	311	BCL	C4-C3-C2	-5.15	113.32	123.52
8	M	311	BCL	OBB-CAB-C3B	5.10	127.73	120.07
10	L	502	U10	C25-C24-C26	5.05	123.07	115.39

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	800	CDL	CA4
9	L	402	BPH	C8
9	L	402	BPH	C13
9	M	401	BPH	C8
9	M	401	BPH	C13

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	L	281/281 (100%)	0.79	36 (12%) 4 4	54, 62, 73, 80	0
2	M	302/307 (98%)	0.82	50 (16%) 2 2	54, 62, 73, 94	0
3	H	241/260 (92%)	0.34	13 (5%) 25 25	54, 62, 73, 100	0
All	All	824/848 (97%)	0.67	99 (12%) 4 5	54, 62, 73, 100	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	277	GLY	6.8
3	H	251	VAL	5.5
2	M	80	TRP	5.2
1	L	281	GLY	5.0
1	L	278	GLY	4.9

### 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
14	LDA	H	903	16/16	1.40	26.02	73,75,78,78	16
14	LDA	M	907	16/16	0.48	15.70	69,72,77,77	16
14	LDA	M	902	16/16	0.81	15.33	66,71,75,79	16
14	LDA	H	904	16/16	0.72	14.40	76,79,86,86	16
12	PGT	H	801[A]	51/51	1.22	12.49	45,73,81,82	51
12	PGT	H	801[B]	51/51	1.22	12.47	47,76,84,85	51
15	GOL	L	709	6/6	0.68	8.36	65,66,68,70	6
15	GOL	H	706	6/6	0.54	6.68	72,72,73,74	6
10	U10	L	502	48/63	0.60	6.20	53,68,86,90	48
14	LDA	M	920	16/16	0.53	5.79	41,60,78,80	16
15	GOL	L	708	6/6	0.33	4.83	60,66,68,68	6
13	PGK	M	802	53/53	0.62	4.23	61,67,76,77	53
11	CDL	M	800	81/100	0.43	3.98	49,74,88,90	81
14	LDA	H	901	16/16	0.40	3.29	72,77,86,88	16
7	PO4	M	705	5/5	0.26	2.31	63,64,65,65	5
15	GOL	L	707	6/6	0.42	2.12	65,67,68,68	6
7	PO4	H	704	5/5	0.25	1.92	61,61,63,63	5
10	U10	M	501	48/63	0.32	1.87	56,69,90,93	0
7	PO4	M	702	5/5	0.28	1.25	69,71,74,77	5
8	BCL	L	314	66/66	0.23	1.24	50,59,75,80	0
6	CL	M	701	1/1	0.21	0.97	73,73,73,73	1
8	BCL	M	313	66/66	0.19	0.77	51,59,84,95	0
8	BCL	M	311	66/66	0.23	0.73	55,62,119,120	0
8	BCL	L	312	66/66	0.19	0.34	49,59,70,78	0
9	BPH	M	401	65/65	0.20	0.26	56,62,116,118	0
9	BPH	L	402	65/65	0.18	0.21	50,62,66,68	0
4	FE	M	500	1/1	0.20	-0.84	59,59,59,59	0
7	PO4	M	703	5/5	0.18	-1.63	59,59,63,64	5
5	K	H	700	1/1	0.09	-2.19	58,58,58,58	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.