



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:48 AM GMT

PDB ID : 2HG9
Title : Reaction centre from Rhodobacter sphaeroides strain R-26.1 complexed with
tetrabrominated phosphatidylcholine
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2006-06-26
Resolution : 2.45 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

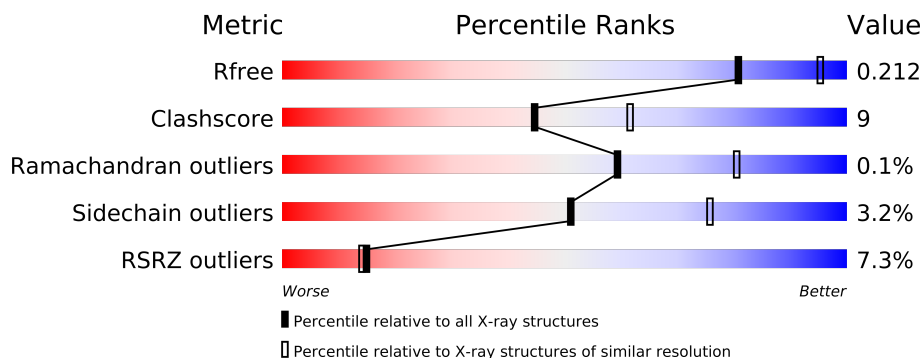
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.45 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	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

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 ≥ 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	PC7	H	801	-	X
13	PCK	M	802	-	X
14	LDA	H	901	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
14	LDA	H	903	-	X
14	LDA	H	904	-	X
14	LDA	H	908	-	X
14	LDA	M	902	-	X
14	LDA	M	907	-	X
14	LDA	M	920	-	X
15	GOL	H	705	-	X
15	GOL	H	706	-	X
15	GOL	H	708	-	X
15	GOL	M	707	-	X
15	GOL	M	710	-	X
6	PO4	H	704	-	X
6	PO4	L	703	-	X
7	CL	L	712	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7843 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	3	0
			2237	1511	356	362	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	12	0
			2450	1631	402	406	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	9	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 PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

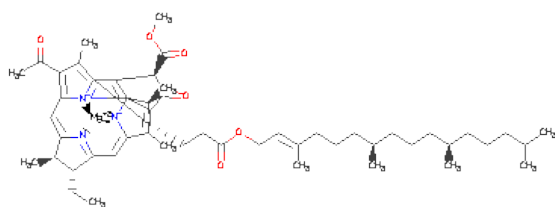


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		
6	L	1	Total	O	P	0	0
			5	4	1		
6	H	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

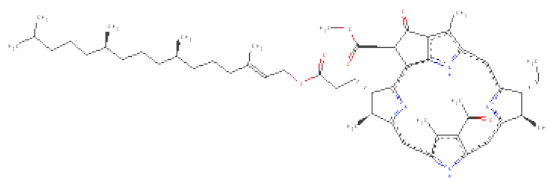
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	1	Total	Cl	0	0
			1	1		
7	M	1	Total	Cl	0	0
			1	1		

- Molecule 8 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



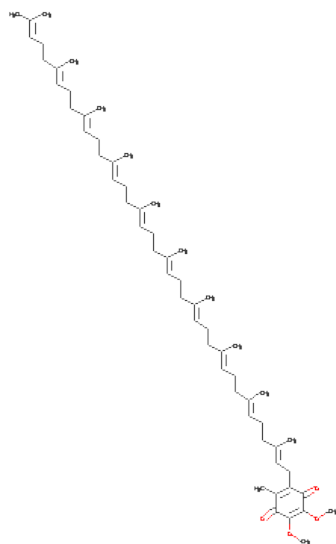
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
8	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



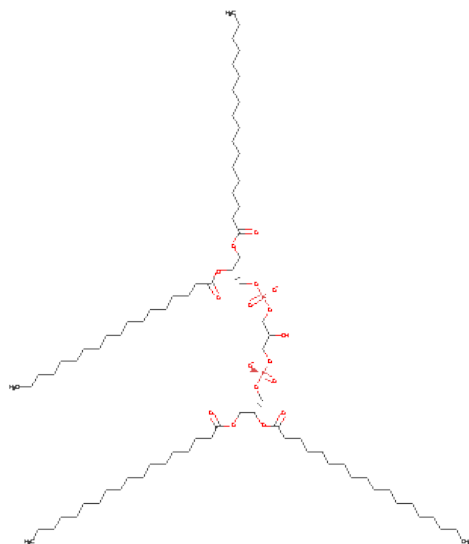
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	M	1	Total	C	N	O	0	0
			65	55	4	6		
9	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



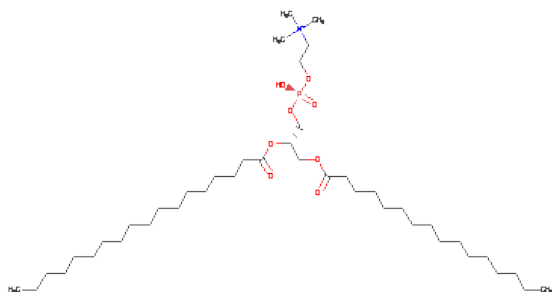
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			48	44	4		
10	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

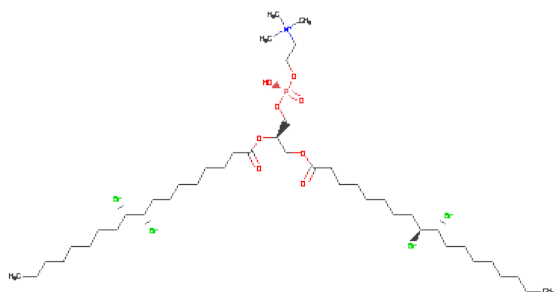
- Molecule 12 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM4-OXIDE (three-letter code: PC7) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	H	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

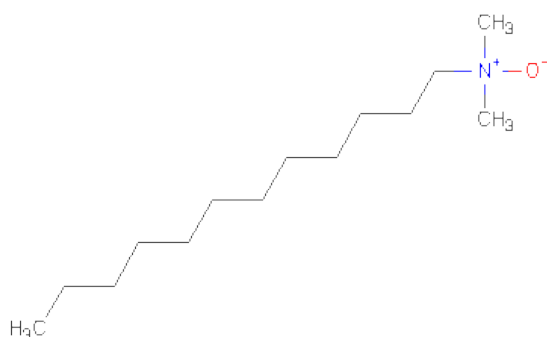
- Molecule 13 is (7R,18S,19R)-18,19-DIBROMO-7-{[(9S,10S)-9,10-DIBROMOOCTADECAN

OYL]OXY}-4-HYDROXY-N,N,N-TRIMETHYL-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOSAN-1-AMINIUM4-OXIDE (three-letter code: PCK) (formula: $C_{44}H_{85}Br_4NO_8P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	M	1	Total	Br	C	N	O	P	0	0
			58	4	44	1	8	1		

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



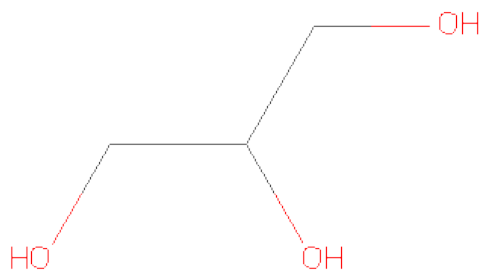
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	H	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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		

- 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	H	1	Total	C	O	0	0
			6	3	3		
15	M	1	Total	C	O	0	0
			6	3	3		
15	H	1	Total	C	O	0	0
			6	3	3		
15	H	1	Total	C	O	0	0
			6	3	3		

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

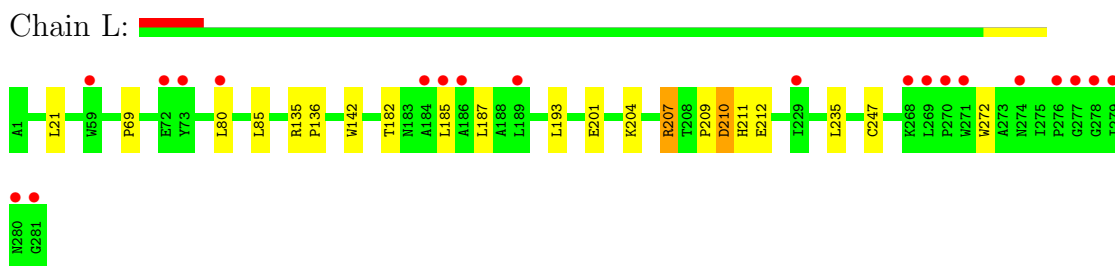
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	H	208	Total	O	0	0
			208	208		
16	L	100	Total	O	0	0
			100	100		
16	M	133	Total	O	0	0
			133	133		

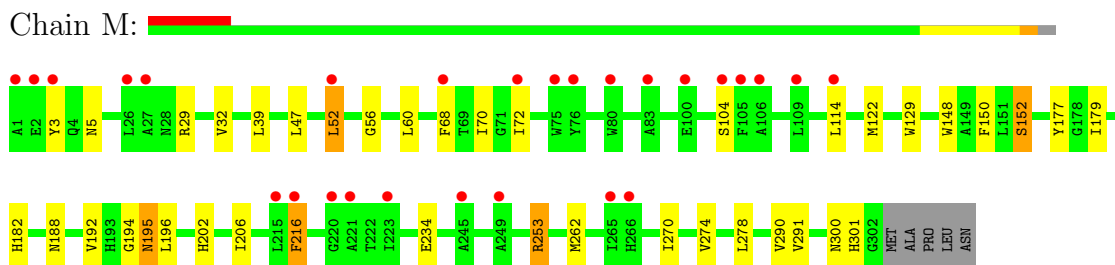
3 Residue-property plots

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.

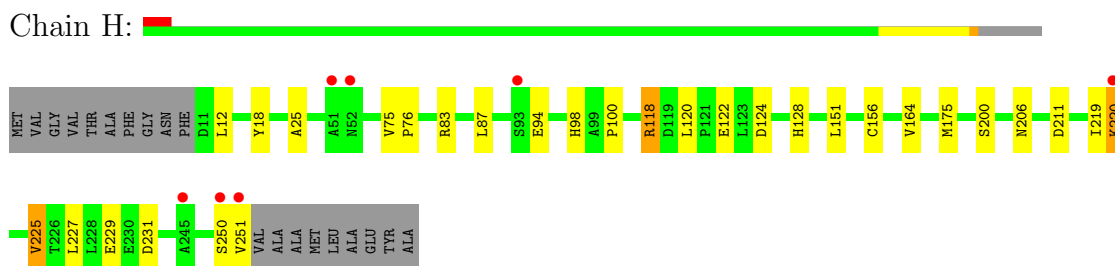
• Molecule 1: Reaction center protein L chain



• 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, α , β , γ	139.55Å 139.55Å 184.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.36 – 2.45 39.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.36-2.45) 98.0 (39.36-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.179 , 0.209 0.185 , 0.212	Depositor DCC
R_{free} test set	3708 reflections (4.93%)	DCC
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.4	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 75227 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7843	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, PC7, PCK, 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	0.90	0/2342	0.73	1/3205 (0.0%)
2	M	0.90	1/2601 (0.0%)	0.80	3/3548 (0.1%)
3	H	0.95	3/1961 (0.2%)	0.84	4/2663 (0.2%)
All	All	0.92	4/6904 (0.1%)	0.79	8/9416 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	94	GLU	CG-CD	6.20	1.61	1.51
3	H	94	GLU	CB-CG	5.59	1.62	1.52
3	H	94	GLU	CD-OE2	5.30	1.31	1.25
2	M	152	SER	CB-OG	5.05	1.48	1.42

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	124	ASP	CB-CG-OD1	7.74	125.27	118.30
3	H	124	ASP	CB-CG-OD2	-6.80	112.18	118.30
2	M	253[A]	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	M	253[B]	ARG	NE-CZ-NH2	6.00	123.30	120.30
3	H	83	ARG	NE-CZ-NH2	-5.78	117.41	120.30

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	L	2237	0	2202	10	0
2	M	2450	0	2370	38	0
3	H	1862	0	1884	21	0
4	M	1	0	0	0	0
5	H	1	0	0	0	0
6	H	5	0	0	0	0
6	L	5	0	0	0	0
6	M	10	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	1	0
8	L	132	0	148	8	0
8	M	132	0	148	20	0
9	L	65	0	75	3	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	2	0
12	H	52	0	84	6	0
13	M	58	0	80	24	0
14	H	64	0	124	19	0
14	M	48	0	93	9	0
15	H	24	0	32	2	0
15	M	12	0	16	0	0
16	H	208	0	0	0	0
16	L	100	0	0	0	0
16	M	133	0	0	7	0
All	All	7843	0	7564	128	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 128 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:M:902:LDA:H121	14:H:908:LDA:H121	1.37	1.04
2:M:47[A]:LEU:HD22	13:M:802:PCK:BR4	2.11	1.04
10:L:502:U10:H351	10:L:502:U10:H38	1.41	1.03
13:M:802:PCK:H252	13:M:802:PCK:H211	1.35	1.02
2:M:122:MET:SD	14:M:920:LDA:H122	2.01	1.01

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	312/307 (102%)	300 (96%)	11 (4%)	1 (0%)	50	70
3	H	248/260 (95%)	245 (99%)	3 (1%)	0	100	100
All	All	842/848 (99%)	820 (97%)	21 (2%)	1 (0%)	59	80

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	223/220 (101%)	216 (97%)	7 (3%)	52	77
2	M	248/240 (103%)	239 (96%)	9 (4%)	47	71
3	H	205/208 (99%)	198 (97%)	7 (3%)	49	74
All	All	676/668 (101%)	653 (97%)	23 (3%)	51	74

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	114	LEU
2	M	192	VAL

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Mol	Chain	Res	Type
3	H	225	VAL
2	M	182	HIS
2	M	196	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
3	H	68	HIS

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 32 ligands modelled in this entry, 4 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	PO4	H	704	-	4,4,4	0.16	0	6,6,6	0.33	0
15	GOL	H	705	-	5,5,5	0.49	0	5,5,5	0.68	0
15	GOL	H	706	-	5,5,5	0.28	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	GOL	H	708	-	5,5,5	0.26	0	5,5,5	0.53	0
15	GOL	H	709	-	5,5,5	0.43	0	5,5,5	0.41	0
12	PC7	H	801	-	51,51,51	0.84	2 (3%)	59,59,59	0.90	3 (5%)
14	LDA	H	901	-	15,15,15	3.78	2 (13%)	17,17,17	0.84	0
14	LDA	H	903	-	15,15,15	3.70	1 (6%)	17,17,17	0.74	0
14	LDA	H	904	-	15,15,15	3.68	2 (13%)	17,17,17	0.88	1 (5%)
14	LDA	H	908	-	15,15,15	3.76	1 (6%)	17,17,17	1.11	1 (5%)
8	BCL	L	312	1	74,74,74	1.31	9 (12%)	97,115,115	1.52	18 (18%)
8	BCL	L	314	1	74,74,74	1.48	8 (10%)	97,115,115	1.61	24 (24%)
9	BPH	L	402	-	70,70,70	1.36	8 (11%)	94,101,101	1.19	10 (10%)
10	U10	L	502	-	48,48,63	1.15	5 (10%)	59,61,79	1.88	16 (27%)
6	PO4	L	703	-	4,4,4	0.17	0	6,6,6	0.31	0
8	BCL	M	311	2	74,74,74	1.38	10 (13%)	97,115,115	1.59	21 (21%)
8	BCL	M	313	2	74,74,74	1.40	10 (13%)	97,115,115	1.69	20 (20%)
9	BPH	M	401	-	70,70,70	1.40	8 (11%)	94,101,101	1.39	14 (14%)
10	U10	M	501	-	48,48,63	1.00	5 (10%)	59,61,79	1.69	13 (22%)
6	PO4	M	701	-	4,4,4	0.29	0	6,6,6	0.34	0
6	PO4	M	702	-	4,4,4	0.30	0	6,6,6	0.34	0
15	GOL	M	707	-	5,5,5	0.47	0	5,5,5	0.39	0
15	GOL	M	710	-	5,5,5	0.38	0	5,5,5	0.44	0
11	CDL	M	800	-	80,80,99	1.46	7 (8%)	92,92,111	1.18	8 (8%)
13	PCK	M	802	-	57,57,57	0.76	0	69,69,69	1.05	4 (5%)
14	LDA	M	902	-	15,15,15	3.78	2 (13%)	17,17,17	1.69	3 (17%)
14	LDA	M	907	-	15,15,15	3.78	2 (13%)	17,17,17	0.87	2 (11%)
14	LDA	M	920	-	15,15,15	3.71	1 (6%)	17,17,17	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PO4	H	704	-	-	0/0/0/0	0/0/0/0
15	GOL	H	705	-	-	0/4/4/4	0/0/0/0
15	GOL	H	706	-	-	0/4/4/4	0/0/0/0
15	GOL	H	708	-	-	0/4/4/4	0/0/0/0
15	GOL	H	709	-	-	0/4/4/4	0/0/0/0
12	PC7	H	801	-	-	0/55/55/55	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
14	LDA	H	908	-	-	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
6	PO4	L	703	-	-	0/0/0/0	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
6	PO4	M	701	-	-	0/0/0/0	0/0/0/0
6	PO4	M	702	-	-	0/0/0/0	0/0/0/0
15	GOL	M	707	-	-	0/4/4/4	0/0/0/0
15	GOL	M	710	-	-	0/4/4/4	0/0/0/0
11	CDL	M	800	-	1/1/9/9	0/91/91/110	0/0/0/0
13	PCK	M	802	-	-	0/67/67/67	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 83 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	H	901	LDA	O1-N1	-14.36	1.25	1.39
14	H	908	LDA	O1-N1	-14.34	1.25	1.39
14	M	907	LDA	O1-N1	-14.33	1.25	1.39
14	H	903	LDA	O1-N1	-14.12	1.26	1.39
14	M	902	LDA	O1-N1	-14.10	1.26	1.39

The worst 5 of 158 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	800	CDL	OA6-CA5-C11	4.84	122.17	111.56
8	M	311	BCL	C4-C3-C2	-4.75	114.11	123.52
10	M	501	U10	C32-C33-C34	-4.58	117.92	127.80
8	M	313	BCL	CMB-C2B-C1B	-4.54	121.64	128.62
10	L	502	U10	C30-C29-C31	4.52	122.27	115.39

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	800	CDL	CA4
9	M	401	BPH	C8
9	M	401	BPH	C13
9	L	402	BPH	C8
9	L	402	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, 95th 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 ²)	Q<0.9
1	L	281/281 (100%)	0.28	20 (7%)	16 15	43, 53, 66, 82	0
2	M	302/307 (98%)	0.38	27 (8%)	10 9	43, 53, 65, 89	0
3	H	241/260 (92%)	-0.13	7 (2%)	49 50	44, 53, 61, 95	0
All	All	824/848 (97%)	0.20	54 (6%)	15 17	43, 53, 65, 95	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	9.7
3	H	251	VAL	8.0
1	L	277	GLY	6.2
2	M	2[A]	GLU	5.1
3	H	250	SER	5.0

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, 95th 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(\AA^2)	Q<0.9
14	LDA	H	904	16/16	0.53	23.28	53,54,58,58	16
15	GOL	H	708	6/6	0.61	18.70	47,49,50,52	6
12	PC7	H	801	52/52	0.65	15.40	24,60,69,69	52
14	LDA	M	902	16/16	0.53	15.05	59,64,67,68	16
14	LDA	H	908	16/16	0.79	12.92	45,51,61,61	16
15	GOL	H	705	6/6	0.38	11.73	48,58,59,61	6
14	LDA	M	920	16/16	0.59	10.81	42,46,59,59	16
14	LDA	H	903	16/16	0.48	10.07	56,61,64,65	16
14	LDA	M	907	16/16	0.47	9.84	56,59,65,66	16
11	CDL	M	800	81/100	0.52	6.96	43,67,79,82	81
6	PO4	H	704	5/5	0.31	6.66	71,73,74,75	5
15	GOL	M	710	6/6	0.43	6.62	55,57,58,60	6
13	PCK	M	802	58/58	0.59	6.05	60,69,82,84	58
10	U10	L	502	48/63	0.52	4.58	40,55,73,75	48
7	CL	L	712	1/1	0.38	4.36	66,66,66,66	1
15	GOL	M	707	6/6	0.28	3.55	49,50,52,52	6
15	GOL	H	706	6/6	0.34	2.69	71,72,73,74	6
14	LDA	H	901	16/16	0.26	2.66	61,63,66,68	16
6	PO4	L	703	5/5	0.34	2.00	61,61,62,65	5
8	BCL	M	311	66/66	0.25	1.45	46,54,119,120	0
9	BPH	M	401	65/65	0.25	0.93	45,55,106,107	0
10	U10	M	501	48/63	0.26	0.87	49,61,81,84	0
8	BCL	L	312	66/66	0.18	0.87	42,50,63,67	0
8	BCL	M	313	66/66	0.20	0.80	42,50,79,87	0
8	BCL	L	314	66/66	0.19	0.64	41,48,67,71	0
9	BPH	L	402	65/65	0.18	0.56	40,52,60,61	0
7	CL	M	711	1/1	0.19	0.10	74,74,74,74	1
15	GOL	H	709	6/6	0.18	-0.39	55,56,57,58	6
6	PO4	M	701	5/5	0.18	-0.52	57,58,62,62	5
6	PO4	M	702	5/5	0.11	-1.11	53,53,54,55	5
5	K	H	700	1/1	0.06	-1.50	57,57,57,57	0
4	FE	M	500	1/1	0.21	-2.52	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.