



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:05 PM GMT

PDB ID : 1RZH
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TRIGONAL FORM)
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Deposited on : 2003-12-24
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

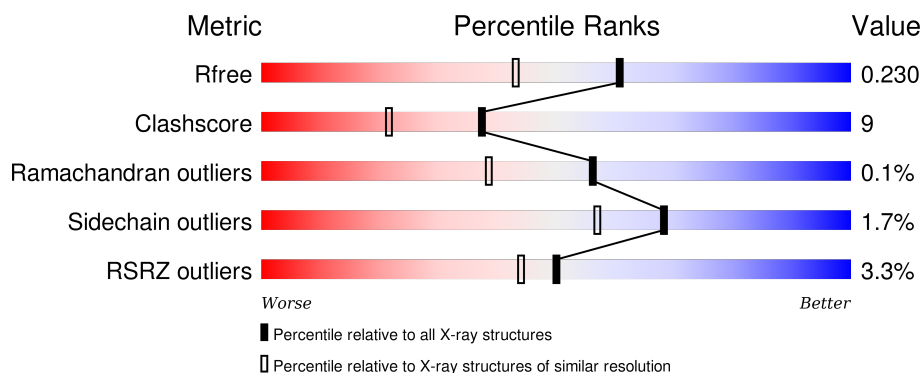
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>4%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	M	307	<div> <div>4%</div> <div>80%</div> <div>18%</div> <div>.</div> </div>
3	H	260	<div> <div>2%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SPO	M	860	-	-	-	X
11	LDA	H	862	-	-	-	X
11	LDA	M	861	-	-	-	X
11	LDA	M	863	-	-	-	X
12	CDL	M	900	-	-	-	X
13	GOL	M	867	-	X	-	-
4	BCL	M	851	X	-	-	X
4	BCL	M	853	-	-	-	X
5	BPH	L	856	X	-	-	-
5	BPH	M	855	X	-	-	-
6	U10	L	859[A]	-	-	-	X
6	U10	M	858	-	-	-	X
7	HTO	L	865	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7586 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	1	0
			2238	1510	357	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	ENGINEERED	UNP P02954

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2399	1602	390	396	11			

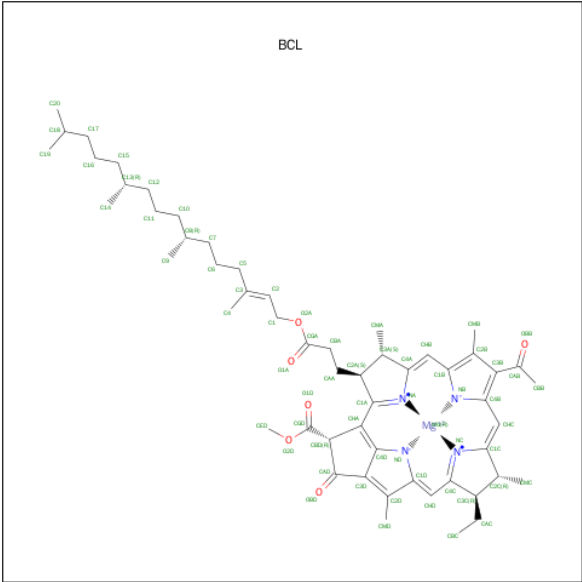
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	ENGINEERED	UNP P02953

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

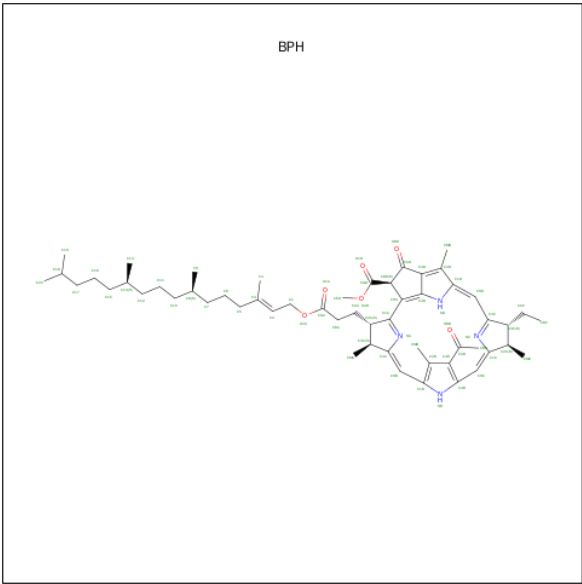
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	1	0
			1822	1165	312	335	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



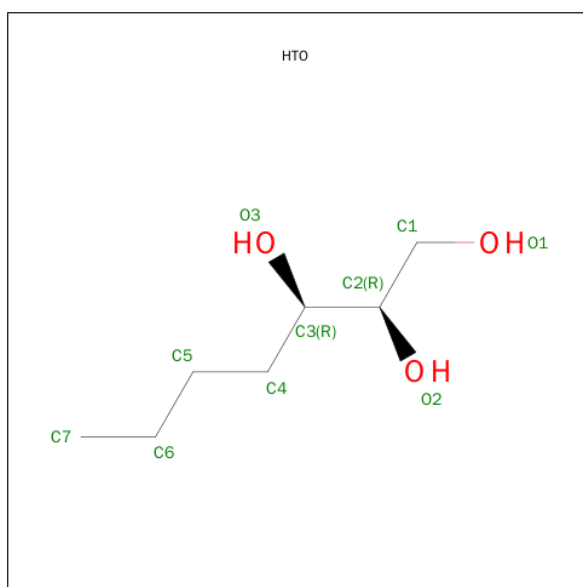
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	1
			33	29	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

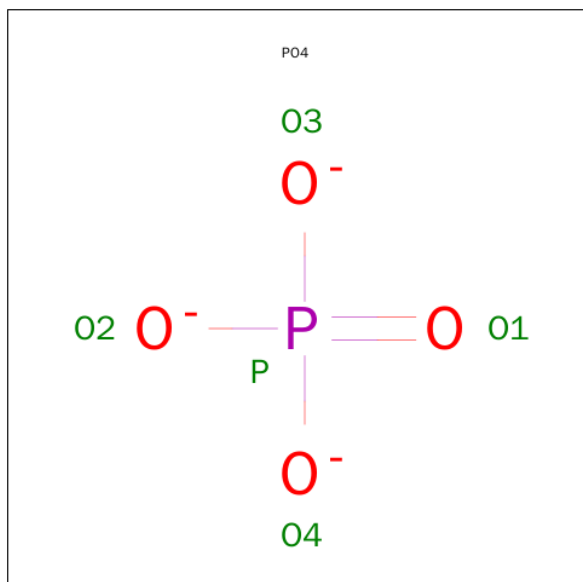


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

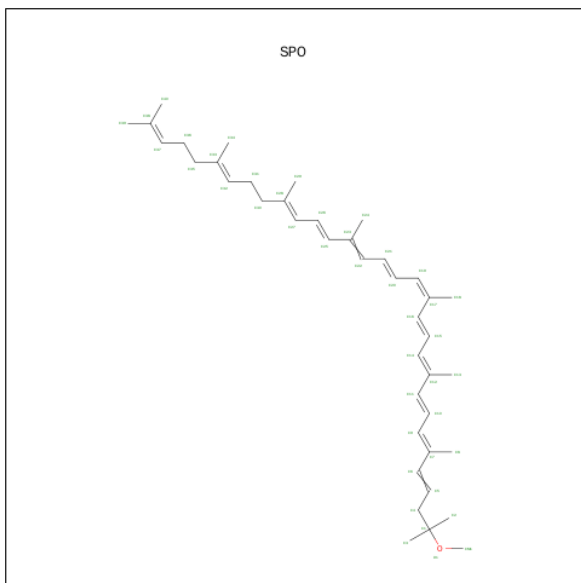
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



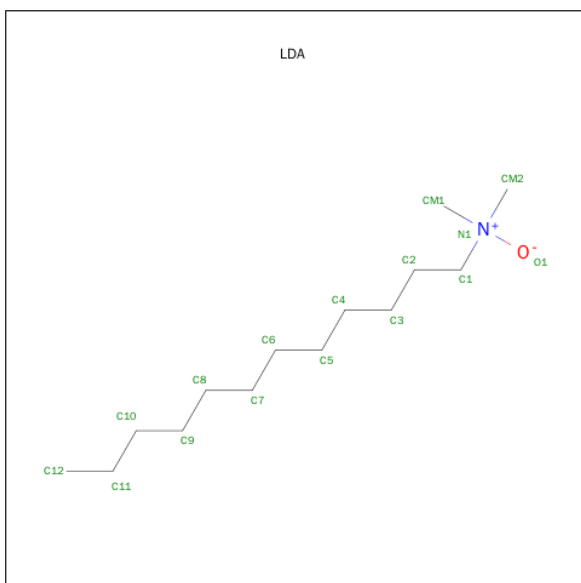
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



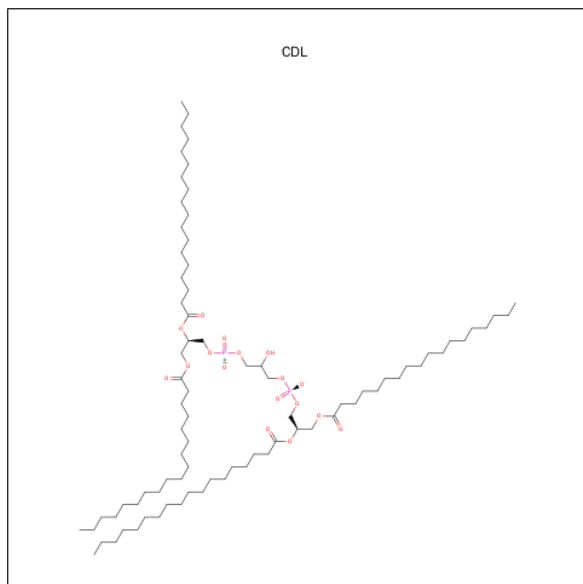
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	M	1	Total	C	O	P	0	0
			69	50	17	2		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

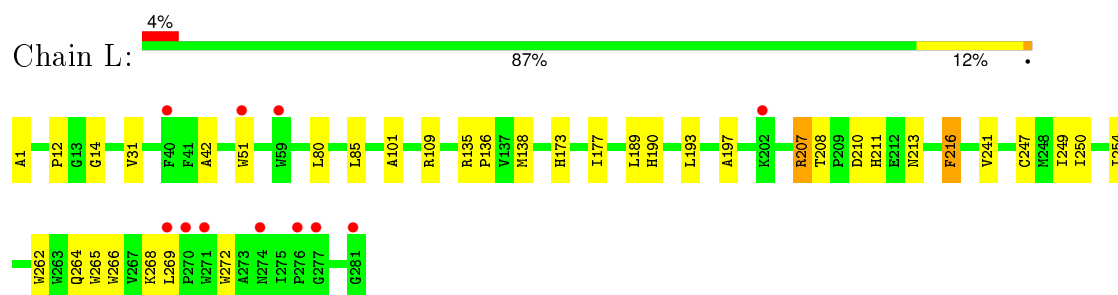
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	124	Total	O	0	2
			124	124		
14	M	138	Total	O	0	0
			138	138		
14	H	209	Total	O	0	0
			209	209		

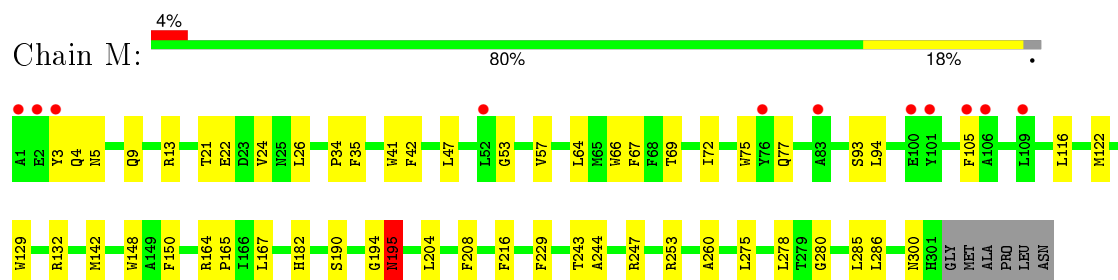
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

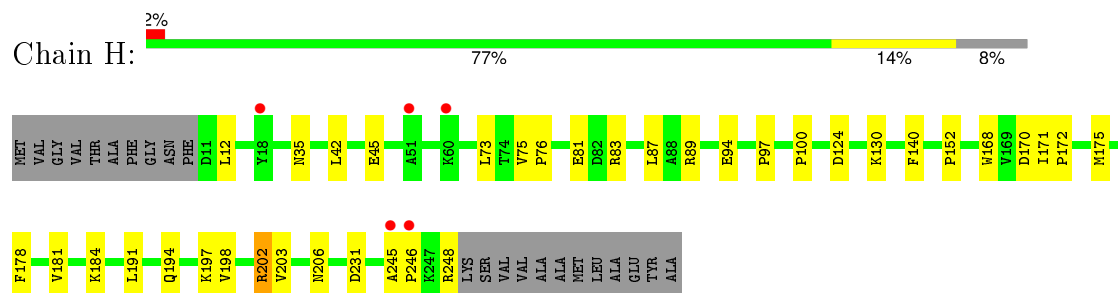
• Molecule 1: Reaction center protein L chain



• 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, α , β , γ	139.35Å 139.35Å 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.31 – 1.80 39.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.31-1.80) 98.3 (39.31-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.233 0.218 , 0.230	Depositor DCC
R_{free} test set	9418 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 188308 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, FE2, SPO, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L	0.36	0/2326	0.55	0/3183
2	M	0.35	0/2491	0.53	0/3402
3	H	0.30	0/1870	0.59	0/2544
All	All	0.34	0/6687	0.56	0/9129

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2238	0	2193	36	0
2	M	2399	0	2310	53	0
3	H	1822	0	1826	29	0
4	L	132	0	148	4	0
4	M	132	0	148	21	0
5	L	65	0	74	5	0
5	M	55	0	53	3	0
6	L	33	0	39	8	0
6	M	48	0	61	3	0
7	L	20	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	5	0	0	0	0
10	M	42	0	60	7	0
11	H	16	0	31	2	0
11	M	32	0	62	5	0
12	M	69	0	82	2	0
13	M	6	0	4	0	0
14	H	209	0	0	1	0
14	L	124	0	0	0	0
14	M	138	0	0	0	0
All	All	7586	0	7123	132	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 132 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:851:BCL:H121	4:M:851:BCL:C9	1.41	1.43
4:M:851:BCL:C12	4:M:851:BCL:H91	1.36	1.39
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.46	0.97
4:M:851:BCL:H91	4:M:851:BCL:H122	1.54	0.90
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.53	0.90

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	273 (98%)	7 (2%)	0	100 100
2	M	299/307 (97%)	292 (98%)	6 (2%)	1 (0%)	46 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	H	237/260 (91%)	236 (100%)	1 (0%)	0	100	100
All	All	816/848 (96%)	801 (98%)	14 (2%)	1 (0%)	56	38

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%)	217 (98%)	4 (2%)	66	54
2	M	236/240 (98%)	233 (99%)	3 (1%)	76	68
3	H	194/208 (93%)	190 (98%)	4 (2%)	61	47
All	All	651/668 (98%)	640 (98%)	11 (2%)	68	57

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	94	LEU
2	M	195	ASN
3	H	175	MET
1	L	272	TRP
3	H	73	LEU

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

Mol	Chain	Res	Type
2	M	77	GLN
3	H	206	ASN
2	M	299	GLN
1	L	213	ASN

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Mol	Chain	Res	Type
2	M	195	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	LDA	H	862	-	15,15,15	4.18	2 (13%)	16,17,17	2.75	4 (25%)
4	BCL	L	852	-	53,74,74	1.05	2 (3%)	57,115,115	1.71	13 (22%)
4	BCL	L	854	-	53,74,74	1.43	9 (16%)	57,115,115	1.99	14 (24%)
5	BPH	L	856	-	64,70,70	1.46	9 (14%)	73,101,101	2.13	17 (23%)
6	U10	L	859[A]	-	33,33,63	2.09	12 (36%)	40,43,79	1.93	10 (25%)
7	HTO	L	865	-	9,9,9	1.23	1 (11%)	8,10,10	0.39	0
7	HTO	L	866	-	9,9,9	1.23	1 (11%)	8,10,10	0.39	0
4	BCL	M	851	-	53,74,74	1.29	7 (13%)	57,115,115	2.35	16 (28%)
4	BCL	M	853	-	53,74,74	1.32	7 (13%)	57,115,115	1.96	13 (22%)
5	BPH	M	855	-	54,60,70	1.38	7 (12%)	61,89,101	2.31	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	U10	M	858	-	48,48,63	2.26	19 (39%)	58,61,79	3.59	18 (31%)
10	SPO	M	860	-	40,41,41	3.39	23 (57%)	45,50,50	2.54	13 (28%)
11	LDA	M	861	-	15,15,15	4.09	2 (13%)	16,17,17	2.33	3 (18%)
11	LDA	M	863	-	15,15,15	3.74	2 (13%)	16,17,17	2.54	4 (25%)
9	PO4	M	864	-	4,4,4	1.18	0	6,6,6	0.27	0
13	GOL	M	867	-	5,5,5	4.78	5 (100%)	5,5,5	5.70	3 (60%)
12	CDL	M	900	-	68,68,99	0.74	2 (2%)	70,80,111	0.98	4 (5%)

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
11	LDA	H	862	-	-	0/13/13/13	0/0/0/0
4	BCL	L	852	-	-	0/37/137/137	0/0/9/9
4	BCL	L	854	-	-	0/37/137/137	0/0/9/9
5	BPH	L	856	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	859[A]	-	-	0/27/51/87	0/1/1/1
7	HTO	L	865	-	-	0/10/10/10	0/0/0/0
7	HTO	L	866	-	-	0/10/10/10	0/0/0/0
4	BCL	M	851	-	2/2/21/25	0/37/137/137	0/0/9/9
4	BCL	M	853	-	-	0/37/137/137	0/0/9/9
5	BPH	M	855	-	1/1/16/22	0/42/93/105	0/1/6/6
6	U10	M	858	-	-	0/45/69/87	0/1/1/1
10	SPO	M	860	-	-	0/47/47/47	0/0/0/0
11	LDA	M	861	-	-	0/13/13/13	0/0/0/0
11	LDA	M	863	-	-	0/13/13/13	0/0/0/0
9	PO4	M	864	-	-	0/0/0/0	0/0/0/0
13	GOL	M	867	-	-	0/4/4/4	0/0/0/0
12	CDL	M	900	-	-	0/79/79/110	0/0/0/0

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	862	LDA	O1-N1	-15.06	1.25	1.39
11	M	861	LDA	O1-N1	-14.66	1.25	1.39
11	M	863	LDA	O1-N1	-13.94	1.26	1.39
13	M	867	GOL	C3-C2	-8.06	1.21	1.52
6	M	858	U10	C37-C38	-5.52	1.35	1.50

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	H	862	LDA	CM2-N1-CM1	-8.10	99.69	108.83
10	M	860	SPO	O1-C1-C4	-8.03	86.23	105.87
11	M	863	LDA	CM2-N1-CM1	-7.46	100.41	108.83
4	M	851	BCL	C4-C3-C5	-6.65	105.25	115.41
11	M	861	LDA	CM2-N1-CM1	-6.39	101.62	108.83

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	856	BPH	C8
5	L	856	BPH	C13
4	M	851	BCL	C8
4	M	851	BCL	C13
5	M	855	BPH	C8

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	862	LDA	2	0
4	L	852	BCL	1	0
4	L	854	BCL	3	0
5	L	856	BPH	5	0
6	L	859[A]	U10	8	0
7	L	865	HTO	1	0
7	L	866	HTO	1	0
4	M	851	BCL	15	0
4	M	853	BCL	7	0
5	M	855	BPH	3	0
6	M	858	U10	3	0
10	M	860	SPO	7	0
11	M	861	LDA	2	0
11	M	863	LDA	3	0
12	M	900	CDL	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.05	11 (3%) 43 37	15, 22, 46, 59	0
2	M	301/307 (98%)	0.02	11 (3%) 45 39	13, 25, 47, 63	0
3	H	238/260 (91%)	-0.24	5 (2%) 67 62	17, 25, 38, 51	0
All	All	820/848 (96%)	-0.08	27 (3%) 50 44	13, 24, 45, 63	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.4
1	L	281	GLY	5.0
1	L	51	TRP	4.3
1	L	276	PRO	3.8
2	M	2	GLU	3.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	U10	L	859[A]	33/63	0.71	0.65	14.40	45,50,52,53	33
11	LDA	M	861	16/16	0.63	0.31	13.98	57,63,67,68	0
7	HTO	L	865	10/10	0.69	0.25	13.07	61,63,64,64	0
12	CDL	M	900	69/100	0.68	0.37	4.90	49,71,77,78	0
11	LDA	M	863	16/16	0.70	0.27	4.90	70,70,74,74	0
11	LDA	H	862	16/16	0.75	0.22	4.67	61,62,66,67	0
6	U10	M	858	48/63	0.89	0.19	2.88	16,29,61,63	0
4	BCL	M	851	66/66	0.91	0.16	2.51	17,22,66,68	0
10	SPO	M	860	42/42	0.75	0.19	2.44	25,32,50,52	0
4	BCL	M	853	66/66	0.92	0.14	2.20	13,18,38,44	0
4	BCL	L	852	66/66	0.93	0.12	1.48	15,17,29,32	0
9	PO4	M	864	5/5	0.89	0.17	1.38	72,73,73,73	0
5	BPH	L	856	65/65	0.92	0.13	1.33	13,17,33,36	0
4	BCL	L	854	66/66	0.93	0.12	1.12	12,17,40,44	0
5	BPH	M	855	55/65	0.93	0.13	0.96	19,22,63,66	0
8	FE2	M	857	1/1	0.98	0.09	-4.56	14,14,14,14	0
7	HTO	L	866	10/10	0.58	0.35	-	66,68,69,69	0
13	GOL	M	867	6/6	0.86	0.20	-	51,55,56,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.