



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 11:29 AM GMT

PDB ID : 1RVJ
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM
RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH
ASN AND ARG H177 REPLACED WITH HIS
Authors : Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher,
G.
Deposited on : 2003-12-14
Resolution : 2.75 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>

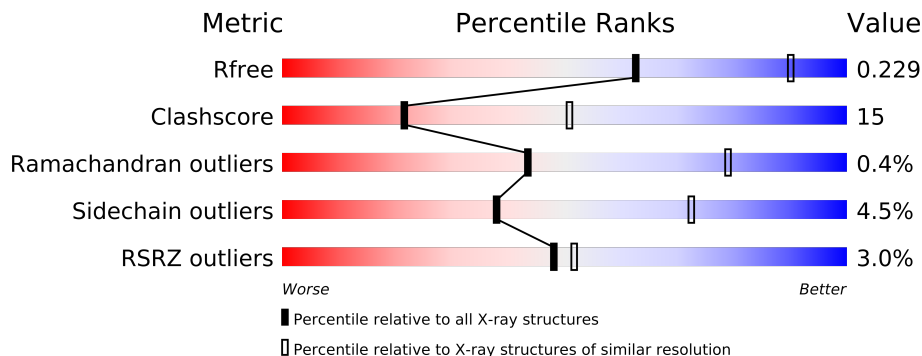
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.75 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	2406 (2.80-2.72)
Clashscore	79885	2995 (2.80-2.72)
Ramachandran outliers	78287	2941 (2.80-2.72)
Sidechain outliers	78261	2944 (2.80-2.72)
RSRZ outliers	66119	2409 (2.80-2.72)

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	LDA	M	861	-	X
10	LDA	M	863	-	X
11	CDL	M	900	-	X
6	U10	L	859	-	X
9	SPO	M	860	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7210 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	0	0
			2232	1507	356	361	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
			2404	1605	393	396	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	ALA	-	CLONING ARTIFACT	UNP P02953

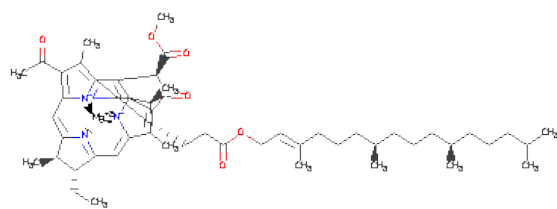
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1813	1160	310	334	9			

There are 2 discrepancies between the modelled and reference sequences:

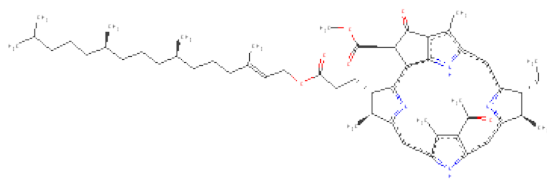
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	ENGINEERED	UNP P11846
H	177	HIS	ARG	ENGINEERED	UNP P11846

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



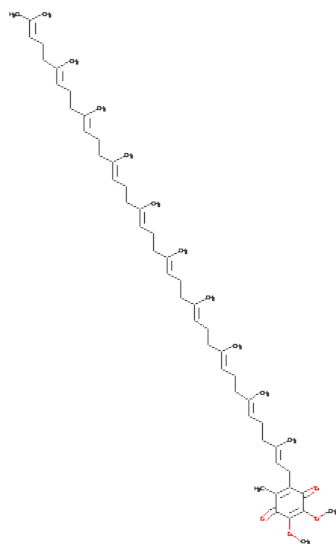
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is 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
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).

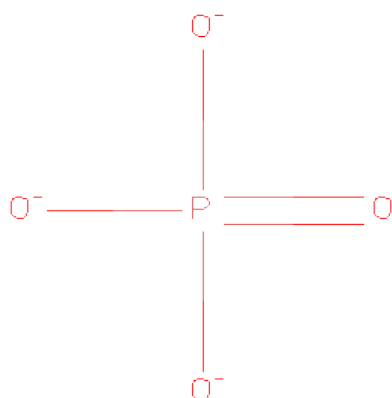


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			44	40	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

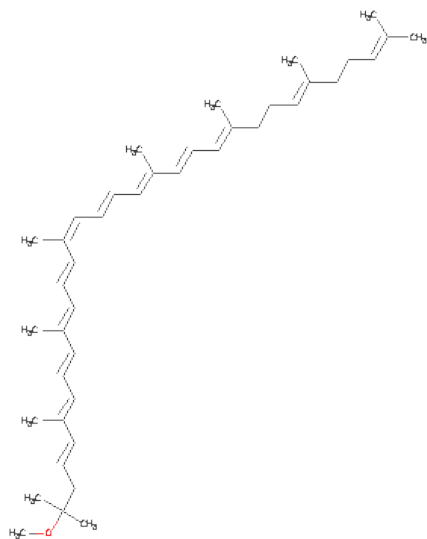
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



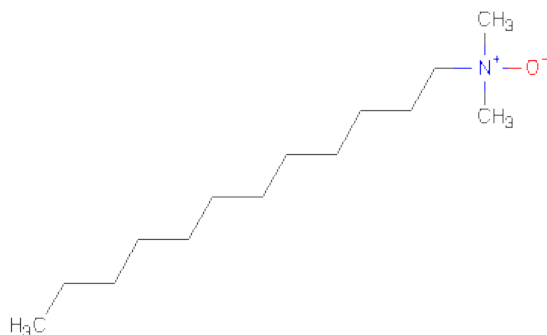
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



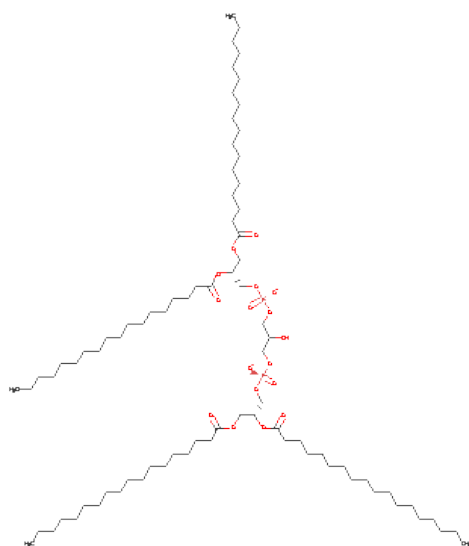
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- 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
			69	50	17	2		

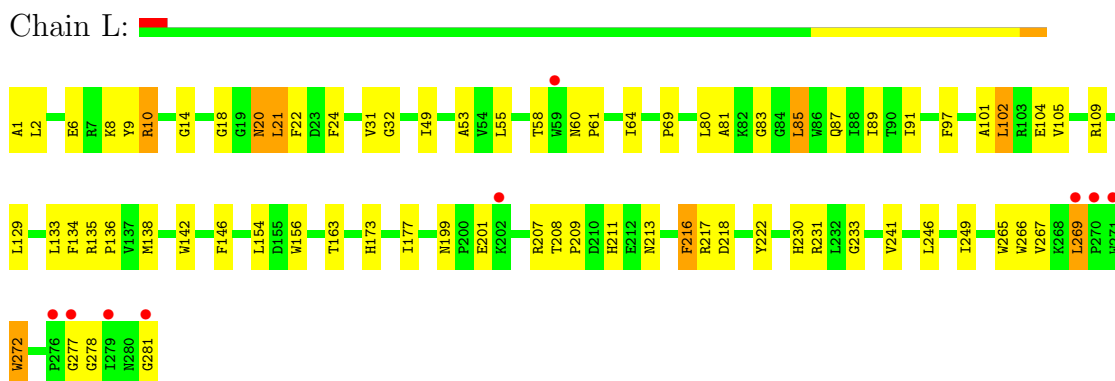
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	40	Total 40	O 40	0	0
12	M	43	Total 43	O 43	0	0
12	H	42	Total 42	O 42	0	0

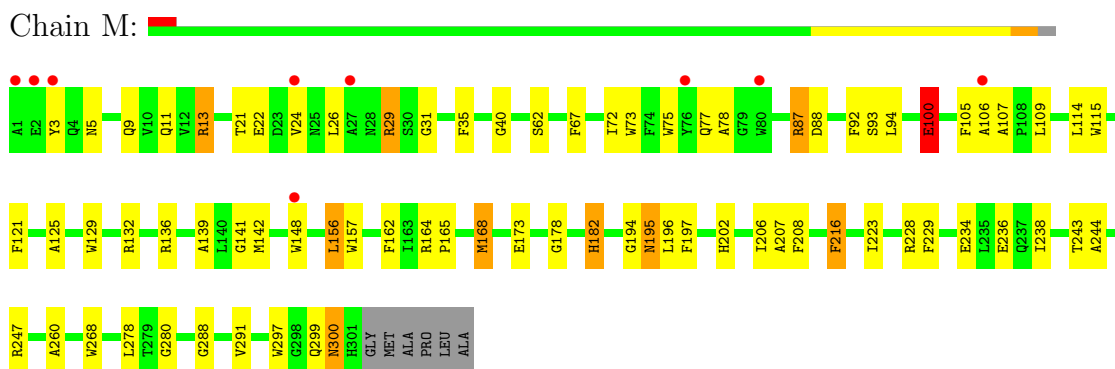
3 Residue-property plots

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.

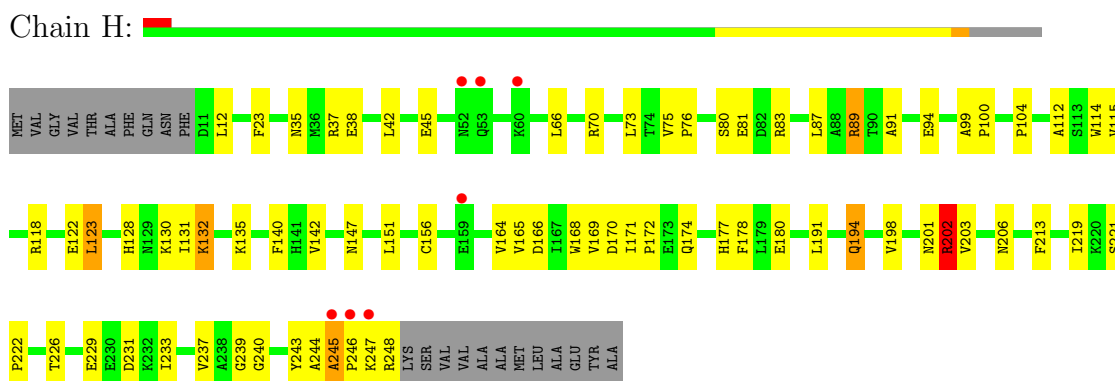
- Molecule 1: Reaction center protein L chain



- 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	138.24Å 138.24Å 184.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 2.75 39.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.00-2.75) 99.5 (39.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.237 0.208 , 0.229	Depositor DCC
R_{free} test set	2685 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 53193 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7210	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, LDA, CDL, BPH, PO4, 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	0.40	0/2320	0.59	0/3175
2	M	0.39	0/2496	0.57	0/3408
3	H	0.36	0/1862	0.63	0/2535
All	All	0.39	0/6678	0.60	0/9118

There are no bond length outliers.

There are no bond angle outliers.

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	2232	0	2189	57	0
2	M	2404	0	2318	95	0
3	H	1813	0	1812	65	0
4	L	117	0	115	12	0
4	M	132	0	147	13	0
5	L	65	0	74	5	0
5	M	65	0	74	13	0
6	L	44	0	57	1	0
6	M	48	0	62	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	1	0	0	0	0
8	M	5	0	0	0	0
9	M	42	0	60	9	0
10	H	16	0	31	1	0
10	M	32	0	62	2	0
11	M	69	0	82	6	0
12	H	42	0	0	0	0
12	L	40	0	0	0	0
12	M	43	0	0	2	0
All	All	7210	0	7083	215	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 15.

The worst 5 of 215 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:M:855:BPH:H121	5:M:855:BPH:H9C1	1.40	0.99
2:M:300:ASN:HD22	2:M:300:ASN:N	1.64	0.93
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.55	0.87
2:M:9:GLN:HE22	3:H:198:VAL:H	1.23	0.86
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.59	0.84

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	279/281 (99%)	266 (95%)	13 (5%)	0	100	100
2	M	299/307 (97%)	285 (95%)	13 (4%)	1 (0%)	50	83
3	H	236/260 (91%)	227 (96%)	7 (3%)	2 (1%)	27	63
All	All	814/848 (96%)	778 (96%)	33 (4%)	3 (0%)	43	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	245	ALA
2	M	100	GLU
3	H	202	ARG

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	220/220 (100%)	211 (96%)	9 (4%)	41	76
2	M	236/239 (99%)	226 (96%)	10 (4%)	40	75
3	H	193/209 (92%)	183 (95%)	10 (5%)	32	66
All	All	649/668 (97%)	620 (96%)	29 (4%)	38	72

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	156	LEU
2	M	195	ASN
3	H	194	GLN
2	M	168	MET
2	M	216	PHE

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	M	5	ASN
2	M	9	GLN
2	M	300	ASN
1	L	264	GLN
2	M	195	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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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	$\# Z > 2$
10	LDA	H	862	-	15,15,15	3.85	2 (13%)	17,17,17	2.51	5 (29%)
4	BCL	L	851	-	59,59,74	2.37	14 (23%)	77,97,115	2.13	22 (28%)
4	BCL	L	852	-	74,74,74	2.12	12 (16%)	97,115,115	1.86	27 (27%)
5	BPH	L	856	-	70,70,70	1.74	13 (18%)	94,101,101	2.02	26 (27%)
6	U10	L	859	-	44,44,63	1.87	11 (25%)	55,56,79	1.37	4 (7%)
4	BCL	M	853	-	74,74,74	2.14	13 (17%)	97,115,115	2.51	28 (28%)
4	BCL	M	854	-	74,74,74	2.12	13 (17%)	97,115,115	2.29	24 (24%)
5	BPH	M	855	-	70,70,70	1.73	14 (20%)	94,101,101	2.10	30 (31%)
6	U10	M	858	-	48,48,63	2.20	18 (37%)	59,61,79	3.52	17 (28%)
9	SPO	M	860	-	41,41,41	3.41	26 (63%)	50,50,50	4.05	17 (34%)
10	LDA	M	861	-	15,15,15	3.92	2 (13%)	17,17,17	2.29	2 (11%)
10	LDA	M	863	-	15,15,15	4.14	2 (13%)	17,17,17	2.72	6 (35%)
8	PO4	M	864	-	4,4,4	0.84	0	6,6,6	0.31	0
11	CDL	M	900	-	68,68,99	1.82	11 (16%)	80,80,111	1.91	17 (21%)

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
10	LDA	H	862	-	-	0/13/13/13	0/0/0/0
4	BCL	L	851	-	-	0/23/119/137	0/0/9/9
4	BCL	L	852	-	-	0/41/137/137	0/0/9/9
5	BPH	L	856	-	-	0/49/105/105	0/0/6/6
6	U10	L	859	-	-	0/41/65/87	0/1/1/1
4	BCL	M	853	-	-	0/41/137/137	0/0/9/9
4	BCL	M	854	-	-	0/41/137/137	0/0/9/9
5	BPH	M	855	-	-	0/49/105/105	0/0/6/6
6	U10	M	858	-	-	0/45/69/87	0/1/1/1
9	SPO	M	860	-	-	0/47/47/47	0/0/0/0
10	LDA	M	861	-	-	0/13/13/13	0/0/0/0
10	LDA	M	863	-	-	0/13/13/13	0/0/0/0
8	PO4	M	864	-	-	0/0/0/0	0/0/0/0
11	CDL	M	900	-	1/1/9/9	0/79/79/110	0/0/0/0

The worst 5 of 151 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	863	LDA	O1-N1	-15.40	1.24	1.39
10	M	861	LDA	O1-N1	-14.31	1.25	1.39
10	H	862	LDA	O1-N1	-14.12	1.26	1.39
4	M	854	BCL	C1B-C2B	9.68	1.52	1.40
4	L	852	BCL	C3B-C4B	9.41	1.55	1.40

The worst 5 of 225 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	858	U10	C32-C33-C34	20.45	171.91	127.80
9	M	860	SPO	C2-C1-C4	-19.42	78.90	110.97
4	M	853	BCL	C1-C2-C3	12.35	148.15	126.19
9	M	860	SPO	C3-C1-C4	-10.94	92.89	110.97
4	M	854	BCL	CAC-C3C-C4C	-10.41	89.47	112.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	M	900	CDL	CA4

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%)	-0.07	9 (3%)	45	49	40, 52, 77, 92	0
2	M	301/307 (98%)	-0.01	9 (2%)	48	52	39, 55, 80, 112	0
3	H	238/260 (91%)	-0.06	7 (2%)	49	53	43, 55, 69, 111	0
All	All	820/848 (96%)	-0.04	25 (3%)	48	52	39, 54, 77, 112	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	8.3
3	H	246	PRO	6.3
2	M	3	TYR	4.5
1	L	277	GLY	4.3
3	H	247	LYS	4.3

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
10	LDA	M	863	16/16	0.39	13.39	93,95,103,104	0
6	U10	L	859	44/63	0.47	5.15	92,100,103,107	0
9	SPO	M	860	42/42	0.33	3.67	48,67,86,88	0
11	CDL	M	900	69/100	0.38	3.00	93,106,120,122	0
10	LDA	M	861	16/16	0.26	2.08	60,69,80,81	0
6	U10	M	858	48/63	0.26	1.89	47,59,84,85	0
5	BPH	M	855	65/65	0.23	1.43	46,51,100,102	0
4	BCL	M	853	66/66	0.20	1.07	44,50,63,70	0
4	BCL	L	851	51/66	0.21	0.97	39,45,68,70	0
10	LDA	H	862	16/16	0.23	0.93	66,68,78,79	0
5	BPH	L	856	65/65	0.18	0.48	37,43,52,54	0
4	BCL	L	852	66/66	0.18	0.43	38,49,52,53	0
4	BCL	M	854	66/66	0.17	0.16	35,40,62,64	0
8	PO4	M	864	5/5	0.13	-1.17	91,93,94,94	0
7	FE2	M	857	1/1	0.15	-2.55	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.