



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 02:25 PM GMT

PDB ID : 1K6N
Title : E(L212)A,D(L213)A Double Mutant Structure of Photosynthetic Reaction Center from Rhodobacter Sphaeroides
Authors : Pokkuluri, P.R.; Laible, P.D.; Deng, Y.-L.; Wong, T.N.; Hanson, D.K.; Schiffer, M.
Deposited on : 2001-10-16
Resolution : 3.10 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>

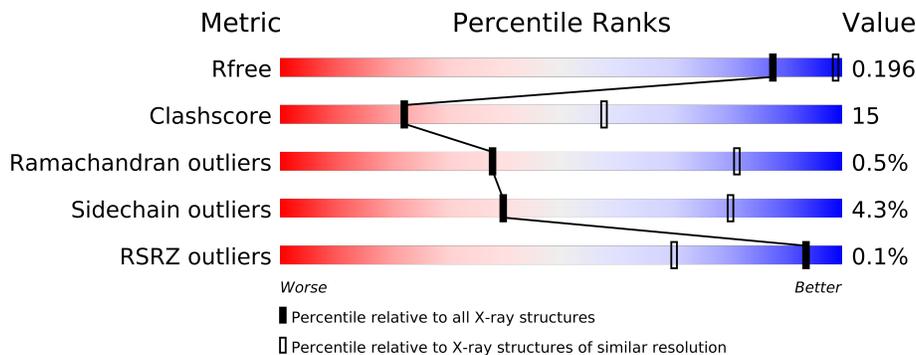
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.10 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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	314	
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	H	703	-	X
10	LDA	L	709	-	X
10	LDA	M	701	-	X
10	LDA	M	704	-	X
5	BCL	M	501	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	BPH	L	402	-	X
7	U10	L	502	-	X
8	SPN	M	600	-	X
9	CDL	M	800	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7270 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 PHOTOSYNTHETIC REACTION CENTER L SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	281	2225	1504	355	358	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	212	ALA	GLU	ENGINEERED	UNP P02954
L	213	ALA	ASP	ENGINEERED	UNP P02954

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	M	302	2408	1607	394	397	10	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	308	HIS	-	EXPRESSION TAG	UNP P02953
M	309	HIS	-	EXPRESSION TAG	UNP P02953
M	310	HIS	-	EXPRESSION TAG	UNP P02953
M	311	HIS	-	EXPRESSION TAG	UNP P02953
M	312	HIS	-	EXPRESSION TAG	UNP P02953
M	313	HIS	-	EXPRESSION TAG	UNP P02953
M	314	HIS	-	EXPRESSION TAG	UNP P02953

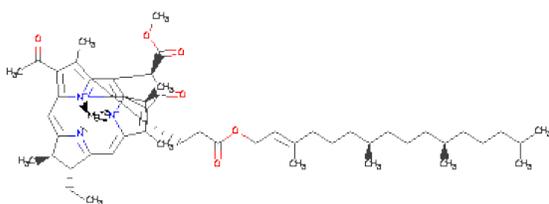
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	240	1829	1169	314	337	9	0	0	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

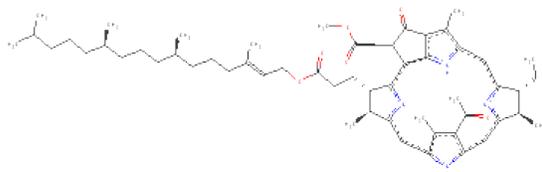
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total Fe 1 1	0	0

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



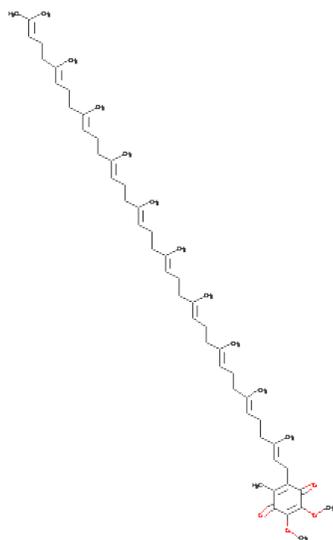
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0
5	M	1	Total C Mg N O 66 55 1 4 6	0	0
5	L	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C₅₅H₇₆N₄O₆).



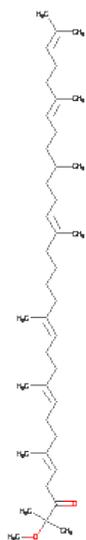
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	M	1	65	55	4	6	10	0
6	L	1	65	55	4	6	0	0

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: C₅₉H₉₀O₄).



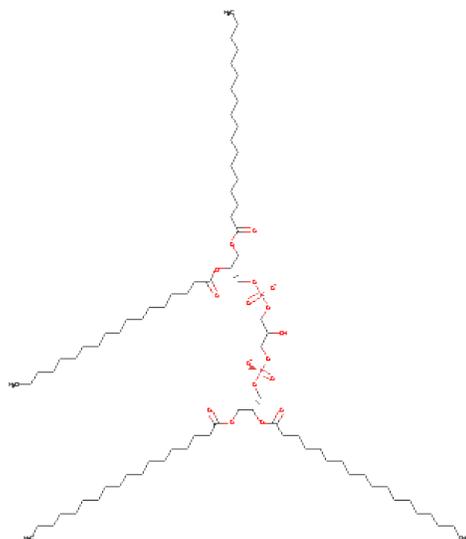
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	M	1	48	44	4	0	0
7	L	1	48	44	4	0	0

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	M	1	43	41	2	0	0

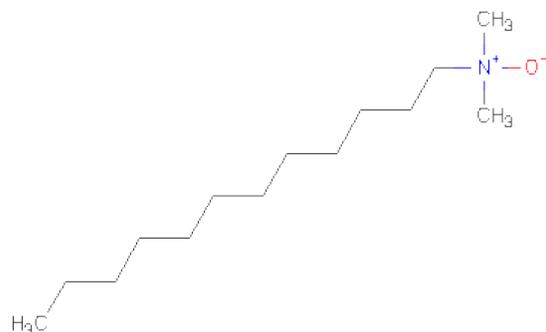
- Molecule 9 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	51	Total	O	0	0
			51	51		
11	L	34	Total	O	0	0
			34	34		
11	M	44	Total	O	0	0
			44	44		

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.50Å 141.50Å 187.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 3.10 14.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.10) 88.4 (14.99-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 3.12Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	0.203 , 0.207 0.192 , 0.196	Depositor DCC
R_{free} test set	2439 reflections (7.50%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.4	EDS
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 34959 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7270	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, LDA, CDL, BPH, FE, SPN, 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	0.95	0/2313	1.09	13/3166 (0.4%)
2	M	1.04	0/2500	1.10	16/3413 (0.5%)
3	H	0.94	1/1877 (0.1%)	1.21	20/2553 (0.8%)
All	All	0.98	1/6690 (0.0%)	1.13	49/9132 (0.5%)

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
1	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	250	SER	C-O	5.48	1.33	1.23

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	103	ARG	NE-CZ-NH1	11.02	125.81	120.30
3	H	154	ARG	NE-CZ-NH2	7.36	123.98	120.30
3	H	117	ARG	NE-CZ-NH2	7.36	123.98	120.30
2	M	13	ARG	NE-CZ-NH2	7.33	123.96	120.30
2	M	247	ARG	NE-CZ-NH2	7.33	123.96	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	280	ASN	Mainchain

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	2225	0	2187	86	0
2	M	2408	0	2321	76	0
3	H	1829	0	1836	47	0
4	M	1	0	0	0	0
5	L	132	0	148	16	0
5	M	132	0	148	20	0
6	L	65	0	76	2	0
6	M	65	0	76	1	0
7	L	48	0	62	11	0
7	M	48	0	63	6	0
8	M	43	0	69	1	0
9	M	81	0	106	1	0
10	H	16	0	31	4	0
10	L	16	0	31	4	0
10	M	32	0	62	4	0
11	H	51	0	0	3	0
11	L	34	0	0	1	0
11	M	44	0	0	0	0
All	All	7270	0	7216	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)
3:H:33:THR:O	3:H:59:PRO:HG3	1.69	0.91
1:L:34:PHE:O	1:L:38:THR:HG23	1.71	0.89
7:M:503:U10:H202	10:H:703:LDA:H112	1.54	0.88
1:L:204:LYS:HD3	1:L:207:ARG:HH22	1.36	0.87
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.56	0.85

There are no symmetry-related clashes.

5.3 Torsion angles

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	279/281 (99%)	264 (95%)	15 (5%)	0	100	100
2	M	300/314 (96%)	286 (95%)	10 (3%)	4 (1%)	18	60
3	H	238/260 (92%)	227 (95%)	11 (5%)	0	100	100
All	All	817/855 (96%)	777 (95%)	36 (4%)	4 (0%)	38	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
2	M	22	GLU
2	M	52	LEU
2	M	34	PRO

5.3.2 Protein sidechains [i](#)

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	218/218 (100%)	208 (95%)	10 (5%)	37	78
2	M	236/247 (96%)	229 (97%)	7 (3%)	53	87
3	H	195/208 (94%)	184 (94%)	11 (6%)	30	70
All	All	649/673 (96%)	621 (96%)	28 (4%)	40	80

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	152	SER
2	M	216	PHE
3	H	225	VAL
2	M	196	LEU
2	M	204	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	280	ASN
2	M	4	GLN
2	M	188	ASN
3	H	206	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	703	-	15,15,15	4.76	4 (26%)	17,17,17	1.25	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	BCL	L	302	1	74,74,74	1.61	13 (17%)	97,115,115	1.90	17 (17%)
5	BCL	L	304	1	74,74,74	1.57	14 (18%)	97,115,115	1.71	15 (15%)
6	BPH	L	402	-	70,70,70	1.47	13 (18%)	94,101,101	1.79	22 (23%)
7	U10	L	502	-	48,48,63	1.91	14 (29%)	59,61,79	2.99	17 (28%)
10	LDA	L	709	-	15,15,15	4.58	2 (13%)	17,17,17	3.73	1 (5%)
6	BPH	M	401	-	70,70,70	1.56	13 (18%)	94,101,101	2.13	34 (36%)
5	BCL	M	501	2	74,74,74	1.56	15 (20%)	97,115,115	2.14	24 (24%)
5	BCL	M	502	2	74,74,74	1.43	11 (14%)	97,115,115	1.46	14 (14%)
7	U10	M	503	-	48,48,63	2.60	23 (47%)	59,61,79	1.39	10 (16%)
8	SPN	M	600	-	42,42,42	4.15	17 (40%)	52,52,52	2.73	18 (34%)
10	LDA	M	701	-	15,15,15	4.88	2 (13%)	17,17,17	5.44	1 (5%)
10	LDA	M	704	-	15,15,15	3.74	1 (6%)	17,17,17	4.37	1 (5%)
9	CDL	M	800	-	80,80,99	1.36	4 (5%)	92,92,111	0.99	3 (3%)

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	703	-	-	0/13/13/13	0/0/0/0
5	BCL	L	302	1	-	0/41/137/137	0/0/9/9
5	BCL	L	304	1	1/1/21/25	0/41/137/137	0/0/9/9
6	BPH	L	402	-	2/2/18/22	0/49/105/105	0/0/6/6
7	U10	L	502	-	-	0/45/69/87	0/1/1/1
10	LDA	L	709	-	-	0/13/13/13	0/0/0/0
6	BPH	M	401	-	1/1/18/22	0/49/105/105	0/0/6/6
5	BCL	M	501	2	2/2/21/25	1/41/137/137	0/0/9/9
5	BCL	M	502	2	-	0/41/137/137	0/0/9/9
7	U10	M	503	-	-	0/45/69/87	0/1/1/1
8	SPN	M	600	-	-	0/51/51/51	0/0/0/0
10	LDA	M	701	-	-	0/13/13/13	0/0/0/0
10	LDA	M	704	-	-	0/13/13/13	0/0/0/0
9	CDL	M	800	-	1/1/9/9	0/91/91/110	0/0/0/0

The worst 5 of 146 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-18.69	1.21	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	703	LDA	O1-N1	-17.65	1.22	1.39
10	L	709	LDA	O1-N1	-17.50	1.22	1.39
10	M	704	LDA	O1-N1	-14.40	1.25	1.39
8	M	600	SPN	C4-C5	10.60	1.54	1.32

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	701	LDA	C2-C1-N1	22.33	152.29	113.80
10	M	704	LDA	C2-C1-N1	17.84	144.55	113.80
7	L	502	U10	C32-C33-C34	16.29	162.93	127.80
10	L	709	LDA	C2-C1-N1	15.21	140.02	113.80
5	L	302	BCL	OBB-CAB-C3B	10.98	136.55	120.07

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	304	BCL	C13
9	M	800	CDL	CA4
5	M	501	BCL	C8
5	M	501	BCL	C13
6	M	401	BPH	C13

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	501	BCL	C1-C2-C3-C4

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 [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%)	-0.55	0 100 100	10, 27, 66, 94	0
2	M	302/314 (96%)	-0.54	1 (0%) 91 53	11, 32, 68, 97	0
3	H	240/260 (92%)	-0.49	0 100 100	13, 29, 58, 95	0
All	All	823/855 (96%)	-0.53	1 (0%) 93 70	10, 29, 66, 97	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	2.3

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	U10	L	502	48/63	0.45	13.90	43,72,101,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
10	LDA	L	709	16/16	0.47	8.03	67,85,95,97	0
10	LDA	M	704	16/16	0.33	7.85	48,75,109,109	0
10	LDA	H	703	16/16	0.26	4.11	34,50,64,67	0
9	CDL	M	800	81/100	0.38	3.51	41,62,76,77	81
6	BPH	L	402	65/65	0.17	2.56	23,27,38,40	0
10	LDA	M	701	16/16	0.18	2.53	29,44,52,58	0
5	BCL	M	501	66/66	0.17	2.26	27,32,92,94	0
8	SPN	M	600	43/43	0.21	2.12	36,47,64,67	0
7	U10	M	503	48/63	0.15	1.59	15,29,60,62	0
5	BCL	M	502	66/66	0.12	0.44	10,19,52,68	0
5	BCL	L	304	66/66	0.12	0.08	2,14,40,49	0
6	BPH	M	401	65/65	0.13	-0.02	29,33,63,67	10
5	BCL	L	302	66/66	0.10	-0.50	5,17,40,54	0
4	FE	M	500	1/1	0.02	-2.98	18,18,18,18	0

6.5 Other polymers

There are no such residues in this entry.