



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:07 AM GMT

PDB ID : 3DTA
Title : E(L212)Q, N(M44)D double mutant structure of photosynthetic reaction center from Rhodobacter sphaeroides
Authors : Pokkuluri, P.R.; Schiffer, M.
Deposited on : 2008-07-14
Resolution : 3.20 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>

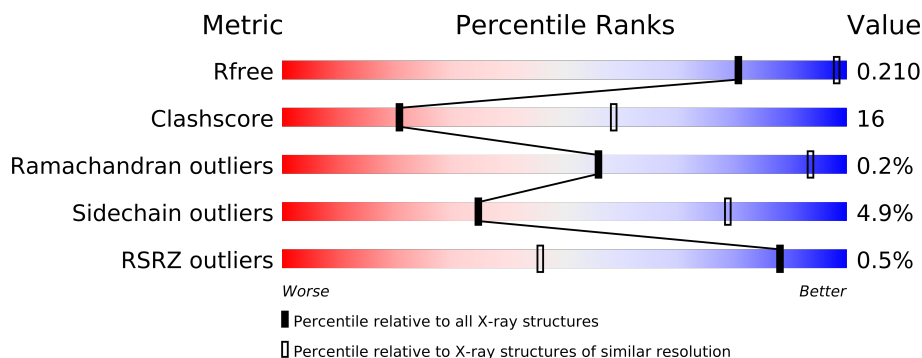
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	CDL	M	800	-	X
5	BCL	M	501	-	X
7	U10	L	504	-	X
8	LDA	H	703	-	X
8	LDA	L	709	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
8	LDA	M	704	-	X
9	SPN	M	600	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7296 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	212	GLN	GLU	ENGINEERED	UNP P0C0Y8

- 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	0	0
			2408	1607	393	398	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	44	ASP	ASN	ENGINEERED	UNP P0C0Y9
M	308	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	309	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	310	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	311	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	312	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	313	HIS	-	EXPRESSION TAG	UNP P0C0Y9
M	314	HIS	-	EXPRESSION TAG	UNP P0C0Y9

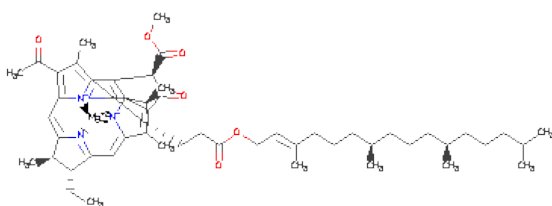
- Molecule 3 is a protein called Reaction center protein H chain.

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

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

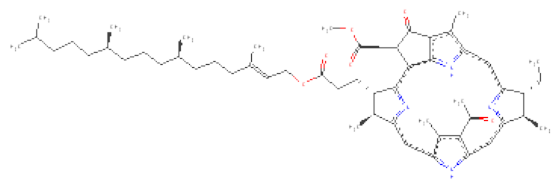
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



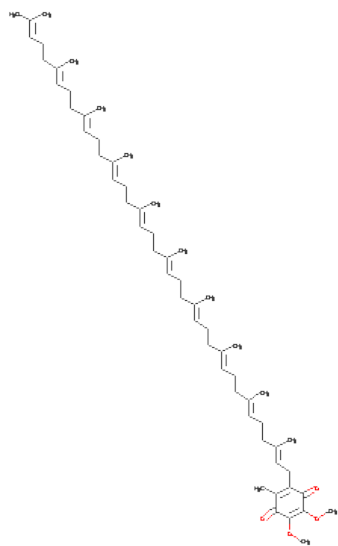
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



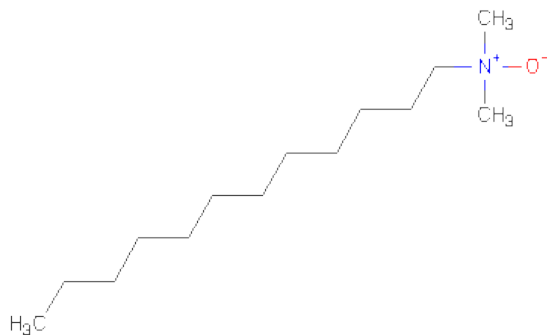
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	M	1	Total	C	N	O	10	0
			65	55	4	6		

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



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

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



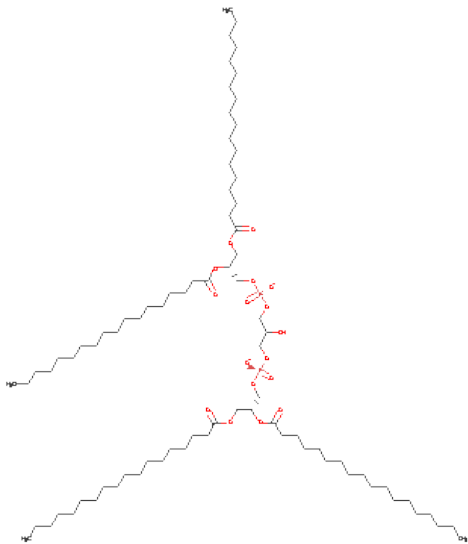
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

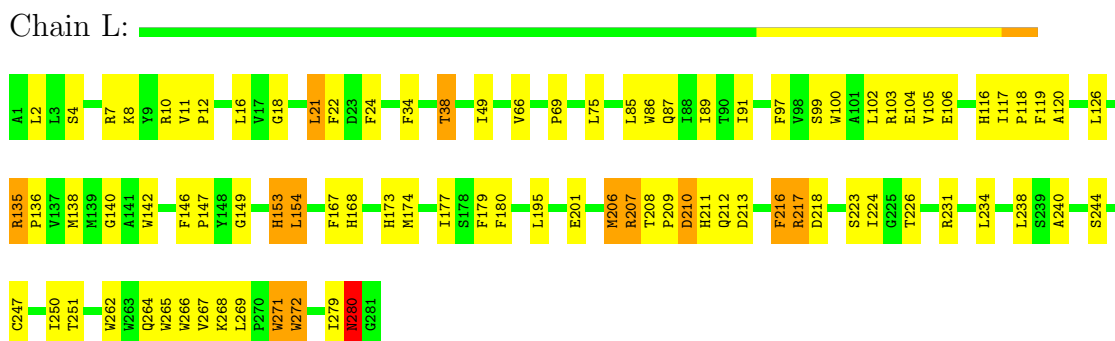
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	64	Total 64	O 64	0	0
11	L	40	Total 40	O 40	0	0
11	M	44	Total 44	O 44	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.

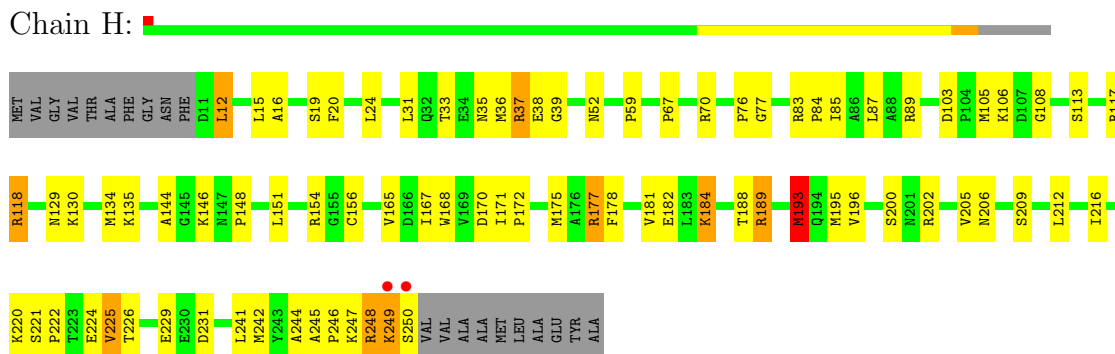
• Molecule 1: Reaction center protein L chain



• 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	141.50Å 141.50Å 187.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.20 28.52 – 3.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 89.9 (28.52-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.17Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.203 0.206 , 0.210	Depositor DCC
R_{free} test set	2275 reflections (7.51%)	DCC
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.4	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 34465 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7296	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, 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	0/2320	1.08	13/3175 (0.4%)
2	M	1.08	3/2500 (0.1%)	1.17	21/3413 (0.6%)
3	H	0.95	2/1877 (0.1%)	1.25	21/2553 (0.8%)
All	All	1.00	5/6697 (0.1%)	1.17	55/9141 (0.6%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	76	PRO	C-N	-6.35	1.21	1.33
2	M	14	GLY	N-CA	5.91	1.54	1.46
3	H	77	GLY	N-CA	5.73	1.54	1.46
2	M	247	ARG	CG-CD	-5.41	1.38	1.51
2	M	301	HIS	CA-C	-5.14	1.39	1.52

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	248	ARG	CD-NE-CZ	13.08	141.92	123.60
2	M	247	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	L	103	ARG	NE-CZ-NH1	11.02	125.81	120.30
3	H	250	SER	CA-C-O	-8.25	102.78	120.10
1	L	207	ARG	NE-CZ-NH2	7.67	124.13	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	2232	0	2189	79	0
2	M	2408	0	2319	86	0
3	H	1829	0	1836	46	0
4	M	1	0	0	0	0
5	L	132	0	148	16	0
5	M	132	0	148	19	0
6	L	65	0	76	2	0
6	M	65	0	76	1	0
7	L	48	0	63	7	0
7	M	48	0	63	6	0
8	H	16	0	31	4	0
8	L	16	0	31	3	0
8	M	32	0	62	4	0
9	M	43	0	69	1	0
10	M	81	0	106	1	0
11	H	64	0	0	3	0
11	L	40	0	0	1	0
11	M	44	0	0	3	0
All	All	7296	0	7217	223	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 16.

The worst 5 of 223 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:13:ARG:HD3	2:M:35:PHE:CD2	1.72	1.23
2:M:13:ARG:CD	2:M:35:PHE:CD2	2.43	1.02

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:13:ARG:HD3	2:M:35:PHE:CE2	1.94	1.00
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

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%)	262 (94%)	16 (6%)	1 (0%)	43	88
2	M	300/314 (96%)	285 (95%)	14 (5%)	1 (0%)	50	91
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	817/855 (96%)	776 (95%)	39 (5%)	2 (0%)	56	93

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
1	L	210	ASP

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%)	208 (94%)	12 (6%)	30	75
2	M	236/247 (96%)	227 (96%)	9 (4%)	44	84
3	H	195/208 (94%)	184 (94%)	11 (6%)	30	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	651/675 (96%)	619 (95%)	32 (5%)	35 79

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	144	LYS
2	M	204	LEU
3	H	225	VAL
2	M	196	LEU
2	M	216	PHE

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

Mol	Chain	Res	Type
1	L	280	ASN
2	M	4	GLN
2	M	188	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$
8	LDA	H	703	-	15,15,15	4.75	4 (26%)	17,17,17	1.24	1 (5%)
5	BCL	L	501	1	74,74,74	1.57	14 (18%)	97,115,115	1.71	15 (15%)
5	BCL	L	502	1	74,74,74	1.61	13 (17%)	97,115,115	1.90	17 (17%)
6	BPH	L	503	-	70,70,70	1.48	13 (18%)	94,101,101	1.80	22 (23%)
7	U10	L	504	-	48,48,63	2.23	20 (41%)	59,61,79	1.05	3 (5%)
8	LDA	L	709	-	15,15,15	4.60	2 (13%)	17,17,17	3.74	1 (5%)
5	BCL	M	501	2	74,74,74	1.55	14 (18%)	97,115,115	2.14	24 (24%)
5	BCL	M	502	2	74,74,74	1.42	11 (14%)	97,115,115	1.46	15 (15%)
6	BPH	M	503	-	70,70,70	1.57	13 (18%)	94,101,101	2.13	34 (36%)
7	U10	M	504	-	48,48,63	2.61	23 (47%)	59,61,79	1.39	11 (18%)
9	SPN	M	600	-	42,42,42	4.14	17 (40%)	52,52,52	2.73	19 (36%)
8	LDA	M	701	-	15,15,15	4.89	2 (13%)	17,17,17	5.44	1 (5%)
8	LDA	M	704	-	15,15,15	3.74	1 (6%)	17,17,17	4.38	1 (5%)
10	CDL	M	800	-	80,80,99	1.35	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
8	LDA	H	703	-	-	0/13/13/13	0/0/0/0
5	BCL	L	501	1	1/1/21/25	0/41/137/137	0/0/9/9
5	BCL	L	502	1	-	0/41/137/137	0/0/9/9
6	BPH	L	503	-	2/2/18/22	0/49/105/105	0/0/6/6
7	U10	L	504	-	-	0/45/69/87	0/1/1/1
8	LDA	L	709	-	-	0/13/13/13	0/0/0/0
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
6	BPH	M	503	-	1/1/18/22	0/49/105/105	0/0/6/6
7	U10	M	504	-	-	0/45/69/87	0/1/1/1
9	SPN	M	600	-	-	0/51/51/51	0/0/0/0
8	LDA	M	701	-	-	0/13/13/13	0/0/0/0
8	LDA	M	704	-	-	0/13/13/13	0/0/0/0
10	CDL	M	800	-	1/1/9/9	0/91/91/110	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)
8	M	701	LDA	O1-N1	-18.71	1.21	1.39
8	H	703	LDA	O1-N1	-17.59	1.22	1.39
8	L	709	LDA	O1-N1	-17.55	1.22	1.39
8	M	704	LDA	O1-N1	-14.40	1.25	1.39
9	M	600	SPN	C4-C5	10.60	1.54	1.32

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	701	LDA	C2-C1-N1	22.35	152.32	113.80
8	M	704	LDA	C2-C1-N1	17.90	144.66	113.80
8	L	709	LDA	C2-C1-N1	15.25	140.08	113.80
5	L	502	BCL	OBB-CAB-C3B	10.94	136.49	120.07
9	M	600	SPN	CM6-C18-C17	7.66	127.03	115.39

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	M	800	CDL	CA4
5	M	501	BCL	C8
5	M	501	BCL	C13
6	L	503	BPH	C8
6	L	503	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 ⓘ

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%)	-0.41	0 100 100	26, 44, 79, 100	0
2	M	302/314 (96%)	-0.33	1 (0%) 91 58	25, 52, 87, 106	0
3	H	240/260 (92%)	-0.31	2 (0%) 83 35	29, 49, 70, 110	0
All	All	823/855 (96%)	-0.35	3 (0%) 88 51	25, 48, 83, 110	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	249	LYS	2.9
2	M	1	ALA	2.4
3	H	250	SER	2.1

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
7	U10	L	504	48/63	0.79	16.60	97,99,105,105	0
8	LDA	M	704	16/16	0.43	8.05	78,97,117,117	0
8	LDA	L	709	16/16	0.68	5.64	105,107,110,110	0
9	SPN	M	600	43/43	0.36	4.08	52,67,84,85	0
10	CDL	M	800	81/100	0.43	4.03	56,75,87,90	81
5	BCL	M	501	66/66	0.21	3.34	32,40,106,107	0
8	LDA	H	703	16/16	0.30	2.40	64,66,72,73	0
7	U10	M	504	48/63	0.22	1.96	36,40,77,78	0
8	LDA	M	701	16/16	0.23	1.95	53,61,72,73	0
6	BPH	L	503	65/65	0.16	1.01	31,40,48,49	0
6	BPH	M	503	65/65	0.19	0.71	42,55,69,73	10
5	BCL	L	502	66/66	0.16	0.14	22,27,51,52	0
5	BCL	L	501	66/66	0.16	0.02	17,25,56,59	0
5	BCL	M	502	66/66	0.16	-0.05	26,31,64,69	0
4	FE	M	500	1/1	0.07	-2.33	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.