



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:50 am GMT

PDB ID : 1E14
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M197 REPLACED WITH ARG (CHAIN M, FM197R) AND GLY M203 REPLACED WITH ASP (CHAIN M, GM203D)
Authors : Fyfe, P.K.; Ridge, J.P.; Mcauley, K.E.; Cogdell, R.J.; Isaacs, N.W.; Jones, M.R.
Deposited on : 2000-04-18
Resolution : 2.70 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

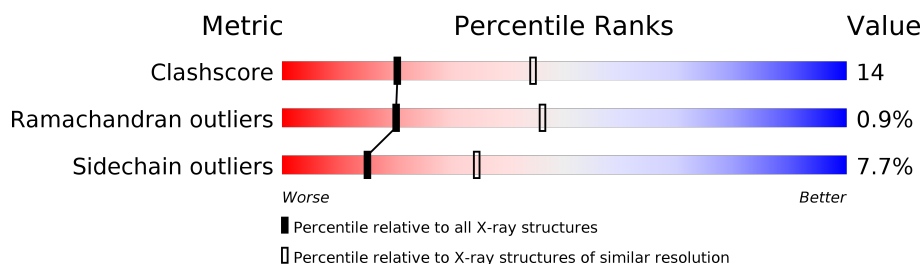
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	260	
2	L	281	
3	M	307	

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
4	BCL	M	1301	X	-	-	-
5	BPH	L	401	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7250 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 PHOTOSYNTHETIC REACTION CENTER H SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	1
			1830	1169	315	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

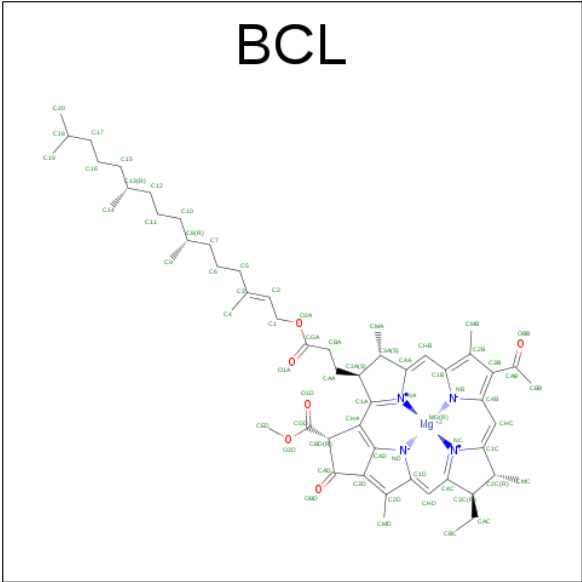
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2413	1606	398	399	10			

There are 2 discrepancies between the modelled and reference sequences:

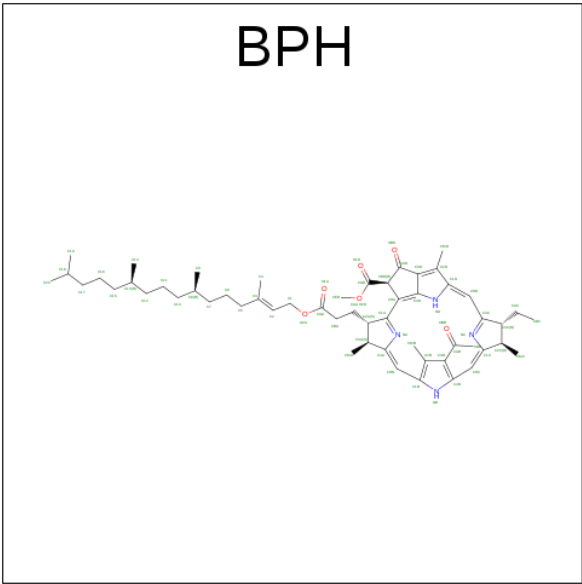
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	ENGINEERED MUTATION	UNP P02953
M	203	ASP	GLY	ENGINEERED MUTATION	UNP P02953

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



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

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

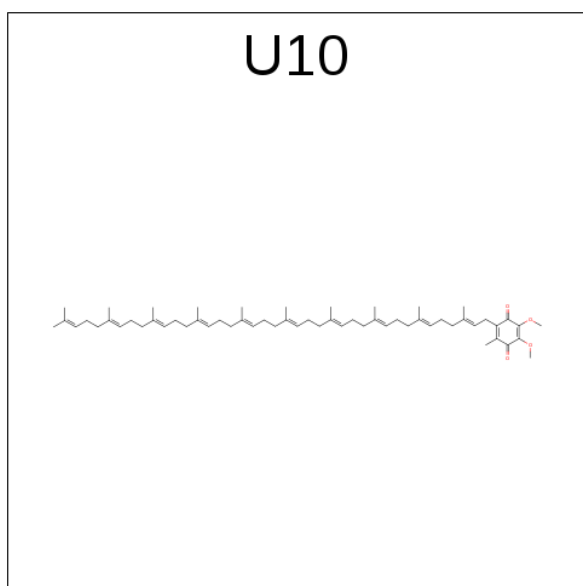


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

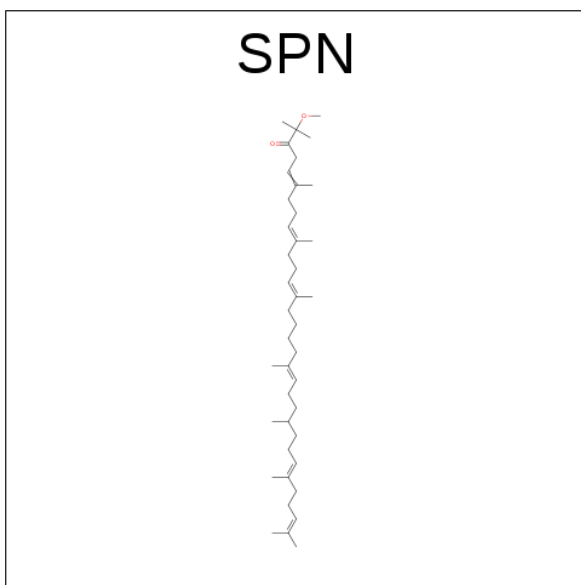
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

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



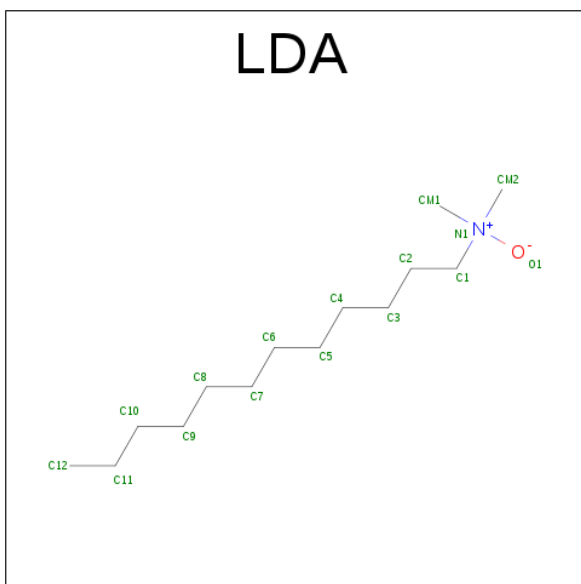
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	22	0
			48	44	4		
7	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: C₄₁H₇₀O₂).



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

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



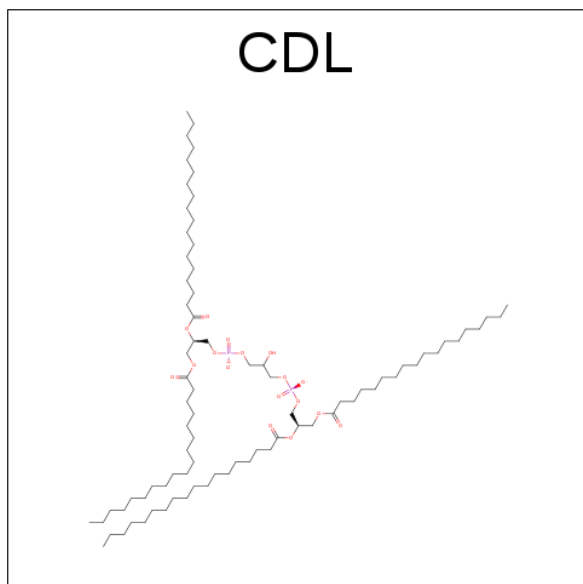
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	H	1	Total	C	N	O	0	0
			16	14	1	1		
9	M	1	Total	C	N	O	0	0
			16	14	1	1		

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

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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	42	Total	O	0	0
			42	42		
11	L	28	Total	O	0	0
			28	28		
11	M	42	Total	O	0	0
			42	42		

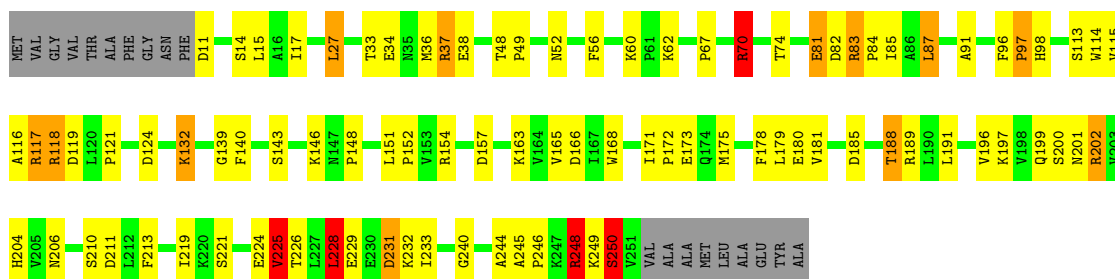
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

Note EDS was not executed.

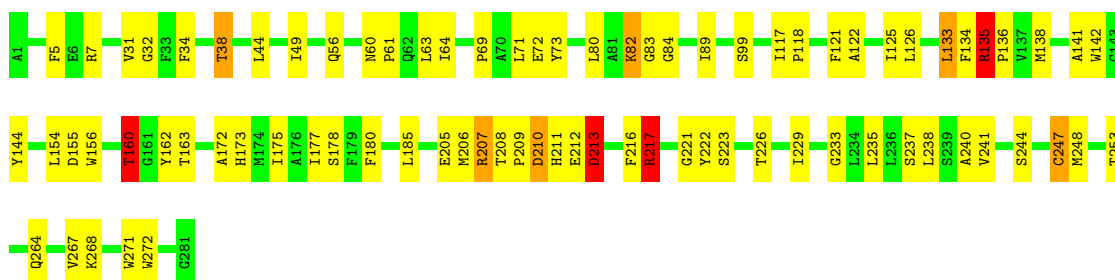
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H: 



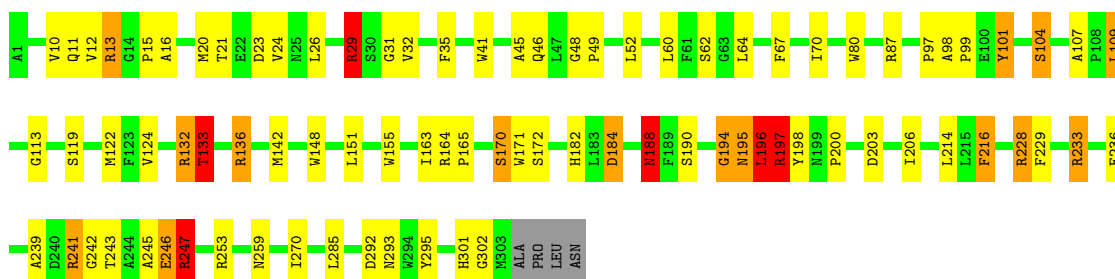
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L: 



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.00 Å 140.00 Å 184.60 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.6 (30.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.268	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

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	H	0.66	0/1878	1.75	30/2555 (1.2%)
2	L	0.63	0/2320	1.48	12/3175 (0.4%)
3	M	0.61	0/2504	1.56	36/3419 (1.1%)
All	All	0.63	0/6702	1.59	78/9149 (0.9%)

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	H	0	7
2	L	0	5
3	M	0	2
All	All	0	14

There are no bond length outliers.

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	NE-CZ-NH2	-21.92	109.34	120.30
3	M	247	ARG	NE-CZ-NH1	17.87	129.24	120.30
2	L	135	ARG	NE-CZ-NH1	16.24	128.42	120.30
2	L	135	ARG	CD-NE-CZ	15.24	144.93	123.60
2	L	135	ARG	NE-CZ-NH2	-14.98	112.81	120.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	113	SER	Mainchain
1	H	114	TRP	Mainchain
1	H	115	VAL	Mainchain
1	H	87	LEU	Mainchain
1	H	91	ALA	Mainchain

5.2 Too-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 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	H	1830	0	1836	61	0
2	L	2232	0	2187	59	0
3	M	2413	0	2326	58	0
4	L	132	0	148	15	0
4	M	132	0	148	10	0
5	L	65	0	76	10	0
5	M	65	0	76	3	0
6	M	1	0	0	0	0
7	L	48	0	58	1	0
7	M	48	0	63	0	0
8	M	43	0	69	5	0
9	H	16	0	31	0	0
9	M	32	0	62	5	0
10	M	81	0	106	16	0
11	H	42	0	0	3	0
11	L	28	0	0	1	0
11	M	42	0	0	1	0
All	All	7250	0	7186	200	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 14.

The worst 5 of 200 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)
10:M:800:CDL:CA6	10:M:800:CDL:HB4	1.62	1.28
10:M:800:CDL:HA61	10:M:800:CDL:HB4	1.10	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:M:800:CDL:CB4	10:M:800:CDL:HA61	1.83	1.08
1:H:27:LEU:HD23	10:M:800:CDL:H132	1.51	0.92
2:L:206:MET:HE1	3:M:239:ALA:HB2	1.51	0.89

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	H	239/260 (92%)	224 (94%)	13 (5%)	2 (1%)	22	49
2	L	279/281 (99%)	262 (94%)	17 (6%)	0	100	100
3	M	301/307 (98%)	275 (91%)	21 (7%)	5 (2%)	11	27
All	All	819/848 (97%)	761 (93%)	51 (6%)	7 (1%)	20	46

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	250	SER
1	H	116	ALA
3	M	195	ASN
3	M	301	HIS
3	M	80	TRP

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	H	195/208 (94%)	182 (93%)	13 (7%)	19	42
2	L	220/220 (100%)	199 (90%)	21 (10%)	10	23
3	M	237/241 (98%)	221 (93%)	16 (7%)	18	41
All	All	652/669 (98%)	602 (92%)	50 (8%)	15	34

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	185	LEU
2	L	217	ARG
3	M	197	ARG
2	L	205	GLU
2	L	210	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	126	HIS
1	H	199	GLN
1	H	204	HIS
1	H	206	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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$
9	LDA	H	701	-	13,15,15	2.87	2 (15%)	14,17,17	0.97	2 (14%)
4	BCL	L	1302	2	55,74,74	1.66	8 (14%)	65,115,115	2.00	18 (27%)
4	BCL	L	1304	2	55,74,74	1.66	6 (10%)	65,115,115	2.57	20 (30%)
5	BPH	L	401	-	65,70,70	1.40	6 (9%)	75,101,101	2.52	21 (28%)
7	U10	L	501	-	47,47,63	1.97	10 (21%)	55,58,79	2.53	20 (36%)
4	BCL	M	1301	3	55,74,74	1.68	6 (10%)	65,115,115	2.13	22 (33%)
4	BCL	M	1303	3	55,74,74	1.61	8 (14%)	65,115,115	1.70	18 (27%)
5	BPH	M	402	-	65,70,70	1.23	8 (12%)	75,101,101	2.56	23 (30%)
7	U10	M	502	-	48,48,63	1.74	14 (29%)	58,61,79	1.43	10 (17%)
8	SPN	M	600	-	40,42,42	3.64	19 (47%)	48,52,52	2.92	19 (39%)
9	LDA	M	702	-	13,15,15	2.87	2 (15%)	14,17,17	0.85	1 (7%)
9	LDA	M	703	-	13,15,15	2.86	2 (15%)	14,17,17	0.95	1 (7%)
10	CDL	M	800	-	80,80,99	0.50	0	82,92,111	0.91	4 (4%)

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
9	LDA	H	701	-	-	0/13/13/13	0/0/0/0
4	BCL	L	1302	2	-	0/37/137/137	0/0/9/9
4	BCL	L	1304	2	-	0/37/137/137	0/0/9/9
5	BPH	L	401	-	2/2/18/22	0/54/105/105	0/1/6/6
7	U10	L	501	-	-	0/41/65/87	0/1/1/1
4	BCL	M	1301	3	1/1/21/25	0/37/137/137	0/0/9/9
4	BCL	M	1303	3	-	0/37/137/137	0/0/9/9
5	BPH	M	402	-	-	0/54/105/105	0/1/6/6
7	U10	M	502	-	-	0/45/69/87	0/1/1/1
8	SPN	M	600	-	-	0/50/51/51	0/0/0/0
9	LDA	M	702	-	-	0/13/13/13	0/0/0/0
9	LDA	M	703	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CDL	M	800	-	-	0/91/91/110	0/0/0/0

The worst 5 of 91 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	H	701	LDA	O1-N1	-10.07	1.22	1.42
9	M	702	LDA	O1-N1	-10.06	1.22	1.42
9	M	703	LDA	O1-N1	-9.94	1.22	1.42
8	M	600	SPN	C3-C4	-6.45	1.40	1.50
8	M	600	SPN	C10-C9	-6.25	1.37	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	401	BPH	O1D-CGD-CBD	-7.30	111.50	124.60
8	M	600	SPN	C7-C8-C9	-6.72	110.81	127.68
5	M	402	BPH	O2D-CGD-O1D	-6.40	110.94	123.82
5	M	402	BPH	OBD-CAD-CBD	-6.30	116.44	125.94
4	M	1301	BCL	CMB-C2B-C1B	-5.81	119.54	128.46

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	1301	BCL	C13
5	L	401	BPH	C8
5	L	401	BPH	C13

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1302	BCL	9	0
4	L	1304	BCL	8	0
5	L	401	BPH	10	0
7	L	501	U10	1	0
4	M	1301	BCL	5	0
4	M	1303	BCL	6	0
5	M	402	BPH	3	0
8	M	600	SPN	5	0
9	M	702	LDA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	703	LDA	2	0
10	M	800	CDL	16	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.