



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:57 am GMT

PDB ID : 1F6N  
Title : CRYSTAL STRUCTURE ANALYSIS OF THE MUTANT REACTION CENTER PRO L209-> TYR FROM THE PHOTOSYNTHETIC PURPLE BACTERIUM RHODOBACTER SPHAEROIDES  
Authors : Kuglstatter, A.; Ermler, U.; Michel, H.; Baciou, L.; Fritzsche, G.  
Deposited on : 2000-06-22  
Resolution : 2.80 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](mailto: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.

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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

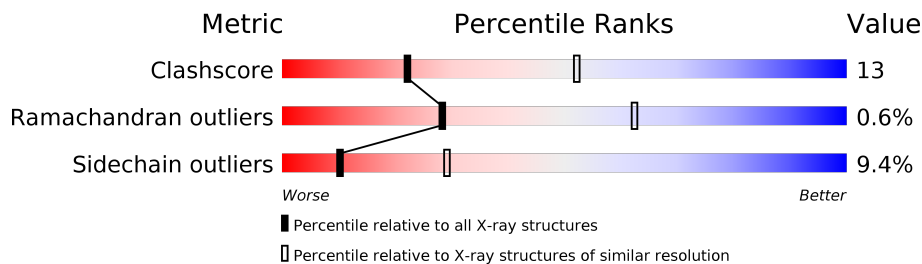
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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  $\geq 3$ , 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	L	281	
2	M	307	
3	H	260	

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
6	BCL	L	301	X	-	-	-
6	BCL	L	304	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7186 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	0	0
			2237	1511	355	363	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	209	TYR	PRO	ENGINEERED	UNP P02954

- 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
			2404	1603	394	397	10			

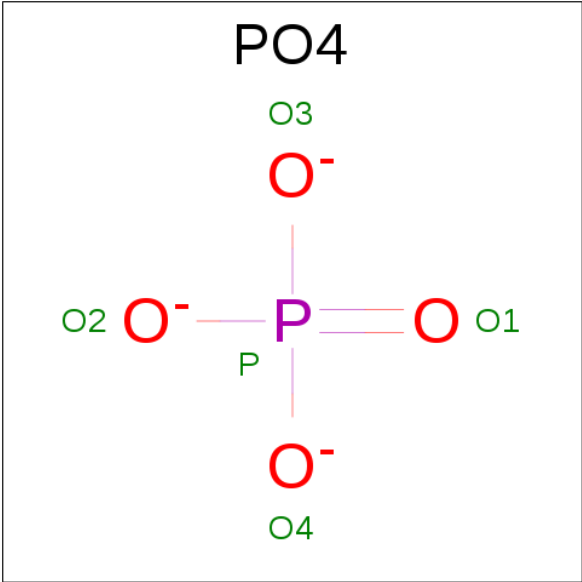
- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

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).

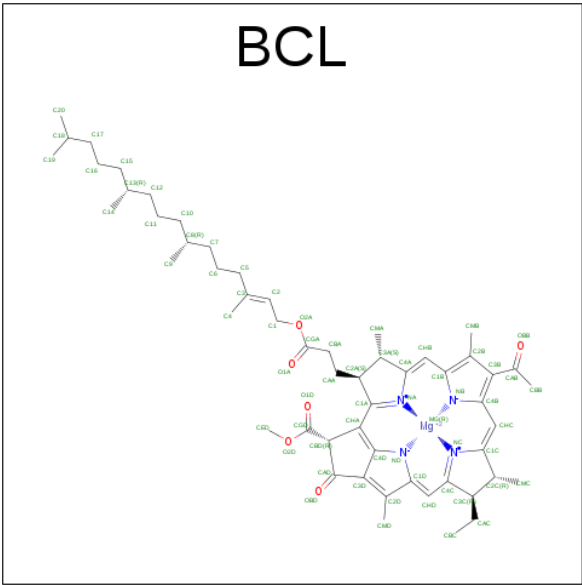
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



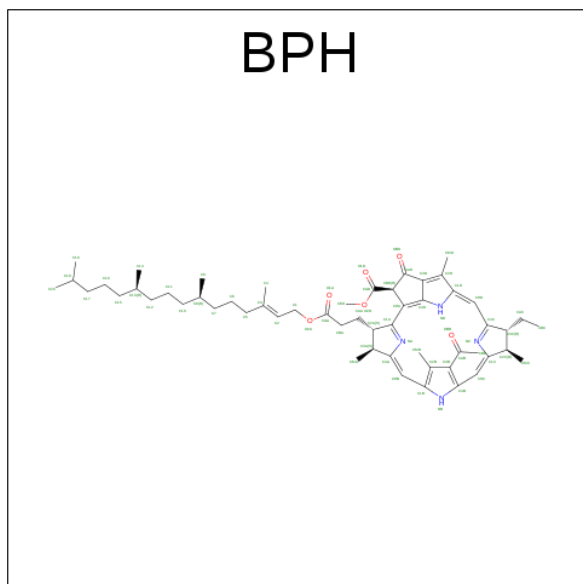
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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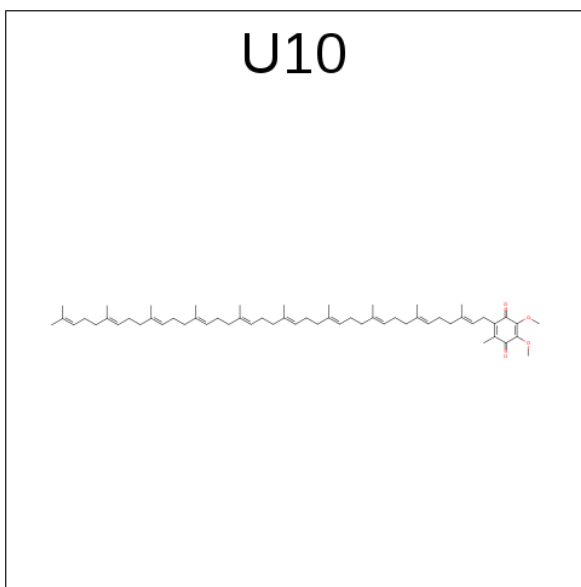
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).



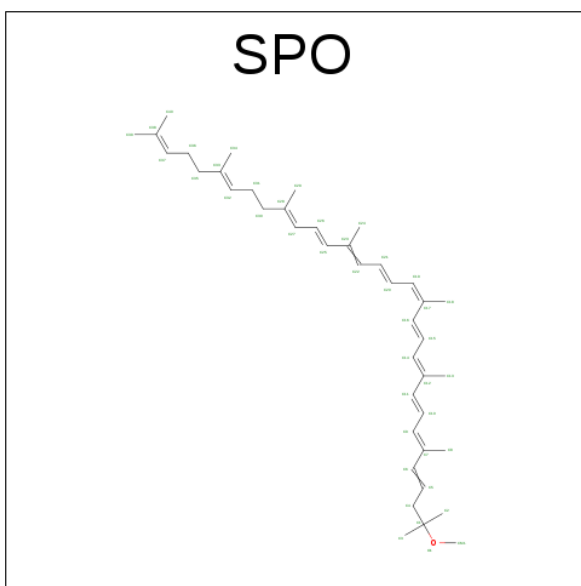
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



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

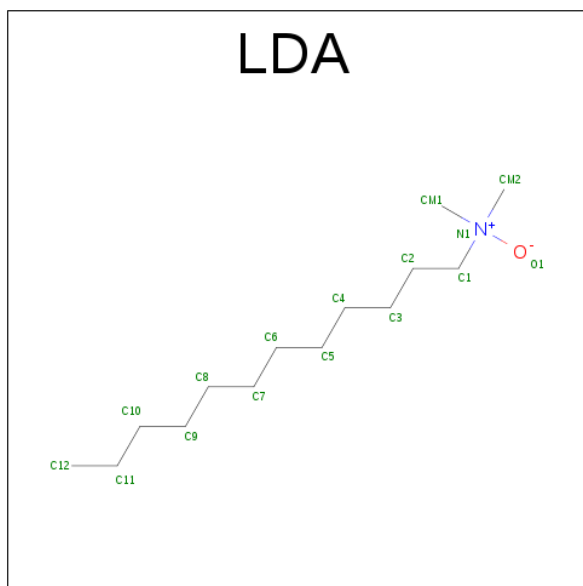
- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



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<sub>14</sub>H<sub>31</sub>NO).



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	L	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 water.

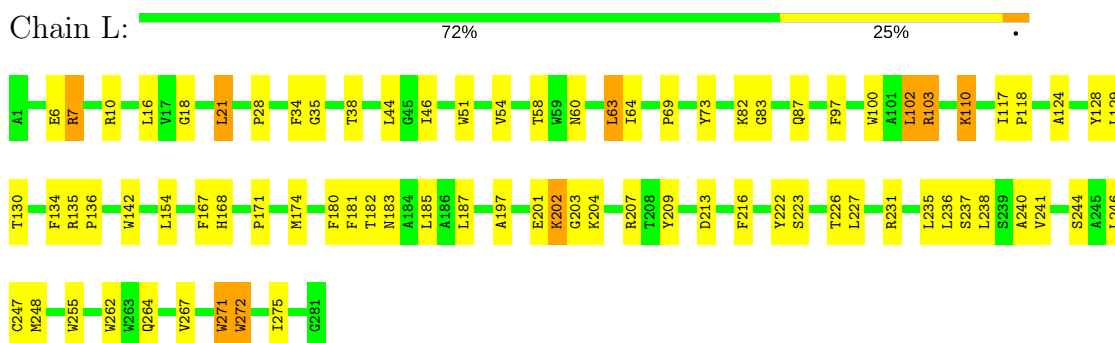
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	49	Total	O	0	0
			49	49		
11	L	22	Total	O	0	0
			22	22		
11	M	27	Total	O	0	0
			27	27		

### 3 Residue-property plots [i](#)

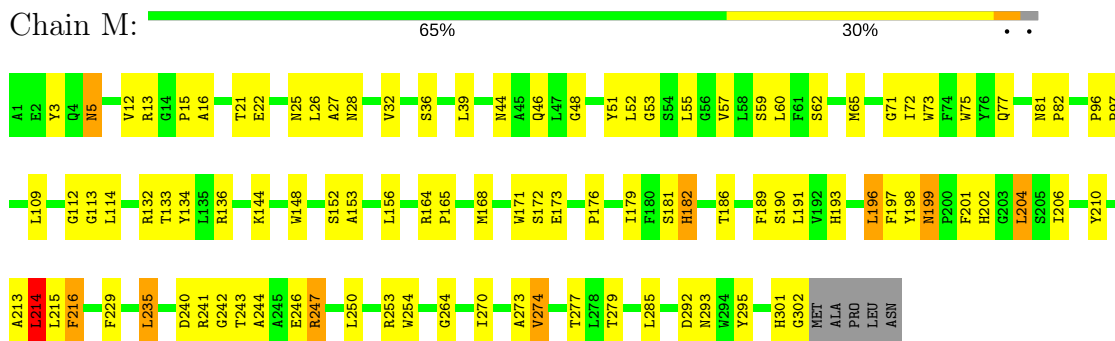
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

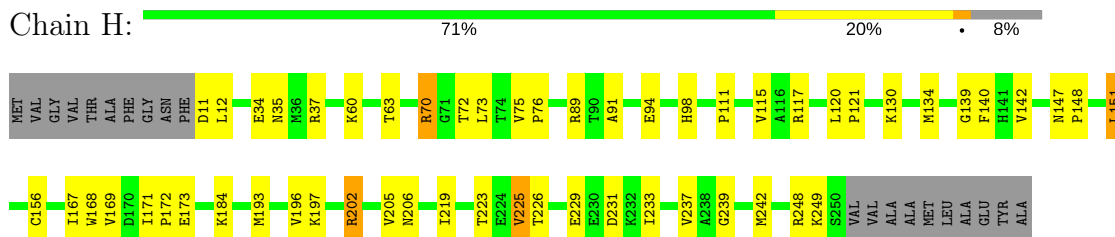
#### • Molecule 1: REACTION CENTER PROTEIN L CHAIN



#### • Molecule 2: REACTION CENTER PROTEIN M CHAIN



#### • Molecule 3: REACTION CENTER PROTEIN H CHAIN





## 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, $\alpha$ , $\beta$ , $\gamma$	141.53Å 141.53Å 187.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	93.1 (50.00-2.80)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.221 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7186	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	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, BPH, PO4, FE, 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	0.45	0/2325	0.51	0/3181
2	M	0.44	0/2496	0.51	1/3407 (0.0%)
3	H	0.43	0/1877	0.54	0/2553
All	All	0.44	0/6698	0.52	1/9141 (0.0%)

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	3
2	M	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	214	LEU	CA-CB-CG	6.79	130.91	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	103	ARG	Sidechain
1	L	216	PHE	Sidechain
1	L	73	TYR	Sidechain
2	M	198	TYR	Sidechain

## 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	L	2237	0	2189	60	0
2	M	2404	0	2311	70	0
3	H	1829	0	1836	41	0
4	M	1	0	0	0	0
5	M	5	0	0	0	0
6	L	198	0	221	30	0
6	M	66	0	74	15	0
7	L	65	0	76	10	0
7	M	65	0	76	10	0
8	L	48	0	63	0	0
8	M	48	0	63	1	0
9	M	42	0	60	4	0
10	H	32	0	62	1	0
10	L	16	0	31	3	0
10	M	32	0	62	0	0
11	H	49	0	0	2	0
11	L	22	0	0	4	0
11	M	27	0	0	1	0
All	All	7186	0	7124	187	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 13.

The worst 5 of 187 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)
6:L:301:BCL:HHC	6:L:301:BCL:HBB2	1.40	1.02
7:L:402:BPH:HHC	7:L:402:BPH:HBB3	1.42	1.01
6:L:302:BCL:HBB3	6:L:302:BCL:HHC	1.49	0.93
2:M:153:ALA:HB2	7:M:401:BPH:HAC1	1.50	0.91
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.59	0.83

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	279/281 (99%)	263 (94%)	15 (5%)	1 (0%)	38	72
2	M	300/307 (98%)	283 (94%)	13 (4%)	4 (1%)	14	41
3	H	238/260 (92%)	228 (96%)	10 (4%)	0	100	100
All	All	817/848 (96%)	774 (95%)	38 (5%)	5 (1%)	28	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	113	GLY
2	M	301	HIS
1	L	202	LYS
2	M	5	ASN
2	M	22	GLU

### 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	220/220 (100%)	199 (90%)	21 (10%)	10	28
2	M	235/240 (98%)	210 (89%)	25 (11%)	8	23
3	H	195/208 (94%)	180 (92%)	15 (8%)	15	39
All	All	650/668 (97%)	589 (91%)	61 (9%)	10	29

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	109	LEU
2	M	196	LEU
3	H	223	THR
2	M	133	THR
2	M	156	LEU

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	81	ASN
2	M	193	HIS
3	H	98	HIS
2	M	44	ASN
2	M	299	GLN

### 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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	702	-	13,15,15	3.04	2 (15%)	14,17,17	0.62	0
10	LDA	H	705	-	13,15,15	2.69	1 (7%)	14,17,17	0.58	0
6	BCL	L	301	2	55,74,74	1.48	6 (10%)	65,115,115	1.68	8 (12%)
6	BCL	L	302	1	55,74,74	1.58	7 (12%)	65,115,115	1.45	8 (12%)
6	BCL	L	304	1	55,74,74	1.68	6 (10%)	65,115,115	4.02	15 (23%)
7	BPH	L	402	-	65,70,70	1.14	5 (7%)	75,101,101	1.69	13 (17%)
8	U10	L	502	-	48,48,63	1.75	14 (29%)	58,61,79	1.10	5 (8%)
10	LDA	L	703	-	13,15,15	2.60	1 (7%)	14,17,17	0.67	0
7	BPH	M	401	-	65,70,70	1.29	5 (7%)	75,101,101	1.75	15 (20%)
8	U10	M	501	-	48,48,63	2.09	15 (31%)	58,61,79	0.98	2 (3%)
9	SPO	M	600	-	40,41,41	3.19	24 (60%)	49,50,50	2.13	11 (22%)
10	LDA	M	701	-	13,15,15	2.71	1 (7%)	14,17,17	0.64	0
10	LDA	M	704	-	13,15,15	2.69	2 (15%)	14,17,17	0.77	1 (7%)
5	PO4	M	800	-	4,4,4	1.59	1 (25%)	6,6,6	0.45	0
6	BCL	M	801	2	55,74,74	1.39	6 (10%)	65,115,115	1.65	11 (16%)

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	702	-	-	0/13/13/13	0/0/0/0
10	LDA	H	705	-	-	0/13/13/13	0/0/0/0
6	BCL	L	301	2	1/1/21/25	0/37/137/137	0/0/9/9
6	BCL	L	302	1	-	0/37/137/137	0/0/9/9
6	BCL	L	304	1	1/1/21/25	0/37/137/137	0/0/9/9
7	BPH	L	402	-	-	0/54/105/105	0/1/6/6
8	U10	L	502	-	-	0/45/69/87	0/1/1/1
10	LDA	L	703	-	-	0/13/13/13	0/0/0/0
7	BPH	M	401	-	-	0/54/105/105	0/1/6/6
8	U10	M	501	-	-	0/45/69/87	0/1/1/1
9	SPO	M	600	-	-	0/47/47/47	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
5	PO4	M	800	-	-	0/0/0/0	0/0/0/0
6	BCL	M	801	2	-	0/37/137/137	0/0/9/9

The worst 5 of 96 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	H	702	LDA	O1-N1	-10.62	1.21	1.42
10	M	701	LDA	O1-N1	-9.60	1.23	1.42
10	H	705	LDA	O1-N1	-9.59	1.23	1.42
10	M	704	LDA	O1-N1	-9.39	1.23	1.42
10	L	703	LDA	O1-N1	-9.29	1.23	1.42

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	BCL	CHB-C4A-NA	-16.62	101.53	124.51
9	M	600	SPO	C15-C14-C12	-7.49	116.63	127.31
6	L	304	BCL	O1D-CGD-CBD	-6.89	112.22	124.60
7	M	401	BPH	O1D-CGD-CBD	-6.16	113.53	124.60
7	L	402	BPH	O1D-CGD-CBD	-6.10	113.64	124.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	304	BCL	C13
6	L	301	BCL	C8

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	702	LDA	1	0
6	L	301	BCL	11	0
6	L	302	BCL	12	0
6	L	304	BCL	8	0
7	L	402	BPH	10	0
10	L	703	LDA	3	0
7	M	401	BPH	10	0
8	M	501	U10	1	0
9	M	600	SPO	4	0
6	M	801	BCL	15	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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.