



# wwPDB X-ray Structure Validation Summary Report

Jan 31, 2016 – 07:08 PM GMT

PDB ID : 1E6D  
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH TRP M115 REPLACED WITH PHE (CHAIN M, WM115F) PHE M197 REPLACED WITH ARG (CHAIN M, FM197R)  
Authors : Ridge, J.P.; Fyfe, P.K.; Mcauley, K.E.; Van Brederode, M.E.; Robert, B.; Van Grondelle, R.; Isaacs, N.W.; Cogdell, R.J.; Jones, M.R.  
Deposited on : 2000-08-11  
Resolution : 2.30 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 (RC4), CSD as536be (2015)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

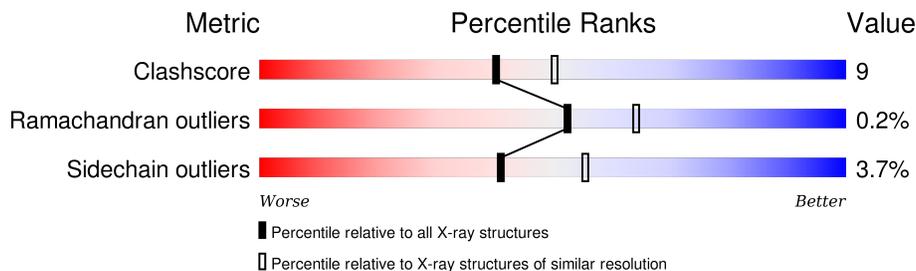
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	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
10	PO4	M	1801	-	-	X	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	BCL	L	1304	X	-	-	-
4	BCL	M	1301	X	-	-	-
5	BPH	M	1401	X	-	-	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7334 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
			Total	C	N	O	S			
1	H	240	1829	1169	314	337	9	0	0	0

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

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

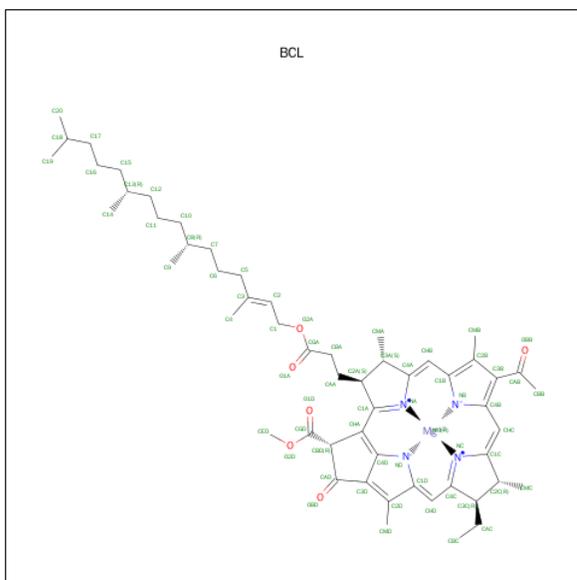
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER M SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	302	2405	1602	396	397	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

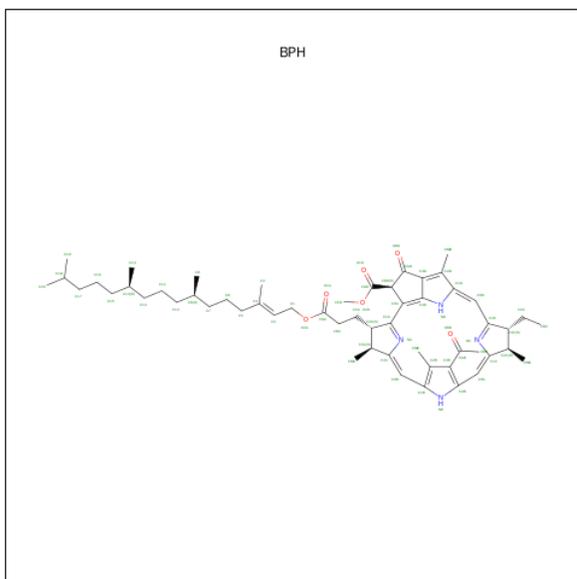
Chain	Residue	Modelled	Actual	Comment	Reference
M	197	ARG	PHE	ENGINEERED MUTATION	UNP P02953
M	115	PHE	TRP	ENGINEERED MUTATION	UNP P02953

- Molecule 4 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	
			Total	C	Mg	N			O
4	M	1	Total	C	Mg	N	O	0	0
			66	55	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	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ).

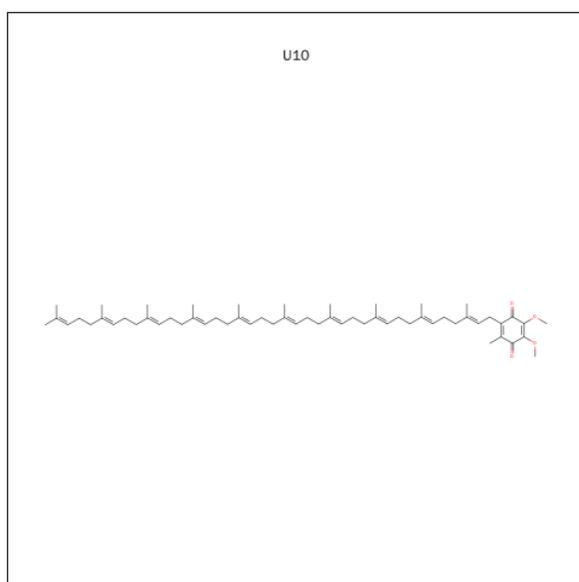


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			65	55	4	6		
5	L	1	Total	C	N	O	0	0
			65	55	4	6		

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

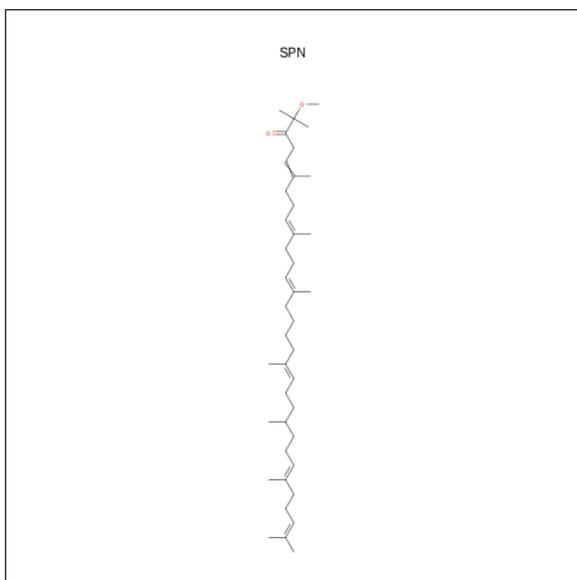
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Fe	0	0
			1	1		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



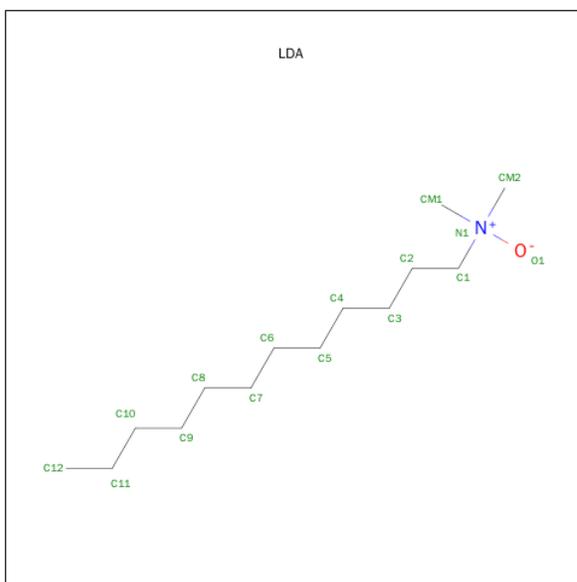
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			48	44	4		
7	L	1	Total	C	O	0	0
			48	44	4		

- Molecule 8 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).



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

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



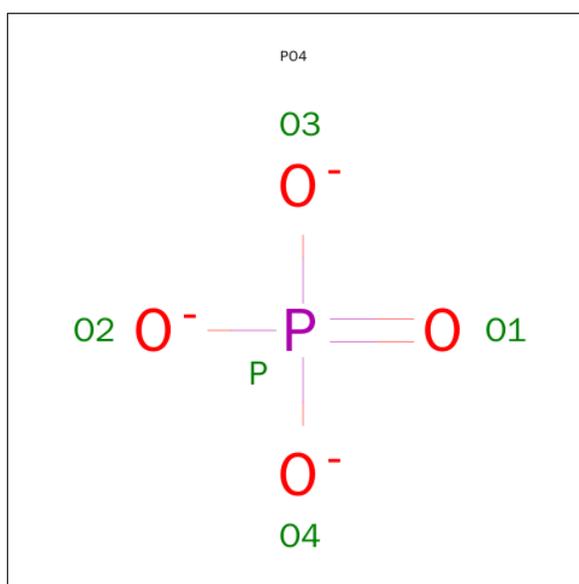
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	M	1	16	14	1	1	0	0
9	M	1	16	14	1	1	0	0

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

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	1	Total	O	0	0
			1	1		
11	M	2	Total	O	0	0
			2	2		

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
11	L	1	Total 1	O 1	0	0
11	H	1	Total 1	O 1	0	0
11	M	1	Total 1	O 1	0	0
11	H	94	Total 94	O 94	0	0
11	L	47	Total 47	O 47	0	0
11	M	65	Total 65	O 65	0	0

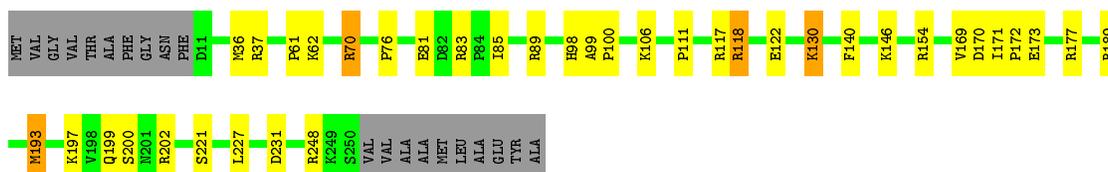
### 3 Residue-property plots

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.

Note EDS was not executed.

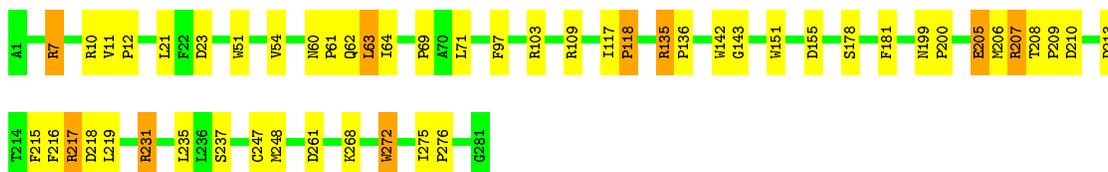
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER H SUBUNIT

Chain H: 



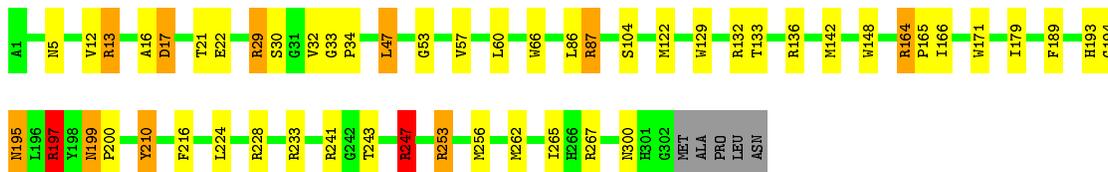
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER L SUBUNIT

Chain L: 



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER M SUBUNIT

Chain M: 



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.20Å 141.20Å 187.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.40 – 2.30	Depositor
% Data completeness (in resolution range)	94.5 (26.40-2.30)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.174 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

## 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, BPH, PO4, 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	0.74	0/1877	1.29	14/2553 (0.5%)
2	L	0.73	1/2320 (0.0%)	1.12	15/3175 (0.5%)
3	M	0.70	0/2495	1.11	17/3404 (0.5%)
All	All	0.72	1/6692 (0.0%)	1.17	46/9132 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	237	SER	CA-CB	5.00	1.60	1.52

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	ARG	CD-NE-CZ	18.85	149.99	123.60
2	L	135	ARG	NE-CZ-NH2	-10.14	115.23	120.30
3	M	210	TYR	CB-CG-CD1	8.25	125.95	121.00
3	M	247	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	H	117	ARG	NE-CZ-NH2	7.22	123.91	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	1829	0	1836	17	0
2	L	2232	0	2187	36	0
3	M	2405	0	2324	44	0
4	L	132	0	148	5	0
4	M	132	0	148	14	0
5	L	65	0	75	6	0
5	M	65	0	76	10	0
6	M	1	0	0	0	0
7	L	48	0	63	9	0
7	M	48	0	63	3	0
8	M	43	0	69	2	0
9	H	32	0	62	0	0
9	M	80	0	155	11	0
10	M	10	0	0	3	0
11	H	95	0	0	1	0
11	L	49	0	0	8	0
11	M	68	0	0	1	0
All	All	7334	0	7206	124	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 9.

The worst 5 of 124 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)
3:M:243:THR:O	3:M:247:ARG:HG2	1.58	1.02
4:M:1303:BCL:H191	9:M:1706:LDA:H121	1.47	0.97
5:L:1402:BPH:HHC	5:L:1402:BPH:HBB3	1.51	0.93
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.50	0.93
9:M:1701:LDA:H91	9:M:1702:LDA:H121	1.54	0.88

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	238/260 (92%)	233 (98%)	5 (2%)	0	100	100
2	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
3	M	300/307 (98%)	290 (97%)	8 (3%)	2 (1%)	26	31
All	All	817/848 (96%)	794 (97%)	21 (3%)	2 (0%)	52	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	30	SER
3	M	195	ASN

### 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%)	189 (97%)	6 (3%)	47	64
2	L	220/220 (100%)	211 (96%)	9 (4%)	37	50
3	M	236/240 (98%)	227 (96%)	9 (4%)	40	54
All	All	651/668 (98%)	627 (96%)	24 (4%)	41	55

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	216	PHE
2	L	268	LYS
3	M	247	ARG
2	L	235	LEU
2	L	247	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	28	ASN
3	M	299	GLN
3	M	193	HIS
2	L	199	ASN
3	M	187	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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	1704	-	15,15,15	4.37	2 (13%)	16,17,17	0.89	1 (6%)
9	LDA	H	1707	-	15,15,15	4.35	2 (13%)	16,17,17	0.95	0
4	BCL	L	1302	2	53,74,74	1.26	6 (11%)	57,115,115	2.09	16 (28%)
4	BCL	L	1304	2	53,74,74	1.43	7 (13%)	57,115,115	2.34	15 (26%)
5	BPH	L	1402	-	64,70,70	1.48	11 (17%)	73,101,101	2.13	18 (24%)
7	U10	L	1502	-	48,48,63	2.13	16 (33%)	58,61,79	1.75	12 (20%)
4	BCL	M	1301	3	53,74,74	1.40	6 (11%)	57,115,115	2.24	17 (29%)
4	BCL	M	1303	3	53,74,74	1.30	7 (13%)	57,115,115	1.96	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	BPH	M	1401	-	64,70,70	1.35	11 (17%)	73,101,101	2.34	16 (21%)
7	U10	M	1501	-	48,48,63	2.00	16 (33%)	58,61,79	1.65	12 (20%)
8	SPN	M	1600	-	41,42,42	4.37	19 (46%)	41,52,52	2.80	19 (46%)
9	LDA	M	1701	-	15,15,15	4.39	3 (20%)	16,17,17	1.02	1 (6%)
9	LDA	M	1702	-	15,15,15	4.88	3 (20%)	16,17,17	0.80	1 (6%)
9	LDA	M	1703	-	15,15,15	4.36	3 (20%)	16,17,17	1.07	2 (12%)
9	LDA	M	1705	-	15,15,15	4.33	4 (26%)	16,17,17	1.08	1 (6%)
9	LDA	M	1706	-	15,15,15	4.73	2 (13%)	16,17,17	0.96	1 (6%)
10	PO4	M	1800	-	4,4,4	1.66	1 (25%)	6,6,6	0.41	0
10	PO4	M	1801	-	4,4,4	1.00	0	6,6,6	0.35	0

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	1704	-	-	0/13/13/13	0/0/0/0
9	LDA	H	1707	-	-	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	1/1/21/25	0/37/137/137	0/0/9/9
5	BPH	L	1402	-	-	0/54/105/105	0/1/6/6
7	U10	L	1502	-	-	0/45/69/87	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	1401	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	M	1501	-	-	0/45/69/87	0/1/1/1
8	SPN	M	1600	-	-	0/50/51/51	0/0/0/0
9	LDA	M	1701	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1702	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1703	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1705	-	-	0/13/13/13	0/0/0/0
9	LDA	M	1706	-	-	0/13/13/13	0/0/0/0
10	PO4	M	1800	-	-	0/0/0/0	0/0/0/0
10	PO4	M	1801	-	-	0/0/0/0	0/0/0/0

The worst 5 of 119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1702	LDA	O1-N1	-18.37	1.22	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1706	LDA	O1-N1	-17.90	1.22	1.39
9	M	1703	LDA	O1-N1	-16.45	1.23	1.39
9	H	1707	LDA	O1-N1	-16.41	1.23	1.39
9	M	1701	LDA	O1-N1	-16.37	1.23	1.39

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	1401	BPH	O1D-CGD-CBD	-7.15	114.37	124.62
4	L	1304	BCL	O1D-CGD-CBD	-6.63	115.13	124.62
8	M	1600	SPN	C7-C8-C9	-5.64	115.50	127.76
8	M	1600	SPN	C10-C9-C8	-5.62	110.39	121.05
4	M	1303	BCL	CAC-C3C-C4C	-5.43	100.52	112.58

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	1301	BCL	C13
4	L	1304	BCL	C13
5	M	1401	BPH	C8

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1302	BCL	4	0
4	L	1304	BCL	1	0
5	L	1402	BPH	6	0
7	L	1502	U10	9	0
4	M	1301	BCL	11	0
4	M	1303	BCL	4	0
5	M	1401	BPH	10	0
7	M	1501	U10	3	0
8	M	1600	SPN	2	0
9	M	1701	LDA	2	0
9	M	1702	LDA	2	0
9	M	1703	LDA	5	0
9	M	1706	LDA	4	0
10	M	1800	PO4	1	0
10	M	1801	PO4	2	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.