



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 06:24 PM GMT

PDB ID : 1AIJ
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER
SPHAEROIDES IN THE CHARGE-NEUTRAL DQAQB STATE
Authors : Stowell, M.H.B.; Mcphillips, T.M.; Soltis, S.M.; Rees, D.C.; Abresch, E.; Fe-
her, G.
Deposited on : 1997-04-18
Resolution : 2.20 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 (RC4), CSD as536be (2015)
Xtriage (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

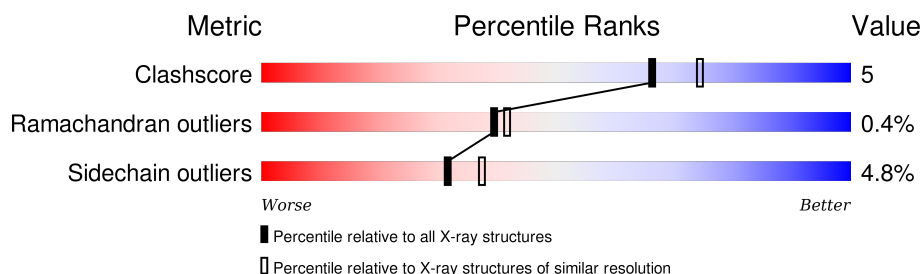
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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	L	281	
1	R	281	
2	M	307	
2	S	307	
3	H	260	
3	T	260	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14393 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 (L SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			
1	R	281	Total	C	N	O	S	4	0	0
			2232	1507	355	362	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2404	1605	393	396	10			
2	S	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	246	Total	C	N	O	S	4	0	0
			1869	1196	320	343	10			
3	T	246	Total	C	N	O	S	0	0	0
			1869	1196	320	343	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	CONFLICT	UNP P11846
T	8	GLN	GLY	CONFLICT	UNP P11846

- Molecule 4 is FE (II) ION (three-letter code: FE2) (formula: Fe).

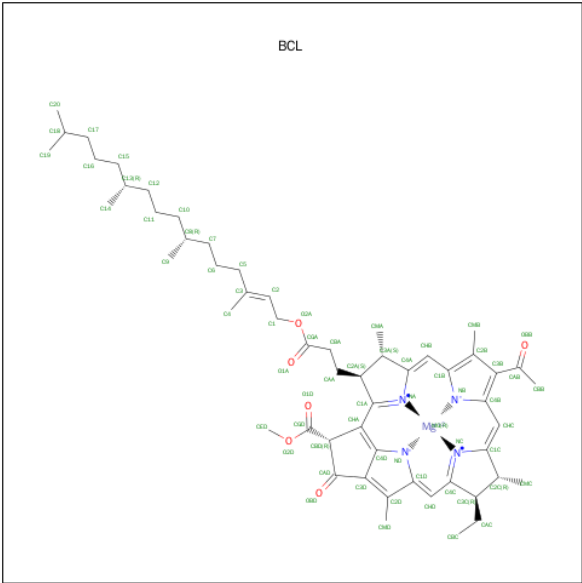
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	S	1	Total	Fe	0	0
			1	1		

Continued on next page...

Continued from previous page...

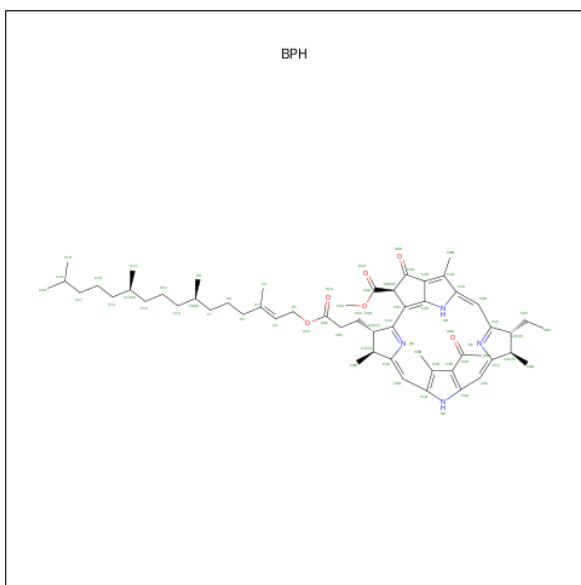
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

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



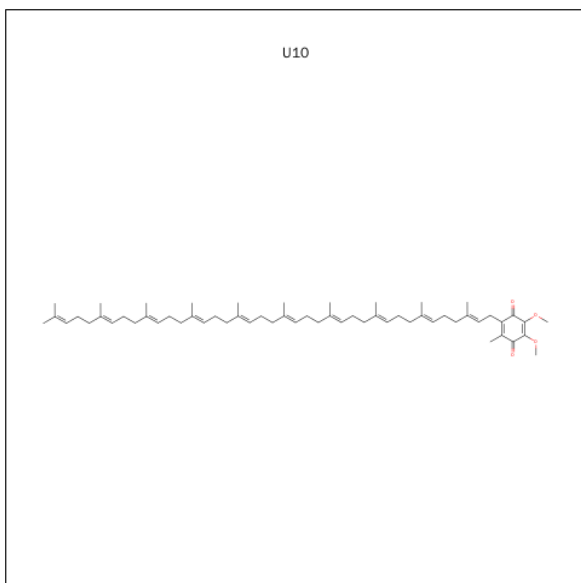
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	S	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	S	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	R	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



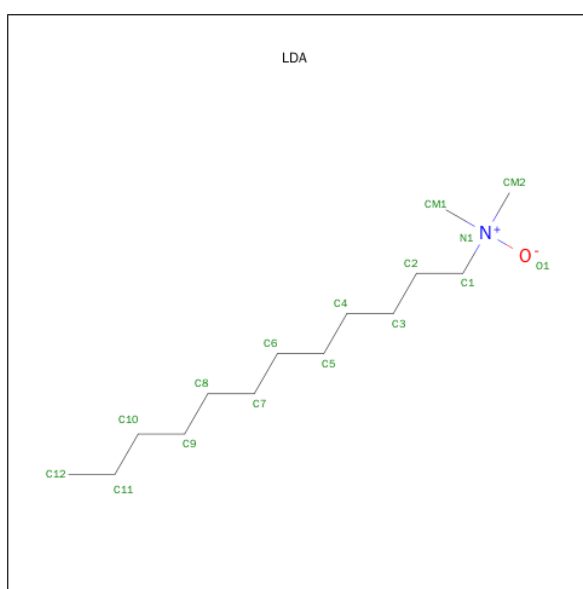
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	0	0
			51	41	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	S	1	Total	C	N	O	0	0
			52	42	4	6		
6	R	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 7 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			38	34	4		
7	L	1	Total	C	O	0	0
			44	40	4		
7	S	1	Total	C	O	0	0
			32	28	4		
7	R	1	Total	C	O	0	0
			18	14	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	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	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		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	105	Total	O	0	0
			105	105		

Continued on next page...

Continued from previous page...

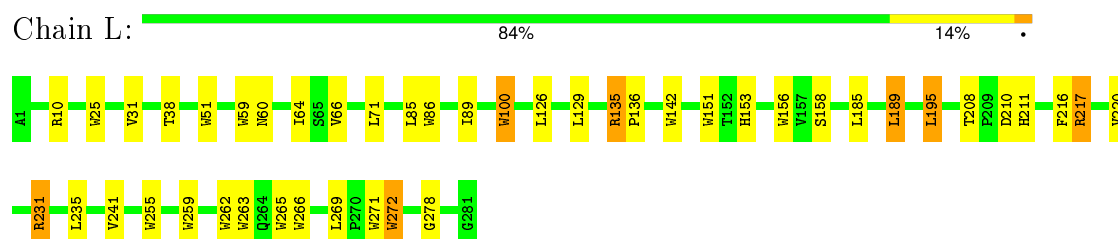
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	L	67	Total 67	O 67	0	0
9	M	91	Total 91	O 91	0	0
9	R	56	Total 56	O 56	0	0
9	S	85	Total 85	O 85	0	0
9	T	64	Total 64	O 64	0	0

3 Residue-property plots

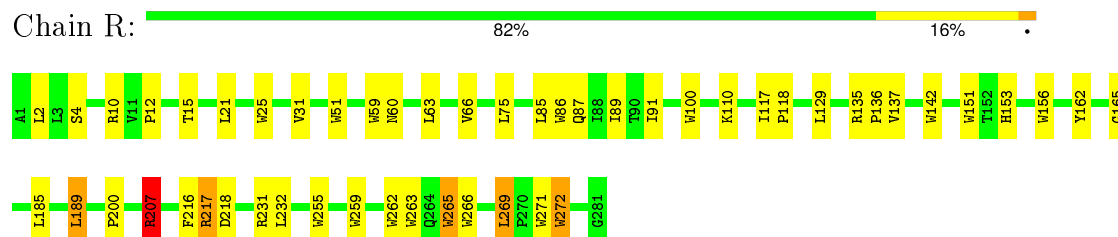
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

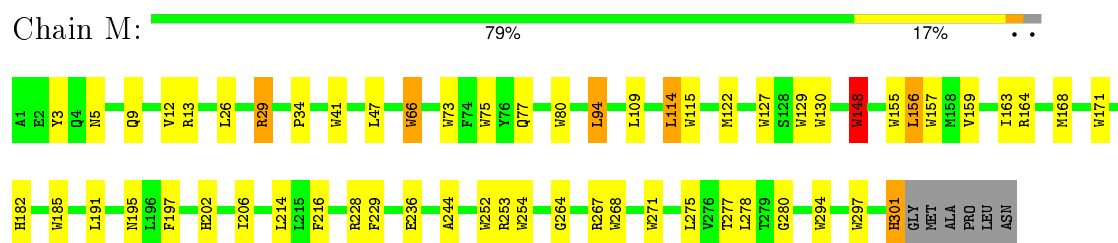
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



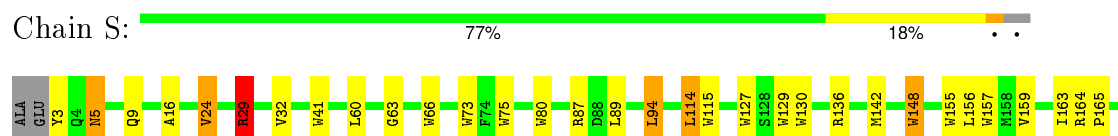
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

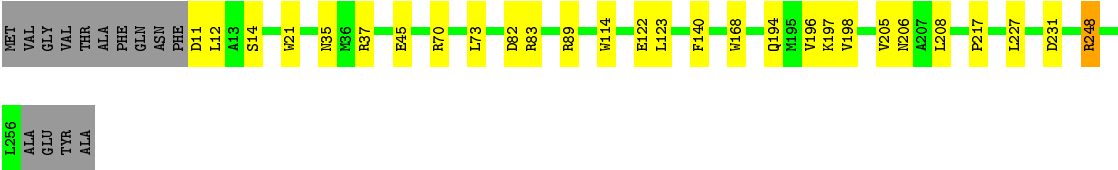
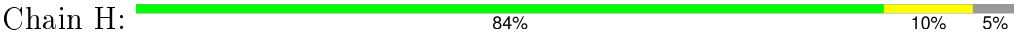


• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

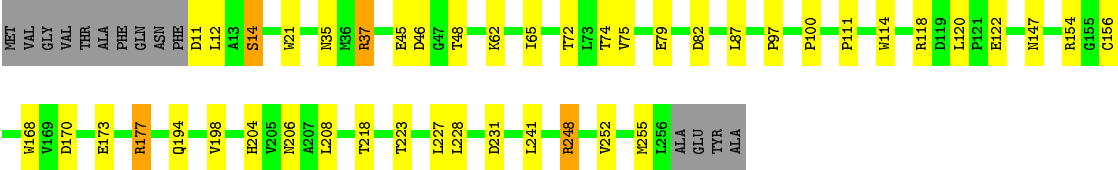




● Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



● Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.08 Å 140.08 Å 271.63 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.216 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14393	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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, BPH, LDA, FE2, 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	0.78	0/2320	1.48	59/3175 (1.9%)
1	R	0.78	0/2320	1.45	53/3175 (1.7%)
2	M	0.79	0/2496	1.51	67/3408 (2.0%)
2	S	0.80	0/2482	1.54	74/3389 (2.2%)
3	H	0.66	0/1917	1.21	13/2608 (0.5%)
3	T	0.66	0/1917	1.20	13/2608 (0.5%)
All	All	0.75	0/13452	1.42	279/18363 (1.5%)

There are no bond length outliers.

The worst 5 of 279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	231	ARG	NE-CZ-NH1	9.91	125.26	120.30
3	H	248	ARG	NE-CZ-NH1	9.33	124.96	120.30
1	L	10	ARG	NE-CZ-NH1	9.18	124.89	120.30
2	S	41	TRP	CD1-CG-CD2	9.09	113.57	106.30
3	T	248	ARG	NE-CZ-NH1	8.90	124.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2232	0	2187	13	0
1	R	2232	0	2187	20	0
2	M	2404	0	2318	27	0
2	S	2390	0	2304	22	0
3	H	1869	0	1884	11	0
3	T	1869	0	1884	25	0
4	M	1	0	0	0	0
4	S	1	0	0	0	0
5	L	132	0	148	10	0
5	M	117	0	115	11	0
5	R	132	0	148	9	0
5	S	117	0	115	11	0
6	L	116	0	121	5	0
6	R	65	0	76	4	0
6	S	52	0	47	2	0
7	L	44	0	57	1	0
7	M	38	0	47	1	0
7	R	18	0	15	2	0
7	S	32	0	39	0	0
8	M	64	0	124	4	0
9	H	105	0	0	0	0
9	L	67	0	0	0	0
9	M	91	0	0	2	0
9	R	56	0	0	0	0
9	S	85	0	0	1	0
9	T	64	0	0	1	0
All	All	14393	0	13816	135	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 5.

The worst 5 of 135 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)
5:M:309:BCL:HBB3	5:M:310:BCL:H41	1.46	0.96
5:S:309:BCL:HBB3	5:S:310:BCL:H41	1.69	0.74
2:S:208:PHE:HD1	2:S:272:MET:HE3	1.52	0.74
6:R:284:BPH:HHC	6:R:284:BPH:HBB3	1.70	0.73
2:S:63:GLY:HA3	6:S:311:BPH:H5C2	1.70	0.73

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%)	271 (97%)	6 (2%)	2 (1%)	26	25
1	R	279/281 (99%)	271 (97%)	6 (2%)	2 (1%)	26	25
2	M	299/307 (97%)	290 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	287 (97%)	9 (3%)	1 (0%)	46	50
3	H	244/260 (94%)	239 (98%)	4 (2%)	1 (0%)	39	42
3	T	244/260 (94%)	234 (96%)	9 (4%)	1 (0%)	39	42
All	All	1642/1696 (97%)	1592 (97%)	43 (3%)	7 (0%)	39	42

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	71	LEU
3	H	45	GLU
3	T	45	GLU
1	R	2	LEU
2	S	195	ASN

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%)	27	30
1	R	220/220 (100%)	212 (96%)	8 (4%)	42	52
2	M	236/240 (98%)	224 (95%)	12 (5%)	29	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	235/240 (98%)	223 (95%)	12 (5%)	29	34
3	H	199/209 (95%)	192 (96%)	7 (4%)	43	53
3	T	199/209 (95%)	187 (94%)	12 (6%)	24	26
All	All	1309/1338 (98%)	1246 (95%)	63 (5%)	31	37

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	208	LEU
1	R	207	ARG
3	T	208	LEU
3	H	217	PRO
1	R	15	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	206	ASN
1	R	87	GLN
3	T	147	ASN
3	H	194	GLN
2	S	9	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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
5	BCL	L	282	1	53,74,74	1.02	5 (9%)	57,115,115	1.46	13 (22%)
5	BCL	L	283	1	53,74,74	1.04	5 (9%)	57,115,115	1.70	10 (17%)
6	BPH	L	284	-	50,56,70	1.27	5 (10%)	56,84,101	1.84	10 (17%)
6	BPH	L	285	-	64,70,70	1.19	6 (9%)	73,101,101	1.72	11 (15%)
7	U10	L	286	-	44,44,63	1.75	10 (22%)	53,56,79	1.39	5 (9%)
5	BCL	M	309	2	38,59,74	1.16	4 (10%)	40,97,115	1.77	9 (22%)
5	BCL	M	310	2	53,74,74	0.98	5 (9%)	57,115,115	1.60	11 (19%)
7	U10	M	311	-	38,38,63	1.68	9 (23%)	46,49,79	1.16	3 (6%)
8	LDA	M	312	-	15,15,15	4.74	3 (20%)	16,17,17	3.11	3 (18%)
8	LDA	M	313	-	15,15,15	4.91	3 (20%)	16,17,17	3.08	5 (31%)
8	LDA	M	314	-	15,15,15	4.78	3 (20%)	16,17,17	3.14	5 (31%)
8	LDA	M	315	-	15,15,15	4.78	3 (20%)	16,17,17	3.08	5 (31%)
5	BCL	R	282	1	53,74,74	1.00	5 (9%)	57,115,115	1.45	11 (19%)
5	BCL	R	283	1	53,74,74	1.03	5 (9%)	57,115,115	1.54	9 (15%)
6	BPH	R	284	-	64,70,70	1.12	5 (7%)	73,101,101	1.69	12 (16%)
7	U10	R	285	-	18,18,63	1.76	5 (27%)	22,25,79	0.99	0
5	BCL	S	309	2	38,59,74	1.15	5 (13%)	40,97,115	1.88	8 (20%)
5	BCL	S	310	2	53,74,74	0.98	5 (9%)	57,115,115	1.57	11 (19%)
6	BPH	S	311	-	51,57,70	1.26	5 (9%)	57,85,101	1.87	10 (17%)
7	U10	S	312	-	32,32,63	1.69	7 (21%)	38,41,79	1.09	2 (5%)

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
5	BCL	L	282	1	-	0/37/137/137	0/0/9/9
5	BCL	L	283	1	-	0/37/137/137	0/0/9/9
6	BPH	L	284	-	-	0/38/89/105	0/1/6/6
6	BPH	L	285	-	-	0/54/105/105	0/1/6/6
7	U10	L	286	-	-	0/41/65/87	0/1/1/1
5	BCL	M	309	2	-	0/19/119/137	0/0/9/9
5	BCL	M	310	2	-	0/37/137/137	0/0/9/9
7	U10	M	311	-	-	0/33/57/87	0/1/1/1
8	LDA	M	312	-	-	0/13/13/13	0/0/0/0
8	LDA	M	313	-	-	0/13/13/13	0/0/0/0
8	LDA	M	314	-	-	0/13/13/13	0/0/0/0
8	LDA	M	315	-	-	0/13/13/13	0/0/0/0
5	BCL	R	282	1	-	0/37/137/137	0/0/9/9
5	BCL	R	283	1	-	0/37/137/137	0/0/9/9
6	BPH	R	284	-	-	0/54/105/105	0/1/6/6
7	U10	R	285	-	-	0/9/33/87	0/1/1/1
5	BCL	S	309	2	-	0/19/119/137	0/0/9/9
5	BCL	S	310	2	-	0/37/137/137	0/0/9/9
6	BPH	S	311	-	-	0/39/90/105	0/1/6/6
7	U10	S	312	-	-	0/26/50/87	0/1/1/1

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	313	LDA	O1-N1	-18.38	1.22	1.39
8	M	314	LDA	O1-N1	-17.88	1.22	1.39
8	M	315	LDA	O1-N1	-17.82	1.22	1.39
8	M	312	LDA	O1-N1	-17.71	1.22	1.39
6	L	285	BPH	C3D-CAD	-3.69	1.39	1.46

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	314	LDA	CM2-N1-CM1	-10.86	96.58	108.83
8	M	312	LDA	CM2-N1-CM1	-10.65	96.82	108.83
8	M	313	LDA	CM2-N1-CM1	-10.61	96.86	108.83
8	M	315	LDA	CM2-N1-CM1	-10.53	96.95	108.83
6	S	311	BPH	C4D-C3D-C2D	-5.79	99.60	107.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	282	BCL	7	0
5	L	283	BCL	6	0
6	L	284	BPH	1	0
6	L	285	BPH	4	0
7	L	286	U10	1	0
5	M	309	BCL	5	0
5	M	310	BCL	7	0
7	M	311	U10	1	0
8	M	312	LDA	2	0
8	M	314	LDA	1	0
8	M	315	LDA	1	0
5	R	282	BCL	7	0
5	R	283	BCL	6	0
6	R	284	BPH	4	0
7	R	285	U10	2	0
5	S	309	BCL	5	0
5	S	310	BCL	8	0
6	S	311	BPH	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.