



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:43 am GMT

PDB ID : 1AIG
Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE D+QB-CHARGE SEPARATED STATE
Authors : Stowell, M.H.B.; Mcphillips, T.M.; Soltis, S.M.; Rees, D.C.; Abresch, E.; Fehrer, G.
Deposited on : 1997-04-17
Resolution : 2.60 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

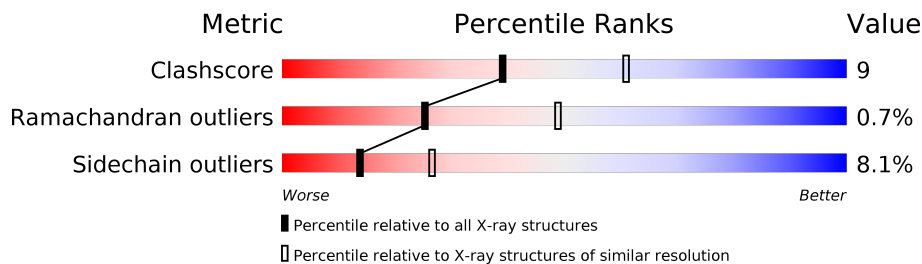
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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	N	281	
2	M	307	
2	O	307	
3	H	260	
3	P	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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	M	309	X	-	-	-
5	BCL	M	310	X	-	-	-
5	BCL	N	282	X	-	-	-
5	BCL	O	309	X	-	-	-
6	BPH	L	284	X	-	-	-
6	BPH	L	285	X	-	-	-
6	BPH	N	285	X	-	-	-
6	BPH	O	310	X	-	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14138 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	N	281	Total	C	N	O	S	0	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	299	Total	C	N	O	S	0	0	0
			2390	1597	391	392	10			
2	O	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	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			
3	P	248	Total	C	N	O	S	0	0	0
			1883	1204	322	347	10			

There are 2 discrepancies between the modelled and reference sequences:

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

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

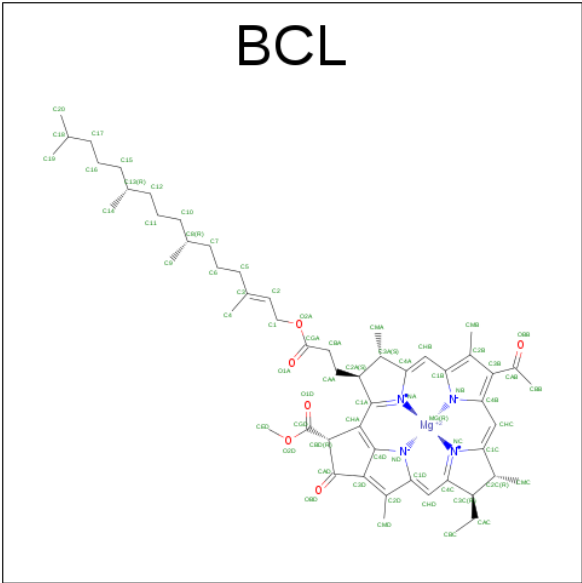
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total	Fe	0	0
			1	1		

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

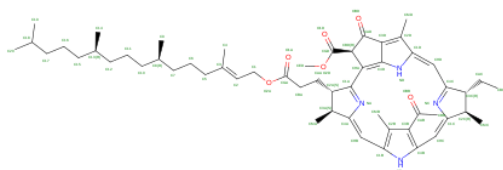
- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			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	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	N	1	Total	C	Mg	N	O	12	0
			66	55	1	4	6		
5	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	O	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	N	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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

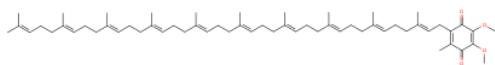
BPH



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	1	Total	C	N	O	14	0
			65	55	4	6		
6	L	1	Total	C	N	O	0	0
			65	55	4	6		
6	O	1	Total	C	N	O	0	0
			65	55	4	6		
6	N	1	Total	C	N	O	0	0
			65	55	4	6		

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

U10



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			63	59	4		
7	L	1	Total	C	O	0	0
			63	59	4		
7	O	1	Total	C	O	0	0
			63	59	4		
7	N	1	Total	C	O	19	0
			63	59	4		

- Molecule 8 is water.

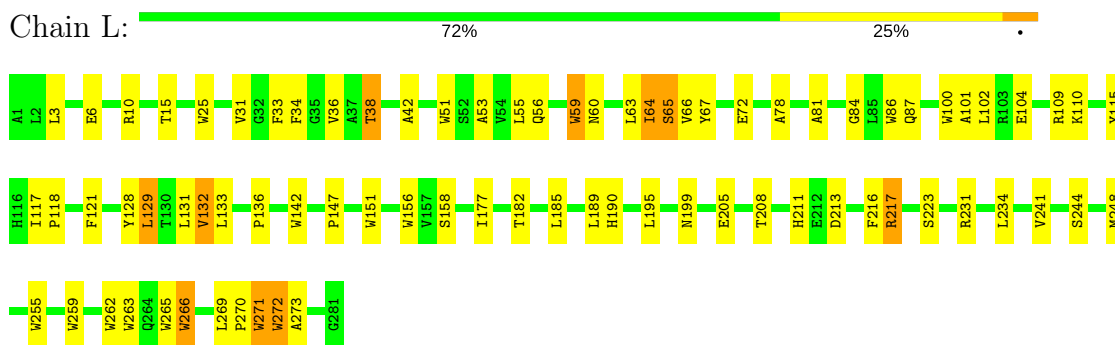
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	13	Total	O	0	0
			13	13		
8	L	19	Total	O	0	0
			19	19		
8	M	21	Total	O	0	0
			21	21		
8	N	13	Total	O	0	0
			13	13		
8	O	15	Total	O	0	0
			15	15		
8	P	5	Total	O	0	0
			5	5		

3 Residue-property plots [i](#)

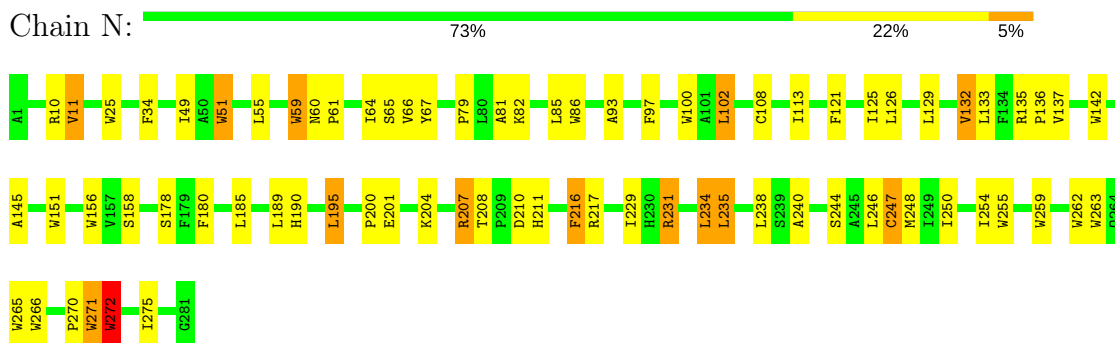
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

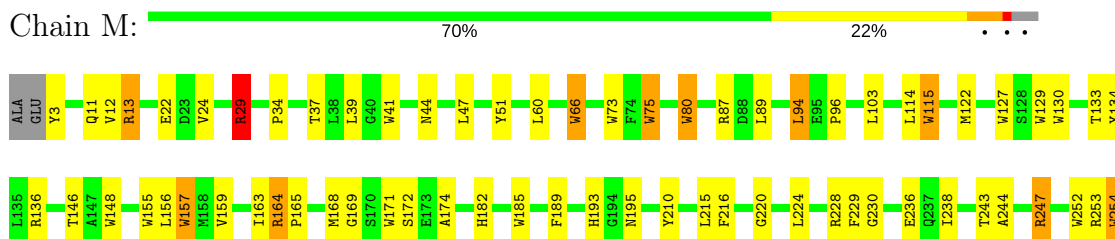
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



• Molecule 1: PHOTOSYNTHETIC REACTION CENTER (L SUBUNIT)



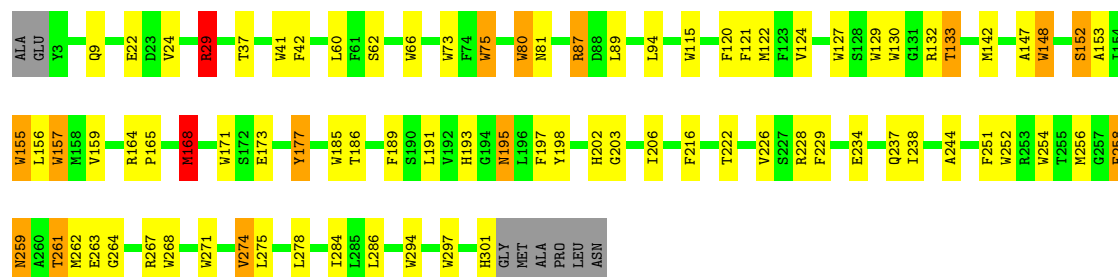
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)





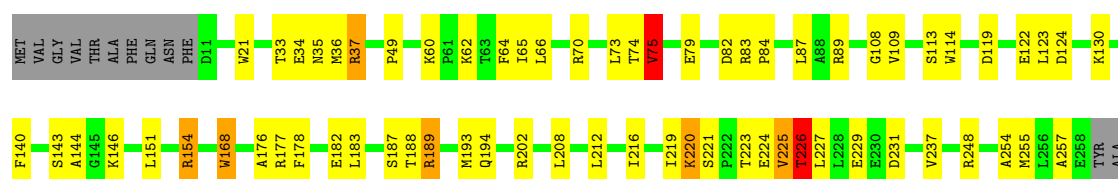
• Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)

Chain O: 70% 22% 5% ..



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain H: 70% 23% .. 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.10Å 140.10Å 271.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	88.0 (30.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	X-PLOR 3.89	Depositor
R, R_{free}	0.215 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14138	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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, BPH, 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	0.87	0/2320	1.65	69/3175 (2.2%)
1	N	0.85	0/2320	1.59	53/3175 (1.7%)
2	M	0.90	0/2482	1.68	81/3389 (2.4%)
2	O	0.89	0/2482	1.60	68/3389 (2.0%)
3	H	0.76	0/1931	1.44	23/2627 (0.9%)
3	P	0.75	0/1931	1.38	15/2627 (0.6%)
All	All	0.85	0/13466	1.57	309/18382 (1.7%)

There are no bond length outliers.

The worst 5 of 309 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	217	ARG	NE-CZ-NH1	9.66	125.13	120.30
2	M	41	TRP	CD1-CG-CD2	9.54	113.93	106.30
2	O	297	TRP	CD1-CG-CD2	9.42	113.83	106.30
1	N	231	ARG	NE-CZ-NH1	9.41	125.01	120.30
3	H	37	ARG	NE-CZ-NH2	-9.33	115.64	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	L	2232	0	2187	39	0
1	N	2232	0	2187	40	0
2	M	2390	0	2304	36	0
2	O	2390	0	2304	47	0
3	H	1883	0	1895	30	0
3	P	1883	0	1895	30	0
4	M	1	0	0	0	0
4	O	1	0	0	0	0
5	L	132	0	148	11	0
5	M	132	0	148	12	0
5	N	198	0	222	18	0
5	O	66	0	74	9	0
6	L	130	0	152	11	0
6	N	65	0	76	7	0
6	O	65	0	76	3	0
7	L	63	0	90	4	0
7	M	63	0	90	1	0
7	N	63	0	90	6	0
7	O	63	0	90	2	0
8	H	13	0	0	3	0
8	L	19	0	0	4	0
8	M	21	0	0	0	0
8	N	13	0	0	0	0
8	O	15	0	0	1	0
8	P	5	0	0	0	0
All	All	14138	0	14028	238	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 238 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)
2:M:275:LEU:O	2:M:279:THR:HB	1.86	0.75
5:N:282:BCL:HBB3	5:O:309:BCL:H41	1.71	0.72
5:N:284:BCL:HED2	2:O:203:GLY:HA3	1.72	0.70
2:M:261:THR:HG22	2:M:264:GLY:H	1.55	0.70
3:H:226:THR:HG22	3:H:229:GLU:H	1.55	0.70

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%)	261 (94%)	14 (5%)	4 (1%)	13	26
1	N	279/281 (99%)	261 (94%)	15 (5%)	3 (1%)	17	35
2	M	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	25	49
2	O	297/307 (97%)	284 (96%)	11 (4%)	2 (1%)	25	49
3	H	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
3	P	246/260 (95%)	238 (97%)	7 (3%)	1 (0%)	38	63
All	All	1644/1696 (97%)	1566 (95%)	66 (4%)	12 (1%)	25	49

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	270	PRO
2	M	259	ASN
2	O	259	ASN
1	L	271	TRP
2	M	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%)	25	49
1	N	220/220 (100%)	201 (91%)	19 (9%)	12	23
2	M	235/240 (98%)	218 (93%)	17 (7%)	17	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	235/240 (98%)	220 (94%)	15 (6%)	20	40
3	H	200/209 (96%)	179 (90%)	21 (10%)	8	15
3	P	200/209 (96%)	178 (89%)	22 (11%)	7	13
All	All	1310/1338 (98%)	1204 (92%)	106 (8%)	14	26

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	227	LEU
1	N	189	LEU
3	P	208	LEU
3	H	255	MET
1	N	64	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	87	GLN
1	N	183	ASN
2	O	145	HIS
3	H	204	HIS
2	O	193	HIS

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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	55,74,74	1.44	8 (14%)	65,115,115	1.51	13 (20%)
5	BCL	L	283	1	55,74,74	1.28	7 (12%)	65,115,115	1.72	14 (21%)
6	BPH	L	284	-	65,70,70	1.18	6 (9%)	75,101,101	1.83	13 (17%)
6	BPH	L	285	-	65,70,70	1.11	6 (9%)	75,101,101	1.91	17 (22%)
7	U10	L	286	-	63,63,63	1.66	14 (22%)	76,79,79	1.31	7 (9%)
5	BCL	M	309	2	55,74,74	1.36	7 (12%)	65,115,115	1.84	16 (24%)
5	BCL	M	310	2	55,74,74	1.32	7 (12%)	65,115,115	1.70	15 (23%)
7	U10	M	311	-	63,63,63	1.66	13 (20%)	76,79,79	1.26	6 (7%)
5	BCL	N	282	2	55,74,74	1.56	11 (20%)	65,115,115	1.69	14 (21%)
5	BCL	N	283	1,5	55,74,74	1.42	8 (14%)	65,115,115	1.69	17 (26%)
5	BCL	N	284	1	55,74,74	1.35	8 (14%)	65,115,115	1.68	18 (27%)
6	BPH	N	285	-	65,70,70	1.10	5 (7%)	75,101,101	1.98	14 (18%)
7	U10	N	286	-	63,63,63	1.62	13 (20%)	76,79,79	1.53	10 (13%)
5	BCL	O	309	2,5	55,74,74	1.35	7 (12%)	65,115,115	1.48	9 (13%)
6	BPH	O	310	-	65,70,70	1.13	5 (7%)	75,101,101	1.93	13 (17%)
7	U10	O	311	-	63,63,63	1.51	14 (22%)	76,79,79	1.13	9 (11%)

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	-	2/2/18/22	0/54/105/105	0/1/6/6
6	BPH	L	285	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	L	286	-	-	0/63/87/87	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BCL	M	309	2	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	M	310	2	2/2/21/25	0/37/137/137	0/0/9/9
7	U10	M	311	-	-	0/63/87/87	0/1/1/1
5	BCL	N	282	2	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	N	283	1,5	-	0/37/137/137	0/0/9/9
5	BCL	N	284	1	-	0/37/137/137	0/0/9/9
6	BPH	N	285	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	N	286	-	-	0/63/87/87	0/1/1/1
5	BCL	O	309	2,5	1/1/21/25	0/37/137/137	0/0/9/9
6	BPH	O	310	-	1/1/18/22	0/54/105/105	0/1/6/6
7	U10	O	311	-	-	0/63/87/87	0/1/1/1

The worst 5 of 139 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	286	U10	C7-C8	-4.75	1.43	1.50
7	M	311	U10	C7-C8	-4.59	1.43	1.50
7	N	286	U10	C7-C8	-4.19	1.44	1.50
5	L	282	BCL	O2D-CGD	-4.17	1.22	1.33
6	N	285	BPH	C3D-CAD	-3.93	1.38	1.47

The worst 5 of 205 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	285	BPH	C4D-C3D-CAD	-8.73	102.79	107.78
6	L	284	BPH	C4D-C3D-CAD	-7.86	103.28	107.78
6	O	310	BPH	C4D-C3D-CAD	-7.38	103.56	107.78
6	N	285	BPH	C4D-C3D-CAD	-6.66	103.97	107.78
6	O	310	BPH	O1D-CGD-CBD	-5.81	114.17	124.60

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	O	310	BPH	C13
6	L	284	BPH	C8
6	L	284	BPH	C13
6	N	285	BPH	C8
5	O	309	BCL	C8

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 75 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	282	BCL	8	0
5	L	283	BCL	6	0
6	L	284	BPH	2	0
6	L	285	BPH	9	0
7	L	286	U10	4	0
5	M	309	BCL	7	0
5	M	310	BCL	5	0
7	M	311	U10	1	0
5	N	282	BCL	7	0
5	N	283	BCL	6	0
5	N	284	BCL	7	0
6	N	285	BPH	7	0
7	N	286	U10	6	0
5	O	309	BCL	9	0
6	O	310	BPH	3	0
7	O	311	U10	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 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.