



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:31 am GMT

PDB ID : 4RCR  
Title : STRUCTURE OF THE REACTION CENTER FROM RHODOBACTER SPHAEROIDES R-26 AND 2.4.1: PROTEIN-COFACTOR (BACTERIOCHLOROPHYLL, BACTERIOPHEOPHYTIN, AND CAROTENOID) INTERACTIONS  
Authors : Komiya, H.; Yeates, T.O.; Chirino, A.J.; Rees, D.C.; Allen, J.P.; Feher, G.  
Deposited on : 1991-09-09  
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

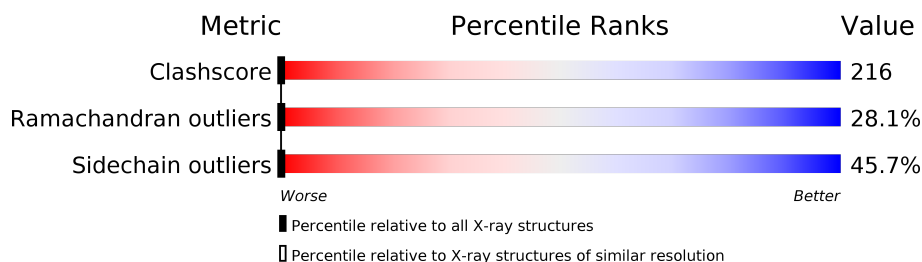
# 1 Overall quality at a glance

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
4	BOG	M	308	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCL	L	283	-	-	X	-
6	BCL	M	310	-	-	X	-
6	BCL	M	311	-	-	X	-
7	BPH	L	284	-	-	X	-
7	BPH	M	312	-	-	X	-
8	U10	L	285	-	-	X	-
8	U10	M	313	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6764 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	266	Total	C	N	O	S	0	0	0
			2120	1433	336	343	8			

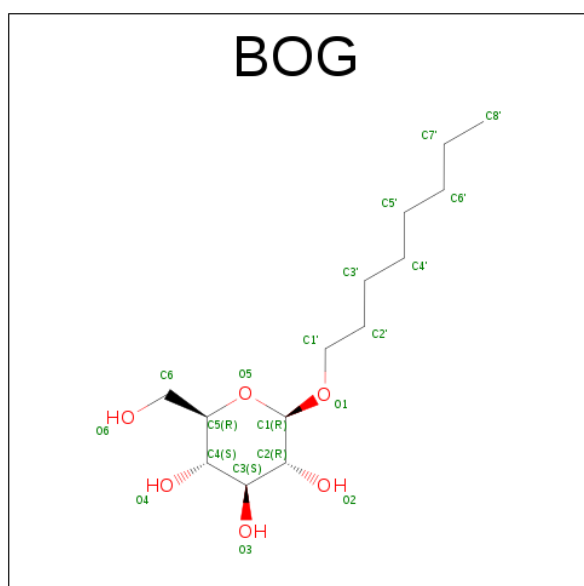
- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	296	Total	C	N	O	S	0	0	0
			2361	1579	386	386	10			

- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	237	Total	C	N	O	S	0	0	0
			1806	1156	310	331	9			

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).

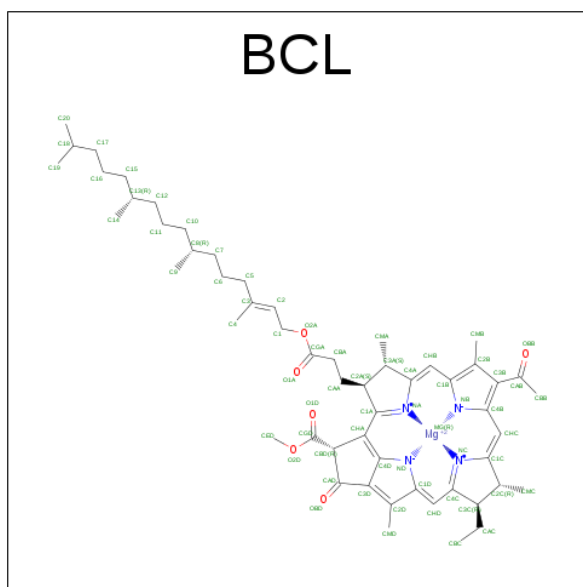


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	M	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

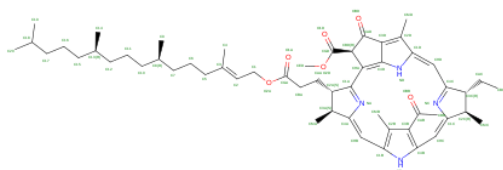
- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $\text{C}_{55}\text{H}_{74}\text{MgN}_4\text{O}_6$ ).



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

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $\text{C}_{55}\text{H}_{76}\text{N}_4\text{O}_6$ ).

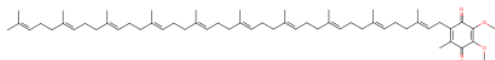
## BPH



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:  $C_{59}H_{90}O_4$ ).

## U10



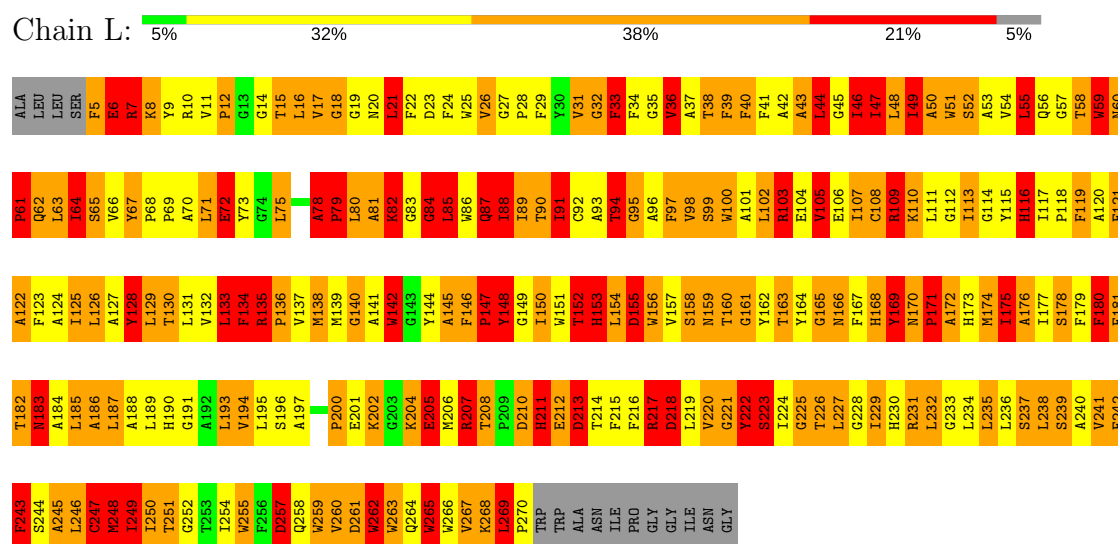
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			51	47	4		
8	L	1	Total	C	O	0	0
			41	37	4		

### 3 Residue-property plots

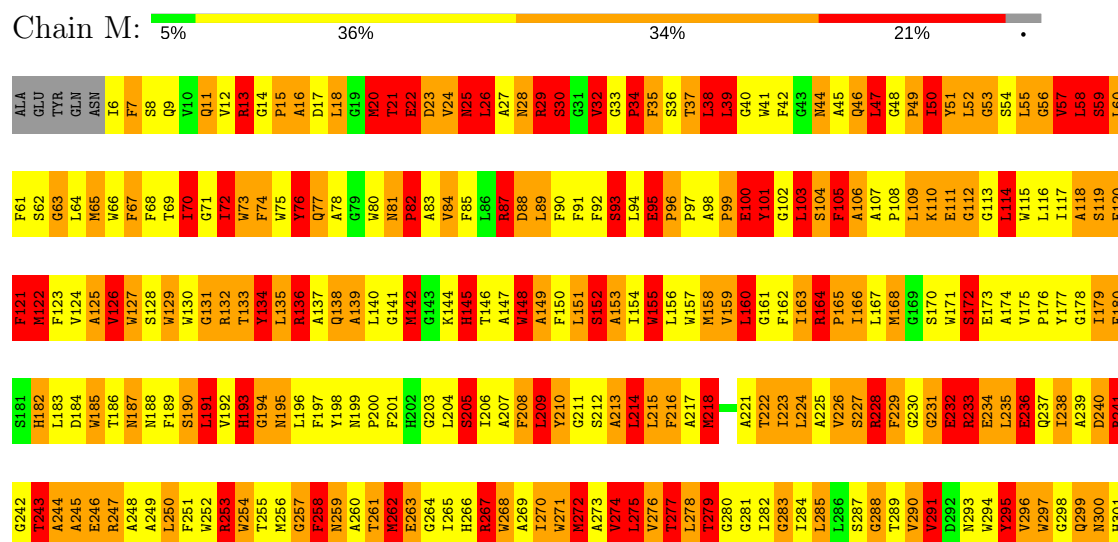
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

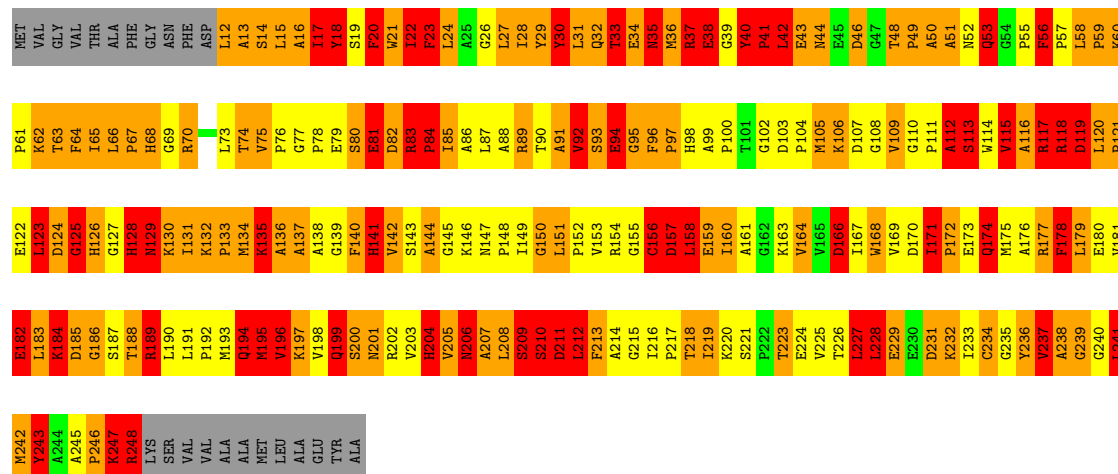
Note EDS was not executed.

#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER



#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER







## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.00Å 77.50Å 141.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.227 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	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, U10, FE, BOG

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	1.01	1/2203 (0.0%)	1.69	48/3014 (1.6%)
2	M	1.03	0/2452	1.71	52/3348 (1.6%)
3	H	1.16	4/1854 (0.2%)	1.95	48/2523 (1.9%)
All	All	1.06	5/6509 (0.1%)	1.78	148/8885 (1.7%)

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	36
2	M	0	29
3	H	2	39
All	All	2	104

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	53	GLN	C-N	17.61	1.64	1.33
3	H	56	PHE	C-N	-12.37	1.10	1.34
3	H	248	ARG	CD-NE	-6.33	1.35	1.46
3	H	248	ARG	NE-CZ	-5.38	1.26	1.33
1	L	94	THR	CA-CB	5.02	1.66	1.53

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	248	ARG	CD-NE-CZ	40.26	179.96	123.60
2	M	13	ARG	NE-CZ-NH1	14.66	127.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	13	ARG	NE-CZ-NH2	-11.69	114.46	120.30
3	H	177	ARG	NE-CZ-NH1	-10.41	115.10	120.30
3	H	248	ARG	NE-CZ-NH1	9.76	125.18	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	141	HIS	CA
3	H	204	HIS	CA

5 of 104 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	36	VAL	Mainchain
1	L	44	LEU	Mainchain
1	L	46	ILE	Mainchain
1	L	6	GLU	Mainchain
1	L	7	ARG	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	2120	0	2077	1093	0
2	M	2361	0	2279	1145	0
3	H	1806	0	1814	771	0
4	M	20	0	28	7	0
5	M	1	0	0	0	0
6	L	117	0	115	116	0
6	M	117	0	113	93	0
7	L	65	0	76	44	0
7	M	65	0	76	47	0
8	L	41	0	52	31	0
8	M	51	0	68	43	0
All	All	6764	0	6698	2900	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 216.

The worst 5 of 2900 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:73:TRP:CD1	2:M:114:LEU:HG	1.20	1.64
7:M:312:BPH:C11	7:M:312:BPH:C10	1.76	1.61
7:M:312:BPH:C6	7:M:312:BPH:C7	1.78	1.60
1:L:175:ILE:HG21	1:L:243:PHE:CD2	1.24	1.60
2:M:197:PHE:CZ	6:M:310:BCL:HBB2	1.33	1.57

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	264/281 (94%)	118 (45%)	65 (25%)	81 (31%)	0	0
2	M	294/307 (96%)	141 (48%)	74 (25%)	79 (27%)	0	0
3	H	235/260 (90%)	107 (46%)	65 (28%)	63 (27%)	0	0
All	All	793/848 (94%)	366 (46%)	204 (26%)	223 (28%)	0	0

5 of 223 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	6	GLU
1	L	7	ARG
1	L	18	GLY
1	L	21	LEU
1	L	31	VAL

### 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	210/220 (96%)	124 (59%)	86 (41%)	0	0
2	M	232/240 (97%)	128 (55%)	104 (45%)	0	0
3	H	192/208 (92%)	92 (48%)	100 (52%)	0	0
All	All	634/668 (95%)	344 (54%)	290 (46%)	0	0

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	119	SER
2	M	227	SER
3	H	204	HIS
2	M	126	VAL
2	M	165	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	44	ASN
2	M	77	GLN
3	H	98	HIS
2	M	28	ASN
3	H	199	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 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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$
6	BCL	L	282	2	40,59,74	1.91	5 (12%)	47,97,115	2.35	14 (29%)
6	BCL	L	283	1	55,74,74	1.62	6 (10%)	65,115,115	2.22	21 (32%)
7	BPH	L	284	-	65,70,70	2.20	9 (13%)	75,101,101	3.79	23 (30%)
8	U10	L	285	-	41,41,63	0.97	0	49,52,79	1.82	13 (26%)
4	BOG	M	308	-	20,20,20	0.67	0	25,25,25	1.43	3 (12%)
6	BCL	M	310	2	55,74,74	1.59	5 (9%)	65,115,115	2.04	15 (23%)
6	BCL	M	311	-	40,59,74	2.72	9 (22%)	47,97,115	2.44	17 (36%)
7	BPH	M	312	2	65,70,70	1.56	7 (10%)	75,101,101	3.68	21 (28%)
8	U10	M	313	-	51,51,63	0.92	1 (1%)	61,64,79	1.93	20 (32%)

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
6	BCL	L	282	2	-	0/19/119/137	0/0/9/9
6	BCL	L	283	1	-	0/37/137/137	0/0/9/9
7	BPH	L	284	-	-	0/54/105/105	0/1/6/6
8	U10	L	285	-	-	0/37/61/87	0/1/1/1
4	BOG	M	308	-	1/1/5/5	0/11/31/31	0/1/1/1
6	BCL	M	310	2	-	0/37/137/137	0/0/9/9
6	BCL	M	311	-	-	0/19/119/137	0/0/9/9
7	BPH	M	312	2	-	2/54/105/105	0/1/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	U10	M	313	-	-	0/49/73/87	0/1/1/1

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	311	BCL	CHB-C4A	-11.51	1.19	1.33
7	L	284	BPH	O2D-CGD	-4.69	1.21	1.33
7	M	312	BPH	O2D-CGD	-4.63	1.21	1.33
6	M	310	BCL	O2D-CGD	-3.96	1.23	1.33
6	M	311	BCL	CMA-C3A	-3.63	1.45	1.53

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	312	BPH	C4D-C3D-CAD	-25.19	93.37	107.78
7	L	284	BPH	C4D-C3D-CAD	-23.99	94.06	107.78
7	L	284	BPH	CHB-C1B-NB	-9.92	105.20	124.64
6	L	283	BCL	CMB-C2B-C1B	-6.31	118.76	128.46
7	L	284	BPH	O1D-CGD-CBD	-5.96	113.89	124.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	M	308	BOG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	312	BPH	OBB-CAB-C3B-C4B
7	M	312	BPH	C4B-C3B-CAB-CBB

There are no ring outliers.

9 monomers are involved in 327 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	282	BCL	19	0
6	L	283	BCL	100	0
7	L	284	BPH	44	0
8	L	285	U10	31	0
4	M	308	BOG	7	0
6	M	310	BCL	68	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	311	BCL	25	0
7	M	312	BPH	47	0
8	M	313	U10	43	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.