W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:52 PM GMT

PDB ID : 1YST
Title : STRUCTURE OF THE PHOTOCHEMICAL REACTION CENTER OF A SPHEROIDENE CONTAINING PURPLE BACTERIUM, RHODOBACTER SPHAEROIDES Y, AT 3 ANGSTROMS RESOLUTION
Authors : Arnoux, B.; Gaucher, J.F.; Ducruix, A.; Reiss-Husson, F.
Deposited on : 1994-12-07
Resolution : 3.00 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Clashscore		46
Ramachandran outliers		14.1%
Sidechain outliers		28.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
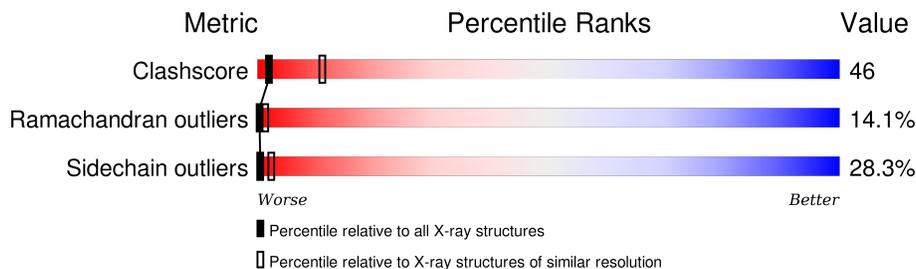
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 <=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	273	32% 41% 22% 5%
2	M	305	35% 46% 17% •
3	H	260	31% 46% 20% •

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
5	BCL	L	274	X	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BCL	M	307	X	-	X	-
6	BPH	L	276	X	-	X	-
6	BPH	M	309	X	-	-	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7136 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	273	Total 2181	C 1476	N 345	O 352	S 8	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	305	Total 2429	C 1619	N 397	O 401	S 12	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	260	Total 1973	C 1264	N 335	O 363	S 11	0	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).
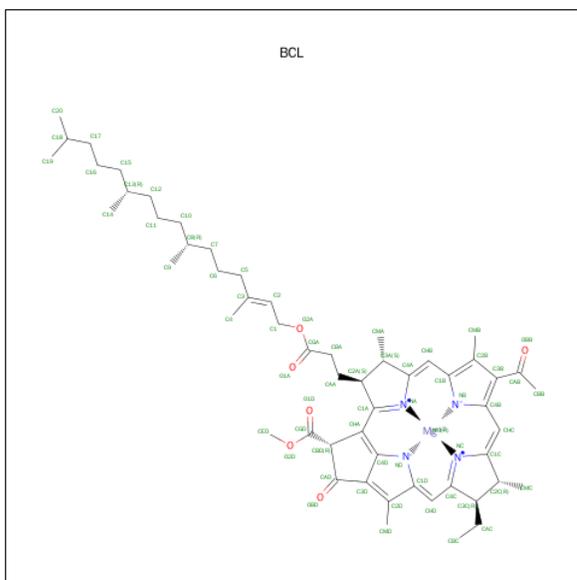
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).
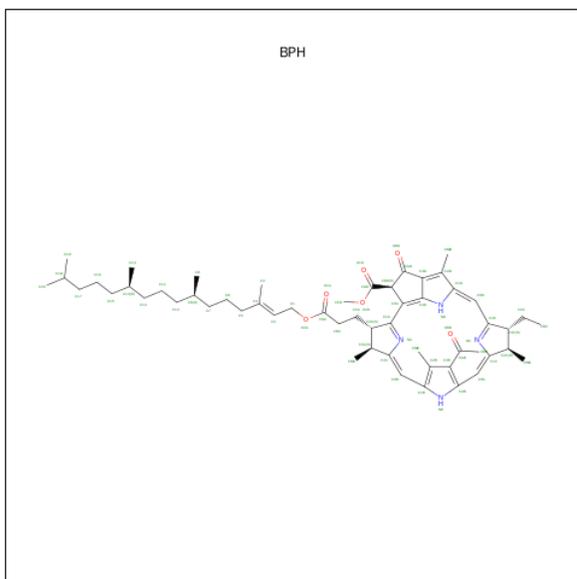
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	M	1	Total 65	C 55	N 4	O 6	0	0
6	L	1	Total 65	C 55	N 4	O 6	0	0

• Molecule 7 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).
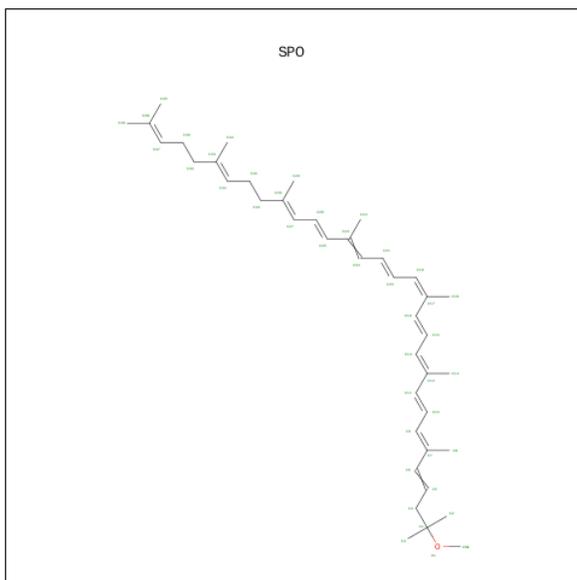
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total 42	C 41	O 1	0	0

• Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).
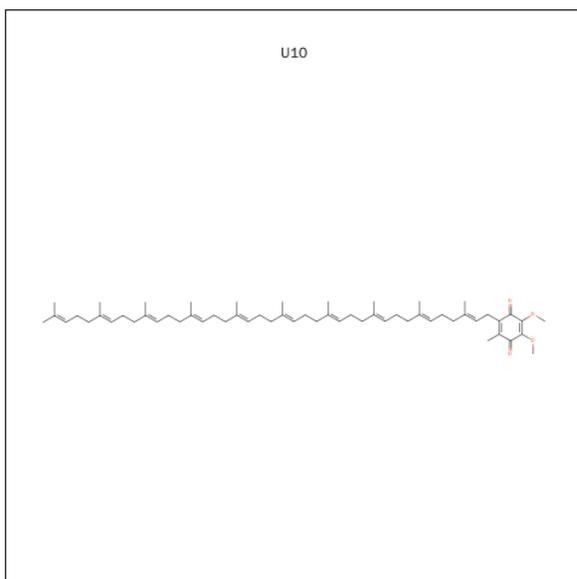
| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total 58	C 54	O 4	0	0
8	L	1	Total 58	C 54	O 4	0	0

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)
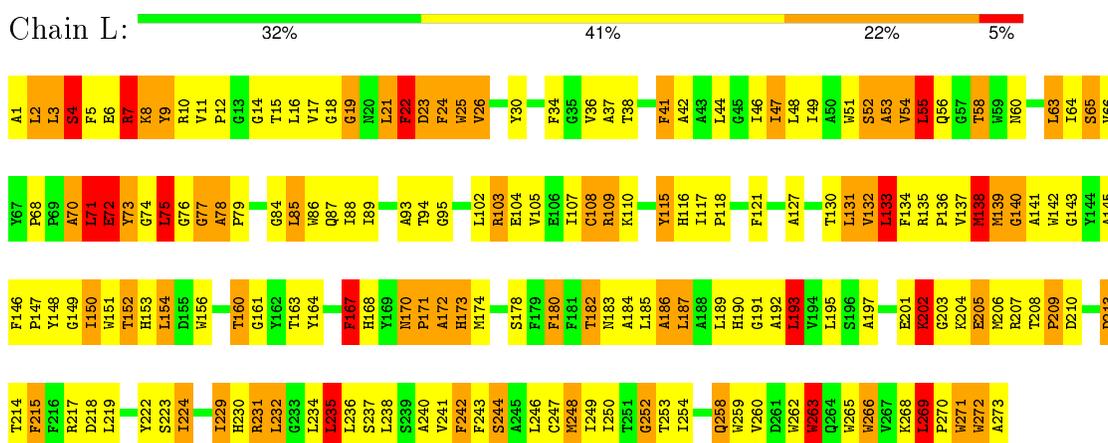
● Molecule 2: PHOTOSYNTHETIC REACTION CENTER (M SUBUNIT)
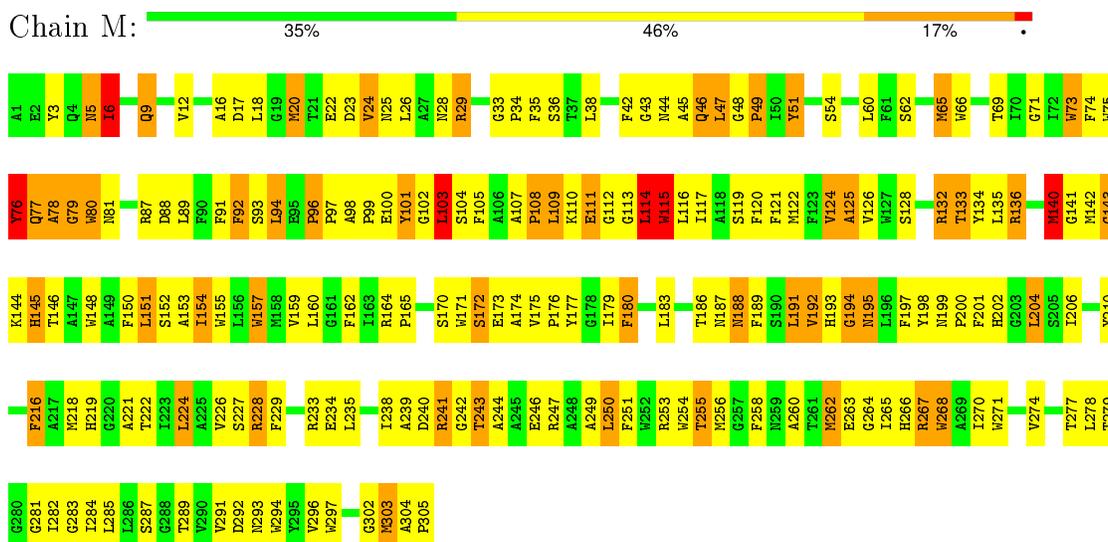
● Molecule 3: PHOTOSYNTHETIC REACTION CENTER (H SUBUNIT)

Chain H:
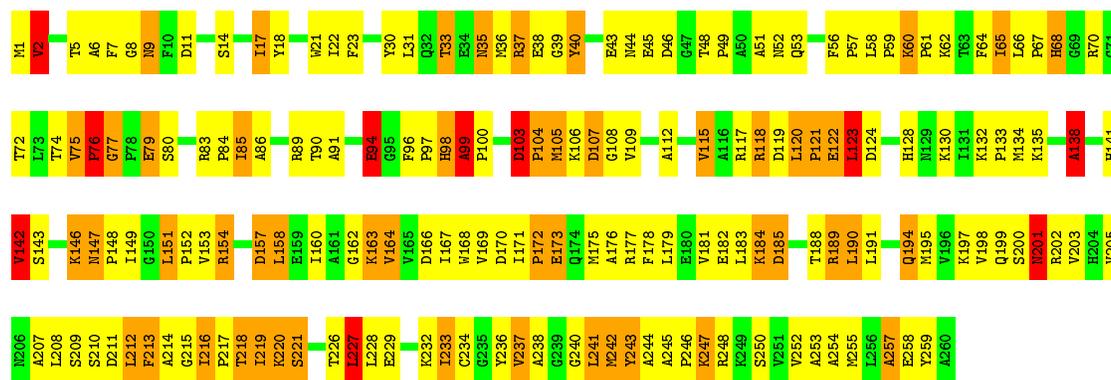
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	143.70Å　　139.80Å　　78.65Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	7.00　　–　　3.00	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.234　　,　　(Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7136	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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, MN, U10, SPO

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	1/2268 (0.0%)	1.04	11/3104 (0.4%)
2	M	0.85	4/2522 (0.2%)	1.41	10/3441 (0.3%)
3	H	0.92	2/2024 (0.1%)	1.16	8/2752 (0.3%)
All	All	0.87	7/6814 (0.1%)	1.22	29/9297 (0.3%)

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
3	H	0	4
All	All	0	7

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	76	PRO	C-N	18.97	1.67	1.33
1	L	252	GLY	C-N	-14.31	1.01	1.34
2	M	228	ARG	CD-NE	-11.97	1.26	1.46
2	M	228	ARG	NE-CZ	-9.37	1.20	1.33
3	H	99	ALA	C-N	6.71	1.47	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	M	228	ARG	NE-CZ-NH2	37.25	138.92	120.30
2	M	228	ARG	NE-CZ-NH1	-33.24	103.68	120.30
2	M	228	ARG	CD-NE-CZ	28.33	163.26	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	76	PRO	C-N-CA	9.99	143.28	122.30
1	L	133	LEU	CA-CB-CG	8.18	134.11	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	138	ALA	Mainchain
3	H	99	ALA	Mainchain
1	L	153	HIS	Mainchain
1	L	252	GLY	Mainchain
1	L	263	TRP	Mainchain

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	2181	0	2136	239	0
2	M	2429	0	2339	202	0
3	H	1973	0	1981	197	0
4	M	1	0	0	0	0
5	L	132	0	145	28	0
5	M	132	0	148	36	0
6	L	65	0	76	23	0
6	M	65	0	76	11	0
7	M	42	0	60	13	0
8	L	58	0	79	16	0
8	M	58	0	79	19	0
All	All	7136	0	7119	661	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 46.

The worst 5 of 661 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)
8:L:277:U10:C27	8:L:277:U10:C28	1.79	1.56
6:L:276:BPH:C2A	6:L:276:BPH:CAA	1.75	1.54
1:L:78:ALA:HB1	1:L:79:PRO:CD	1.69	1.21
1:L:78:ALA:CB	1:L:79:PRO:HD3	1.74	1.15
1:L:78:ALA:CB	1:L:79:PRO:CD	2.25	1.15

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	271/273 (99%)	166 (61%)	63 (23%)	42 (16%)	0	1
2	M	303/305 (99%)	201 (66%)	70 (23%)	32 (11%)	0	3
3	H	258/260 (99%)	151 (58%)	64 (25%)	43 (17%)	0	1
All	All	832/838 (99%)	518 (62%)	197 (24%)	117 (14%)	0	1

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	3	LEU
1	L	4	SER
1	L	65	SER
1	L	70	ALA
1	L	71	LEU

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	215/215 (100%)	156 (73%)	59 (27%)	0	2
2	M	238/238 (100%)	173 (73%)	65 (27%)	0	2
3	H	208/208 (100%)	145 (70%)	63 (30%)	0	2
All	All	661/661 (100%)	474 (72%)	187 (28%)	0	2

5 of 187 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	101	TYR
2	M	187	ASN
3	H	197	LYS
2	M	114	LEU
2	M	136	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	M	46	GLN
2	M	188	ASN
3	H	194	GLN
2	M	81	ASN
2	M	145	HIS

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
5	BCL	L	274	1	53,74,74	4.07	22 (41%)	57,115,115	1.70	10 (17%)
5	BCL	L	275	1	53,74,74	2.73	21 (39%)	57,115,115	1.43	10 (17%)
6	BPH	L	276	-	64,70,70	2.28	16 (25%)	73,101,101	1.41	9 (12%)
8	U10	L	277	-	58,58,63	4.12	35 (60%)	70,73,79	1.76	14 (20%)
5	BCL	M	307	2	53,74,74	2.36	13 (24%)	57,115,115	1.86	12 (21%)
5	BCL	M	308	2	53,74,74	2.52	17 (32%)	57,115,115	1.59	13 (22%)
6	BPH	M	309	-	64,70,70	2.60	20 (31%)	73,101,101	1.46	11 (15%)
7	SPO	M	310	-	40,41,41	3.20	21 (52%)	45,50,50	1.73	11 (24%)
8	U10	M	311	-	58,58,63	3.36	29 (50%)	70,73,79	1.59	13 (18%)

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	274	1	1/1/21/25	0/37/137/137	0/0/9/9
5	BCL	L	275	1	-	0/37/137/137	0/0/9/9
6	BPH	L	276	-	1/1/18/22	0/54/105/105	0/1/6/6
8	U10	L	277	-	-	0/57/81/87	0/1/1/1
5	BCL	M	307	2	2/2/21/25	0/37/137/137	0/0/9/9
5	BCL	M	308	2	-	0/37/137/137	0/0/9/9
6	BPH	M	309	-	1/1/18/22	0/54/105/105	0/1/6/6
7	SPO	M	310	-	-	0/47/47/47	0/0/0/0
8	U10	M	311	-	-	0/57/81/87	0/1/1/1

The worst 5 of 194 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	311	U10	C18-C19	-9.54	1.14	1.33
5	L	274	BCL	CBB-CAB	-9.31	1.21	1.49
5	M	308	BCL	C3C-C4C	-8.75	1.40	1.51
5	M	308	BCL	C2C-C3C	-6.89	1.33	1.54
5	L	275	BCL	CMD-C2D	-6.70	1.37	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	274	BCL	CHC-C1C-NC	-6.47	115.56	124.51
5	L	274	BCL	OBB-CAB-C3B	-5.41	111.44	120.00
6	L	276	BPH	CBB-CAB-C3B	-5.34	108.66	120.52
8	M	311	U10	C17-C18-C19	-5.11	116.65	127.76
8	M	311	U10	C21-C19-C18	-4.76	112.02	121.05

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	M	307	BCL	C8
5	M	307	BCL	C13
6	L	276	BPH	C8
5	L	274	BCL	C2C
6	M	309	BPH	C3C

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 136 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	274	BCL	22	0
5	L	275	BCL	9	0
6	L	276	BPH	23	0
8	L	277	U10	16	0
5	M	307	BCL	23	0
5	M	308	BCL	17	0
6	M	309	BPH	11	0
7	M	310	SPO	13	0
8	M	311	U10	19	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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