WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:03 PM GMT

PDB ID : 1DS8

Title : PHOTOSYNTHETIC REACTION CENTER FROM RHODOBACTER SPHAEROIDES IN THE CHARGE-NEUTRAL DQAQB STATE WITH THE PROTON TRANSFER INHIBITOR CD2+

Authors : Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.

Deposited on : 2000-01-07
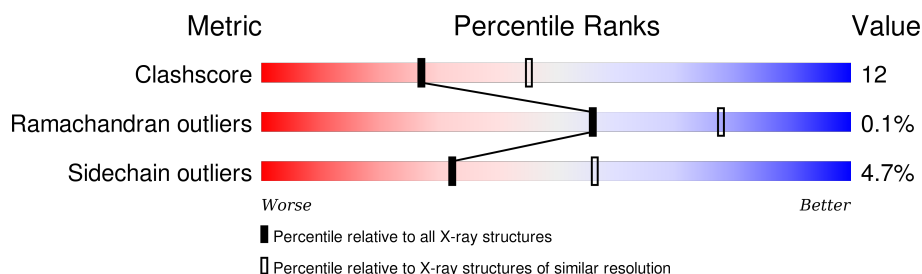
Resolution : 2.50 Å(reported)

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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 2.50 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		12
Ramachandran outliers		0.1%
Sidechain outliers		4.7%

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	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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	281	72% 26% •
1	R	281	72% 26% •
2	M	307	79% 17% • •
2	S	307	79% 17% • •
3	H	260	73% 20% • 5%
3	T	260	72% 21% • 5%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 14529 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 REACTION CENTER PROTEIN L CHAIN.

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

- Molecule 2 is a protein called REACTION CENTER PROTEIN M CHAIN.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	ALA	ASN	CONFLICT	UNP P02953
S	307	ALA	ASN	CONFLICT	UNP P02953

- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

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

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 1	Fe 1	0	0
4	M	1	Total 1	Fe 1	0	0

- Molecule 5 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	Cd 1	0	0
5	T	1	Total 1	Cd 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	S	1	Total 1	Cl 1	0	0
6	M	1	Total 1	Cl 1	0	0

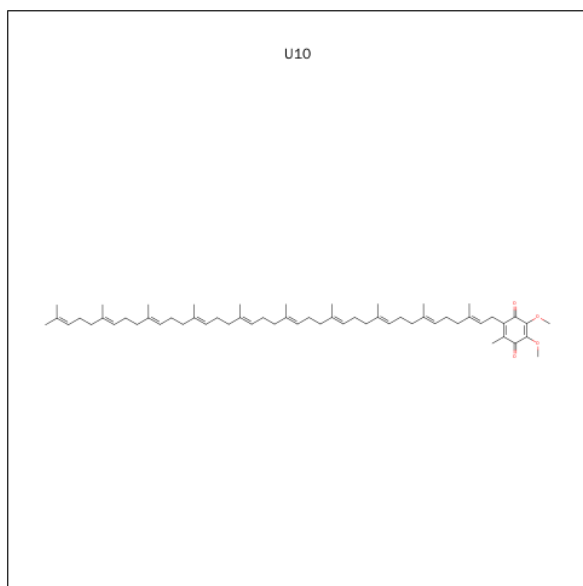- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).
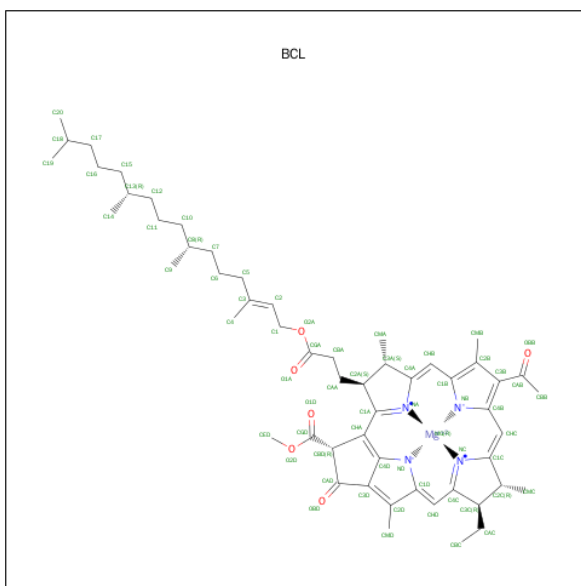
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	R	1	Total 51	C 40	Mg 1	N 4	O 6	0	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).
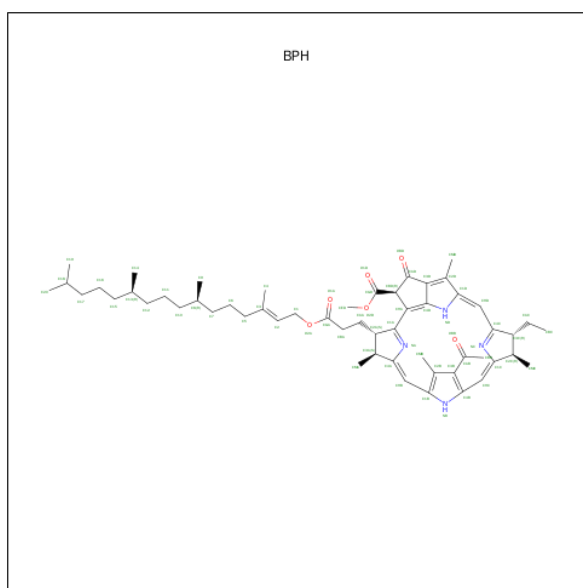
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	M	1	Total 51	C 41	N 4	O 6	0	0
8	L	1	Total 65	C 55	N 4	O 6	0	0
8	S	1	Total 52	C 42	N 4	O 6	0	0
8	R	1	Total 65	C 55	N 4	O 6	0	0

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

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

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).
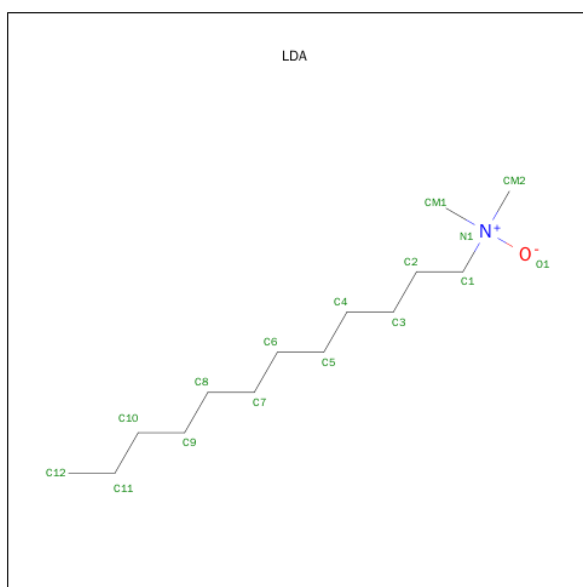
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total 16	C 14	N 1	O 1	0	0
10	M	1	Total 16	C 14	N 1	O 1	0	0
10	M	1	Total 16	C 14	N 1	O 1	0	0
10	S	1	Total 16	C 14	N 1	O 1	0	0
10	S	1	Total 16	C 14	N 1	O 1	0	0
10	S	1	Total 16	C 14	N 1	O 1	0	0

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	122	Total 122	O 122	0	0
11	L	88	Total 88	O 88	0	0
11	M	133	Total 133	O 133	0	0
11	R	62	Total 62	O 62	0	0
11	S	92	Total 92	O 92	0	0
11	T	85	Total 85	O 85	0	0

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 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.
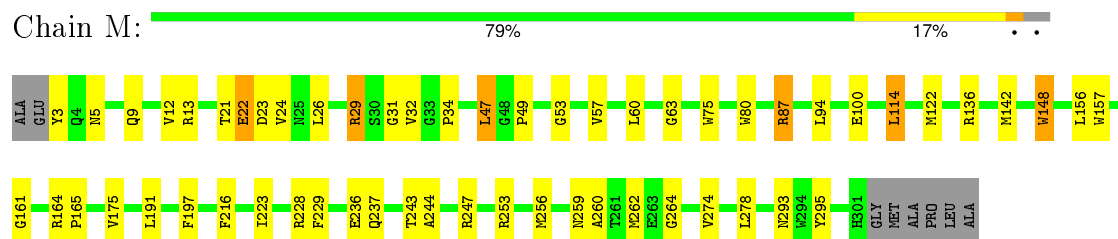
Note EDS was not executed.

- Molecule 1: REACTION CENTER PROTEIN L CHAIN
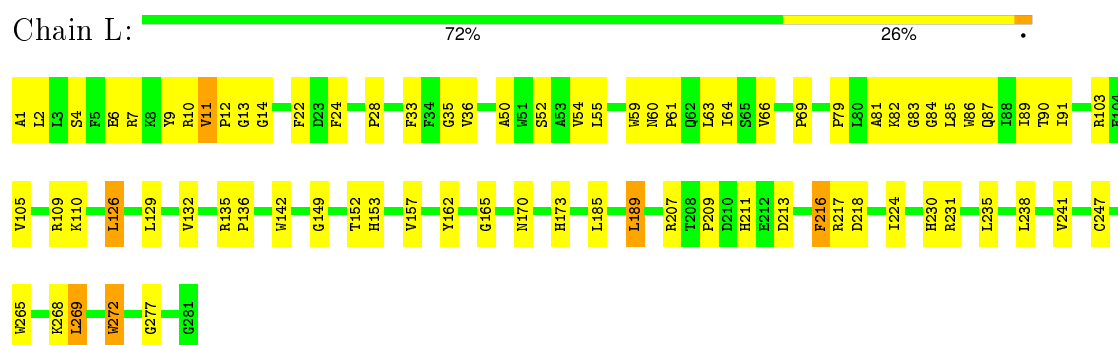
- Molecule 1: REACTION CENTER PROTEIN L CHAIN
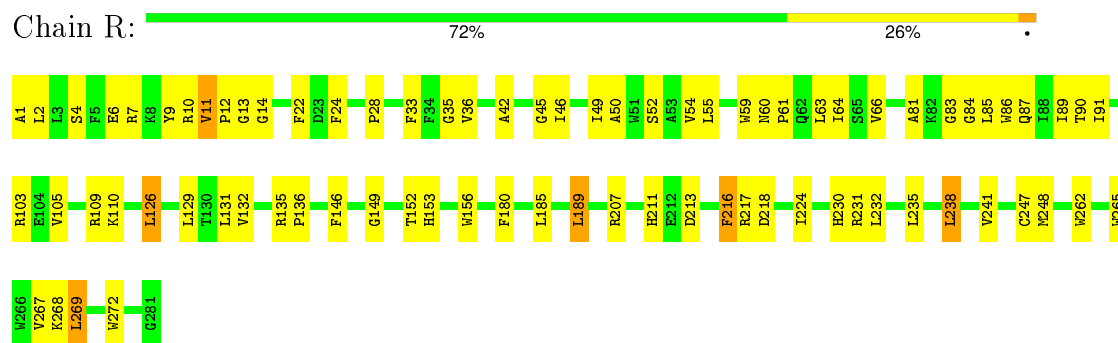
- Molecule 2: REACTION CENTER PROTEIN M CHAIN

- Molecule 2: REACTION CENTER PROTEIN M CHAIN

Chain S:
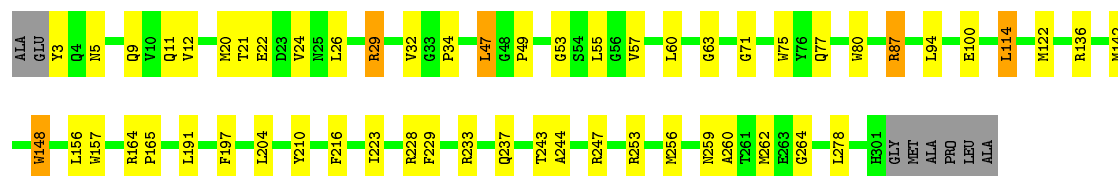
● Molecule 3: REACTION CENTER PROTEIN H CHAIN

Chain H:
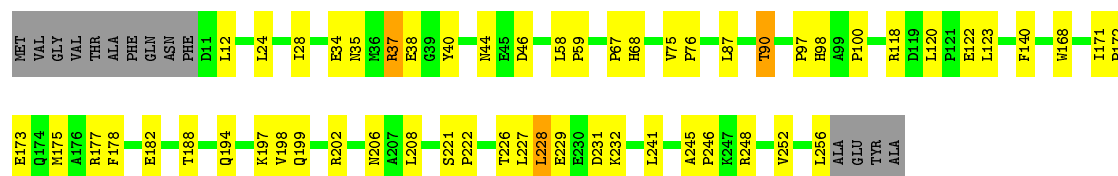
● Molecule 3: REACTION CENTER PROTEIN H CHAIN

Chain T:
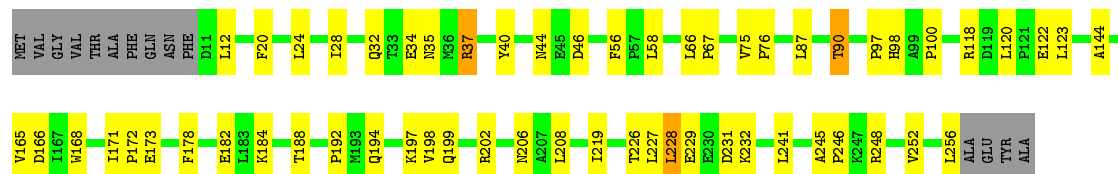
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	139.59Å 139.59Å 272.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50	Depositor
% Data completeness (in resolution range)	99.8 (50.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.227 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14529	wwPDB-VP
Average B, all atoms (Å^2)	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, CL, BPH, CD, 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	0.39	0/2320	0.55	0/3175
1	R	0.40	0/2320	0.55	0/3175
2	M	0.41	0/2482	0.54	0/3389
2	S	0.40	0/2482	0.54	0/3389
3	H	0.35	0/1917	0.60	0/2608
3	T	0.35	0/1917	0.60	0/2608
All	All	0.39	0/13438	0.56	0/18344

There are no bond length outliers.

There are no bond angle outliers.

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	59	0
1	R	2232	0	2187	63	0
2	M	2390	0	2304	53	0
2	S	2390	0	2304	49	0
3	H	1869	0	1884	49	0
3	T	1869	0	1884	45	0
4	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S	1	0	0	0	0
5	H	1	0	0	0	0
5	T	1	0	0	0	0
6	M	1	0	0	0	0
6	S	1	0	0	0	0
7	L	183	0	189	17	0
7	M	66	0	73	8	0
7	R	183	0	189	17	0
7	S	66	0	74	6	0
8	L	65	0	76	5	0
8	M	51	0	45	5	0
8	R	65	0	76	14	0
8	S	52	0	47	4	0
9	L	44	0	57	2	0
9	M	38	0	47	2	0
9	R	18	0	15	3	0
9	S	32	0	39	2	0
10	M	48	0	93	7	0
10	S	48	0	93	5	0
11	H	122	0	0	6	0
11	L	88	0	0	7	0
11	M	133	0	0	2	0
11	R	62	0	0	2	0
11	S	92	0	0	3	0
11	T	85	0	0	3	0
All	All	14529	0	13863	333	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 12.

The worst 5 of 333 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:197:PHE:HZ	7:M:1003:BCL:HBB2	1.34	0.91
2:M:197:PHE:CZ	7:M:1003:BCL:HBB2	2.11	0.86
1:L:217:ARG:HD2	11:M:1108:HOH:O	1.77	0.85
2:M:161:GLY:HA3	10:M:1014:LDA:HM12	1.62	0.82
1:R:131:LEU:HD21	7:R:2002:BCL:HED2	1.64	0.80

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	279/281 (99%)	266 (95%)	12 (4%)	1 (0%)	39	61
1	R	279/281 (99%)	266 (95%)	12 (4%)	1 (0%)	39	61
2	M	297/307 (97%)	288 (97%)	9 (3%)	0	100	100
2	S	297/307 (97%)	289 (97%)	8 (3%)	0	100	100
3	H	244/260 (94%)	236 (97%)	8 (3%)	0	100	100
3	T	244/260 (94%)	234 (96%)	10 (4%)	0	100	100
All	All	1640/1696 (97%)	1579 (96%)	59 (4%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	4	SER
1	L	4	SER

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	220/220 (100%)	209 (95%)	11 (5%)	30	53
1	R	220/220 (100%)	209 (95%)	11 (5%)	30	53
2	M	235/239 (98%)	222 (94%)	13 (6%)	27	48
2	S	235/239 (98%)	222 (94%)	13 (6%)	27	48
3	H	199/209 (95%)	192 (96%)	7 (4%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	T	199/209 (95%)	192 (96%)	7 (4%)	43	70
All	All	1308/1336 (98%)	1246 (95%)	62 (5%)	32	56

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	208	LEU
1	R	129	LEU
3	T	90	THR
1	R	7	ARG
1	R	216	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
3	H	199	GLN
3	H	206	ASN
2	S	300	ASN
3	H	194	GLN
3	T	194	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 28 ligands modelled in this entry, 6 are monoatomic - leaving 22 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	#$|Z| > 2$
7	BCL	L	1001	2	38,59,74	1.06	4 (10%)	40,97,115	1.65	11 (27%)
7	BCL	L	1002	1	53,74,74	0.93	4 (7%)	57,115,115	1.38	11 (19%)
7	BCL	L	1004	1	53,74,74	0.97	4 (7%)	57,115,115	1.55	11 (19%)
8	BPH	L	1006	-	64,70,70	1.25	8 (12%)	73,101,101	1.56	10 (13%)
9	U10	L	1009	-	44,44,63	1.77	9 (20%)	53,56,79	1.53	10 (18%)
7	BCL	M	1003	2	53,74,74	0.97	5 (9%)	57,115,115	1.44	12 (21%)
8	BPH	M	1005	-	50,56,70	1.17	7 (14%)	56,84,101	1.93	10 (17%)
9	U10	M	1008	-	38,38,63	1.85	11 (28%)	46,49,79	1.30	4 (8%)
10	LDA	M	1012	-	15,15,15	4.14	3 (20%)	16,17,17	3.28	3 (18%)
10	LDA	M	1013	-	15,15,15	4.46	3 (20%)	16,17,17	3.13	3 (18%)
10	LDA	M	1014	-	15,15,15	4.54	2 (13%)	16,17,17	2.92	4 (25%)
7	BCL	R	2001	2	38,59,74	1.03	5 (13%)	40,97,115	1.68	7 (17%)
7	BCL	R	2002	1	53,74,74	0.99	3 (5%)	57,115,115	1.34	8 (14%)
7	BCL	R	2004	1	53,74,74	1.00	5 (9%)	57,115,115	1.57	8 (14%)
8	BPH	R	2006	-	64,70,70	1.07	5 (7%)	73,101,101	1.48	9 (12%)
9	U10	R	2009	-	18,18,63	1.80	3 (16%)	22,25,79	1.34	3 (13%)
7	BCL	S	2003	2	53,74,74	0.99	5 (9%)	57,115,115	1.52	11 (19%)
8	BPH	S	2005	-	51,57,70	1.26	5 (9%)	57,85,101	1.74	11 (19%)
9	U10	S	2008	-	32,32,63	1.69	7 (21%)	38,41,79	1.18	4 (10%)
10	LDA	S	2012	-	15,15,15	4.63	3 (20%)	16,17,17	3.29	2 (12%)
10	LDA	S	2013	-	15,15,15	4.39	3 (20%)	16,17,17	3.32	2 (12%)
10	LDA	S	2014	-	15,15,15	4.77	2 (13%)	16,17,17	2.93	3 (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
7	BCL	L	1001	2	-	0/19/119/137	0/0/9/9
7	BCL	L	1002	1	-	0/37/137/137	0/0/9/9
7	BCL	L	1004	1	-	0/37/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BPH	L	1006	-	-	0/54/105/105	0/1/6/6
9	U10	L	1009	-	-	0/41/65/87	0/1/1/1
7	BCL	M	1003	2	-	0/37/137/137	0/0/9/9
8	BPH	M	1005	-	-	0/38/89/105	0/1/6/6
9	U10	M	1008	-	-	0/33/57/87	0/1/1/1
10	LDA	M	1012	-	-	0/13/13/13	0/0/0/0
10	LDA	M	1013	-	-	0/13/13/13	0/0/0/0
10	LDA	M	1014	-	-	0/13/13/13	0/0/0/0
7	BCL	R	2001	2	-	0/19/119/137	0/0/9/9
7	BCL	R	2002	1	-	0/37/137/137	0/0/9/9
7	BCL	R	2004	1	-	0/37/137/137	0/0/9/9
8	BPH	R	2006	-	-	0/54/105/105	0/1/6/6
9	U10	R	2009	-	-	0/9/33/87	0/1/1/1
7	BCL	S	2003	2	-	0/37/137/137	0/0/9/9
8	BPH	S	2005	-	-	0/39/90/105	0/1/6/6
9	U10	S	2008	-	-	0/26/50/87	0/1/1/1
10	LDA	S	2012	-	-	0/13/13/13	0/0/0/0
10	LDA	S	2013	-	-	0/13/13/13	0/0/0/0
10	LDA	S	2014	-	-	0/13/13/13	0/0/0/0

The worst 5 of 106 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	S	2014	LDA	O1-N1	-18.09	1.22	1.39
10	S	2012	LDA	O1-N1	-17.32	1.23	1.39
10	M	1014	LDA	O1-N1	-17.26	1.23	1.39
10	M	1013	LDA	O1-N1	-16.79	1.23	1.39
10	S	2013	LDA	O1-N1	-16.59	1.23	1.39

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	S	2012	LDA	CM2-N1-CM1	-11.49	95.87	108.83
10	S	2013	LDA	CM2-N1-CM1	-11.30	96.08	108.83
10	M	1012	LDA	CM2-N1-CM1	-11.27	96.11	108.83
10	M	1013	LDA	CM2-N1-CM1	-10.85	96.59	108.83
10	S	2014	LDA	CM2-N1-CM1	-10.43	97.06	108.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	1001	BCL	4	0
7	L	1002	BCL	9	0
7	L	1004	BCL	7	0
8	L	1006	BPH	5	0
9	L	1009	U10	2	0
7	M	1003	BCL	8	0
8	M	1005	BPH	5	0
9	M	1008	U10	2	0
10	M	1012	LDA	1	0
10	M	1013	LDA	1	0
10	M	1014	LDA	5	0
7	R	2001	BCL	3	0
7	R	2002	BCL	9	0
7	R	2004	BCL	6	0
8	R	2006	BPH	14	0
9	R	2009	U10	3	0
7	S	2003	BCL	6	0
8	S	2005	BPH	4	0
9	S	2008	U10	2	0
10	S	2012	LDA	2	0
10	S	2013	LDA	1	0
10	S	2014	LDA	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 (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.