



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:30 PM GMT

PDB ID : 1PCR
Title : STRUCTURE OF THE PHOTOSYNTHETIC REACTION CENTRE FROM
RHODOBACTER SPHAEROIDES AT 2.65 ANGSTROMS RESOLUTION:
COFACTORS AND PROTEIN-COFACTOR INTERACTIONS
Authors : Ermler, U.; Fritzsche, G.; Michel, H.
Deposited on : 1994-11-10
Resolution : 2.65 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

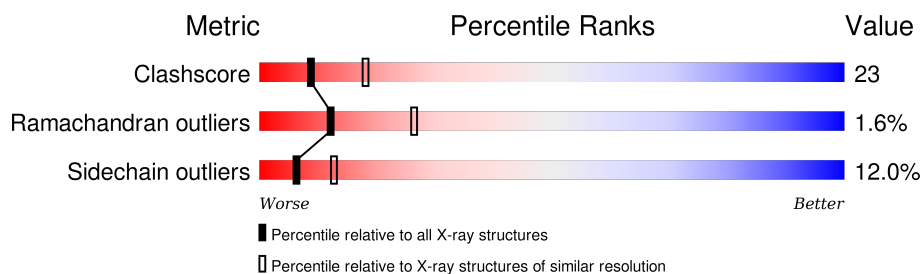
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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	
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
6	BCL	L	301	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCL	L	304	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7311 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	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2408	1607	394	397	10			

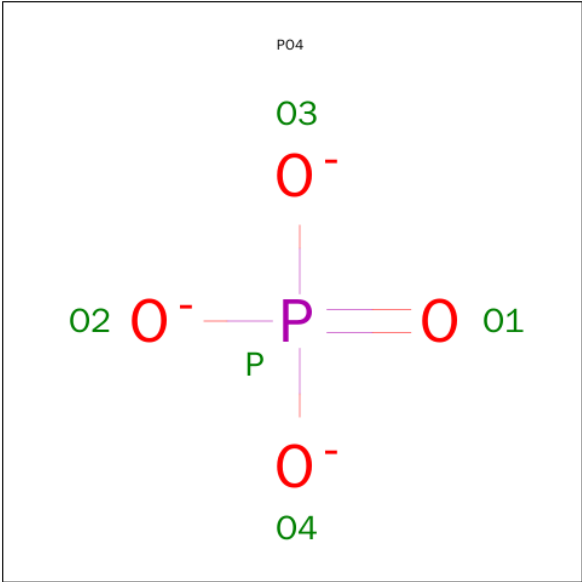
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	240	Total	C	N	O	S	0	0	0
			1829	1169	314	337	9			

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

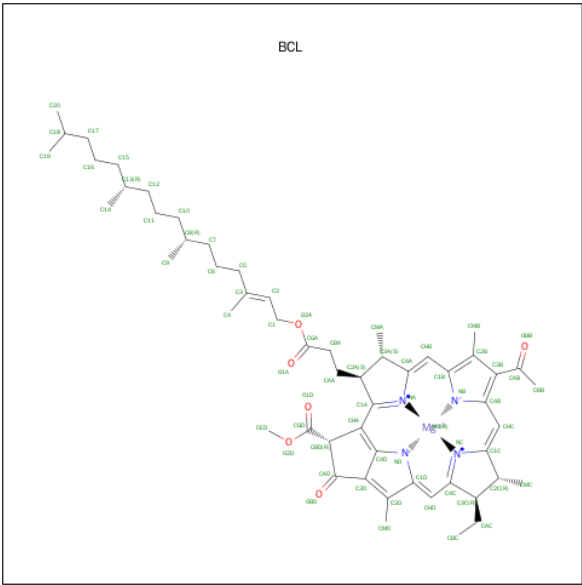
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



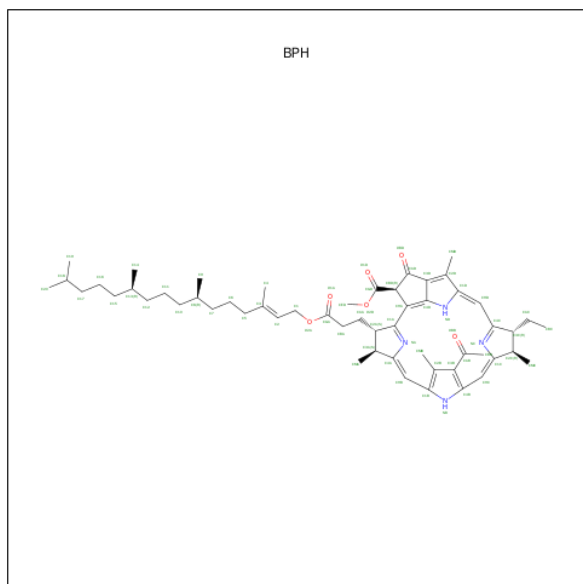
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

Continued on next page...

Continued from previous page...

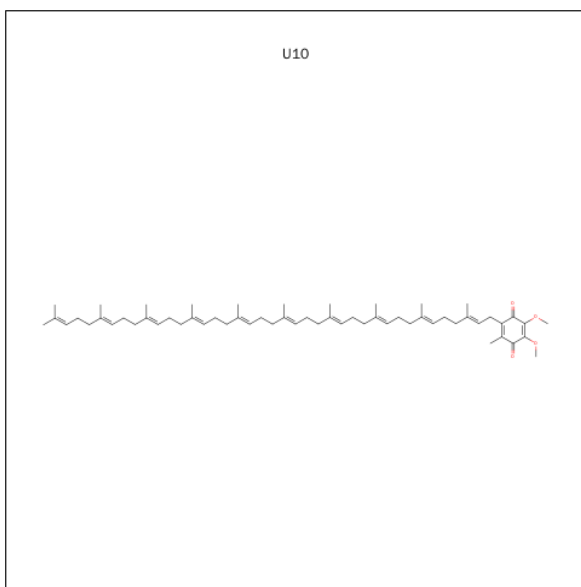
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



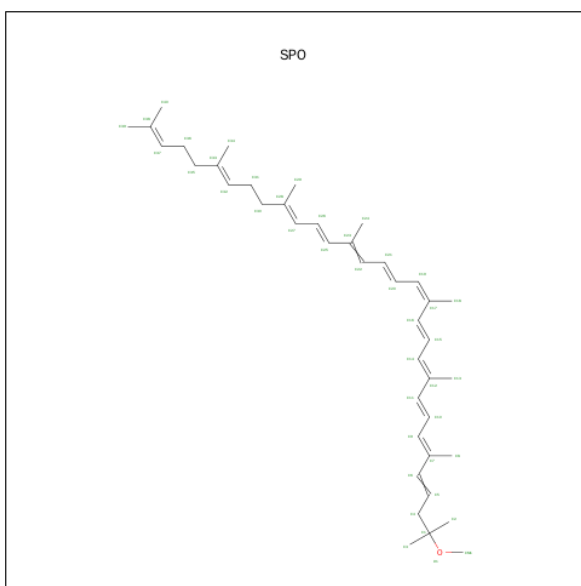
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			48	44	4		
8	L	1	Total	C	O	0	0
			48	44	4		

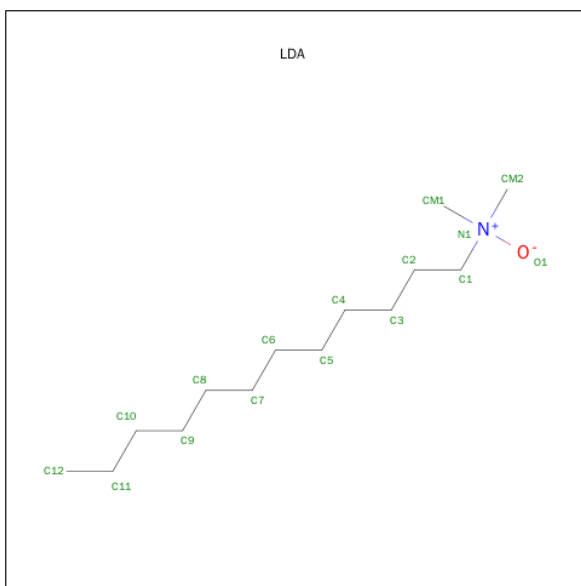
- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	M	1	Total	C	N	O	0	0
			16	14	1	1		
10	L	1	Total	C	N	O	0	0
			16	14	1	1		
10	L	1	Total	C	N	O	0	0
			16	14	1	1		
10	L	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	70	Total	O	0	0
			70	70		
11	L	40	Total	O	0	0
			40	40		

Continued on next page...

Continued from previous page...

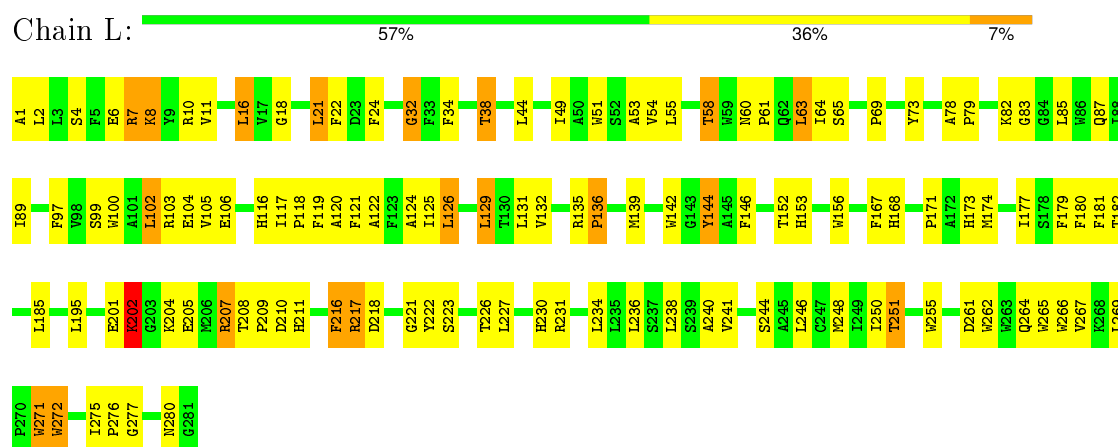
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	M	50	Total	O	0	0
			50	50		

3 Residue-property plots

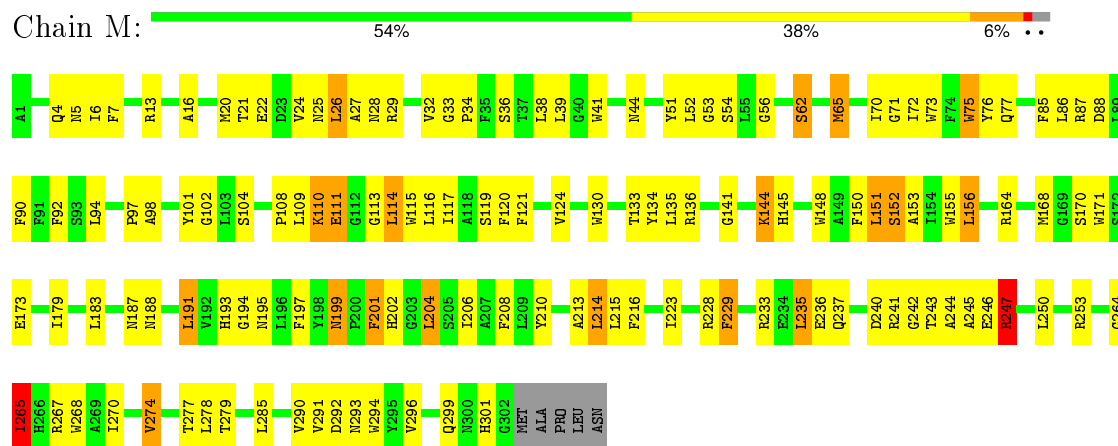
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

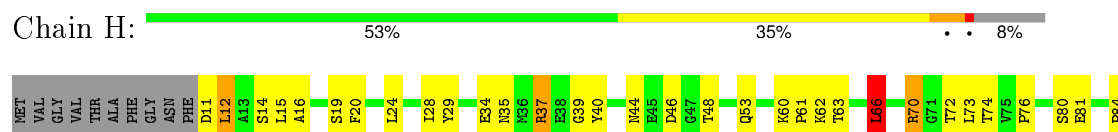
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



I85	I86	I87	H98	D103	K106	P111	V115	A116	R117	R118	D119	L120	P121	D124	M129	K130	I131	K132	P133	M134	K135	F140	H141	V142	N147	P148	L151	P152	C156	I160	V165	D166	I167	H168	V169	D170	I171	A176	A177	V181	H182	L183	K184	D185							
T188	R189	I190	L191	P192	M193	V196	K197	V198	Q199	S200	N201	R202	V203	H204	V205	N206	S209	L212	I219	K220	S221	P222	T223	E224	V225	T226	E229	E230	D231	K232	L233	V237	L241	A245	P246	K247	R248	K249	S250	VAL	VAL	ALA	ALA	ALA	ALA	MET	LEU	ALA	GLU	TYR	ALA

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.30 Å 141.30 Å 187.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	88.9 (10.00-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7311	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, LDA, BPH, PO4, FE, SPO, 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	0.64	0/2320	0.71	0/3175
2	M	0.61	0/2500	0.69	1/3413 (0.0%)
3	H	0.63	0/1877	0.74	0/2553
All	All	0.63	0/6697	0.71	1/9141 (0.0%)

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	6
2	M	0	4
3	H	0	4
All	All	0	14

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	M	156	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	103	ARG	Sidechain
1	L	144	TYR	Sidechain
1	L	167	PHE	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	L	32	GLY	Peptide
1	L	73	TYR	Sidechain

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	105	0
2	M	2408	0	2321	142	0
3	H	1829	0	1836	73	0
4	M	1	0	0	0	0
5	M	5	0	0	0	0
6	L	198	0	222	21	0
6	M	66	0	74	14	0
7	L	65	0	76	12	0
7	M	65	0	76	8	0
8	L	48	0	63	8	0
8	M	48	0	63	8	0
9	M	42	0	60	7	0
10	L	48	0	93	2	0
10	M	96	0	186	25	0
11	H	70	0	0	7	0
11	L	40	0	0	2	0
11	M	50	0	0	3	0
All	All	7311	0	7257	338	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 23.

The worst 5 of 338 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)
6:M:801:BCL:HBB3	6:M:801:BCL:HHC	1.35	1.09
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.39	1.01
2:M:119:SER:HB2	9:M:600:SPO:H342	1.47	0.93
3:H:44:ASN:HD22	3:H:48:THR:HB	1.36	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.54	0.88

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%)	261 (94%)	15 (5%)	3 (1%)	17	38
2	M	300/307 (98%)	278 (93%)	18 (6%)	4 (1%)	15	33
3	H	238/260 (92%)	215 (90%)	17 (7%)	6 (2%)	7	15
All	All	817/848 (96%)	754 (92%)	50 (6%)	13 (2%)	12	26

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	202	LYS
2	M	54	SER
3	H	116	ALA
1	L	207	ARG
3	H	124	ASP

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%)	196 (89%)	24 (11%)	8	16
2	M	236/240 (98%)	206 (87%)	30 (13%)	5	11
3	H	195/208 (94%)	171 (88%)	24 (12%)	6	12
All	All	651/668 (98%)	573 (88%)	78 (12%)	6	13

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	151	LEU
2	M	215	LEU
3	H	221	SER
2	M	152	SER
2	M	191	LEU

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

Mol	Chain	Res	Type
2	M	77	GLN
2	M	193	HIS
3	H	44	ASN
2	M	44	ASN
2	M	301	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 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 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	301	2	53,74,74	1.25	4 (7%)	57,115,115	1.89	9 (15%)
6	BCL	L	302	1,6	53,74,74	1.37	7 (13%)	57,115,115	1.88	10 (17%)
6	BCL	L	304	1	53,74,74	1.17	5 (9%)	57,115,115	2.62	12 (21%)
7	BPH	L	402	-	64,70,70	1.18	5 (7%)	73,101,101	1.71	8 (10%)
8	U10	L	502	-	48,48,63	2.24	21 (43%)	58,61,79	1.05	4 (6%)
10	LDA	L	707	-	15,15,15	4.40	2 (13%)	16,17,17	0.58	0
10	LDA	L	708	-	15,15,15	4.13	1 (6%)	16,17,17	0.61	0
10	LDA	L	709	-	15,15,15	4.62	2 (13%)	16,17,17	0.59	0
7	BPH	M	401	-	64,70,70	1.25	8 (12%)	73,101,101	1.84	11 (15%)
8	U10	M	501	-	48,48,63	2.61	21 (43%)	58,61,79	1.40	10 (17%)
9	SPO	M	600	-	40,41,41	3.40	22 (55%)	45,50,50	2.11	14 (31%)
10	LDA	M	701	-	15,15,15	4.89	2 (13%)	16,17,17	0.52	0
10	LDA	M	702	-	15,15,15	4.85	1 (6%)	16,17,17	1.04	1 (6%)
10	LDA	M	703	-	15,15,15	4.78	4 (26%)	16,17,17	0.85	0
10	LDA	M	704	-	15,15,15	3.75	1 (6%)	16,17,17	0.60	0
10	LDA	M	705	-	15,15,15	4.28	4 (26%)	16,17,17	0.57	0
10	LDA	M	706	-	15,15,15	4.52	2 (13%)	16,17,17	0.61	0
5	PO4	M	800	-	4,4,4	1.33	0	6,6,6	0.31	0
6	BCL	M	801	2,6	53,74,74	0.96	3 (5%)	57,115,115	1.76	8 (14%)

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	301	2	2/2/21/25	0/37/137/137	0/0/9/9
6	BCL	L	302	1,6	-	0/37/137/137	0/0/9/9
6	BCL	L	304	1	1/1/21/25	0/37/137/137	0/0/9/9
7	BPH	L	402	-	-	0/54/105/105	0/1/6/6
8	U10	L	502	-	-	0/45/69/87	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LDA	L	707	-	-	0/13/13/13	0/0/0/0
10	LDA	L	708	-	-	0/13/13/13	0/0/0/0
10	LDA	L	709	-	-	0/13/13/13	0/0/0/0
7	BPH	M	401	-	-	0/54/105/105	0/1/6/6
8	U10	M	501	-	-	0/45/69/87	0/1/1/1
9	SPO	M	600	-	-	0/47/47/47	0/0/0/0
10	LDA	M	701	-	-	0/13/13/13	0/0/0/0
10	LDA	M	702	-	-	0/13/13/13	0/0/0/0
10	LDA	M	703	-	-	0/13/13/13	0/0/0/0
10	LDA	M	704	-	-	0/13/13/13	0/0/0/0
10	LDA	M	705	-	-	0/13/13/13	0/0/0/0
10	LDA	M	706	-	-	0/13/13/13	0/0/0/0
5	PO4	M	800	-	-	0/0/0/0	0/0/0/0
6	BCL	M	801	2,6	-	0/37/137/137	0/0/9/9

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-18.73	1.21	1.39
10	M	702	LDA	O1-N1	-18.56	1.21	1.39
10	M	703	LDA	O1-N1	-17.68	1.22	1.39
10	L	709	LDA	O1-N1	-17.65	1.22	1.39
10	M	706	LDA	O1-N1	-17.22	1.23	1.39

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	BCL	CBB-CAB-C3B	-8.17	96.08	120.33
6	L	304	BCL	O1D-CGD-CBD	-7.96	113.22	124.62
7	M	401	BPH	O1D-CGD-CBD	-7.18	114.34	124.62
6	L	301	BCL	O1D-CGD-CBD	-6.74	114.96	124.62
7	L	402	BPH	O1D-CGD-CBD	-6.71	115.00	124.62

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	301	BCL	C8
6	L	301	BCL	C13
6	L	304	BCL	C13

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	301	BCL	9	0
6	L	302	BCL	10	0
6	L	304	BCL	5	0
7	L	402	BPH	12	0
8	L	502	U10	8	0
10	L	707	LDA	1	0
10	L	708	LDA	1	0
7	M	401	BPH	8	0
8	M	501	U10	8	0
9	M	600	SPO	7	0
10	M	701	LDA	4	0
10	M	702	LDA	6	0
10	M	703	LDA	8	0
10	M	705	LDA	4	0
10	M	706	LDA	5	0
6	M	801	BCL	14	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.