



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:56 PM GMT

PDB ID : 1MPS
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH PHE M 197 REPLACED WITH ARG AND TYR M 177 REPLACED WITH PHE (CHAIN M, Y177F, F197R)
Authors : Mcauley-Hecht, K.E.; Fyfe, P.K.; Ridge, J.P.; Prince, S.; Hunter, C.N.; Isaacs, N.W.; Cogdell, R.J.; Jones, M.R.
Deposited on : 1998-03-09
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

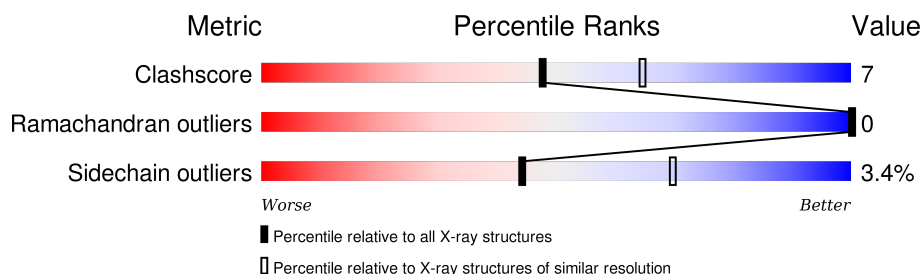
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)

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 $\leq 5\%$. 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	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCL	M	802	X	-	-	-
7	BPH	L	401	X	-	-	-
7	BPH	L	402	X	-	-	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7155 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
			2407	1604	397	396	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	177	PHE	TYR	ENGINEERED MUTATION	UNP P02953
M	197	ARG	PHE	ENGINEERED MUTATION	UNP P02953

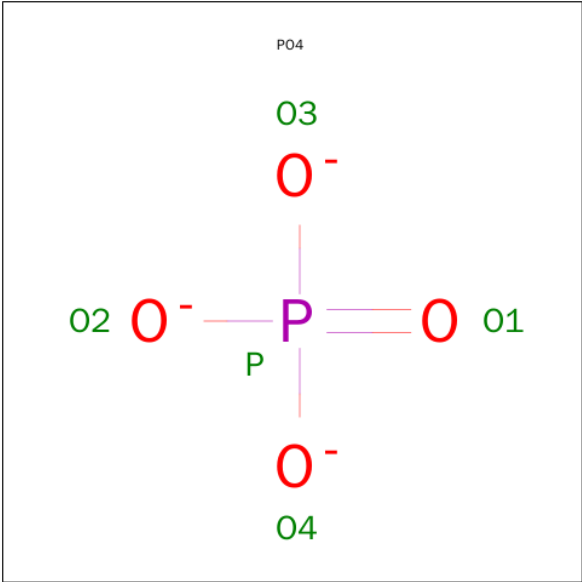
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

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 (II) ION (three-letter code: FE2) (formula: Fe).

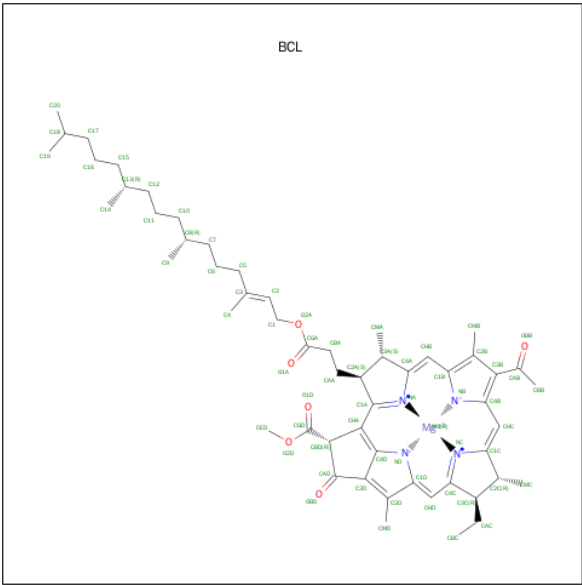
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- 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).



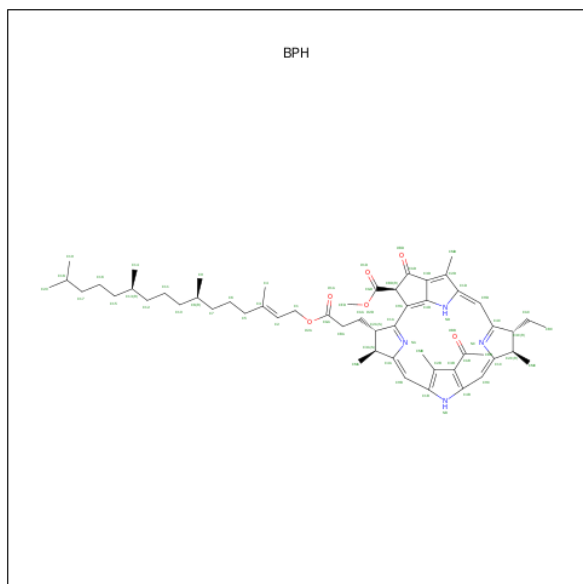
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	M	1	Total	C	Mg	N	O	17	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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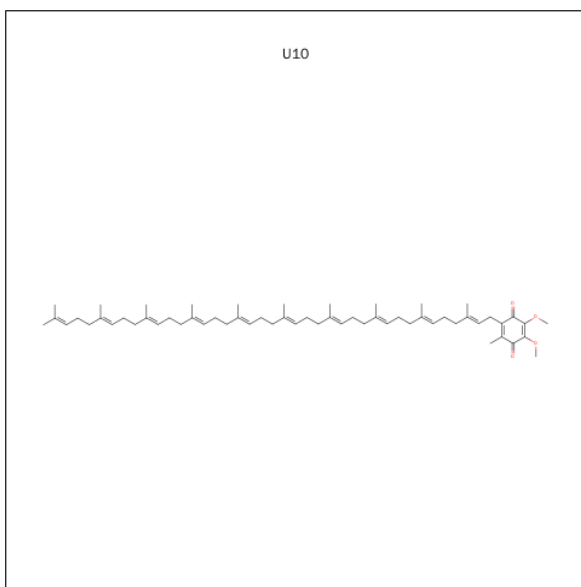
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



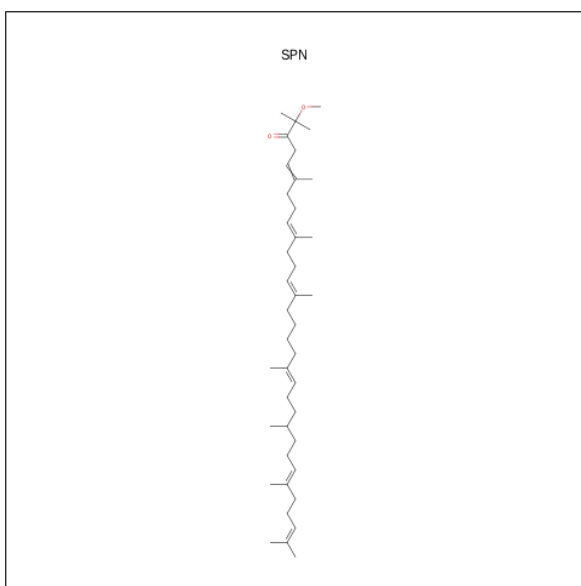
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	N	O	17	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- 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	48	0
			48	44	4		

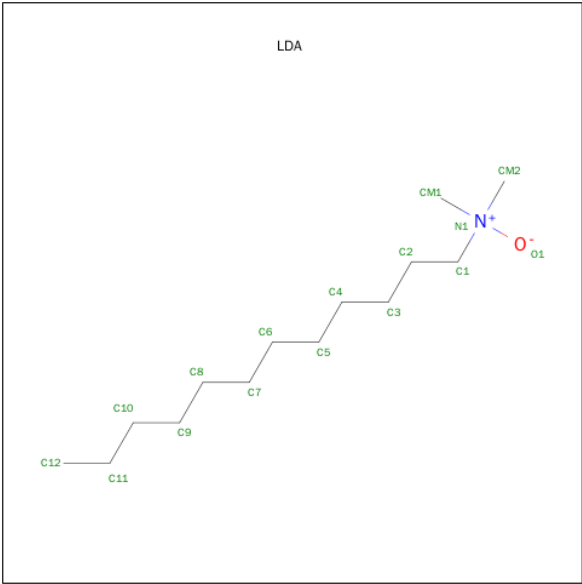
- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	11	0
			43	41	2		

- 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		

- Molecule 11 is water.

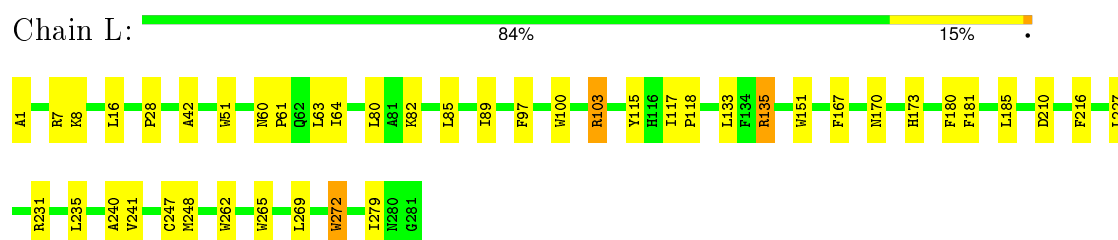
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	37	Total	O	0	0
			37	37		
11	L	28	Total	O	0	0
			28	28		
11	M	35	Total	O	0	0
			35	35		

3 Residue-property plots [i](#)

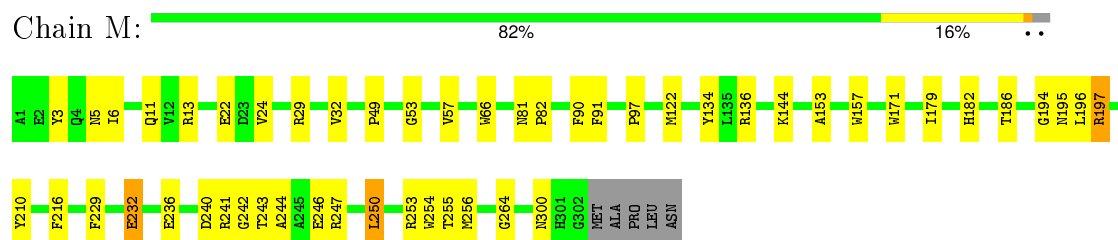
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

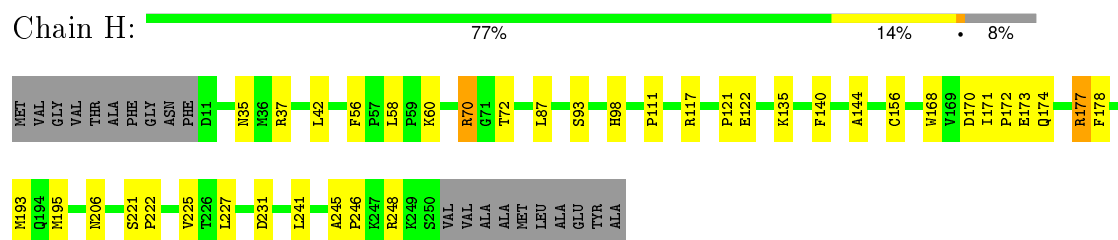
• Molecule 1: PHOTOSYNTHETIC REACTION CENTER



• Molecule 2: PHOTOSYNTHETIC REACTION CENTER



• Molecule 3: PHOTOSYNTHETIC REACTION CENTER



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	141.90 Å 141.90 Å 187.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	11.00 – 2.55	Depositor
% Data completeness (in resolution range)	76.5 (11.00-2.55)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.194 , 0.217	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7155	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, LDA, BPH, PO4, FE2, SPN, 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	0.41	0/2320	0.56	0/3175
2	M	0.40	0/2498	0.53	0/3409
3	H	0.37	0/1877	0.64	2/2553 (0.1%)
All	All	0.40	0/6695	0.57	2/9137 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	195	MET	CG-SD-CE	5.78	109.44	100.20
3	H	193	MET	CG-SD-CE	5.30	108.69	100.20

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	34	0
2	M	2407	0	2325	42	0
3	H	1829	0	1836	26	0
4	M	1	0	0	0	0
5	M	5	0	0	0	0
6	L	132	0	148	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	132	0	148	8	0
7	L	130	0	152	15	0
8	L	48	0	63	0	0
8	M	48	0	63	3	0
9	M	43	0	69	1	0
10	M	48	0	93	2	0
11	H	37	0	0	3	0
11	L	28	0	0	1	0
11	M	35	0	0	1	0
All	All	7155	0	7084	103	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 7.

All (103) 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)
1:L:241:VAL:HG21	7:L:402:BPH:HAC2	1.61	0.83
7:L:402:BPH:HHC	7:L:402:BPH:HBB3	1.65	0.78
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.68	0.76
7:L:401:BPH:HHC	7:L:401:BPH:HBB3	1.67	0.76
2:M:253:ARG:HD3	11:M:829:HOH:O	1.88	0.73
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.23	0.69
7:L:401:BPH:HAC1	2:M:153:ALA:HB2	1.76	0.68
1:L:103:ARG:HG2	11:L:507:HOH:O	2.01	0.60
7:L:402:BPH:CHC	7:L:402:BPH:HBB3	2.31	0.59
1:L:151:TRP:HE3	2:M:197:ARG:HH21	1.50	0.59
7:L:402:BPH:HBB2	2:M:210:TYR:HB3	1.83	0.58
1:L:181:PHE:CD2	7:L:401:BPH:HBB1	2.39	0.58
1:L:167:PHE:HB3	6:L:302:BCL:HMC3	1.85	0.58
1:L:135:ARG:HD3	1:L:248:MET:O	2.04	0.58
1:L:115:TYR:O	1:L:118:PRO:HD2	2.04	0.57
6:L:302:BCL:HMB1	6:L:302:BCL:CBB	2.35	0.56
3:H:170:ASP:HB2	3:H:177:ARG:HD2	1.87	0.56
1:L:8:LYS:HA	3:H:87:LEU:HD11	1.87	0.56
6:M:802:BCL:HBB3	6:M:802:BCL:HMB1	1.87	0.55
7:L:402:BPH:CBB	2:M:210:TYR:HB3	2.36	0.55
2:M:13:ARG:O	3:H:140:PHE:HA	2.07	0.55
2:M:240:ASP:O	3:H:117:ARG:NH1	2.40	0.54
1:L:97:PHE:CE1	6:L:302:BCL:H121	2.43	0.54
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:70:ARG:NH2	3:H:121:PRO:O	2.42	0.53
6:M:801:BCL:CBB	6:M:801:BCL:HMB1	2.38	0.53
2:M:243:THR:OG1	2:M:247:ARG:HD2	2.09	0.53
2:M:53:GLY:O	2:M:57:VAL:HG23	2.08	0.53
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.91	0.52
3:H:177:ARG:NH1	11:H:295:HOH:O	2.40	0.52
8:M:501:U10:H202	10:M:701:LDA:H121	1.91	0.52
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.10	0.52
1:L:42:ALA:HA	7:L:402:BPH:H9C3	1.91	0.52
1:L:1:ALA:HB1	3:H:42:LEU:HB3	1.92	0.52
6:M:802:BCL:HMB1	6:M:802:BCL:CBB	2.40	0.51
3:H:241:LEU:HB2	11:H:296:HOH:O	2.10	0.51
6:L:304:BCL:OBB	6:L:304:BCL:HHC	2.11	0.50
2:M:194:GLY:O	2:M:195:ASN:HB3	2.10	0.50
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.93	0.50
6:L:304:BCL:CBB	6:L:304:BCL:HMB1	2.41	0.50
7:L:401:BPH:CHC	7:L:401:BPH:HBB3	2.41	0.49
2:M:24:VAL:HG11	2:M:29:ARG:NH2	2.27	0.49
2:M:24:VAL:HG11	2:M:29:ARG:HH21	1.77	0.48
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.95	0.48
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.94	0.48
1:L:180:PHE:CD2	1:L:240:ALA:HB1	2.48	0.47
1:L:100:TRP:HZ3	8:M:501:U10:H362	1.78	0.47
1:L:181:PHE:HB3	7:L:401:BPH:CBB	2.45	0.47
2:M:90:PHE:CD1	2:M:179:ILE:HD13	2.50	0.47
2:M:179:ILE:HG13	6:M:801:BCL:HED1	1.97	0.47
3:H:122:GLU:HB2	3:H:227:LEU:HD21	1.98	0.46
6:L:302:BCL:HHC	6:L:302:BCL:OBB	2.14	0.46
6:L:304:BCL:HMB1	6:L:304:BCL:HBB2	1.97	0.45
2:M:256:MET:CE	8:M:501:U10:H102	2.46	0.45
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.98	0.45
2:M:157:TRP:CE2	9:M:600:SPN:HM73	2.52	0.45
1:L:170:ASN:HB3	1:L:173:HIS:HB3	1.99	0.45
1:L:231:ARG:HD2	2:M:6:ILE:O	2.17	0.45
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.53	0.44
3:H:37:ARG:NH2	3:H:60:LYS:O	2.50	0.44
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.52	0.44
1:L:60:ASN:O	1:L:64:ILE:HG13	2.17	0.44
1:L:227:LEU:HD13	2:M:232:GLU:HG2	2.00	0.44
6:L:304:BCL:HMD2	6:M:802:BCL:HBB3	2.00	0.43
2:M:247:ARG:NH2	3:H:111:PRO:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.36	0.43
10:M:701:LDA:H52	3:H:56:PHE:CE2	2.53	0.43
1:L:28:PRO:HB2	2:M:253:ARG:HG3	2.00	0.43
1:L:28:PRO:O	2:M:254:TRP:HA	2.18	0.43
6:M:801:BCL:HHC	6:M:801:BCL:OBB	2.19	0.43
6:M:801:BCL:HBB2	6:M:801:BCL:HMB1	2.00	0.43
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.54	0.43
2:M:136:ARG:HA	2:M:136:ARG:NE	2.34	0.42
6:L:302:BCL:HBB3	6:L:302:BCL:HMB1	2.00	0.42
1:L:82:LYS:HE2	1:L:82:LYS:HB3	1.86	0.42
7:L:402:BPH:H101	7:L:402:BPH:H142	2.00	0.42
1:L:103:ARG:NH2	2:M:255:THR:O	2.51	0.42
1:L:60:ASN:HB3	1:L:63:LEU:HD12	2.01	0.42
3:H:135:LYS:HB3	3:H:135:LYS:HE2	1.81	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.19	0.42
1:L:51:TRP:CH2	1:L:80:LEU:HD13	2.55	0.42
2:M:97:PRO:HG2	2:M:171:TRP:HB2	2.02	0.41
2:M:236:GLU:HB3	11:H:292:HOH:O	2.20	0.41
3:H:221:SER:HA	3:H:222:PRO:HD3	1.94	0.41
2:M:250:LEU:HD12	2:M:250:LEU:HA	1.90	0.41
3:H:58:LEU:HD12	3:H:58:LEU:HA	1.91	0.41
7:L:402:BPH:HBB1	2:M:210:TYR:CD2	2.56	0.41
7:L:402:BPH:HBC3	7:L:402:BPH:HHD	2.03	0.41
1:L:185:LEU:HD13	7:L:401:BPH:ND	2.36	0.41
2:M:186:THR:HG23	6:M:802:BCL:HMD2	2.03	0.41
2:M:81:ASN:HA	2:M:82:PRO:HD2	1.90	0.41
1:L:85:LEU:HD23	1:L:85:LEU:HA	1.96	0.41
1:L:85:LEU:O	1:L:89:ILE:HG13	2.21	0.41
2:M:196:LEU:HD23	2:M:196:LEU:HA	1.86	0.41
3:H:245:ALA:N	3:H:246:PRO:HD2	2.36	0.41
1:L:231:ARG:HD3	2:M:5:ASN:O	2.20	0.40
1:L:279:ILE:HG21	2:M:91:PHE:HB3	2.02	0.40
3:H:156:CYS:HB2	3:H:248:ARG:HG3	2.04	0.40
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.85	0.40
2:M:241:ARG:HD3	2:M:246:GLU:HG2	2.04	0.40
3:H:173:GLU:O	3:H:174:GLN:C	2.58	0.40
2:M:134:TYR:CE2	2:M:144:LYS:HG3	2.56	0.40
1:L:262:TRP:O	1:L:265:TRP:HD1	2.04	0.40

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%)	267 (96%)	12 (4%)	0	100	100
2	M	300/307 (98%)	288 (96%)	12 (4%)	0	100	100
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100
All	All	817/848 (96%)	784 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	211 (96%)	9 (4%)	37	61
2	M	236/240 (98%)	229 (97%)	7 (3%)	48	74
3	H	195/208 (94%)	189 (97%)	6 (3%)	47	73
All	All	651/668 (98%)	629 (97%)	22 (3%)	44	70

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	16	LEU
1	L	103	ARG
1	L	133	LEU
1	L	135	ARG
1	L	210	ASP

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Mol	Chain	Res	Type
1	L	216	PHE
1	L	235	LEU
1	L	247	CYS
1	L	272	TRP
2	M	22	GLU
2	M	182	HIS
2	M	197	ARG
2	M	216	PHE
2	M	232	GLU
2	M	250	LEU
2	M	300	ASN
3	H	70	ARG
3	H	72	THR
3	H	93	SER
3	H	177	ARG
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
1	L	159	ASN
1	L	183	ASN
1	L	264	GLN
2	M	299	GLN
2	M	300	ASN
3	H	98	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 14 ligands modelled in this entry, 1 is monoatomic - leaving 13 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	302	1	53,74,74	1.26	5 (9%)	57,115,115	1.79	11 (19%)
6	BCL	L	304	1	53,74,74	1.07	4 (7%)	57,115,115	2.04	9 (15%)
7	BPH	L	401	-	64,70,70	1.12	4 (6%)	73,101,101	1.88	11 (15%)
7	BPH	L	402	-	64,70,70	1.15	4 (6%)	73,101,101	1.76	10 (13%)
8	U10	L	502	-	48,48,63	1.90	12 (25%)	58,61,79	1.20	5 (8%)
8	U10	M	501	-	48,48,63	1.97	16 (33%)	58,61,79	1.04	5 (8%)
9	SPN	M	600	-	41,42,42	4.25	20 (48%)	41,52,52	2.50	20 (48%)
10	LDA	M	701	-	15,15,15	4.99	3 (20%)	16,17,17	0.71	0
10	LDA	M	702	-	15,15,15	4.11	4 (26%)	16,17,17	0.64	0
10	LDA	M	703	-	15,15,15	4.12	4 (26%)	16,17,17	0.59	0
5	PO4	M	800	-	4,4,4	1.35	0	6,6,6	0.28	0
6	BCL	M	801	2	53,74,74	1.24	4 (7%)	57,115,115	2.08	12 (21%)
6	BCL	M	802	2	53,74,74	1.21	4 (7%)	57,115,115	1.95	11 (19%)

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	302	1	1/1/21/25	0/37/137/137	0/0/9/9
6	BCL	L	304	1	-	0/37/137/137	0/0/9/9
7	BPH	L	401	-	2/2/18/22	0/54/105/105	0/1/6/6
7	BPH	L	402	-	1/1/18/22	0/54/105/105	0/1/6/6
8	U10	L	502	-	-	0/45/69/87	0/1/1/1
8	U10	M	501	-	-	0/45/69/87	0/1/1/1
9	SPN	M	600	-	-	0/50/51/51	0/0/0/0
10	LDA	M	701	-	-	0/13/13/13	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LDA	M	702	-	-	0/13/13/13	0/0/0/0
10	LDA	M	703	-	-	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	-	0/37/137/137	0/0/9/9
6	BCL	M	802	2	1/1/21/25	0/37/137/137	0/0/9/9

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-18.70	1.21	1.39
10	M	703	LDA	O1-N1	-15.52	1.24	1.39
10	M	702	LDA	O1-N1	-15.19	1.25	1.39
9	M	600	SPN	C3-C4	-7.34	1.39	1.50
9	M	600	SPN	C17-C18	-5.40	1.39	1.51
9	M	600	SPN	C14-C13	-5.37	1.39	1.51
9	M	600	SPN	C6-C5	-5.30	1.39	1.51
9	M	600	SPN	C10-C9	-4.95	1.40	1.51
9	M	600	SPN	C20-C19	-4.08	1.39	1.50
9	M	600	SPN	C11-C12	-4.08	1.39	1.50
6	M	801	BCL	O2D-CED	-4.04	1.35	1.45
6	M	802	BCL	O2D-CED	-3.96	1.35	1.45
9	M	600	SPN	C7-C8	-3.93	1.39	1.50
6	L	302	BCL	O2D-CED	-3.79	1.36	1.45
10	M	701	LDA	C1-N1	-3.68	1.44	1.51
8	M	501	U10	O3-C3M	-3.65	1.36	1.45
10	M	702	LDA	CM1-N1	-3.21	1.44	1.49
6	L	304	BCL	O2D-CED	-3.11	1.37	1.45
8	M	501	U10	O4-C4M	-3.00	1.38	1.45
10	M	701	LDA	CM1-N1	-2.92	1.45	1.49
8	L	502	U10	O4-C4M	-2.88	1.38	1.45
8	M	501	U10	C7-C8	-2.88	1.46	1.50
8	L	502	U10	C7-C8	-2.84	1.46	1.50
10	M	702	LDA	C1-N1	-2.66	1.46	1.51
8	M	501	U10	C27-C28	-2.59	1.43	1.50
7	L	401	BPH	O2D-CED	-2.46	1.39	1.45
9	M	600	SPN	C21-C22	-2.44	1.40	1.52
8	M	501	U10	C17-C18	-2.24	1.44	1.50
8	L	502	U10	O3-C3M	-2.22	1.39	1.45
10	M	703	LDA	C1-N1	-2.15	1.47	1.51
9	M	600	SPN	C16-C15	-2.10	1.39	1.51
10	M	703	LDA	CM2-N1	-2.08	1.46	1.49
7	L	402	BPH	O2D-CED	-2.07	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	703	LDA	CM1-N1	-2.04	1.46	1.49
10	M	702	LDA	CM2-N1	-2.03	1.46	1.49
8	M	501	U10	C30-C29	2.00	1.55	1.50
8	M	501	U10	C10-C9	2.08	1.55	1.50
6	L	302	BCL	C4-C3	2.13	1.55	1.50
9	M	600	SPN	CM4-C9	2.23	1.56	1.50
9	M	600	SPN	O1-C1	2.27	1.53	1.41
9	M	600	SPN	C29-C30	2.29	1.39	1.32
8	M	501	U10	C38-C39	2.37	1.39	1.32
8	L	502	U10	C38-C39	2.42	1.39	1.32
6	L	304	BCL	O2A-CGA	2.44	1.40	1.33
6	L	302	BCL	O2A-CGA	2.71	1.41	1.33
7	L	402	BPH	O2D-CGD	3.00	1.40	1.33
6	L	304	BCL	C2-C3	3.00	1.38	1.33
7	L	401	BPH	O2D-CGD	3.01	1.40	1.33
9	M	600	SPN	O1-CMA	3.18	1.53	1.43
6	L	302	BCL	C2-C3	3.24	1.39	1.33
8	M	501	U10	C18-C19	3.26	1.39	1.33
8	M	501	U10	O4-C4	3.28	1.45	1.37
8	M	501	U10	C13-C14	3.34	1.39	1.33
8	L	502	U10	C8-C9	3.38	1.39	1.33
8	L	502	U10	C33-C34	3.38	1.39	1.33
8	M	501	U10	C28-C29	3.41	1.39	1.33
6	M	801	BCL	C2-C3	3.41	1.39	1.33
9	M	600	SPN	C25-C26	3.42	1.39	1.33
8	L	502	U10	C23-C24	3.44	1.39	1.33
8	L	502	U10	C18-C19	3.44	1.39	1.33
8	M	501	U10	C23-C24	3.45	1.39	1.33
8	M	501	U10	C8-C9	3.45	1.39	1.33
6	M	802	BCL	O2D-CGD	3.46	1.42	1.33
7	L	401	BPH	O2A-CGA	3.46	1.43	1.33
8	L	502	U10	C28-C29	3.47	1.39	1.33
8	L	502	U10	C13-C14	3.47	1.39	1.33
6	M	802	BCL	C2-C3	3.48	1.39	1.33
8	L	502	U10	O4-C4	3.49	1.46	1.37
7	L	401	BPH	C2-C3	3.58	1.40	1.33
7	L	402	BPH	O2A-CGA	3.60	1.44	1.33
7	L	402	BPH	C2-C3	3.60	1.40	1.33
8	M	501	U10	O3-C3	3.63	1.46	1.37
6	M	801	BCL	O2D-CGD	3.66	1.42	1.33
8	M	501	U10	C33-C34	3.67	1.40	1.33
6	L	304	BCL	O2D-CGD	3.82	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	802	BCL	O2A-CGA	3.99	1.45	1.33
8	L	502	U10	O3-C3	4.13	1.47	1.37
6	M	801	BCL	O2A-CGA	4.27	1.46	1.33
6	L	302	BCL	O2D-CGD	4.90	1.45	1.33
9	M	600	SPN	C3-C2	6.02	1.59	1.52
9	M	600	SPN	C12-C13	10.15	1.52	1.33
9	M	600	SPN	C19-C18	10.19	1.53	1.33
9	M	600	SPN	C4-C5	10.42	1.53	1.33
9	M	600	SPN	C8-C9	10.51	1.53	1.33

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	401	BPH	O1D-CGD-CBD	-7.33	114.12	124.62
6	L	304	BCL	O1D-CGD-CBD	-6.87	114.78	124.62
7	L	402	BPH	O1D-CGD-CBD	-6.76	114.93	124.62
6	M	802	BCL	O1D-CGD-CBD	-6.58	115.19	124.62
6	M	801	BCL	O1D-CGD-CBD	-6.47	115.35	124.62
6	M	801	BCL	CMB-C2B-C1B	-4.64	120.69	128.36
6	L	302	BCL	O1D-CGD-CBD	-4.57	118.08	124.62
6	L	304	BCL	CMB-C2B-C1B	-3.60	122.41	128.36
6	L	302	BCL	CMB-C2B-C1B	-3.43	122.70	128.36
9	M	600	SPN	C11-C12-C13	-3.38	120.41	127.76
9	M	600	SPN	C3-C4-C5	-3.34	121.04	126.70
7	L	402	BPH	OBD-CAD-CBD	-3.12	121.23	125.94
9	M	600	SPN	C20-C19-C18	-3.09	121.04	127.76
6	M	802	BCL	CMB-C2B-C1B	-3.08	123.27	128.36
9	M	600	SPN	C7-C8-C9	-3.08	121.07	127.76
6	M	802	BCL	OBD-CAD-CBD	-3.08	121.29	125.94
7	L	401	BPH	OBD-CAD-CBD	-3.01	121.39	125.94
9	M	600	SPN	C17-C18-C19	-2.92	115.51	121.05
6	L	304	BCL	OBD-CAD-CBD	-2.92	121.54	125.94
6	L	302	BCL	OBD-CAD-CBD	-2.88	121.60	125.94
9	M	600	SPN	C10-C9-C8	-2.83	115.69	121.05
7	L	401	BPH	C3A-C4A-NA	-2.79	108.69	113.57
6	M	801	BCL	OBD-CAD-CBD	-2.79	121.73	125.94
9	M	600	SPN	C14-C13-C12	-2.77	115.81	121.05
9	M	600	SPN	C6-C5-C4	-2.63	116.06	121.05
6	M	801	BCL	C4-C3-C5	-2.51	111.57	115.41
7	L	401	BPH	CBB-CAB-C3B	-2.44	115.10	120.52
7	L	402	BPH	C3A-C4A-NA	-2.32	109.50	113.57
7	L	402	BPH	C4-C3-C5	-2.26	111.95	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	501	U10	C25-C24-C26	-2.26	111.96	115.41
7	L	402	BPH	O2A-CGA-O1A	-2.22	117.75	123.49
8	M	501	U10	C35-C34-C36	-2.20	112.05	115.41
7	L	401	BPH	C2A-C1A-NA	-2.18	109.29	112.08
6	M	802	BCL	CAC-C3C-C4C	-2.17	107.77	112.58
6	M	801	BCL	O2A-CGA-O1A	-2.17	117.89	123.49
8	M	501	U10	C20-C19-C21	-2.14	112.14	115.41
6	M	802	BCL	O2A-CGA-O1A	-2.11	118.04	123.49
6	L	302	BCL	CAC-C3C-C4C	-2.09	107.94	112.58
8	L	502	U10	C20-C19-C21	-2.08	112.24	115.41
7	L	402	BPH	CBB-CAB-C3B	-2.03	116.00	120.52
6	L	302	BCL	O2A-CGA-O1A	-2.01	118.30	123.49
7	L	402	BPH	OBb-CAB-C3B	2.00	124.17	120.31
7	L	402	BPH	C3A-C4A-CHB	2.02	125.58	121.84
6	M	802	BCL	OBb-CAB-C3B	2.08	123.30	120.00
6	M	802	BCL	CMB-C2B-C3B	2.10	129.19	125.09
9	M	600	SPN	C21-C20-C19	2.12	118.33	112.40
7	L	401	BPH	C3A-C4A-CHB	2.23	125.97	121.84
8	L	502	U10	C7-C6-C5	2.26	121.22	118.56
6	M	801	BCL	C2A-C1A-CHA	2.28	128.09	123.89
6	M	801	BCL	CMD-C2D-C3D	2.37	129.72	125.09
6	L	302	BCL	CMB-C2B-C3B	2.39	129.76	125.09
6	L	302	BCL	CED-O2D-CGD	2.40	121.62	115.99
8	M	501	U10	C7-C8-C9	2.41	130.78	126.70
6	M	802	BCL	CED-O2D-CGD	2.49	121.84	115.99
9	M	600	SPN	C10-C11-C12	2.51	118.26	111.69
6	L	304	BCL	CMB-C2B-C3B	2.52	130.02	125.09
7	L	401	BPH	CMD-C2D-C3D	2.53	130.03	125.09
9	M	600	SPN	C6-C7-C8	2.65	118.62	111.69
9	M	600	SPN	C7-C6-C5	2.69	121.46	112.71
9	M	600	SPN	C11-C10-C9	2.70	121.51	112.71
7	L	401	BPH	C4A-NA-C1A	2.77	110.69	108.21
8	L	502	U10	C7-C8-C9	2.87	131.57	126.70
7	L	401	BPH	O2A-CGA-CBA	2.88	120.67	111.90
8	L	502	U10	C4M-O4-C4	2.90	126.91	116.61
6	L	304	BCL	CMD-C2D-C3D	2.90	130.76	125.09
8	M	501	U10	C4M-O4-C4	2.92	126.99	116.61
6	L	302	BCL	C4A-NA-C1A	2.99	110.22	106.36
6	M	801	BCL	C4A-NA-C1A	3.02	110.27	106.36
6	L	304	BCL	O2A-CGA-CBA	3.06	121.22	111.90
6	L	304	BCL	C4A-NA-C1A	3.08	110.34	106.36
7	L	401	BPH	OBb-CAB-C3B	3.12	126.33	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	302	BCL	O2A-CGA-CBA	3.27	121.88	111.90
6	M	802	BCL	C4A-NA-C1A	3.30	110.62	106.36
6	M	801	BCL	CMB-C2B-C3B	3.31	131.57	125.09
8	L	502	U10	C3M-O3-C3	3.43	128.82	116.61
7	L	402	BPH	O2A-CGA-CBA	3.50	122.56	111.90
6	L	304	BCL	OBB-CAB-C3B	3.53	125.59	120.00
9	M	600	SPN	CM7-C22-C21	3.56	124.76	111.08
6	M	801	BCL	O2A-CGA-CBA	3.78	123.41	111.90
6	M	802	BCL	O2A-CGA-CBA	3.82	123.55	111.90
9	M	600	SPN	C15-C14-C13	4.19	121.69	112.48
9	M	600	SPN	C16-C17-C18	4.22	121.75	112.48
9	M	600	SPN	CM3-C5-C6	4.33	122.01	115.41
6	M	801	BCL	OBB-CAB-C3B	4.43	127.02	120.00
6	L	302	BCL	OBB-CAB-C3B	4.61	127.31	120.00
9	M	600	SPN	CM6-C18-C17	4.66	122.53	115.41
9	M	600	SPN	CM5-C13-C14	4.71	122.60	115.41
9	M	600	SPN	CM4-C9-C10	4.79	122.73	115.41
6	L	302	BCL	O2D-CGD-CBD	6.87	120.72	111.30
6	M	801	BCL	O2D-CGD-CBD	8.36	122.77	111.30
6	M	802	BCL	O2D-CGD-CBD	8.53	123.01	111.30
7	L	402	BPH	O2D-CGD-CBD	8.82	123.40	111.30
6	L	304	BCL	O2D-CGD-CBD	9.26	124.01	111.30
7	L	401	BPH	O2D-CGD-CBD	9.99	125.01	111.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	M	802	BCL	C13
7	L	402	BPH	C8
6	L	302	BCL	C13
7	L	401	BPH	C8
7	L	401	BPH	C13

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	302	BCL	5	0
6	L	304	BCL	4	0
7	L	401	BPH	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	402	BPH	9	0
8	M	501	U10	3	0
9	M	600	SPN	1	0
10	M	701	LDA	2	0
6	M	801	BCL	4	0
6	M	802	BCL	4	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.