



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:26 PM GMT

PDB ID : 1FNP  
Title : CRYSTAL STRUCTURE ANALYSIS OF THE MUTANT REACTION CENTER PRO L209-> PHE FROM THE PHOTOSYNTHETIC PURPLE BACTERIUM RHODOBACTER SPHAEROIDES  
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Deposited on : 2000-08-23  
Resolution : 2.60 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](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 (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

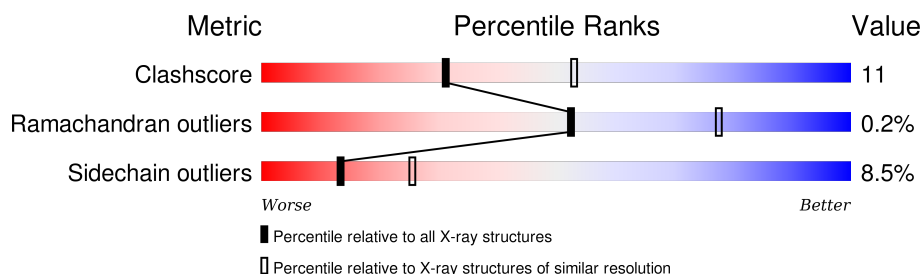
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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
6	BCL	L	304	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	BCL	M	801	X	-	-	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7256 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	C	N	O	S	0	0	0
			2236	1511	355	362	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	209	PHE	PRO	ENGINEERED	UNP P02954

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2399	1600	393	396	10			

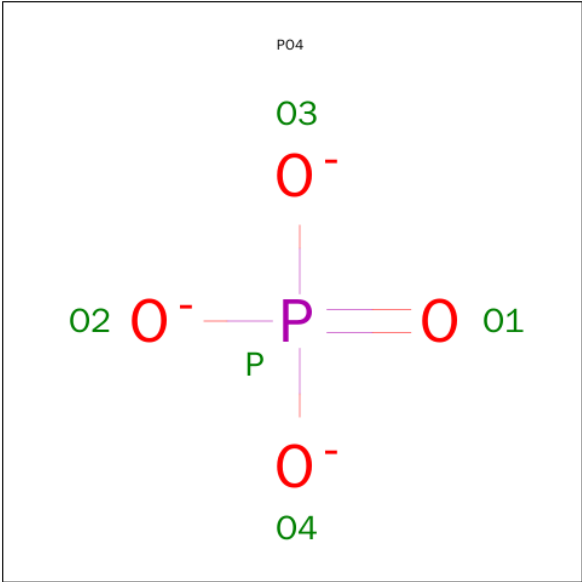
- Molecule 3 is a protein called REACTION CENTER PROTEIN H CHAIN.

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).

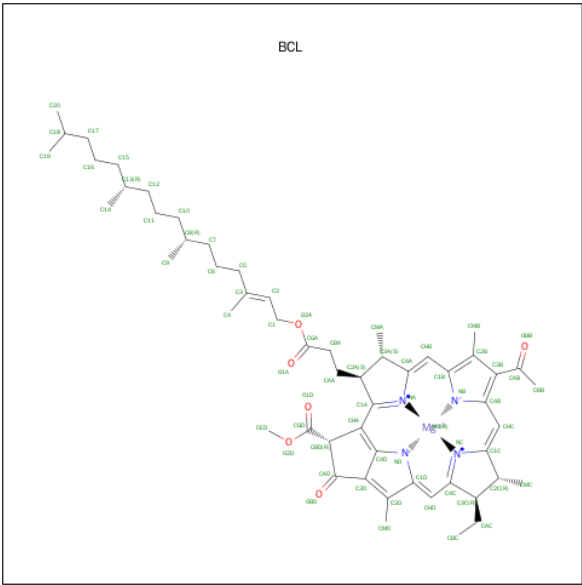
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	1	Total	Fe	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



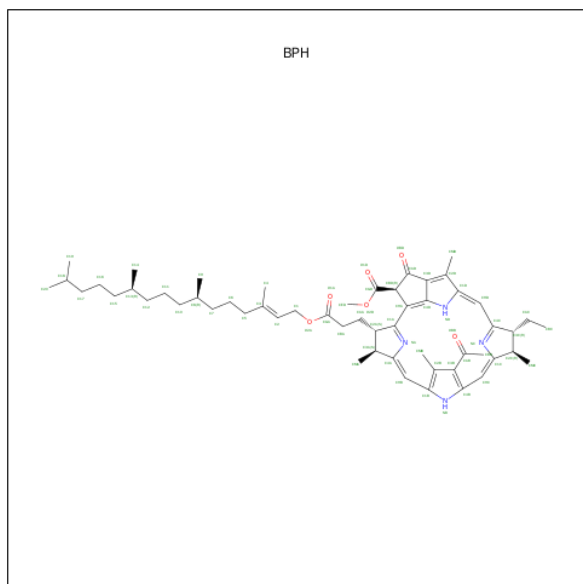
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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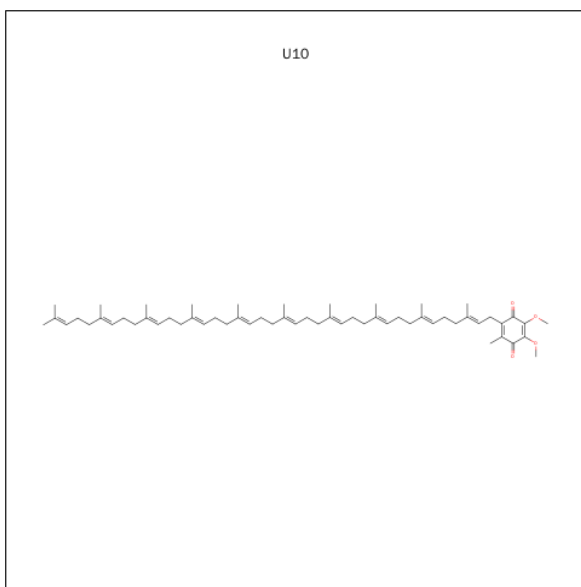
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



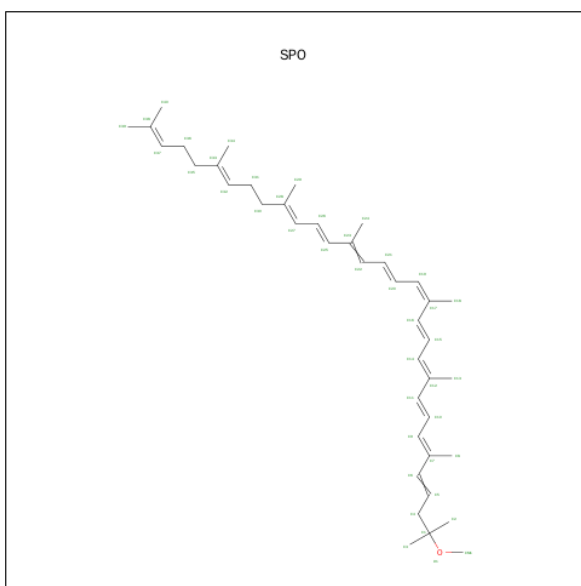
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- 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		

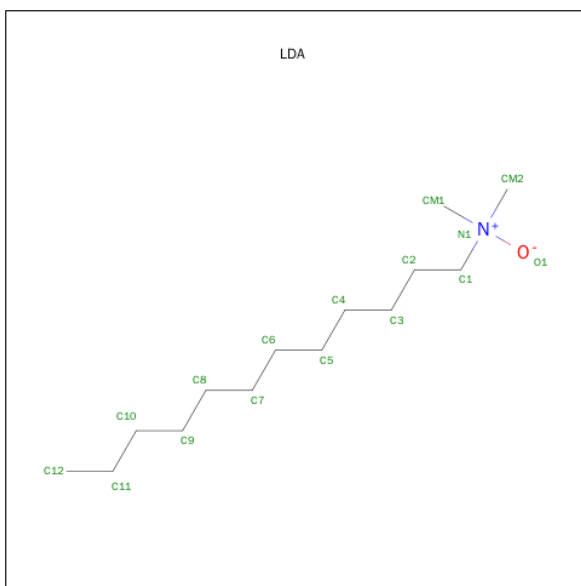
- Molecule 9 is SPHEROIDENE (three-letter code: SPO) (formula:  $C_{41}H_{60}O$ ).



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:

C<sub>14</sub>H<sub>31</sub>NO).



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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	H	65	Total O 65 65	0	0
11	L	38	Total O 38 38	0	0
11	M	39	Total O 39 39	0	0

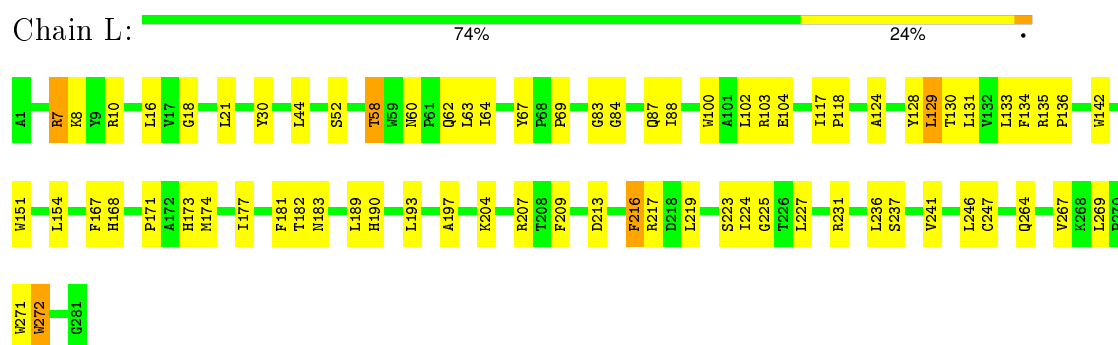


### 3 Residue-property plots

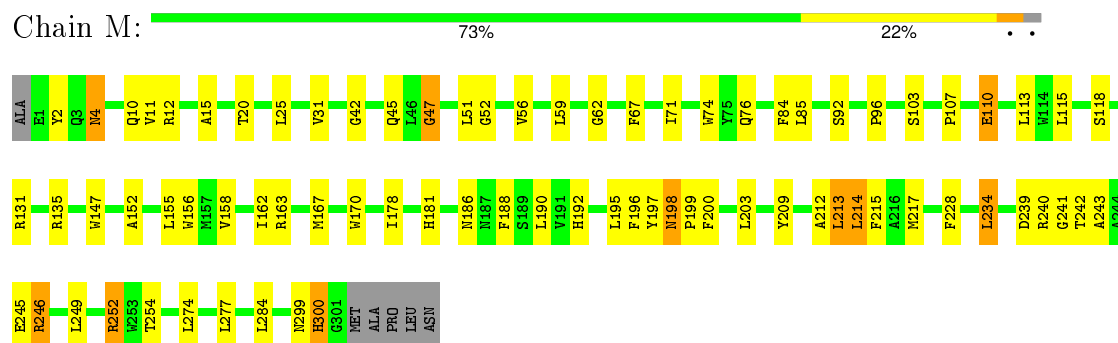
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

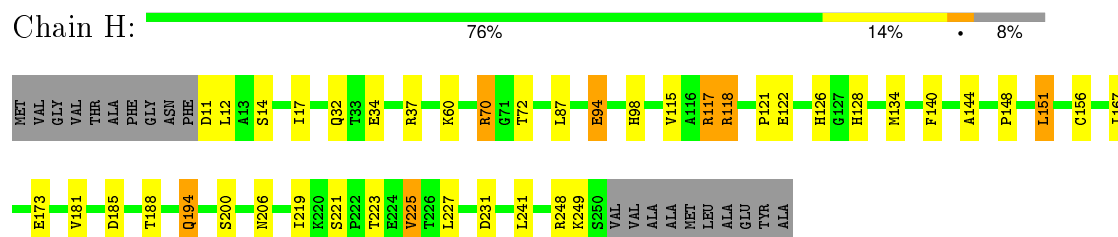
#### • Molecule 1: REACTION CENTER PROTEIN L CHAIN



#### • Molecule 2: REACTION CENTER PROTEIN M CHAIN



#### • Molecule 3: REACTION CENTER PROTEIN H CHAIN



## 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, $\alpha$ , $\beta$ , $\gamma$	141.75Å 141.75Å 187.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	92.2 (50.00-2.60)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.216 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	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	0.44	0/2324	0.48	0/3179
2	M	0.43	0/2491	0.49	1/3400 (0.0%)
3	H	0.42	0/1877	0.53	0/2553
All	All	0.43	0/6692	0.50	1/9132 (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	1
2	M	0	3
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	213	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	10	ARG	Sidechain
2	M	197	TYR	Sidechain
2	M	252	ARG	Sidechain
2	M	47	GLY	Peptide

## 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	2236	0	2189	53	0
2	M	2399	0	2306	59	0
3	H	1829	0	1836	34	0
4	M	1	0	0	0	0
5	M	5	0	0	1	0
6	L	132	0	148	12	0
6	M	132	0	148	12	0
7	L	65	0	76	8	0
7	M	65	0	76	11	0
8	L	48	0	63	8	0
8	M	48	0	63	2	0
9	M	42	0	60	1	0
10	H	32	0	62	2	0
10	L	16	0	31	0	0
10	M	64	0	124	1	0
11	H	65	0	0	4	0
11	L	38	0	0	6	0
11	M	39	0	0	0	0
All	All	7256	0	7182	154	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 11.

All (154) 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:L:304:BCL:HBB2	6:L:304:BCL:HHC	1.42	1.02
7:L:402:BPH:HHC	7:L:402:BPH:HBB3	1.48	0.95
6:M:801:BCL:HHC	6:M:801:BCL:HBB2	1.49	0.92
2:M:152:ALA:HB2	7:M:401:BPH:HAC1	1.54	0.90
3:H:194:GLN:H	3:H:194:GLN:HE21	1.21	0.85
6:L:302:BCL:HHC	6:L:302:BCL:CBB	2.10	0.82
11:L:731:HOH:O	2:M:217:MET:SD	2.39	0.81
11:L:706:HOH:O	2:M:252:ARG:HD3	1.82	0.79
6:M:802:BCL:HHC	6:M:802:BCL:CBB	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:802:BCL:HHC	6:M:802:BCL:HBB3	1.67	0.77
7:L:402:BPH:HBB2	2:M:209:TYR:HB3	1.68	0.76
6:M:801:BCL:HHC	6:M:801:BCL:CBB	2.17	0.73
2:M:214:LEU:HA	2:M:217:MET:HE2	1.69	0.73
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.71	0.72
2:M:196:PHE:CZ	6:M:802:BCL:HBB2	2.26	0.71
1:L:167:PHE:HB3	6:L:302:BCL:HMC3	1.72	0.71
2:M:45:GLN:HE21	2:M:47:GLY:HA3	1.56	0.71
1:L:241:VAL:HG21	7:L:402:BPH:HAC2	1.70	0.70
2:M:196:PHE:HZ	6:M:802:BCL:HBB2	1.56	0.69
6:L:304:BCL:CBB	6:L:304:BCL:HHC	2.20	0.68
6:M:801:BCL:HBB3	6:M:802:BCL:H41	1.76	0.66
1:L:30:TYR:O	1:L:103:ARG:NH2	2.29	0.66
1:L:209:PHE:CE2	3:H:173:GLU:HG3	2.30	0.66
6:L:302:BCL:HBB2	6:L:302:BCL:HHC	1.77	0.66
3:H:94:GLU:HG3	11:H:744:HOH:O	1.95	0.65
1:L:131:LEU:HD11	6:L:302:BCL:HED3	1.79	0.65
2:M:242:THR:O	2:M:246:ARG:HG2	1.96	0.65
1:L:190:HIS:HD1	8:L:502:U10:H4M1	1.62	0.64
1:L:168:HIS:NE2	6:L:302:BCL:HBB2	2.14	0.63
7:M:401:BPH:HHC	7:M:401:BPH:HBB3	1.80	0.62
3:H:148:PRO:O	3:H:151:LEU:HB2	1.99	0.62
2:M:118:SER:HB3	9:M:600:SPO:H311	1.82	0.62
1:L:197:ALA:HB1	2:M:234:LEU:HD21	1.82	0.61
1:L:7:ARG:HH21	3:H:98:HIS:CD2	2.18	0.61
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.82	0.60
7:L:402:BPH:CHC	7:L:402:BPH:HBB3	2.28	0.60
3:H:14:SER:HA	3:H:17:ILE:HG22	1.82	0.59
6:L:302:BCL:H52	6:L:304:BCL:HBB3	1.83	0.59
2:M:20:THR:HG23	2:M:25:LEU:HD21	1.84	0.58
3:H:37:ARG:NH1	3:H:60:LYS:O	2.35	0.58
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.86	0.58
2:M:241:GLY:CA	3:H:117:ARG:HD2	2.34	0.58
1:L:182:THR:HG22	1:L:236:LEU:HD13	1.86	0.58
2:M:198:ASN:HD22	2:M:198:ASN:C	2.06	0.58
6:L:302:BCL:HBB3	6:L:302:BCL:HHC	1.84	0.57
2:M:228:PHE:HB2	2:M:243:ALA:HB2	1.86	0.57
2:M:178:ILE:HG23	6:M:801:BCL:HED1	1.87	0.57
2:M:156:TRP:HB2	6:M:802:BCL:H62	1.85	0.57
1:L:103:ARG:HG3	11:L:711:HOH:O	2.04	0.57
1:L:171:PRO:HA	1:L:174:MET:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:501:U10:H202	10:H:702:LDA:H121	1.86	0.56
1:L:7:ARG:NH2	3:H:98:HIS:CD2	2.74	0.56
1:L:103:ARG:NH1	2:M:254:THR:O	2.39	0.56
3:H:173:GLU:HG2	11:H:750:HOH:O	2.05	0.56
2:M:242:THR:OG1	2:M:246:ARG:HD3	2.05	0.55
6:M:801:BCL:HBB3	6:M:802:BCL:C4	2.37	0.55
1:L:124:ALA:HB2	7:L:402:BPH:HAC1	1.89	0.54
1:L:62:GLN:HE21	1:L:151:TRP:HE1	1.53	0.54
2:M:10:GLN:HB2	3:H:144:ALA:HB3	1.90	0.53
5:M:800:PO4:O3	10:M:704:LDA:HM23	2.08	0.53
2:M:62:GLY:HA3	7:M:401:BPH:H6C1	1.91	0.53
2:M:239:ASP:O	3:H:117:ARG:NH2	2.42	0.53
1:L:181:PHE:CD2	7:M:401:BPH:HBB1	2.43	0.53
1:L:197:ALA:CB	2:M:234:LEU:HD21	2.39	0.52
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.91	0.52
3:H:206:ASN:HD21	3:H:248:ARG:HD2	1.74	0.52
2:M:147:TRP:HA	2:M:147:TRP:CE3	2.45	0.52
2:M:76:GLN:HE22	2:M:92:SER:H	1.58	0.51
3:H:70:ARG:NH1	3:H:121:PRO:O	2.42	0.51
2:M:107:PRO:HG2	2:M:110:GLU:HB2	1.92	0.51
3:H:34:GLU:O	3:H:37:ARG:HG3	2.11	0.51
2:M:84:PHE:HD2	2:M:85:LEU:HD12	1.76	0.50
3:H:32:GLN:NE2	10:H:702:LDA:H22	2.27	0.50
2:M:96:PRO:HG2	2:M:170:TRP:HB2	1.94	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.94	0.50
2:M:31:VAL:HG13	2:M:47:GLY:HA2	1.94	0.50
2:M:147:TRP:HA	2:M:147:TRP:HE3	1.77	0.50
1:L:69:PRO:HD3	1:L:83:GLY:O	2.12	0.49
7:L:402:BPH:HMC3	2:M:212:ALA:HB3	1.93	0.49
7:L:402:BPH:HMC3	2:M:212:ALA:CB	2.43	0.49
2:M:198:ASN:HD22	2:M:200:PHE:H	1.60	0.49
1:L:190:HIS:HA	8:L:502:U10:H4M1	1.95	0.49
1:L:231:ARG:HD3	2:M:4:ASN:O	2.13	0.49
1:L:227:LEU:O	1:L:231:ARG:HG3	2.13	0.48
2:M:241:GLY:HA2	3:H:117:ARG:HD2	1.94	0.48
2:M:198:ASN:ND2	2:M:200:PHE:H	2.11	0.48
2:M:2:TYR:CZ	2:M:4:ASN:HA	2.49	0.48
3:H:156:CYS:HB3	3:H:206:ASN:O	2.14	0.48
7:M:401:BPH:H4C1	7:M:401:BPH:H7C1	1.96	0.47
1:L:131:LEU:HD11	6:L:302:BCL:CED	2.44	0.47
3:H:219:ILE:HG21	3:H:225:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:223:SER:HA	8:L:502:U10:H1M2	1.96	0.47
2:M:214:LEU:HD23	2:M:217:MET:CE	2.45	0.47
2:M:234:LEU:HA	2:M:234:LEU:HD12	1.74	0.47
2:M:214:LEU:HD23	2:M:217:MET:HE3	1.96	0.47
1:L:181:PHE:HB3	7:M:401:BPH:CBB	2.44	0.46
7:L:402:BPH:HH3	7:L:402:BPH:CBB	2.30	0.46
1:L:129:LEU:O	1:L:133:LEU:HB3	2.15	0.46
2:M:240:ARG:HD3	2:M:245:GLU:HG2	1.99	0.45
1:L:87:GLN:NE2	1:L:142:TRP:CD1	2.85	0.45
1:L:18:GLY:O	1:L:21:LEU:HB2	2.16	0.45
2:M:45:GLN:HG2	2:M:47:GLY:H	1.82	0.45
2:M:158:VAL:HA	2:M:162:ILE:HB	1.97	0.45
2:M:15:ALA:HB1	2:M:31:VAL:HG21	1.99	0.45
3:H:121:PRO:HB3	3:H:225:VAL:O	2.16	0.45
3:H:70:ARG:HB3	3:H:118:ARG:HH12	1.80	0.45
8:L:502:U10:H121	8:L:502:U10:H101	1.53	0.44
1:L:104:GLU:HB3	1:L:118:PRO:HG3	1.99	0.44
3:H:241:LEU:HB2	11:H:707:HOH:O	2.17	0.44
1:L:130:THR:HA	1:L:134:PHE:HB2	1.99	0.44
3:H:117:ARG:NH1	3:H:227:LEU:HD22	2.33	0.44
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.53	0.44
3:H:134:MET:HB2	3:H:167:ILE:O	2.18	0.43
2:M:51:LEU:HD23	2:M:51:LEU:HA	1.85	0.43
3:H:194:GLN:HE21	3:H:194:GLN:N	2.03	0.43
2:M:62:GLY:CA	7:M:401:BPH:H6C1	2.48	0.43
1:L:60:ASN:O	1:L:64:ILE:HG13	2.17	0.43
1:L:225:GLY:H	8:L:502:U10:H3M2	1.84	0.43
3:H:122:GLU:HB2	3:H:227:LEU:HD21	2.00	0.43
1:L:183:ASN:ND2	1:L:237:SER:OG	2.51	0.43
1:L:58:THR:HG22	11:L:723:HOH:O	2.18	0.43
1:L:193:LEU:HD23	8:L:502:U10:H4M3	2.01	0.43
1:L:227:LEU:HD21	2:M:4:ASN:OD1	2.19	0.43
2:M:52:GLY:O	2:M:56:VAL:HG23	2.19	0.43
1:L:84:GLY:O	1:L:88:ILE:HG13	2.19	0.43
3:H:126:HIS:HB2	3:H:128:HIS:CD2	2.53	0.42
6:L:304:BCL:CHC	6:L:304:BCL:CBB	2.90	0.42
7:M:401:BPH:H6C2	7:M:401:BPH:H102	1.88	0.42
1:L:7:ARG:HH21	3:H:98:HIS:CG	2.38	0.42
2:M:163:ARG:O	2:M:167:MET:HG2	2.19	0.42
1:L:224:ILE:HG13	2:M:42:GLY:HA3	2.02	0.42
2:M:12:ARG:O	3:H:140:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:11:ASP:HA	11:H:745:HOH:O	2.20	0.42
1:L:128:TYR:HD1	6:L:304:BCL:HBB1	1.84	0.42
2:M:274:LEU:HD23	2:M:277:LEU:HD23	2.01	0.42
2:M:188:PHE:O	2:M:192:HIS:HD2	2.02	0.42
1:L:100:TRP:CZ2	8:M:501:U10:H251	2.55	0.41
1:L:189:LEU:HD13	1:L:216:PHE:HZ	1.84	0.41
2:M:113:LEU:HD23	2:M:113:LEU:HA	1.93	0.41
2:M:186:ASN:HA	6:M:802:BCL:HBC3	2.03	0.41
1:L:190:HIS:HD1	8:L:502:U10:C4M	2.32	0.41
7:M:401:BPH:H4C1	7:M:401:BPH:C7	2.48	0.41
2:M:4:ASN:ND2	3:H:194:GLN:HG3	2.35	0.41
2:M:198:ASN:HD22	2:M:199:PRO:N	2.19	0.41
3:H:181:VAL:O	3:H:188:THR:HA	2.21	0.41
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.04	0.41
2:M:67:PHE:O	2:M:71:ILE:HG12	2.21	0.41
8:L:502:U10:H72	8:L:502:U10:H1M1	1.68	0.40
1:L:269:LEU:HB2	1:L:272:TRP:NE1	2.37	0.40
6:M:801:BCL:O2A	7:M:401:BPH:HBB2	2.21	0.40
7:M:401:BPH:HBB3	7:M:401:BPH:CHC	2.50	0.40
1:L:217:ARG:HD2	11:L:724:HOH:O	2.20	0.40
1:L:219:LEU:HD12	2:M:131:ARG:NH2	2.36	0.40
1:L:67:TYR:HE1	11:L:722:HOH:O	2.04	0.40

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%)	269 (96%)	10 (4%)	0	100	100
2	M	299/307 (97%)	283 (95%)	14 (5%)	2 (1%)	26	51
3	H	238/260 (92%)	229 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	816/848 (96%)	781 (96%)	33 (4%)	2 (0%)	52	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	4	ASN
2	M	300	HIS

### 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%)	203 (92%)	17 (8%)	16	31
2	M	235/240 (98%)	213 (91%)	22 (9%)	11	20
3	H	195/208 (94%)	179 (92%)	16 (8%)	14	27
All	All	650/668 (97%)	595 (92%)	55 (8%)	13	25

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	ARG
1	L	16	LEU
1	L	44	LEU
1	L	52	SER
1	L	58	THR
1	L	63	LEU
1	L	102	LEU
1	L	129	LEU
1	L	154	LEU
1	L	204	LYS
1	L	207	ARG
1	L	213	ASP
1	L	216	PHE
1	L	246	LEU

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Mol	Chain	Res	Type
1	L	247	CYS
1	L	271	TRP
1	L	272	TRP
2	M	11	VAL
2	M	59	LEU
2	M	74	TRP
2	M	103	SER
2	M	110	GLU
2	M	115	LEU
2	M	135	ARG
2	M	155	LEU
2	M	181	HIS
2	M	190	LEU
2	M	195	LEU
2	M	198	ASN
2	M	203	LEU
2	M	213	LEU
2	M	214	LEU
2	M	215	PHE
2	M	234	LEU
2	M	246	ARG
2	M	249	LEU
2	M	284	LEU
2	M	299	ASN
2	M	300	HIS
3	H	12	LEU
3	H	70	ARG
3	H	72	THR
3	H	94	GLU
3	H	115	VAL
3	H	117	ARG
3	H	118	ARG
3	H	151	LEU
3	H	185	ASP
3	H	194	GLN
3	H	200	SER
3	H	221	SER
3	H	223	THR
3	H	225	VAL
3	H	231	ASP
3	H	249	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
1	L	159	ASN
1	L	173	HIS
1	L	183	ASN
2	M	24	ASN
2	M	43	ASN
2	M	45	GLN
2	M	76	GLN
2	M	192	HIS
2	M	198	ASN
3	H	98	HIS
3	H	128	HIS
3	H	194	GLN
3	H	206	ASN

### 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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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
10	LDA	H	702	-	15,15,15	4.67	2 (13%)	16,17,17	0.56	0
10	LDA	H	706	-	15,15,15	4.34	3 (20%)	16,17,17	0.67	0
6	BCL	L	302	1	53,74,74	1.20	5 (9%)	57,115,115	1.87	8 (14%)
6	BCL	L	304	1	53,74,74	1.43	4 (7%)	57,115,115	2.15	9 (15%)
7	BPH	L	402	-	64,70,70	1.14	4 (6%)	73,101,101	1.81	7 (9%)
8	U10	L	502	-	48,48,63	2.00	13 (27%)	58,61,79	1.32	6 (10%)
10	LDA	L	705	-	15,15,15	4.67	3 (20%)	16,17,17	0.61	0
7	BPH	M	401	-	64,70,70	1.20	4 (6%)	73,101,101	1.85	12 (16%)
8	U10	M	501	-	48,48,63	2.21	18 (37%)	58,61,79	1.07	4 (6%)
9	SPO	M	600	-	40,41,41	3.20	21 (52%)	45,50,50	2.05	12 (26%)
10	LDA	M	701	-	15,15,15	4.77	2 (13%)	16,17,17	0.41	0
10	LDA	M	703	-	15,15,15	4.77	4 (26%)	16,17,17	0.55	0
10	LDA	M	704	-	15,15,15	4.62	3 (20%)	16,17,17	0.76	1 (6%)
10	LDA	M	707	-	15,15,15	4.22	2 (13%)	16,17,17	0.58	0
5	PO4	M	800	-	4,4,4	1.38	0	6,6,6	0.30	0
6	BCL	M	801	2	53,74,74	1.17	4 (7%)	57,115,115	1.99	7 (12%)
6	BCL	M	802	2	53,74,74	1.18	5 (9%)	57,115,115	1.86	7 (12%)

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
10	LDA	H	702	-	-	0/13/13/13	0/0/0/0
10	LDA	H	706	-	-	0/13/13/13	0/0/0/0
6	BCL	L	302	1	-	1/37/137/137	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
10	LDA	L	705	-	-	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	703	-	-	0/13/13/13	0/0/0/0
10	LDA	M	704	-	-	0/13/13/13	0/0/0/0
10	LDA	M	707	-	-	0/13/13/13	0/0/0/0
5	PO4	M	800	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	M	801	2	1/1/21/25	0/37/137/137	0/0/9/9
6	BCL	M	802	2	-	0/37/137/137	0/0/9/9

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	701	LDA	O1-N1	-18.16	1.22	1.39
10	M	703	LDA	O1-N1	-17.61	1.22	1.39
10	H	702	LDA	O1-N1	-17.57	1.22	1.39
10	L	705	LDA	O1-N1	-17.48	1.22	1.39
10	M	704	LDA	O1-N1	-16.96	1.23	1.39
10	H	706	LDA	O1-N1	-16.29	1.24	1.39
10	M	707	LDA	O1-N1	-15.98	1.24	1.39
8	M	501	U10	C7-C8	-6.25	1.41	1.50
10	M	704	LDA	CM2-N1	-4.92	1.41	1.49
8	L	502	U10	C7-C8	-4.54	1.43	1.50
6	L	302	BCL	O2D-CED	-4.13	1.35	1.45
8	M	501	U10	C27-C28	-3.92	1.39	1.50
8	M	501	U10	O4-C4M	-3.63	1.36	1.45
8	M	501	U10	C22-C23	-3.63	1.40	1.50
10	M	703	LDA	CM1-N1	-3.52	1.44	1.49
10	H	702	LDA	C1-N1	-3.45	1.45	1.51
10	M	703	LDA	C1-N1	-3.39	1.45	1.51
7	M	401	BPH	O2D-CED	-3.34	1.37	1.45
10	L	705	LDA	CM2-N1	-3.12	1.44	1.49
6	M	801	BCL	O2D-CED	-3.03	1.37	1.45
9	M	600	SPO	C11-C12	-3.01	1.39	1.45
9	M	600	SPO	C25-C23	-2.99	1.39	1.45
6	M	802	BCL	O2D-CED	-2.90	1.38	1.45
7	L	402	BPH	O2D-CED	-2.82	1.38	1.45
10	H	706	LDA	CM1-N1	-2.79	1.45	1.49
8	M	501	U10	O3-C3M	-2.77	1.38	1.45
10	L	705	LDA	C1-N1	-2.75	1.46	1.51
9	M	600	SPO	C16-C17	-2.69	1.39	1.45
10	M	704	LDA	C1-N1	-2.61	1.46	1.51
10	M	703	LDA	CM2-N1	-2.61	1.45	1.49
8	M	501	U10	C17-C18	-2.58	1.43	1.50
9	M	600	SPO	C6-C7	-2.56	1.40	1.45
10	M	707	LDA	C1-N1	-2.41	1.47	1.51
6	L	302	BCL	C1-C2	-2.37	1.41	1.49
10	H	706	LDA	C1-N1	-2.34	1.47	1.51
6	L	304	BCL	C1-C2	-2.34	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	L	502	U10	O4-C4M	-2.33	1.39	1.45
10	M	701	LDA	CM2-N1	-2.25	1.46	1.49
8	L	502	U10	O3-C3M	-2.19	1.40	1.45
6	M	802	BCL	C1-C2	-2.09	1.42	1.49
8	M	501	U10	C12-C13	-2.06	1.44	1.50
8	L	502	U10	O2-C2	-2.05	1.18	1.23
8	M	501	U10	C37-C38	-2.01	1.44	1.50
8	M	501	U10	C30-C29	2.08	1.55	1.50
9	M	600	SPO	C8-C7	2.16	1.55	1.50
9	M	600	SPO	C22-C23	2.35	1.38	1.35
7	L	402	BPH	O2A-CGA	2.37	1.40	1.33
9	M	600	SPO	C15-C14	2.41	1.51	1.43
9	M	600	SPO	C26-C27	2.45	1.51	1.43
8	L	502	U10	C38-C39	2.46	1.39	1.32
8	M	501	U10	C38-C39	2.50	1.39	1.32
9	M	600	SPO	C37-C38	2.54	1.40	1.32
6	L	302	BCL	O2A-CGA	2.68	1.41	1.33
8	M	501	U10	C8-C9	2.85	1.38	1.33
8	M	501	U10	C28-C29	2.85	1.38	1.33
6	M	802	BCL	C2-C3	2.89	1.38	1.33
9	M	600	SPO	C10-C9	2.90	1.52	1.43
7	M	401	BPH	O2D-CGD	2.98	1.40	1.33
8	L	502	U10	O4-C4	2.98	1.44	1.37
9	M	600	SPO	C19-C17	2.98	1.39	1.35
8	M	501	U10	C23-C24	3.04	1.38	1.33
9	M	600	SPO	C14-C12	3.10	1.39	1.35
8	M	501	U10	O4-C4	3.15	1.45	1.37
6	L	304	BCL	C2-C3	3.15	1.39	1.33
8	M	501	U10	C18-C19	3.16	1.39	1.33
9	M	600	SPO	C9-C7	3.22	1.40	1.35
8	M	501	U10	C13-C14	3.26	1.39	1.33
6	M	802	BCL	O2A-CGA	3.26	1.43	1.33
6	M	801	BCL	C2-C3	3.26	1.39	1.33
8	L	502	U10	C8-C9	3.30	1.39	1.33
8	L	502	U10	C18-C19	3.33	1.39	1.33
6	L	302	BCL	C2-C3	3.34	1.39	1.33
9	M	600	SPO	C32-C33	3.38	1.39	1.33
7	L	402	BPH	C2-C3	3.47	1.39	1.33
7	M	401	BPH	C2-C3	3.48	1.39	1.33
9	M	600	SPO	O1-CM1	3.54	1.54	1.43
8	L	502	U10	C13-C14	3.55	1.39	1.33
8	L	502	U10	C28-C29	3.55	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	801	BCL	O2D-CGD	3.60	1.42	1.33
8	L	502	U10	C23-C24	3.63	1.40	1.33
8	L	502	U10	C33-C34	3.64	1.40	1.33
6	L	302	BCL	O2D-CGD	3.69	1.42	1.33
8	M	501	U10	C33-C34	3.81	1.40	1.33
7	L	402	BPH	O2D-CGD	3.90	1.43	1.33
7	M	401	BPH	O2A-CGA	3.95	1.45	1.33
8	M	501	U10	O3-C3	4.02	1.47	1.37
6	M	801	BCL	O2A-CGA	4.10	1.45	1.33
6	M	802	BCL	O2D-CGD	4.34	1.44	1.33
8	L	502	U10	O3-C3	4.43	1.48	1.37
9	M	600	SPO	C27-C28	4.50	1.39	1.34
6	L	304	BCL	O2A-CGA	4.73	1.47	1.33
9	M	600	SPO	C26-C25	5.10	1.47	1.34
9	M	600	SPO	C21-C20	5.21	1.49	1.35
6	L	304	BCL	O2D-CGD	6.82	1.50	1.33
9	M	600	SPO	C15-C16	7.36	1.53	1.34
9	M	600	SPO	C10-C11	7.77	1.54	1.34
9	M	600	SPO	C6-C5	8.32	1.55	1.31

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	BCL	O1D-CGD-CBD	-8.07	113.05	124.62
7	M	401	BPH	O1D-CGD-CBD	-7.65	113.65	124.62
6	M	801	BCL	O1D-CGD-CBD	-7.59	113.74	124.62
7	L	402	BPH	O1D-CGD-CBD	-7.52	113.84	124.62
6	M	802	BCL	O1D-CGD-CBD	-6.68	115.05	124.62
9	M	600	SPO	C15-C14-C12	-6.02	118.50	127.20
6	L	302	BCL	O1D-CGD-CBD	-5.89	116.18	124.62
9	M	600	SPO	C4-C5-C6	-4.22	118.67	124.67
9	M	600	SPO	C20-C19-C17	-4.15	121.20	127.20
9	M	600	SPO	C25-C23-C22	-3.92	112.67	118.98
9	M	600	SPO	C20-C21-C22	-3.79	115.01	123.39
7	L	402	BPH	OBD-CAD-CBD	-3.54	120.60	125.94
9	M	600	SPO	C15-C16-C17	-3.29	116.65	126.32
6	M	801	BCL	OBD-CAD-CBD	-3.26	121.01	125.94
7	M	401	BPH	OBD-CAD-CBD	-3.24	121.05	125.94
6	L	302	BCL	OBD-CAD-CBD	-3.24	121.06	125.94
6	L	304	BCL	CMB-C2B-C1B	-3.21	123.06	128.36
6	M	802	BCL	OBD-CAD-CBD	-3.09	121.27	125.94
9	M	600	SPO	C6-C7-C9	-2.96	114.21	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	304	BCL	OBD-CAD-CBD	-2.72	121.84	125.94
6	M	802	BCL	CMB-C2B-C1B	-2.67	123.94	128.36
9	M	600	SPO	C21-C22-C23	-2.59	123.45	127.20
7	L	402	BPH	C3A-C4A-NA	-2.56	109.09	113.57
7	M	401	BPH	C3A-C4A-NA	-2.51	109.17	113.57
7	L	402	BPH	O2A-CGA-O1A	-2.51	117.02	123.49
9	M	600	SPO	C10-C9-C7	-2.49	123.60	127.20
6	L	302	BCL	CMB-C2B-C1B	-2.44	124.33	128.36
6	L	302	BCL	O2A-CGA-O1A	-2.41	117.26	123.49
7	M	401	BPH	CBB-CAB-C3B	-2.37	115.25	120.52
7	M	401	BPH	O2A-CGA-O1A	-2.32	117.49	123.49
9	M	600	SPO	C34-C33-C35	-2.26	111.95	115.41
6	M	801	BCL	CMB-C2B-C1B	-2.23	124.67	128.36
8	M	501	U10	O3-C3-C2	-2.14	109.59	116.41
7	M	401	BPH	C2A-C1A-NA	-2.10	109.39	112.08
8	L	502	U10	C25-C24-C26	-2.03	112.31	115.41
8	L	502	U10	C32-C33-C34	2.01	132.14	127.76
8	L	502	U10	C22-C23-C24	2.06	132.24	127.76
6	L	304	BCL	CMB-C2B-C3B	2.10	129.20	125.09
6	L	304	BCL	CED-O2D-CGD	2.12	120.95	115.99
8	M	501	U10	C27-C28-C29	2.12	132.38	127.76
6	M	801	BCL	CMD-C2D-C3D	2.18	129.34	125.09
10	M	704	LDA	O1-N1-CM1	2.20	111.99	109.05
7	M	401	BPH	CMD-C2D-C3D	2.20	129.40	125.09
6	L	302	BCL	CED-O2D-CGD	2.21	121.18	115.99
6	M	802	BCL	CED-O2D-CGD	2.24	121.24	115.99
7	M	401	BPH	CED-O2D-CGD	2.27	121.32	115.99
9	M	600	SPO	C24-C23-C25	2.37	122.05	118.10
7	M	401	BPH	C4A-NA-C1A	2.39	110.34	108.21
8	L	502	U10	C4M-O4-C4	2.39	125.11	116.61
8	M	501	U10	C4M-O4-C4	2.41	125.18	116.61
7	L	402	BPH	C4A-NA-C1A	2.50	110.44	108.21
6	L	304	BCL	CMD-C2D-C3D	2.54	130.06	125.09
7	M	401	BPH	OBB-CAB-C3B	2.63	125.39	120.31
9	M	600	SPO	C8-C7-C6	2.69	122.57	118.10
8	M	501	U10	C7-C8-C9	2.69	131.26	126.70
6	L	302	BCL	C4A-NA-C1A	2.96	110.19	106.36
6	M	802	BCL	C4A-NA-C1A	3.01	110.25	106.36
6	M	801	BCL	O2A-CGA-CBA	3.08	121.27	111.90
6	M	801	BCL	C4A-NA-C1A	3.08	110.33	106.36
6	L	304	BCL	O2A-CGA-CBA	3.11	121.37	111.90
6	L	304	BCL	C4A-NA-C1A	3.11	110.38	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	402	BPH	O2A-CGA-CBA	3.43	122.36	111.90
6	M	802	BCL	O2A-CGA-CBA	3.48	122.50	111.90
6	L	302	BCL	O2A-CGA-CBA	3.61	122.90	111.90
7	M	401	BPH	O2A-CGA-CBA	3.69	123.14	111.90
8	L	502	U10	C7-C6-C5	4.00	123.27	118.56
8	L	502	U10	C3M-O3-C3	5.08	134.69	116.61
6	M	802	BCL	O2D-CGD-CBD	8.41	122.84	111.30
6	L	302	BCL	O2D-CGD-CBD	8.80	123.37	111.30
7	M	401	BPH	O2D-CGD-CBD	9.12	123.82	111.30
6	M	801	BCL	O2D-CGD-CBD	9.39	124.18	111.30
7	L	402	BPH	O2D-CGD-CBD	9.49	124.32	111.30
6	L	304	BCL	O2D-CGD-CBD	10.27	125.40	111.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	L	304	BCL	C13
6	M	801	BCL	C8

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	302	BCL	CED-O2D-CGD-CBD

There are no ring outliers.

12 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	702	LDA	2	0
6	L	302	BCL	8	0
6	L	304	BCL	5	0
7	L	402	BPH	8	0
8	L	502	U10	8	0
7	M	401	BPH	11	0
8	M	501	U10	2	0
9	M	600	SPO	1	0
10	M	704	LDA	1	0
5	M	800	PO4	1	0
6	M	801	BCL	6	0
6	M	802	BCL	8	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.