



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:51 AM GMT

PDB ID : 1KBY  
Title : Structure of Photosynthetic Reaction Center with bacteriochlorophyll-bacteriopheophytin heterodimer  
Authors : Camara-Artigas, A.; Magee, C.; Goetsch, A.; Allen, J.P.  
Deposited on : 2001-11-07  
Resolution : 2.50 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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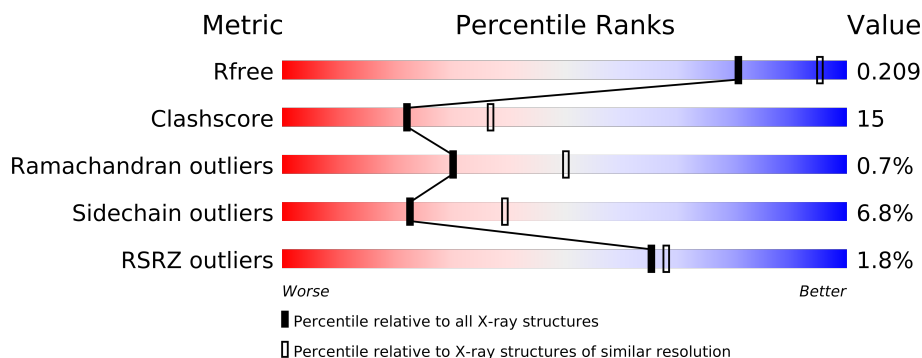
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	281	
2	M	307	
3	H	260	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	CL	M	6000	-	X
6	BCL	L	850	-	X
6	BCL	L	851	-	X
7	BPH	L	854	-	X
7	BPH	M	852	-	X
9	SPO	M	859	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7220 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN L CHAIN.

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 PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	302	Total	C	N	O	S	0	0	0
			2406	1607	392	397	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	202	LEU	HIS	ENGINEERED	UNP P02953

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	236	Total	C	N	O	S	0	0	0
			1794	1148	305	332	9			

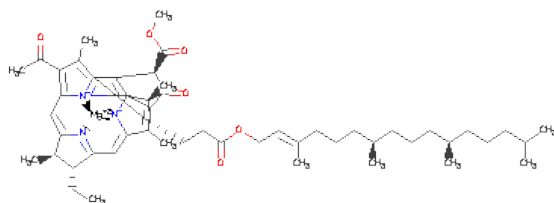
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

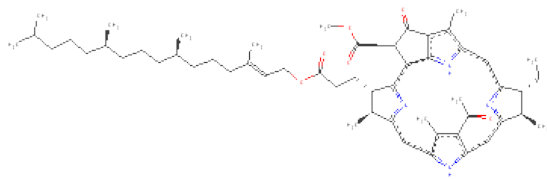
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Cl	0	0
			1	1		

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula:  $C_{55}H_{74}MgN_4O_6$ ).



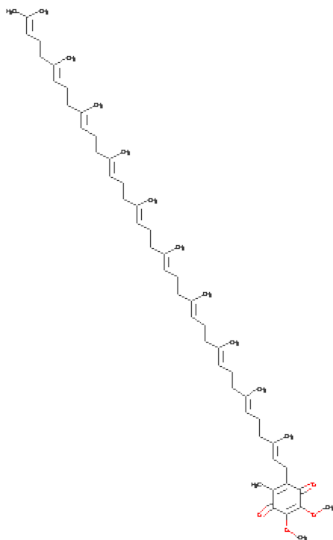
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



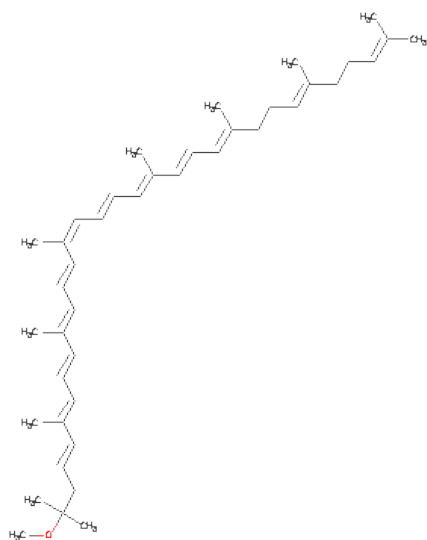
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



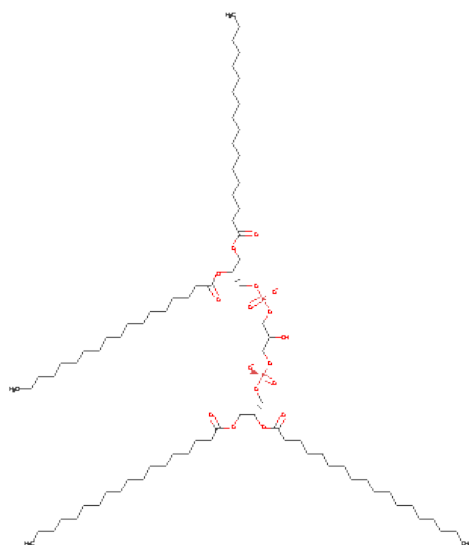
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			48	44	4		

- 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 CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is water.

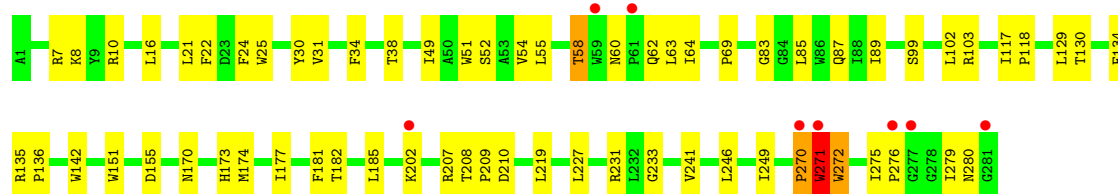
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	77	Total 77	O 77	0	0
11	L	74	Total 74	O 74	0	0
11	M	71	Total 71	O 71	0	0

### 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.

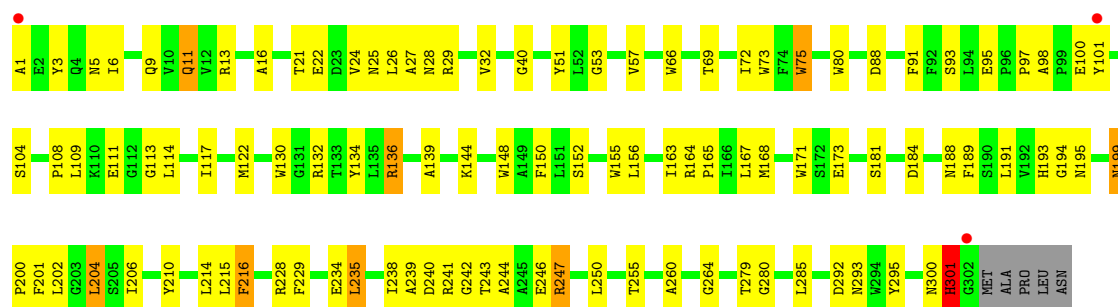
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER PROTEIN L CHAIN

Chain L: 



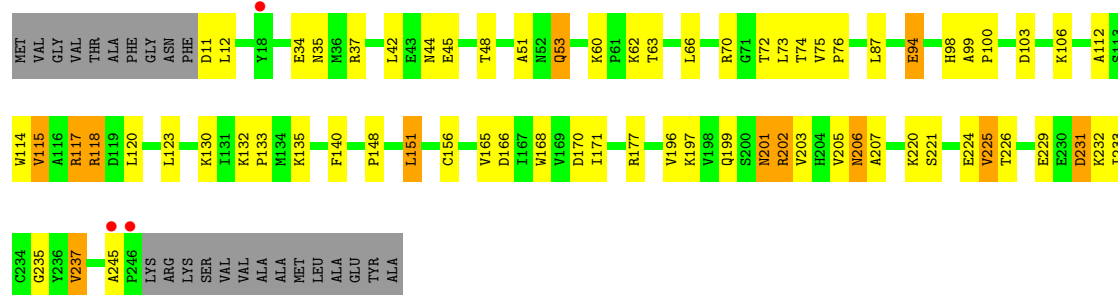
#### • Molecule 2: PHOTOSYNTHETIC REACTION CENTER PROTEIN M CHAIN

Chain M: 



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

Chain H: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.31Å 142.31Å 187.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.07 – 2.50 27.07 – 2.56	Depositor EDS
% Data completeness (in resolution range)	81.4 (27.07-2.50) 83.8 (27.07-2.56)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.195 , 0.224 0.193 , 0.209	Depositor DCC
$R_{free}$ test set	6034 reflections (11.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.0	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 59548 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, CL, CDL, BPH, 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	0.43	0/2320	0.61	0/3175
2	M	0.43	0/2497	0.60	0/3409
3	H	0.39	0/1842	0.66	0/2509
All	All	0.42	0/6659	0.62	0/9093

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2232	0	2187	60	0
2	M	2406	0	2325	78	0
3	H	1794	0	1792	64	0
4	M	1	0	0	0	0
5	M	1	0	0	0	0
6	L	198	0	222	16	0
7	L	130	0	152	17	0
7	M	65	0	76	9	0
8	M	48	0	63	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	42	0	60	1	0
10	M	81	0	106	1	0
11	H	77	0	0	1	0
11	L	74	0	0	2	0
11	M	71	0	0	3	0
All	All	7220	0	6983	210	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (210) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:272:TRP:HA	1:L:275:ILE:HD13	1.42	1.00
7:M:852:BPH:HBD	7:M:852:BPH:HAA2	1.47	0.96
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.45	0.95
1:L:34:PHE:O	1:L:38:THR:HG23	1.74	0.88
6:L:850:BCL:H93	7:M:852:BPH:H203	1.56	0.87
2:M:108:PRO:HG2	2:M:111:GLU:HB2	1.57	0.86
1:L:38:THR:HG22	1:L:99:SER:HB2	1.56	0.85
7:M:852:BPH:CBD	7:M:852:BPH:HAA2	2.02	0.83
2:M:202:LEU:O	2:M:206:ILE:HG12	1.79	0.81
1:L:58:THR:HG21	1:L:63:LEU:HD23	1.64	0.79
3:H:70:ARG:HH21	3:H:120:LEU:HB3	1.49	0.78
1:L:271:TRP:CD1	1:L:271:TRP:N	2.49	0.77
1:L:38:THR:HG22	1:L:99:SER:CB	2.15	0.76
1:L:271:TRP:HD1	1:L:271:TRP:H	1.30	0.75
2:M:75:TRP:HD1	2:M:80:TRP:HA	1.52	0.74
1:L:181:PHE:CD2	7:L:854:BPH:HBB1	2.23	0.74
3:H:45:GLU:HG3	3:H:94:GLU:HG2	1.71	0.73
2:M:240:ASP:O	3:H:117:ARG:NH1	2.21	0.71
7:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.73	0.70
3:H:70:ARG:NH2	3:H:120:LEU:HB3	2.07	0.70
6:L:850:BCL:H11	7:L:854:BPH:HBB2	1.74	0.69
2:M:72:ILE:HD12	2:M:73:TRP:N	2.08	0.68
3:H:201:ASN:H	3:H:201:ASN:HD22	1.41	0.68
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.76	0.67
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.76	0.67
2:M:242:GLY:HA2	3:H:117:ARG:HD2	1.75	0.66
2:M:144:LYS:N	2:M:144:LYS:HD2	2.11	0.66
3:H:148:PRO:HA	3:H:151:LEU:HD22	1.77	0.66
1:L:69:PRO:HG2	1:L:142:TRP:HB2	1.77	0.65
1:L:51:TRP:O	1:L:54:VAL:HG22	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:7:ARG:NH1	3:H:98:HIS:CD2	2.65	0.64
2:M:199:ASN:HD22	2:M:199:ASN:C	2.00	0.64
2:M:11:GLN:OE1	2:M:40:GLY:HA3	1.96	0.64
1:L:7:ARG:HH12	3:H:98:HIS:CD2	2.16	0.63
6:L:850:BCL:HMB2	7:L:854:BPH:HMB3	1.81	0.63
2:M:243:THR:O	2:M:247:ARG:HG2	1.99	0.63
1:L:117:ILE:HB	1:L:118:PRO:HD3	1.81	0.63
3:H:70:ARG:HH12	3:H:123:LEU:HD11	1.63	0.62
2:M:241:ARG:HD3	2:M:246:GLU:HG2	1.80	0.62
1:L:275:ILE:H	1:L:275:ILE:HD12	1.65	0.62
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.34	0.62
2:M:168:MET:HG3	2:M:173:GLU:HG2	1.82	0.62
1:L:275:ILE:N	1:L:275:ILE:HD12	2.15	0.61
2:M:93:SER:HB2	2:M:181:SER:OG	2.00	0.61
2:M:75:TRP:CD1	2:M:80:TRP:HA	2.35	0.61
3:H:156:CYS:HB3	3:H:206:ASN:O	2.00	0.61
2:M:242:GLY:CA	3:H:117:ARG:HD2	2.30	0.61
3:H:148:PRO:O	3:H:151:LEU:HB2	2.00	0.61
2:M:164:ARG:HH12	2:M:173:GLU:HG3	1.66	0.61
2:M:199:ASN:ND2	2:M:201:PHE:H	1.99	0.60
3:H:70:ARG:NH1	3:H:123:LEU:HD11	2.17	0.60
3:H:37:ARG:NH2	3:H:60:LYS:O	2.35	0.60
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.85	0.59
1:L:241:VAL:HG21	7:L:855:BPH:HAC2	1.83	0.59
1:L:246:LEU:O	1:L:249:ILE:HG22	2.02	0.59
1:L:275:ILE:CD1	1:L:275:ILE:H	2.15	0.58
2:M:113:GLY:O	2:M:117:ILE:HD13	2.03	0.58
1:L:60:ASN:O	1:L:64:ILE:HG13	2.03	0.58
2:M:164:ARG:NH1	2:M:173:GLU:HG3	2.19	0.58
11:M:1152:HOH:O	3:H:118:ARG:HD3	2.03	0.58
1:L:30:TYR:O	1:L:103:ARG:NH1	2.37	0.57
3:H:130:LYS:HE3	3:H:170:ASP:OD2	2.04	0.57
6:L:850:BCL:CBB	6:L:850:BCL:HHC	2.34	0.57
2:M:101:TYR:O	2:M:104:SER:HB3	2.05	0.57
1:L:181:PHE:HB3	7:L:854:BPH:CBB	2.35	0.57
1:L:208:THR:HB	1:L:209:PRO:HD2	1.86	0.56
2:M:204:LEU:CB	2:M:279:THR:HG21	2.36	0.56
2:M:199:ASN:HD22	2:M:200:PRO:N	2.04	0.55
2:M:136:ARG:NE	2:M:136:ARG:HA	2.21	0.55
1:L:181:PHE:HB3	7:L:854:BPH:HBB2	1.88	0.55
1:L:52:SER:HB2	1:L:85:LEU:HD13	1.89	0.55
7:L:854:BPH:H4C2	7:M:852:BPH:H141	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:103:ARG:HG3	11:L:1016:HOH:O	2.07	0.55
3:H:202:ARG:HG2	3:H:203:VAL:N	2.21	0.55
6:L:850:BCL:HHC	6:L:850:BCL:HBB3	1.90	0.54
3:H:133:PRO:HG3	3:H:168:TRP:CZ2	2.42	0.54
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.08	0.53
3:H:103:ASP:HB3	3:H:106:LYS:HB2	1.91	0.53
1:L:22:PHE:O	1:L:31:VAL:O	2.27	0.53
2:M:22:GLU:HB3	2:M:139:ALA:O	2.08	0.53
3:H:201:ASN:HD22	3:H:201:ASN:N	2.03	0.52
1:L:54:VAL:HG23	1:L:55:LEU:N	2.25	0.52
2:M:204:LEU:HB3	2:M:279:THR:HG21	1.91	0.52
3:H:45:GLU:CG	3:H:94:GLU:HG2	2.37	0.52
2:M:152:SER:O	2:M:155:TRP:HB3	2.10	0.52
3:H:135:LYS:HE2	3:H:166:ASP:OD2	2.10	0.52
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.45	0.52
1:L:174:MET:HB3	6:L:850:BCL:O1D	2.09	0.52
3:H:221:SER:HB3	3:H:224:GLU:HG2	1.92	0.52
2:M:53:GLY:O	2:M:57:VAL:HG23	2.11	0.51
2:M:163:ILE:O	2:M:167:LEU:HG	2.10	0.51
2:M:1:ALA:HB3	3:H:197:LYS:NZ	2.25	0.51
3:H:42:LEU:N	3:H:53:GLN:OE1	2.43	0.51
1:L:182:THR:OG1	6:L:850:BCL:H42	2.10	0.51
1:L:177:ILE:HG12	6:L:851:BCL:HMB3	1.93	0.51
7:L:855:BPH:HHC	7:L:855:BPH:HBB3	1.92	0.50
3:H:133:PRO:HG3	3:H:168:TRP:CE2	2.46	0.50
3:H:233:ILE:O	3:H:237:VAL:HG13	2.11	0.50
2:M:134:TYR:CE2	2:M:144:LYS:HG2	2.47	0.50
3:H:207:ALA:HB1	3:H:237:VAL:O	2.11	0.50
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.47	0.50
2:M:130:TRP:HD1	2:M:150:PHE:CD2	2.30	0.49
6:L:853:BCL:HAA2	6:L:853:BCL:HBD	1.95	0.48
11:M:1055:HOH:O	3:H:34:GLU:HG3	2.13	0.48
1:L:103:ARG:NH2	2:M:255:THR:O	2.46	0.48
3:H:201:ASN:H	3:H:201:ASN:ND2	2.07	0.48
1:L:246:LEU:C	1:L:246:LEU:HD13	2.33	0.48
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.28	0.48
2:M:13:ARG:O	3:H:140:PHE:HA	2.14	0.48
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.13	0.48
1:L:280:ASN:ND2	2:M:88:ASP:OD1	2.46	0.48
2:M:194:GLY:O	2:M:195:ASN:HB3	2.12	0.47
1:L:83:GLY:O	1:L:87:GLN:HG3	2.15	0.47
3:H:11:ASP:HB2	11:H:1139:HOH:O	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:239:ALA:O	3:H:73:LEU:HD22	2.14	0.47
3:H:70:ARG:NH1	3:H:123:LEU:CD1	2.77	0.47
6:L:851:BCL:HAA2	6:L:853:BCL:HBC1	1.96	0.47
1:L:275:ILE:CD1	1:L:275:ILE:N	2.76	0.47
3:H:44:ASN:ND2	3:H:48:THR:HG22	2.30	0.47
1:L:58:THR:HG21	1:L:63:LEU:CD2	2.41	0.47
1:L:231:ARG:HD2	2:M:6:ILE:O	2.15	0.47
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.96	0.47
2:M:97:PRO:CG	2:M:171:TRP:HB2	2.43	0.46
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.30	0.46
2:M:228:ARG:HG3	2:M:229:PHE:CE1	2.50	0.46
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.16	0.46
2:M:1:ALA:HB3	3:H:197:LYS:HZ3	1.79	0.46
3:H:63:THR:HA	3:H:73:LEU:O	2.16	0.46
8:M:857:U10:H201	8:M:857:U10:H222	1.66	0.46
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.50	0.46
3:H:196:VAL:HG12	3:H:205:VAL:HG22	1.97	0.46
6:L:853:BCL:H193	7:L:855:BPH:H111	1.96	0.46
3:H:201:ASN:ND2	3:H:201:ASN:N	2.63	0.46
2:M:72:ILE:C	2:M:72:ILE:HD12	2.36	0.45
3:H:34:GLU:OE2	3:H:37:ARG:NH1	2.49	0.45
1:L:22:PHE:HA	1:L:24:PHE:HE2	1.81	0.45
6:L:851:BCL:CAA	6:L:853:BCL:HBC1	2.46	0.45
2:M:109:LEU:HD12	2:M:109:LEU:N	2.32	0.45
1:L:38:THR:HG22	1:L:99:SER:HB3	1.97	0.45
1:L:85:LEU:O	1:L:89:ILE:HG13	2.17	0.45
3:H:34:GLU:O	3:H:37:ARG:HG3	2.17	0.45
2:M:204:LEU:HB2	2:M:279:THR:HG21	1.98	0.45
3:H:199:GLN:OE1	3:H:202:ARG:HD2	2.17	0.45
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.52	0.45
3:H:132:LYS:HD2	3:H:171:ILE:CD1	2.46	0.45
2:M:28:ASN:HB2	2:M:51:TYR:CE2	2.52	0.44
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.17	0.44
11:M:1077:HOH:O	3:H:70:ARG:HD3	2.17	0.44
2:M:101:TYR:CD1	2:M:101:TYR:N	2.85	0.44
3:H:115:VAL:HG13	3:H:231:ASP:OD2	2.18	0.44
1:L:130:THR:HA	1:L:134:PHE:HB2	2.00	0.44
2:M:229:PHE:HB2	2:M:244:ALA:HB2	2.00	0.44
2:M:75:TRP:HZ3	9:M:859:SPO:O1	2.01	0.44
1:L:170:ASN:HB3	1:L:173:HIS:CB	2.48	0.44
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.85	0.44
1:L:270:PRO:HB2	1:L:271:TRP:HD1	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:L:855:BPH:HMB1	7:L:855:BPH:HHB	1.80	0.43
2:M:189:PHE:O	2:M:193:HIS:HD2	2.01	0.43
1:L:34:PHE:HB2	11:L:1016:HOH:O	2.18	0.43
2:M:184:ASP:O	2:M:188:ASN:HB2	2.18	0.43
1:L:60:ASN:HB3	1:L:63:LEU:HB2	2.00	0.43
3:H:75:VAL:HA	3:H:76:PRO:C	2.38	0.43
7:L:854:BPH:HHB	7:L:854:BPH:HMB1	1.78	0.43
2:M:11:GLN:HB2	2:M:11:GLN:HE21	1.66	0.43
3:H:165:VAL:O	3:H:166:ASP:HB2	2.17	0.43
8:M:857:U10:H251	8:M:857:U10:H271	1.71	0.43
3:H:45:GLU:HG3	3:H:94:GLU:CG	2.44	0.42
1:L:8:LYS:HA	3:H:87:LEU:HD11	2.01	0.42
6:L:851:BCL:HAA2	6:L:851:BCL:HBD	2.01	0.42
2:M:199:ASN:C	2:M:199:ASN:ND2	2.71	0.42
2:M:109:LEU:HA	2:M:113:GLY:HA3	2.01	0.42
1:L:227:LEU:O	1:L:231:ARG:HG3	2.19	0.42
3:H:148:PRO:HA	3:H:151:LEU:CD2	2.46	0.42
2:M:206:ILE:HG23	7:M:852:BPH:HMB2	2.01	0.42
2:M:234:GLU:O	2:M:238:ILE:HG13	2.20	0.42
7:L:854:BPH:HBB3	7:L:854:BPH:HHC	2.02	0.42
1:L:279:ILE:HG21	2:M:91:PHE:HB3	2.01	0.42
1:L:202:LYS:HG3	1:L:202:LYS:H	1.54	0.42
3:H:45:GLU:CD	3:H:94:GLU:HG2	2.40	0.42
1:L:170:ASN:HB3	1:L:173:HIS:HB3	2.02	0.42
1:L:62:GLN:NE2	1:L:151:TRP:HE1	2.18	0.42
3:H:112:ALA:HA	3:H:235:GLY:O	2.20	0.42
7:L:854:BPH:H7C2	7:M:852:BPH:H192	2.01	0.41
3:H:114:TRP:CZ2	3:H:232:LYS:HE2	2.54	0.41
3:H:44:ASN:HD22	3:H:48:THR:HG22	1.84	0.41
1:L:272:TRP:HA	1:L:275:ILE:CD1	2.30	0.41
2:M:280:GLY:O	7:M:852:BPH:HED3	2.20	0.41
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.20	0.41
3:H:62:LYS:O	3:H:74:THR:HA	2.20	0.41
2:M:235:LEU:HD12	2:M:235:LEU:HA	1.82	0.41
6:L:851:BCL:H122	7:L:855:BPH:H3A	2.03	0.41
2:M:148:TRP:CD2	10:M:5000:CDL:H511	2.56	0.41
2:M:199:ASN:HD22	2:M:201:PHE:H	1.68	0.41
2:M:98:ALA:HB1	2:M:100:GLU:OE1	2.20	0.41
2:M:242:GLY:O	2:M:246:GLU:HG3	2.20	0.41
3:H:66:LEU:HD23	3:H:66:LEU:N	2.36	0.41
7:L:854:BPH:H8	7:M:852:BPH:H191	2.03	0.41
3:H:118:ARG:HB3	3:H:120:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.55	0.41
3:H:132:LYS:HD2	3:H:171:ILE:HD11	2.03	0.41
1:L:10:ARG:NH2	1:L:25:TRP:HB2	2.36	0.41
2:M:300:ASN:O	2:M:301:HIS:C	2.59	0.41
6:L:850:BCL:HBB3	6:L:850:BCL:CHC	2.48	0.41
8:M:857:U10:H71	8:M:857:U10:H1M1	1.87	0.41
7:M:852:BPH:HBC2	7:M:852:BPH:H2C	1.95	0.40
2:M:73:TRP:CE3	2:M:114:LEU:HD12	2.56	0.40
6:L:850:BCL:H2	7:L:854:BPH:HMB2	2.03	0.40
2:M:69:THR:O	2:M:72:ILE:HG13	2.21	0.40
1:L:49:ILE:HG13	1:L:89:ILE:HD13	2.03	0.40
1:L:275:ILE:HA	1:L:276:PRO:HD3	1.96	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%)	262 (94%)	15 (5%)	2 (1%)	30	50
2	M	300/307 (98%)	286 (95%)	13 (4%)	1 (0%)	50	73
3	H	234/260 (90%)	222 (95%)	9 (4%)	3 (1%)	18	29
All	All	813/848 (96%)	770 (95%)	37 (5%)	6 (1%)	30	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS
3	H	220	LYS
3	H	51	ALA
1	L	270	PRO
1	L	271	TRP
3	H	245	ALA



### 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%)	209 (95%)	11 (5%)	34	58
2	M	236/240 (98%)	218 (92%)	18 (8%)	19	33
3	H	191/208 (92%)	176 (92%)	15 (8%)	18	31
All	All	647/668 (97%)	603 (93%)	44 (7%)	22	39

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	16	LEU
1	L	21	LEU
1	L	58	THR
1	L	102	LEU
1	L	129	LEU
1	L	155	ASP
1	L	185	LEU
1	L	207	ARG
1	L	210	ASP
1	L	271	TRP
1	L	272	TRP
2	M	9	GLN
2	M	11	GLN
2	M	75	TRP
2	M	95	GLU
2	M	136	ARG
2	M	156	LEU
2	M	191	LEU
2	M	199	ASN
2	M	204	LEU
2	M	214	LEU
2	M	215	LEU
2	M	216	PHE
2	M	235	LEU
2	M	247	ARG
2	M	250	LEU
2	M	285	LEU

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Mol	Chain	Res	Type
2	M	292	ASP
2	M	301	HIS
3	H	12	LEU
3	H	53	GLN
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	177	ARG
3	H	201	ASN
3	H	202	ARG
3	H	206	ASN
3	H	225	VAL
3	H	231	ASP
3	H	237	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
1	L	159	ASN
1	L	264	GLN
2	M	11	GLN
2	M	28	ASN
2	M	193	HIS
2	M	199	ASN
2	M	299	GLN
3	H	44	ASN
3	H	98	HIS
3	H	201	ASN
3	H	206	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
6	BCL	L	850	-	74,74,74	2.29	14 (18%)	97,115,115	5.14	29 (29%)
6	BCL	L	851	-	74,74,74	1.49	11 (14%)	97,115,115	1.91	23 (23%)
6	BCL	L	853	-	74,74,74	1.55	14 (18%)	97,115,115	2.15	27 (27%)
7	BPH	L	854	-	70,70,70	1.57	8 (11%)	94,101,101	1.98	21 (22%)
7	BPH	L	855	-	70,70,70	1.44	10 (14%)	94,101,101	2.06	22 (23%)
10	CDL	M	5000	-	80,80,99	1.23	5 (6%)	92,92,111	1.04	7 (7%)
7	BPH	M	852	-	70,70,70	1.61	11 (15%)	94,101,101	2.63	26 (27%)
8	U10	M	857	-	48,48,63	2.30	14 (29%)	59,61,79	2.35	24 (40%)
9	SPO	M	859	-	41,41,41	3.53	27 (65%)	50,50,50	2.87	17 (34%)

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	850	-	-	0/41/137/137	0/0/9/9
6	BCL	L	851	-	-	0/41/137/137	0/0/9/9
6	BCL	L	853	-	-	0/41/137/137	0/0/9/9
7	BPH	L	854	-	2/2/18/22	0/49/105/105	0/0/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BPH	L	855	-	2/2/18/22	0/49/105/105	0/0/6/6
10	CDL	M	5000	-	1/1/9/9	0/91/91/110	0/0/0/0
7	BPH	M	852	-	2/2/18/22	0/49/105/105	0/0/6/6
8	U10	M	857	-	-	0/45/69/87	0/1/1/1
9	SPO	M	859	-	-	0/47/47/47	0/0/0/0

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	850	BCL	C3B-C4B	11.36	1.58	1.40
6	L	850	BCL	C1B-NB	-8.91	1.24	1.34
9	M	859	SPO	C15-C16	8.90	1.58	1.34
8	M	857	U10	C6-C1	7.59	1.54	1.35
9	M	859	SPO	C10-C11	6.93	1.53	1.34
7	L	854	BPH	C1D-CHD	6.89	1.43	1.35
9	M	859	SPO	C6-C5	6.50	1.50	1.31
7	L	855	BPH	C1D-CHD	5.91	1.42	1.35
10	M	5000	CDL	C43-C42	-5.74	1.52	1.55
9	M	859	SPO	C21-C20	5.73	1.51	1.35
6	L	850	BCL	C3B-C2B	5.60	1.57	1.40
9	M	859	SPO	C27-C28	5.56	1.40	1.34
9	M	859	SPO	C13-C12	5.35	1.60	1.51
6	L	853	BCL	C2-C3	5.13	1.43	1.32
7	M	852	BPH	C2-C3	5.02	1.43	1.32
7	L	854	BPH	C3B-C4B	4.99	1.48	1.40
10	M	5000	CDL	C58-C57	-4.79	1.53	1.55
9	M	859	SPO	C26-C25	4.78	1.47	1.34
8	M	857	U10	C7-C8	-4.78	1.43	1.50
6	L	850	BCL	C2-C3	4.66	1.42	1.32
7	M	852	BPH	C3B-C4B	4.64	1.47	1.40
7	L	855	BPH	C3B-C4B	4.63	1.47	1.40
6	L	851	BCL	C1A-NA	4.50	1.42	1.32
9	M	859	SPO	C14-C12	4.46	1.41	1.35
8	M	857	U10	C4-C3	4.20	1.54	1.35
7	M	852	BPH	C3D-CAD	-4.11	1.39	1.47
6	L	850	BCL	C3B-CAB	4.10	1.60	1.49
6	L	853	BCL	C1A-NA	4.05	1.41	1.32
6	L	851	BCL	C3B-C4B	4.03	1.46	1.40
9	M	859	SPO	O1-CM1	4.01	1.56	1.43
7	M	852	BPH	C1D-CHD	4.01	1.39	1.35
6	L	850	BCL	C1A-NA	3.99	1.41	1.32
10	M	5000	CDL	C84-C83	-3.98	1.53	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	859	SPO	C15-C14	3.97	1.55	1.43
9	M	859	SPO	C32-C33	3.96	1.40	1.32
7	L	854	BPH	C2-C3	3.95	1.40	1.32
8	M	857	U10	C33-C34	3.77	1.40	1.32
6	L	853	BCL	C3B-C4B	3.69	1.46	1.40
9	M	859	SPO	C19-C17	3.69	1.40	1.35
6	L	850	BCL	C3D-C2D	3.68	1.51	1.40
8	M	857	U10	C6-C5	3.67	1.57	1.46
7	M	852	BPH	CMB-C2B	3.65	1.59	1.51
8	M	857	U10	C7-C6	3.64	1.58	1.51
6	L	851	BCL	C2-C3	3.60	1.40	1.32
8	M	857	U10	C28-C29	3.55	1.40	1.32
9	M	859	SPO	C8-C7	3.51	1.57	1.51
6	L	850	BCL	C4C-NC	3.51	1.40	1.32
10	M	5000	CDL	C24-C23	-3.44	1.53	1.55
7	M	852	BPH	O2A-CGA	-3.43	1.22	1.33
8	M	857	U10	C23-C24	3.42	1.39	1.32
6	L	851	BCL	C4C-NC	3.38	1.39	1.32
6	L	851	BCL	C3D-C2D	3.38	1.50	1.40
9	M	859	SPO	C31-C32	-3.38	1.40	1.50
8	M	857	U10	C18-C19	3.37	1.39	1.32
8	M	857	U10	C13-C14	3.36	1.39	1.32
9	M	859	SPO	C22-C23	3.36	1.40	1.35
7	L	855	BPH	CMB-C2B	3.32	1.58	1.51
9	M	859	SPO	C10-C9	3.28	1.53	1.43
6	L	853	BCL	C4C-NC	3.25	1.39	1.32
6	L	853	BCL	C3C-C4C	-3.20	1.47	1.51
6	L	851	BCL	C4B-NB	3.19	1.38	1.34
9	M	859	SPO	C4-C5	-3.16	1.45	1.50
9	M	859	SPO	C35-C33	3.14	1.58	1.51
7	L	854	BPH	CMB-C2B	3.11	1.58	1.51
9	M	859	SPO	C11-C12	-3.07	1.39	1.45
7	L	855	BPH	C2-C3	3.05	1.39	1.32
7	M	852	BPH	C3B-CAB	3.03	1.57	1.49
6	L	853	BCL	CMB-C2B	3.02	1.58	1.51
9	M	859	SPO	C37-C38	2.98	1.42	1.32
7	M	852	BPH	C3B-C2B	2.98	1.49	1.40
6	L	851	BCL	CMB-C2B	2.93	1.57	1.51
9	M	859	SPO	C24-C23	2.93	1.56	1.51
6	L	853	BCL	C3D-C2D	2.91	1.49	1.40
10	M	5000	CDL	CB3-CB4	2.84	1.58	1.50
6	L	853	BCL	C3B-C2B	2.82	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	853	BCL	C3B-CAB	2.81	1.56	1.49
6	L	851	BCL	C3B-C2B	2.77	1.48	1.40
9	M	859	SPO	O1-C1	2.73	1.58	1.41
6	L	853	BCL	C4B-NB	2.72	1.38	1.34
8	M	857	U10	C38-C39	2.71	1.39	1.34
6	L	851	BCL	C3D-CAD	-2.69	1.41	1.47
6	L	850	BCL	C4B-CHC	2.68	1.47	1.39
7	L	854	BPH	C3D-C2D	2.67	1.48	1.40
7	L	855	BPH	C3D-CAD	-2.66	1.41	1.47
6	L	851	BCL	C3B-CAB	2.65	1.56	1.49
7	L	855	BPH	C3D-C2D	2.64	1.48	1.40
9	M	859	SPO	C9-C7	2.64	1.39	1.35
6	L	850	BCL	OBD-CAD	2.62	1.26	1.22
8	M	857	U10	O4-C4	2.51	1.43	1.36
9	M	859	SPO	C29-C28	2.50	1.57	1.50
7	L	854	BPH	C3D-CAD	-2.41	1.42	1.47
7	L	855	BPH	C3A-C2A	-2.39	1.47	1.54
6	L	853	BCL	MG-NB	2.39	2.10	2.05
6	L	853	BCL	C3D-CAD	-2.38	1.42	1.47
8	M	857	U10	C41-C39	2.34	1.53	1.40
6	L	850	BCL	CMB-C2B	2.30	1.56	1.51
6	L	853	BCL	OBD-CAD	2.28	1.25	1.22
7	M	852	BPH	C1C-NC	-2.28	1.33	1.38
9	M	859	SPO	C18-C17	2.27	1.54	1.51
7	L	854	BPH	C1B-CHB	-2.24	1.37	1.46
6	L	850	BCL	MG-NB	2.20	2.09	2.05
7	M	852	BPH	O2A-C1	-2.19	1.39	1.46
6	L	850	BCL	C3A-C2A	-2.19	1.48	1.54
9	M	859	SPO	C25-C23	-2.18	1.41	1.45
7	M	852	BPH	C4-C3	2.18	1.56	1.50
7	L	855	BPH	O2A-CGA	-2.17	1.26	1.33
6	L	853	BCL	C3A-C2A	-2.08	1.48	1.54
7	L	855	BPH	C3B-C2B	2.06	1.46	1.40
6	L	851	BCL	CBB-CAB	2.05	1.56	1.49
9	M	859	SPO	C6-C7	-2.03	1.41	1.45
6	L	850	BCL	O2D-CGD	-2.01	1.27	1.33
7	L	855	BPH	C4-C3	2.00	1.55	1.50
8	M	857	U10	C36-C34	2.00	1.56	1.51
7	L	854	BPH	C3A-C2A	-2.00	1.48	1.54

All (196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	850	BCL	OBB-CAB-C3B	28.58	162.96	120.07
6	L	850	BCL	C4B-C3B-C2B	-23.38	78.68	106.97
6	L	850	BCL	C3B-C4B-NB	18.30	126.43	108.64
6	L	850	BCL	OBB-CAB-CBB	-16.90	78.14	120.13
6	L	850	BCL	CBB-CAB-C3B	-12.14	84.83	120.30
9	M	859	SPO	C25-C23-C22	-11.16	101.83	118.97
6	L	850	BCL	CMB-C2B-C1B	-8.75	115.16	128.62
6	L	853	BCL	CAA-C2A-C1A	-8.14	91.32	111.62
7	M	852	BPH	C4B-C3B-C2B	-7.92	101.86	107.60
9	M	859	SPO	C26-C27-C28	-7.71	120.54	127.91
6	L	850	BCL	CHC-C4B-NB	-7.59	111.90	124.58
7	M	852	BPH	CBA-CAA-C2A	7.32	135.73	114.01
7	M	852	BPH	CAA-C2A-C1A	-7.26	93.62	112.72
7	L	855	BPH	C4B-C3B-C2B	-6.94	102.57	107.60
6	L	853	BCL	CMB-C2B-C1B	-6.72	118.29	128.62
6	L	851	BCL	CMB-C2B-C1B	-6.66	118.37	128.62
7	L	854	BPH	C4B-C3B-C2B	-6.59	102.82	107.60
8	M	857	U10	C7-C6-C5	6.57	125.89	118.75
7	M	852	BPH	CMB-C2B-C1B	-6.57	118.65	128.65
7	M	852	BPH	C4-C3-C5	6.34	125.03	115.39
7	M	852	BPH	CMB-C2B-C3B	6.30	134.89	124.97
6	L	850	BCL	C4D-C3D-C2D	-6.17	99.88	107.42
9	M	859	SPO	C18-C17-C19	-6.01	114.39	122.92
6	L	853	BCL	C4D-C3D-C2D	-5.99	100.10	107.42
7	L	855	BPH	C4-C3-C5	5.99	124.50	115.39
7	L	854	BPH	CMB-C2B-C1B	-5.91	119.65	128.65
7	L	855	BPH	CMB-C2B-C1B	-5.88	119.70	128.65
6	L	851	BCL	C4D-C3D-C2D	-5.86	100.26	107.42
6	L	850	BCL	CAA-C2A-C1A	-5.84	97.06	111.62
6	L	853	BCL	CMB-C2B-C3B	5.79	134.10	124.97
7	M	852	BPH	C5-C3-C2	-5.75	110.02	121.08
7	L	854	BPH	CMB-C2B-C3B	5.74	134.01	124.97
6	L	851	BCL	CMB-C2B-C3B	5.70	133.94	124.97
7	L	855	BPH	CMB-C2B-C3B	5.49	133.62	124.97
7	L	854	BPH	C1-O2A-CGA	5.47	132.29	116.98
8	M	857	U10	C15-C14-C13	-5.41	112.80	123.52
8	M	857	U10	C10-C9-C8	-5.32	112.98	123.52
7	M	852	BPH	C6-C5-C3	5.20	125.14	112.78
8	M	857	U10	C15-C14-C16	5.14	123.20	115.39
7	L	855	BPH	C1-O2A-CGA	5.01	131.01	116.98
7	M	852	BPH	C3B-C4B-NB	5.00	112.74	107.10
7	L	855	BPH	C4D-C3D-C2D	-4.94	101.39	107.37
9	M	859	SPO	C20-C21-C22	-4.93	112.44	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	852	BPH	C1-O2A-CGA	4.93	130.79	116.98
7	M	852	BPH	C1-C2-C3	4.83	134.77	126.19
7	L	854	BPH	O2A-C1-C2	-4.81	98.13	108.55
6	L	853	BCL	C4B-C3B-C2B	-4.76	101.20	106.97
6	L	851	BCL	C4B-C3B-C2B	-4.52	101.50	106.97
7	L	854	BPH	C4D-C3D-C2D	-4.52	101.91	107.37
9	M	859	SPO	C24-C23-C22	-4.50	116.53	122.92
6	L	853	BCL	CHC-C4B-NB	-4.46	117.12	124.58
7	M	852	BPH	CAA-CBA-CGA	4.44	127.57	113.27
7	L	855	BPH	C6-C5-C3	4.39	123.22	112.78
8	M	857	U10	C35-C34-C33	-4.38	114.84	123.52
7	M	852	BPH	C7-C6-C5	-4.30	100.34	113.01
6	L	850	BCL	C4B-C3B-CAB	4.28	145.84	127.09
7	L	855	BPH	C5-C3-C2	-4.22	112.96	121.08
6	L	851	BCL	CHC-C4B-NB	-4.21	117.55	124.58
7	M	852	BPH	C4D-C3D-C2D	-4.11	102.40	107.37
6	L	853	BCL	C3B-C4B-NB	4.11	112.64	108.64
6	L	851	BCL	C2A-C3A-C4A	4.07	107.65	101.40
9	M	859	SPO	C8-C7-C9	4.02	128.62	122.92
7	L	855	BPH	C3B-C4B-NB	4.01	111.63	107.10
7	L	854	BPH	C4B-CHC-C1C	4.01	140.35	127.62
9	M	859	SPO	C11-C12-C14	-4.00	112.82	118.97
7	M	852	BPH	C4B-CHC-C1C	3.93	140.10	127.62
7	M	852	BPH	CAA-C2A-C3A	3.90	122.26	113.04
8	M	857	U10	C25-C24-C23	-3.86	115.87	123.52
10	M	5000	CDL	OB8-CB6-CB4	3.85	118.92	108.83
7	L	854	BPH	C3B-C4B-NB	3.84	111.44	107.10
9	M	859	SPO	C15-C14-C12	-3.82	121.78	127.29
6	L	850	BCL	C4B-CHC-C1C	3.74	137.85	130.06
7	L	854	BPH	C4-C3-C5	3.72	121.04	115.39
6	L	853	BCL	CED-O2D-CGD	3.70	124.83	116.02
7	L	855	BPH	C4B-CHC-C1C	3.68	139.29	127.62
6	L	851	BCL	CED-O2D-CGD	3.67	124.75	116.02
9	M	859	SPO	C4-C5-C6	-3.57	119.05	124.95
6	L	850	BCL	C2A-C3A-C4A	3.53	106.83	101.40
6	L	851	BCL	C3B-C4B-NB	3.52	112.06	108.64
8	M	857	U10	C20-C19-C18	-3.51	116.57	123.52
6	L	851	BCL	OBD-CAD-C3D	-3.48	121.43	127.91
6	L	853	BCL	CBA-CAA-C2A	3.45	124.24	114.01
6	L	850	BCL	CED-O2D-CGD	3.41	124.14	116.02
6	L	850	BCL	C3B-C2B-C1B	3.41	120.01	109.98
6	L	853	BCL	C2A-C3A-C4A	3.39	106.62	101.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	857	U10	C11-C9-C8	3.36	127.55	121.08
6	L	853	BCL	OBD-CAD-C3D	-3.34	121.69	127.91
8	M	857	U10	C25-C24-C26	3.29	120.40	115.39
6	L	851	BCL	CGD-CBD-CHA	3.29	122.14	110.96
6	L	850	BCL	C6-C5-C3	3.25	120.52	112.78
9	M	859	SPO	C15-C16-C17	-3.23	117.15	126.38
6	L	850	BCL	C2B-C3B-CAB	-3.17	116.61	127.43
7	L	854	BPH	O2D-CGD-CBD	3.12	117.69	111.33
6	L	850	BCL	OBD-CAD-C3D	-3.12	122.11	127.91
7	M	852	BPH	C4D-CHA-CBD	-3.10	102.47	110.15
6	L	853	BCL	CAC-C3C-C2C	-3.08	106.83	113.89
7	L	855	BPH	O1D-CGD-CBD	-3.07	118.13	124.42
7	M	852	BPH	O2A-C1-C2	-3.07	101.91	108.55
7	L	854	BPH	O1D-CGD-CBD	-3.07	118.14	124.42
6	L	850	BCL	C2A-C1A-CHA	3.03	129.09	123.83
7	L	855	BPH	O2A-C1-C2	-3.02	102.00	108.55
7	M	852	BPH	CED-O2D-CGD	3.00	123.16	116.02
8	M	857	U10	C30-C29-C31	2.98	119.92	115.39
8	M	857	U10	C7-C8-C9	2.97	131.77	126.76
6	L	851	BCL	CHA-C1A-NA	-2.92	120.22	126.22
9	M	859	SPO	C16-C17-C19	2.87	123.38	118.97
9	M	859	SPO	C2-C1-C4	-2.84	106.28	110.97
8	M	857	U10	C35-C34-C36	2.80	119.64	115.39
8	M	857	U10	C7-C6-C1	-2.79	116.50	123.35
6	L	853	BCL	O2A-CGA-CBA	2.77	120.66	111.94
7	L	855	BPH	CED-O2D-CGD	2.76	122.58	116.02
7	L	854	BPH	C3C-C4C-CHD	2.75	127.55	121.83
7	M	852	BPH	C6-C7-C8	2.75	123.06	115.14
7	L	854	BPH	C3D-CAD-CBD	2.75	111.48	107.60
7	L	855	BPH	O2D-CGD-CBD	2.73	116.90	111.33
6	L	850	BCL	CHA-C1A-NA	-2.71	120.65	126.22
8	M	857	U10	C4M-O4-C4	2.70	125.64	116.48
8	M	857	U10	C10-C9-C11	2.68	119.47	115.39
6	L	851	BCL	C2D-C1D-ND	2.67	111.42	109.41
6	L	853	BCL	C2C-C3C-C4C	2.65	104.72	101.05
10	M	5000	CDL	OA4-PA1-OA3	-2.64	110.75	118.72
7	L	854	BPH	CHD-C4C-NC	-2.60	119.83	124.54
6	L	853	BCL	C6-C5-C3	2.59	118.94	112.78
6	L	850	BCL	CBA-CAA-C2A	2.58	121.68	114.01
6	L	851	BCL	C2A-C1A-CHA	2.57	128.29	123.83
9	M	859	SPO	C18-C17-C16	2.56	122.23	118.09
7	M	852	BPH	C3D-CAD-CBD	2.55	111.21	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	857	U10	C11-C12-C13	2.54	118.88	111.62
7	M	852	BPH	C11-C12-C13	2.54	122.45	115.14
8	M	857	U10	O5-C5-C4	-2.53	115.35	120.96
6	L	850	BCL	O2A-CGA-CBA	2.51	119.84	111.94
8	M	857	U10	C40-C39-C38	-2.51	117.61	123.62
6	L	853	BCL	CAA-C2A-C3A	-2.48	107.17	113.04
6	L	853	BCL	C4B-CHC-C1C	2.48	135.23	130.06
7	L	855	BPH	C4D-CHA-CBD	-2.47	104.03	110.15
6	L	853	BCL	O1D-CGD-CBD	-2.46	119.38	124.42
9	M	859	SPO	C13-C12-C11	2.46	122.07	118.09
7	L	855	BPH	C3C-C4C-CHD	2.45	126.92	121.83
6	L	851	BCL	C4B-CHC-C1C	2.44	135.15	130.06
8	M	857	U10	C30-C29-C28	-2.44	118.69	123.52
7	L	854	BPH	C4D-CHA-CBD	-2.44	104.12	110.15
6	L	850	BCL	C2D-C3D-CAD	2.43	154.82	138.46
6	L	853	BCL	CHA-C1A-NA	-2.42	121.25	126.22
10	M	5000	CDL	OB4-PB2-OB3	-2.42	111.43	118.72
8	M	857	U10	C31-C32-C33	-2.40	104.75	111.62
8	M	857	U10	C21-C19-C18	2.39	125.69	121.08
10	M	5000	CDL	CB6-CB4-CB3	-2.39	106.41	111.86
7	L	854	BPH	CED-O2D-CGD	2.39	121.71	116.02
6	L	853	BCL	C2D-C3D-CAD	2.38	154.44	138.46
6	L	851	BCL	C2D-C3D-CAD	2.37	154.38	138.46
7	L	854	BPH	C2B-C1B-NB	2.37	112.76	108.16
6	L	851	BCL	C6-C5-C3	2.36	118.38	112.78
6	L	850	BCL	C4B-NB-C1B	-2.34	103.68	106.76
6	L	853	BCL	C2B-C1B-NB	2.34	111.18	109.41
7	L	855	BPH	C3D-CAD-CBD	2.33	110.89	107.60
6	L	853	BCL	O2D-CGD-CBD	2.33	116.08	111.33
6	L	851	BCL	CAA-C2A-C1A	-2.32	105.83	111.62
6	L	851	BCL	C3B-C4B-CHC	2.31	130.38	126.00
6	L	850	BCL	CAA-C2A-C3A	-2.31	107.59	113.04
6	L	850	BCL	C3B-C4B-CHC	-2.31	121.63	126.00
8	M	857	U10	C36-C34-C33	2.30	125.52	121.08
6	L	851	BCL	C2B-C1B-NB	2.28	111.14	109.41
7	L	855	BPH	C2D-C3D-CAD	2.28	153.78	138.46
6	L	853	BCL	C2D-C1D-ND	2.27	111.12	109.41
10	M	5000	CDL	OB6-CB5-C51	2.25	116.48	111.56
6	L	850	BCL	C4D-C3D-CAD	-2.23	105.31	108.05
6	L	853	BCL	C3B-C4B-CHC	2.23	130.24	126.00
6	L	851	BCL	C2C-C3C-C4C	2.23	104.13	101.05
6	L	853	BCL	C2A-C1A-CHA	2.22	127.68	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	854	BPH	C2D-C3D-CAD	2.22	153.40	138.46
7	M	852	BPH	CHD-C4C-NC	-2.22	120.53	124.54
10	M	5000	CDL	CB4-OB6-CB5	2.20	123.33	117.92
8	M	857	U10	C27-C28-C29	-2.20	123.06	127.80
6	L	851	BCL	C4D-C3D-CAD	-2.19	105.36	108.05
9	M	859	SPO	C8-C7-C6	-2.19	114.56	118.09
7	L	855	BPH	CAC-C3C-C2C	-2.18	108.89	113.89
6	L	850	BCL	C2D-C1D-ND	2.17	111.05	109.41
6	L	851	BCL	C4D-CHA-CBD	-2.15	104.31	109.37
6	L	851	BCL	C3D-CAD-CBD	2.13	110.60	107.60
9	M	859	SPO	C9-C10-C11	-2.12	116.07	123.24
6	L	853	BCL	C4D-C3D-CAD	-2.11	105.46	108.05
8	M	857	U10	C1-C6-C5	-2.11	117.61	120.26
7	M	852	BPH	O1D-CGD-CBD	-2.09	120.13	124.42
7	L	855	BPH	CHD-C4C-NC	-2.09	120.75	124.54
7	L	855	BPH	C2B-C1B-NB	2.08	112.21	108.16
7	M	852	BPH	C3C-C4C-CHD	2.08	126.15	121.83
7	L	854	BPH	CBB-CAB-C3B	-2.08	114.23	120.30
7	L	854	BPH	C6-C7-C8	2.07	121.10	115.14
6	L	853	BCL	CGD-CBD-CHA	2.06	117.98	110.96
7	M	852	BPH	C3A-C2A-C1A	-2.04	99.31	101.91
10	M	5000	CDL	OA8-CA6-CA4	-2.03	103.51	108.83
6	L	850	BCL	C2C-C1C-NC	2.03	113.42	110.95
7	L	855	BPH	C3D-C4D-ND	2.02	114.89	108.80
9	M	859	SPO	C34-C33-C35	-2.02	112.32	115.39
7	L	854	BPH	C2A-C3A-C4A	2.01	105.64	101.11
6	L	850	BCL	C2C-C3C-C4C	2.00	103.83	101.05

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	L	855	BPH	C8
7	L	855	BPH	C13
10	M	5000	CDL	CA4
7	M	852	BPH	C8
7	M	852	BPH	C13
7	L	854	BPH	C8
7	L	854	BPH	C13

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	L	281/281 (100%)	-0.49	8 (2%)	50	53	24, 39, 73, 82	0
2	M	302/307 (98%)	-0.47	3 (0%)	79	81	23, 45, 74, 89	0
3	H	236/260 (90%)	-0.51	3 (1%)	74	76	28, 45, 65, 85	0
All	All	819/848 (96%)	-0.49	14 (1%)	65	69	23, 44, 72, 89	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.5
1	L	59	TRP	4.5
3	H	245	ALA	3.2
2	M	302	GLY	3.0
3	H	246	PRO	2.7
1	L	277	GLY	2.7
3	H	18	TYR	2.6
1	L	202	LYS	2.4
2	M	101	TYR	2.3
1	L	270	PRO	2.3
1	L	276	PRO	2.3
1	L	271	TRP	2.1
1	L	281	GLY	2.1
1	L	61	PRO	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	CL	M	6000	1/1	0.45	6.88	100,100,100,100	0
6	BCL	L	850	66/66	0.22	3.21	35,46,96,98	0
9	SPO	M	859	42/42	0.25	2.90	47,62,74,75	0
7	BPH	M	852	65/65	0.18	2.88	33,37,66,76	0
7	BPH	L	854	65/65	0.19	2.71	39,44,95,98	0
6	BCL	L	851	66/66	0.16	2.02	30,37,47,60	0
8	U10	M	857	48/63	0.16	1.64	41,51,69,70	0
10	CDL	M	5000	81/100	0.20	1.36	59,76,86,90	0
7	BPH	L	855	65/65	0.14	1.35	26,35,46,53	0
6	BCL	L	853	66/66	0.14	0.87	24,30,60,66	0
4	FE	M	856	1/1	0.08	-1.32	28,28,28,28	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.