



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM 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 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

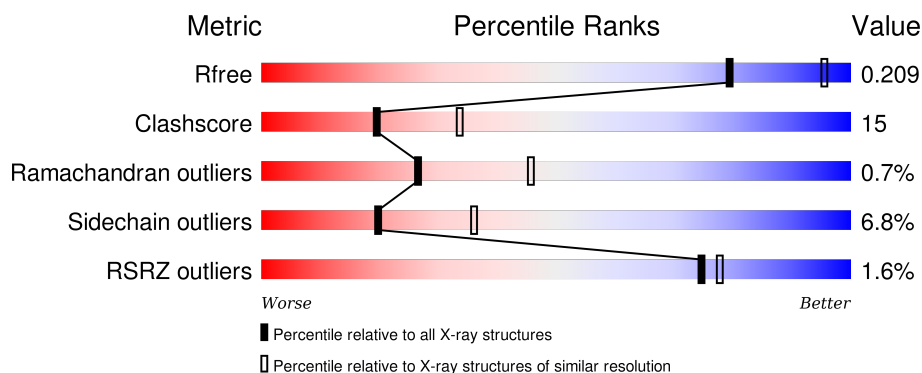
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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.

Mol	Chain	Length	Quality of chain
1	L	281	<div> <div>2%</div> <div>77%</div> <div>22%</div> <div>.</div> </div>
2	M	307	<div> <div>%</div> <div>64%</div> <div>31%</div> <div>..</div> </div>
3	H	260	<div> <div>%</div> <div>64%</div> <div>22%</div> <div>5%</div> <div>9%</div> </div>

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	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 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 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			

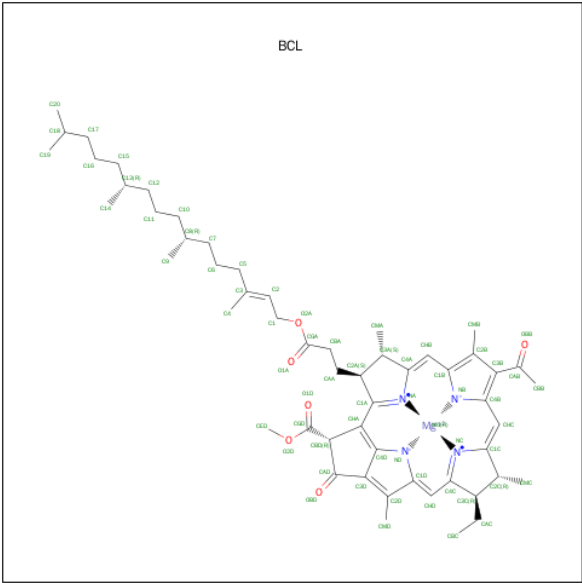
- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

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).

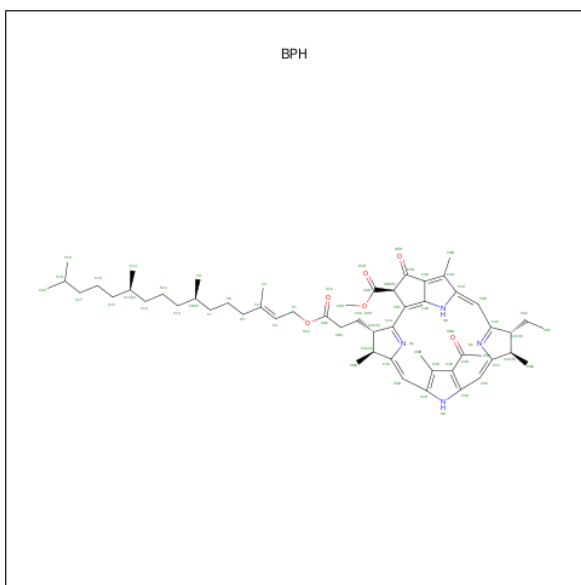
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	Cl			0	0
			1	1				

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C<sub>55</sub>H<sub>74</sub>MgN<sub>4</sub>O<sub>6</sub>).



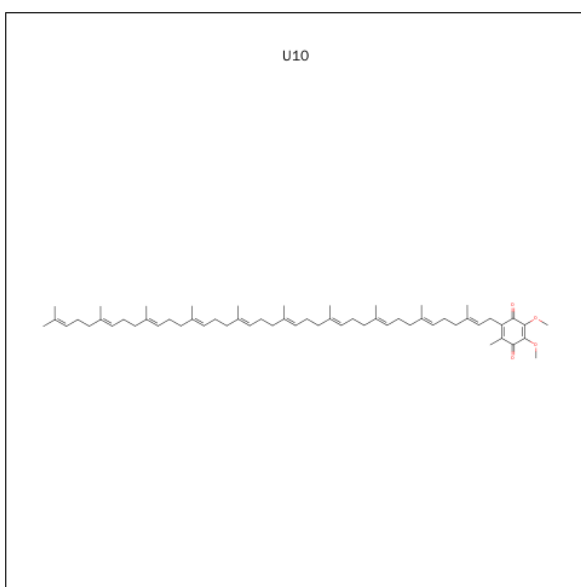
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
6	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



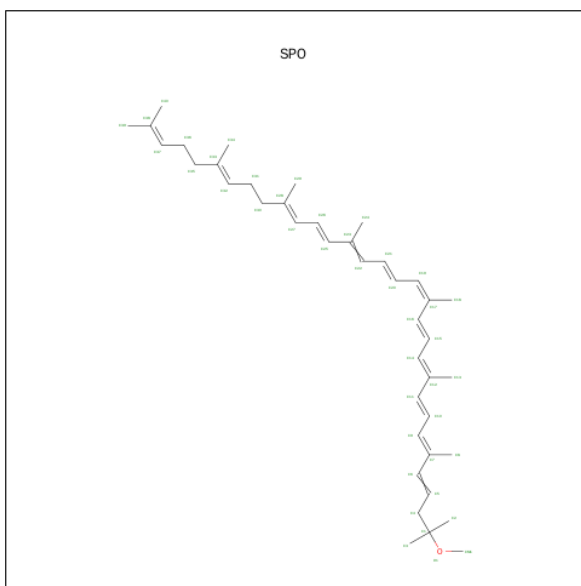
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



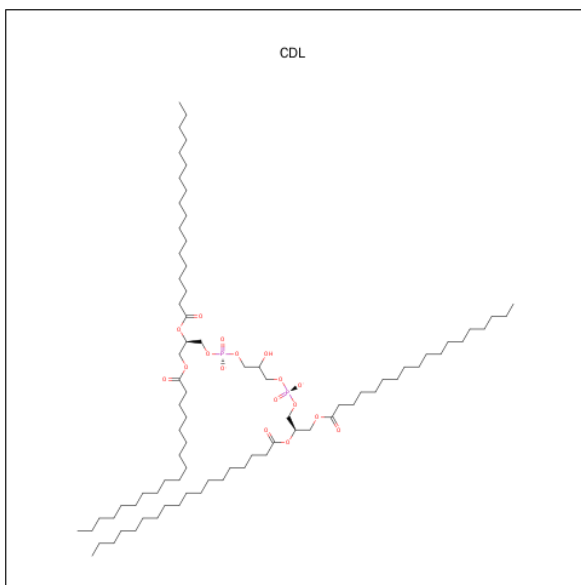
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			48	44	4		

- 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.

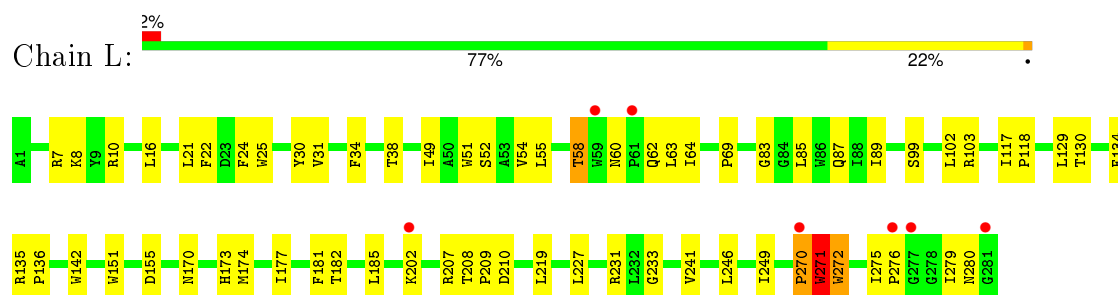
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	77	Total 77	O 77	0	0
11	L	74	Total 74	O 74	0	0
11	M	71	Total 71	O 71	0	0



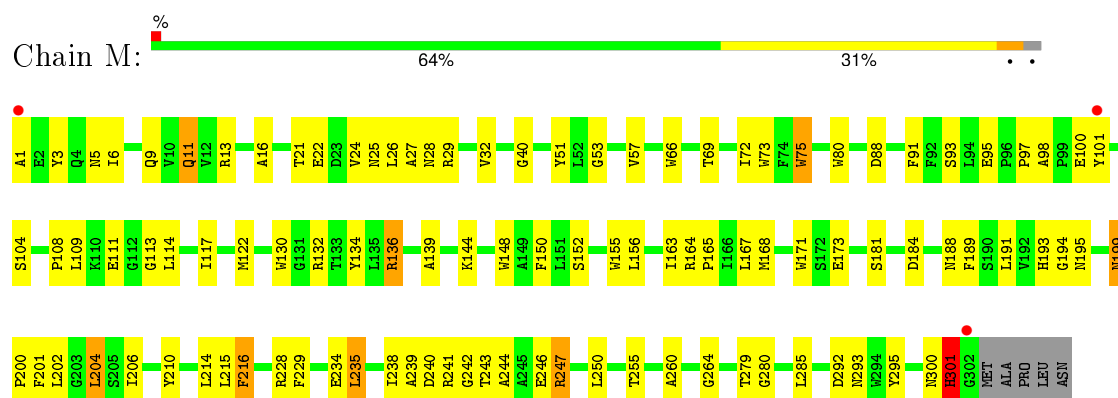
### 3 Residue-property plots

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.

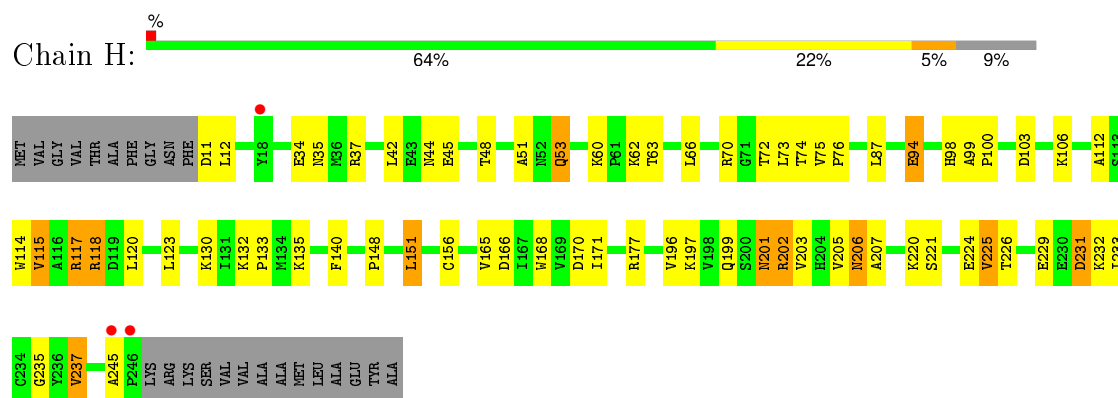
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER PROTEIN L CHAIN



- Molecule 2: PHOTOSYNTHETIC REACTION CENTER PROTEIN M CHAIN



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER PROTEIN H CHAIN



## 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> )	0.32 , 73.9	EDS
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 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, 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 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	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
9	M	42	0	60	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 15.

All (210) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:TRP:O	1:L:54:VAL:HG22	1.96	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	26	46
2	M	300/307 (98%)	286 (95%)	13 (4%)	1 (0%)	46	68
3	H	234/260 (90%)	222 (95%)	9 (4%)	3 (1%)	15	26
All	All	813/848 (96%)	770 (95%)	37 (5%)	6 (1%)	26	46

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%)	30	53
2	M	236/240 (98%)	218 (92%)	18 (8%)	16	30
3	H	191/208 (92%)	176 (92%)	15 (8%)	15	28
All	All	647/668 (97%)	603 (93%)	44 (7%)	20	36

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
3	H	206	ASN

### 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 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	-	53,74,74	1.79	9 (16%)	57,115,115	4.90	14 (24%)
6	BCL	L	851	-	53,74,74	1.45	7 (13%)	57,115,115	1.61	8 (14%)
6	BCL	L	853	-	53,74,74	1.57	9 (16%)	57,115,115	2.03	13 (22%)
7	BPH	L	854	-	64,70,70	1.41	8 (12%)	73,101,101	1.65	13 (17%)
7	BPH	L	855	-	64,70,70	1.36	12 (18%)	73,101,101	1.85	14 (19%)
10	CDL	M	5000	-	80,80,99	0.73	1 (1%)	82,92,111	0.96	4 (4%)
7	BPH	M	852	-	64,70,70	1.68	12 (18%)	73,101,101	2.49	22 (30%)
8	U10	M	857	-	48,48,63	2.34	13 (27%)	58,61,79	2.32	22 (37%)
9	SPO	M	859	-	40,41,41	3.54	25 (62%)	45,50,50	2.71	16 (35%)

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	-	-	0/37/137/137	0/0/9/9
6	BCL	L	851	-	-	0/37/137/137	0/0/9/9
6	BCL	L	853	-	-	0/37/137/137	0/0/9/9
7	BPH	L	854	-	-	0/54/105/105	0/1/6/6
7	BPH	L	855	-	-	0/54/105/105	0/1/6/6
10	CDL	M	5000	-	-	0/91/91/110	0/0/0/0
7	BPH	M	852	-	-	0/54/105/105	0/1/6/6
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 (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	857	U10	C7-C8	-4.96	1.43	1.50
7	M	852	BPH	C3D-CAD	-3.88	1.39	1.46
7	M	852	BPH	O2A-CGA	-3.61	1.22	1.33
9	M	859	SPO	C4-C5	-3.57	1.45	1.50
9	M	859	SPO	C31-C32	-3.48	1.40	1.50
6	L	853	BCL	C3C-C4C	-3.20	1.47	1.51
9	M	859	SPO	C11-C12	-3.07	1.39	1.45
7	L	854	BPH	C1B-C2B	-2.57	1.40	1.45
7	L	855	BPH	C3D-CAD	-2.42	1.41	1.46
7	L	855	BPH	C3A-C2A	-2.37	1.47	1.54
7	L	855	BPH	C1B-C2B	-2.36	1.40	1.45
7	M	852	BPH	O2A-C1	-2.30	1.39	1.46
7	L	855	BPH	O2A-CGA	-2.30	1.26	1.33
9	M	859	SPO	C25-C23	-2.18	1.41	1.45
7	L	854	BPH	C3D-CAD	-2.18	1.42	1.46
6	L	850	BCL	C3A-C2A	-2.17	1.48	1.54
6	L	850	BCL	O2D-CGD	-2.10	1.27	1.33
6	L	853	BCL	C3A-C2A	-2.06	1.48	1.54
9	M	859	SPO	C6-C7	-2.03	1.41	1.45
6	L	853	BCL	CMD-C2D	2.05	1.56	1.51
7	M	852	BPH	C3D-C2D	2.08	1.45	1.40
7	L	855	BPH	C4-C3	2.11	1.55	1.50
8	M	857	U10	C36-C34	2.12	1.56	1.51
6	L	851	BCL	CBB-CAB	2.15	1.56	1.49
6	L	851	BCL	CMD-C2D	2.15	1.56	1.51
6	L	853	BCL	OBD-CAD	2.16	1.25	1.22
7	L	854	BPH	CHA-C1A	2.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	852	BPH	CMD-C2D	2.29	1.56	1.51
7	M	852	BPH	C4-C3	2.29	1.56	1.50
7	M	852	BPH	CBB-CAB	2.30	1.55	1.50
8	M	857	U10	O4-C4	2.33	1.43	1.37
6	L	850	BCL	CMB-C2B	2.34	1.56	1.51
7	L	855	BPH	CMD-C2D	2.37	1.56	1.51
7	L	855	BPH	CHA-C1A	2.41	1.42	1.37
9	M	859	SPO	C24-C23	2.41	1.56	1.50
7	L	855	BPH	C3B-CAB	2.42	1.54	1.46
6	L	850	BCL	OBD-CAD	2.49	1.26	1.22
8	M	857	U10	C38-C39	2.51	1.39	1.32
7	L	854	BPH	CMD-C2D	2.56	1.56	1.51
9	M	859	SPO	C9-C7	2.62	1.39	1.35
9	M	859	SPO	C29-C28	2.63	1.57	1.50
6	L	850	BCL	C4B-CHC	2.68	1.47	1.39
7	L	854	BPH	C3B-C2B	2.68	1.46	1.38
6	L	851	BCL	C3B-CAB	2.73	1.56	1.49
10	M	5000	CDL	CB3-CB4	2.81	1.58	1.50
7	L	855	BPH	C3B-C2B	2.86	1.46	1.38
6	L	853	BCL	C3B-CAB	2.89	1.56	1.49
9	M	859	SPO	C8-C7	2.89	1.57	1.50
6	L	851	BCL	CMB-C2B	2.98	1.57	1.51
6	L	853	BCL	CMB-C2B	3.08	1.58	1.51
7	L	855	BPH	C2-C3	3.12	1.39	1.33
9	M	859	SPO	C10-C9	3.13	1.53	1.43
9	M	859	SPO	C37-C38	3.16	1.42	1.32
9	M	859	SPO	C35-C33	3.33	1.58	1.51
9	M	859	SPO	C22-C23	3.34	1.40	1.35
7	M	852	BPH	C3B-CAB	3.39	1.57	1.46
7	L	855	BPH	C3D-C2D	3.43	1.48	1.40
8	M	857	U10	C13-C14	3.44	1.39	1.33
8	M	857	U10	C18-C19	3.45	1.39	1.33
7	L	854	BPH	C3D-C2D	3.46	1.48	1.40
7	L	854	BPH	CMB-C2B	3.47	1.58	1.50
8	M	857	U10	C23-C24	3.51	1.39	1.33
6	L	851	BCL	C3B-C2B	3.59	1.48	1.40
8	M	857	U10	C28-C29	3.64	1.40	1.33
6	L	853	BCL	C3B-C2B	3.65	1.48	1.40
9	M	859	SPO	C19-C17	3.67	1.40	1.35
7	L	855	BPH	CMB-C2B	3.68	1.58	1.50
6	L	851	BCL	C2-C3	3.69	1.40	1.33
8	M	857	U10	C6-C5	3.75	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	853	BCL	C3D-C2D	3.77	1.49	1.40
9	M	859	SPO	C15-C14	3.80	1.55	1.43
7	M	852	BPH	C3B-C2B	3.84	1.49	1.38
8	M	857	U10	C7-C6	3.84	1.58	1.51
8	M	857	U10	C33-C34	3.86	1.40	1.33
7	M	852	BPH	CMB-C2B	4.01	1.59	1.50
7	L	854	BPH	C2-C3	4.06	1.40	1.33
9	M	859	SPO	C32-C33	4.07	1.40	1.33
9	M	859	SPO	O1-CM1	4.07	1.56	1.43
6	L	850	BCL	C3B-CAB	4.19	1.60	1.49
8	M	857	U10	C4-C3	4.29	1.54	1.35
6	L	851	BCL	C3D-C2D	4.35	1.50	1.40
9	M	859	SPO	C13-C12	4.40	1.60	1.50
7	M	852	BPH	CHA-C1A	4.44	1.47	1.37
9	M	859	SPO	C14-C12	4.44	1.41	1.35
6	L	850	BCL	C3D-C2D	4.74	1.51	1.40
6	L	850	BCL	C2-C3	4.78	1.42	1.33
9	M	859	SPO	C26-C25	4.96	1.47	1.34
7	M	852	BPH	C2-C3	5.16	1.43	1.33
6	L	853	BCL	C2-C3	5.26	1.43	1.33
9	M	859	SPO	C27-C28	5.32	1.40	1.34
9	M	859	SPO	C21-C20	5.64	1.51	1.35
9	M	859	SPO	C6-C5	6.82	1.50	1.31
6	L	850	BCL	C3B-C2B	7.15	1.57	1.40
9	M	859	SPO	C10-C11	7.18	1.53	1.34
8	M	857	U10	C6-C1	7.91	1.54	1.35
9	M	859	SPO	C15-C16	9.21	1.58	1.34

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	850	BCL	OBB-CAB-CBB	-17.52	78.14	120.13
6	L	850	BCL	CBB-CAB-C3B	-11.96	84.83	120.33
9	M	859	SPO	C25-C23-C22	-10.65	101.83	118.98
6	L	850	BCL	CMB-C2B-C1B	-7.98	115.16	128.36
7	M	852	BPH	CAA-C2A-C1A	-7.31	93.62	112.86
6	L	853	BCL	CMB-C2B-C1B	-6.09	118.29	128.36
6	L	851	BCL	CMB-C2B-C1B	-6.04	118.37	128.36
6	L	853	BCL	CAA-C2A-C1A	-6.00	91.32	112.47
7	M	852	BPH	C5-C3-C2	-5.82	110.02	121.05
9	M	859	SPO	C18-C17-C19	-5.76	114.39	122.90
8	M	857	U10	C15-C14-C13	-5.45	112.80	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	857	U10	C10-C9-C8	-5.36	112.98	123.50
9	M	859	SPO	C20-C21-C22	-4.95	112.44	123.39
7	L	855	BPH	O1D-CGD-CBD	-4.53	118.13	124.62
7	L	854	BPH	O1D-CGD-CBD	-4.52	118.14	124.62
8	M	857	U10	C35-C34-C33	-4.41	114.84	123.50
7	L	855	BPH	C4D-C3D-C2D	-4.41	101.39	107.08
6	L	850	BCL	CAA-C2A-C1A	-4.37	97.06	112.47
9	M	859	SPO	C24-C23-C22	-4.31	116.53	122.90
7	M	852	BPH	C7-C6-C5	-4.31	100.34	113.06
7	L	855	BPH	C5-C3-C2	-4.27	112.96	121.05
7	L	854	BPH	C4D-C3D-C2D	-4.01	101.91	107.08
9	M	859	SPO	C4-C5-C6	-3.95	119.05	124.67
7	M	852	BPH	CMB-C2B-C1B	-3.93	118.65	125.06
8	M	857	U10	C25-C24-C23	-3.89	115.87	123.50
9	M	859	SPO	C11-C12-C14	-3.82	112.82	118.98
7	L	855	BPH	CHC-C4B-NB	-3.81	117.66	124.91
9	M	859	SPO	C15-C14-C12	-3.75	121.78	127.20
6	L	853	BCL	O1D-CGD-CBD	-3.66	119.38	124.62
7	M	852	BPH	C4D-C3D-C2D	-3.63	102.40	107.08
8	M	857	U10	C20-C19-C18	-3.53	116.57	123.50
6	L	851	BCL	OBD-CAD-C3D	-3.39	121.43	128.35
7	L	854	BPH	CHC-C4B-NB	-3.38	118.47	124.91
7	L	854	BPH	CMB-C2B-C1B	-3.32	119.65	125.06
7	L	855	BPH	CMB-C2B-C1B	-3.29	119.70	125.06
6	L	853	BCL	OBD-CAD-C3D	-3.27	121.69	128.35
7	M	852	BPH	O1D-CGD-CBD	-3.13	120.13	124.62
7	M	852	BPH	CHC-C4B-NB	-3.13	118.95	124.91
9	M	859	SPO	C15-C16-C17	-3.12	117.15	126.32
6	L	850	BCL	OBD-CAD-C3D	-3.06	122.11	128.35
6	L	853	BCL	CAC-C3C-C2C	-2.90	106.83	114.13
7	L	854	BPH	CBB-CAB-C3B	-2.83	114.23	120.52
6	L	850	BCL	O1D-CGD-CBD	-2.77	120.64	124.62
8	M	857	U10	C31-C32-C33	-2.65	104.75	111.69
8	M	857	U10	O5-C5-C4	-2.51	115.35	120.79
8	M	857	U10	C30-C29-C28	-2.45	118.69	123.50
10	M	5000	CDL	CB6-CB4-CB3	-2.42	106.41	112.07
6	L	851	BCL	CHA-C1A-NA	-2.37	120.22	126.06
9	M	859	SPO	C9-C10-C11	-2.31	116.07	123.13
8	M	857	U10	C1-C6-C5	-2.20	117.61	120.12
6	L	850	BCL	CHA-C1A-NA	-2.20	120.65	126.06
8	M	857	U10	C27-C28-C29	-2.16	123.06	127.76
9	M	859	SPO	C8-C7-C6	-2.13	114.56	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	853	BCL	CAA-C2A-C3A	-2.10	107.17	113.22
7	L	855	BPH	CBB-CAB-C3B	-2.08	115.89	120.52
7	L	855	BPH	CAC-C3C-C2C	-2.08	108.89	114.13
7	M	852	BPH	C1C-NC-C4C	-2.04	108.35	110.44
9	M	859	SPO	C34-C33-C35	-2.02	112.32	115.41
7	L	854	BPH	C2B-C1B-NB	2.02	112.76	109.73
6	L	853	BCL	C2A-C1A-CHA	2.06	127.68	123.89
7	M	852	BPH	C11-C12-C13	2.10	122.45	115.49
7	L	854	BPH	C6-C5-C3	2.10	117.10	112.48
6	L	851	BCL	C3D-CAD-CBD	2.13	110.60	107.60
9	M	859	SPO	O1-C1-C4	2.27	111.42	105.87
10	M	5000	CDL	CB4-OB6-CB5	2.27	123.33	117.89
7	M	852	BPH	C3A-C4A-CHB	2.27	126.06	121.84
10	M	5000	CDL	OB6-CB5-C51	2.28	116.48	111.53
7	M	852	BPH	C6-C7-C8	2.28	123.06	115.49
6	L	850	BCL	O2D-CGD-CBD	2.29	114.43	111.30
7	L	855	BPH	C3D-CAD-CBD	2.33	110.89	107.60
8	M	857	U10	C36-C34-C33	2.36	125.52	121.05
9	M	859	SPO	C13-C12-C11	2.39	122.07	118.10
6	L	851	BCL	C2A-C1A-CHA	2.39	128.29	123.89
7	L	855	BPH	CMB-C2B-C3B	2.40	133.62	128.04
7	L	854	BPH	CED-O2D-CGD	2.44	121.71	115.99
8	M	857	U10	C21-C19-C18	2.44	125.69	121.05
9	M	859	SPO	C18-C17-C16	2.48	122.23	118.10
8	M	857	U10	C4M-O4-C4	2.54	125.64	116.61
7	M	852	BPH	C3D-CAD-CBD	2.55	111.21	107.60
7	L	854	BPH	CMB-C2B-C3B	2.56	134.01	128.04
7	M	852	BPH	C2A-C1A-NA	2.57	115.37	112.08
6	L	850	BCL	O2A-CGA-CBA	2.61	119.84	111.90
8	M	857	U10	C10-C9-C11	2.66	119.47	115.41
7	M	852	BPH	O2D-CGD-CBD	2.67	114.96	111.30
6	L	851	BCL	C6-C5-C3	2.69	118.38	112.48
9	M	859	SPO	C16-C17-C19	2.73	123.38	118.98
8	M	857	U10	C11-C12-C13	2.74	118.88	111.69
7	L	854	BPH	C3D-CAD-CBD	2.75	111.48	107.60
8	M	857	U10	C35-C34-C36	2.77	119.64	115.41
7	L	855	BPH	CED-O2D-CGD	2.81	122.58	115.99
6	L	850	BCL	CBA-CAA-C2A	2.82	121.68	113.73
6	L	850	BCL	C2A-C1A-CHA	2.82	129.09	123.89
6	L	853	BCL	O2A-CGA-CBA	2.88	120.66	111.90
6	L	853	BCL	C6-C5-C3	2.94	118.94	112.48
7	M	852	BPH	CMB-C2B-C3B	2.94	134.89	128.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	857	U10	C30-C29-C31	2.95	119.92	115.41
8	M	857	U10	C7-C8-C9	2.99	131.77	126.70
7	M	852	BPH	CED-O2D-CGD	3.06	123.16	115.99
7	M	852	BPH	CAA-C2A-C3A	3.15	122.26	113.22
8	M	857	U10	C25-C24-C26	3.27	120.40	115.41
8	M	857	U10	C11-C9-C8	3.43	127.55	121.05
6	L	850	BCL	CED-O2D-CGD	3.48	124.14	115.99
6	L	853	BCL	O2D-CGD-CBD	3.48	116.08	111.30
6	L	850	BCL	C6-C5-C3	3.66	120.52	112.48
7	L	854	BPH	C4-C3-C5	3.69	121.04	115.41
6	L	853	BCL	CBA-CAA-C2A	3.72	124.24	113.73
6	L	851	BCL	CED-O2D-CGD	3.74	124.75	115.99
6	L	853	BCL	CED-O2D-CGD	3.77	124.83	115.99
10	M	5000	CDL	OB8-CB6-CB4	3.80	118.92	108.69
9	M	859	SPO	C8-C7-C9	3.87	128.62	122.90
7	L	855	BPH	O2D-CGD-CBD	4.08	116.90	111.30
7	L	855	BPH	C3C-C4C-NC	4.38	112.32	107.93
6	L	851	BCL	CMB-C2B-C3B	4.53	133.94	125.09
6	L	853	BCL	CMB-C2B-C3B	4.61	134.10	125.09
7	L	854	BPH	O2D-CGD-CBD	4.66	117.69	111.30
7	L	854	BPH	C3C-C4C-NC	4.68	112.61	107.93
7	M	852	BPH	CAA-CBA-CGA	4.87	127.57	113.32
7	L	855	BPH	C6-C5-C3	4.89	123.22	112.48
8	M	857	U10	C15-C14-C16	5.11	123.20	115.41
7	M	852	BPH	C3C-C4C-NC	5.39	113.33	107.93
7	M	852	BPH	C6-C5-C3	5.77	125.14	112.48
7	L	855	BPH	C4-C3-C5	5.95	124.50	115.41
8	M	857	U10	C7-C6-C5	6.23	125.89	118.56
7	M	852	BPH	C4-C3-C5	6.30	125.03	115.41
7	M	852	BPH	CBA-CAA-C2A	7.80	135.73	113.73
6	L	850	BCL	OB8-CAB-C3B	27.12	162.96	120.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	850	BCL	9	0
6	L	851	BCL	5	0
6	L	853	BCL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	854	BPH	11	0
7	L	855	BPH	6	0
10	M	5000	CDL	1	0
7	M	852	BPH	9	0
8	M	857	U10	3	0
9	M	859	SPO	1	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](#)

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%)	-0.54	7 (2%) 61 65	24, 39, 73, 82	0
2	M	302/307 (98%)	-0.52	3 (0%) 84 86	23, 45, 74, 89	0
3	H	236/260 (90%)	-0.54	3 (1%) 79 82	28, 45, 65, 85	0
All	All	819/848 (96%)	-0.54	13 (1%) 74 78	23, 44, 72, 89	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	5.8
1	L	59	TRP	4.9
3	H	245	ALA	3.8
1	L	277	GLY	3.5
1	L	276	PRO	3.2
3	H	246	PRO	2.9
2	M	302	GLY	2.7
2	M	101	TYR	2.7
1	L	61	PRO	2.6
1	L	281	GLY	2.6
1	L	202	LYS	2.5
3	H	18	TYR	2.5
1	L	270	PRO	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	BCL	L	850	66/66	0.89	0.23	3.52	35,46,96,98	0
7	BPH	M	852	65/65	0.94	0.18	2.85	33,37,66,76	0
9	SPO	M	859	42/42	0.86	0.24	2.74	47,62,74,75	0
7	BPH	L	854	65/65	0.87	0.19	2.62	39,44,95,98	0
6	BCL	L	851	66/66	0.95	0.17	2.14	30,37,47,60	0
8	U10	M	857	48/63	0.94	0.16	1.58	41,51,69,70	0
10	CDL	M	5000	81/100	0.90	0.21	1.47	59,76,86,90	0
7	BPH	L	855	65/65	0.95	0.14	1.44	26,35,46,53	0
6	BCL	L	853	66/66	0.95	0.14	0.94	24,30,60,66	0
4	FE	M	856	1/1	0.99	0.07	-1.37	28,28,28,28	0
5	CL	M	6000	1/1	0.72	0.35	-	100,100,100,100	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.