



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:48 PM GMT

PDB ID : 1M3X  
Title : Photosynthetic Reaction Center From Rhodobacter Sphaeroides  
Authors : Camara-Artigas, A.; Brune, D.; Allen, J.P.  
Deposited on : 2002-07-01  
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

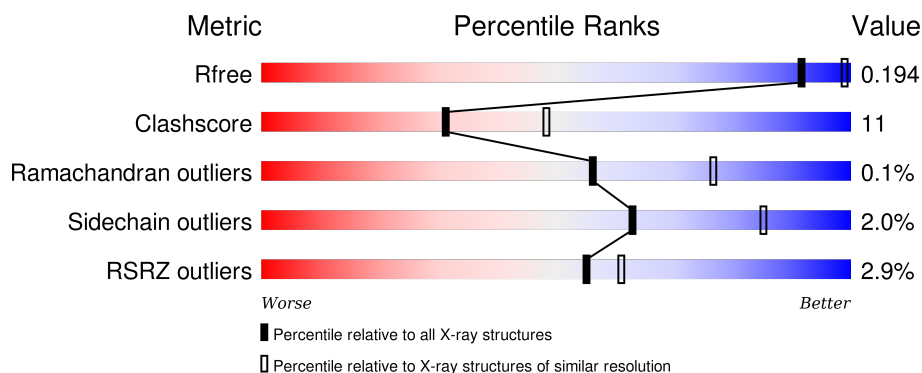
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>4%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	M	307	<div> <div>3%</div> <div>77%</div> <div>21%</div> <div>..</div> </div>
3	H	260	<div> <div>2%</div> <div>78%</div> <div>13%</div> <div>8%</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
11	PC1	L	901	-	-	-	X
12	GGD	M	902	-	-	-	X
6	BCL	L	850	-	-	-	X
6	BCL	L	851	-	-	-	X
6	BCL	L	853	-	-	-	X
6	BCL	M	852	-	-	-	X
7	BPH	L	855	-	-	-	X
7	BPH	M	854	-	-	-	X
8	U10	L	858	-	-	-	X
8	U10	M	857	-	-	-	X
9	SPO	M	859	-	-	-	X

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7323 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
			2408	1607	394	397	10			

- Molecule 3 is a protein called Photosynthetic Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1814	1160	311	334	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).

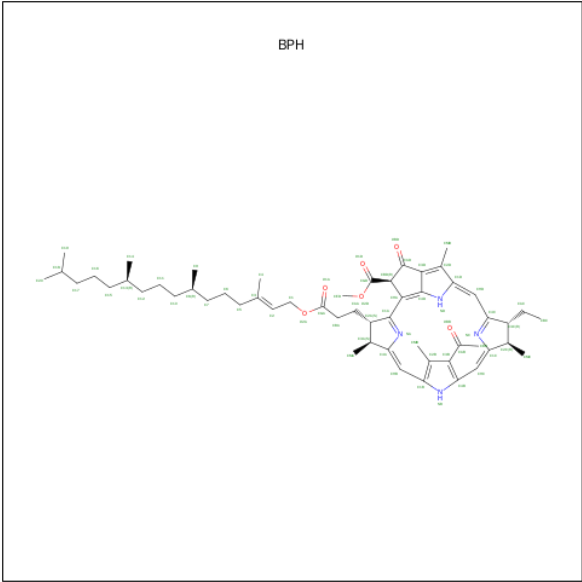
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Cl	0	0
			1	1		

- 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
			52	41	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		
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>).



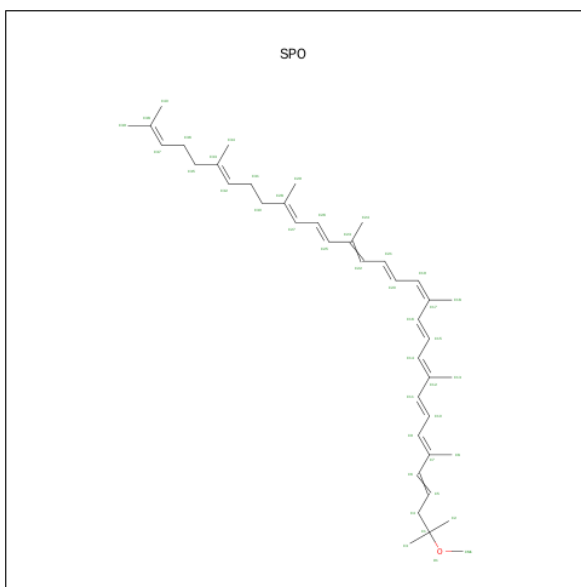
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	N	O	0	0
			65	55	4	6		
7	L	1	Total	C	N	O	0	0
			65	55	4	6		

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



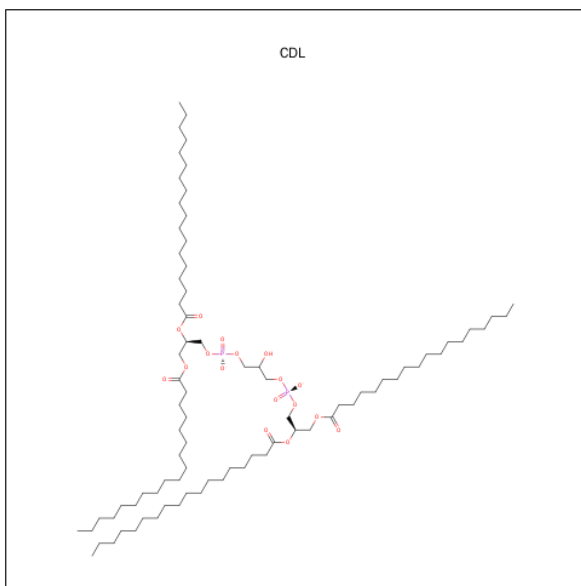
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	C	O	0	0
			48	44	4		
8	L	1	Total	C	O	0	0
			13	9	4		

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



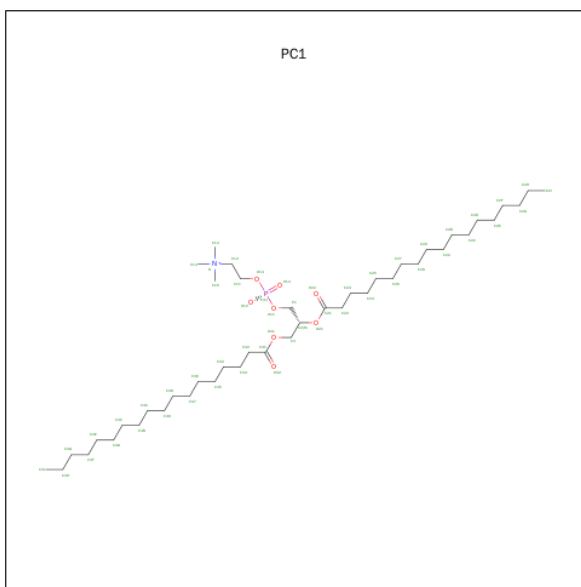
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 10 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



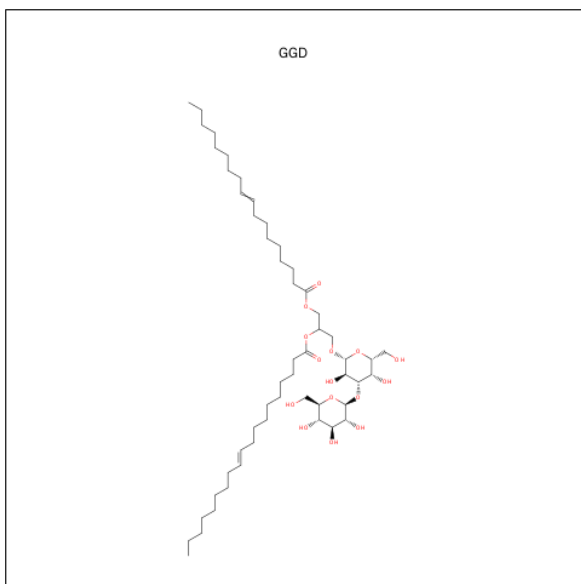
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 11 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	N	O	P	0	0
			43	33	1	8	1		

- Molecule 12 is NONADEC-10-ENOIC ACID 2-[3,4-DIHYDROXY-6-HYDROXYMETHYL-L-5-(3,4,5-TRIHYDROXY-6-HYDROXYMETHYL-TETRAHYDRO-PYRAN-2-YLOXY)-TETRAHYDRO-PYRAN-2-YLOXY]-1-OCTADEC-9-ENOYLOXYMETHYL-ETHYL ESTER (three-letter code: GGD) (formula:  $C_{52}H_{94}O_{15}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	M	1	Total	C	O	0	0
			57	42	15		



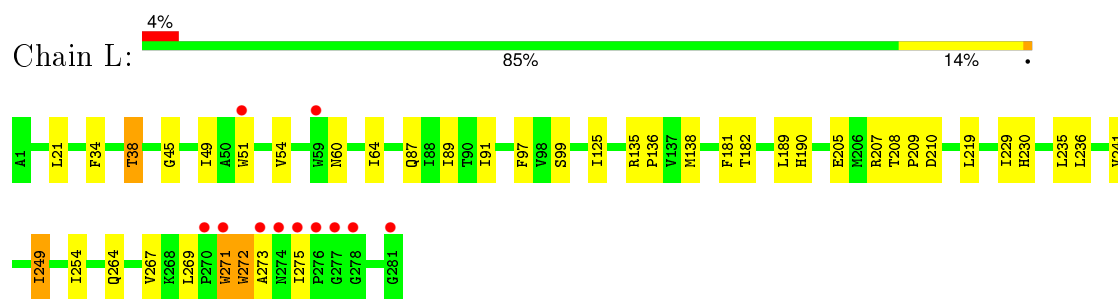
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	72	Total 72	O 72	0	0
13	L	63	Total 63	O 63	0	0
13	M	68	Total 68	O 68	0	0

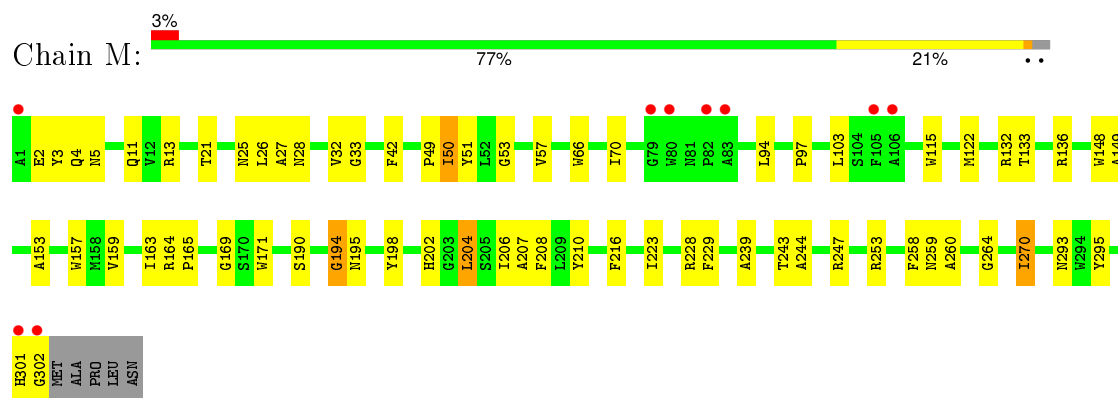
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

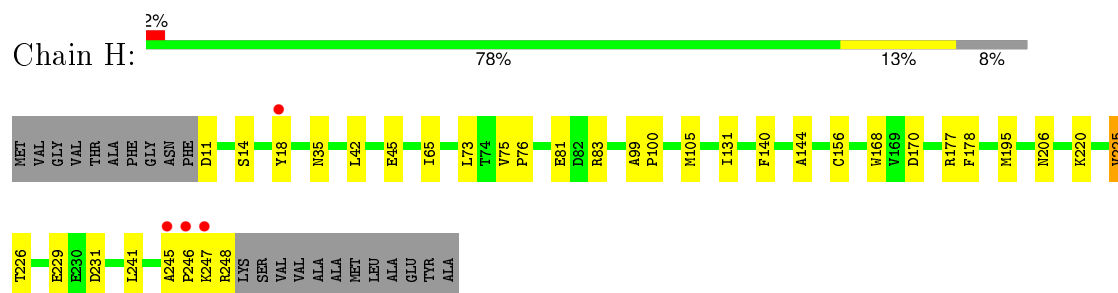
- Molecule 1: Photosynthetic Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	141.80Å 141.80Å 187.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.91 – 2.55 30.84 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.91-2.55) 96.9 (30.84-2.55)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.185 , 0.209 0.179 , 0.194	Depositor DCC
$R_{free}$ test set	6974 reflections (11.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 72.5	EDS
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 68925 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7323	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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, PC1, GGD, 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	0.40	0/2320	0.56	0/3175
2	M	0.40	0/2500	0.55	1/3413 (0.0%)
3	H	0.35	0/1862	0.61	0/2534
All	All	0.38	0/6682	0.57	1/9122 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	194	GLY	N-CA-C	-5.64	99.00	113.10

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	46	0
2	M	2408	0	2321	62	0
3	H	1814	0	1818	34	0
4	M	1	0	0	0	0
5	M	1	0	0	0	0
6	L	184	0	191	14	0
6	M	66	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	65	0	76	6	0
7	M	65	0	76	7	0
8	L	13	0	9	2	0
8	M	48	0	63	4	0
9	M	42	0	60	0	0
10	M	81	0	106	0	0
11	L	43	0	60	8	0
12	M	57	0	65	16	0
13	H	72	0	0	3	0
13	L	63	0	0	1	0
13	M	68	0	0	2	0
All	All	7323	0	7106	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)
11:L:901:PC1:C1	11:L:901:PC1:C2	1.74	1.64
11:L:901:PC1:C1	11:L:901:PC1:O11	1.74	1.35
2:M:202:HIS:O	2:M:206:ILE:HD13	1.78	0.84
11:L:901:PC1:C1	11:L:901:PC1:P	2.76	0.74
2:M:207:ALA:CB	12:M:902:GGD:OB3	2.36	0.73
2:M:253:ARG:HH22	12:M:902:GGD:C24	2.01	0.73
2:M:50:ILE:HD13	2:M:51:TYR:N	2.02	0.73
1:L:97:PHE:HB3	1:L:125:ILE:HD12	1.69	0.73
11:L:901:PC1:C1	11:L:901:PC1:C3	2.66	0.73
3:H:14:SER:O	3:H:18:TYR:HD1	1.72	0.73
1:L:49:ILE:HD13	1:L:89:ILE:HD13	1.70	0.72
1:L:34:PHE:O	1:L:38:THR:HG23	1.89	0.72
1:L:219:LEU:HD12	2:M:132:ARG:NH1	2.06	0.71
2:M:207:ALA:HB1	12:M:902:GGD:OB3	1.91	0.70
2:M:50:ILE:HD13	2:M:51:TYR:H	1.56	0.70
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.73	0.69
1:L:264:GLN:HA	1:L:267:VAL:HG12	1.75	0.68
6:L:853:BCL:HBA1	12:M:902:GGD:OB3	1.94	0.67
1:L:241:VAL:HG21	7:L:855:BPH:HAC2	1.76	0.67
2:M:228:ARG:NE	3:H:195:MET:HE3	2.10	0.66
1:L:271:TRP:N	1:L:271:TRP:CD1	2.61	0.65
2:M:195:ASN:HB3	2:M:198:TYR:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:TRP:O	1:L:54:VAL:HG22	1.97	0.64
1:L:235:LEU:HD22	2:M:42:PHE:CZ	2.32	0.64
7:L:855:BPH:HBB2	2:M:210:TYR:HB3	1.80	0.63
2:M:204:LEU:O	2:M:207:ALA:HB3	1.98	0.63
1:L:97:PHE:HB3	1:L:125:ILE:CD1	2.29	0.62
6:L:850:BCL:H2	7:M:854:BPH:HMB2	1.82	0.61
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.82	0.60
1:L:219:LEU:HA	2:M:132:ARG:HH12	1.65	0.60
12:M:902:GGD:C24	3:H:42:LEU:HD11	2.31	0.60
2:M:32:VAL:HG22	2:M:49:PRO:HD3	1.84	0.59
2:M:302:GLY:HA2	3:H:11:ASP:OD1	2.01	0.59
1:L:38:THR:HG22	1:L:99:SER:HB3	1.85	0.59
11:L:901:PC1:H11	11:L:901:PC1:C2	2.18	0.59
2:M:11:GLN:HB2	3:H:144:ALA:HB3	1.84	0.59
6:L:853:BCL:HMD2	6:M:852:BCL:HBB3	1.85	0.58
1:L:45:GLY:O	1:L:49:ILE:HG12	2.04	0.58
1:L:38:THR:HG22	1:L:99:SER:CB	2.35	0.57
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.85	0.57
2:M:207:ALA:HB2	12:M:902:GGD:OB3	2.04	0.57
7:L:855:BPH:HH1	7:L:855:BPH:HBB3	1.87	0.56
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.46	0.56
12:M:902:GGD:C24	3:H:42:LEU:HD21	2.36	0.56
1:L:190:HIS:HB2	1:L:229:ILE:HD11	1.88	0.55
6:L:850:BCL:HBB2	6:M:852:BCL:H111	1.88	0.55
1:L:219:LEU:HD12	2:M:132:ARG:HH11	1.72	0.55
6:L:853:BCL:H193	7:L:855:BPH:H111	1.88	0.55
2:M:243:THR:O	2:M:247:ARG:HG3	2.07	0.54
3:H:131:ILE:HD13	3:H:170:ASP:HA	1.89	0.54
2:M:190:SER:O	2:M:194:GLY:O	2.25	0.54
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.08	0.54
2:M:13:ARG:O	3:H:140:PHE:HA	2.07	0.54
2:M:97:PRO:HG2	2:M:171:TRP:HB2	1.90	0.54
2:M:253:ARG:HB2	2:M:259:ASN:HD22	1.72	0.54
2:M:208:PHE:CE1	12:M:902:GGD:OA4	2.61	0.53
1:L:181:PHE:HB3	7:M:854:BPH:CBB	2.38	0.53
8:M:857:U10:H202	12:M:902:GGD:HC31	1.90	0.53
2:M:28:ASN:HB2	2:M:51:TYR:CE1	2.43	0.53
2:M:208:PHE:HE1	12:M:902:GGD:OA4	1.92	0.53
1:L:264:GLN:HA	1:L:267:VAL:CG1	2.39	0.53
2:M:258:PHE:CE1	12:M:902:GGD:H151	2.44	0.52
2:M:25:ASN:OD1	2:M:27:ALA:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:LEU:HB3	8:L:858:U10:H4M3	1.91	0.52
1:L:272:TRP:HA	1:L:275:ILE:HG12	1.92	0.52
2:M:264:GLY:HA3	3:H:35:ASN:OD1	2.09	0.52
3:H:220:LYS:HE3	13:H:1054:HOH:O	2.10	0.52
3:H:65:ILE:HD12	3:H:65:ILE:N	2.24	0.52
1:L:49:ILE:CD1	1:L:89:ILE:HD13	2.37	0.52
1:L:219:LEU:O	2:M:132:ARG:NH1	2.41	0.52
3:H:45:GLU:HG3	13:H:1081:HOH:O	2.09	0.52
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.46	0.51
1:L:181:PHE:CD2	7:M:854:BPH:HBB1	2.45	0.51
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.46	0.51
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.92	0.51
11:L:901:PC1:H12	11:L:901:PC1:C2	2.18	0.51
2:M:206:ILE:HD12	6:M:852:BCL:HMA3	1.94	0.50
1:L:190:HIS:HB2	1:L:229:ILE:CD1	2.41	0.50
2:M:94:LEU:HD21	2:M:115:TRP:HA	1.93	0.50
1:L:181:PHE:HB3	7:M:854:BPH:HBB2	1.94	0.50
1:L:60:ASN:O	1:L:64:ILE:HG12	2.10	0.50
3:H:81:GLU:O	3:H:83:ARG:HG2	2.12	0.50
1:L:269:LEU:HD12	1:L:272:TRP:CZ2	2.47	0.50
2:M:149:ALA:HB2	2:M:270:ILE:HD11	1.94	0.49
1:L:219:LEU:HD11	2:M:133:THR:HG22	1.95	0.49
2:M:253:ARG:NH2	12:M:902:GGD:C24	2.74	0.49
3:H:248:ARG:O	3:H:248:ARG:HG2	2.12	0.49
3:H:105:MET:HE2	3:H:105:MET:HA	1.93	0.49
1:L:219:LEU:HA	2:M:132:ARG:NH1	2.27	0.48
1:L:34:PHE:O	1:L:38:THR:CG2	2.60	0.48
1:L:235:LEU:HD22	2:M:42:PHE:HZ	1.78	0.48
11:L:901:PC1:H2	11:L:901:PC1:C1	2.19	0.48
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.95	0.48
3:H:248:ARG:NH1	3:H:248:ARG:HB2	2.29	0.47
6:L:851:BCL:H122	7:L:855:BPH:H3A	1.97	0.47
3:H:241:LEU:HB2	13:H:1089:HOH:O	2.15	0.47
1:L:254:ILE:HD12	1:L:254:ILE:C	2.36	0.47
1:L:138:MET:SD	1:L:249:ILE:HD11	2.55	0.46
6:L:850:BCL:HAA2	6:L:850:BCL:HBD	1.98	0.46
2:M:21:THR:HG23	2:M:26:LEU:HD21	1.95	0.46
8:M:857:U10:H222	8:M:857:U10:H201	1.59	0.46
2:M:208:PHE:HE1	12:M:902:GGD:HO41	1.56	0.46
1:L:208:THR:HB	1:L:209:PRO:HD2	1.98	0.46
13:M:1166:HOH:O	3:H:195:MET:HE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:854:BPH:HHB	7:M:854:BPH:HMB1	1.79	0.45
2:M:208:PHE:HE1	12:M:902:GGD:HA62	1.81	0.45
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.98	0.45
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.52	0.45
1:L:235:LEU:HD23	11:L:901:PC1:C2B	2.47	0.45
1:L:229:ILE:O	1:L:229:ILE:HG12	2.16	0.45
6:M:852:BCL:HBD	6:M:852:BCL:HAA2	1.98	0.45
1:L:219:LEU:CA	2:M:132:ARG:HH12	2.29	0.45
6:L:850:BCL:HMD2	6:L:851:BCL:HBB3	1.99	0.44
2:M:153:ALA:HB2	7:M:854:BPH:HAC1	1.98	0.44
2:M:132:ARG:O	2:M:136:ARG:HG2	2.17	0.44
2:M:32:VAL:HG12	2:M:33:GLY:O	2.16	0.44
3:H:75:VAL:HA	3:H:76:PRO:C	2.38	0.44
3:H:131:ILE:CD1	3:H:177:ARG:HD2	2.47	0.44
6:L:853:BCL:HBA1	12:M:902:GGD:CB3	2.47	0.44
3:H:156:CYS:SG	3:H:248:ARG:HA	2.58	0.44
7:L:855:BPH:HHB	7:L:855:BPH:HMB1	1.85	0.43
6:L:850:BCL:H11	7:M:854:BPH:HBB2	2.01	0.43
2:M:66:TRP:O	2:M:70:ILE:HG12	2.18	0.43
2:M:239:ALA:O	3:H:73:LEU:HD22	2.17	0.43
6:L:850:BCL:HBB1	2:M:157:TRP:CD1	2.54	0.43
3:H:206:ASN:O	3:H:248:ARG:HD3	2.19	0.43
2:M:159:VAL:HA	2:M:163:ILE:HB	1.99	0.43
2:M:53:GLY:O	2:M:57:VAL:HG23	2.18	0.43
8:M:857:U10:H1M1	8:M:857:U10:H71	1.84	0.43
1:L:205:GLU:HG3	13:L:1122:HOH:O	2.18	0.43
2:M:293:ASN:OD1	2:M:295:TYR:HB3	2.19	0.43
2:M:202:HIS:O	2:M:206:ILE:CD1	2.58	0.42
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.54	0.42
1:L:229:ILE:HD12	8:L:858:U10:O4	2.19	0.42
6:L:853:BCL:H61	8:M:857:U10:H203	2.01	0.42
2:M:2:GLU:HG3	2:M:4:GLN:NE2	2.34	0.42
1:L:269:LEU:HD12	1:L:272:TRP:HZ2	1.84	0.42
3:H:168:TRP:CZ3	3:H:225:VAL:HG22	2.54	0.42
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.86	0.42
2:M:49:PRO:HG2	13:M:1045:HOH:O	2.19	0.41
2:M:103:LEU:HG	2:M:169:GLY:O	2.20	0.41
1:L:87:GLN:O	1:L:91:ILE:HG12	2.21	0.41
1:L:182:THR:HG22	1:L:236:LEU:HD13	2.03	0.41
2:M:195:ASN:HB3	2:M:198:TYR:CE2	2.55	0.41
6:L:851:BCL:H112	6:L:853:BCL:HBB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.21	0.41
6:M:852:BCL:HBC2	6:M:852:BCL:H2C	1.94	0.41
12:M:902:GGD:HC32	12:M:902:GGD:OC7	2.21	0.41
6:L:850:BCL:HMD2	6:L:851:BCL:CBB	2.51	0.41
3:H:156:CYS:HB3	3:H:206:ASN:O	2.21	0.40
1:L:269:LEU:O	1:L:273:ALA:HB2	2.21	0.40
3:H:245:ALA:C	3:H:247:LYS:H	2.23	0.40
1:L:190:HIS:ND1	1:L:229:ILE:HD13	2.37	0.40
3:H:131:ILE:HD12	3:H:177:ARG:HD2	2.03	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%)	267 (96%)	12 (4%)	0	100	100
2	M	300/307 (98%)	289 (96%)	10 (3%)	1 (0%)	46	66
3	H	236/260 (91%)	227 (96%)	9 (4%)	0	100	100
All	All	815/848 (96%)	783 (96%)	31 (4%)	1 (0%)	56	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	301	HIS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	220/220 (100%)	213 (97%)	7 (3%)	46	72
2	M	236/240 (98%)	232 (98%)	4 (2%)	68	88
3	H	193/208 (93%)	191 (99%)	2 (1%)	82	94
All	All	649/668 (97%)	636 (98%)	13 (2%)	63	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	LEU
1	L	38	THR
1	L	207	ARG
1	L	210	ASP
1	L	249	ILE
1	L	271	TRP
1	L	272	TRP
2	M	50	ILE
2	M	204	LEU
2	M	216	PHE
2	M	270	ILE
3	H	225	VAL
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	4	GLN
2	M	28	ASN
2	M	188	ASN
2	M	259	ASN
2	M	299	GLN

### 5.3.3 RNA ⓘ

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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	2	39,60,74	1.64	8 (20%)	40,98,115	2.08	11 (27%)
6	BCL	L	851	1	53,74,74	1.45	11 (20%)	57,115,115	1.67	10 (17%)
6	BCL	L	853	1	53,74,74	1.57	9 (16%)	57,115,115	2.16	14 (24%)
7	BPH	L	855	-	64,70,70	1.29	10 (15%)	73,101,101	1.84	14 (19%)
8	U10	L	858	-	13,13,63	2.99	4 (30%)	18,18,79	1.57	4 (22%)
11	PC1	L	901	-	42,42,53	2.40	12 (28%)	46,50,61	1.64	11 (23%)
6	BCL	M	852	2	53,74,74	1.36	7 (13%)	57,115,115	1.69	10 (17%)
7	BPH	M	854	-	64,70,70	1.36	9 (14%)	73,101,101	1.66	12 (16%)
8	U10	M	857	-	48,48,63	2.30	13 (27%)	58,61,79	2.35	21 (36%)
9	SPO	M	859	-	40,41,41	3.55	24 (60%)	45,50,50	2.71	16 (35%)
10	CDL	M	900	-	80,80,99	0.68	2 (2%)	82,92,111	0.93	3 (3%)
12	GGD	M	902	-	58,58,68	2.87	20 (34%)	72,72,82	4.26	35 (48%)

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	2	-	0/21/121/137	0/0/9/9
6	BCL	L	851	1	-	0/37/137/137	0/0/9/9
6	BCL	L	853	1	-	0/37/137/137	0/0/9/9
7	BPH	L	855	-	-	0/54/105/105	0/1/6/6
8	U10	L	858	-	-	0/4/24/87	0/1/1/1
11	PC1	L	901	-	-	0/46/46/57	0/0/0/0
6	BCL	M	852	2	-	0/37/137/137	0/0/9/9
7	BPH	M	854	-	-	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
10	CDL	M	900	-	-	0/91/91/110	0/0/0/0
12	GGD	M	902	-	-	1/47/87/97	0/2/2/2

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	902	GGD	OC6-CC4	-12.01	1.16	1.46
8	M	857	U10	C7-C8	-4.76	1.43	1.50
12	M	902	GGD	C24-C23	-4.04	1.31	1.49
12	M	902	GGD	OB6-CB6	-3.90	1.25	1.42
9	M	859	SPO	C4-C5	-3.78	1.44	1.50
11	L	901	PC1	P-O12	-3.48	1.40	1.54
9	M	859	SPO	C31-C32	-3.35	1.41	1.50
9	M	859	SPO	C11-C12	-3.19	1.38	1.45
12	M	902	GGD	CC6-CC4	-2.82	1.42	1.50
6	L	853	BCL	C3C-C4C	-2.81	1.48	1.51
7	L	855	BPH	C3D-CAD	-2.75	1.41	1.46
6	L	853	BCL	C3A-C2A	-2.68	1.46	1.54
12	M	902	GGD	OB3-CB3	-2.62	1.36	1.43
7	L	855	BPH	O2A-CGA	-2.41	1.26	1.33
7	M	854	BPH	C3D-CAD	-2.36	1.42	1.46
6	L	851	BCL	C3C-C4C	-2.36	1.48	1.51
7	M	854	BPH	C1B-C2B	-2.27	1.40	1.45
6	L	850	BCL	C3A-C2A	-2.19	1.48	1.54
7	L	855	BPH	C3A-C2A	-2.16	1.48	1.54
6	L	853	BCL	CAA-CBA	-2.15	1.45	1.52
12	M	902	GGD	OA1-CA1	-2.14	1.36	1.40
6	L	850	BCL	O2D-CGD	-2.09	1.27	1.33
9	M	859	SPO	C25-C23	-2.08	1.41	1.45
11	L	901	PC1	P-O11	-2.03	1.49	1.59
6	L	851	BCL	O2A-CGA	-2.02	1.27	1.33
11	L	901	PC1	C12-N	-2.01	1.44	1.51
7	M	854	BPH	O2A-CGA	-2.01	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	853	BCL	C3B-CAB	2.04	1.54	1.49
6	L	853	BCL	OBD-CAD	2.04	1.25	1.22
6	L	851	BCL	CBB-CAB	2.06	1.55	1.49
6	L	850	BCL	OBD-CAD	2.06	1.25	1.22
6	L	851	BCL	C3B-CAB	2.07	1.54	1.49
6	M	852	BCL	CBB-CAB	2.10	1.56	1.49
8	M	857	U10	C8-C9	2.10	1.37	1.33
8	M	857	U10	O4-C4	2.11	1.42	1.37
12	M	902	GGD	C22-C23	2.11	1.45	1.29
10	M	900	CDL	OA8-CA7	2.12	1.39	1.33
6	L	851	BCL	CAC-C3C	2.16	1.58	1.54
11	L	901	PC1	C2A-C29	2.17	1.67	1.51
6	L	851	BCL	OBD-CAD	2.19	1.25	1.22
7	M	854	BPH	CHA-C1A	2.21	1.42	1.37
7	L	855	BPH	C3B-CAB	2.22	1.53	1.46
6	L	851	BCL	CMD-C2D	2.24	1.56	1.51
10	M	900	CDL	CB3-CB4	2.30	1.57	1.50
6	L	850	BCL	C3B-CAB	2.33	1.55	1.49
7	L	855	BPH	CMD-C2D	2.34	1.56	1.51
9	M	859	SPO	C24-C23	2.35	1.55	1.50
6	M	852	BCL	C3B-CAB	2.48	1.55	1.49
12	M	902	GGD	OB1-CA3	2.50	1.50	1.43
9	M	859	SPO	C22-C23	2.52	1.39	1.35
11	L	901	PC1	O31-C3	2.53	1.50	1.45
6	M	852	BCL	CMD-C2D	2.55	1.57	1.51
7	L	855	BPH	CHA-C1A	2.56	1.43	1.37
8	L	858	U10	C4-C5	2.57	1.52	1.46
12	M	902	GGD	OC7-CC5	2.60	1.30	1.22
7	M	854	BPH	C3B-C2B	2.60	1.45	1.38
8	M	857	U10	C38-C39	2.60	1.40	1.32
7	M	854	BPH	CMD-C2D	2.61	1.57	1.51
7	L	855	BPH	C3B-C2B	2.68	1.46	1.38
11	L	901	PC1	C3-C2	2.68	1.58	1.50
9	M	859	SPO	C9-C7	2.71	1.39	1.35
7	L	855	BPH	C3D-C2D	2.72	1.46	1.40
12	M	902	GGD	C15-C14	2.74	1.62	1.52
9	M	859	SPO	C29-C28	2.77	1.57	1.50
6	M	852	BCL	CMB-C2B	2.81	1.57	1.51
12	M	902	GGD	CB4-CB5	2.83	1.59	1.53
9	M	859	SPO	C8-C7	2.85	1.57	1.50
11	L	901	PC1	P-O14	2.87	1.61	1.51
11	L	901	PC1	O22-C21	2.89	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	850	BCL	CMB-C2B	2.91	1.57	1.51
6	L	853	BCL	CMB-C2B	2.93	1.57	1.51
6	L	853	BCL	C3B-C2B	3.03	1.47	1.40
6	L	851	BCL	CMB-C2B	3.16	1.58	1.51
9	M	859	SPO	C37-C38	3.22	1.42	1.32
9	M	859	SPO	C10-C9	3.24	1.53	1.43
7	L	855	BPH	CMB-C2B	3.25	1.57	1.50
6	L	850	BCL	C3B-C2B	3.27	1.48	1.40
8	L	858	U10	C6-C5	3.27	1.54	1.44
7	M	854	BPH	C3D-C2D	3.34	1.48	1.40
6	L	851	BCL	C3B-C2B	3.35	1.48	1.40
9	M	859	SPO	C35-C33	3.35	1.58	1.51
7	L	855	BPH	C2-C3	3.38	1.39	1.33
12	M	902	GGD	C39-C38	3.40	1.51	1.31
6	M	852	BCL	C3B-C2B	3.42	1.48	1.40
8	M	857	U10	C23-C24	3.52	1.39	1.33
12	M	902	GGD	CA4-CA5	3.52	1.60	1.53
8	M	857	U10	C13-C14	3.53	1.39	1.33
12	M	902	GGD	C31-CC7	3.56	1.61	1.50
7	M	854	BPH	CMB-C2B	3.59	1.58	1.50
7	M	854	BPH	C2-C3	3.63	1.40	1.33
6	L	851	BCL	C2-C3	3.72	1.40	1.33
6	M	852	BCL	C2-C3	3.76	1.40	1.33
8	M	857	U10	C6-C5	3.77	1.57	1.46
8	L	858	U10	C4-C3	3.80	1.52	1.35
8	M	857	U10	C33-C34	3.81	1.40	1.33
9	M	859	SPO	C15-C14	3.84	1.55	1.43
6	L	850	BCL	C3D-C2D	3.84	1.49	1.40
9	M	859	SPO	O1-CM1	3.85	1.55	1.43
9	M	859	SPO	C19-C17	3.88	1.40	1.35
6	M	852	BCL	C3D-C2D	3.91	1.49	1.40
11	L	901	PC1	O31-C31	3.95	1.45	1.33
8	M	857	U10	C18-C19	4.03	1.40	1.33
8	M	857	U10	C7-C6	4.03	1.58	1.51
8	M	857	U10	C4-C3	4.04	1.53	1.35
8	M	857	U10	C28-C29	4.05	1.40	1.33
6	L	853	BCL	C3D-C2D	4.09	1.50	1.40
9	M	859	SPO	C14-C12	4.21	1.41	1.35
9	M	859	SPO	C32-C33	4.21	1.41	1.33
9	M	859	SPO	C13-C12	4.33	1.60	1.50
12	M	902	GGD	OB5-CB1	4.36	1.53	1.41
12	M	902	GGD	OB2-CB2	4.39	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	851	BCL	C3D-C2D	4.43	1.50	1.40
6	L	850	BCL	C2-C3	4.74	1.42	1.33
11	L	901	PC1	O21-C21	4.90	1.49	1.34
9	M	859	SPO	C26-C25	4.91	1.47	1.34
12	M	902	GGD	OC6-CC5	4.98	1.49	1.34
12	M	902	GGD	OB4-CB4	5.10	1.55	1.43
6	L	853	BCL	C2-C3	5.36	1.43	1.33
9	M	859	SPO	C27-C28	5.52	1.40	1.34
9	M	859	SPO	C21-C20	5.86	1.51	1.35
12	M	902	GGD	OB5-CB5	5.91	1.59	1.44
9	M	859	SPO	C6-C5	6.89	1.51	1.31
9	M	859	SPO	C10-C11	7.13	1.53	1.34
11	L	901	PC1	O11-C1	7.32	1.74	1.44
8	M	857	U10	C6-C1	7.49	1.52	1.35
12	M	902	GGD	OA1-CC3	8.09	1.58	1.43
8	L	858	U10	C6-C1	8.42	1.52	1.35
11	L	901	PC1	C1-C2	8.48	1.74	1.50
9	M	859	SPO	C15-C16	9.27	1.58	1.34

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	859	SPO	C25-C23-C22	-10.87	101.47	118.98
12	M	902	GGD	CC3-OA1-CA1	-7.37	98.34	113.82
6	L	853	BCL	CAA-C2A-C1A	-6.96	87.93	112.47
12	M	902	GGD	CA1-CA2-CA3	-6.62	98.08	110.00
6	L	850	BCL	CMB-C2B-C1B	-6.11	118.25	128.36
6	L	851	BCL	CMB-C2B-C1B	-5.96	118.51	128.36
6	L	853	BCL	CMB-C2B-C1B	-5.80	118.78	128.36
9	M	859	SPO	C18-C17-C19	-5.79	114.34	122.90
12	M	902	GGD	OB1-CA3-CA2	-5.70	92.45	107.17
6	M	852	BCL	CMB-C2B-C1B	-5.66	119.00	128.36
8	M	857	U10	C10-C9-C8	-5.55	112.61	123.50
12	M	902	GGD	C21-C22-C23	-5.50	80.89	133.31
8	M	857	U10	C15-C14-C13	-5.46	112.79	123.50
9	M	859	SPO	C20-C21-C22	-4.92	112.50	123.39
6	L	850	BCL	CAA-C2A-C1A	-4.66	96.05	112.47
7	L	855	BPH	O1D-CGD-CBD	-4.49	118.19	124.62
7	M	854	BPH	O1D-CGD-CBD	-4.45	118.24	124.62
9	M	859	SPO	C24-C23-C22	-4.41	116.38	122.90
8	M	857	U10	C25-C24-C23	-4.24	115.18	123.50
7	L	855	BPH	C4D-C3D-C2D	-4.08	101.82	107.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	857	U10	C35-C34-C33	-4.06	115.53	123.50
7	M	854	BPH	C4D-C3D-C2D	-3.97	101.95	107.08
6	L	853	BCL	CAA-C2A-C3A	-3.97	101.80	113.22
7	L	855	BPH	C5-C3-C2	-3.91	113.63	121.05
9	M	859	SPO	C4-C5-C6	-3.77	119.31	124.67
9	M	859	SPO	C11-C12-C14	-3.68	113.05	118.98
7	L	855	BPH	CHC-C4B-NB	-3.66	117.94	124.91
8	M	857	U10	C20-C19-C18	-3.56	116.51	123.50
9	M	859	SPO	C15-C14-C12	-3.55	122.06	127.20
12	M	902	GGD	CB6-CB5-CB4	-3.55	104.26	113.02
11	L	901	PC1	C25-C24-C23	-3.52	96.38	114.53
6	L	853	BCL	CAC-C3C-C2C	-3.51	105.31	114.13
6	L	853	BCL	O1D-CGD-CBD	-3.48	119.64	124.62
11	L	901	PC1	O21-C21-O22	-3.43	114.47	123.67
6	L	851	BCL	OBD-CAD-C3D	-3.42	121.38	128.35
6	L	853	BCL	OBD-CAD-C3D	-3.40	121.42	128.35
7	M	854	BPH	CHC-C4B-NB	-3.31	118.61	124.91
6	M	852	BCL	OBD-CAD-C3D	-3.31	121.61	128.35
8	L	858	U10	O5-C5-C4	-3.26	116.62	121.59
12	M	902	GGD	CB3-CB4-CB5	-3.21	104.60	110.20
12	M	902	GGD	OB5-CB5-CB4	-3.10	103.86	109.68
7	M	854	BPH	CMB-C2B-C1B	-3.10	120.01	125.06
12	M	902	GGD	OC9-CC7-C31	-3.08	111.39	123.72
6	L	850	BCL	O1D-CGD-CBD	-3.05	120.25	124.62
6	L	850	BCL	OBD-CAD-C3D	-3.02	122.19	128.35
12	M	902	GGD	C37-C38-C39	-2.98	104.61	125.34
7	L	855	BPH	CMB-C2B-C1B	-2.97	120.21	125.06
11	L	901	PC1	C28-C27-C26	-2.93	99.37	114.53
9	M	859	SPO	C15-C16-C17	-2.92	117.72	126.32
12	M	902	GGD	OB5-CB1-CB2	-2.74	104.65	110.28
12	M	902	GGD	OC6-CC5-OC7	-2.69	116.45	123.67
6	M	852	BCL	CHA-C1A-NA	-2.69	119.44	126.06
7	M	854	BPH	CBB-CAB-C3B	-2.69	114.55	120.52
12	M	902	GGD	C36-C35-C34	-2.63	100.93	114.53
8	M	857	U10	C30-C29-C28	-2.47	118.66	123.50
8	M	857	U10	O5-C5-C4	-2.45	115.48	120.79
6	L	851	BCL	CHA-C1A-NA	-2.44	120.06	126.06
8	M	857	U10	C1-C6-C5	-2.43	117.35	120.12
12	M	902	GGD	OB3-CB3-CB4	-2.41	104.92	110.34
11	L	901	PC1	C3-C2-C1	-2.39	106.47	112.07
10	M	900	CDL	CB6-CB4-CB3	-2.37	106.52	112.07
7	L	855	BPH	CBB-CAB-C3B	-2.30	115.41	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	859	SPO	C34-C33-C35	-2.24	111.98	115.41
8	M	857	U10	C31-C32-C33	-2.20	105.92	111.69
9	M	859	SPO	C10-C9-C7	-2.19	124.03	127.20
12	M	902	GGD	OB2-CB2-CB1	-2.15	105.31	110.02
6	L	851	BCL	CMA-C3A-C2A	-2.14	104.87	114.35
12	M	902	GGD	C35-C34-C33	-2.13	103.53	114.53
6	L	850	BCL	CHA-C1A-NA	-2.13	120.82	126.06
9	M	859	SPO	C8-C7-C6	-2.09	114.62	118.10
7	L	855	BPH	C1C-NC-C4C	-2.09	108.30	110.44
6	M	852	BCL	CAC-C3C-C2C	-2.06	108.95	114.13
12	M	902	GGD	OB1-CB1-CB2	-2.04	103.13	108.10
11	L	901	PC1	C23-C22-C21	-2.02	105.64	113.59
6	M	852	BCL	O2A-CGA-CBA	2.01	118.01	111.90
6	M	852	BCL	C2A-C1A-CHA	2.12	127.78	123.89
6	L	851	BCL	CBC-CAC-C3C	2.12	118.75	113.57
11	L	901	PC1	C2B-C2A-C29	2.15	130.34	113.44
6	L	851	BCL	O2A-CGA-CBA	2.18	118.55	111.90
8	L	858	U10	C4M-O4-C4	2.19	124.38	116.61
12	M	902	GGD	CA3-CA4-CA5	2.19	114.58	109.61
12	M	902	GGD	C20-C21-C22	2.19	123.94	112.45
8	M	857	U10	C36-C34-C33	2.20	125.22	121.05
9	M	859	SPO	C13-C12-C11	2.23	121.80	118.10
12	M	902	GGD	C16-C15-C14	2.23	121.48	113.29
6	L	850	BCL	O2A-CGA-CBA	2.23	118.71	111.90
7	L	855	BPH	CMB-C2B-C3B	2.24	133.25	128.04
6	L	850	BCL	C2A-C1A-CHA	2.24	128.02	123.89
7	L	855	BPH	C3D-CAD-CBD	2.25	110.78	107.60
11	L	901	PC1	O12-P-O11	2.25	119.83	108.46
6	M	852	BCL	C3D-CAD-CBD	2.34	110.91	107.60
7	M	854	BPH	CMB-C2B-C3B	2.38	133.59	128.04
10	M	900	CDL	CB4-OB6-CB5	2.39	123.63	117.89
6	L	851	BCL	C2A-C1A-CHA	2.40	128.30	123.89
7	M	854	BPH	CED-O2D-CGD	2.42	121.67	115.99
7	L	855	BPH	CED-O2D-CGD	2.45	121.73	115.99
8	M	857	U10	C10-C9-C11	2.46	119.17	115.41
6	L	853	BCL	C3A-C2A-C1A	2.47	105.69	101.50
8	L	858	U10	C6-C5-C4	2.48	121.33	115.45
9	M	859	SPO	C18-C17-C16	2.51	122.27	118.10
12	M	902	GGD	OA5-CA5-CA4	2.51	114.39	109.68
8	M	857	U10	C35-C34-C36	2.51	119.25	115.41
8	L	858	U10	C1M-C1-C2	2.56	119.39	117.50
8	M	857	U10	C4M-O4-C4	2.56	125.70	116.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	902	GGD	OB1-CB1-OB5	2.56	117.17	110.68
9	M	859	SPO	O1-C1-C4	2.58	112.19	105.87
8	M	857	U10	C11-C12-C13	2.63	118.58	111.69
8	M	857	U10	C30-C29-C31	2.65	119.45	115.41
6	L	853	BCL	C2A-C1A-CHA	2.65	128.76	123.89
7	M	854	BPH	C6-C5-C3	2.70	118.40	112.48
9	M	859	SPO	C16-C17-C19	2.73	123.39	118.98
8	M	857	U10	C21-C19-C18	2.74	126.24	121.05
7	M	854	BPH	C3D-CAD-CBD	2.76	111.50	107.60
6	L	850	BCL	O2D-CGD-CBD	2.76	115.08	111.30
6	L	853	BCL	CBA-CAA-C2A	3.01	122.22	113.73
8	M	857	U10	C25-C24-C26	3.02	120.02	115.41
12	M	902	GGD	CB4-CB3-CB2	3.07	116.51	110.79
6	L	851	BCL	C6-C5-C3	3.07	119.22	112.48
6	L	850	BCL	CBA-CAA-C2A	3.13	122.57	113.73
11	L	901	PC1	C24-C23-C22	3.14	124.81	113.29
6	L	853	BCL	C6-C5-C3	3.14	119.38	112.48
11	L	901	PC1	P-O13-C11	3.14	139.45	121.50
6	L	853	BCL	O2A-CGA-CBA	3.37	122.16	111.90
6	L	853	BCL	O2D-CGD-CBD	3.38	115.94	111.30
6	L	850	BCL	CED-O2D-CGD	3.40	123.97	115.99
11	L	901	PC1	O21-C2-C1	3.49	120.65	108.36
9	M	859	SPO	C8-C7-C9	3.50	128.07	122.90
8	M	857	U10	C7-C8-C9	3.56	132.73	126.70
12	M	902	GGD	OB5-CB5-CB6	3.59	115.43	106.36
12	M	902	GGD	OC6-CC5-C14	3.60	119.35	111.53
10	M	900	CDL	OB8-CB6-CB4	3.62	118.44	108.69
8	M	857	U10	C11-C9-C8	3.78	128.22	121.05
6	L	853	BCL	CED-O2D-CGD	3.80	124.91	115.99
11	L	901	PC1	O21-C21-C22	3.94	120.10	111.53
6	L	851	BCL	CED-O2D-CGD	4.05	125.48	115.99
7	L	855	BPH	O2D-CGD-CBD	4.06	116.87	111.30
6	M	852	BCL	CED-O2D-CGD	4.10	125.61	115.99
12	M	902	GGD	OC6-CC4-CC3	4.12	122.87	108.36
6	M	852	BCL	CMB-C2B-C3B	4.27	133.44	125.09
12	M	902	GGD	OC8-CC6-CC4	4.29	120.25	108.69
7	M	854	BPH	C4-C3-C5	4.30	121.98	115.41
6	L	851	BCL	CMB-C2B-C3B	4.54	133.97	125.09
6	L	853	BCL	CMB-C2B-C3B	4.55	133.98	125.09
6	L	850	BCL	CMB-C2B-C3B	4.62	134.13	125.09
7	M	854	BPH	O2D-CGD-CBD	4.63	117.66	111.30
7	M	854	BPH	C3C-C4C-NC	4.64	112.58	107.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	852	BCL	C6-C5-C3	4.66	122.72	112.48
12	M	902	GGD	OB1-CA3-CA4	4.72	119.35	107.17
12	M	902	GGD	OC8-CC7-C31	4.88	126.78	111.90
7	L	855	BPH	C3C-C4C-NC	4.91	112.85	107.93
8	M	857	U10	C15-C14-C16	5.07	123.16	115.41
12	M	902	GGD	OC6-CC4-CC6	5.15	126.51	108.36
7	L	855	BPH	C6-C5-C3	5.20	123.89	112.48
7	L	855	BPH	C4-C3-C5	6.04	124.63	115.41
12	M	902	GGD	CC6-OC8-CC7	6.49	135.00	116.85
8	M	857	U10	C7-C6-C5	6.55	126.26	118.56
12	M	902	GGD	C15-C14-CC5	7.16	141.73	113.59
12	M	902	GGD	C32-C31-CC7	7.38	142.59	113.59
12	M	902	GGD	CC4-OC6-CC5	9.52	140.74	117.89
12	M	902	GGD	OA1-CC3-CC4	16.66	150.62	110.99
12	M	902	GGD	CB1-OB1-CA3	18.28	165.77	118.01

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	902	GGD	CA1-OA1-CC3-CC4

There are no ring outliers.

10 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	850	BCL	7	0
6	L	851	BCL	4	0
6	L	853	BCL	6	0
7	L	855	BPH	6	0
8	L	858	U10	2	0
11	L	901	PC1	8	0
6	M	852	BCL	5	0
7	M	854	BPH	7	0
8	M	857	U10	4	0
12	M	902	GGD	16	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 ⓘ

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%)	-0.47	11 (3%) 43 49	15, 29, 64, 80	0
2	M	302/307 (98%)	-0.31	9 (2%) 54 60	13, 34, 67, 79	0
3	H	238/260 (91%)	-0.46	4 (1%) 73 77	20, 33, 53, 80	0
All	All	821/848 (96%)	-0.41	24 (2%) 55 61	13, 32, 64, 80	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	281	GLY	5.2
3	H	18	TYR	5.2
2	M	1	ALA	4.9
2	M	302	GLY	4.9
1	L	59	TRP	4.6
3	H	246	PRO	4.0
3	H	247	LYS	3.6
1	L	276	PRO	3.5
1	L	270	PRO	3.4
3	H	245	ALA	3.1
1	L	271	TRP	3.1
2	M	301	HIS	3.0
2	M	82	PRO	2.9
1	L	277	GLY	2.7
1	L	278	GLY	2.7
2	M	105	PHE	2.6
1	L	275	ILE	2.5
1	L	51	TRP	2.4
2	M	80	TRP	2.4
2	M	83	ALA	2.3
1	L	274	ASN	2.3
2	M	106	ALA	2.1
2	M	79	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	273	ALA	2.0

## 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 [i](#)

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
8	U10	L	858	13/63	0.78	0.46	17.23	55,56,57,59	13
12	GGD	M	902	57/67	0.66	0.36	9.16	66,79,80,80	0
11	PC1	L	901	43/54	0.77	0.43	7.66	65,79,80,80	0
7	BPH	M	854	65/65	0.88	0.21	4.10	30,35,80,80	0
6	BCL	L	850	52/66	0.94	0.18	3.54	23,28,54,56	0
8	U10	M	857	48/63	0.90	0.23	2.96	27,39,67,68	0
6	BCL	L	853	66/66	0.94	0.19	2.90	11,17,52,59	0
7	BPH	L	855	65/65	0.95	0.17	2.60	18,23,33,43	0
6	BCL	L	851	66/66	0.95	0.17	2.59	16,23,36,44	0
9	SPO	M	859	42/42	0.84	0.24	2.31	34,47,65,68	0
6	BCL	M	852	66/66	0.95	0.17	2.30	19,24,56,69	0
10	CDL	M	900	81/100	0.89	0.19	1.37	55,67,78,80	0
4	FE	M	856	1/1	1.00	0.06	-3.56	18,18,18,18	0
5	CL	M	2000	1/1	0.88	0.26	-	80,80,80,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.