



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:58 AM GMT

PDB ID : 2JJ0  
Title : PHOTOSYNTHETIC REACTION CENTER MUTANT WITH ALA M248  
REPLACED WITH TRP (CHAIN M, AM248W)  
Authors : Fyfe, P.K.; Potter, J.A.; Cheng, J.; Williams, C.M.; Watson, A.J.; Jones, M.R.  
Deposited on : 2007-07-03  
Resolution : 2.80 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

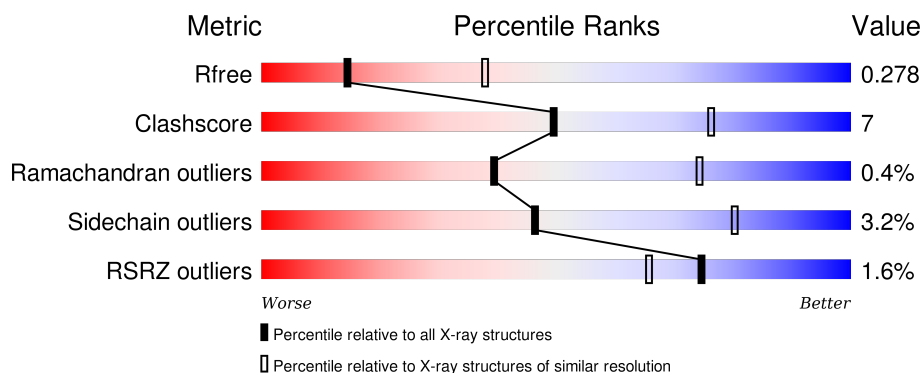
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	H	260	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 79%; height: 10px; background-color: green;"></div> <div style="width: 10%; height: 10px; background-color: yellow;"></div> <div style="width: 10%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>79%</span> <span>10%</span> <span>10%</span> </div> </div>
2	L	281	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>2%</span> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 15%; height: 10px; background-color: yellow;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>84%</span> <span>15%</span> <span>.</span> </div> </div>
3	M	308	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>%</span> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <div style="display: flex; justify-content: space-between; align-items: center;"> <span>87%</span> <span>11%</span> <span>.</span> </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	U10	L	1286	-	-	-	X
7	CDL	M	1305	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7111 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called REACTION CENTER PROTEIN H CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	235	Total	C	N	O	S	0	1	0
			1796	1148	305	334	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	1	0
			2244	1516	356	364	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	301	Total	C	N	O	S	0	0	0
			2412	1612	394	396	10			

There is a discrepancy between the modelled and reference sequences:

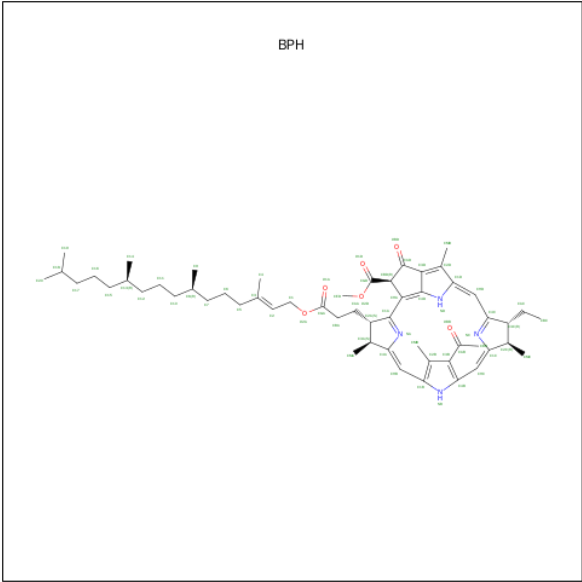
Chain	Residue	Modelled	Actual	Comment	Reference
M	248	TRP	ALA	ENGINEERED MUTATION	UNP P0C0Y9

- Molecule 4 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
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
4	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: C<sub>55</sub>H<sub>76</sub>N<sub>4</sub>O<sub>6</sub>).



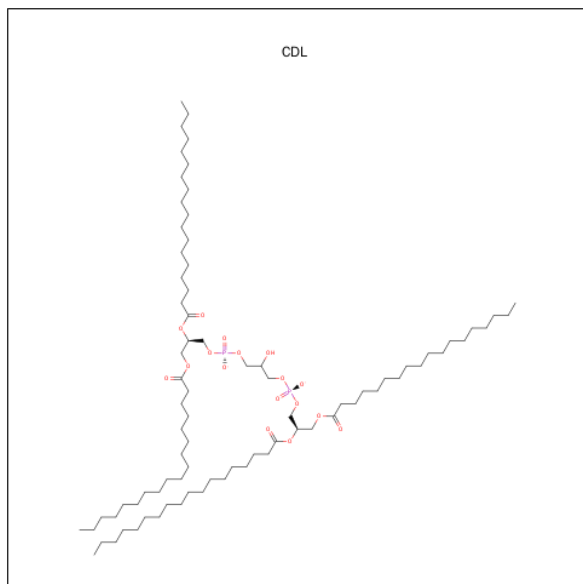
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 6 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			17	13	4		

- Molecule 7 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).

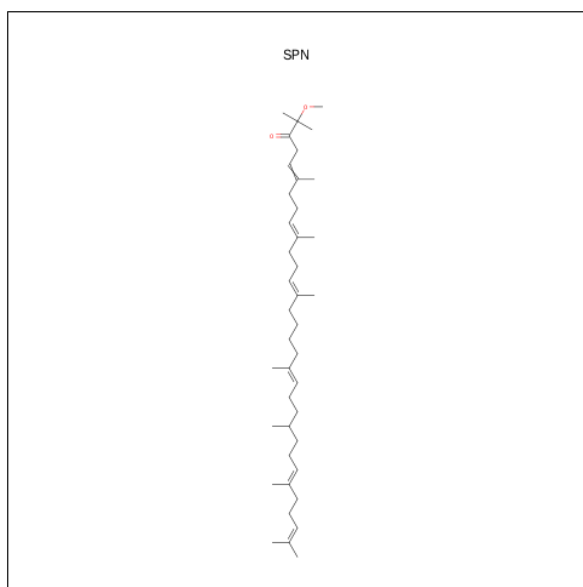


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	M	1	Total	C	O	P	0	0
			81	62	17	2		

- Molecule 8 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 9 is SPEROIDENONE (three-letter code: SPN) (formula: C<sub>41</sub>H<sub>70</sub>O<sub>2</sub>).



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

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	H	55	Total	O	0	0
			55	55		

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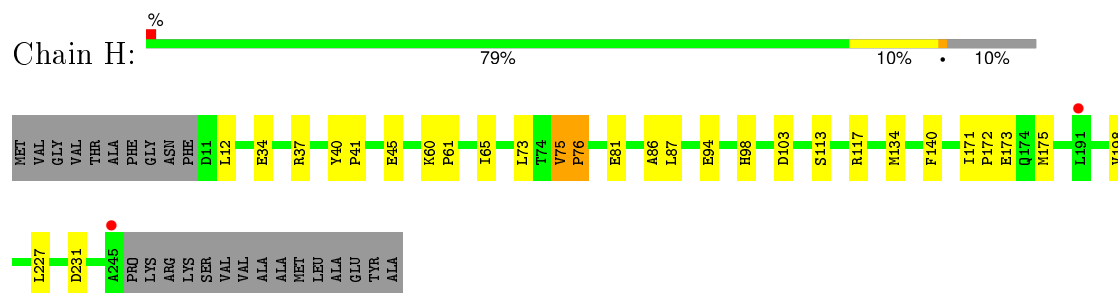
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	L	23	Total 23	O 23	0	0
11	M	44	Total 44	O 44	0	0



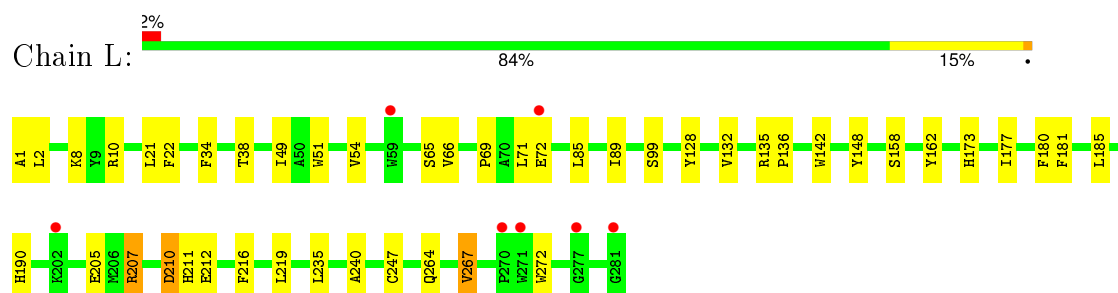
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

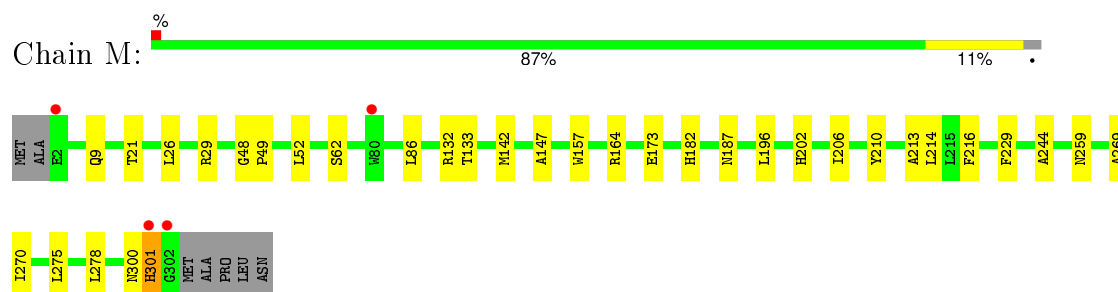
#### • Molecule 1: REACTION CENTER PROTEIN H CHAIN



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.81Å 139.81Å 185.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.90 – 2.80 25.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (27.90-2.80) 99.0 (25.41-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.203 , 0.245 0.238 , 0.278	Depositor DCC
$R_{free}$ test set	2573 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.8	EDS
Estimated twinning fraction	0.019 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 51452 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7111	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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

### 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, SPN, U10

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	H	0.64	0/1843	0.74	1/2509 (0.0%)
2	L	0.61	0/2333	0.63	0/3194
3	M	0.59	0/2506	0.65	1/3422 (0.0%)
All	All	0.61	0/6682	0.67	2/9125 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	2
3	M	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	103	ASP	CB-CG-OD1	5.17	122.95	118.30
3	M	29	ARG	NE-CZ-NH2	-5.13	117.74	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	40	TYR	Peptide
1	H	75	VAL	Peptide
3	M	300	ASN	Peptide

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Mol	Chain	Res	Type	Group
3	M	48	GLY	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1796	0	1790	20	0
2	L	2244	0	2196	33	0
3	M	2412	0	2318	28	0
4	L	198	0	222	17	0
4	M	66	0	74	7	0
5	L	65	0	76	7	0
5	M	65	0	76	8	0
6	L	17	0	15	2	0
7	M	81	0	106	2	0
8	M	1	0	0	0	0
9	M	43	0	69	9	0
10	M	1	0	0	0	0
11	H	55	0	0	1	0
11	L	23	0	0	0	0
11	M	44	0	0	1	0
All	All	7111	0	6942	99	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (99) 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)
3:M:275:LEU:HD23	3:M:278:LEU:HD23	1.53	0.88
4:L:1283:BCL:HMB1	4:L:1283:BCL:HBB3	1.61	0.80
5:L:1285:BPH:HHC	5:L:1285:BPH:HBB3	1.62	0.80
5:M:1307:BPH:HHC	5:M:1307:BPH:HBB3	1.64	0.79
2:L:181:PHE:CD2	5:M:1307:BPH:HBB1	2.20	0.77
1:H:41:PRO:HD2	11:H:2008:HOH:O	1.85	0.77
2:L:181:PHE:HB3	5:M:1307:BPH:HBB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1285:BPH:HBB2	3:M:210:TYR:HB3	1.71	0.73
4:L:1283:BCL:HMB1	4:L:1283:BCL:CBB	2.18	0.73
3:M:157:TRP:CD1	9:M:1308:SPN:H202	2.24	0.73
1:H:173[B]:GLU:OE2	1:H:175:MET:HE3	1.91	0.70
1:H:198:VAL:H	3:M:9:GLN:HE22	1.39	0.69
1:H:198:VAL:H	3:M:9:GLN:NE2	1.91	0.67
3:M:133:THR:HG21	3:M:147:ALA:HA	1.78	0.66
4:L:1284:BCL:HMD1	3:M:206:ILE:HD13	1.78	0.66
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.77	0.65
2:L:264:GLN:HA	2:L:267:VAL:HG13	1.77	0.65
1:H:61:PRO:HA	1:H:76:PRO:HD3	1.77	0.65
2:L:21:LEU:HD23	2:L:22:PHE:CE1	2.33	0.63
4:L:1284:BCL:CBB	4:L:1284:BCL:HMB1	2.28	0.63
2:L:38:THR:HG22	2:L:99:SER:HB2	1.80	0.62
3:M:133:THR:CG2	3:M:147:ALA:HA	2.30	0.61
4:L:1284:BCL:HBB2	4:L:1284:BCL:HMB1	1.82	0.61
1:H:37:ARG:NH2	1:H:60:LYS:O	2.33	0.61
2:L:71:LEU:H	2:L:71:LEU:HD12	1.66	0.60
2:L:190:HIS:HA	6:L:1286:U10:O2	2.03	0.59
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.86	0.58
1:H:173[B]:GLU:OE2	1:H:175:MET:CE	2.51	0.58
4:L:1282:BCL:H62	4:M:1304:BCL:H203	1.84	0.58
2:L:51:TRP:O	2:L:54:VAL:HG22	2.04	0.57
4:L:1282:BCL:C6	4:M:1304:BCL:H203	2.34	0.57
3:M:157:TRP:NE1	9:M:1308:SPN:H202	2.19	0.56
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.87	0.56
4:L:1282:BCL:HMB1	4:L:1282:BCL:HBB2	1.88	0.55
3:M:133:THR:HG22	3:M:147:ALA:HB2	1.87	0.55
1:H:34:GLU:O	1:H:37:ARG:HG3	2.08	0.54
4:M:1304:BCL:CBB	4:M:1304:BCL:HMB1	2.38	0.54
4:L:1282:BCL:HMB1	4:L:1282:BCL:CBB	2.38	0.53
2:L:38:THR:HG22	2:L:99:SER:CB	2.37	0.53
1:H:117:ARG:NH2	1:H:227:LEU:HD22	2.25	0.52
2:L:128:TYR:CE2	2:L:132:VAL:HG21	2.44	0.52
9:M:1308:SPN:H32	9:M:1308:SPN:HMA3	1.91	0.52
1:H:86:ALA:O	1:H:87:LEU:HD23	2.10	0.52
4:L:1282:BCL:CAB	9:M:1308:SPN:H162	2.40	0.52
2:L:207:ARG:HG3	3:M:142:MET:HG2	1.92	0.51
3:M:164:ARG:HH12	3:M:173:GLU:HG3	1.75	0.51
1:H:45:GLU:HG3	1:H:94:GLU:OE2	2.11	0.51
4:L:1282:BCL:C3B	9:M:1308:SPN:H152	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:1285:BPH:HBB1	3:M:210:TYR:CD2	2.46	0.51
4:L:1282:BCL:H141	9:M:1308:SPN:H101	1.92	0.50
4:M:1304:BCL:H202	5:M:1307:BPH:HMA3	1.92	0.50
2:L:219:LEU:HD12	3:M:132:ARG:NH1	2.27	0.50
3:M:270:ILE:HD13	7:M:1305:CDL:H311	1.94	0.50
3:M:157:TRP:CE2	9:M:1308:SPN:HM73	2.47	0.49
2:L:181:PHE:HB3	5:M:1307:BPH:CBB	2.40	0.48
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.46	0.48
2:L:177:ILE:HG12	4:L:1283:BCL:HMB3	1.95	0.47
5:L:1285:BPH:CMC	3:M:213:ALA:HB3	2.44	0.47
3:M:278:LEU:HD13	7:M:1305:CDL:H391	1.97	0.47
1:H:87:LEU:HD13	1:H:98:HIS:HB2	1.95	0.47
3:M:206:ILE:HG12	4:M:1304:BCL:HMB3	1.97	0.47
2:L:34:PHE:O	2:L:38:THR:HG23	2.14	0.47
1:H:140:PHE:CE2	1:H:171:ILE:HG23	2.50	0.47
2:L:85:LEU:O	2:L:89:ILE:HG13	2.15	0.47
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.49	0.47
1:H:65:ILE:HB	2:L:205:GLU:HA	1.98	0.46
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.97	0.46
2:L:210:ASP:OD1	2:L:210:ASP:N	2.49	0.46
2:L:173:HIS:CE1	2:L:177:ILE:HD11	2.51	0.46
1:H:61:PRO:HA	1:H:76:PRO:CD	2.46	0.46
2:L:207:ARG:HB3	2:L:211:HIS:CG	2.51	0.46
4:L:1282:BCL:OBB	9:M:1308:SPN:HM63	2.16	0.45
2:L:66:VAL:HG11	2:L:89:ILE:HD12	1.97	0.45
5:L:1285:BPH:HHC	5:L:1285:BPH:CBB	2.40	0.45
1:H:117:ARG:CZ	1:H:227:LEU:HD22	2.47	0.45
2:L:1:ALA:O	2:L:2:LEU:HD23	2.17	0.44
1:H:73:LEU:HG	1:H:75:VAL:HG13	2.00	0.44
1:H:171:ILE:HB	1:H:172:PRO:CD	2.48	0.43
4:L:1282:BCL:C14	9:M:1308:SPN:H101	2.49	0.42
3:M:133:THR:HG22	3:M:147:ALA:CB	2.49	0.42
5:M:1307:BPH:CBB	5:M:1307:BPH:HHC	2.44	0.42
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.55	0.42
4:L:1284:BCL:CMD	3:M:206:ILE:HD13	2.47	0.42
5:L:1285:BPH:CHC	5:L:1285:BPH:HBB3	2.43	0.42
3:M:259:ASN:ND2	11:M:2036:HOH:O	2.52	0.42
4:M:1304:BCL:HBB3	4:M:1304:BCL:HMB1	2.02	0.41
2:L:128:TYR:O	2:L:132:VAL:HG22	2.20	0.41
5:M:1307:BPH:HBB3	5:M:1307:BPH:CHC	2.43	0.41
4:L:1282:BCL:H61	4:M:1304:BCL:H203	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:202:HIS:CE1	3:M:206:ILE:HD11	2.55	0.41
2:L:2:LEU:CD2	2:L:10:ARG:CZ	2.98	0.41
1:H:75:VAL:O	1:H:75:VAL:HG23	2.20	0.41
2:L:212:GLU:OE2	6:L:1286:U10:H3M2	2.21	0.41
1:H:81:GLU:OE2	2:L:8:LYS:NZ	2.31	0.41
5:M:1307:BPH:H4C1	5:M:1307:BPH:H6C1	1.58	0.41
2:L:65:SER:HA	2:L:148:TYR:O	2.20	0.41
5:L:1285:BPH:ND	3:M:214:LEU:HD13	2.36	0.40
3:M:269:ALA:O	3:M:270:ILE:C	2.59	0.40
2:L:49:ILE:HG13	2:L:89:ILE:HD13	2.03	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	H	234/260 (90%)	224 (96%)	9 (4%)	1 (0%)	39	74
2	L	280/281 (100%)	265 (95%)	15 (5%)	0	100	100
3	M	299/308 (97%)	284 (95%)	13 (4%)	2 (1%)	26	62
All	All	813/849 (96%)	773 (95%)	37 (5%)	3 (0%)	39	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	49	PRO
3	M	301	HIS
1	H	76	PRO

### 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	H	191/208 (92%)	187 (98%)	4 (2%)	61	90
2	L	221/220 (100%)	211 (96%)	10 (4%)	34	68
3	M	237/242 (98%)	230 (97%)	7 (3%)	48	82
All	All	649/670 (97%)	628 (97%)	21 (3%)	46	80

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	12	LEU
1	H	113	SER
1	H	134	MET
1	H	231	ASP
2	L	72	GLU
2	L	158	SER
2	L	185	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	235	LEU
2	L	247	CYS
2	L	267	VAL
2	L	272	TRP
3	M	52	LEU
3	M	62	SER
3	M	86	LEU
3	M	182	HIS
3	M	196	LEU
3	M	216	PHE
3	M	301	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:



Mol	Chain	Res	Type
1	H	68	HIS
2	L	183	ASN
2	L	280	ASN
3	M	4	GLN
3	M	9	GLN
3	M	28	ASN
3	M	187	ASN
3	M	193	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	$\# Z  > 2$
4	BCL	L	1282	3	53,74,74	0.68	0	57,115,115	1.51	13 (22%)
4	BCL	L	1283	2	53,74,74	0.71	0	57,115,115	0.97	3 (5%)
4	BCL	L	1284	2	53,74,74	0.87	1 (1%)	57,115,115	1.86	12 (21%)
5	BPH	L	1285	-	64,70,70	0.73	0	73,101,101	1.24	6 (8%)
6	U10	L	1286	-	17,17,63	1.81	2 (11%)	19,23,79	1.24	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	BCL	M	1304	3	53,74,74	0.70	1 (1%)	57,115,115	1.19	6 (10%)
7	CDL	M	1305	-	80,80,99	1.08	4 (5%)	82,92,111	1.13	7 (8%)
5	BPH	M	1307	-	64,70,70	0.76	1 (1%)	73,101,101	1.50	11 (15%)
9	SPN	M	1308	-	41,42,42	3.79	15 (36%)	41,52,52	2.51	20 (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
4	BCL	L	1282	3	-	0/37/137/137	0/0/9/9
4	BCL	L	1283	2	-	0/37/137/137	0/0/9/9
4	BCL	L	1284	2	-	0/37/137/137	0/0/9/9
5	BPH	L	1285	-	-	0/54/105/105	0/1/6/6
6	U10	L	1286	-	-	0/8/32/87	0/1/1/1
4	BCL	M	1304	3	-	0/37/137/137	0/0/9/9
7	CDL	M	1305	-	-	0/91/91/110	0/0/0/0
5	BPH	M	1307	-	-	0/54/105/105	0/1/6/6
9	SPN	M	1308	-	-	0/50/51/51	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	1308	SPN	C3-C4	-8.90	1.36	1.50
9	M	1308	SPN	C10-C9	-7.18	1.35	1.51
9	M	1308	SPN	C14-C13	-6.85	1.36	1.51
9	M	1308	SPN	C6-C5	-6.75	1.36	1.51
9	M	1308	SPN	C17-C18	-6.45	1.36	1.51
9	M	1308	SPN	C7-C8	-5.31	1.35	1.50
9	M	1308	SPN	C11-C12	-5.26	1.35	1.50
9	M	1308	SPN	C20-C19	-4.90	1.36	1.50
9	M	1308	SPN	C21-C22	-3.37	1.35	1.52
9	M	1308	SPN	C16-C15	-2.61	1.36	1.51
4	L	1284	BCL	C3C-C4C	-2.49	1.48	1.51
4	M	1304	BCL	C1B-CHB	-2.03	1.34	1.39
9	M	1308	SPN	C6-C7	-2.02	1.46	1.53
5	M	1307	BPH	CHC-C1C	3.12	1.42	1.36
6	L	1286	U10	C4-C3	3.15	1.49	1.35
7	M	1305	CDL	OB6-CB5	3.81	1.45	1.34
7	M	1305	CDL	OA8-CA7	3.93	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	1305	CDL	OA6-CA5	4.36	1.47	1.34
7	M	1305	CDL	OB8-CB7	4.66	1.47	1.33
6	L	1286	U10	C6-C1	6.22	1.50	1.35
9	M	1308	SPN	C12-C13	6.72	1.46	1.33
9	M	1308	SPN	C8-C9	7.13	1.47	1.33
9	M	1308	SPN	C19-C18	7.25	1.47	1.33
9	M	1308	SPN	C4-C5	7.41	1.47	1.33

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1284	BCL	O1D-CGD-CBD	-6.20	115.73	124.62
4	L	1282	BCL	CMB-C2B-C1B	-4.44	121.01	128.36
4	L	1284	BCL	CAC-C3C-C2C	-3.48	105.39	114.13
4	L	1284	BCL	CAC-C3C-C4C	-3.41	105.01	112.58
4	L	1282	BCL	O1D-CGD-CBD	-3.37	119.80	124.62
5	M	1307	BPH	OBD-CAD-CBD	-3.27	121.00	125.94
4	L	1282	BCL	OBD-CAD-CBD	-3.27	121.00	125.94
4	L	1284	BCL	CMB-C2B-C1B	-3.20	123.08	128.36
4	L	1284	BCL	CAA-C2A-C3A	-3.12	104.23	113.22
5	M	1307	BPH	C3B-C4B-NB	-3.05	103.50	109.98
4	L	1284	BCL	C5-C3-C2	-3.01	115.33	121.05
5	M	1307	BPH	O1D-CGD-CBD	-2.98	120.36	124.62
4	M	1304	BCL	CMB-C2B-C1B	-2.97	123.46	128.36
4	M	1304	BCL	CHA-C1A-NA	-2.92	118.87	126.06
5	M	1307	BPH	CAA-C2A-C3A	-2.83	105.08	113.22
4	L	1283	BCL	CAA-C2A-C3A	-2.82	105.12	113.22
9	M	1308	SPN	C3-C4-C5	-2.73	122.06	126.70
4	M	1304	BCL	CAC-C3C-C4C	-2.70	106.59	112.58
9	M	1308	SPN	C10-C9-C8	-2.63	116.06	121.05
5	M	1307	BPH	C4-C3-C2	-2.62	118.36	123.50
7	M	1305	CDL	OB6-CB5-OB7	-2.60	116.69	123.67
4	L	1282	BCL	CAA-C2A-C3A	-2.54	105.90	113.22
5	L	1285	BPH	CMA-C3A-C4A	-2.53	104.76	113.01
9	M	1308	SPN	C14-C13-C12	-2.51	116.30	121.05
5	M	1307	BPH	C2B-C1B-NB	-2.42	106.09	109.73
4	L	1284	BCL	C6-C5-C3	-2.41	107.20	112.48
4	M	1304	BCL	CAC-C3C-C2C	-2.40	108.10	114.13
4	L	1282	BCL	CHA-C1A-NA	-2.37	120.22	126.06
9	M	1308	SPN	C7-C8-C9	-2.36	122.62	127.76
6	L	1286	U10	O5-C5-C6	-2.31	117.34	121.68
7	M	1305	CDL	OA8-CA7-OA9	-2.31	117.54	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	1283	BCL	CHA-C1A-NA	-2.30	120.39	126.06
4	L	1282	BCL	CMA-C3A-C2A	-2.30	104.16	114.35
7	M	1305	CDL	CB4-OB6-CB5	-2.23	112.53	117.89
4	L	1284	BCL	CHA-C1A-NA	-2.15	120.78	126.06
5	L	1285	BPH	C3B-C4B-NB	-2.15	105.42	109.98
4	M	1304	BCL	OBD-CAD-CBD	-2.11	122.75	125.94
4	L	1282	BCL	CAC-C3C-C2C	-2.08	108.90	114.13
4	L	1282	BCL	C4-C3-C2	-2.04	119.50	123.50
4	L	1283	BCL	CMA-C3A-C2A	-2.02	105.43	114.35
9	M	1308	SPN	C10-C11-C12	2.01	116.96	111.69
4	L	1282	BCL	OBB-CAB-C3B	2.01	123.19	120.00
4	M	1304	BCL	O2D-CGD-CBD	2.05	114.11	111.30
9	M	1308	SPN	CMB-C30-CM9	2.11	119.83	114.64
5	L	1285	BPH	CAC-C3C-C2C	2.18	119.61	114.13
4	L	1282	BCL	CAA-CBA-CGA	2.18	119.71	113.32
5	M	1307	BPH	CAA-CBA-CGA	2.21	119.79	113.32
9	M	1308	SPN	C21-C20-C19	2.22	118.62	112.40
9	M	1308	SPN	CM7-C22-C23	2.25	119.73	111.08
4	L	1284	BCL	OBB-CAB-C3B	2.34	123.71	120.00
4	L	1282	BCL	C5-C3-C2	2.43	125.66	121.05
5	L	1285	BPH	C1B-NB-C4B	2.48	111.41	106.51
7	M	1305	CDL	OB8-CB7-C71	2.57	119.74	111.90
7	M	1305	CDL	OA8-CA7-C31	2.61	119.86	111.90
4	L	1284	BCL	C2C-C3C-C4C	2.62	105.94	101.50
9	M	1308	SPN	CM7-C22-C21	2.63	121.18	111.08
4	L	1284	BCL	CAA-CBA-CGA	2.73	121.32	113.32
5	M	1307	BPH	C5-C3-C2	2.78	126.33	121.05
9	M	1308	SPN	C6-C7-C8	2.79	119.00	111.69
9	M	1308	SPN	C16-C15-C14	3.07	124.54	113.29
5	M	1307	BPH	C1B-NB-C4B	3.16	112.76	106.51
5	M	1307	BPH	C3C-C4C-NC	3.35	111.28	107.93
5	L	1285	BPH	O2D-CGD-CBD	3.35	115.89	111.30
9	M	1308	SPN	C7-C6-C5	3.35	123.63	112.71
9	M	1308	SPN	C15-C16-C17	3.36	125.61	113.29
4	L	1282	BCL	CMB-C2B-C3B	3.42	131.78	125.09
9	M	1308	SPN	C11-C10-C9	3.45	123.94	112.71
4	L	1282	BCL	O2D-CGD-CBD	3.65	116.30	111.30
9	M	1308	SPN	CM4-C9-C10	3.78	121.19	115.41
9	M	1308	SPN	CM3-C5-C6	3.84	121.27	115.41
5	L	1285	BPH	C3C-C4C-NC	4.00	111.93	107.93
7	M	1305	CDL	OB6-CB5-C51	4.09	120.43	111.53
7	M	1305	CDL	OA6-CA5-C11	4.27	120.80	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	1308	SPN	CM6-C18-C17	4.39	122.11	115.41
9	M	1308	SPN	C16-C17-C18	4.55	122.48	112.48
9	M	1308	SPN	C15-C14-C13	4.73	122.86	112.48
9	M	1308	SPN	CM5-C13-C14	5.39	123.64	115.41
5	M	1307	BPH	O2D-CGD-CBD	5.67	119.08	111.30
4	L	1284	BCL	O2D-CGD-CBD	6.37	120.04	111.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1282	BCL	10	0
4	L	1283	BCL	3	0
4	L	1284	BCL	4	0
5	L	1285	BPH	7	0
6	L	1286	U10	2	0
4	M	1304	BCL	7	0
7	M	1305	CDL	2	0
5	M	1307	BPH	8	0
9	M	1308	SPN	9	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	H	235/260 (90%)	-0.29	2 (0%) 85 79	36, 43, 53, 58	4 (1%)
2	L	281/281 (100%)	-0.16	7 (2%) 61 48	32, 44, 56, 63	1 (0%)
3	M	301/308 (97%)	-0.28	4 (1%) 79 71	36, 44, 54, 79	1 (0%)
All	All	817/849 (96%)	-0.24	13 (1%) 74 66	32, 44, 54, 79	6 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	245	ALA	3.9
2	L	59	TRP	3.8
3	M	302	GLY	3.7
2	L	281	GLY	3.1
2	L	270	PRO	2.8
2	L	277	GLY	2.7
3	M	301	HIS	2.6
3	M	80	TRP	2.4
2	L	202	LYS	2.3
2	L	72	GLU	2.2
3	M	2	GLU	2.2
2	L	271	TRP	2.1
1	H	191	LEU	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
6	U10	L	1286	17/63	0.83	0.56	9.60	29,32,33,33	17
7	CDL	M	1305	81/100	0.83	0.33	2.19	24,39,52,54	81
4	BCL	L	1282	66/66	0.93	0.20	1.81	37,44,69,69	0
5	BPH	M	1307	65/65	0.87	0.23	1.62	38,44,85,86	0
4	BCL	M	1304	66/66	0.95	0.22	1.57	36,40,51,54	0
9	SPN	M	1308	43/43	0.89	0.22	1.33	37,43,51,52	0
4	BCL	L	1283	66/66	0.95	0.21	1.31	29,39,53,56	0
4	BCL	L	1284	66/66	0.95	0.17	0.15	29,36,50,54	0
5	BPH	L	1285	65/65	0.97	0.15	-0.17	33,40,43,46	0
8	FE	M	1306	1/1	0.98	0.15	-1.01	44,44,44,44	0
10	CL	M	1309	1/1	0.99	0.13	-1.57	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.