



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:53 am GMT

PDB ID : 1RVJ  
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG H177 REPLACED WITH HIS  
Authors : Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.  
Deposited on : 2003-12-14  
Resolution : 2.75 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

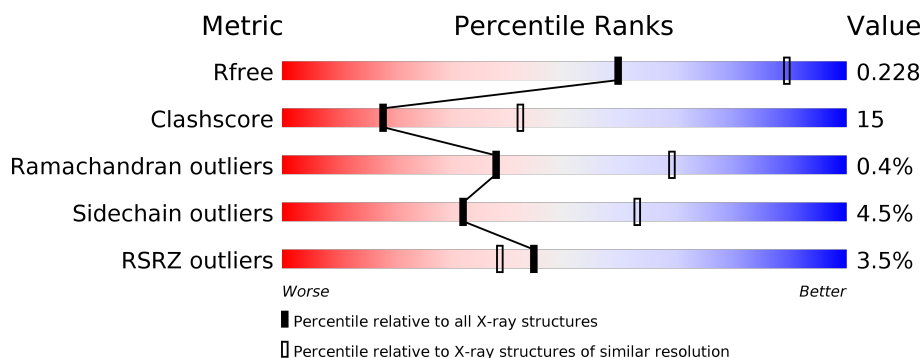
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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> <div></div> <div>74%</div> <div>23%</div> <div>•</div> </div> </div>
2	M	307	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
3	H	260	<div> <div>3%</div> <div> <div></div> <div>63%</div> <div>26%</div> <div>• 8%</div> </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
10	LDA	M	861	-	-	-	X
11	CDL	M	900	-	-	-	X
5	BPH	L	856	X	-	-	-
5	BPH	M	855	X	-	-	-
6	U10	L	859	-	-	-	X
9	SPO	M	860	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7210 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	281	Total	C	N	O	S	0	0	0
			2232	1507	356	361	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	213	ASN	ASP	ENGINEERED	UNP P02954

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	301	Total	C	N	O	S	0	0	0
			2404	1605	393	396	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	307	ALA	-	CLONING ARTIFACT	UNP P02953

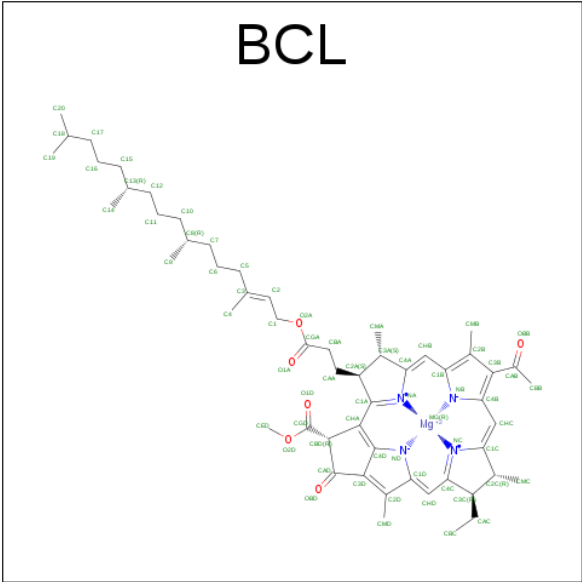
- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	0	0
			1813	1160	310	334	9			

There are 2 discrepancies between the modelled and reference sequences:

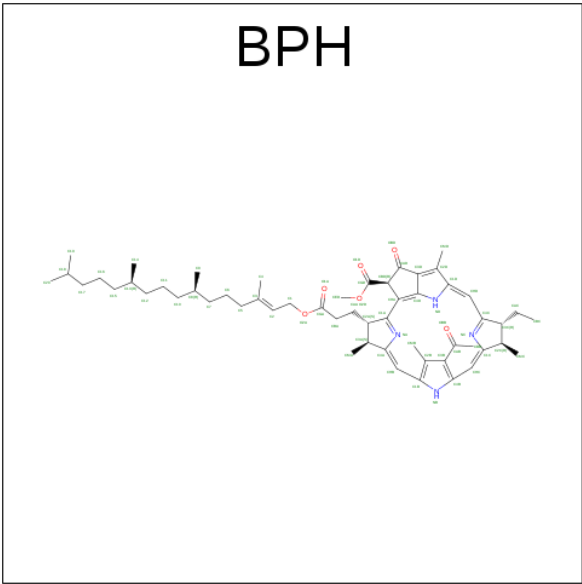
Chain	Residue	Modelled	Actual	Comment	Reference
H	8	GLN	GLY	ENGINEERED	UNP P11846
H	177	HIS	ARG	ENGINEERED	UNP P11846

- 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>).



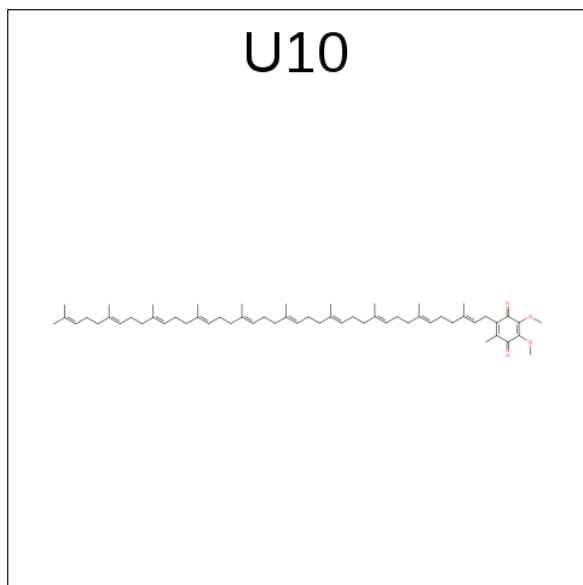
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- 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<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	L	1	Total	C	O	0	0
			44	40	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is FE (II) ION (three-letter code: FE2) (formula: Fe).

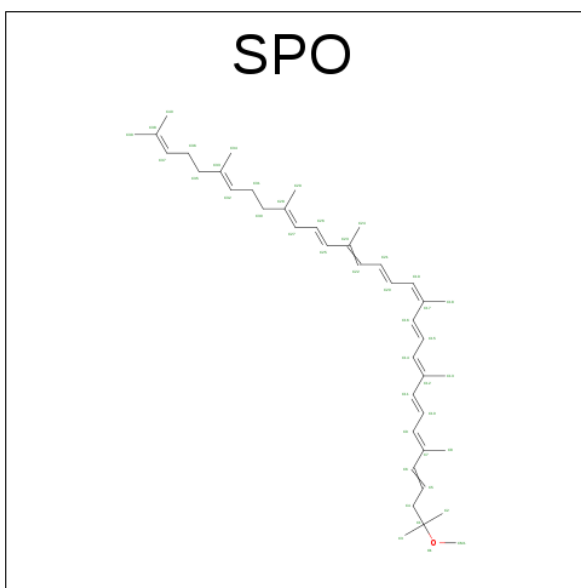
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	M	1	Total	Fe	0	0
			1	1		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



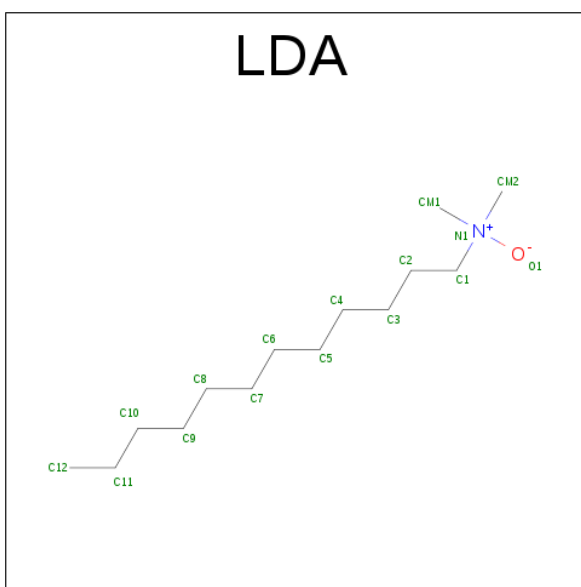
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	P	0	0
			5	4	1		

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



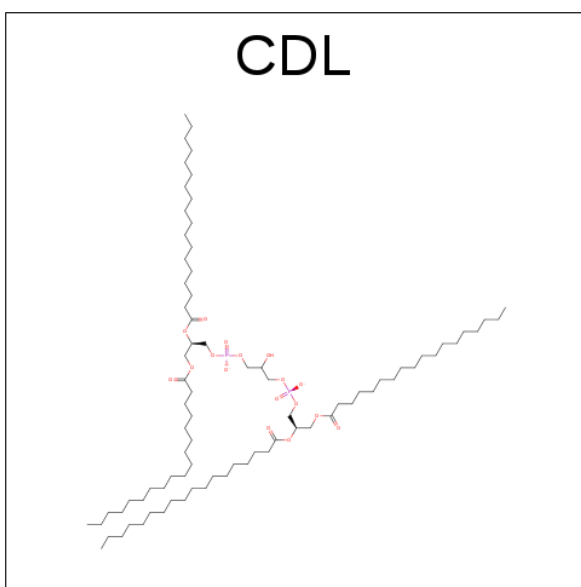
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	C	O	0	0
			42	41	1		

- Molecule 10 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



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

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	O	P	0	0
			69	50	17	2		



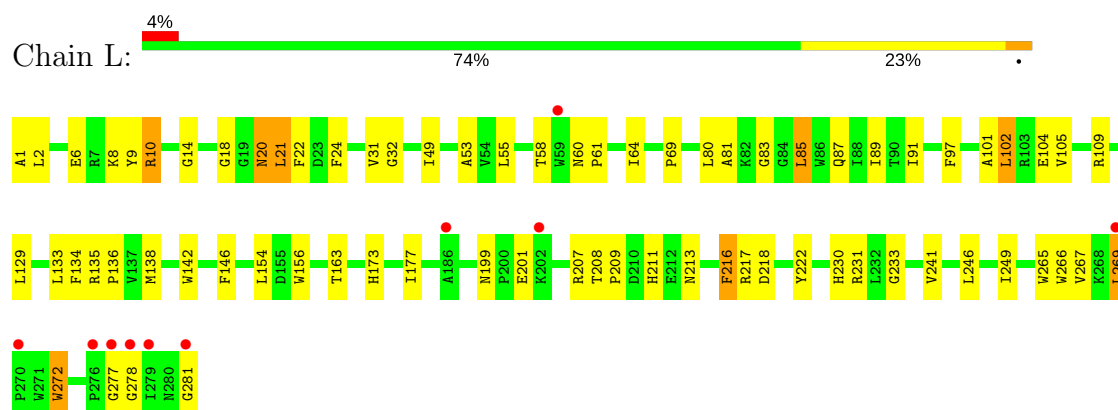
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	L	40	Total 40	O 40	0	0
12	M	43	Total 43	O 43	0	0
12	H	42	Total 42	O 42	0	0

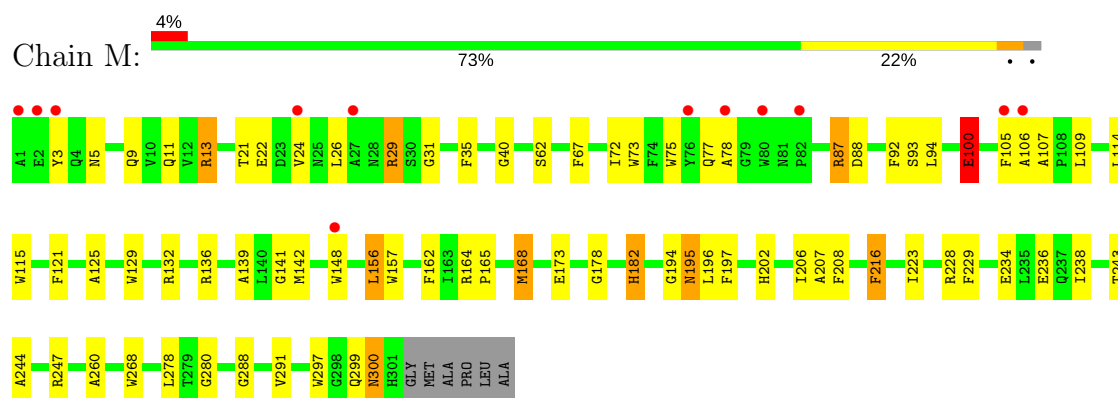
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

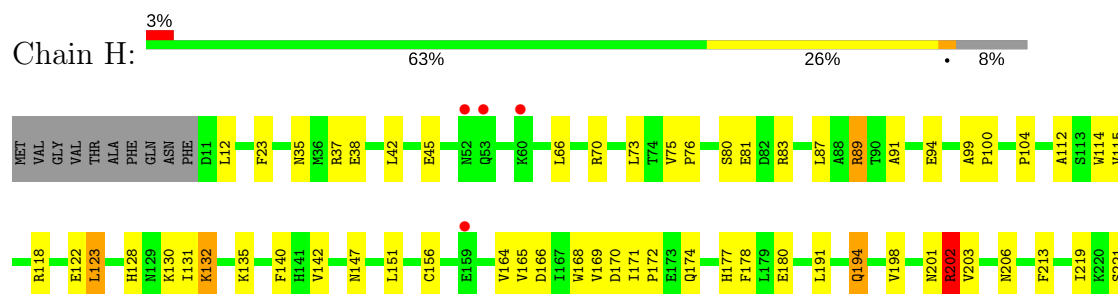
#### • Molecule 1: Reaction center protein L chain

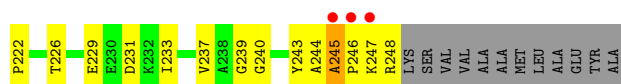


#### • Molecule 2: Reaction center protein M chain



#### • Molecule 3: 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, $\alpha$ , $\beta$ , $\gamma$	138.24Å 138.24Å 184.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.00 – 2.75 39.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.00-2.75) 99.5 (39.00-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.77Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.237 0.208 , 0.228	Depositor DCC
$R_{free}$ test set	2685 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, LDA, CDL, BPH, PO4, FE2, 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	0.59	0/3175
2	M	0.39	0/2496	0.57	0/3408
3	H	0.36	0/1862	0.63	0/2535
All	All	0.39	0/6678	0.60	0/9118

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	2189	57	0
2	M	2404	0	2318	95	0
3	H	1813	0	1812	65	0
4	L	117	0	115	12	0
4	M	132	0	147	13	0
5	L	65	0	74	5	0
5	M	65	0	74	13	0
6	L	44	0	57	1	0
6	M	48	0	62	3	0
7	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	5	0	0	0	0
9	M	42	0	60	9	0
10	H	16	0	31	1	0
10	M	32	0	62	2	0
11	M	69	0	82	6	0
12	H	42	0	0	0	0
12	L	40	0	0	0	0
12	M	43	0	0	2	0
All	All	7210	0	7083	215	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 (215) 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)
5:M:855:BPH:H121	5:M:855:BPH:H9C1	1.40	0.99
2:M:300:ASN:HD22	2:M:300:ASN:N	1.64	0.93
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.55	0.87
2:M:9:GLN:HE22	3:H:198:VAL:H	1.23	0.86
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.59	0.84
5:M:855:BPH:C12	5:M:855:BPH:H9C1	2.09	0.82
2:M:236:GLU:HG3	3:H:122:GLU:CD	2.06	0.76
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.20	0.75
2:M:228:ARG:HA	3:H:194:GLN:HG3	1.68	0.74
2:M:300:ASN:ND2	2:M:300:ASN:N	2.36	0.73
2:M:195:ASN:ND2	2:M:197:PHE:H	1.88	0.71
2:M:156:LEU:HD13	4:M:853:BCL:H43	1.73	0.71
6:M:858:U10:H202	10:H:862:LDA:H123	1.73	0.71
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.72	0.70
2:M:9:GLN:NE2	3:H:198:VAL:H	1.89	0.70
3:H:202:ARG:HG2	3:H:203:VAL:N	2.05	0.69
2:M:195:ASN:HD22	2:M:195:ASN:C	1.95	0.69
2:M:243:THR:O	2:M:247:ARG:HG3	1.93	0.68
2:M:75:TRP:HE1	9:M:860:SPO:H32A	1.57	0.68
2:M:278:LEU:HD21	11:M:900:CDL:H382	1.77	0.66
2:M:236:GLU:HG3	3:H:122:GLU:CG	2.26	0.66
2:M:207:ALA:HA	4:M:854:BCL:O1A	1.96	0.65
2:M:168:MET:HG2	2:M:173:GLU:HG3	1.79	0.65
3:H:132:LYS:HG3	3:H:171:ILE:HD13	1.80	0.63
1:L:265:TRP:O	1:L:269:LEU:HD13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:194:GLY:O	2:M:195:ASN:HB3	1.99	0.63
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.80	0.62
1:L:218:ASP:OD1	2:M:29:ARG:HD2	1.99	0.62
2:M:67:PHE:CG	5:M:855:BPH:H9C2	2.34	0.62
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.80	0.62
2:M:228:ARG:HA	3:H:194:GLN:CG	2.29	0.62
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.35	0.62
3:H:66:LEU:CD1	3:H:118:ARG:HH22	2.11	0.62
4:L:851:BCL:HBC1	4:M:853:BCL:CAD	2.30	0.61
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.35	0.61
5:M:855:BPH:H121	5:M:855:BPH:C9	2.24	0.61
1:L:105:VAL:O	1:L:109:ARG:HG3	2.01	0.61
2:M:9:GLN:HE22	3:H:198:VAL:N	1.95	0.61
2:M:236:GLU:HG3	3:H:122:GLU:HG3	1.82	0.60
3:H:132:LYS:HG3	3:H:171:ILE:CD1	2.31	0.60
1:L:231:ARG:HD2	2:M:5:ASN:O	2.01	0.60
3:H:140:PHE:CE2	3:H:174:GLN:HG2	2.37	0.60
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.67	0.60
1:L:18:GLY:O	1:L:21:LEU:HB2	2.02	0.60
2:M:75:TRP:NE1	9:M:860:SPO:H32A	2.17	0.60
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.84	0.59
2:M:13:ARG:O	3:H:140:PHE:HA	2.02	0.59
2:M:168:MET:CG	2:M:173:GLU:HG3	2.33	0.59
2:M:208:PHE:HE1	10:M:861:LDA:H111	1.68	0.59
1:L:1:ALA:O	1:L:2:LEU:HD12	2.04	0.58
2:M:228:ARG:CA	3:H:194:GLN:HG3	2.34	0.58
2:M:178:GLY:O	2:M:182:HIS:HB3	2.04	0.58
3:H:165:VAL:CG2	3:H:180:GLU:HG2	2.34	0.57
1:L:80:LEU:HB3	1:L:85:LEU:HD13	1.86	0.57
3:H:37:ARG:O	3:H:38:GLU:HG2	2.04	0.57
2:M:109:LEU:HB3	2:M:114:LEU:CD1	2.35	0.57
3:H:140:PHE:HE2	3:H:174:GLN:HG2	1.69	0.56
1:L:101:ALA:O	1:L:104:GLU:HB2	2.05	0.56
2:M:77:GLN:HE22	2:M:93:SER:H	1.52	0.56
2:M:5:ASN:HD22	3:H:194:GLN:HB3	1.69	0.56
2:M:299:GLN:C	2:M:300:ASN:HD22	2.09	0.56
1:L:14:GLY:O	1:L:109:ARG:HD3	2.05	0.56
3:H:165:VAL:O	3:H:166:ASP:HB2	2.05	0.56
4:M:854:BCL:HAA2	10:M:861:LDA:H32	1.87	0.56
2:M:109:LEU:HB3	2:M:114:LEU:HD13	1.87	0.55
1:L:87:GLN:O	1:L:91:ILE:HG12	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:O	1:L:64:ILE:HG13	2.07	0.55
1:L:230:HIS:CD2	2:M:223:ILE:HG13	2.42	0.54
3:H:201:ASN:O	3:H:202:ARG:HB3	2.07	0.54
3:H:104:PRO:HB2	3:H:243:TYR:CE2	2.43	0.54
1:L:207:ARG:HG3	1:L:211:HIS:CG	2.42	0.54
1:L:22:PHE:HA	1:L:24:PHE:CE2	2.42	0.54
2:M:21:THR:CG2	2:M:26:LEU:HD11	2.36	0.54
9:M:860:SPO:HM12	9:M:860:SPO:H5	1.90	0.54
4:L:851:BCL:HBB2	9:M:860:SPO:H243	1.90	0.54
1:L:222:TYR:HA	12:M:1103:HOH:O	2.07	0.53
2:M:26:LEU:HD12	2:M:26:LEU:H	1.73	0.53
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.74	0.53
2:M:195:ASN:HD22	2:M:196:LEU:N	2.07	0.53
3:H:156:CYS:SG	3:H:248:ARG:HB2	2.49	0.52
3:H:89:ARG:HG2	3:H:91:ALA:O	2.10	0.52
2:M:234:GLU:O	2:M:238:ILE:HG13	2.10	0.52
4:L:852:BCL:H42	4:M:854:BCL:HBC2	1.91	0.52
3:H:248:ARG:HB2	3:H:248:ARG:NH1	2.25	0.52
1:L:241:VAL:CG2	5:L:856:BPH:HAC1	2.33	0.52
3:H:70:ARG:NH2	3:H:123:LEU:HD22	2.26	0.51
4:L:851:BCL:HBB1	2:M:157:TRP:HD1	1.74	0.51
4:M:854:BCL:H61	6:M:858:U10:H203	1.92	0.51
5:L:856:BPH:H7C2	4:M:854:BCL:H193	1.93	0.51
3:H:229:GLU:O	3:H:233:ILE:HG13	2.10	0.51
1:L:266:TRP:HE1	2:M:87:ARG:HA	1.76	0.51
2:M:280:GLY:HA2	4:M:853:BCL:HED2	1.93	0.51
5:M:855:BPH:C14	5:M:855:BPH:H172	2.40	0.50
2:M:125:ALA:HB1	5:M:855:BPH:H2	1.93	0.50
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.10	0.50
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.93	0.49
3:H:112:ALA:HB2	3:H:239:GLY:HA3	1.94	0.49
1:L:207:ARG:HG3	1:L:211:HIS:ND1	2.27	0.49
2:M:75:TRP:HE1	9:M:860:SPO:HM13	1.76	0.49
1:L:49:ILE:CG1	1:L:89:ILE:HD13	2.43	0.49
1:L:208:THR:H	1:L:211:HIS:CD2	2.31	0.48
2:M:195:ASN:C	2:M:195:ASN:ND2	2.64	0.48
5:M:855:BPH:C14	5:M:855:BPH:C17	2.90	0.48
2:M:202:HIS:CE1	2:M:206:ILE:HD11	2.49	0.48
2:M:67:PHE:CG	5:M:855:BPH:C9	2.96	0.48
1:L:49:ILE:HG12	1:L:89:ILE:HD13	1.95	0.48
2:M:164:ARG:O	2:M:168:MET:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:233:GLY:HA3	2:M:216:PHE:CE1	2.48	0.48
1:L:272:TRP:CE2	2:M:87:ARG:HB3	2.49	0.48
11:M:900:CDL:H381	3:H:23:PHE:CZ	2.49	0.48
4:L:851:BCL:HBC1	4:M:853:BCL:CB	2.43	0.47
1:L:1:ALA:HB1	3:H:42:LEU:HB3	1.96	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.95	0.47
3:H:170:ASP:O	3:H:174:GLN:N	2.48	0.47
1:L:69:PRO:HD2	1:L:142:TRP:HB2	1.97	0.47
3:H:130:LYS:HG2	3:H:131:ILE:HD12	1.96	0.47
1:L:6:GLU:OE2	1:L:10:ARG:HD3	2.15	0.47
4:L:852:BCL:H122	5:L:856:BPH:H3A	1.97	0.47
1:L:267:VAL:HG13	2:M:87:ARG:HD2	1.96	0.47
2:M:195:ASN:HD22	2:M:197:PHE:H	1.59	0.47
2:M:73:TRP:NE1	2:M:77:GLN:NE2	2.62	0.46
2:M:67:PHE:CD1	5:M:855:BPH:H9C2	2.51	0.46
3:H:81:GLU:O	3:H:83:ARG:HG2	2.16	0.46
1:L:213:ASN:O	1:L:217:ARG:HB2	2.15	0.46
2:M:62:SER:HB3	2:M:121:PHE:O	2.14	0.46
2:M:100:GLU:H	2:M:100:GLU:HG3	1.48	0.46
3:H:245:ALA:HA	3:H:248:ARG:NH2	2.31	0.46
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.97	0.46
1:L:80:LEU:HD22	1:L:85:LEU:CD1	2.46	0.45
2:M:3:TYR:CD2	3:H:194:GLN:HA	2.50	0.45
1:L:208:THR:HB	1:L:209:PRO:HD2	1.99	0.45
2:M:129:TRP:O	2:M:132:ARG:HB3	2.17	0.45
5:M:855:BPH:H142	5:M:855:BPH:H172	1.98	0.45
3:H:201:ASN:O	3:H:202:ARG:CB	2.64	0.45
1:L:216:PHE:HE1	12:M:1087:HOH:O	1.98	0.45
2:M:291:VAL:HG13	2:M:297:TRP:HB2	1.99	0.45
1:L:102:LEU:HD12	1:L:102:LEU:HA	1.74	0.45
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.51	0.45
4:L:852:BCL:CGA	4:M:854:BCL:HBC1	2.47	0.45
2:M:78:ALA:HB2	2:M:92:PHE:CZ	2.52	0.45
3:H:170:ASP:HB2	3:H:177:HIS:HD2	1.81	0.45
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.17	0.44
3:H:131:ILE:C	3:H:132:LYS:HG2	2.36	0.44
3:H:191:LEU:HD11	3:H:213:PHE:CE2	2.51	0.44
1:L:55:LEU:HD13	1:L:81:ALA:HB2	1.98	0.44
3:H:244:ALA:O	3:H:246:PRO:N	2.51	0.44
4:L:851:BCL:H2C	4:L:851:BCL:HBC2	1.67	0.44
1:L:85:LEU:O	1:L:89:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:148:TRP:HB3	11:M:900:CDL:H741	2.00	0.44
5:M:855:BPH:C17	5:M:855:BPH:H141	2.46	0.44
2:M:148:TRP:CD1	11:M:900:CDL:OB6	2.71	0.44
2:M:148:TRP:CE2	11:M:900:CDL:H511	2.52	0.44
4:L:851:BCL:CBB	9:M:860:SPO:H243	2.47	0.44
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.89	0.44
1:L:20:ASN:HD22	1:L:20:ASN:N	2.16	0.44
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.99	0.44
2:M:87:ARG:HG3	2:M:88:ASP:N	2.33	0.44
1:L:163:THR:O	1:L:163:THR:HG22	2.17	0.44
3:H:247:LYS:HD2	3:H:247:LYS:N	2.33	0.44
6:L:859:U10:H311	2:M:31:GLY:O	2.17	0.44
1:L:277:GLY:N	1:L:281:GLY:O	2.51	0.44
2:M:106:ALA:O	2:M:107:ALA:C	2.56	0.44
4:M:854:BCL:H3A	4:M:854:BCL:HBA2	1.75	0.44
2:M:105:PHE:N	2:M:105:PHE:CD2	2.86	0.43
3:H:131:ILE:HA	3:H:169:VAL:O	2.17	0.43
2:M:168:MET:HE3	2:M:288:GLY:O	2.18	0.43
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.18	0.43
1:L:278:GLY:HA2	2:M:77:GLN:O	2.19	0.43
2:M:24:VAL:HG11	2:M:29:ARG:NH1	2.34	0.43
3:H:219:ILE:HA	3:H:229:GLU:OE2	2.18	0.43
1:L:53:ALA:HB1	1:L:58:THR:O	2.18	0.43
3:H:221:SER:HA	3:H:222:PRO:HD3	1.87	0.43
3:H:75:VAL:HA	3:H:76:PRO:C	2.39	0.43
2:M:182:HIS:CG	9:M:860:SPO:H181	2.54	0.43
2:M:162:PHE:HB2	9:M:860:SPO:H291	2.00	0.42
2:M:3:TYR:HD2	3:H:194:GLN:HA	1.84	0.42
2:M:75:TRP:CD1	9:M:860:SPO:H32A	2.53	0.42
3:H:151:LEU:O	3:H:164:VAL:HG23	2.19	0.42
2:M:94:LEU:CD2	2:M:115:TRP:HB2	2.50	0.42
3:H:156:CYS:HB3	3:H:206:ASN:O	2.18	0.42
5:M:855:BPH:C12	5:M:855:BPH:C9	2.80	0.42
1:L:60:ASN:HA	1:L:61:PRO:HD3	1.84	0.42
2:M:157:TRP:HB2	4:M:853:BCL:H62	2.02	0.42
3:H:123:LEU:HA	3:H:128:HIS:O	2.20	0.42
1:L:8:LYS:HE2	1:L:9:TYR:CZ	2.55	0.42
1:L:83:GLY:O	1:L:87:GLN:HG3	2.19	0.42
4:L:852:BCL:H2C	4:M:853:BCL:H2C	2.01	0.42
2:M:24:VAL:HG22	2:M:139:ALA:HB1	2.01	0.42
1:L:272:TRP:CD2	2:M:87:ARG:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:140:PHE:CE1	3:H:171:ILE:HG13	2.55	0.41
4:L:851:BCL:HBB2	4:L:851:BCL:HHC	2.01	0.41
3:H:114:TRP:HE3	3:H:115:VAL:O	2.03	0.41
3:H:142:VAL:HG21	3:H:147:ASN:ND2	2.34	0.41
1:L:134:PHE:O	1:L:138:MET:HG3	2.20	0.41
2:M:132:ARG:O	2:M:136:ARG:HG2	2.20	0.41
1:L:97:PHE:CE1	4:L:852:BCL:H121	2.55	0.41
2:M:109:LEU:O	2:M:114:LEU:HD13	2.20	0.41
3:H:219:ILE:HD12	3:H:221:SER:O	2.21	0.41
1:L:201:GLU:HG3	2:M:141:GLY:O	2.21	0.41
3:H:171:ILE:HB	3:H:172:PRO:HD3	2.02	0.41
1:L:246:LEU:HA	1:L:249:ILE:HG22	2.02	0.41
3:H:240:GLY:O	3:H:244:ALA:HB3	2.21	0.41
2:M:11:GLN:OE1	2:M:40:GLY:HA3	2.19	0.41
2:M:268:TRP:CD1	6:M:858:U10:H111	2.56	0.41
5:L:856:BPH:HMB1	5:L:856:BPH:HHB	1.92	0.41
1:L:129:LEU:O	1:L:133:LEU:HB3	2.21	0.41
2:M:87:ARG:NE	2:M:88:ASP:OD1	2.55	0.40
1:L:31:VAL:HG12	1:L:32:GLY:N	2.36	0.40
2:M:72:ILE:HG23	2:M:73:TRP:N	2.37	0.40
3:H:169:VAL:CG1	3:H:170:ASP:N	2.84	0.40
3:H:233:ILE:O	3:H:237:VAL:HG23	2.22	0.40
2:M:67:PHE:CB	5:M:855:BPH:C9	2.99	0.40
1:L:20:ASN:HD22	1:L:20:ASN:H	1.70	0.40
1:L:146:PHE:HB3	1:L:156:TRP:CD2	2.57	0.40
1:L:199:ASN:O	11:M:900:CDL:H1	2.20	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%)	266 (95%)	13 (5%)	0	100	100
2	M	299/307 (97%)	285 (95%)	13 (4%)	1 (0%)	44	75
3	H	236/260 (91%)	227 (96%)	7 (3%)	2 (1%)	22	52
All	All	814/848 (96%)	778 (96%)	33 (4%)	3 (0%)	38	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	245	ALA
2	M	100	GLU
3	H	202	ARG

### 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%)	211 (96%)	9 (4%)	35	67
2	M	236/239 (99%)	226 (96%)	10 (4%)	34	66
3	H	193/209 (92%)	183 (95%)	10 (5%)	27	57
All	All	649/668 (97%)	620 (96%)	29 (4%)	32	63

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	10	ARG
1	L	20	ASN
1	L	21	LEU
1	L	85	LEU
1	L	102	LEU
1	L	154	LEU
1	L	216	PHE
1	L	269	LEU
1	L	272	TRP
2	M	13	ARG

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Mol	Chain	Res	Type
2	M	29	ARG
2	M	87	ARG
2	M	100	GLU
2	M	156	LEU
2	M	168	MET
2	M	182	HIS
2	M	195	ASN
2	M	216	PHE
2	M	300	ASN
3	H	12	LEU
3	H	73	LEU
3	H	80	SER
3	H	89	ARG
3	H	123	LEU
3	H	132	LYS
3	H	135	LYS
3	H	194	GLN
3	H	202	ARG
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	20	ASN
1	L	87	GLN
1	L	211	HIS
1	L	264	GLN
2	M	5	ASN
2	M	9	GLN
2	M	77	GLN
2	M	195	ASN
2	M	300	ASN
3	H	177	HIS
3	H	194	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 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
10	LDA	H	862	-	13,15,15	2.31	1 (7%)	14,17,17	2.30	5 (35%)
4	BCL	L	851	-	40,59,74	1.53	3 (7%)	47,97,115	2.22	13 (27%)
4	BCL	L	852	-	55,74,74	1.29	4 (7%)	65,115,115	1.77	20 (30%)
5	BPH	L	856	-	65,70,70	1.48	10 (15%)	75,101,101	2.14	17 (22%)
6	U10	L	859	-	44,44,63	1.57	10 (22%)	53,56,79	1.26	5 (9%)
4	BCL	M	853	-	55,74,74	1.40	7 (12%)	65,115,115	2.64	21 (32%)
4	BCL	M	854	-	55,74,74	1.35	7 (12%)	65,115,115	2.20	14 (21%)
5	BPH	M	855	-	65,70,70	1.48	9 (13%)	75,101,101	2.28	25 (33%)
6	U10	M	858	-	48,48,63	2.01	16 (33%)	58,61,79	3.11	14 (24%)
9	SPO	M	860	-	40,41,41	3.43	24 (60%)	49,50,50	3.95	16 (32%)
10	LDA	M	861	-	13,15,15	2.40	1 (7%)	14,17,17	2.17	4 (28%)
10	LDA	M	863	-	13,15,15	2.49	1 (7%)	14,17,17	2.15	4 (28%)
8	PO4	M	864	-	4,4,4	1.32	0	6,6,6	0.39	0
11	CDL	M	900	-	68,68,99	1.33	8 (11%)	70,80,111	1.79	15 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LDA	H	862	-	-	0/13/13/13	0/0/0/0
4	BCL	L	851	-	-	0/19/119/137	0/0/9/9
4	BCL	L	852	-	-	0/37/137/137	0/0/9/9
5	BPH	L	856	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	L	859	-	-	0/41/65/87	0/1/1/1
4	BCL	M	853	-	-	0/37/137/137	0/0/9/9
4	BCL	M	854	-	-	0/37/137/137	0/0/9/9
5	BPH	M	855	-	2/2/18/22	0/54/105/105	0/1/6/6
6	U10	M	858	-	-	0/45/69/87	0/1/1/1
9	SPO	M	860	-	-	0/47/47/47	0/0/0/0
10	LDA	M	861	-	-	0/13/13/13	0/0/0/0
10	LDA	M	863	-	-	0/13/13/13	0/0/0/0
8	PO4	M	864	-	-	0/0/0/0	0/0/0/0
11	CDL	M	900	-	-	0/79/79/110	0/0/0/0

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	863	LDA	O1-N1	-8.78	1.24	1.42
10	M	861	LDA	O1-N1	-8.24	1.25	1.42
10	H	862	LDA	O1-N1	-8.14	1.26	1.42
5	M	855	BPH	C11-C10	-5.28	1.28	1.52
5	L	856	BPH	C11-C10	-5.17	1.29	1.52
4	L	851	BCL	C3C-C4C	-4.64	1.45	1.51
6	M	858	U10	C7-C8	-4.57	1.43	1.50
5	L	856	BPH	O2D-CED	-2.96	1.38	1.45
6	M	858	U10	C37-C38	-2.87	1.40	1.50
6	L	859	U10	C3-C2	-2.87	1.40	1.48
6	M	858	U10	O3-C3M	-2.75	1.38	1.45
6	L	859	U10	C7-C8	-2.67	1.46	1.50
9	M	860	SPO	C11-C12	-2.60	1.40	1.45
5	M	855	BPH	O2D-CED	-2.56	1.39	1.45
9	M	860	SPO	C25-C23	-2.52	1.40	1.45
6	L	859	U10	C4-C5	-2.50	1.41	1.48
11	M	900	CDL	OB2-CB2	-2.46	1.35	1.44
4	M	853	BCL	C2-C3	-2.43	1.26	1.33
9	M	860	SPO	C6-C7	-2.30	1.40	1.45
4	M	853	BCL	C3C-C4C	-2.21	1.48	1.51
4	L	852	BCL	C3C-C4C	-2.17	1.48	1.51
4	M	854	BCL	C3D-CAD	-2.11	1.40	1.46
4	M	854	BCL	C3C-C4C	-2.11	1.48	1.51
5	M	855	BPH	C2C-C3C	-2.06	1.48	1.54
6	M	858	U10	C18-C19	2.03	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	855	BPH	CHC-C1C	2.05	1.40	1.36
6	M	858	U10	C8-C9	2.06	1.38	1.33
4	M	854	BCL	C6-C5	2.07	1.59	1.52
11	M	900	CDL	PB2-OB5	2.07	1.68	1.59
4	M	853	BCL	CBB-CAB	2.08	1.56	1.49
9	M	860	SPO	C22-C23	2.11	1.38	1.35
4	M	853	BCL	C3A-C2A	2.14	1.60	1.54
4	M	853	BCL	CMD-C2D	2.14	1.56	1.51
5	L	856	BPH	C2A-C1A	2.15	1.55	1.51
4	L	852	BCL	CBB-CAB	2.16	1.56	1.49
6	M	858	U10	C31-C29	2.19	1.56	1.51
4	M	854	BCL	C4-C3	2.19	1.56	1.50
6	M	858	U10	C15-C14	2.25	1.56	1.50
6	M	858	U10	C30-C29	2.25	1.56	1.50
5	L	856	BPH	C3D-C4D	2.27	1.44	1.41
5	L	856	BPH	CAA-C2A	2.31	1.58	1.54
4	M	854	BCL	CBB-CAB	2.34	1.56	1.49
9	M	860	SPO	C35-C33	2.36	1.56	1.51
6	L	859	U10	C23-C24	2.38	1.38	1.33
6	M	858	U10	C36-C34	2.44	1.56	1.51
6	L	859	U10	C13-C14	2.45	1.39	1.33
5	L	856	BPH	CHC-C1C	2.48	1.41	1.36
5	L	856	BPH	O1D-CGD	2.49	1.27	1.21
9	M	860	SPO	C15-C14	2.52	1.51	1.43
5	M	855	BPH	C2A-C1A	2.53	1.55	1.51
9	M	860	SPO	C24-C23	2.55	1.56	1.50
6	L	859	U10	C33-C34	2.55	1.39	1.33
5	M	855	BPH	C2-C3	2.59	1.39	1.33
9	M	860	SPO	C8-C7	2.60	1.56	1.50
9	M	860	SPO	C13-C12	2.63	1.56	1.50
9	M	860	SPO	O1-C1	2.68	1.58	1.41
5	L	856	BPH	C2-C3	2.69	1.39	1.33
6	M	858	U10	C23-C24	2.72	1.39	1.33
6	L	859	U10	C28-C29	2.72	1.39	1.33
9	M	860	SPO	C32-C33	2.73	1.39	1.33
6	L	859	U10	C18-C19	2.75	1.39	1.33
9	M	860	SPO	C37-C38	2.76	1.40	1.32
9	M	860	SPO	C26-C27	2.79	1.52	1.43
6	M	858	U10	O3-C3	2.82	1.43	1.36
11	M	900	CDL	OA6-CA5	2.88	1.42	1.34
6	L	859	U10	C8-C9	2.92	1.40	1.33
4	L	852	BCL	CHB-C4A	2.93	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	900	CDL	OA8-CA6	2.93	1.51	1.45
5	M	855	BPH	CAA-C2A	2.94	1.59	1.54
6	M	858	U10	C6-C1	3.08	1.42	1.35
9	M	860	SPO	C10-C9	3.09	1.53	1.43
6	L	859	U10	C6-C1	3.22	1.42	1.35
11	M	900	CDL	C11-CA5	3.22	1.60	1.50
6	M	858	U10	C13-C14	3.23	1.41	1.33
4	M	854	BCL	CHC-C1C	3.30	1.37	1.33
11	M	900	CDL	OA6-CA4	3.36	1.55	1.46
4	L	851	BCL	CHB-C4A	3.40	1.37	1.33
5	L	856	BPH	O2D-CGD	3.48	1.42	1.33
11	M	900	CDL	OA8-CA7	3.65	1.44	1.33
6	M	858	U10	C33-C34	3.82	1.42	1.33
9	M	860	SPO	O1-CM1	3.84	1.55	1.43
4	L	851	BCL	CHC-C1C	3.88	1.38	1.33
9	M	860	SPO	C19-C17	3.94	1.41	1.35
9	M	860	SPO	C9-C7	4.06	1.41	1.35
6	M	858	U10	C28-C29	4.07	1.43	1.33
11	M	900	CDL	CA3-CA4	4.07	1.62	1.50
9	M	860	SPO	C14-C12	4.12	1.41	1.35
5	L	856	BPH	O2A-CGA	4.27	1.45	1.33
4	M	853	BCL	CHB-C4A	4.37	1.39	1.33
4	M	854	BCL	CHB-C4A	4.46	1.39	1.33
5	M	855	BPH	O2A-CGA	4.50	1.46	1.33
5	M	855	BPH	O2D-CGD	4.54	1.44	1.33
4	M	853	BCL	CHC-C1C	4.63	1.39	1.33
4	L	852	BCL	CHC-C1C	4.66	1.39	1.33
6	M	858	U10	O4-C4	4.96	1.49	1.36
9	M	860	SPO	C26-C25	5.14	1.47	1.34
9	M	860	SPO	C21-C20	5.25	1.49	1.35
9	M	860	SPO	C27-C28	5.85	1.40	1.34
9	M	860	SPO	C15-C16	7.57	1.54	1.34
9	M	860	SPO	C10-C11	8.19	1.55	1.34
9	M	860	SPO	C6-C5	8.72	1.55	1.31

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	860	SPO	C2-C1-C4	-18.82	78.90	110.90
9	M	860	SPO	C3-C1-C4	-10.59	92.89	110.90
4	M	854	BCL	CAC-C3C-C4C	-10.41	89.47	112.58
4	L	851	BCL	CBC-CAC-C3C	-8.08	95.21	113.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	860	SPO	O1-C1-C4	-7.00	87.50	106.29
9	M	860	SPO	C15-C14-C12	-6.10	118.61	127.31
4	M	853	BCL	C5-C3-C2	-5.94	108.95	121.10
10	H	862	LDA	CM2-N1-CM1	-5.72	100.04	110.99
9	M	860	SPO	C20-C21-C22	-5.72	111.25	123.46
10	M	861	LDA	CM2-N1-CM1	-5.54	100.39	110.99
10	M	863	LDA	CM2-N1-CM1	-5.42	100.61	110.99
9	M	860	SPO	C25-C23-C22	-5.39	110.67	118.94
11	M	900	CDL	OA2-PA1-OA3	-4.62	90.60	109.25
4	M	853	BCL	C16-C15-C13	-4.58	100.69	115.73
11	M	900	CDL	CB2-C1-CA2	-4.52	99.17	112.73
4	L	851	BCL	C1-C2-C3	-4.38	119.75	126.68
5	M	855	BPH	O1D-CGD-CBD	-4.28	116.91	124.60
4	M	853	BCL	OBB-CAB-CBB	-4.27	110.42	120.16
4	M	854	BCL	OBB-CAB-CBB	-4.27	110.43	120.16
4	L	852	BCL	OBB-CAB-CBB	-4.11	110.78	120.16
5	L	856	BPH	O2D-CGD-O1D	-4.05	115.68	123.82
4	L	851	BCL	OBB-CAB-CBB	-3.90	111.28	120.16
6	M	858	U10	O5-C5-C6	-3.81	114.80	121.82
9	M	860	SPO	C18-C17-C19	-3.72	117.71	122.92
10	H	862	LDA	CM1-N1-C1	-3.63	102.61	110.23
11	M	900	CDL	CB6-CB4-CB3	-3.57	103.81	111.86
9	M	860	SPO	C4-C5-C6	-3.55	119.48	124.57
11	M	900	CDL	OA5-PA1-OA3	-3.54	94.95	109.25
4	L	852	BCL	OBD-CAD-CBD	-3.53	120.61	125.94
5	L	856	BPH	O1D-CGD-CBD	-3.48	118.34	124.60
4	M	853	BCL	OBD-CAD-CBD	-3.48	120.69	125.94
9	M	860	SPO	C15-C16-C17	-3.48	116.65	126.42
4	L	851	BCL	CAC-C3C-C4C	-3.47	104.87	112.58
4	M	853	BCL	CMB-C2B-C1B	-3.46	123.14	128.46
4	L	851	BCL	CAA-C2A-C3A	-3.45	103.36	112.81
4	M	854	BCL	C11-C12-C13	-3.41	104.53	115.73
4	L	852	BCL	C1-C2-C3	-3.37	119.74	125.96
4	M	854	BCL	C3C-C2C-C1C	-3.34	96.47	101.87
6	M	858	U10	C30-C29-C31	-3.33	109.50	115.29
5	M	855	BPH	O2D-CGD-O1D	-3.31	117.16	123.82
4	M	853	BCL	C12-C11-C10	-3.26	97.48	113.25
4	L	851	BCL	OBD-CAD-CBD	-3.23	121.06	125.94
10	M	861	LDA	CM1-N1-C1	-3.18	103.55	110.23
6	M	858	U10	C20-C19-C21	-3.16	109.81	115.29
9	M	860	SPO	C6-C7-C9	-3.12	114.16	118.94
4	M	853	BCL	C1-O2A-CGA	-3.05	109.46	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	900	CDL	O1-C1-CA2	-3.03	98.17	109.34
11	M	900	CDL	OB6-CB5-OB7	-3.03	116.12	123.68
10	M	863	LDA	C5-C4-C3	-3.02	98.88	114.45
6	M	858	U10	O2-C2-C3	-2.97	114.64	120.95
4	L	852	BCL	O2D-CGD-CBD	-2.97	105.99	111.30
4	L	852	BCL	CMB-C2B-C1B	-2.92	123.98	128.46
4	M	853	BCL	C20-C18-C19	-2.89	96.85	110.50
5	M	855	BPH	CAA-C2A-C3A	-2.87	104.95	112.81
10	M	863	LDA	C9-C8-C7	-2.79	100.06	114.45
5	M	855	BPH	OBD-CAD-CBD	-2.74	121.80	125.94
5	M	855	BPH	C4B-C3B-CAB	-2.74	119.99	130.09
6	M	858	U10	C35-C34-C36	-2.67	110.65	115.29
5	L	856	BPH	C7-C6-C5	-2.66	105.73	113.11
4	M	854	BCL	OBD-CAD-CBD	-2.65	121.94	125.94
5	L	856	BPH	C4B-C3B-CAB	-2.64	120.34	130.09
4	L	851	BCL	CHA-C1A-NA	-2.64	120.05	126.18
4	M	853	BCL	C7-C6-C5	-2.63	105.81	113.11
4	M	853	BCL	CAC-C3C-C4C	-2.61	106.79	112.58
6	L	859	U10	C7-C8-C9	-2.61	122.35	126.71
4	M	853	BCL	CHA-C1A-NA	-2.56	120.23	126.18
4	L	852	BCL	C7-C6-C5	-2.51	106.13	113.11
4	M	854	BCL	C14-C13-C15	-2.50	102.23	111.36
4	L	852	BCL	CAA-C2A-C3A	-2.50	105.96	112.81
5	M	855	BPH	C5-C3-C2	-2.46	116.07	121.10
5	M	855	BPH	C4D-CHA-C1A	-2.45	123.98	130.23
5	L	856	BPH	O2A-CGA-O1A	-2.45	117.48	123.55
9	M	860	SPO	C10-C9-C7	-2.43	123.84	127.31
5	L	856	BPH	C4D-CHA-C1A	-2.43	124.05	130.23
4	L	852	BCL	CAC-C3C-C4C	-2.41	107.23	112.58
11	M	900	CDL	OA4-PA1-OA3	-2.38	99.94	112.28
4	L	852	BCL	CHA-C1A-NA	-2.38	120.66	126.18
10	H	862	LDA	C9-C8-C7	-2.37	102.26	114.45
9	M	860	SPO	C20-C19-C17	-2.33	123.99	127.31
4	L	852	BCL	C16-C15-C13	-2.32	108.13	115.73
4	L	852	BCL	C11-C12-C13	-2.32	108.13	115.73
5	M	855	BPH	C6-C7-C8	-2.31	108.15	115.73
4	M	854	BCL	CHA-C1A-NA	-2.30	120.84	126.18
5	M	855	BPH	C2A-C1A-NA	-2.26	109.16	111.91
5	M	855	BPH	O2A-CGA-O1A	-2.26	117.94	123.55
5	L	856	BPH	CAA-C2A-C3A	-2.24	106.66	112.81
5	M	855	BPH	CMA-C3A-C2A	-2.23	104.71	113.77
4	M	854	BCL	CMB-C2B-C1B	-2.22	125.05	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	853	BCL	O2A-CGA-O1A	-2.19	118.12	123.55
4	L	852	BCL	CBC-CAC-C3C	-2.16	108.62	113.51
5	L	856	BPH	CMA-C3A-C2A	-2.15	105.06	113.77
5	M	855	BPH	CBB-CAB-C3B	-2.14	115.94	120.52
11	M	900	CDL	CA6-CA4-CA3	-2.07	107.19	111.86
4	L	852	BCL	CBA-CAA-C2A	2.05	119.92	113.80
11	M	900	CDL	C52-C51-CB5	2.10	121.26	113.58
4	L	852	BCL	CED-O2D-CGD	2.16	121.03	115.97
5	M	855	BPH	C3A-C2A-C1A	2.17	104.23	101.68
4	L	852	BCL	C3D-CAD-CBD	2.18	110.68	107.60
6	M	858	U10	C16-C14-C13	2.23	125.67	121.10
5	M	855	BPH	C4-C3-C5	2.24	119.18	115.29
11	M	900	CDL	OA6-CA5-C11	2.31	116.34	111.55
11	M	900	CDL	OA4-PA1-OA5	2.31	119.07	108.14
11	M	900	CDL	OA4-PA1-OA2	2.32	119.11	108.14
4	M	854	BCL	CMB-C2B-C3B	2.33	129.21	124.89
5	M	855	BPH	C3C-C2C-C1C	2.33	105.63	101.87
6	M	858	U10	C7-C8-C9	2.35	130.64	126.71
4	M	854	BCL	CBA-CAA-C2A	2.35	120.82	113.80
4	L	851	BCL	CBB-CAB-C3B	2.35	127.22	120.39
4	L	851	BCL	CMB-C2B-C3B	2.36	129.26	124.89
10	M	863	LDA	O1-N1-C1	2.39	115.12	109.27
4	L	852	BCL	C2C-C3C-C4C	2.40	104.94	101.34
4	M	853	BCL	CED-O2D-CGD	2.41	121.61	115.97
5	L	856	BPH	C3C-C2C-C1C	2.44	105.81	101.87
10	M	861	LDA	O1-N1-C1	2.46	115.30	109.27
10	H	862	LDA	CM2-N1-C1	2.48	115.44	110.23
4	L	851	BCL	C3D-CAD-CBD	2.48	111.11	107.60
6	M	858	U10	C21-C19-C18	2.49	126.19	121.10
5	M	855	BPH	CMD-C2D-C3D	2.51	129.55	124.89
4	L	851	BCL	CHD-C4C-NC	2.51	127.87	125.08
6	L	859	U10	C3M-O3-C3	2.56	125.61	116.44
4	L	852	BCL	CBB-CAB-C3B	2.69	128.21	120.39
4	M	853	BCL	C6-C5-C3	2.71	118.79	112.66
6	L	859	U10	C30-C29-C31	2.74	120.05	115.29
10	H	862	LDA	O1-N1-C1	2.76	116.04	109.27
10	M	861	LDA	CM2-N1-C1	2.77	116.05	110.23
6	L	859	U10	C35-C34-C36	2.82	119.18	115.85
11	M	900	CDL	OB2-PB2-OB3	2.83	120.67	109.25
4	M	853	BCL	CBB-CAB-C3B	2.84	128.64	120.39
9	M	860	SPO	C8-C7-C6	2.84	122.63	118.10
6	M	858	U10	C31-C32-C33	2.85	121.75	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	856	BPH	C2C-C3C-C4C	2.94	105.75	101.34
5	M	855	BPH	C2C-C3C-C4C	2.99	105.81	101.34
4	M	854	BCL	CBB-CAB-C3B	3.01	129.14	120.39
6	L	859	U10	C25-C24-C26	3.13	120.72	115.29
9	M	860	SPO	C3-C1-C2	3.21	116.65	110.31
4	M	853	BCL	O2A-CGA-CBA	3.23	121.29	111.90
4	M	853	BCL	C2C-C3C-C4C	3.23	106.18	101.34
4	L	852	BCL	O1D-CGD-CBD	3.25	130.45	124.60
4	L	852	BCL	CMB-C2B-C3B	3.42	131.25	124.89
4	M	853	BCL	CMB-C2B-C3B	3.45	131.30	124.89
6	M	858	U10	C31-C29-C28	3.52	128.31	121.10
5	M	855	BPH	CBC-CAC-C3C	3.59	121.66	113.51
5	M	855	BPH	C11-C10-C8	3.68	127.83	115.73
5	L	856	BPH	CED-O2D-CGD	3.73	124.71	115.97
9	M	860	SPO	C1-C4-C5	3.76	122.57	112.87
4	L	852	BCL	CMD-C2D-C3D	3.80	131.94	124.89
4	L	851	BCL	C2C-C3C-C4C	3.87	107.13	101.34
4	M	853	BCL	CMD-C2D-C3D	3.90	132.13	124.89
9	M	860	SPO	C24-C23-C25	3.93	124.36	118.10
5	L	856	BPH	C11-C10-C8	4.01	128.89	115.73
4	M	854	BCL	CMD-C2D-C3D	4.15	132.59	124.89
6	M	858	U10	C36-C34-C33	4.33	129.97	121.10
5	M	855	BPH	CED-O2D-CGD	4.36	126.18	115.97
4	L	851	BCL	CMD-C2D-C3D	4.37	133.00	124.89
5	L	856	BPH	C1-C2-C3	4.58	134.40	125.96
5	M	855	BPH	C6-C5-C3	4.71	123.33	112.66
5	L	856	BPH	C4A-NA-C1A	4.87	112.10	108.16
5	M	855	BPH	C4A-NA-C1A	4.93	112.15	108.16
5	M	855	BPH	C7-C6-C5	4.95	126.88	113.11
5	L	856	BPH	CBC-CAC-C3C	5.10	125.06	113.51
4	M	854	BCL	C1-O2A-CGA	5.14	129.09	116.77
4	M	854	BCL	C2C-C3C-C4C	5.30	109.27	101.34
11	M	900	CDL	OB6-CB5-C51	5.34	122.65	111.55
4	M	853	BCL	C4-C3-C5	5.48	124.79	115.29
11	M	900	CDL	OB8-CB6-CB4	5.81	123.25	108.66
5	L	856	BPH	C6-C5-C3	5.83	125.88	112.66
6	M	858	U10	C3M-O3-C3	5.96	137.78	116.44
5	M	855	BPH	C1-C2-C3	6.13	137.26	125.96
6	M	858	U10	C27-C28-C29	7.77	147.19	127.68
5	M	855	BPH	O2D-CGD-CBD	8.16	125.89	111.30
5	L	856	BPH	O2D-CGD-CBD	8.20	125.95	111.30
4	M	853	BCL	C1-C2-C3	12.05	148.15	125.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	858	U10	C32-C33-C34	17.61	171.91	127.68

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	856	BPH	C8
5	L	856	BPH	C13
5	M	855	BPH	C8
5	M	855	BPH	C13

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	862	LDA	1	0
4	L	851	BCL	7	0
4	L	852	BCL	5	0
5	L	856	BPH	5	0
6	L	859	U10	1	0
4	M	853	BCL	6	0
4	M	854	BCL	7	0
5	M	855	BPH	13	0
6	M	858	U10	3	0
9	M	860	SPO	9	0
10	M	861	LDA	2	0
11	M	900	CDL	6	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

### 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%)	-0.07	10 (3%) 43 37	40, 52, 77, 92	0
2	M	301/307 (98%)	0.00	12 (3%) 39 33	39, 55, 80, 112	0
3	H	238/260 (91%)	-0.04	7 (2%) 52 46	43, 55, 69, 111	0
All	All	820/848 (96%)	-0.03	29 (3%) 44 38	39, 54, 77, 112	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	6.7
3	H	246	PRO	6.4
1	L	277	GLY	5.0
3	H	245	ALA	4.5
2	M	3	TYR	4.2
3	H	247	LYS	3.9
1	L	281	GLY	3.3
2	M	76	TYR	3.2
1	L	59	TRP	3.1
2	M	80	TRP	3.1
1	L	276	PRO	3.0
1	L	270	PRO	3.0
3	H	53	GLN	2.7
2	M	27	ALA	2.7
1	L	279	ILE	2.6
2	M	2	GLU	2.4
2	M	106	ALA	2.3
3	H	60	LYS	2.2
3	H	52	ASN	2.2
1	L	202	LYS	2.2
1	L	269	LEU	2.2
2	M	105	PHE	2.2
1	L	278	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	82	PRO	2.1
2	M	24	VAL	2.1
2	M	148	TRP	2.1
3	H	159	GLU	2.1
1	L	186	ALA	2.0
2	M	78	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
6	U10	L	859	44/63	0.65	0.46	4.67	92,100,103,107	0
11	CDL	M	900	69/100	0.81	0.38	3.29	93,106,120,122	0
9	SPO	M	860	42/42	0.88	0.34	3.24	48,67,86,88	0
10	LDA	M	861	16/16	0.85	0.27	2.59	60,69,80,81	0
6	U10	M	858	48/63	0.91	0.27	1.86	47,59,84,85	0
5	BPH	M	855	65/65	0.89	0.25	1.49	46,51,100,102	0
4	BCL	M	853	66/66	0.96	0.21	1.30	44,50,63,70	0
4	BCL	L	851	51/66	0.95	0.23	1.07	39,45,68,70	0
5	BPH	L	856	65/65	0.95	0.20	0.73	37,43,52,54	0
10	LDA	H	862	16/16	0.93	0.23	0.63	66,68,78,79	0
4	BCL	L	852	66/66	0.95	0.18	0.56	38,49,52,53	0
4	BCL	M	854	66/66	0.95	0.18	0.51	35,40,62,64	0
8	PO4	M	864	5/5	0.93	0.14	-0.91	91,93,94,94	0
7	FE2	M	857	1/1	0.99	0.16	-2.17	45,45,45,45	0
10	LDA	M	863	16/16	0.76	0.42	-	93,95,103,104	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.