Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:04 PM GMT

PDB ID	:	1RY5
Title	:	PHOTOSYNTHETIC REACTION CENTER MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN
Authors	:	Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on	:	2003-12-19
Resolution	:	2.10 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

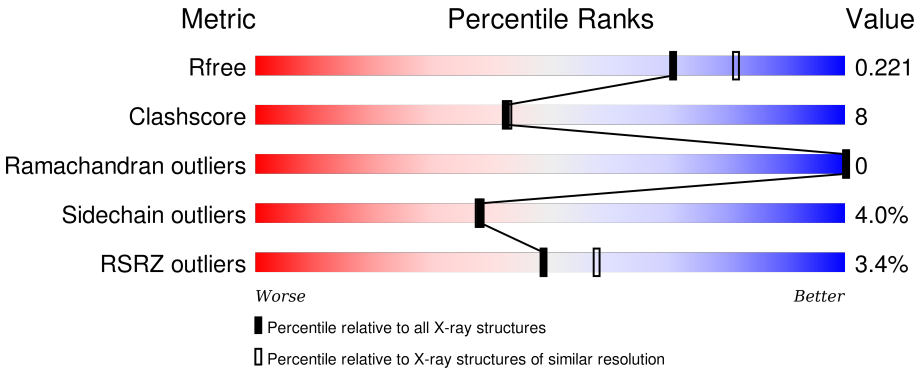
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 >=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 <=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	3% 87% 11%
2	M	307	4% 80% 16%
3	H	260	3% 73% 17% 8%

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	SPO	M	860	-	-	-	X
11	LDA	H	861	-	-	-	X
11	LDA	M	862	-	-	-	X
11	LDA	M	863	-	-	-	X
12	CDL	M	900	-	-	-	X
5	BPH	L	856	X	-	-	-
6	U10	L	859	-	-	-	X
7	GOL	L	866	-	X	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7504 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

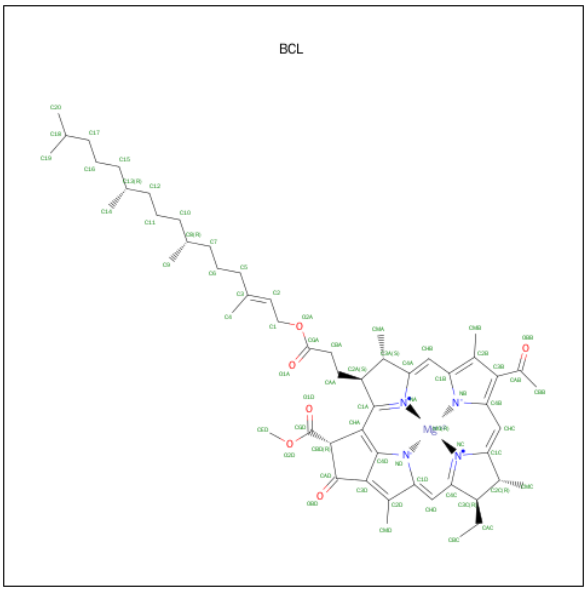
- Molecule 2 is a protein called Reaction center protein M chain.

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

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

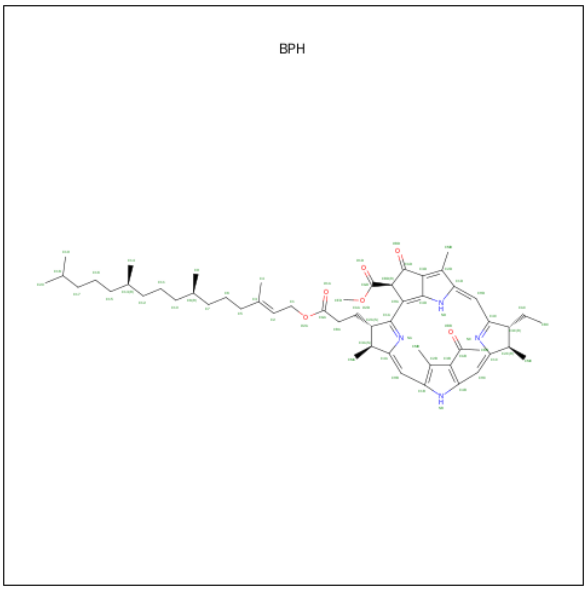
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	239	Total	C	N	O	S	0	1	0
			1832	1171	314	338	9			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



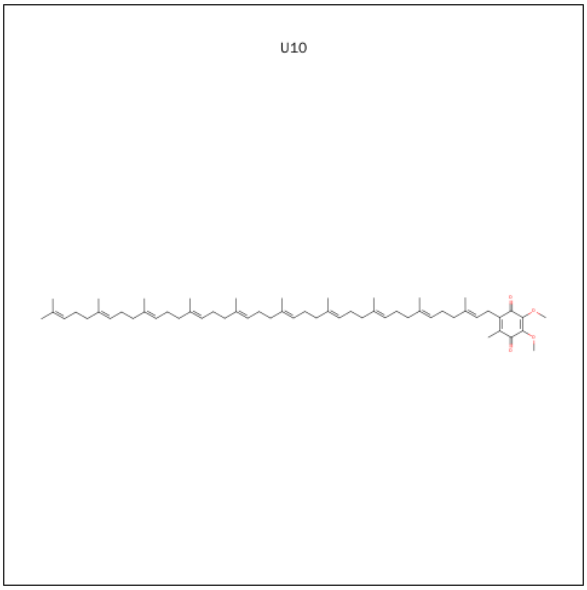
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	L	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
4	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 5 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



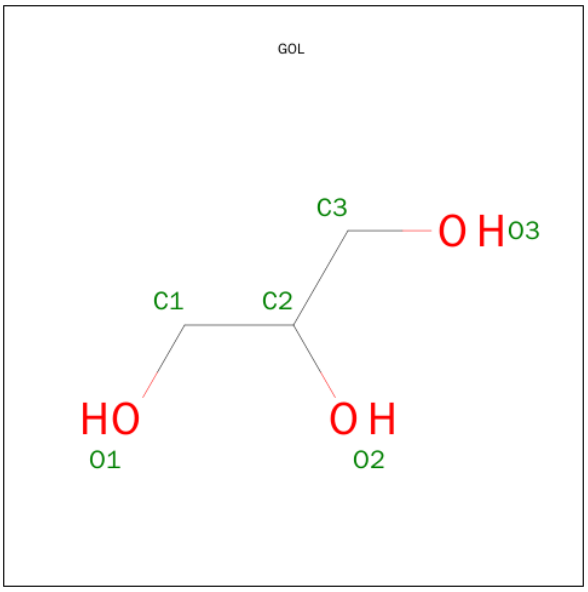
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			51	41	4	6		

- 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
			24	20	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

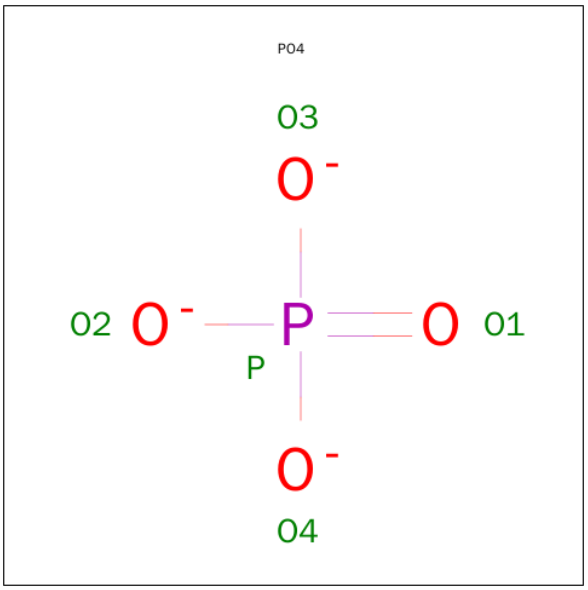


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C O 6 3 3	0	0

- Molecule 8 is FE (II) ION (three-letter code: FE2) (formula: Fe).

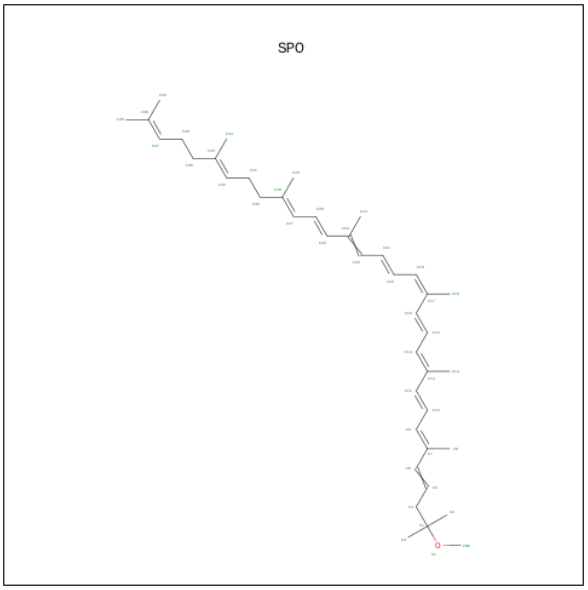
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total Fe 1 1	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



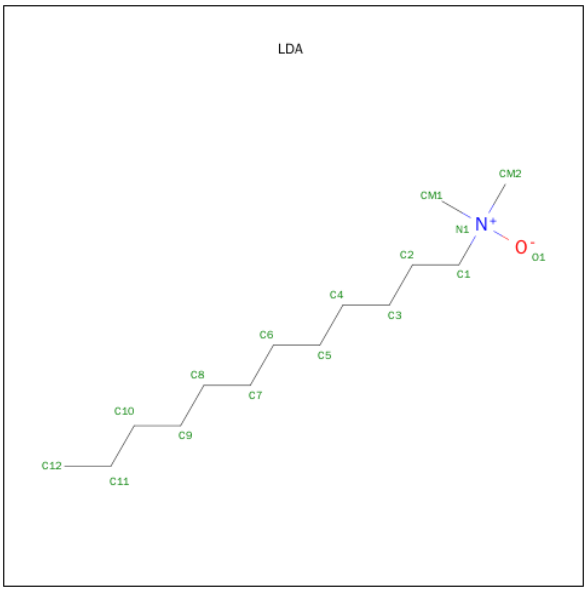
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total O P 5 4 1	0	0
9	M	1	Total O P 5 4 1	0	0

- Molecule 10 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



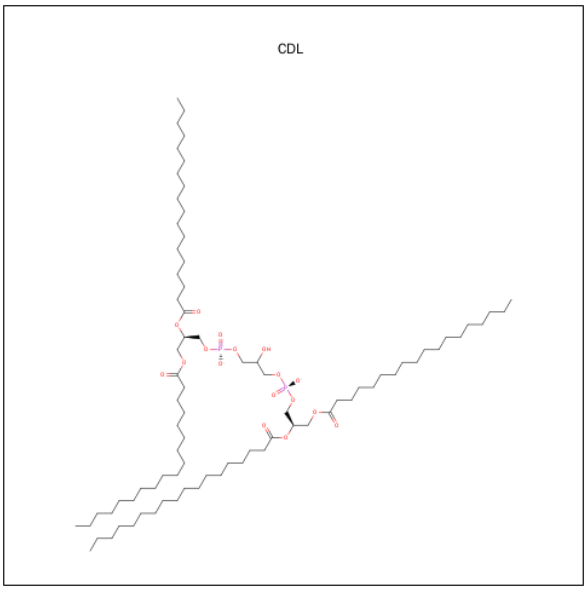
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total C O 42 41 1	0	0

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



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

- Molecule 13 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	1	Total K 1 1	0	0

- Molecule 14 is water.

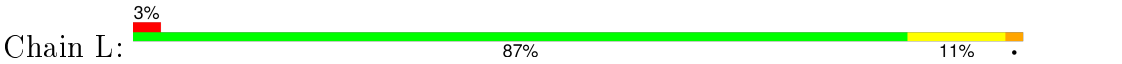
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	L	107	Total O 107 107	0	0
14	M	130	Total O 130 130	0	1
14	H	173	Total O 173 173	0	1

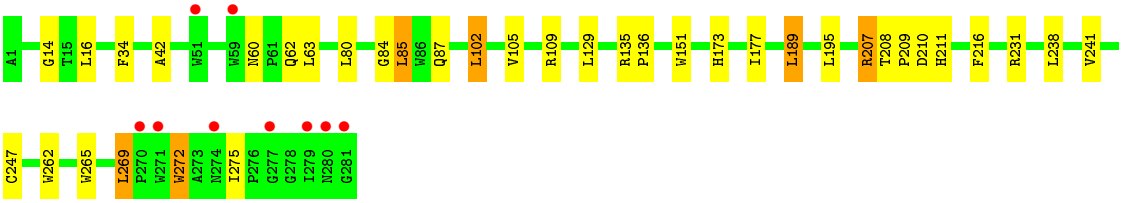
3 Residue-property plots (i)

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 L chain

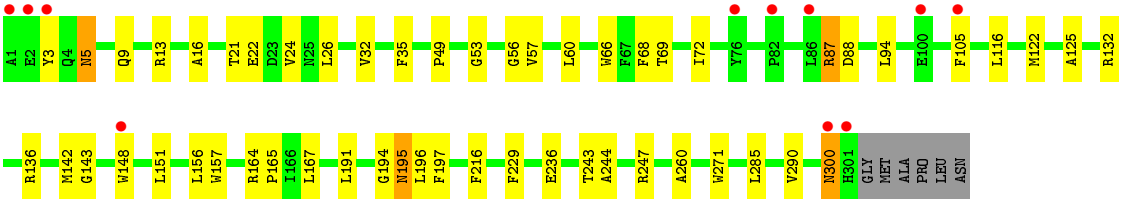
Chain L:





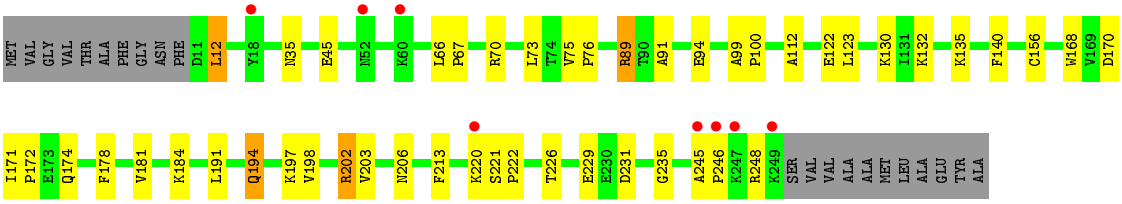
- Molecule 2: Reaction center protein M chain

Chain M:



- Molecule 3: Reaction center protein H chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	139.07Å 139.07Å 184.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.23 – 2.10 39.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.23-2.10) 98.8 (39.23-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.226 0.207 , 0.221	Depositor DCC
R_{free} test set	6001 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 70.3	EDS
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 119000 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7504	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GOL, LDA, CDL, BPH, K, FE2, SPO, U10, PO4

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	0.37	0/2320	0.55	0/3175
2	M	0.37	0/2496	0.53	0/3408
3	H	0.32	0/1880	0.59	0/2557
All	All	0.36	0/6696	0.56	0/9140

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

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	26	0
2	M	2404	0	2318	48	0
3	H	1832	0	1836	42	0
4	L	183	0	189	13	0
4	M	66	0	74	4	0
5	L	65	0	74	6	0
5	M	51	0	45	2	0
6	L	24	0	25	1	0
6	M	48	0	62	0	0
7	L	6	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	M	1	0	0	0	0
9	M	10	0	0	0	0
10	M	42	0	60	0	0
11	H	16	0	31	0	0
11	M	32	0	62	0	0
12	M	81	0	106	1	0
13	H	1	0	0	0	0
14	H	173	0	0	3	0
14	L	107	0	0	1	0
14	M	130	0	0	2	0
All	All	7504	0	7075	117	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 8.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:241:VAL:HG21	5:L:856:BPH:HAC2	1.35	1.03
2:M:157:TRP:HB2	4:M:853:BCL:H62	1.54	0.90
2:M:236:GLU:HG3	3:H:122:GLU:CD	1.98	0.84
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.65	0.78
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.23	0.74
3:H:194:GLN:H	3:H:194:GLN:NE2	1.88	0.72
3:H:89:ARG:HG3	14:H:875:HOH:O	1.92	0.69
3:H:245:ALA:HA	3:H:248:ARG:NH1	2.08	0.68
2:M:16:ALA:HB1	2:M:32:VAL:HG11	1.74	0.68
2:M:300:ASN:N	2:M:300:ASN:HD22	1.92	0.68
1:L:62:GLN:HE21	1:L:151:TRP:HE1	1.40	0.67
14:L:922:HOH:O	2:M:143:GLY:HA2	1.95	0.66
2:M:105:PHE:HD1	2:M:116:LEU:HD13	1.60	0.66
2:M:9:GLN:NE2	3:H:198:VAL:H	1.94	0.66
4:L:852:BCL:H42	4:L:854:BCL:HBC3	1.79	0.65
2:M:9:GLN:HE22	3:H:198:VAL:H	1.43	0.65
3:H:202:ARG:HG2	3:H:203:VAL:N	2.13	0.64
3:H:206:ASN:HD21	3:H:248:ARG:HD3	1.61	0.64
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.80	0.63
3:H:130:LYS:HE3	3:H:170:ASP:OD2	1.99	0.62
3:H:181:VAL:HG21	3:H:191:LEU:HD12	1.82	0.62
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.83	0.61
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:60:ASN:CG	1:L:63:LEU:HD23	2.21	0.60
1:L:189:LEU:HG	1:L:216:PHE:HZ	1.67	0.60
2:M:136:ARG:HA	2:M:136:ARG:NE	2.19	0.58
2:M:13:ARG:O	3:H:140:PHE:HA	2.04	0.58
1:L:208:THR:H	1:L:211:HIS:CD2	2.22	0.57
1:L:231:ARG:HH21	2:M:5:ASN:ND2	2.01	0.57
1:L:62:GLN:NE2	1:L:151:TRP:HE1	2.01	0.57
3:H:112:ALA:HA	3:H:235:GLY:O	2.05	0.57
3:H:89:ARG:HG2	3:H:91:ALA:O	2.05	0.56
4:L:851:BCL:HBC1	4:M:853:BCL:HBD	1.87	0.56
2:M:26:LEU:HD12	2:M:26:LEU:H	1.70	0.56
3:H:140:PHE:CE2	3:H:174:GLN:HG2	2.40	0.56
2:M:60:LEU:HA	5:M:855:BPH:H4C2	1.88	0.55
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.06	0.55
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.88	0.55
2:M:236:GLU:HG3	3:H:122:GLU:CG	2.37	0.54
3:H:132:LYS:HG2	14:H:933:HOH:O	2.08	0.54
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.42	0.54
1:L:265:TRP:O	1:L:269:LEU:HD13	2.07	0.54
2:M:243:THR:O	2:M:247:ARG:HG3	2.08	0.53
3:H:140:PHE:HE2	3:H:174:GLN:HG2	1.74	0.52
4:L:854:BCL:HMA1	4:L:854:BCL:H121	1.92	0.52
1:L:105:VAL:O	1:L:109:ARG:HG3	2.10	0.52
1:L:14:GLY:O	1:L:109:ARG:HD3	2.10	0.51
1:L:80:LEU:HB3	1:L:85:LEU:HD13	1.93	0.51
4:L:851:BCL:HBC3	4:M:853:BCL:CAD	2.41	0.51
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.92	0.51
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.94	0.51
4:L:854:BCL:H151	5:L:856:BPH:H171	1.93	0.51
3:H:156:CYS:HB2	3:H:248:ARG:HG3	1.93	0.51
2:M:68:PHE:HA	14:M:1025:HOH:O	2.11	0.50
2:M:300:ASN:N	2:M:300:ASN:ND2	2.56	0.50
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.94	0.50
4:L:851:BCL:CBC	4:M:853:BCL:HBD	2.42	0.50
2:M:26:LEU:N	2:M:26:LEU:HD12	2.27	0.50
3:H:75:VAL:HA	3:H:76:PRO:C	2.33	0.49
2:M:194:GLY:O	2:M:195:ASN:HB3	2.11	0.49
6:L:859:U10:H3M1	14:M:923:HOH:O	2.13	0.49
3:H:245:ALA:HB3	3:H:246:PRO:HD3	1.94	0.48
1:L:16:LEU:HD23	1:L:109:ARG:NH1	2.27	0.48
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:236:GLU:HG3	3:H:122:GLU:HG3	1.95	0.48
2:M:125:ALA:HB1	5:M:855:BPH:H2	1.95	0.48
3:H:226:THR:OG1	3:H:229:GLU:HG3	2.14	0.48
3:H:135:LYS:HD2	14:H:904:HOH:O	2.13	0.48
2:M:271:TRP:HH2	12:M:900:CDL:H342	1.78	0.47
3:H:194:GLN:H	3:H:194:GLN:HE21	1.59	0.47
2:M:32:VAL:HG12	2:M:49:PRO:HD3	1.94	0.47
1:L:208:THR:H	1:L:211:HIS:HD2	1.61	0.47
1:L:208:THR:HB	1:L:209:PRO:HD2	1.96	0.47
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.50	0.47
4:L:854:BCL:H193	4:L:854:BCL:H162	1.80	0.47
3:H:168:TRP:HB2	3:H:178:PHE:HB2	1.96	0.47
2:M:56:GLY:HA2	2:M:132:ARG:HD2	1.97	0.47
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.97	0.46
4:L:854:BCL:HBB3	5:L:856:BPH:H141	1.98	0.46
4:L:852:BCL:H122	5:L:856:BPH:H3A	1.97	0.46
2:M:69:THR:O	2:M:72:ILE:HG22	2.16	0.46
4:L:852:BCL:CGA	4:L:854:BCL:HBC1	2.46	0.46
2:M:195:ASN:HD22	2:M:195:ASN:C	2.19	0.46
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.51	0.46
2:M:24:VAL:O	2:M:26:LEU:HD12	2.16	0.46
4:L:852:BCL:HBD	4:L:854:BCL:HAC1	1.98	0.46
1:L:84:GLY:HA2	1:L:87:GLN:HE21	1.81	0.45
3:H:245:ALA:HA	3:H:248:ARG:HH12	1.81	0.45
1:L:238:LEU:HD23	5:L:856:BPH:CBC	2.47	0.45
1:L:34:PHE:CE1	1:L:102:LEU:HD23	2.52	0.45
3:H:170:ASP:OD1	3:H:172:PRO:HD2	2.17	0.44
3:H:206:ASN:HD21	3:H:248:ARG:CD	2.29	0.44
3:H:184:LYS:N	3:H:184:LYS:HD2	2.32	0.44
2:M:148:TRP:HA	2:M:148:TRP:HE3	1.82	0.44
2:M:53:GLY:O	2:M:57:VAL:HG23	2.18	0.44
1:L:208:THR:HB	1:L:209:PRO:CD	2.48	0.43
3:H:66:LEU:HA	3:H:67:PRO:HD3	1.86	0.43
1:L:42:ALA:HA	5:L:856:BPH:H9C3	2.01	0.43
2:M:236:GLU:HG3	3:H:122:GLU:OE2	2.19	0.43
2:M:195:ASN:ND2	2:M:197:PHE:H	2.17	0.43
2:M:194:GLY:O	2:M:195:ASN:CB	2.67	0.43
2:M:26:LEU:CD1	2:M:26:LEU:H	2.31	0.42
2:M:290:VAL:HG11	3:H:12:LEU:HB3	2.01	0.42
3:H:191:LEU:HD11	3:H:213:PHE:HE2	1.84	0.42
3:H:99:ALA:HA	3:H:100:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.83	0.42
4:L:851:BCL:H2C	4:L:851:BCL:HBC2	1.87	0.42
3:H:70:ARG:HH22	3:H:123:LEU:HD13	1.85	0.42
1:L:272:TRP:HA	1:L:275:ILE:HG13	2.01	0.42
2:M:56:GLY:O	2:M:60:LEU:HD13	2.20	0.41
3:H:220:LYS:HG3	3:H:229:GLU:OE2	2.19	0.41
1:L:60:ASN:CB	1:L:63:LEU:HD23	2.51	0.41
3:H:221:SER:HA	3:H:222:PRO:HD3	1.84	0.41
3:H:220:LYS:HE3	3:H:220:LYS:HB2	1.78	0.41
4:L:854:BCL:H141	4:L:854:BCL:H161	1.87	0.40
1:L:262:TRP:O	1:L:265:TRP:HD1	2.05	0.40
2:M:87:ARG:HG3	2:M:88:ASP:N	2.35	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%)	270 (97%)	9 (3%)	0	100	100
2	M	299/307 (97%)	292 (98%)	7 (2%)	0	100	100
3	H	238/260 (92%)	234 (98%)	4 (2%)	0	100	100
All	All	816/848 (96%)	796 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	210 (96%)	10 (4%)	34	32
2	M	236/240 (98%)	226 (96%)	10 (4%)	36	35
3	H	195/208 (94%)	189 (97%)	6 (3%)	47	50
All	All	651/668 (98%)	625 (96%)	26 (4%)	38	38

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	85	LEU
1	L	102	LEU
1	L	129	LEU
1	L	189	LEU
1	L	195	LEU
1	L	207	ARG
1	L	210	ASP
1	L	247	CYS
1	L	269	LEU
1	L	272	TRP
2	M	5	ASN
2	M	87	ARG
2	M	94	LEU
2	M	151	LEU
2	M	156	LEU
2	M	191	LEU
2	M	195	ASN
2	M	196	LEU
2	M	216	PHE
2	M	300	ASN
3	H	12	LEU
3	H	73	LEU
3	H	89	ARG
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	62	GLN
1	L	87	GLN
1	L	211	HIS
1	L	213	ASN
2	M	5	ASN
2	M	9	GLN
2	M	195	ASN
2	M	300	ASN
3	H	194	GLN
3	H	206	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
11	LDA	H	861	-	15,15,15	3.92	2 (13%)	16,17,17	2.65	4 (25%)
4	BCL	L	851	-	38,59,74	1.17	1 (2%)	40,97,115	2.05	12 (30%)
4	BCL	L	852	-	53,74,74	1.06	2 (3%)	57,115,115	1.75	14 (24%)
4	BCL	L	854	-	53,74,74	1.13	3 (5%)	57,115,115	1.69	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	BPH	L	856	-	64,70,70	1.47	9 (14%)	73,101,101	2.12	16 (21%)
6	U10	L	859	-	24,24,63	2.14	8 (33%)	29,32,79	2.04	7 (24%)
7	GOL	L	866	-	5,5,5	4.80	5 (100%)	5,5,5	5.64	3 (60%)
4	BCL	M	853	-	53,74,74	1.01	2 (3%)	57,115,115	1.95	17 (29%)
5	BPH	M	855	-	50,56,70	1.42	7 (14%)	56,84,101	2.32	16 (28%)
6	U10	M	858	-	48,48,63	2.07	17 (35%)	58,61,79	2.93	14 (24%)
10	SPO	M	860	-	40,41,41	3.45	23 (57%)	45,50,50	2.49	14 (31%)
11	LDA	M	862	-	15,15,15	3.93	2 (13%)	16,17,17	2.62	4 (25%)
11	LDA	M	863	-	15,15,15	3.97	2 (13%)	16,17,17	2.60	4 (25%)
9	PO4	M	864	-	4,4,4	1.12	0	6,6,6	0.27	0
9	PO4	M	865	-	4,4,4	1.15	0	6,6,6	0.27	0
12	CDL	M	900	-	80,80,99	0.81	2 (2%)	82,92,111	0.99	5 (6%)

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
11	LDA	H	861	-	-	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
4	BCL	L	854	-	-	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	-	-	0/17/41/87	0/1/1/1
7	GOL	L	866	-	-	0/4/4/4	0/0/0/0
4	BCL	M	853	-	-	0/37/137/137	0/0/9/9
5	BPH	M	855	-	-	1/38/89/105	0/1/6/6
6	U10	M	858	-	-	1/45/69/87	0/1/1/1
10	SPO	M	860	-	-	0/47/47/47	0/0/0/0
11	LDA	M	862	-	-	0/13/13/13	0/0/0/0
11	LDA	M	863	-	-	0/13/13/13	0/0/0/0
9	PO4	M	864	-	-	0/0/0/0	0/0/0/0
9	PO4	M	865	-	-	0/0/0/0	0/0/0/0
12	CDL	M	900	-	-	0/91/91/110	0/0/0/0

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	863	LDA	O1-N1	-14.63	1.25	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	862	LDA	O1-N1	-14.46	1.25	1.39
11	H	861	LDA	O1-N1	-14.42	1.25	1.39
7	L	866	GOL	C3-C2	-8.18	1.21	1.52
5	L	856	BPH	C11-C10	-4.99	1.29	1.52
11	H	861	LDA	CM2-N1	-4.03	1.43	1.49
11	M	862	LDA	CM2-N1	-3.98	1.43	1.49
11	M	863	LDA	CM2-N1	-3.96	1.43	1.49
6	L	859	U10	C7-C8	-3.38	1.45	1.50
6	M	858	U10	C7-C8	-3.36	1.45	1.50
7	L	866	GOL	C1-C2	-3.12	1.40	1.52
6	M	858	U10	C32-C33	-2.99	1.42	1.50
10	M	860	SPO	C25-C23	-2.91	1.39	1.45
6	M	858	U10	O3-C3M	-2.90	1.38	1.45
7	L	866	GOL	O2-C2	-2.89	1.34	1.43
6	L	859	U10	O3-C3M	-2.81	1.38	1.45
4	L	851	BCL	C3C-C4C	-2.66	1.48	1.51
5	M	855	BPH	O2D-CED	-2.55	1.39	1.45
5	L	856	BPH	O2D-CED	-2.44	1.39	1.45
6	M	858	U10	C27-C28	-2.33	1.44	1.50
10	M	860	SPO	C11-C12	-2.22	1.41	1.45
10	M	860	SPO	C6-C7	-2.09	1.41	1.45
5	M	855	BPH	C2C-C3C	-2.02	1.48	1.54
6	M	858	U10	C20-C19	2.00	1.55	1.50
6	M	858	U10	C30-C29	2.01	1.55	1.50
5	L	856	BPH	O1D-CGD	2.07	1.26	1.21
6	M	858	U10	C33-C34	2.11	1.37	1.33
5	L	856	BPH	C2A-C1A	2.11	1.55	1.51
10	M	860	SPO	C24-C23	2.13	1.55	1.50
10	M	860	SPO	C22-C23	2.13	1.38	1.35
5	L	856	BPH	CHC-C1C	2.17	1.40	1.36
4	L	854	BCL	C4-C3	2.21	1.56	1.50
4	M	853	BCL	C4-C3	2.22	1.56	1.50
4	L	854	BCL	CAA-C2A	2.22	1.58	1.54
5	M	855	BPH	C2A-C1A	2.25	1.55	1.51
4	M	853	BCL	CBB-CAB	2.25	1.56	1.49
5	L	856	BPH	CAA-C2A	2.29	1.58	1.54
4	L	852	BCL	CBB-CAB	2.29	1.56	1.49
4	L	854	BCL	CAA-CBA	2.36	1.60	1.52
6	L	859	U10	C6-C1	2.37	1.40	1.35
10	M	860	SPO	C26-C27	2.37	1.51	1.43
4	L	852	BCL	C4-C3	2.38	1.56	1.50
5	M	855	BPH	CAA-C2A	2.39	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	859	U10	C15-C14	2.39	1.56	1.50
6	M	858	U10	C15-C14	2.45	1.56	1.50
10	M	860	SPO	C13-C12	2.53	1.56	1.50
6	M	858	U10	C38-C39	2.53	1.40	1.32
12	M	900	CDL	CB3-CB4	2.55	1.57	1.50
6	M	858	U10	C6-C1	2.55	1.41	1.35
10	M	860	SPO	C8-C7	2.61	1.56	1.50
10	M	860	SPO	C15-C14	2.68	1.52	1.43
10	M	860	SPO	C37-C38	2.70	1.40	1.32
12	M	900	CDL	OA8-CA7	2.72	1.41	1.33
6	M	858	U10	C28-C29	2.84	1.38	1.33
6	M	858	U10	O3-C3	2.96	1.44	1.37
10	M	860	SPO	C10-C9	3.07	1.53	1.43
6	M	858	U10	C18-C19	3.18	1.39	1.33
6	L	859	U10	O3-C3	3.21	1.45	1.37
7	L	866	GOL	O3-C3	3.22	1.56	1.42
5	M	855	BPH	C2-C3	3.23	1.39	1.33
6	M	858	U10	C8-C9	3.39	1.39	1.33
5	L	856	BPH	C2-C3	3.39	1.39	1.33
10	M	860	SPO	C32-C33	3.60	1.40	1.33
5	L	856	BPH	O2D-CGD	3.70	1.42	1.33
6	L	859	U10	C8-C9	3.71	1.40	1.33
10	M	860	SPO	C19-C17	3.84	1.40	1.35
5	L	856	BPH	O2A-CGA	3.86	1.45	1.33
5	M	855	BPH	O2D-CGD	3.88	1.43	1.33
5	M	855	BPH	O2A-CGA	3.99	1.45	1.33
6	M	858	U10	C23-C24	3.99	1.40	1.33
6	L	859	U10	O4-C4	4.07	1.47	1.37
10	M	860	SPO	C4-C1	4.15	1.59	1.53
10	M	860	SPO	O1-CM1	4.28	1.56	1.43
10	M	860	SPO	C9-C7	4.34	1.41	1.35
6	M	858	U10	C13-C14	4.37	1.41	1.33
7	L	866	GOL	O1-C1	4.46	1.61	1.42
10	M	860	SPO	C14-C12	4.65	1.41	1.35
10	M	860	SPO	C26-C25	4.71	1.46	1.34
6	M	858	U10	O4-C4	4.80	1.49	1.37
10	M	860	SPO	C27-C28	4.90	1.39	1.34
6	L	859	U10	C13-C14	5.00	1.42	1.33
10	M	860	SPO	C21-C20	5.24	1.49	1.35
10	M	860	SPO	C15-C16	7.71	1.54	1.34
10	M	860	SPO	C10-C11	8.16	1.55	1.34
10	M	860	SPO	C6-C5	8.55	1.55	1.31

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	861	LDA	CM2-N1-CM1	-7.66	100.19	108.83
11	M	862	LDA	CM2-N1-CM1	-7.65	100.20	108.83
11	M	863	LDA	CM2-N1-CM1	-7.61	100.25	108.83
10	M	860	SPO	O1-C1-C4	-7.42	87.71	105.87
10	M	860	SPO	C15-C14-C12	-6.08	118.42	127.20
4	L	851	BCL	CAC-C3C-C4C	-5.69	99.94	112.58
10	M	860	SPO	C20-C21-C22	-5.26	111.77	123.39
5	M	855	BPH	O1D-CGD-CBD	-5.23	117.13	124.62
10	M	860	SPO	C25-C23-C22	-4.99	110.95	118.98
5	L	856	BPH	O1D-CGD-CBD	-4.66	117.94	124.62
4	M	853	BCL	C5-C3-C2	-4.56	112.40	121.05
6	M	858	U10	C30-C29-C31	-3.99	109.32	115.41
4	M	853	BCL	OBD-CAD-CBD	-3.87	120.10	125.94
10	M	860	SPO	C18-C17-C19	-3.81	117.28	122.90
4	L	854	BCL	OBB-CAB-CBB	-3.80	111.03	120.13
4	L	852	BCL	OBB-CAB-CBB	-3.78	111.08	120.13
4	M	853	BCL	OBB-CAB-CBB	-3.77	111.11	120.13
4	L	851	BCL	OBB-CAB-CBB	-3.76	111.13	120.13
6	L	859	U10	O5-C5-C6	-3.59	114.94	121.68
4	M	853	BCL	C11-C12-C13	-3.58	103.62	115.49
10	M	860	SPO	C4-C5-C6	-3.56	119.61	124.67
4	L	851	BCL	OBD-CAD-CBD	-3.39	120.83	125.94
5	L	856	BPH	O2D-CGD-O1D	-3.38	116.81	123.79
6	M	858	U10	O5-C5-C6	-3.38	115.33	121.68
6	L	859	U10	O2-C2-C3	-3.33	113.57	120.79
4	L	854	BCL	OBD-CAD-CBD	-3.33	120.92	125.94
4	L	854	BCL	C11-C12-C13	-3.32	104.46	115.49
4	L	852	BCL	O2D-CGD-CBD	-3.31	106.76	111.30
6	M	858	U10	C20-C19-C21	-3.29	110.38	115.41
4	L	852	BCL	C7-C6-C5	-3.27	103.41	113.06
5	M	855	BPH	O2D-CGD-O1D	-3.27	117.05	123.79
4	L	851	BCL	C1-C2-C3	-3.24	121.39	126.71
10	M	860	SPO	C15-C16-C17	-3.20	116.89	126.32
4	L	852	BCL	CAC-C3C-C4C	-3.13	105.64	112.58
4	L	854	BCL	CAA-C2A-C3A	-3.06	104.42	113.22
4	L	852	BCL	CAA-C2A-C3A	-3.00	104.58	113.22
4	L	852	BCL	CMB-C2B-C1B	-3.00	123.40	128.36
4	L	852	BCL	OBD-CAD-CBD	-2.96	121.48	125.94
4	L	851	BCL	CAA-C2A-C3A	-2.92	104.82	113.22
10	M	860	SPO	C6-C7-C9	-2.91	114.30	118.98
6	L	859	U10	C1-C6-C5	-2.85	116.87	120.12
4	M	853	BCL	CMB-C2B-C1B	-2.81	123.71	128.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	851	BCL	CMB-C2B-C1B	-2.77	123.78	128.36
6	M	858	U10	O2-C2-C3	-2.68	114.98	120.79
4	M	853	BCL	CAA-C2A-C3A	-2.65	105.61	113.22
4	L	854	BCL	C7-C6-C5	-2.62	105.33	113.06
6	L	859	U10	C15-C14-C16	-2.61	112.73	115.68
12	M	900	CDL	CB6-CB4-CB3	-2.57	106.05	112.07
4	M	853	BCL	CHA-C1A-NA	-2.57	119.73	126.06
4	L	851	BCL	CHA-C1A-NA	-2.52	119.86	126.06
10	M	860	SPO	C10-C9-C7	-2.51	123.57	127.20
6	M	858	U10	C1-C6-C5	-2.51	117.26	120.12
4	L	854	BCL	CHA-C1A-NA	-2.50	119.91	126.06
4	L	854	BCL	CMB-C2B-C1B	-2.49	124.25	128.36
4	M	853	BCL	C16-C15-C13	-2.48	107.27	115.49
5	M	855	BPH	CAA-C2A-C3A	-2.47	106.13	113.22
5	L	856	BPH	C7-C6-C5	-2.44	105.86	113.06
4	M	853	BCL	C11-C10-C8	-2.43	107.43	115.49
5	L	856	BPH	O2A-CGA-O1A	-2.40	117.28	123.49
5	M	855	BPH	C2A-C1A-NA	-2.39	109.02	112.08
5	L	856	BPH	CAA-C2A-C3A	-2.37	106.40	113.22
4	L	852	BCL	CHA-C1A-NA	-2.35	120.29	126.06
4	L	854	BCL	CAC-C3C-C4C	-2.31	107.46	112.58
11	H	861	LDA	C9-C8-C7	-2.30	102.63	114.53
4	L	852	BCL	C11-C12-C13	-2.30	107.85	115.49
11	M	862	LDA	C9-C8-C7	-2.25	102.91	114.53
5	L	856	BPH	CAC-C3C-C2C	-2.23	108.52	114.13
5	M	855	BPH	CBB-CAB-C3B	-2.22	115.59	120.52
10	M	860	SPO	C27-C26-C25	-2.20	116.42	123.13
11	H	861	LDA	CM1-N1-C1	-2.19	102.72	109.77
11	M	862	LDA	CM1-N1-C1	-2.16	102.81	109.77
5	L	856	BPH	C5-C3-C2	-2.16	116.95	121.05
11	M	863	LDA	C9-C8-C7	-2.16	103.39	114.53
6	L	859	U10	C7-C6-C5	-2.13	116.05	118.56
5	M	855	BPH	O2A-CGA-O1A	-2.11	118.04	123.49
12	M	900	CDL	CA6-CA4-CA3	-2.11	107.13	112.07
5	L	856	BPH	OBD-CAD-CBD	-2.08	122.80	125.94
11	M	863	LDA	CM1-N1-C1	-2.07	103.09	109.77
5	L	856	BPH	CAA-C2A-C1A	-2.06	107.43	112.86
10	M	860	SPO	C20-C19-C17	-2.06	124.22	127.20
5	M	855	BPH	C5-C3-C2	-2.05	116.17	120.74
4	L	854	BCL	C12-C11-C10	-2.05	102.84	112.99
4	L	854	BCL	C16-C15-C13	-2.04	108.71	115.49
5	M	855	BPH	C3A-C4A-NA	-2.04	110.00	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	855	BPH	OBD-CAD-CBD	-2.03	122.87	125.94
4	M	853	BCL	CAC-C3C-C2C	-2.03	109.03	114.13
5	M	855	BPH	CMD-C2D-C3D	2.03	129.06	125.09
6	M	858	U10	C17-C18-C19	2.04	132.19	127.76
4	M	853	BCL	C3D-CAD-CBD	2.05	110.49	107.60
6	M	858	U10	C7-C8-C9	2.09	130.25	126.70
12	M	900	CDL	C52-C51-CB5	2.10	121.84	113.59
4	L	852	BCL	CED-O2D-CGD	2.14	121.00	115.99
4	L	851	BCL	C3D-CAD-CBD	2.16	110.65	107.60
4	L	854	BCL	C3D-CAD-CBD	2.23	110.75	107.60
4	M	853	BCL	C6-C5-C3	2.31	117.55	112.48
5	M	855	BPH	C2C-C3C-C4C	2.38	105.54	101.50
4	M	853	BCL	CED-O2D-CGD	2.41	121.65	115.99
5	L	856	BPH	C2C-C3C-C4C	2.43	105.62	101.50
4	L	854	BCL	CBB-CAB-C3B	2.47	127.64	120.33
6	M	858	U10	C21-C19-C18	2.52	125.83	121.05
4	L	852	BCL	CBB-CAB-C3B	2.62	128.09	120.33
6	M	858	U10	C16-C14-C13	2.65	126.08	121.05
6	M	858	U10	C31-C32-C33	2.66	118.65	111.69
4	L	851	BCL	CBB-CAB-C3B	2.67	128.25	120.33
4	L	854	BCL	C2C-C3C-C4C	2.68	106.05	101.50
6	M	858	U10	C31-C29-C28	2.70	126.16	121.05
10	M	860	SPO	C8-C7-C6	2.76	122.69	118.10
4	M	853	BCL	CBB-CAB-C3B	2.78	128.58	120.33
5	M	855	BPH	C4-C3-C5	2.84	118.90	115.68
4	L	854	BCL	CMB-C2B-C3B	2.87	130.69	125.09
6	L	859	U10	C16-C14-C13	2.88	127.16	120.74
4	M	853	BCL	CMB-C2B-C3B	2.97	130.90	125.09
4	L	851	BCL	CMB-C2B-C3B	3.16	131.27	125.09
4	L	852	BCL	CMD-C2D-C3D	3.18	131.31	125.09
12	M	900	CDL	CB4-OB6-CB5	3.20	125.57	117.89
7	L	866	GOL	O1-C1-C2	3.25	125.93	110.18
4	M	853	BCL	CMD-C2D-C3D	3.31	131.56	125.09
5	M	855	BPH	CBC-CAC-C3C	3.34	121.73	113.57
4	L	852	BCL	CMB-C2B-C3B	3.38	131.69	125.09
4	L	852	BCL	O1D-CGD-CBD	3.40	129.50	124.62
10	M	860	SPO	C3-C1-C2	3.48	117.25	110.22
5	L	856	BPH	CBC-CAC-C3C	3.50	122.13	113.57
4	L	851	BCL	CMD-C2D-C3D	3.55	132.04	125.09
4	L	854	BCL	CMD-C2D-C3D	3.67	132.26	125.09
4	L	851	BCL	C2C-C3C-C4C	3.73	107.82	101.50
5	L	856	BPH	C11-C10-C8	3.77	128.00	115.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	860	SPO	C24-C23-C25	3.90	124.58	118.10
5	L	856	BPH	C4A-NA-C1A	4.04	111.81	108.21
5	L	856	BPH	CED-O2D-CGD	4.16	125.75	115.99
12	M	900	CDL	OB8-CB6-CB4	4.22	120.05	108.69
5	M	855	BPH	CED-O2D-CGD	4.29	126.05	115.99
5	M	855	BPH	C4A-NA-C1A	4.59	112.31	108.21
4	M	853	BCL	C4-C3-C5	4.74	122.65	115.41
11	M	862	LDA	O1-N1-C1	5.23	116.16	110.27
11	M	863	LDA	O1-N1-C1	5.27	116.20	110.27
11	H	861	LDA	O1-N1-C1	5.32	116.26	110.27
5	L	856	BPH	C6-C5-C3	5.38	124.29	112.48
6	L	859	U10	C3M-O3-C3	6.14	138.43	116.61
6	M	858	U10	C3M-O3-C3	6.33	139.11	116.61
7	L	866	GOL	O2-C2-C3	6.65	139.13	108.65
6	M	858	U10	C27-C28-C29	7.12	143.24	127.76
5	L	856	BPH	O2D-CGD-CBD	10.13	125.20	111.30
7	L	866	GOL	O3-C3-C2	10.18	159.56	110.18
5	M	855	BPH	O2D-CGD-CBD	10.57	125.80	111.30
6	M	858	U10	C32-C33-C34	16.51	163.67	127.76

All (2) chirality outliers are listed below:

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

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	855	BPH	C1-C2-C3-C4
6	M	858	U10	C34-C33-C32-C31

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	851	BCL	4	0
4	L	852	BCL	4	0
4	L	854	BCL	8	0
5	L	856	BPH	6	0
6	L	859	U10	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	853	BCL	4	0
5	M	855	BPH	2	0
12	M	900	CDL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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^{th} 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^2)	Q<0.9
1	L	281/281 (100%)	-0.24	9 (3%) 51 60	22, 31, 55, 82	0
2	M	301/307 (98%)	-0.08	11 (3%) 45 54	21, 35, 57, 79	0
3	H	239/260 (91%)	-0.28	8 (3%) 50 59	24, 35, 49, 84	0
All	All	821/848 (96%)	-0.19	28 (3%) 49 58	21, 34, 54, 84	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.0
1	L	59	TRP	4.6
2	M	3	TYR	4.5
3	H	249	LYS	4.4
1	L	277	GLY	4.2
1	L	279	ILE	4.0
3	H	245	ALA	4.0
2	M	301	HIS	3.8
2	M	2	GLU	3.7
1	L	271	TRP	3.1
3	H	18	TYR	3.0
2	M	100	GLU	3.0
2	M	82	PRO	2.9
1	L	280	ASN	2.9
1	L	270	PRO	2.9
2	M	148	TRP	2.9
3	H	247	LYS	2.7
1	L	281	GLY	2.7
2	M	86	LEU	2.5
3	H	52	ASN	2.5
2	M	105	PHE	2.4
1	L	274	ASN	2.3
3	H	246	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	300	ASN	2.2
3	H	220	LYS	2.1
1	L	51	TRP	2.1
3	H	60	LYS	2.0
2	M	76	TYR	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^{th} 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^2)	Q<0.9
11	LDA	M	863	16/16	0.67	0.27	8.88	67,72,73,73	0
11	LDA	M	862	16/16	0.69	0.28	5.72	74,75,82,82	0
6	U10	L	859	24/63	0.69	0.28	3.85	43,53,58,58	0
12	CDL	M	900	81/100	0.79	0.27	3.35	61,75,84,86	0
7	GOL	L	866	6/6	0.86	0.12	2.73	47,52,53,54	0
10	SPO	M	860	42/42	0.80	0.20	2.60	34,46,62,64	0
11	LDA	H	861	16/16	0.84	0.17	2.46	63,65,68,69	0
4	BCL	M	853	66/66	0.92	0.15	1.91	19,26,56,62	0
4	BCL	L	854	66/66	0.92	0.15	1.80	22,29,54,57	0
6	U10	M	858	48/63	0.91	0.19	1.67	25,41,69,69	0
4	BCL	L	851	51/66	0.93	0.15	1.51	24,29,55,57	0
5	BPH	M	855	51/65	0.94	0.15	1.27	28,33,56,59	0
5	BPH	L	856	65/65	0.95	0.12	0.90	22,26,50,51	0
4	BCL	L	852	66/66	0.95	0.11	0.46	21,26,41,47	0
9	PO4	M	865	5/5	0.95	0.14	-0.04	70,71,71,71	0
9	PO4	M	864	5/5	0.97	0.12	-0.05	67,68,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	K	H	867	1/1	0.96	0.06	-1.75	36,36,36,36	0
8	FE2	M	857	1/1	0.99	0.10	-2.68	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.