



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:05 PM GMT

PDB ID : 1RZH
Title : PHOTOSYNTHETIC REACTION CENTER DOUBLE MUTANT FROM RHODOBACTER SPHAEROIDES WITH ASP L213 REPLACED WITH ASN AND ARG M233 REPLACED WITH CYS IN THE CHARGE-NEUTRAL DQAQB STATE (TRIGONAL FORM)
Authors : Xu, Q.; Axelrod, H.L.; Abresch, E.C.; Paddock, M.L.; Okamura, M.Y.; Feher, G.
Deposited on : 2003-12-24
Resolution : 1.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

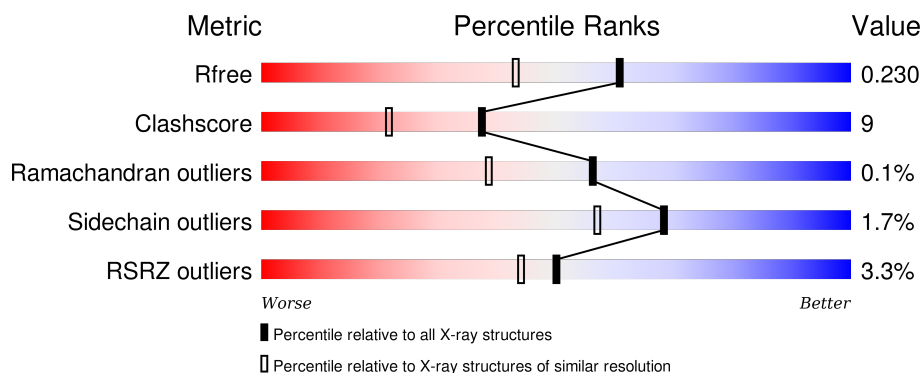
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 ≥ 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>87%</div> <div>12%</div> </div>
2	M	307	<div> <div>4%</div> <div>80%</div> <div>18%</div> </div>
3	H	260	<div> <div>2%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SPO	M	860	-	-	-	X
11	LDA	H	862	-	-	-	X
11	LDA	M	861	-	-	-	X
11	LDA	M	863	-	-	-	X
12	CDL	M	900	-	-	-	X
13	GOL	M	867	-	X	-	-
4	BCL	M	851	X	-	-	X
4	BCL	M	853	-	-	-	X
5	BPH	L	856	X	-	-	-
5	BPH	M	855	X	-	-	-
6	U10	L	859[A]	-	-	-	X
6	U10	M	858	-	-	-	X
7	HTO	L	865	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 7586 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	1	0
			2238	1510	357	363	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
			2399	1602	390	396	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	233	CYS	ARG	ENGINEERED	UNP P02953

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

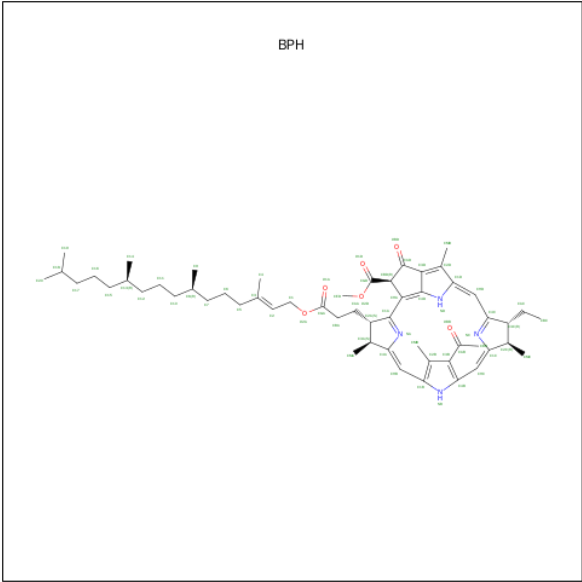
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	238	Total	C	N	O	S	0	1	0
			1822	1165	312	335	10			

- Molecule 4 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: C₅₅H₇₄MgN₄O₆).



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	M	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: C₅₅H₇₆N₄O₆).



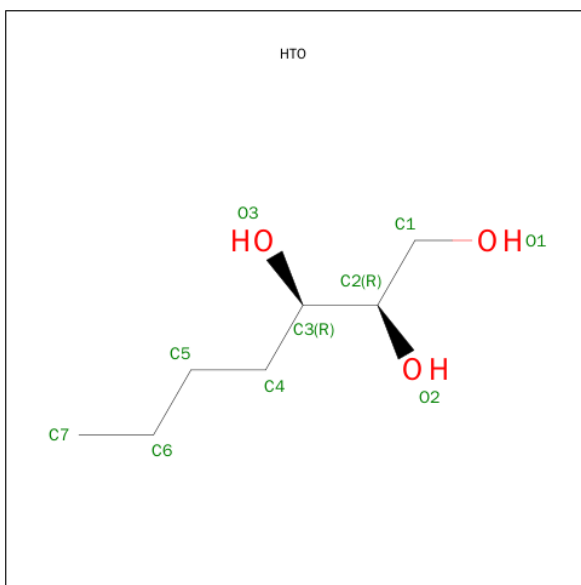
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	L	1	Total	C	N	O	0	0
			65	55	4	6		
5	M	1	Total	C	N	O	0	0
			55	45	4	6		

- 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	1
			33	29	4		
6	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).

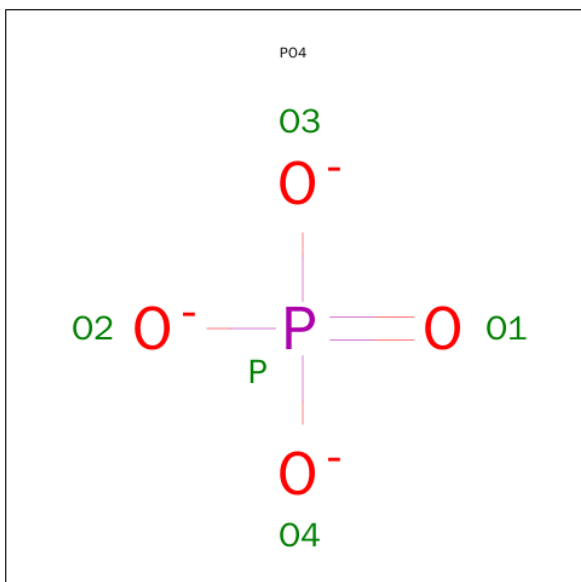


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	L	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		

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

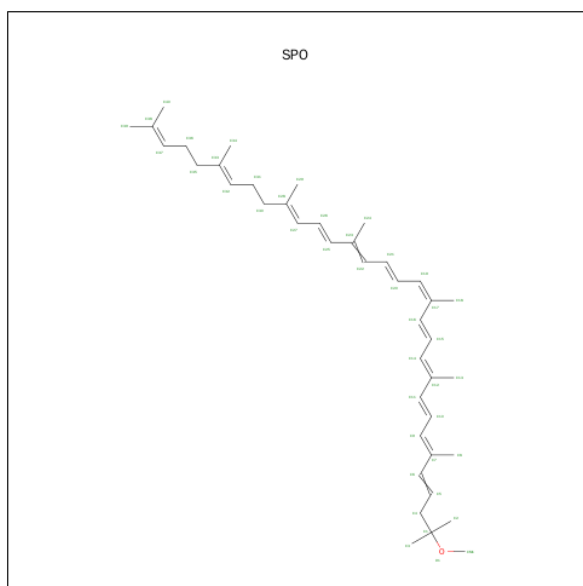
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	M	1	Total	Fe	0	0
			1	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



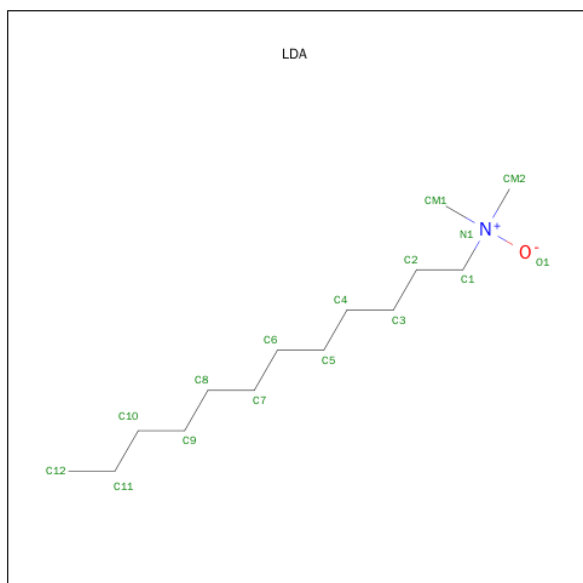
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	M	1	Total	O	P	0	0
			5	4	1		

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



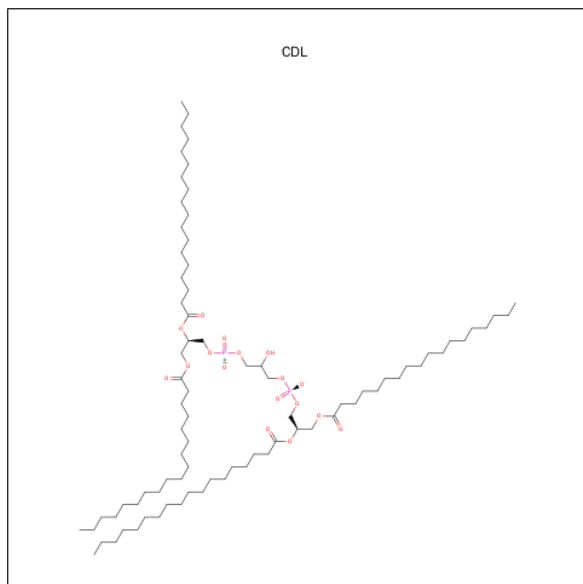
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	M	1	Total	C	O	0	0
			42	41	1		

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



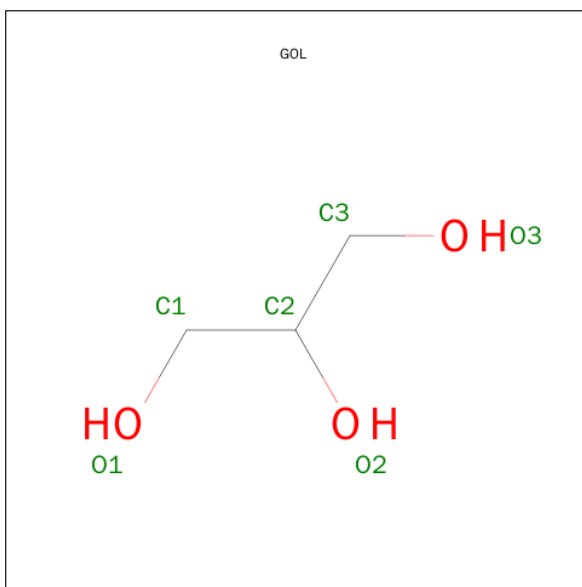
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	M	1	Total	C	N	O	0	0
			16	14	1	1		
11	M	1	Total	C	N	O	0	0
			16	14	1	1		
11	H	1	Total	C	N	O	0	0
			16	14	1	1		

- 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
			69	50	17	2		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	M	1	Total	C	O	0	0
			6	3	3		

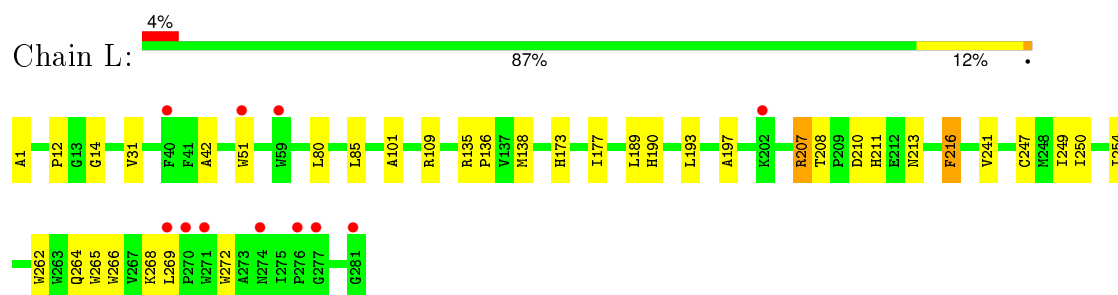
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	L	124	Total	O	0	2
			124	124		
14	M	138	Total	O	0	0
			138	138		
14	H	209	Total	O	0	0
			209	209		

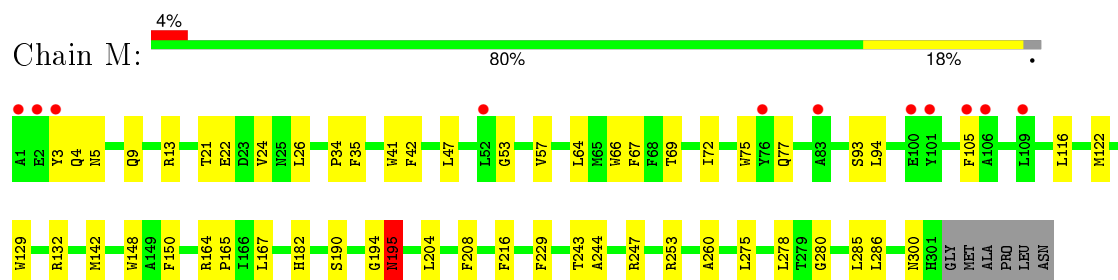
3 Residue-property plots

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

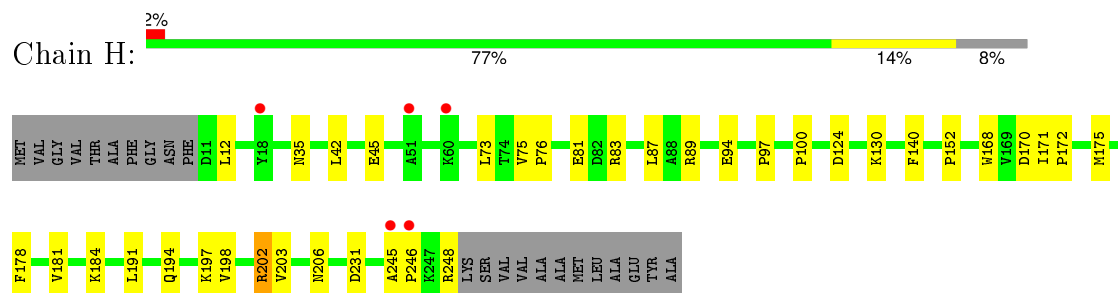
• Molecule 1: Reaction center protein L chain



• 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, α , β , γ	139.35Å 139.35Å 184.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.31 – 1.80 39.31 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.31-1.80) 98.3 (39.31-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.233 0.218 , 0.230	Depositor DCC
R_{free} test set	9418 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 188308 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7586	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, GOL, LDA, CDL, BPH, PO4, HTO, 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	0.36	0/2326	0.55	0/3183
2	M	0.35	0/2491	0.53	0/3402
3	H	0.30	0/1870	0.59	0/2544
All	All	0.34	0/6687	0.56	0/9129

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	2238	0	2193	36	0
2	M	2399	0	2310	53	0
3	H	1822	0	1826	29	0
4	L	132	0	148	4	0
4	M	132	0	148	21	0
5	L	65	0	74	5	0
5	M	55	0	53	3	0
6	L	33	0	39	8	0
6	M	48	0	61	3	0
7	L	20	0	32	2	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	5	0	0	0	0
10	M	42	0	60	7	0
11	H	16	0	31	2	0
11	M	32	0	62	5	0
12	M	69	0	82	2	0
13	M	6	0	4	0	0
14	H	209	0	0	1	0
14	L	124	0	0	0	0
14	M	138	0	0	0	0
All	All	7586	0	7123	132	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 9.

All (132) 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)
4:M:851:BCL:H121	4:M:851:BCL:C9	1.41	1.43
4:M:851:BCL:C12	4:M:851:BCL:H91	1.36	1.39
1:L:241:VAL:HG21	5:L:856:BPH:HAC1	1.46	0.97
4:M:851:BCL:H91	4:M:851:BCL:H122	1.54	0.90
2:M:21:THR:HG23	2:M:26:LEU:HD11	1.53	0.90
3:H:206:ASN:HD21	3:H:248:ARG:HD3	1.49	0.76
2:M:13:ARG:HD2	2:M:35:PHE:CD2	2.21	0.76
1:L:216:PHE:CG	6:L:859[A]:U10:H3M2	2.21	0.74
4:M:851:BCL:H92	4:M:851:BCL:H121	1.67	0.72
4:M:851:BCL:H112	4:M:853:BCL:H171	1.72	0.72
1:L:189:LEU:HB3	6:L:859[A]:U10:H4M3	1.74	0.70
3:H:89:ARG:NH1	3:H:94:GLU:HG2	2.07	0.70
2:M:77:GLN:HE22	2:M:93:SER:H	1.38	0.70
2:M:9:GLN:NE2	3:H:198:VAL:H	1.90	0.68
2:M:9:GLN:HE22	3:H:198:VAL:H	1.43	0.67
4:M:851:BCL:C12	4:M:851:BCL:C9	2.16	0.66
4:M:853:BCL:HMB1	4:M:853:BCL:CBB	2.27	0.65
4:M:851:BCL:H91	4:M:851:BCL:H121	0.66	0.64
3:H:171:ILE:HB	3:H:172:PRO:HD3	1.78	0.64
2:M:64:LEU:HD23	5:M:855:BPH:H9C3	1.79	0.64
2:M:229:PHE:HB2	2:M:244:ALA:HB2	1.80	0.63
1:L:193:LEU:HD22	6:L:859[A]:U10:H3M3	1.79	0.62
3:H:202:ARG:HG2	3:H:203:VAL:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:41:TRP:CG	11:M:863:LDA:HM13	2.36	0.61
3:H:181:VAL:HG21	3:H:191:LEU:HD12	1.83	0.61
2:M:75:TRP:HE1	10:M:860:SPO:HM13	1.66	0.61
1:L:135:ARG:HB3	1:L:136:PRO:HD3	1.82	0.60
2:M:3:TYR:CZ	2:M:5:ASN:HA	2.37	0.60
3:H:87:LEU:HD23	3:H:100:PRO:HA	1.84	0.59
2:M:286:LEU:HD21	3:H:12:LEU:HD12	1.83	0.59
4:M:851:BCL:HMB1	4:M:851:BCL:CBB	2.32	0.59
1:L:266:TRP:O	1:L:269:LEU:HD23	2.02	0.59
2:M:69:THR:O	2:M:72:ILE:HG22	2.02	0.59
2:M:148:TRP:HB3	12:M:900:CDL:H741	1.85	0.58
4:M:851:BCL:HMB1	4:M:851:BCL:HBB2	1.85	0.58
1:L:211:HIS:HE1	2:M:22:GLU:OE1	1.86	0.58
1:L:207:ARG:HG2	2:M:142:MET:HG2	1.84	0.58
1:L:189:LEU:CB	6:L:859[A]:U10:H4M3	2.34	0.57
4:M:853:BCL:HBB3	4:M:853:BCL:HMB1	1.88	0.56
1:L:241:VAL:CG2	5:L:856:BPH:HAC1	2.30	0.56
1:L:265:TRP:O	1:L:269:LEU:HD22	2.05	0.56
4:L:854:BCL:HMB1	4:L:854:BCL:HBB2	1.87	0.56
1:L:208:THR:H	1:L:211:HIS:CD2	2.24	0.56
2:M:204:LEU:HG	11:M:861:LDA:HM22	1.88	0.56
2:M:105:PHE:HD1	2:M:116:LEU:HD13	1.73	0.54
4:L:854:BCL:H61	6:M:858:U10:H203	1.89	0.54
2:M:164:ARG:HB3	2:M:165:PRO:HD3	1.88	0.54
1:L:193:LEU:CD2	6:L:859[A]:U10:H3M3	2.38	0.53
3:H:206:ASN:HD21	3:H:248:ARG:CD	2.21	0.53
2:M:253:ARG:HH12	11:H:862:LDA:HM23	1.73	0.52
1:L:31:VAL:HG22	6:M:858:U10:H403	1.91	0.52
2:M:253:ARG:HH12	11:H:862:LDA:CM2	2.21	0.52
1:L:51:TRP:CZ3	1:L:80:LEU:HD13	2.46	0.51
2:M:66:TRP:CD1	2:M:122:MET:HB2	2.46	0.51
1:L:216:PHE:CD1	6:L:859[A]:U10:H3M2	2.45	0.51
3:H:81:GLU:O	3:H:83:ARG:HG2	2.11	0.50
7:L:866:HTO:H61	6:M:858:U10:H23	1.92	0.50
2:M:275:LEU:HD23	2:M:278:LEU:HD23	1.94	0.50
1:L:189:LEU:HB3	6:L:859[A]:U10:C4M	2.40	0.49
2:M:9:GLN:HE22	3:H:197:LYS:HA	1.76	0.49
2:M:148:TRP:HA	2:M:148:TRP:CE3	2.48	0.48
4:L:852:BCL:H122	5:L:856:BPH:H3A	1.95	0.48
2:M:24:VAL:O	2:M:26:LEU:HD12	2.13	0.48
3:H:75:VAL:HA	3:H:76:PRO:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:194:GLY:O	2:M:195:ASN:HB3	2.13	0.48
2:M:167:LEU:HD12	2:M:285:LEU:HD11	1.95	0.48
3:H:45:GLU:HG3	3:H:94:GLU:OE2	2.14	0.48
1:L:266:TRP:HA	1:L:269:LEU:CD2	2.43	0.47
2:M:26:LEU:N	2:M:26:LEU:HD12	2.29	0.47
3:H:152:PRO:HG2	3:H:202:ARG:HB2	1.96	0.47
1:L:14:GLY:O	1:L:109:ARG:HD3	2.15	0.47
2:M:190:SER:HB2	4:M:853:BCL:H3C	1.97	0.47
2:M:53:GLY:O	2:M:57:VAL:HG23	2.15	0.47
1:L:208:THR:H	1:L:211:HIS:HD2	1.63	0.46
2:M:260:ALA:HB1	3:H:35:ASN:OD1	2.15	0.46
10:M:860:SPO:HM12	10:M:860:SPO:H5	1.97	0.46
1:L:138:MET:SD	1:L:249:ILE:HD11	2.56	0.46
2:M:26:LEU:HD12	2:M:26:LEU:H	1.81	0.46
1:L:264:GLN:O	1:L:268:LYS:HG2	2.16	0.46
2:M:150:PHE:N	5:M:855:BPH:HMD3	2.31	0.46
4:M:851:BCL:H61	4:M:851:BCL:H102	1.40	0.45
2:M:286:LEU:CD2	3:H:12:LEU:HD12	2.45	0.45
3:H:12:LEU:HD13	3:H:12:LEU:O	2.15	0.45
4:M:853:BCL:OBB	4:M:853:BCL:HHC	2.17	0.45
3:H:245:ALA:HA	3:H:248:ARG:NH2	2.32	0.45
2:M:13:ARG:O	3:H:140:PHE:HA	2.17	0.45
2:M:41:TRP:CD2	11:M:863:LDA:CM1	3.00	0.45
1:L:42:ALA:HA	5:L:856:BPH:H9C3	1.97	0.44
2:M:300:ASN:N	2:M:300:ASN:HD22	2.14	0.44
2:M:194:GLY:O	2:M:195:ASN:CB	2.66	0.44
1:L:51:TRP:CE3	1:L:85:LEU:HD21	2.53	0.44
10:M:860:SPO:H15	10:M:860:SPO:H131	1.82	0.43
2:M:243:THR:O	2:M:247:ARG:HG3	2.18	0.43
3:H:130:LYS:NZ	3:H:170:ASP:OD2	2.52	0.43
1:L:262:TRP:O	1:L:265:TRP:HD1	2.02	0.43
4:M:851:BCL:H192	10:M:860:SPO:H81	2.01	0.43
1:L:12:PRO:HG3	3:H:97:PRO:HB2	2.00	0.43
4:M:851:BCL:C19	10:M:860:SPO:C8	2.97	0.43
3:H:194:GLN:CD	3:H:194:GLN:H	2.22	0.43
2:M:182:HIS:CG	10:M:860:SPO:H181	2.54	0.42
2:M:208:PHE:CE1	11:M:861:LDA:H92	2.54	0.42
2:M:190:SER:CB	4:M:853:BCL:H3C	2.49	0.42
4:L:854:BCL:C4A	4:L:854:BCL:HBA1	2.49	0.42
1:L:250:ILE:HB	1:L:254:ILE:HD11	2.01	0.42
2:M:67:PHE:CG	5:M:855:BPH:H9C2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210:ASP:OD1	3:H:124:ASP:HB2	2.20	0.42
3:H:184:LYS:HD3	14:H:913:HOH:O	2.20	0.42
1:L:208:THR:OG1	1:L:211:HIS:HD2	2.03	0.42
2:M:34:PRO:HG2	2:M:47:LEU:HD22	2.01	0.42
2:M:280:GLY:O	4:M:853:BCL:HED3	2.20	0.42
1:L:101:ALA:CB	7:L:865:HTO:H72	2.50	0.42
2:M:42:PHE:HB2	11:M:863:LDA:H72	2.01	0.41
2:M:129:TRP:O	2:M:132:ARG:HB3	2.19	0.41
2:M:75:TRP:HE1	10:M:860:SPO:H32A	1.86	0.41
2:M:195:ASN:HD22	2:M:195:ASN:C	2.24	0.41
4:M:851:BCL:C4	4:M:851:BCL:H72	2.49	0.41
4:M:851:BCL:HHC	4:M:851:BCL:OBB	2.21	0.41
1:L:173:HIS:CE1	1:L:177:ILE:HD11	2.55	0.41
1:L:197:ALA:HA	1:L:207:ARG:HB2	2.02	0.41
1:L:1:ALA:HB1	3:H:42:LEU:HB3	2.02	0.41
3:H:168:TRP:HB2	3:H:178:PHE:HB2	2.02	0.41
2:M:300:ASN:N	2:M:300:ASN:ND2	2.68	0.41
3:H:89:ARG:HH12	3:H:94:GLU:HG2	1.82	0.41
2:M:148:TRP:CE2	12:M:900:CDL:H511	2.56	0.41
4:M:851:BCL:C4	4:M:851:BCL:C7	2.99	0.40
1:L:190:HIS:HA	6:L:859[A]:U10:H4M1	2.04	0.40
2:M:4:GLN:OE1	2:M:4:GLN:HA	2.21	0.40
2:M:26:LEU:CD1	2:M:26:LEU:H	2.34	0.40
3:H:245:ALA:N	3:H:246:PRO:CD	2.84	0.40
1:L:213:ASN:HD22	1:L:213:ASN:HA	1.73	0.40
5:L:856:BPH:OBB	5:L:856:BPH:HHC	2.21	0.40
1:L:269:LEU:HD13	1:L:269:LEU:HA	1.92	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	280/281 (100%)	273 (98%)	7 (2%)	0	100	100
2	M	299/307 (97%)	292 (98%)	6 (2%)	1 (0%)	46	29
3	H	237/260 (91%)	236 (100%)	1 (0%)	0	100	100
All	All	816/848 (96%)	801 (98%)	14 (2%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	195	ASN

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	221/220 (100%)	217 (98%)	4 (2%)	66	54
2	M	236/240 (98%)	233 (99%)	3 (1%)	76	68
3	H	194/208 (93%)	190 (98%)	4 (2%)	61	47
All	All	651/668 (98%)	640 (98%)	11 (2%)	68	57

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	207	ARG
1	L	216	PHE
1	L	247	CYS
1	L	272	TRP
2	M	94	LEU
2	M	195	ASN
2	M	216	PHE
3	H	73	LEU
3	H	175	MET
3	H	202	ARG
3	H	231	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	87	GLN
1	L	211	HIS
1	L	213	ASN
2	M	9	GLN
2	M	77	GLN
2	M	195	ASN
2	M	299	GLN
2	M	300	ASN
3	H	206	ASN

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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	862	-	15,15,15	4.18	2 (13%)	16,17,17	2.75	4 (25%)
4	BCL	L	852	-	53,74,74	1.05	2 (3%)	57,115,115	1.71	13 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BCL	L	854	-	53,74,74	1.43	9 (16%)	57,115,115	1.99	14 (24%)
5	BPH	L	856	-	64,70,70	1.46	9 (14%)	73,101,101	2.13	17 (23%)
6	U10	L	859[A]	-	33,33,63	2.09	12 (36%)	40,43,79	1.93	10 (25%)
7	HTO	L	865	-	9,9,9	1.23	1 (11%)	8,10,10	0.39	0
7	HTO	L	866	-	9,9,9	1.23	1 (11%)	8,10,10	0.39	0
4	BCL	M	851	-	53,74,74	1.29	7 (13%)	57,115,115	2.35	16 (28%)
4	BCL	M	853	-	53,74,74	1.32	7 (13%)	57,115,115	1.96	13 (22%)
5	BPH	M	855	-	54,60,70	1.38	7 (12%)	61,89,101	2.31	15 (24%)
6	U10	M	858	-	48,48,63	2.26	19 (39%)	58,61,79	3.59	18 (31%)
10	SPO	M	860	-	40,41,41	3.39	23 (57%)	45,50,50	2.54	13 (28%)
11	LDA	M	861	-	15,15,15	4.09	2 (13%)	16,17,17	2.33	3 (18%)
11	LDA	M	863	-	15,15,15	3.74	2 (13%)	16,17,17	2.54	4 (25%)
9	PO4	M	864	-	4,4,4	1.18	0	6,6,6	0.27	0
13	GOL	M	867	-	5,5,5	4.78	5 (100%)	5,5,5	5.70	3 (60%)
12	CDL	M	900	-	68,68,99	0.74	2 (2%)	70,80,111	0.98	4 (5%)

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	862	-	-	0/13/13/13	0/0/0/0
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[A]	-	-	0/27/51/87	0/1/1/1
7	HTO	L	865	-	-	0/10/10/10	0/0/0/0
7	HTO	L	866	-	-	0/10/10/10	0/0/0/0
4	BCL	M	851	-	2/2/21/25	0/37/137/137	0/0/9/9
4	BCL	M	853	-	-	0/37/137/137	0/0/9/9
5	BPH	M	855	-	1/1/16/22	0/42/93/105	0/1/6/6
6	U10	M	858	-	-	0/45/69/87	0/1/1/1
10	SPO	M	860	-	-	0/47/47/47	0/0/0/0
11	LDA	M	861	-	-	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
13	GOL	M	867	-	-	0/4/4/4	0/0/0/0
12	CDL	M	900	-	-	0/79/79/110	0/0/0/0

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	862	LDA	O1-N1	-15.06	1.25	1.39
11	M	861	LDA	O1-N1	-14.66	1.25	1.39
11	M	863	LDA	O1-N1	-13.94	1.26	1.39
13	M	867	GOL	C3-C2	-8.06	1.21	1.52
6	M	858	U10	C37-C38	-5.52	1.35	1.50
11	H	862	LDA	CM2-N1	-5.45	1.41	1.49
11	M	861	LDA	CM2-N1	-5.43	1.41	1.49
5	L	856	BPH	C11-C10	-5.07	1.28	1.52
6	M	858	U10	C7-C8	-3.38	1.45	1.50
11	M	863	LDA	CM2-N1	-3.22	1.44	1.49
13	M	867	GOL	C1-C2	-3.17	1.40	1.52
6	L	859[A]	U10	C7-C8	-3.10	1.46	1.50
10	M	860	SPO	C25-C23	-2.85	1.39	1.45
13	M	867	GOL	O2-C2	-2.79	1.35	1.43
6	L	859[A]	U10	O3-C3M	-2.77	1.38	1.45
4	L	854	BCL	C2C-C3C	-2.73	1.46	1.54
10	M	860	SPO	C11-C12	-2.56	1.40	1.45
5	M	855	BPH	O2D-CED	-2.51	1.39	1.45
5	L	856	BPH	O2D-CED	-2.45	1.39	1.45
6	M	858	U10	O3-C3M	-2.45	1.39	1.45
10	M	860	SPO	C6-C7	-2.24	1.40	1.45
4	M	853	BCL	O2D-CED	-2.24	1.39	1.45
4	M	851	BCL	C2C-C3C	-2.22	1.47	1.54
4	L	854	BCL	C3B-C2B	-2.09	1.35	1.40
5	M	855	BPH	C2C-C3C	-2.04	1.48	1.54
6	M	858	U10	C27-C28	-2.02	1.44	1.50
5	L	856	BPH	C2A-C1A	2.02	1.54	1.51
6	L	859[A]	U10	C20-C19	2.02	1.55	1.50
4	M	853	BCL	O1D-CGD	2.02	1.26	1.21
4	M	853	BCL	C3C-C4C	2.03	1.54	1.51
4	M	851	BCL	C4-C3	2.04	1.55	1.50
6	L	859[A]	U10	C7-C6	2.08	1.55	1.51
6	M	858	U10	C6-C5	2.10	1.52	1.46
12	M	900	CDL	OA8-CA7	2.12	1.39	1.33
6	M	858	U10	C36-C34	2.13	1.56	1.51
4	L	854	BCL	CMB-C2B	2.15	1.56	1.51
4	M	853	BCL	C4-C3	2.15	1.55	1.50
5	L	856	BPH	C4C-NC	2.22	1.42	1.37
5	L	856	BPH	CHC-C1C	2.24	1.40	1.36
4	M	851	BCL	CMA-C3A	2.25	1.58	1.53
5	M	855	BPH	CAA-C2A	2.25	1.58	1.54
5	M	855	BPH	O1D-CGD	2.27	1.26	1.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	900	CDL	CB3-CB4	2.28	1.57	1.50
6	M	858	U10	C30-C29	2.31	1.56	1.50
10	M	860	SPO	C22-C23	2.35	1.38	1.35
4	L	854	BCL	O1D-CGD	2.36	1.27	1.21
4	L	852	BCL	CBB-CAB	2.36	1.56	1.49
4	L	854	BCL	CMC-C2C	2.39	1.58	1.53
4	L	854	BCL	CAA-C2A	2.39	1.58	1.54
5	L	856	BPH	CAA-C2A	2.44	1.59	1.54
6	L	859[A]	U10	C15-C14	2.47	1.56	1.50
6	M	858	U10	C15-C14	2.47	1.56	1.50
4	M	851	BCL	CAA-C2A	2.51	1.59	1.54
6	M	858	U10	C25-C24	2.51	1.56	1.50
10	M	860	SPO	C13-C12	2.56	1.56	1.50
10	M	860	SPO	C26-C27	2.58	1.51	1.43
10	M	860	SPO	C24-C23	2.58	1.56	1.50
10	M	860	SPO	C15-C14	2.62	1.51	1.43
4	L	854	BCL	O2A-CGA	2.63	1.41	1.33
10	M	860	SPO	C8-C7	2.64	1.56	1.50
4	L	852	BCL	C4-C3	2.67	1.57	1.50
6	L	859[A]	U10	C6-C1	2.69	1.41	1.35
10	M	860	SPO	C37-C38	2.71	1.40	1.32
6	M	858	U10	C6-C1	2.75	1.41	1.35
10	M	860	SPO	C10-C9	2.76	1.52	1.43
7	L	865	HTO	C3-C2	2.83	1.60	1.52
7	L	866	HTO	C3-C2	2.84	1.60	1.52
4	M	851	BCL	C2-C3	2.91	1.38	1.33
6	L	859[A]	U10	C23-C24	2.91	1.41	1.32
6	M	858	U10	C31-C29	2.95	1.57	1.51
6	M	858	U10	C28-C29	2.97	1.38	1.33
6	M	858	U10	C18-C19	3.06	1.39	1.33
6	M	858	U10	C23-C24	3.07	1.39	1.33
6	M	858	U10	C8-C9	3.08	1.39	1.33
6	L	859[A]	U10	O3-C3	3.08	1.45	1.37
4	L	854	BCL	C2-C3	3.10	1.39	1.33
4	M	853	BCL	O2A-CGA	3.22	1.43	1.33
6	M	858	U10	O3-C3	3.26	1.45	1.37
5	L	856	BPH	C2-C3	3.32	1.39	1.33
5	M	855	BPH	C2-C3	3.38	1.39	1.33
13	M	867	GOL	O3-C3	3.39	1.57	1.42
6	L	859[A]	U10	C18-C19	3.40	1.39	1.33
10	M	860	SPO	C32-C33	3.57	1.40	1.33
10	M	860	SPO	C9-C7	3.59	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	851	BCL	O2A-CGA	3.62	1.44	1.33
5	L	856	BPH	O2D-CGD	3.70	1.42	1.33
10	M	860	SPO	C19-C17	3.73	1.40	1.35
6	L	859[A]	U10	C8-C9	3.73	1.40	1.33
5	M	855	BPH	O2D-CGD	3.77	1.42	1.33
5	L	856	BPH	O2A-CGA	3.77	1.44	1.33
5	M	855	BPH	O2A-CGA	3.91	1.45	1.33
4	M	853	BCL	C2-C3	3.92	1.40	1.33
10	M	860	SPO	O1-CM1	4.03	1.56	1.43
6	M	858	U10	C13-C14	4.34	1.41	1.33
10	M	860	SPO	C14-C12	4.34	1.41	1.35
6	L	859[A]	U10	O4-C4	4.38	1.48	1.37
13	M	867	GOL	O1-C1	4.44	1.61	1.42
6	M	858	U10	O4-C4	4.52	1.48	1.37
4	M	851	BCL	O2D-CGD	4.55	1.44	1.33
10	M	860	SPO	C4-C1	4.56	1.59	1.53
4	M	853	BCL	O2D-CGD	4.65	1.45	1.33
10	M	860	SPO	C26-C25	4.78	1.47	1.34
6	L	859[A]	U10	C13-C14	4.82	1.42	1.33
4	L	854	BCL	O2D-CGD	4.97	1.45	1.33
10	M	860	SPO	C21-C20	5.01	1.49	1.35
10	M	860	SPO	C27-C28	5.28	1.39	1.34
6	M	858	U10	C33-C34	5.44	1.43	1.33
10	M	860	SPO	C15-C16	7.55	1.54	1.34
10	M	860	SPO	C10-C11	7.78	1.54	1.34
10	M	860	SPO	C6-C5	8.26	1.54	1.31

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	862	LDA	CM2-N1-CM1	-8.10	99.69	108.83
10	M	860	SPO	O1-C1-C4	-8.03	86.23	105.87
11	M	863	LDA	CM2-N1-CM1	-7.46	100.41	108.83
4	M	851	BCL	C4-C3-C5	-6.65	105.25	115.41
11	M	861	LDA	CM2-N1-CM1	-6.39	101.62	108.83
6	M	858	U10	C36-C37-C38	-6.17	95.52	111.69
10	M	860	SPO	C15-C14-C12	-6.04	118.47	127.20
10	M	860	SPO	C20-C21-C22	-5.45	111.34	123.39
5	M	855	BPH	O1D-CGD-CBD	-5.13	117.27	124.62
10	M	860	SPO	C25-C23-C22	-4.83	111.21	118.98
5	L	856	BPH	O1D-CGD-CBD	-4.71	117.87	124.62
4	M	851	BCL	O2A-CGA-O1A	-4.48	111.94	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	858	U10	C35-C34-C36	-4.46	108.60	115.41
4	M	851	BCL	OBD-CAD-CBD	-4.45	119.23	125.94
4	M	853	BCL	CAC-C3C-C2C	-3.96	104.17	114.13
4	L	852	BCL	OBB-CAB-CBB	-3.96	110.64	120.13
4	M	853	BCL	O1D-CGD-CBD	-3.88	119.06	124.62
4	M	851	BCL	CAA-C2A-C3A	-3.88	102.07	113.22
10	M	860	SPO	C4-C5-C6	-3.85	119.19	124.67
4	L	852	BCL	CAA-C2A-C3A	-3.74	102.46	113.22
6	L	859[A]	U10	O5-C5-C6	-3.69	114.74	121.68
4	L	854	BCL	CMB-C2B-C1B	-3.68	122.27	128.36
4	L	854	BCL	CAC-C3C-C2C	-3.61	105.05	114.13
10	M	860	SPO	C18-C17-C19	-3.57	117.63	122.90
6	M	858	U10	C20-C19-C21	-3.52	110.02	115.41
6	M	858	U10	C30-C29-C31	-3.34	110.31	115.41
10	M	860	SPO	C6-C7-C9	-3.30	113.67	118.98
4	M	851	BCL	CMB-C2B-C1B	-3.28	122.93	128.36
4	L	852	BCL	C7-C6-C5	-3.25	103.45	113.06
4	L	852	BCL	O2D-CGD-CBD	-3.24	106.85	111.30
5	M	855	BPH	O2D-CGD-O1D	-3.20	117.17	123.79
6	L	859[A]	U10	C20-C19-C21	-3.20	110.52	115.41
6	L	859[A]	U10	O2-C2-C3	-3.20	113.87	120.79
5	L	856	BPH	O2D-CGD-O1D	-3.19	117.21	123.79
4	L	854	BCL	O1D-CGD-CBD	-3.18	120.06	124.62
10	M	860	SPO	C15-C16-C17	-3.17	116.98	126.32
4	M	853	BCL	CAC-C3C-C4C	-3.13	105.65	112.58
4	M	851	BCL	O1D-CGD-CBD	-3.08	120.21	124.62
4	L	854	BCL	O2D-CGD-O1D	-3.07	117.44	123.79
4	M	851	BCL	O2D-CGD-O1D	-3.01	117.56	123.79
4	M	851	BCL	OBB-CAB-CBB	-3.00	112.94	120.13
6	M	858	U10	O5-C5-C6	-2.98	116.08	121.68
6	L	859[A]	U10	C1-C6-C5	-2.97	116.74	120.12
6	M	858	U10	O2-C2-C3	-2.93	114.45	120.79
10	M	860	SPO	C20-C19-C17	-2.84	123.10	127.20
4	L	852	BCL	CMB-C2B-C1B	-2.84	123.67	128.36
4	L	854	BCL	OBD-CAD-CBD	-2.78	121.74	125.94
4	L	852	BCL	OBD-CAD-CBD	-2.78	121.75	125.94
6	M	858	U10	C1-C6-C5	-2.68	117.07	120.12
4	M	851	BCL	CMA-C3A-C2A	-2.67	102.54	114.35
5	L	856	BPH	C7-C6-C5	-2.56	105.50	113.06
5	M	855	BPH	C5-C3-C2	-2.56	116.20	121.05
4	M	853	BCL	O2D-CGD-O1D	-2.53	118.56	123.79
4	L	854	BCL	CAA-C2A-C3A	-2.53	105.95	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	859[A]	U10	C7-C6-C5	-2.52	115.59	118.56
5	L	856	BPH	OBD-CAD-CBD	-2.47	122.20	125.94
4	L	854	BCL	OBB-CAB-CBB	-2.47	114.21	120.13
5	M	855	BPH	CAA-C2A-C3A	-2.42	106.27	113.22
5	L	856	BPH	CAA-C2A-C3A	-2.40	106.32	113.22
5	L	856	BPH	O2A-CGA-O1A	-2.39	117.33	123.49
10	M	860	SPO	C10-C9-C7	-2.37	123.77	127.20
12	M	900	CDL	CB6-CB4-CB3	-2.37	106.53	112.07
11	M	863	LDA	C9-C8-C7	-2.37	102.30	114.53
4	L	852	BCL	CAC-C3C-C4C	-2.34	107.38	112.58
11	H	862	LDA	C9-C8-C7	-2.31	102.63	114.53
5	M	855	BPH	C2A-C1A-NA	-2.29	109.15	112.08
4	M	853	BCL	C4-C3-C5	-2.22	112.02	115.41
4	M	853	BCL	OBD-CAD-CBD	-2.21	122.60	125.94
4	L	852	BCL	CHA-C1A-NA	-2.12	120.85	126.06
5	L	856	BPH	CAA-C2A-C1A	-2.11	107.31	112.86
11	H	862	LDA	CM1-N1-C1	-2.10	103.02	109.77
5	M	855	BPH	O2A-CGA-O1A	-2.09	118.09	123.49
4	M	853	BCL	O2A-CGA-O1A	-2.08	118.12	123.49
11	M	861	LDA	C9-C8-C7	-2.08	103.78	114.53
11	M	863	LDA	CM1-N1-C1	-2.05	103.17	109.77
12	M	900	CDL	CA6-CA4-CA3	-2.02	107.35	112.07
5	L	856	BPH	C5-C3-C2	-2.02	117.23	121.05
6	L	859[A]	U10	C17-C16-C14	2.05	119.39	112.71
6	M	858	U10	C17-C18-C19	2.07	132.27	127.76
5	L	856	BPH	CMD-C2D-C3D	2.08	129.16	125.09
4	M	853	BCL	OBB-CAB-C3B	2.10	123.33	120.00
4	L	852	BCL	C2C-C3C-C4C	2.11	105.07	101.50
5	M	855	BPH	CMD-C2D-C3D	2.17	129.33	125.09
5	L	856	BPH	CAC-C3C-C4C	2.18	118.28	112.67
4	M	851	BCL	C6-C5-C3	2.23	117.38	112.48
4	M	851	BCL	CMD-C2D-C3D	2.25	129.49	125.09
6	L	859[A]	U10	C21-C19-C18	2.28	125.37	121.05
4	L	854	BCL	CHB-C4A-NA	2.38	127.80	124.51
12	M	900	CDL	CB4-OB6-CB5	2.41	123.67	117.89
5	M	855	BPH	C2C-C3C-C4C	2.42	105.61	101.50
5	M	855	BPH	C4-C3-C5	2.43	119.12	115.41
6	M	858	U10	C21-C19-C18	2.47	125.75	121.05
4	L	854	BCL	C4A-NA-C1A	2.51	109.60	106.36
6	M	858	U10	C26-C27-C28	2.54	118.33	111.69
6	M	858	U10	C16-C14-C13	2.54	125.87	121.05
4	M	851	BCL	C2C-C3C-C4C	2.58	105.87	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	856	BPH	C2C-C3C-C4C	2.59	105.90	101.50
6	M	858	U10	C31-C29-C28	2.61	125.99	121.05
4	L	854	BCL	O2A-CGA-CBA	2.61	119.86	111.90
4	L	852	BCL	CBB-CAB-C3B	2.62	128.11	120.33
6	L	859[A]	U10	C17-C18-C19	2.64	133.51	127.76
4	L	854	BCL	CMB-C2B-C3B	2.65	130.28	125.09
4	M	853	BCL	C5-C3-C2	2.93	126.60	121.05
4	L	852	BCL	CMD-C2D-C3D	3.00	130.95	125.09
4	L	852	BCL	CMB-C2B-C3B	3.00	130.96	125.09
10	M	860	SPO	C8-C7-C6	3.05	123.17	118.10
6	L	859[A]	U10	C16-C14-C13	3.11	126.95	121.05
4	M	853	BCL	O2A-CGA-CBA	3.14	121.47	111.90
4	L	852	BCL	O1D-CGD-CBD	3.17	129.17	124.62
10	M	860	SPO	C3-C1-C2	3.18	116.64	110.22
13	M	867	GOL	O1-C1-C2	3.21	125.74	110.18
4	M	853	BCL	CHC-C1C-NC	3.31	129.09	124.51
5	M	855	BPH	CBC-CAC-C3C	3.36	121.79	113.57
5	M	855	BPH	C7-C6-C5	3.39	123.08	113.06
12	M	900	CDL	OB8-CB6-CB4	3.61	118.41	108.69
4	L	854	BCL	CHC-C1C-NC	3.62	129.52	124.51
10	M	860	SPO	C24-C23-C25	3.68	124.23	118.10
5	L	856	BPH	C11-C10-C8	3.75	127.94	115.49
5	L	856	BPH	C4A-NA-C1A	3.96	111.75	108.21
4	M	853	BCL	C4A-NA-C1A	3.97	111.49	106.36
5	L	856	BPH	CED-O2D-CGD	4.01	125.39	115.99
4	L	854	BCL	OB8-CB6-CB4	4.06	126.43	120.00
5	M	855	BPH	CED-O2D-CGD	4.15	125.73	115.99
4	M	851	BCL	C5-C3-C2	4.23	129.08	121.05
6	M	858	U10	C37-C38-C39	4.36	144.53	127.73
5	M	855	BPH	C4A-NA-C1A	4.43	112.17	108.21
5	M	855	BPH	C6-C5-C3	4.49	122.33	112.48
6	M	858	U10	C36-C34-C33	4.55	129.67	121.05
11	M	861	LDA	O1-N1-C1	4.72	115.58	110.27
4	M	851	BCL	O2A-CGA-CBA	4.74	126.34	111.90
5	L	856	BPH	CBC-CAC-C3C	4.79	125.28	113.57
11	M	863	LDA	O1-N1-C1	4.87	115.76	110.27
11	H	862	LDA	O1-N1-C1	5.55	116.52	110.27
5	L	856	BPH	C6-C5-C3	5.64	124.86	112.48
6	M	858	U10	C3M-O3-C3	5.66	136.72	116.61
4	M	851	BCL	O2D-CGD-CBD	5.91	119.41	111.30
6	M	858	U10	C31-C32-C33	6.01	127.42	111.69
6	L	859[A]	U10	C3M-O3-C3	6.25	138.85	116.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	867	GOL	O2-C2-C3	6.63	139.06	108.65
4	M	851	BCL	OBB-CAB-C3B	6.67	130.56	120.00
6	M	858	U10	C27-C28-C29	6.93	142.84	127.76
4	L	854	BCL	O2D-CGD-CBD	7.91	122.15	111.30
4	M	853	BCL	O2D-CGD-CBD	7.92	122.16	111.30
5	L	856	BPH	O2D-CGD-CBD	9.90	124.89	111.30
13	M	867	GOL	O3-C3-C2	10.37	160.46	110.18
5	M	855	BPH	O2D-CGD-CBD	10.39	125.55	111.30
6	M	858	U10	C32-C33-C34	20.30	171.91	127.76

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	L	856	BPH	C8
5	L	856	BPH	C13
4	M	851	BCL	C8
4	M	851	BCL	C13
5	M	855	BPH	C8

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	862	LDA	2	0
4	L	852	BCL	1	0
4	L	854	BCL	3	0
5	L	856	BPH	5	0
6	L	859[A]	U10	8	0
7	L	865	HTO	1	0
7	L	866	HTO	1	0
4	M	851	BCL	15	0
4	M	853	BCL	7	0
5	M	855	BPH	3	0
6	M	858	U10	3	0
10	M	860	SPO	7	0
11	M	861	LDA	2	0
11	M	863	LDA	3	0
12	M	900	CDL	2	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, 95th 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%)	-0.05	11 (3%) 43 37	15, 22, 46, 59	0
2	M	301/307 (98%)	0.02	11 (3%) 45 39	13, 25, 47, 63	0
3	H	238/260 (91%)	-0.24	5 (2%) 67 62	17, 25, 38, 51	0
All	All	820/848 (96%)	-0.08	27 (3%) 50 44	13, 24, 45, 63	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	ALA	10.4
1	L	281	GLY	5.0
1	L	51	TRP	4.3
1	L	276	PRO	3.8
2	M	2	GLU	3.7
1	L	270	PRO	3.5
2	M	105	PHE	3.4
1	L	271	TRP	3.4
3	H	246	PRO	3.1
3	H	245	ALA	3.1
2	M	106	ALA	3.0
1	L	202	LYS	2.9
1	L	274	ASN	2.8
2	M	83	ALA	2.6
1	L	59	TRP	2.6
2	M	76	TYR	2.6
2	M	109	LEU	2.5
1	L	269	LEU	2.5
3	H	60	LYS	2.5
2	M	3	TYR	2.3
2	M	100	GLU	2.3
3	H	18	TYR	2.3
2	M	52	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	40	PHE	2.1
3	H	51	ALA	2.0
1	L	277	GLY	2.0
2	M	101	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, 95th 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
6	U10	L	859[A]	33/63	0.71	0.65	14.40	45,50,52,53	33
11	LDA	M	861	16/16	0.63	0.31	13.98	57,63,67,68	0
7	HTO	L	865	10/10	0.69	0.25	13.07	61,63,64,64	0
12	CDL	M	900	69/100	0.68	0.37	4.90	49,71,77,78	0
11	LDA	M	863	16/16	0.70	0.27	4.90	70,70,74,74	0
11	LDA	H	862	16/16	0.75	0.22	4.67	61,62,66,67	0
6	U10	M	858	48/63	0.89	0.19	2.88	16,29,61,63	0
4	BCL	M	851	66/66	0.91	0.16	2.51	17,22,66,68	0
10	SPO	M	860	42/42	0.75	0.19	2.44	25,32,50,52	0
4	BCL	M	853	66/66	0.92	0.14	2.20	13,18,38,44	0
4	BCL	L	852	66/66	0.93	0.12	1.48	15,17,29,32	0
9	PO4	M	864	5/5	0.89	0.17	1.38	72,73,73,73	0
5	BPH	L	856	65/65	0.92	0.13	1.33	13,17,33,36	0
4	BCL	L	854	66/66	0.93	0.12	1.12	12,17,40,44	0
5	BPH	M	855	55/65	0.93	0.13	0.96	19,22,63,66	0
8	FE2	M	857	1/1	0.98	0.09	-4.56	14,14,14,14	0
7	HTO	L	866	10/10	0.58	0.35	-	66,68,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	GOL	M	867	6/6	0.86	0.20	-	51,55,56,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.