Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BOZ
Title	:	Photosynthetic Reaction Center Mutant With Gly M203 Replaced With Leu
Authors	:	Potter, J.P.; Fyfe, P.K.; Jones, M.R.
Deposited on	:	2005-04-15
Resolution	:	2.40 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:

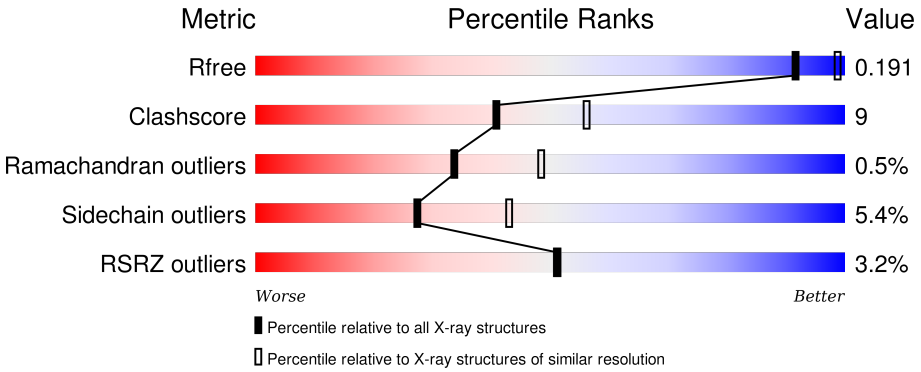
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	H	260	5%, 77%, 12%, 7%
2	L	281	%, 88%, 9%
3	M	307	3%, 81%, 13%

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	PO4	M	1310	-	-	-	X
4	LDA	M	1307	-	-	-	X
8	U10	L	1285	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 7475 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	0	0	1
			1830	1169	315	337	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	281	Total	C	N	O	S	0	0	0
			2232	1507	355	362	8			

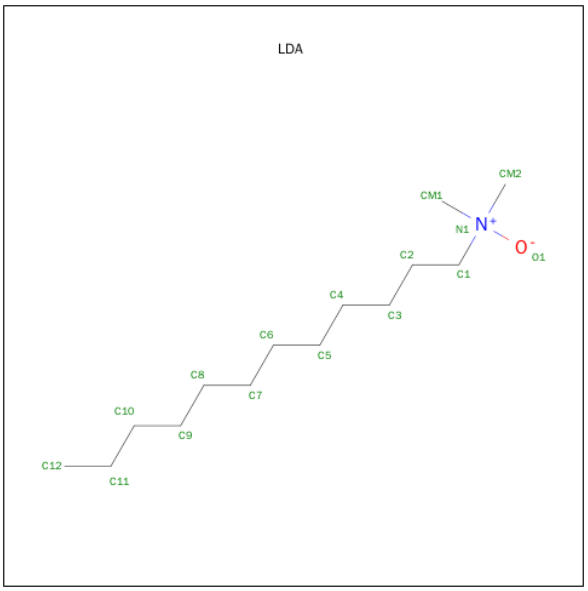
- Molecule 3 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	303	Total	C	N	O	S	0	0	1
			2413	1611	395	397	10			

There is a discrepancy between the modelled and reference sequences:

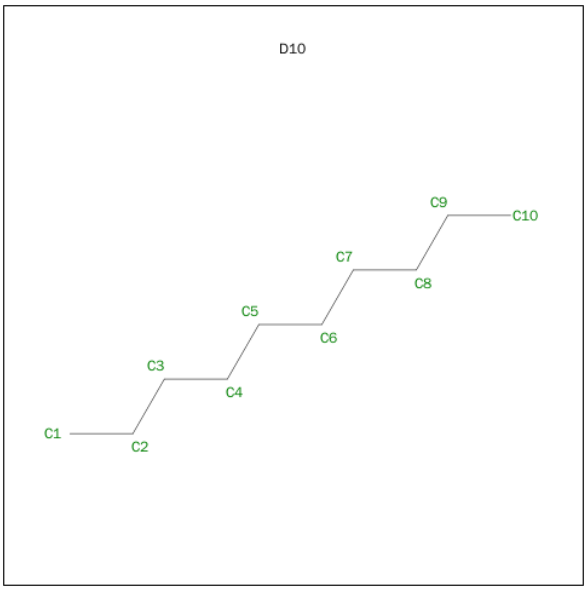
Chain	Residue	Modelled	Actual	Comment	Reference
M	203	LEU	GLY	ENGINEERED MUTATION	UNP P11846

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



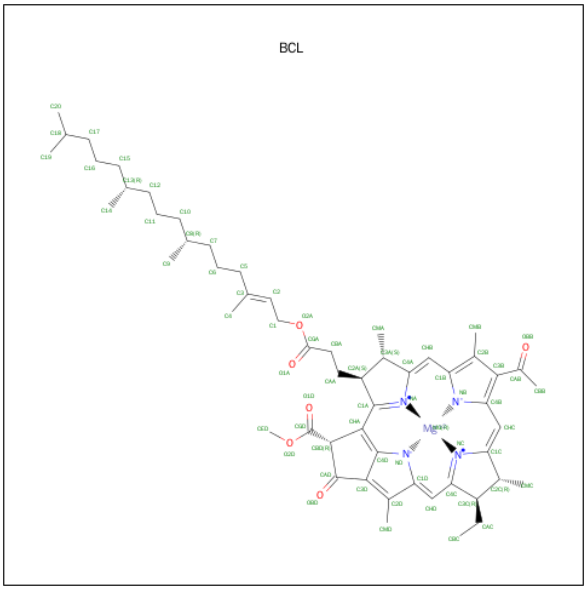
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



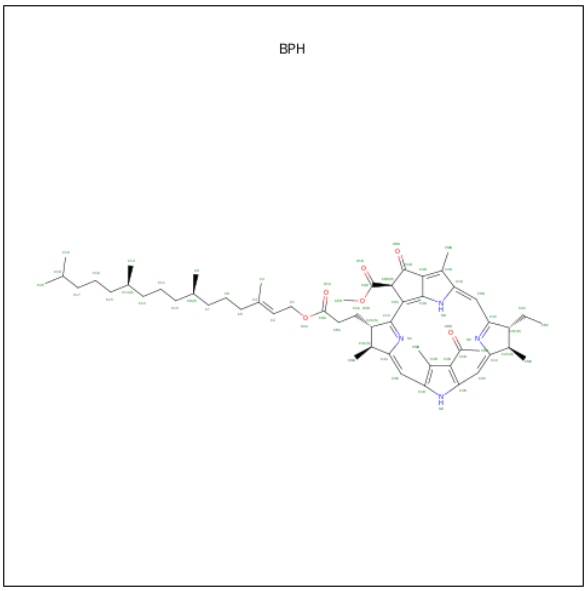
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C 9 9	0	0
5	H	1	Total C 8 8	0	0
5	H	1	Total C 7 7	0	0

- Molecule 6 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



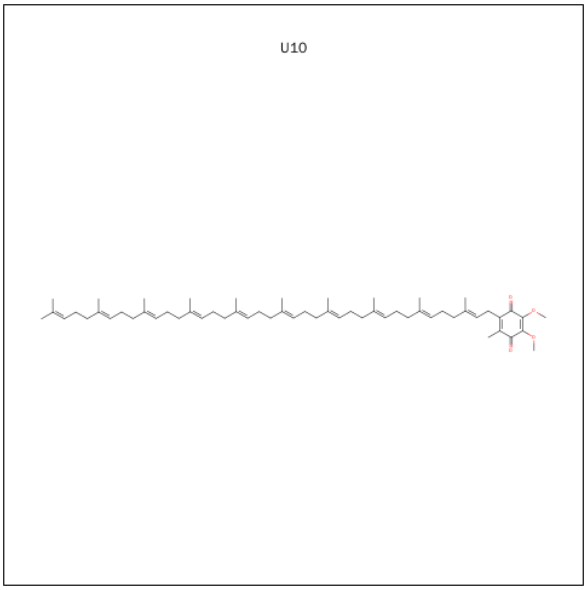
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	L	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0
6	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

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

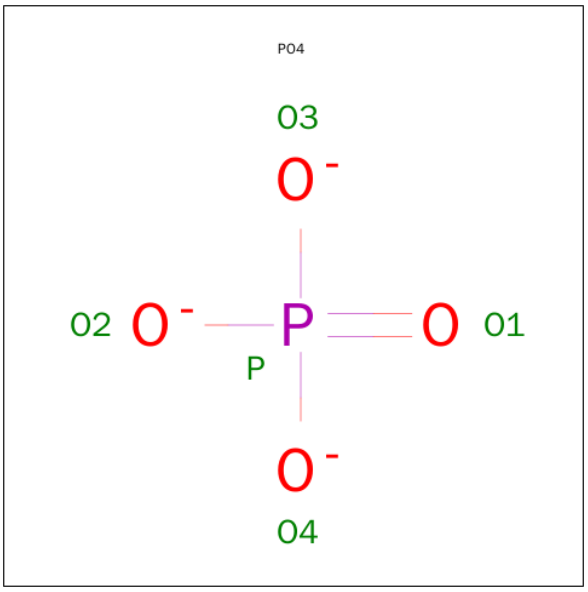


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	L	1	Total	C	O	14	0
			48	44	4		
8	M	1	Total	C	O	0	0
			48	44	4		

- Molecule 9 is FE (III) ION (three-letter code: FE) (formula: Fe).

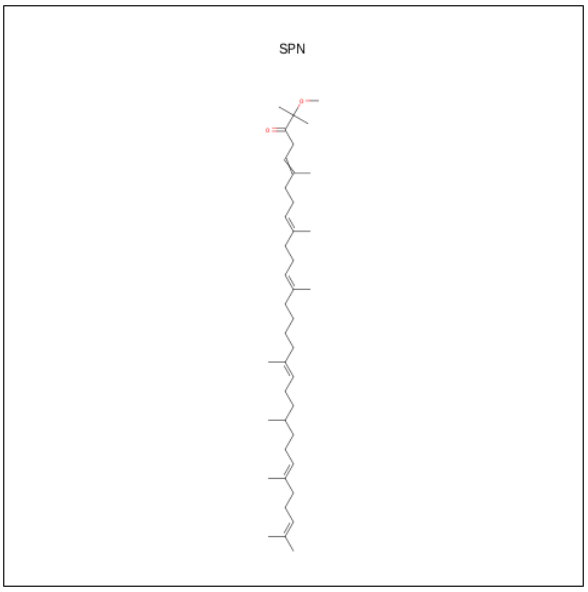
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	M	1	Total Fe 1 1	0	0

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 11 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 12 is water.

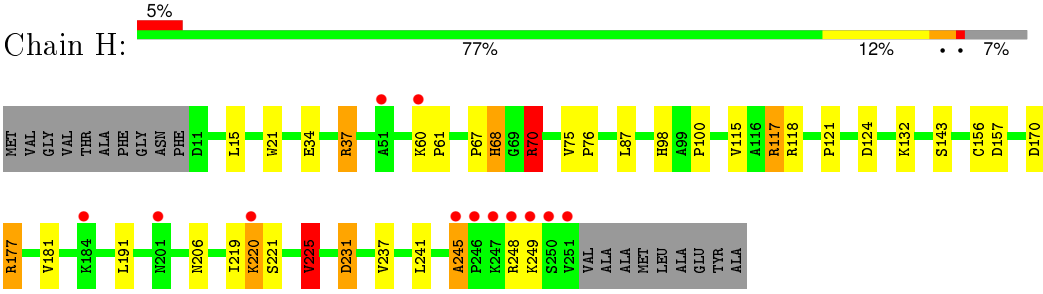
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	H	174	Total O 174 174	0	0
12	L	95	Total O 95 95	0	0
12	M	99	Total O 99 99	0	0

3 Residue-property plots (i)

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

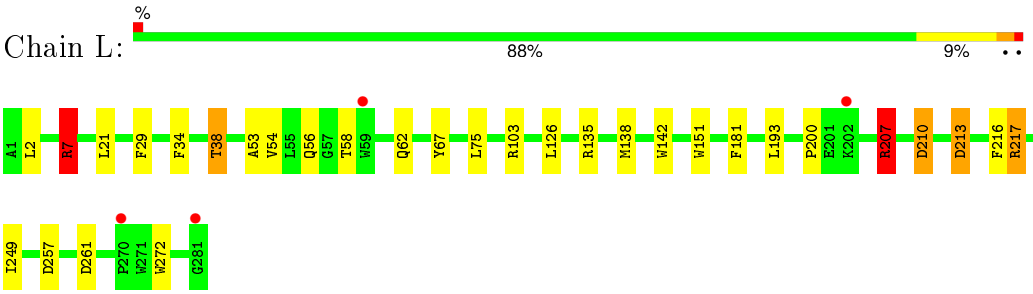
- Molecule 1: REACTION CENTER PROTEIN H CHAIN

Chain H:



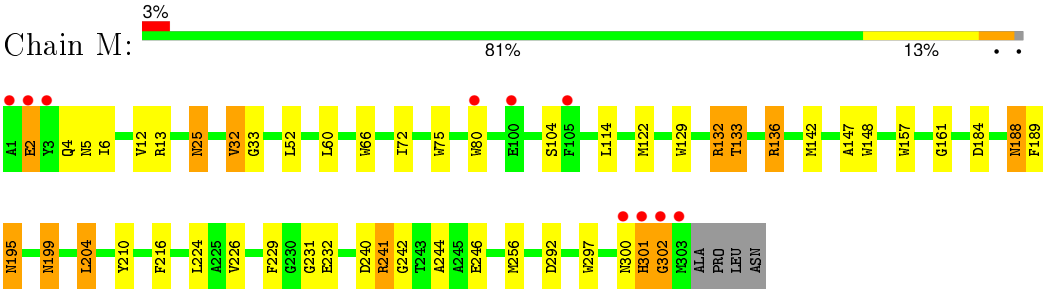
- Molecule 2: REACTION CENTER PROTEIN L CHAIN

Chain L:



- Molecule 3: REACTION CENTER PROTEIN M CHAIN

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.61Å 138.61Å 185.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.96 – 2.40 17.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (17.96-2.40) 99.5 (17.96-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.174 , 0.198 0.167 , 0.191	Depositor DCC
R_{free} test set	3991 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 70.1	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 80240 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7475	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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, LDA, D10, BPH, PO4, FE, SPN, U10

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	H	0.86	1/1878 (0.1%)	1.06	12/2555 (0.5%)
2	L	0.91	0/2320	0.96	17/3175 (0.5%)
3	M	0.83	0/2505	0.88	8/3421 (0.2%)
All	All	0.87	1/6703 (0.0%)	0.96	37/9151 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	68	HIS	N-CA	5.02	1.56	1.46

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	37	ARG	NE-CZ-NH2	-14.39	113.10	120.30
3	M	241	ARG	NE-CZ-NH2	-13.27	113.67	120.30
2	L	103	ARG	NE-CZ-NH2	-12.16	114.22	120.30
2	L	7	ARG	NE-CZ-NH1	12.07	126.34	120.30
3	M	241	ARG	NE-CZ-NH1	11.44	126.02	120.30
2	L	7	ARG	NE-CZ-NH2	-11.25	114.68	120.30
2	L	135	ARG	NE-CZ-NH2	-10.04	115.28	120.30
2	L	207	ARG	NE-CZ-NH2	-8.87	115.87	120.30
2	L	103	ARG	NE-CZ-NH1	8.65	124.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	231	ARG	NE-CZ-NH1	8.64	124.62	120.30
3	M	136	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	H	37	ARG	NE-CZ-NH1	8.62	124.61	120.30
3	M	132	ARG	NE-CZ-NH1	-8.45	116.08	120.30
2	L	231	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	H	37	ARG	CG-CD-NE	-7.89	95.23	111.80
3	M	136	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	H	67	PRO	C-N-CA	-7.45	103.07	121.70
2	L	135	ARG	NE-CZ-NH1	7.43	124.01	120.30
2	L	210	ASP	CB-CG-OD1	7.34	124.91	118.30
1	H	237	VAL	CG1-CB-CG2	6.70	121.62	110.90
1	H	70	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	H	117	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	H	70	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	H	124	ASP	CB-CG-OD1	6.08	123.77	118.30
1	H	157	ASP	CB-CG-OD2	5.96	123.67	118.30
3	M	240	ASP	CB-CG-OD2	5.96	123.66	118.30
2	L	261	ASP	CB-CG-OD2	5.87	123.58	118.30
2	L	2	LEU	CA-CB-CG	5.62	128.24	115.30
2	L	257	ASP	CB-CG-OD2	5.56	123.31	118.30
1	H	225	VAL	CB-CA-C	-5.53	100.90	111.40
1	H	231	ASP	CB-CG-OD2	5.53	123.27	118.30
2	L	207	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	L	213	ASP	CB-CG-OD2	5.49	123.24	118.30
2	L	217	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	L	7	ARG	CD-NE-CZ	5.33	131.06	123.60
3	M	241	ARG	CD-NE-CZ	5.07	130.70	123.60
3	M	292	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	M	300	ASN	Peptide

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	H	1830	0	1836	34	0
2	L	2232	0	2187	24	0
3	M	2413	0	2329	43	0
4	H	16	0	31	3	0
4	M	48	0	93	6	0
5	H	24	0	45	0	0
6	L	132	0	148	5	0
6	M	132	0	148	12	0
7	L	65	0	75	5	0
7	M	65	0	76	10	0
8	L	48	0	60	1	0
8	M	48	0	63	3	0
9	M	1	0	0	0	0
10	M	10	0	0	0	0
11	M	43	0	69	6	0
12	H	174	0	0	4	0
12	L	95	0	0	4	0
12	M	99	0	0	1	0
All	All	7475	0	7160	122	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 (122) 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:H:220:LYS:HE2	12:H:2104:HOH:O	1.30	1.25
7:M:1311:BPH:H171	7:M:1311:BPH:H111	1.22	1.11
4:H:1251:LDA:H121	4:M:1307:LDA:H91	1.40	0.98
3:M:2:GLU:HG2	3:M:4:GLN:HE22	1.29	0.96
7:M:1311:BPH:HBB3	7:M:1311:BPH:HHC	1.45	0.95
3:M:2:GLU:HG2	3:M:4:GLN:NE2	1.86	0.90
1:H:220:LYS:CE	12:H:2104:HOH:O	1.98	0.90
7:M:1311:BPH:C11	7:M:1311:BPH:H171	2.01	0.90
7:L:1284:BPH:HBB3	7:L:1284:BPH:HHC	1.59	0.84
1:H:68:HIS:ND1	12:H:2050:HOH:O	2.10	0.83
1:H:98:HIS:CD2	2:L:7:ARG:HH11	2.01	0.79
2:L:56:GLN:OE1	12:L:2015:HOH:O	2.04	0.75
2:L:67:TYR:HE1	12:L:2022:HOH:O	1.70	0.73
2:L:34:PHE:O	2:L:38:THR:HG22	1.89	0.72
7:L:1284:BPH:HBB2	3:M:210:TYR:HB3	1.72	0.69
3:M:32:VAL:HG13	3:M:33:GLY:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:301:HIS:CD2	3:M:301:HIS:O	2.47	0.68
4:H:1251:LDA:C12	4:M:1307:LDA:H91	2.21	0.66
1:H:175:MET:HE3	12:L:2084:HOH:O	1.95	0.66
2:L:34:PHE:O	2:L:38:THR:CG2	2.44	0.66
2:L:181:PHE:HB3	7:M:1311:BPH:HBB2	1.79	0.65
2:L:231:ARG:HD3	3:M:5:ASN:O	1.98	0.64
2:L:56:GLN:NE2	12:L:2014:HOH:O	2.30	0.63
6:L:1282:BCL:HMB1	6:L:1282:BCL:CBB	2.29	0.63
3:M:189:PHE:O	3:M:193:HIS:HD2	1.82	0.63
2:L:181:PHE:CD2	7:M:1311:BPH:HBB1	2.34	0.62
1:H:156:CYS:SG	1:H:248:ARG:HB2	2.38	0.62
6:M:1304:BCL:CBB	6:M:1304:BCL:HMB1	2.30	0.61
1:H:117:ARG:HD3	3:M:242:GLY:HA2	1.84	0.59
7:M:1311:BPH:CBB	7:M:1311:BPH:HHC	2.28	0.59
7:M:1311:BPH:HBB3	7:M:1311:BPH:CHC	2.27	0.59
6:L:1283:BCL:HBB2	6:L:1283:BCL:HMB1	1.85	0.58
3:M:2:GLU:CG	3:M:4:GLN:HE22	2.10	0.57
1:H:170:ASP:OD2	1:H:177:ARG:NH1	2.31	0.57
1:H:34:GLU:O	1:H:37:ARG:HG3	2.06	0.56
1:H:181:VAL:HG21	1:H:191:LEU:HD12	1.88	0.56
6:M:1303:BCL:CBB	6:M:1303:BCL:HMB1	2.36	0.55
1:H:98:HIS:HD2	2:L:7:ARG:HH11	1.52	0.55
2:L:213:ASP:O	2:L:217:ARG:HG3	2.07	0.55
1:H:117:ARG:HD3	3:M:242:GLY:CA	2.37	0.54
2:L:193:LEU:HD23	8:L:1285:U10:C2	2.38	0.54
6:L:1282:BCL:HBB3	6:L:1282:BCL:HMB1	1.88	0.54
1:H:245:ALA:HB2	1:H:248:ARG:HH21	1.71	0.54
1:H:70:ARG:NH2	1:H:121:PRO:O	2.37	0.54
3:M:184:ASP:O	3:M:188:ASN:HB2	2.08	0.54
1:H:156:CYS:HB2	1:H:248:ARG:HG3	1.90	0.53
3:M:148:TRP:HA	3:M:148:TRP:CE3	2.43	0.53
1:H:241:LEU:O	1:H:248:ARG:NH2	2.42	0.53
3:M:199:ASN:HD22	3:M:199:ASN:C	2.11	0.53
1:H:181:VAL:CG2	1:H:191:LEU:HD12	2.39	0.52
2:L:207:ARG:HG2	3:M:142:MET:HG2	1.92	0.52
2:L:200:PRO:HB3	2:L:207:ARG:HD3	1.90	0.52
1:H:132:LYS:HD2	1:H:171:ILE:CD1	2.40	0.52
1:H:37:ARG:NH2	1:H:60:LYS:O	2.37	0.52
2:L:56:GLN:HG3	2:L:58:THR:HG22	1.91	0.52
1:H:156:CYS:SG	1:H:248:ARG:HA	2.51	0.51
6:M:1304:BCL:HBB3	6:M:1304:BCL:HMB1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:VAL:HG21	1:H:191:LEU:CD1	2.41	0.50
3:M:25:ASN:HD22	3:M:25:ASN:C	2.14	0.49
1:H:21:TRP:HZ2	4:M:1307:LDA:HM11	1.78	0.49
3:M:204:LEU:HD13	4:M:1307:LDA:H12	1.95	0.49
3:M:136:ARG:NE	3:M:136:ARG:HA	2.28	0.48
3:M:133:THR:HG21	3:M:147:ALA:HA	1.96	0.48
6:M:1303:BCL:H71	6:M:1304:BCL:H202	1.96	0.48
1:H:219:ILE:HG21	1:H:225:VAL:HG13	1.95	0.48
3:M:148:TRP:HA	3:M:148:TRP:HE3	1.79	0.47
2:L:181:PHE:HB3	7:M:1311:BPH:CBB	2.45	0.47
6:M:1303:BCL:HBB2	6:M:1303:BCL:HMB1	1.96	0.47
1:H:177:ARG:NH2	3:M:232:GLU:OE2	2.47	0.47
1:H:75:VAL:HA	1:H:76:PRO:C	2.35	0.47
4:H:1251:LDA:H21	4:H:1251:LDA:HM21	1.64	0.47
1:H:156:CYS:SG	1:H:248:ARG:CB	3.03	0.47
3:M:129:TRP:CH2	3:M:132:ARG:NH1	2.82	0.47
7:M:1311:BPH:HHD	7:M:1311:BPH:HBC2	1.97	0.47
6:L:1283:BCL:HMB1	6:L:1283:BCL:CBB	2.45	0.47
6:M:1303:BCL:H91	6:M:1303:BCL:H111	1.71	0.46
6:M:1303:BCL:C3B	11:M:1312:SPN:H152	2.46	0.46
3:M:256:MET:CE	8:M:1313:U10:H102	2.45	0.46
3:M:133:THR:CG2	3:M:147:ALA:HA	2.46	0.46
3:M:2:GLU:HB2	12:M:2015:HOH:O	2.16	0.46
3:M:161:GLY:HA3	11:M:1312:SPN:H201	1.97	0.45
6:M:1303:BCL:CAB	11:M:1312:SPN:H162	2.46	0.45
2:L:138:MET:SD	2:L:249:ILE:HD11	2.56	0.45
3:M:194:GLY:O	3:M:195:ASN:HB3	2.17	0.45
1:H:132:LYS:HB2	1:H:171:ILE:HD11	1.99	0.45
1:H:21:TRP:CZ2	4:M:1307:LDA:HM11	2.52	0.45
7:L:1284:BPH:HBB1	3:M:210:TYR:CD2	2.51	0.45
2:L:231:ARG:HD2	3:M:6:ILE:HA	1.99	0.45
3:M:66:TRP:CD1	3:M:122:MET:HB2	2.52	0.45
2:L:62:GLN:NE2	2:L:151:TRP:HE1	2.15	0.44
7:L:1284:BPH:HHC	7:L:1284:BPH:CBB	2.37	0.44
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.99	0.44
3:M:2:GLU:O	3:M:4:GLN:NE2	2.51	0.44
8:M:1313:U10:H322	8:M:1313:U10:H28	1.74	0.43
2:L:231:ARG:HG2	3:M:224:LEU:HD21	1.98	0.43
6:M:1303:BCL:H141	11:M:1312:SPN:H112	1.99	0.43
3:M:241:ARG:HD3	3:M:246:GLU:HG2	2.01	0.43
6:M:1303:BCL:H141	11:M:1312:SPN:H101	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:133:THR:HG22	3:M:147:ALA:HB2	1.99	0.43
2:L:53:ALA:HB1	2:L:58:THR:O	2.19	0.43
6:L:1282:BCL:NA	6:M:1304:BCL:HBB2	2.34	0.43
1:H:245:ALA:HB2	1:H:248:ARG:NH2	2.33	0.43
3:M:52:LEU:HD12	3:M:52:LEU:HA	1.84	0.43
4:M:1307:LDA:H21	4:M:1307:LDA:HM13	1.42	0.43
1:H:132:LYS:HD2	1:H:171:ILE:HD11	1.99	0.42
6:M:1304:BCL:HAA2	6:M:1304:BCL:HBD	2.02	0.42
2:L:75:LEU:HA	2:L:142:TRP:CD1	2.54	0.42
1:H:87:LEU:HD23	1:H:100:PRO:HA	2.01	0.42
1:H:61:PRO:HA	1:H:76:PRO:HD2	2.01	0.42
1:H:156:CYS:SG	1:H:248:ARG:CA	3.07	0.41
3:M:75:TRP:HB3	3:M:80:TRP:CE3	2.55	0.41
1:H:115:VAL:HG22	1:H:117:ARG:HG2	2.01	0.41
3:M:157:TRP:CE2	11:M:1312:SPN:HM73	2.56	0.41
12:H:2119:HOH:O	3:M:13:ARG:HD2	2.20	0.41
3:M:297:TRP:NE1	3:M:302:GLY:HA2	2.36	0.41
3:M:226:VAL:HG23	3:M:231:GLY:HA3	2.03	0.41
7:L:1284:BPH:NC	7:L:1284:BPH:ND	2.68	0.41
3:M:72:ILE:HD12	3:M:72:ILE:HA	1.96	0.40
3:M:189:PHE:O	3:M:193:HIS:CD2	2.69	0.40
2:L:29:PHE:CE1	8:M:1313:U10:H311	2.56	0.40
7:M:1311:BPH:H4C1	7:M:1311:BPH:H6C1	1.19	0.40
2:L:231:ARG:HD2	3:M:6:ILE:O	2.21	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	H	239/260 (92%)	234 (98%)	4 (2%)	1 (0%)	39 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	L	279/281 (99%)	273 (98%)	6 (2%)	0	100 100
3	M	301/307 (98%)	293 (97%)	5 (2%)	3 (1%)	19 28
All	All	819/848 (97%)	800 (98%)	15 (2%)	4 (0%)	34 48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	245	ALA
3	M	301	HIS
3	M	195	ASN
3	M	302	GLY

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	H	195/208 (94%)	183 (94%)	12 (6%)	23 35
2	L	220/220 (100%)	210 (96%)	10 (4%)	34 52
3	M	237/241 (98%)	224 (94%)	13 (6%)	27 42
All	All	652/669 (98%)	617 (95%)	35 (5%)	27 43

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	15	LEU
1	H	70	ARG
1	H	118	ARG
1	H	143	SER
1	H	175	MET
1	H	177	ARG
1	H	206	ASN
1	H	220	LYS
1	H	221	SER
1	H	225	VAL

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Mol	Chain	Res	Type
1	H	231	ASP
1	H	249	LYS
2	L	7	ARG
2	L	21	LEU
2	L	38	THR
2	L	54	VAL
2	L	126	LEU
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	247	CYS
2	L	272	TRP
3	M	2	GLU
3	M	12	VAL
3	M	25	ASN
3	M	32	VAL
3	M	60	LEU
3	M	104	SER
3	M	114	LEU
3	M	133	THR
3	M	188	ASN
3	M	192	VAL
3	M	199	ASN
3	M	204	LEU
3	M	216	PHE

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

Mol	Chain	Res	Type
1	H	98	HIS
2	L	62	GLN
3	M	4	GLN
3	M	25	ASN
3	M	44	ASN
3	M	193	HIS
3	M	199	ASN
3	M	300	ASN
3	M	301	HIS

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 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	LDA	H	1251	-	15,15,15	4.27	1 (6%)	16,17,17	5.78	6 (37%)
5	D10	H	1252	-	8,8,9	0.27	0	7,7,8	0.47	0
5	D10	H	1253	-	7,7,9	0.24	0	6,6,8	0.68	0
5	D10	H	1254	-	6,6,9	0.70	0	5,5,8	0.53	0
6	BCL	L	1282	2	53,74,74	0.61	0	57,115,115	1.53	13 (22%)
6	BCL	L	1283	2	53,74,74	0.82	1 (1%)	57,115,115	1.65	15 (26%)
7	BPH	L	1284	-	64,70,70	0.87	1 (1%)	73,101,101	1.41	10 (13%)
8	U10	L	1285	-	48,48,63	2.48	5 (10%)	58,61,79	2.75	18 (31%)
6	BCL	M	1303	3	53,74,74	0.68	0	57,115,115	1.69	11 (19%)
6	BCL	M	1304	3	53,74,74	0.75	0	57,115,115	1.37	5 (8%)
4	LDA	M	1305	-	15,15,15	4.21	1 (6%)	16,17,17	5.72	6 (37%)
4	LDA	M	1306	-	15,15,15	3.78	1 (6%)	16,17,17	5.27	6 (37%)
4	LDA	M	1307	-	15,15,15	4.49	1 (6%)	16,17,17	4.76	6 (37%)
10	PO4	M	1309	-	4,4,4	0.90	0	6,6,6	0.30	0
10	PO4	M	1310	-	4,4,4	0.25	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BPH	M	1311	-	64,70,70	0.68	1 (1%)	73,101,101	1.66	18 (24%)
11	SPN	M	1312	-	41,42,42	3.82	15 (36%)	41,52,52	2.46	22 (53%)
8	U10	M	1313	-	48,48,63	1.72	5 (10%)	58,61,79	1.56	10 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LDA	H	1251	-	-	0/13/13/13	0/0/0/0
5	D10	H	1252	-	-	0/6/6/7	0/0/0/0
5	D10	H	1253	-	-	0/5/5/7	0/0/0/0
5	D10	H	1254	-	-	0/4/4/7	0/0/0/0
6	BCL	L	1282	2	-	0/37/137/137	0/0/9/9
6	BCL	L	1283	2	-	0/37/137/137	0/0/9/9
7	BPH	L	1284	-	-	0/54/105/105	0/1/6/6
8	U10	L	1285	-	-	0/45/69/87	0/1/1/1
6	BCL	M	1303	3	-	0/37/137/137	0/0/9/9
6	BCL	M	1304	3	-	0/37/137/137	0/0/9/9
4	LDA	M	1305	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1306	-	-	0/13/13/13	0/0/0/0
4	LDA	M	1307	-	-	0/13/13/13	0/0/0/0
10	PO4	M	1309	-	-	0/0/0/0	0/0/0/0
10	PO4	M	1310	-	-	0/0/0/0	0/0/0/0
7	BPH	M	1311	-	-	0/54/105/105	0/1/6/6
11	SPN	M	1312	-	-	0/50/51/51	0/0/0/0
8	U10	M	1313	-	-	0/45/69/87	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1307	LDA	O1-N1	-17.06	1.23	1.39
4	H	1251	LDA	O1-N1	-16.41	1.23	1.39
4	M	1305	LDA	O1-N1	-16.16	1.24	1.39
4	M	1306	LDA	O1-N1	-14.57	1.25	1.39
8	L	1285	U10	C27-C28	-13.39	1.12	1.50
11	M	1312	SPN	C3-C4	-9.66	1.35	1.50
8	M	1313	U10	C36-C34	-7.02	1.35	1.51
11	M	1312	SPN	C17-C18	-6.83	1.36	1.51
11	M	1312	SPN	C14-C13	-6.54	1.36	1.51
11	M	1312	SPN	C10-C9	-6.21	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	1312	SPN	C6-C5	-6.17	1.37	1.51
8	L	1285	U10	C36-C34	-5.71	1.38	1.51
11	M	1312	SPN	C20-C19	-5.35	1.35	1.50
11	M	1312	SPN	C11-C12	-4.99	1.36	1.50
11	M	1312	SPN	C7-C8	-4.98	1.36	1.50
11	M	1312	SPN	C21-C22	-3.04	1.36	1.52
11	M	1312	SPN	C16-C15	-2.82	1.35	1.51
8	M	1313	U10	O5-C5	2.09	1.28	1.23
6	L	1283	BCL	C2-C3	2.24	1.37	1.33
8	L	1285	U10	C28-C29	2.36	1.37	1.33
7	L	1284	BPH	CHC-C1C	2.41	1.41	1.36
8	M	1313	U10	C13-C14	2.44	1.37	1.33
7	M	1311	BPH	CHC-C1C	2.70	1.41	1.36
11	M	1312	SPN	C25-C26	2.77	1.38	1.33
8	M	1313	U10	C4-C3	3.10	1.49	1.35
8	L	1285	U10	C4-C3	3.37	1.50	1.35
8	L	1285	U10	C6-C1	5.98	1.49	1.35
8	M	1313	U10	C6-C1	6.75	1.51	1.35
11	M	1312	SPN	C4-C5	6.85	1.46	1.33
11	M	1312	SPN	C19-C18	7.11	1.46	1.33
11	M	1312	SPN	C12-C13	7.22	1.47	1.33
11	M	1312	SPN	C8-C9	8.21	1.49	1.33

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1305	LDA	O1-N1-C1	-15.23	93.13	110.27
4	H	1251	LDA	O1-N1-C1	-14.65	93.79	110.27
4	M	1307	LDA	O1-N1-C1	-12.99	95.65	110.27
4	M	1306	LDA	O1-N1-C1	-12.48	96.23	110.27
4	M	1305	LDA	CM1-N1-C1	-6.54	88.69	109.77
4	M	1306	LDA	CM2-N1-C1	-5.77	91.19	109.77
4	H	1251	LDA	CM1-N1-C1	-5.55	91.89	109.77
8	L	1285	U10	C32-C33-C34	-5.47	115.86	127.76
4	H	1251	LDA	CM2-N1-C1	-5.21	92.98	109.77
4	M	1306	LDA	CM1-N1-C1	-5.02	93.59	109.77
6	M	1304	BCL	CAC-C3C-C4C	-4.91	101.70	112.58
6	L	1283	BCL	CMB-C2B-C1B	-4.78	120.45	128.36
6	M	1303	BCL	OBD-CAD-CBD	-4.78	118.73	125.94
6	L	1282	BCL	CAA-C2A-C3A	-4.04	101.60	113.22
6	M	1303	BCL	CMB-C2B-C1B	-4.03	121.69	128.36
4	M	1305	LDA	CM2-N1-C1	-4.03	96.79	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1303	BCL	C4-C3-C2	-3.96	115.72	123.50
7	M	1311	BPH	C6-C5-C3	-3.75	104.26	112.48
7	M	1311	BPH	CAA-C2A-C3A	-3.65	102.71	113.22
8	M	1313	U10	C22-C23-C24	-3.59	119.95	127.76
7	M	1311	BPH	CAA-C2A-C1A	-3.59	103.42	112.86
6	M	1303	BCL	CAA-C2A-C3A	-3.58	102.94	113.22
8	M	1313	U10	C32-C33-C34	-3.55	120.04	127.76
8	L	1285	U10	C35-C34-C33	-3.54	116.56	123.50
4	M	1307	LDA	CM2-N1-C1	-3.50	98.51	109.77
6	L	1283	BCL	CAA-C2A-C3A	-3.47	103.25	113.22
4	M	1307	LDA	CM1-N1-C1	-3.43	98.71	109.77
6	L	1282	BCL	CAA-C2A-C1A	-3.42	100.40	112.47
8	L	1285	U10	O2-C2-C3	-3.33	113.59	120.79
6	L	1283	BCL	CAC-C3C-C4C	-3.29	105.28	112.58
6	L	1283	BCL	CAC-C3C-C2C	-3.24	105.99	114.13
6	M	1304	BCL	CAC-C3C-C2C	-3.17	106.15	114.13
6	M	1304	BCL	CHA-C1A-NA	-3.17	118.26	126.06
6	L	1282	BCL	CMA-C3A-C2A	-3.16	100.38	114.35
7	L	1284	BPH	C1C-NC-C4C	-3.13	107.23	110.44
8	L	1285	U10	C1M-C1-C6	-3.09	117.49	124.10
6	L	1283	BCL	CMC-C2C-C3C	-2.95	101.29	114.35
8	M	1313	U10	C27-C28-C29	-2.93	121.40	127.76
7	L	1284	BPH	CAA-C2A-C3A	-2.90	104.89	113.22
8	L	1285	U10	C22-C23-C24	-2.87	121.52	127.76
6	M	1303	BCL	CMA-C3A-C2A	-2.87	101.66	114.35
8	M	1313	U10	C26-C27-C28	-2.79	104.39	111.69
6	L	1282	BCL	CMB-C2B-C1B	-2.77	123.77	128.36
7	L	1284	BPH	CAA-C2A-C1A	-2.74	105.64	112.86
7	M	1311	BPH	CMA-C3A-C2A	-2.73	102.25	114.35
6	L	1283	BCL	C6-C5-C3	-2.71	106.53	112.48
7	M	1311	BPH	C4-C3-C2	-2.71	118.18	123.50
7	M	1311	BPH	C2B-C1B-NB	-2.66	105.73	109.73
6	L	1282	BCL	CHA-C1A-NA	-2.65	119.53	126.06
7	M	1311	BPH	OBD-CAD-CBD	-2.64	121.96	125.94
7	L	1284	BPH	CMA-C3A-C2A	-2.63	102.72	114.35
6	M	1304	BCL	CMC-C2C-C3C	-2.61	102.81	114.35
11	M	1312	SPN	C17-C18-C19	-2.60	116.11	121.05
6	L	1282	BCL	CAC-C3C-C4C	-2.60	106.81	112.58
7	M	1311	BPH	C2D-C1D-ND	-2.59	106.04	110.29
6	M	1303	BCL	CHA-C1A-NA	-2.58	119.70	126.06
11	M	1312	SPN	CM3-C5-C4	-2.57	118.45	123.50
8	L	1285	U10	C25-C24-C23	-2.55	118.49	123.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1283	BCL	CAA-C2A-C1A	-2.36	104.15	112.47
8	L	1285	U10	C30-C29-C28	-2.34	118.91	123.50
7	M	1311	BPH	C3B-C4B-NB	-2.33	105.03	109.98
6	L	1282	BCL	CAC-C3C-C2C	-2.31	108.31	114.13
7	M	1311	BPH	CBB-CAB-C3B	-2.30	115.40	120.52
6	M	1304	BCL	CMB-C2B-C1B	-2.29	124.57	128.36
6	L	1282	BCL	O2A-CGA-O1A	-2.29	117.59	123.49
6	L	1283	BCL	O2A-CGA-O1A	-2.24	117.71	123.49
11	M	1312	SPN	C3-C4-C5	-2.24	122.91	126.70
7	M	1311	BPH	O1D-CGD-CBD	-2.20	121.47	124.62
6	L	1282	BCL	CMC-C2C-C3C	-2.19	104.64	114.35
11	M	1312	SPN	C7-C8-C9	-2.19	123.00	127.76
6	L	1283	BCL	O2D-CGD-O1D	-2.18	119.29	123.79
6	L	1283	BCL	CMA-C3A-C2A	-2.17	104.76	114.35
11	M	1312	SPN	CM9-C30-C29	-2.11	115.84	122.61
8	L	1285	U10	C12-C13-C14	-2.09	123.22	127.76
8	M	1313	U10	C37-C38-C39	-2.07	119.78	127.73
11	M	1312	SPN	C28-C27-C26	-2.07	105.98	112.71
7	L	1284	BPH	C3B-C4B-NB	-2.04	105.64	109.98
6	M	1303	BCL	C7-C6-C5	2.06	119.15	113.06
11	M	1312	SPN	C15-C16-C17	2.10	120.98	113.29
6	L	1282	BCL	CBA-CAA-C2A	2.13	119.75	113.73
7	M	1311	BPH	CAA-CBA-CGA	2.15	119.62	113.32
6	L	1282	BCL	CMB-C2B-C3B	2.19	129.37	125.09
11	M	1312	SPN	CM7-C22-C23	2.21	119.55	111.08
11	M	1312	SPN	CMA-O1-C1	2.21	124.00	112.20
8	L	1285	U10	C30-C29-C31	2.26	118.86	115.41
6	M	1303	BCL	OBD-CAD-C3D	2.27	133.00	128.35
7	L	1284	BPH	C1B-NB-C4B	2.28	111.02	106.51
6	L	1283	BCL	CBA-CAA-C2A	2.28	120.17	113.73
6	L	1283	BCL	CAA-CBA-CGA	2.33	120.14	113.32
7	M	1311	BPH	C2C-C3C-C4C	2.34	105.47	101.50
6	L	1282	BCL	C1D-CHD-C4C	2.37	129.70	126.07
8	M	1313	U10	C37-C36-C34	2.40	120.53	112.71
11	M	1312	SPN	CMB-C30-CM9	2.41	120.56	114.64
8	L	1285	U10	C3M-O3-C3	2.43	125.25	116.61
11	M	1312	SPN	C10-C11-C12	2.43	118.06	111.69
6	L	1283	BCL	OBB-CAB-C3B	2.45	123.88	120.00
7	L	1284	BPH	CAC-C3C-C4C	2.56	119.24	112.67
6	L	1282	BCL	C4-C3-C5	2.58	119.34	115.41
6	L	1283	BCL	CMB-C2B-C3B	2.76	130.49	125.09
8	L	1285	U10	C15-C14-C16	2.87	119.79	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	1312	SPN	CM7-C22-C21	2.91	122.26	111.08
8	M	1313	U10	C15-C14-C16	2.91	119.86	115.41
7	M	1311	BPH	C1B-NB-C4B	2.93	112.30	106.51
6	M	1303	BCL	CMB-C2B-C3B	2.95	130.86	125.09
7	M	1311	BPH	C5-C3-C2	2.99	126.71	121.05
7	M	1311	BPH	OBB-CAB-C3B	3.00	126.10	120.31
11	M	1312	SPN	C16-C15-C14	3.01	124.34	113.29
8	L	1285	U10	C36-C37-C38	3.03	119.61	111.69
6	L	1283	BCL	O2D-CGD-CBD	3.03	115.45	111.30
8	M	1313	U10	C10-C9-C11	3.07	120.10	115.41
8	L	1285	U10	C31-C32-C33	3.08	119.75	111.69
7	L	1284	BPH	OBB-CAB-C3B	3.14	126.38	120.31
11	M	1312	SPN	C7-C6-C5	3.21	123.17	112.71
7	L	1284	BPH	CAC-C3C-C2C	3.21	122.20	114.13
6	M	1303	BCL	O2D-CGD-CBD	3.25	115.75	111.30
8	M	1313	U10	C35-C34-C36	3.25	120.37	115.41
8	L	1285	U10	C27-C28-C29	3.42	135.21	127.76
8	L	1285	U10	C25-C24-C26	3.48	120.73	115.41
11	M	1312	SPN	C6-C7-C8	3.50	120.84	111.69
11	M	1312	SPN	C16-C17-C18	3.59	120.36	112.48
7	M	1311	BPH	O2D-CGD-CBD	3.59	116.22	111.30
8	M	1313	U10	C30-C29-C31	3.66	121.00	115.41
11	M	1312	SPN	CM5-C13-C14	3.79	121.20	115.41
6	M	1303	BCL	C5-C3-C2	3.80	128.26	121.05
11	M	1312	SPN	C15-C14-C13	3.83	120.89	112.48
8	L	1285	U10	C35-C34-C36	3.99	121.50	115.41
11	M	1312	SPN	CM6-C18-C17	4.10	121.67	115.41
11	M	1312	SPN	CM4-C9-C10	4.26	121.91	115.41
8	L	1285	U10	C37-C36-C34	4.34	126.86	112.71
11	M	1312	SPN	C11-C10-C9	4.56	127.58	112.71
7	M	1311	BPH	CAC-C3C-C4C	4.92	125.31	112.67
11	M	1312	SPN	CM3-C5-C6	5.11	123.21	115.41
7	L	1284	BPH	C3C-C4C-NC	5.59	113.53	107.93
4	M	1306	LDA	O1-N1-CM2	6.35	117.54	109.05
4	H	1251	LDA	O1-N1-CM1	6.60	117.88	109.05
4	H	1251	LDA	O1-N1-CM2	6.64	117.93	109.05
4	M	1305	LDA	O1-N1-CM2	7.02	118.44	109.05
4	M	1307	LDA	O1-N1-CM2	7.04	118.47	109.05
4	M	1307	LDA	O1-N1-CM1	7.09	118.53	109.05
4	M	1307	LDA	CM2-N1-CM1	7.95	117.81	108.83
4	M	1305	LDA	O1-N1-CM1	8.20	120.02	109.05
4	M	1306	LDA	O1-N1-CM1	8.27	120.11	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	1305	LDA	CM2-N1-CM1	10.62	120.81	108.83
4	M	1306	LDA	CM2-N1-CM1	10.91	121.14	108.83
4	H	1251	LDA	CM2-N1-CM1	12.95	123.44	108.83
8	L	1285	U10	C26-C27-C28	14.31	149.16	111.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1251	LDA	3	0
6	L	1282	BCL	3	0
6	L	1283	BCL	2	0
7	L	1284	BPH	5	0
8	L	1285	U10	1	0
6	M	1303	BCL	8	0
6	M	1304	BCL	5	0
4	M	1307	LDA	6	0
7	M	1311	BPH	10	0
11	M	1312	SPN	6	0
8	M	1313	U10	3	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	H	241/260 (92%)	-0.13	12 (4%) 32 33	24, 31, 42, 100	0
2	L	281/281 (100%)	-0.44	4 (1%) 78 77	27, 35, 49, 55	0
3	M	303/307 (98%)	-0.18	10 (3%) 50 50	29, 36, 48, 77	0
All	All	825/848 (97%)	-0.26	26 (3%) 51 51	24, 35, 48, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	251	VAL	13.4
3	M	303	MET	13.3
3	M	1	ALA	11.0
1	H	250	SER	9.6
3	M	302	GLY	9.0
1	H	249	LYS	7.8
1	H	245	ALA	7.6
1	H	246	PRO	6.3
1	H	247	LYS	6.0
3	M	301	HIS	5.3
3	M	2	GLU	4.8
1	H	248	ARG	3.4
2	L	270	PRO	3.3
2	L	59	TRP	3.0
3	M	3	TYR	2.9
2	L	281	GLY	2.7
1	H	60	LYS	2.7
1	H	220	LYS	2.4
1	H	201	ASN	2.4
3	M	100	GLU	2.3
1	H	184	LYS	2.3
1	H	51	ALA	2.3
3	M	105	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	202	LYS	2.2
3	M	80	TRP	2.2
3	M	300	ASN	2.1

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
4	LDA	M	1307	16/16	0.65	0.28	7.02	31,59,69,70	0
8	U10	L	1285	48/63	0.91	0.21	4.74	37,51,81,82	14
10	PO4	M	1310	5/5	0.89	0.35	4.14	74,75,76,77	0
4	LDA	M	1305	16/16	0.89	0.24	1.84	78,80,85,87	0
4	LDA	H	1251	16/16	0.91	0.14	0.71	57,60,65,66	0
7	BPH	M	1311	65/65	0.92	0.12	0.10	22,28,81,82	0
11	SPN	M	1312	43/43	0.91	0.13	-0.20	22,37,59,63	0
8	U10	M	1313	48/63	0.94	0.12	-0.31	12,27,53,55	0
6	BCL	L	1283	66/66	0.97	0.11	-0.36	12,17,38,41	0
6	BCL	M	1303	66/66	0.95	0.11	-0.58	19,23,65,67	0
9	FE	M	1308	1/1	1.00	0.07	-1.06	20,20,20,20	0
7	BPH	L	1284	65/65	0.98	0.08	-1.06	12,19,25,28	0
6	BCL	L	1282	66/66	0.98	0.08	-1.10	15,21,33,41	0
6	BCL	M	1304	66/66	0.98	0.08	-1.36	17,24,38,51	0
5	D10	H	1252	9/10	0.89	0.21	-	74,74,76,76	0
10	PO4	M	1309	5/5	0.99	0.22	-	39,42,44,46	0
5	D10	H	1254	7/10	0.79	0.23	-	77,77,77,78	0
4	LDA	M	1306	16/16	0.60	0.31	-	66,71,91,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	D10	H	1253	8/10	0.83	0.27	-	66,67,71,72	0

6.5 Other polymers (i)

There are no such residues in this entry.