Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:49 PM GMT

PDB ID	:	3V3Z
Title	:	I(L177)H mutant structure of photosynthetic reaction center from Rhodobacter sphaeroides
Authors	:	Gabdulkhakov, A.G.; Fufina, T.Y.; Vasilieva, L.G.; Shuvalov, V.A.
Deposited on	:	2011-12-14
Resolution	:	2.90 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:

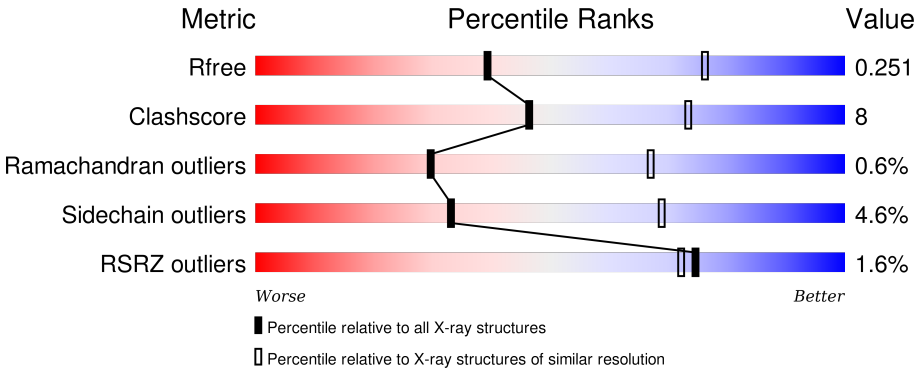
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

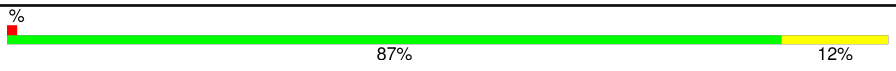
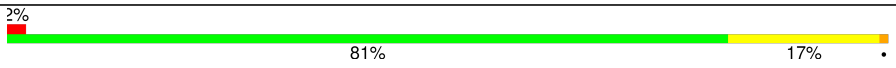
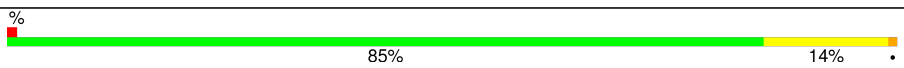
The reported resolution of this entry is 2.90 Å.

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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	241	
2	L	281	
3	M	302	

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	BPH	L	402	X	-	-	-
10	BPH	M	401	X	-	-	-
11	U10	L	502	-	-	-	X
13	SPN	M	600	-	-	-	X
4	LDA	H	704	-	-	-	X
4	LDA	M	701	-	-	-	X
4	LDA	M	702	-	-	-	X
4	LDA	M	703	-	-	-	X
4	LDA	M	705	-	-	-	X
6	HTO	H	2	-	-	-	X
6	HTO	L	282	-	-	-	X
7	DIO	H	251	-	-	X	-
9	BCL	L	301	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 7216 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	0
			1840	1178	315	338	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
			2235	1508	357	362	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	177	HIS	ILE	ENGINEERED MUTATION	UNP P0C0Y8
L	178	THR	SER	SEE REMARK 999	UNP P0C0Y8

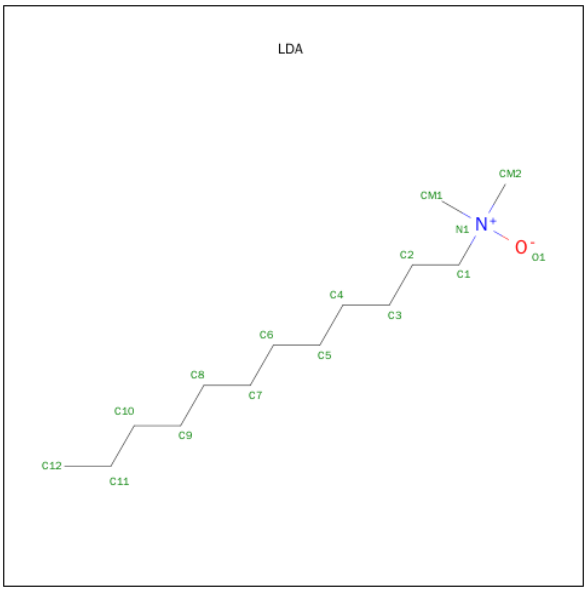
- Molecule 3 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	302	Total	C	N	O	S	0	0	0
			2409	1608	394	397	10			

There is a discrepancy between the modelled and reference sequences:

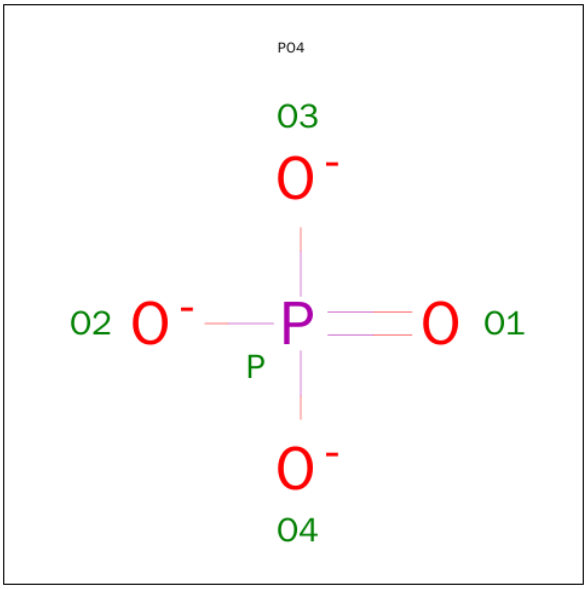
Chain	Residue	Modelled	Actual	Comment	Reference
M	8	THR	SER	SEE REMARK 999	UNP P0C0Y9

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



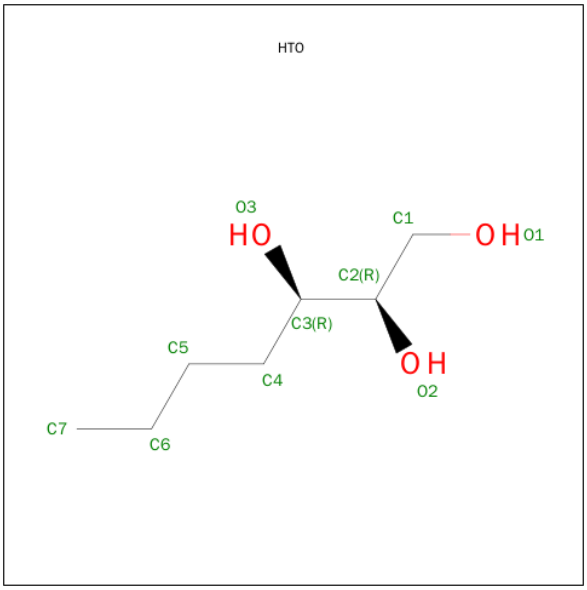
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		
4	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



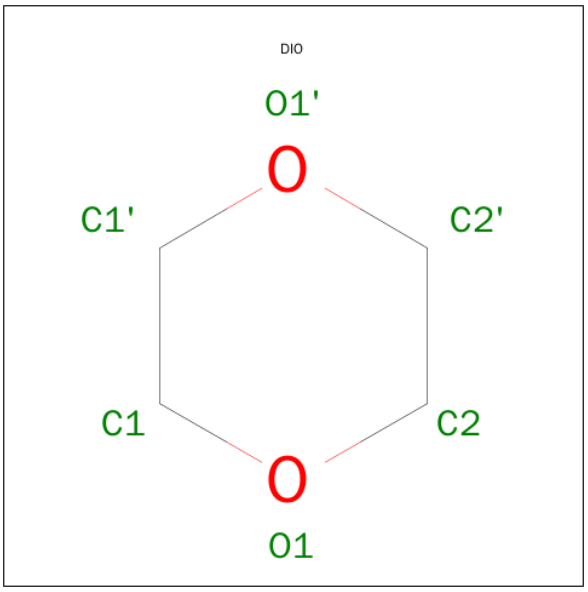
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total O P 5 4 1	0	0
5	H	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0
5	M	1	Total O P 5 4 1	0	0

- Molecule 6 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 7 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).

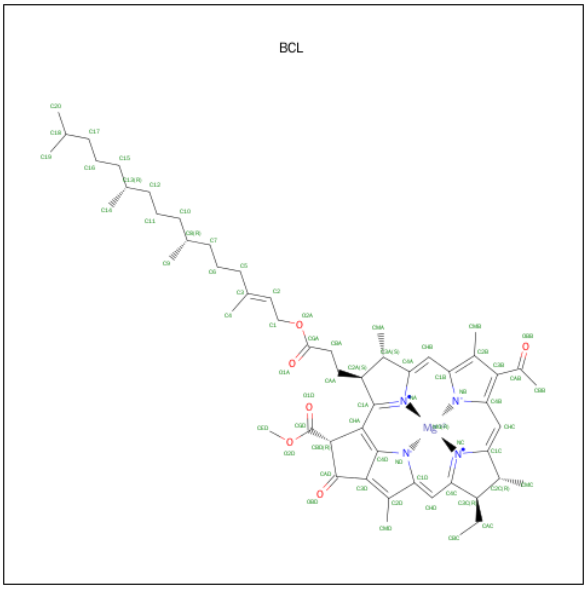


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 6 4 2	0	0
7	L	1	Total C O 6 4 2	0	0

- Molecule 8 is POTASSIUM ION (three-letter code: K) (formula: K).

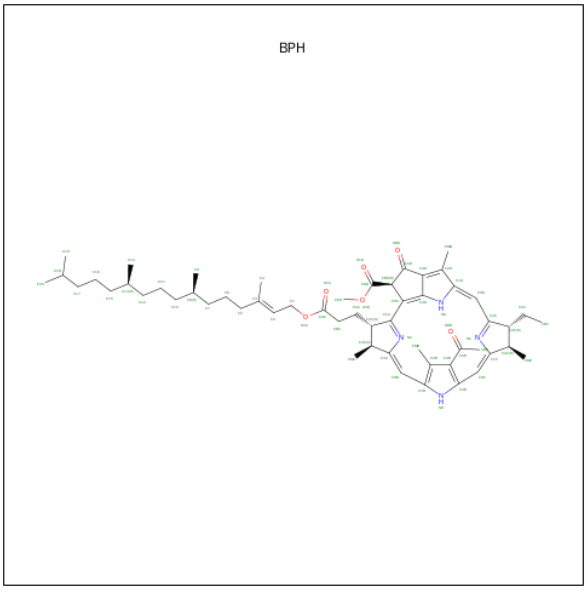
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total K 1 1	0	0

- Molecule 9 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



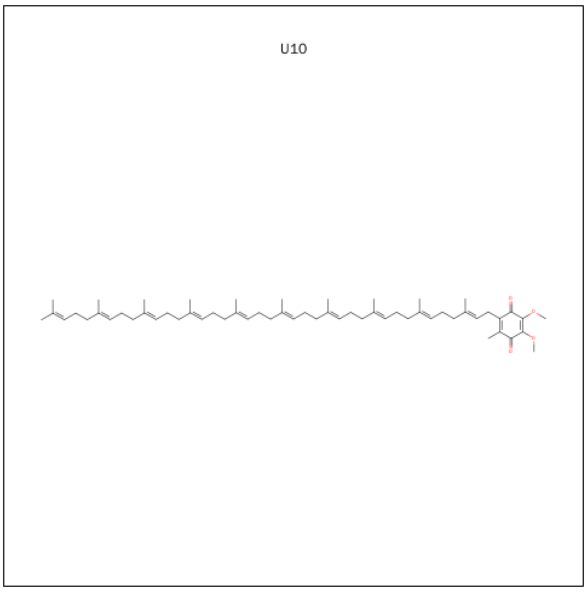
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
9	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 10 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

- Molecule 11 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).

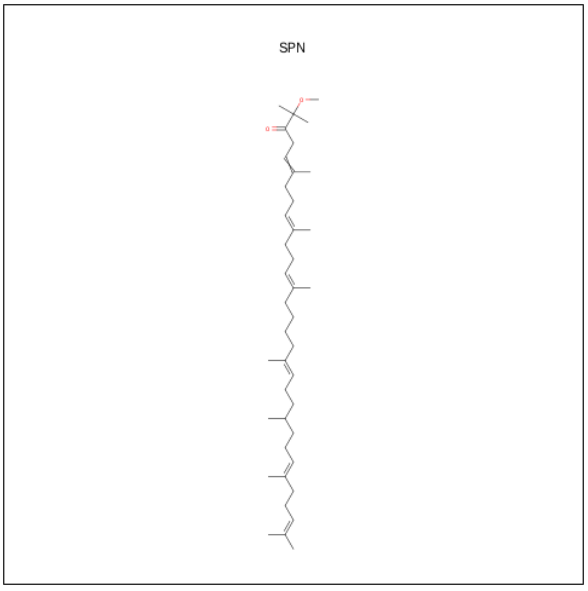


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	1	Total C O 48 44 4	0	0
11	M	1	Total C O 48 44 4	0	0

- Molecule 12 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 13 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$).



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

- Molecule 14 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 15 is water.

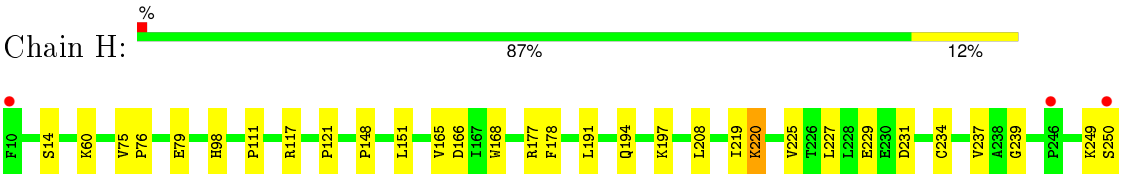
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	13	Total O 13 13	0	0
15	L	19	Total O 19 19	0	0
15	M	17	Total O 17 17	0	0

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.

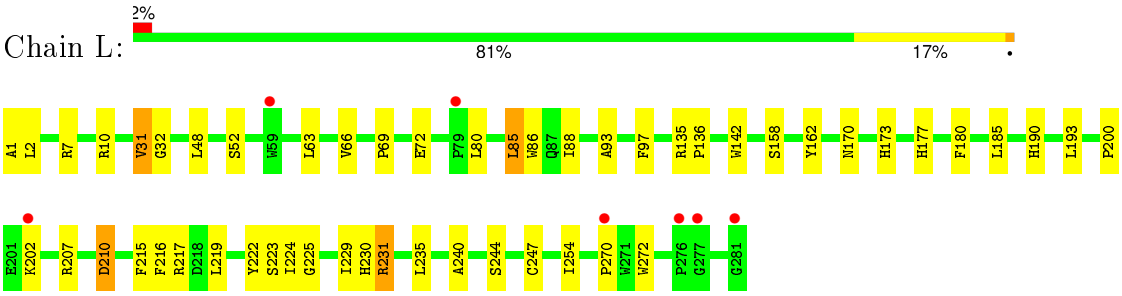
- Molecule 1: Reaction center protein H chain

Chain H:



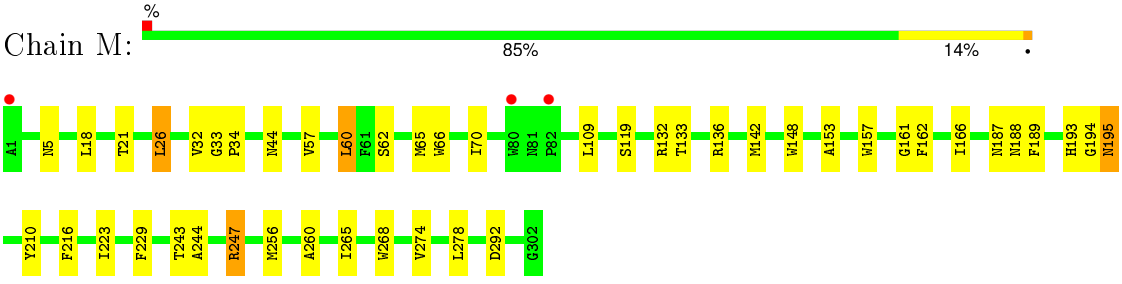
- Molecule 2: Reaction center protein L chain

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	140.13Å 140.13Å 186.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.90 – 2.90 28.90 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.90-2.90) 96.6 (28.90-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.251 0.204 , 0.251	Depositor DCC
R_{free} test set	2286 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 34.0	EDS
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 45707 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7216	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, DIO, CL, HTO, BPH, K, FE, SPN, 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	H	0.53	0/1889	0.62	0/2569
2	L	0.56	0/2324	0.59	0/3181
3	M	0.52	0/2501	0.60	1/3415 (0.0%)
All	All	0.54	0/6714	0.60	1/9165 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	26	LEU	CA-CB-CG	5.02	126.85	115.30

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	H	1840	0	1845	20	0
2	L	2235	0	2185	48	0
3	M	2409	0	2323	32	0
4	H	16	0	31	0	0
4	M	64	0	124	1	0
5	H	10	0	0	0	0
5	M	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	20	0	32	0	0
6	L	10	0	16	0	0
7	H	6	0	8	5	0
7	L	6	0	8	0	0
8	H	1	0	0	0	0
9	L	198	0	222	20	0
9	M	66	0	74	5	0
10	L	65	0	76	7	0
10	M	65	0	76	5	0
11	L	48	0	63	9	0
11	M	48	0	63	2	0
12	M	1	0	0	0	0
13	M	43	0	70	6	0
14	M	1	0	0	0	0
15	H	13	0	0	1	0
15	L	19	0	0	2	0
15	M	17	0	0	0	0
All	All	7216	0	7216	109	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 (109) 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)
2:L:177:HIS:CD2	9:L:302:BCL:HMB3	1.62	1.34
2:L:177:HIS:NE2	9:L:302:BCL:CMB	1.92	1.33
2:L:177:HIS:NE2	9:L:302:BCL:HMB3	1.52	1.16
2:L:177:HIS:NE2	9:L:302:BCL:HMB1	1.81	0.95
2:L:177:HIS:CD2	9:L:302:BCL:CMB	2.42	0.93
9:L:304:BCL:HMB1	9:L:304:BCL:HBB2	1.53	0.88
10:L:402:BPH:HHC	10:L:402:BPH:HBB3	1.57	0.85
9:L:304:BCL:HMB1	9:L:304:BCL:CBB	2.10	0.82
1:H:177:ARG:HD3	7:H:251:DIO:H2'1	1.67	0.77
2:L:225:GLY:H	11:L:502:U10:H3M3	1.55	0.72
3:M:229:PHE:HB2	3:M:244:ALA:HB2	1.71	0.72
3:M:161:GLY:HA3	13:M:600:SPN:H201	1.73	0.71
10:L:402:BPH:HBB2	3:M:210:TYR:HB3	1.73	0.71
2:L:177:HIS:NE2	9:L:302:BCL:C2B	2.54	0.70
9:L:301:BCL:CAB	13:M:600:SPN:H162	2.22	0.70
3:M:189:PHE:O	3:M:193:HIS:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:ARG:HD3	7:H:251:DIO:C2'	2.22	0.69
9:M:303:BCL:HBB3	9:M:303:BCL:HMB1	1.75	0.69
10:M:401:BPH:HHC	10:M:401:BPH:HBB3	1.79	0.65
2:L:52:SER:HB2	2:L:85:LEU:HD12	1.78	0.65
1:H:148:PRO:HA	1:H:151:LEU:HD12	1.78	0.64
2:L:177:HIS:CD2	9:L:302:BCL:C2B	2.81	0.64
3:M:243:THR:O	3:M:247:ARG:HG2	1.99	0.63
3:M:162:PHE:O	3:M:166:ILE:HG12	1.99	0.63
2:L:224:ILE:H	11:L:502:U10:C2	2.12	0.63
2:L:69:PRO:HG2	2:L:142:TRP:HB2	1.81	0.62
2:L:223:SER:HA	11:L:502:U10:O2	2.00	0.62
2:L:177:HIS:CE1	9:L:301:BCL:HMD2	2.35	0.61
9:L:301:BCL:CBB	9:L:301:BCL:HMB1	2.31	0.60
2:L:177:HIS:CE1	9:L:302:BCL:HBB3	2.36	0.60
1:H:111:PRO:HB2	1:H:239:GLY:HA2	1.84	0.59
3:M:157:TRP:HB2	9:M:303:BCL:H62	1.85	0.59
1:H:219:ILE:HG21	1:H:225:VAL:HG23	1.86	0.58
2:L:219:LEU:HA	3:M:132:ARG:HH12	1.68	0.58
9:L:301:BCL:HBB3	9:L:301:BCL:HMB1	1.89	0.55
2:L:97:PHE:CE1	9:L:302:BCL:H121	2.41	0.55
3:M:260:ALA:O	11:M:501:U10:H4M3	2.06	0.55
2:L:225:GLY:N	11:L:502:U10:H3M3	2.21	0.54
2:L:229:ILE:HD13	11:L:502:U10:C5	2.37	0.54
2:L:180:PHE:CE2	2:L:240:ALA:HB1	2.43	0.54
3:M:60:LEU:HA	10:M:401:BPH:H4C2	1.90	0.53
2:L:170:ASN:HB3	2:L:173:HIS:HB3	1.89	0.53
2:L:217:ARG:NH1	15:L:293:HOH:O	2.42	0.52
1:H:121:PRO:HB3	1:H:225:VAL:O	2.10	0.52
2:L:231:ARG:HD3	3:M:5:ASN:O	2.10	0.52
3:M:256:MET:CE	11:M:501:U10:H102	2.41	0.51
2:L:52:SER:HB2	2:L:85:LEU:CD1	2.39	0.51
2:L:135:ARG:HB3	2:L:136:PRO:HD3	1.93	0.51
1:H:98:HIS:CD2	2:L:7:ARG:HH21	2.28	0.51
9:L:301:BCL:OBB	13:M:600:SPN:H162	2.10	0.50
2:L:230:HIS:CD2	3:M:223:ILE:HG13	2.46	0.50
2:L:190:HIS:HA	11:L:502:U10:H4M3	1.94	0.50
1:H:79:GLU:HG2	15:H:256:HOH:O	2.11	0.50
1:H:177:ARG:HH11	7:H:251:DIO:H22	1.75	0.49
10:L:402:BPH:HHC	10:L:402:BPH:CBB	2.35	0.49
2:L:219:LEU:HD11	3:M:133:THR:HG22	1.94	0.49
1:H:208:LEU:HD11	1:H:237:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:220:LYS:HG3	1:H:229:GLU:OE2	2.13	0.49
3:M:189:PHE:O	3:M:193:HIS:CD2	2.62	0.48
9:L:302:BCL:HMB1	9:L:302:BCL:CBB	2.43	0.47
1:H:168:TRP:HB2	1:H:178:PHE:HB2	1.95	0.47
2:L:190:HIS:HD1	11:L:502:U10:H4M1	1.79	0.47
9:M:303:BCL:HAA2	9:M:303:BCL:HBD	1.95	0.47
10:L:402:BPH:CHD	10:L:402:BPH:HBC2	2.44	0.47
3:M:119:SER:CB	13:M:600:SPN:HM82	2.45	0.47
3:M:21:THR:HG23	3:M:26:LEU:HD21	1.97	0.46
2:L:52:SER:CB	2:L:85:LEU:HD12	2.45	0.46
2:L:215:PHE:HB2	3:M:142:MET:HE1	1.98	0.46
10:L:402:BPH:HBC2	10:L:402:BPH:HHD	1.98	0.45
2:L:2:LEU:HD21	2:L:10:ARG:CZ	2.46	0.45
1:H:194:GLN:HE22	7:H:251:DIO:C2	2.29	0.44
1:H:117:ARG:NH1	1:H:227:LEU:HD22	2.32	0.44
2:L:222:TYR:CG	2:L:223:SER:N	2.85	0.44
1:H:98:HIS:HD2	2:L:7:ARG:HH21	1.65	0.44
1:H:208:LEU:HD21	1:H:237:VAL:HA	1.99	0.44
2:L:1:ALA:O	2:L:2:LEU:HD23	2.17	0.44
2:L:219:LEU:O	3:M:132:ARG:NH1	2.47	0.44
2:L:162:TYR:OH	3:M:187:ASN:ND2	2.50	0.44
3:M:32:VAL:HG12	3:M:33:GLY:O	2.18	0.44
3:M:148:TRP:CE3	4:M:703:LDA:H82	2.53	0.43
3:M:194:GLY:O	3:M:195:ASN:HB3	2.17	0.43
9:L:302:BCL:HBB2	9:L:302:BCL:HMB1	2.00	0.43
1:H:75:VAL:HA	1:H:76:PRO:C	2.39	0.43
2:L:180:PHE:CD2	2:L:240:ALA:HB1	2.53	0.43
3:M:157:TRP:CE2	13:M:600:SPN:HM73	2.53	0.43
2:L:66:VAL:O	2:L:86:TRP:HD1	2.02	0.43
15:L:292:HOH:O	3:M:136:ARG:HD3	2.18	0.43
9:M:303:BCL:CBB	9:M:303:BCL:HMB1	2.47	0.42
3:M:62:SER:HA	3:M:65:MET:HB2	2.01	0.42
3:M:119:SER:HB3	13:M:600:SPN:HM82	2.00	0.42
1:H:234:CYS:SG	7:H:251:DIO:H1'1	2.59	0.42
2:L:244:SER:C	9:L:302:BCL:HED3	2.39	0.42
2:L:31:VAL:HG12	2:L:32:GLY:N	2.35	0.42
2:L:223:SER:O	3:M:44:ASN:HB2	2.20	0.42
1:H:249:LYS:O	1:H:250:SER:HB3	2.20	0.41
2:L:210:ASP:OD1	2:L:210:ASP:N	2.53	0.41
3:M:265:ILE:O	3:M:268:TRP:HB2	2.21	0.41
10:M:401:BPH:H4C1	10:M:401:BPH:H6C1	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:66:TRP:NE1	3:M:70:ILE:HD11	2.35	0.41
2:L:185:LEU:HD12	10:M:401:BPH:C1D	2.51	0.41
9:M:303:BCL:HBC2	9:M:303:BCL:H2C	1.73	0.40
2:L:93:ALA:HA	10:L:402:BPH:H9C2	2.03	0.40
10:L:402:BPH:HBB1	3:M:210:TYR:CD2	2.57	0.40
11:L:502:U10:C8	11:L:502:U10:H1M1	2.50	0.40
2:L:193:LEU:CD2	11:L:502:U10:H4M2	2.51	0.40
3:M:153:ALA:HB2	10:M:401:BPH:HBC2	2.03	0.40
2:L:48:LEU:HD11	2:L:88:ILE:HG21	2.04	0.40
2:L:177:HIS:NE2	9:L:302:BCL:HBB3	2.35	0.40
1:H:165:VAL:O	1:H:166:ASP:HB2	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	239/241 (99%)	222 (93%)	17 (7%)	0	100	100
2	L	279/281 (99%)	251 (90%)	25 (9%)	3 (1%)	17	51
3	M	300/302 (99%)	277 (92%)	21 (7%)	2 (1%)	26	63
All	All	818/824 (99%)	750 (92%)	63 (8%)	5 (1%)	30	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	80	LEU
3	M	34	PRO
3	M	195	ASN
2	L	270	PRO
2	L	31	VAL

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	196/196 (100%)	190 (97%)	6 (3%)	47 82
2	L	220/220 (100%)	206 (94%)	14 (6%)	22 53
3	M	236/236 (100%)	226 (96%)	10 (4%)	36 73
All	All	652/652 (100%)	622 (95%)	30 (5%)	33 69

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	14	SER
1	H	60	LYS
1	H	191	LEU
1	H	197	LYS
1	H	220	LYS
1	H	231	ASP
2	L	63	LEU
2	L	72	GLU
2	L	85	LEU
2	L	158	SER
2	L	200	PRO
2	L	202	LYS
2	L	207	ARG
2	L	210	ASP
2	L	216	PHE
2	L	231	ARG
2	L	235	LEU
2	L	247	CYS
2	L	254	ILE
2	L	272	TRP
3	M	18	LEU
3	M	57	VAL
3	M	60	LEU
3	M	109	LEU
3	M	188	ASN
3	M	216	PHE

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Mol	Chain	Res	Type
3	M	247	ARG
3	M	274	VAL
3	M	278	LEU
3	M	292	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	98	HIS
1	H	206	ASN
2	L	183	ASN
3	M	187	ASN
3	M	193	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 27 ligands modelled in this entry, 3 are monoatomic - leaving 24 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	$\#\|Z\|>2$
6	HTO	H	2	-	9,9,9	0.31	0	8,10,10	0.59	0
7	DIO	H	251	-	6,6,6	0.44	0	6,6,6	1.02	0
6	HTO	H	3	-	9,9,9	0.45	0	8,10,10	0.53	0
4	LDA	H	704	-	15,15,15	3.80	1 (6%)	16,17,17	0.84	1 (6%)
5	PO4	H	803	-	4,4,4	0.43	0	6,6,6	0.28	0
5	PO4	H	804	-	4,4,4	0.44	0	6,6,6	0.27	0
6	HTO	L	282	-	9,9,9	0.48	0	8,10,10	0.53	0
7	DIO	L	283	-	6,6,6	0.61	0	6,6,6	0.73	0
9	BCL	L	301	-	53,74,74	0.62	0	57,115,115	1.49	8 (14%)
9	BCL	L	302	-	53,74,74	0.54	1 (1%)	57,115,115	1.60	11 (19%)
9	BCL	L	304	-	53,74,74	0.68	1 (1%)	57,115,115	1.67	10 (17%)
10	BPH	L	402	-	64,70,70	1.40	6 (9%)	73,101,101	1.46	9 (12%)
11	U10	L	502	-	48,48,63	3.26	14 (29%)	58,61,79	1.75	16 (27%)
9	BCL	M	303	-	53,74,74	0.62	1 (1%)	57,115,115	1.54	10 (17%)
10	BPH	M	401	-	64,70,70	1.43	6 (9%)	73,101,101	1.51	12 (16%)
11	U10	M	501	-	48,48,63	3.14	12 (25%)	58,61,79	1.66	14 (24%)
13	SPN	M	600	-	41,42,42	0.63	0	41,52,52	1.68	9 (21%)
4	LDA	M	701	-	15,15,15	3.76	1 (6%)	16,17,17	0.99	2 (12%)
4	LDA	M	702	-	15,15,15	3.60	2 (13%)	16,17,17	0.76	1 (6%)
4	LDA	M	703	-	15,15,15	3.81	1 (6%)	16,17,17	0.72	0
4	LDA	M	705	-	15,15,15	3.87	1 (6%)	16,17,17	0.65	1 (6%)
5	PO4	M	800	-	4,4,4	0.53	0	6,6,6	0.28	0
5	PO4	M	801	-	4,4,4	0.45	0	6,6,6	0.27	0
5	PO4	M	802	-	4,4,4	0.45	0	6,6,6	0.26	0

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
6	HTO	H	2	-	-	0/10/10/10	0/0/0/0
7	DIO	H	251	-	-	0/0/6/6	0/1/1/1
6	HTO	H	3	-	-	0/10/10/10	0/0/0/0
4	LDA	H	704	-	-	0/13/13/13	0/0/0/0
5	PO4	H	803	-	-	0/0/0/0	0/0/0/0
5	PO4	H	804	-	-	0/0/0/0	0/0/0/0
6	HTO	L	282	-	-	0/10/10/10	0/0/0/0
7	DIO	L	283	-	-	0/0/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	BCL	L	301	-	-	0/37/137/137	0/0/9/9
9	BCL	L	302	-	-	0/37/137/137	0/0/9/9
9	BCL	L	304	-	-	0/37/137/137	0/0/9/9
10	BPH	L	402	-	2/2/18/22	0/54/105/105	0/1/6/6
11	U10	L	502	-	-	0/45/69/87	0/1/1/1
9	BCL	M	303	-	-	0/37/137/137	0/0/9/9
10	BPH	M	401	-	2/2/18/22	0/54/105/105	0/1/6/6
11	U10	M	501	-	-	0/45/69/87	0/1/1/1
13	SPN	M	600	-	-	0/50/51/51	0/0/0/0
4	LDA	M	701	-	-	0/13/13/13	0/0/0/0
4	LDA	M	702	-	-	0/13/13/13	0/0/0/0
4	LDA	M	703	-	-	0/13/13/13	0/0/0/0
4	LDA	M	705	-	-	0/13/13/13	0/0/0/0
5	PO4	M	800	-	-	0/0/0/0	0/0/0/0
5	PO4	M	801	-	-	0/0/0/0	0/0/0/0
5	PO4	M	802	-	-	0/0/0/0	0/0/0/0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	705	LDA	O1-N1	-14.74	1.25	1.39
4	M	703	LDA	O1-N1	-14.54	1.25	1.39
4	H	704	LDA	O1-N1	-14.51	1.25	1.39
4	M	701	LDA	O1-N1	-14.28	1.26	1.39
4	M	702	LDA	O1-N1	-13.68	1.26	1.39
11	M	501	U10	O4-C4	-4.76	1.24	1.37
11	L	502	U10	O3-C3	-4.26	1.25	1.37
11	M	501	U10	O3-C3	-4.16	1.26	1.37
11	L	502	U10	O4-C4	-4.00	1.26	1.37
10	M	401	BPH	C4C-NC	-3.49	1.29	1.37
10	L	402	BPH	C1B-C2B	-3.47	1.38	1.45
10	M	401	BPH	C1B-C2B	-3.38	1.38	1.45
10	M	401	BPH	CHB-C4A	-3.04	1.34	1.40
11	L	502	U10	C3-C2	-2.92	1.40	1.48
10	M	401	BPH	C1A-NA	-2.82	1.31	1.37
10	L	402	BPH	CHB-C4A	-2.78	1.35	1.40
10	L	402	BPH	C1A-NA	-2.74	1.31	1.37
10	L	402	BPH	C4C-NC	-2.74	1.31	1.37
11	M	501	U10	C3-C2	-2.73	1.41	1.48
11	L	502	U10	C4-C5	-2.44	1.41	1.48
9	L	302	BCL	CHD-C4C	-2.39	1.34	1.41
9	L	304	BCL	CHD-C4C	-2.37	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	501	U10	C4-C5	-2.31	1.42	1.48
9	M	303	BCL	CHD-C4C	-2.14	1.35	1.41
4	M	702	LDA	C1-N1	-2.12	1.47	1.51
11	M	501	U10	C6-C1	2.11	1.40	1.35
11	L	502	U10	C7-C8	2.19	1.54	1.50
11	L	502	U10	C7-C6	2.34	1.55	1.51
11	L	502	U10	C6-C1	2.61	1.41	1.35
10	M	401	BPH	CHD-C4C	4.58	1.49	1.38
10	L	402	BPH	CHA-C1A	4.92	1.48	1.37
10	M	401	BPH	CHA-C1A	5.12	1.49	1.37
10	L	402	BPH	CHD-C4C	5.13	1.51	1.38
11	M	501	U10	C38-C39	5.25	1.48	1.32
11	L	502	U10	C38-C39	5.26	1.48	1.32
11	M	501	U10	C8-C9	7.22	1.47	1.33
11	L	502	U10	C18-C19	7.55	1.47	1.33
11	M	501	U10	C28-C29	7.84	1.48	1.33
11	M	501	U10	C23-C24	7.84	1.48	1.33
11	L	502	U10	C28-C29	7.90	1.48	1.33
11	M	501	U10	C18-C19	8.05	1.48	1.33
11	M	501	U10	C33-C34	8.08	1.48	1.33
11	M	501	U10	C13-C14	8.16	1.49	1.33
11	L	502	U10	C13-C14	8.27	1.49	1.33
11	L	502	U10	C23-C24	8.29	1.49	1.33
11	L	502	U10	C33-C34	8.31	1.49	1.33
11	L	502	U10	C8-C9	8.61	1.49	1.33

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	L	304	BCL	O1D-CGD-CBD	-4.19	118.62	124.62
11	L	502	U10	O5-C5-C4	-4.11	111.90	120.79
9	L	301	BCL	O1D-CGD-CBD	-3.74	119.26	124.62
9	M	303	BCL	CAA-C2A-C3A	-3.60	102.87	113.22
9	L	302	BCL	C1D-CHD-C4C	-3.56	120.63	126.07
10	L	402	BPH	C2D-C1D-ND	-3.50	104.56	110.29
9	L	302	BCL	CMB-C2B-C1B	-3.36	122.81	128.36
10	M	401	BPH	C2D-C1D-ND	-3.36	104.79	110.29
11	M	501	U10	C22-C23-C24	-3.35	120.47	127.76
11	L	502	U10	C30-C29-C28	-3.28	117.06	123.50
11	M	501	U10	C27-C28-C29	-3.16	120.89	127.76
11	L	502	U10	O2-C2-C3	-3.08	114.11	120.79
11	L	502	U10	C17-C18-C19	-3.04	121.15	127.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	401	BPH	C1C-NC-C4C	-2.96	107.40	110.44
9	L	302	BCL	C11-C12-C13	-2.94	105.74	115.49
11	M	501	U10	C17-C18-C19	-2.85	121.56	127.76
11	M	501	U10	C7-C8-C9	-2.81	121.93	126.70
10	L	402	BPH	C4-C3-C5	-2.71	111.27	115.41
13	M	600	SPN	C3-C4-C5	-2.69	122.14	126.70
11	L	502	U10	C35-C34-C33	-2.69	118.23	123.50
11	M	501	U10	C32-C33-C34	-2.62	122.07	127.76
9	M	303	BCL	O1D-CGD-CBD	-2.55	120.97	124.62
11	L	502	U10	O5-C5-C6	-2.48	117.02	121.68
9	L	302	BCL	O1D-CGD-CBD	-2.40	121.19	124.62
4	M	702	LDA	CM2-N1-CM1	-2.39	106.14	108.83
11	L	502	U10	C27-C28-C29	-2.38	122.59	127.76
9	L	304	BCL	C1D-CHD-C4C	-2.29	122.58	126.07
9	M	303	BCL	C1D-CHD-C4C	-2.29	122.58	126.07
9	L	302	BCL	C6-C7-C8	-2.28	107.91	115.49
11	L	502	U10	C20-C19-C18	-2.28	119.03	123.50
4	H	704	LDA	O1-N1-C1	-2.26	107.73	110.27
9	L	301	BCL	CAC-C3C-C2C	-2.25	108.46	114.13
9	L	304	BCL	C5-C3-C2	-2.24	116.80	121.05
10	L	402	BPH	C2B-C1B-NB	-2.23	106.38	109.73
11	L	502	U10	C1-C6-C5	-2.21	117.60	120.12
10	M	401	BPH	C4-C3-C5	-2.20	112.04	115.41
4	M	705	LDA	O1-N1-CM2	-2.20	106.11	109.05
9	L	301	BCL	C1D-CHD-C4C	-2.12	122.84	126.07
9	L	302	BCL	C3C-C4C-CHD	-2.12	118.61	123.33
4	M	701	LDA	CM2-N1-CM1	-2.11	106.45	108.83
9	L	304	BCL	C3C-C4C-CHD	-2.09	118.66	123.33
9	M	303	BCL	CGD-CBD-CAD	-2.08	103.56	110.62
13	M	600	SPN	C17-C18-C19	-2.07	117.13	121.05
10	M	401	BPH	C2B-C1B-NB	-2.05	106.65	109.73
10	M	401	BPH	C3A-C2A-C1A	-2.04	99.25	101.84
11	M	501	U10	C25-C24-C23	-2.03	119.51	123.50
13	M	600	SPN	C10-C9-C8	-2.03	117.20	121.05
11	M	501	U10	C10-C9-C8	-2.03	119.52	123.50
11	M	501	U10	C30-C29-C28	-2.01	119.56	123.50
13	M	600	SPN	C24-C25-C26	-2.00	123.41	127.76
11	L	502	U10	C4M-O4-C4	2.09	124.03	116.61
11	L	502	U10	C3M-O3-C3	2.09	124.06	116.61
9	L	301	BCL	CHB-C4A-NA	2.10	127.42	124.51
10	L	402	BPH	CHB-C1B-C2B	2.11	130.39	125.61
11	M	501	U10	C25-C24-C26	2.15	118.69	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	402	BPH	CAC-C3C-C4C	2.17	118.25	112.67
11	M	501	U10	C3M-O3-C3	2.19	124.41	116.61
13	M	600	SPN	CMA-O1-C1	2.25	124.19	112.20
9	L	304	BCL	CED-O2D-CGD	2.26	121.28	115.99
10	M	401	BPH	C1B-NB-C4B	2.33	111.12	106.51
9	M	303	BCL	CHB-C4A-NA	2.35	127.76	124.51
9	L	301	BCL	C4-C3-C5	2.40	119.07	115.41
9	L	301	BCL	CHD-C4C-NC	2.40	127.84	125.06
9	L	304	BCL	O2A-CGA-CBA	2.42	119.26	111.90
10	M	401	BPH	OBB-CAB-C3B	2.42	124.99	120.31
9	L	304	BCL	C4-C3-C5	2.47	119.19	115.41
10	L	402	BPH	C1B-NB-C4B	2.52	111.49	106.51
10	M	401	BPH	CMD-C2D-C3D	2.57	130.11	125.09
11	L	502	U10	C15-C14-C16	2.58	119.35	115.41
10	M	401	BPH	C4D-C3D-C2D	2.66	110.51	107.08
9	L	302	BCL	CED-O2D-CGD	2.67	122.25	115.99
9	M	303	BCL	C4-C3-C5	2.70	119.53	115.41
9	L	302	BCL	C4-C3-C5	2.71	119.55	115.41
9	L	302	BCL	CHD-C4C-NC	2.76	128.26	125.06
9	L	304	BCL	CHB-C4A-NA	2.79	128.38	124.51
11	L	502	U10	C25-C24-C26	2.88	119.80	115.41
9	M	303	BCL	O2A-CGA-CBA	2.91	120.77	111.90
4	M	701	LDA	O1-N1-C1	2.92	113.56	110.27
9	L	302	BCL	O2A-CGA-CBA	2.93	120.82	111.90
11	M	501	U10	C30-C29-C31	2.94	119.89	115.41
9	M	303	BCL	CED-O2D-CGD	2.97	122.95	115.99
9	L	301	BCL	O2A-CGA-CBA	2.97	120.96	111.90
11	L	502	U10	C35-C34-C36	3.08	120.11	115.41
11	L	502	U10	C20-C19-C21	3.10	120.15	115.41
9	M	303	BCL	CHD-C4C-NC	3.10	128.66	125.06
10	M	401	BPH	C5-C3-C2	3.12	126.96	121.05
11	M	501	U10	C10-C9-C11	3.26	120.38	115.41
10	L	402	BPH	OBB-CAB-C3B	3.56	127.19	120.31
13	M	600	SPN	CM6-C18-C17	3.59	120.89	115.41
13	M	600	SPN	CM4-C9-C10	3.67	121.02	115.41
9	L	304	BCL	CHD-C4C-NC	3.69	129.34	125.06
13	M	600	SPN	CM3-C5-C6	3.70	121.06	115.41
11	M	501	U10	C15-C14-C16	3.70	121.06	115.41
10	L	402	BPH	C6-C5-C3	3.70	120.61	112.48
11	M	501	U10	C35-C34-C36	3.93	121.41	115.41
13	M	600	SPN	CM5-C13-C14	3.94	121.43	115.41
10	M	401	BPH	C6-C5-C3	4.19	121.67	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	502	U10	C30-C29-C31	4.87	122.84	115.41
10	L	402	BPH	C3C-C4C-NC	5.00	112.94	107.93
9	M	303	BCL	O2D-CGD-CBD	5.24	118.49	111.30
9	L	302	BCL	O2D-CGD-CBD	5.34	118.62	111.30
10	M	401	BPH	C3C-C4C-NC	6.06	114.00	107.93
9	L	301	BCL	O2D-CGD-CBD	6.12	119.70	111.30
9	L	304	BCL	O2D-CGD-CBD	7.43	121.49	111.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	M	401	BPH	C8
10	M	401	BPH	C13
10	L	402	BPH	C8
10	L	402	BPH	C13

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	251	DIO	5	0
9	L	301	BCL	5	0
9	L	302	BCL	13	0
9	L	304	BCL	2	0
10	L	402	BPH	7	0
11	L	502	U10	9	0
9	M	303	BCL	5	0
10	M	401	BPH	5	0
11	M	501	U10	2	0
13	M	600	SPN	6	0
4	M	703	LDA	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	H	241/241 (100%)	-0.38	3 (1%)	81	78	51, 65, 76, 101	0
2	L	281/281 (100%)	-0.43	7 (2%)	61	55	49, 65, 100, 106	0
3	M	302/302 (100%)	-0.45	3 (0%)	84	82	44, 67, 98, 101	0
All	All	824/824 (100%)	-0.42	13 (1%)	74	72	44, 66, 97, 106	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	250	SER	5.1
1	H	10	PHE	4.5
2	L	59	TRP	3.5
3	M	80	TRP	3.4
3	M	1	ALA	3.2
2	L	270	PRO	2.9
2	L	281	GLY	2.9
2	L	202	LYS	2.7
2	L	277	GLY	2.6
2	L	276	PRO	2.2
2	L	79	PRO	2.1
1	H	246	PRO	2.1
3	M	82	PRO	2.1

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

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

6.3 Carbohydrates

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	U10	L	502	48/63	0.69	0.51	14.41	128,135,140,140	0
4	LDA	H	704	16/16	0.67	0.52	6.98	109,114,120,120	0
4	LDA	M	703	16/16	0.69	0.53	6.34	98,102,107,108	0
4	LDA	M	702	16/16	0.78	0.40	4.68	96,109,120,121	0
6	HTO	L	282	10/10	0.86	0.33	4.50	97,98,99,100	0
4	LDA	M	705	16/16	0.90	0.45	4.15	83,90,100,101	0
4	LDA	M	701	16/16	0.87	0.23	3.55	77,85,88,88	0
6	HTO	H	2	10/10	0.83	0.32	3.23	134,136,136,136	0
9	BCL	L	301	66/66	0.95	0.21	3.09	62,71,111,113	0
13	SPN	M	600	43/43	0.89	0.23	2.04	65,76,86,87	0
10	BPH	M	401	65/65	0.89	0.22	1.96	63,73,107,107	0
11	U10	M	501	48/63	0.93	0.20	1.17	53,60,89,89	0
7	DIO	H	251	6/6	0.95	0.23	0.80	84,84,85,86	0
10	BPH	L	402	65/65	0.97	0.16	0.71	48,56,66,66	0
5	PO4	M	801	5/5	0.86	0.28	0.51	140,140,140,140	0
9	BCL	L	302	66/66	0.97	0.17	0.33	45,61,64,65	0
9	BCL	M	303	66/66	0.98	0.15	-0.05	57,60,71,76	0
9	BCL	L	304	66/66	0.98	0.12	-0.78	37,42,64,66	0
5	PO4	M	802	5/5	0.90	0.15	-1.48	110,110,111,111	0
12	FE	M	500	1/1	0.99	0.11	-1.67	55,55,55,55	0
8	K	H	1	1/1	0.95	0.07	-1.83	64,64,64,64	0
6	HTO	H	3	10/10	0.72	0.35	-	113,114,114,115	0
14	CL	M	304	1/1	0.94	0.06	-	83,83,83,83	0
5	PO4	H	803	5/5	0.87	0.19	-	124,124,124,124	0
7	DIO	L	283	6/6	0.63	0.33	-	131,131,131,132	0
5	PO4	H	804	5/5	0.82	0.24	-	123,123,123,123	0
5	PO4	M	800	5/5	0.98	0.08	-	67,67,68,69	0

6.5 Other polymers (i)

There are no such residues in this entry.