Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:37 AM GMT

PDB ID	:	2HVS
Title	:	Structure of T4 RNA Ligase 2 with Nicked 5'-Adenylated nucleic acid duplex containing a 2'-deoxyribonucleotide at the nick
Authors	:	Nandakumar, J.; Lima, C.D.
Deposited on	:	2006-07-30
Resolution	:	2.50 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:

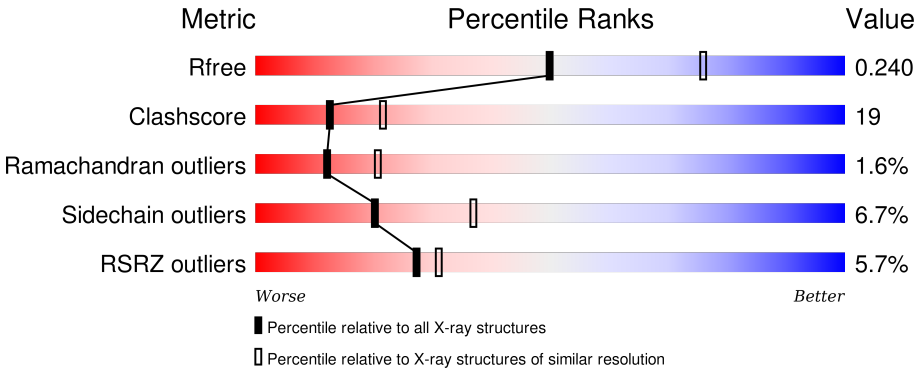
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	C	24	8%, 38%, 63%
1	F	24	42%, 54%, ·
2	D	12	17%, 83%
2	G	12	8%, 17%, 83%
3	E	12	8%, 42%, 58%

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Mol	Chain	Length	Quality of chain
3	H	12	8% 25% 75%
4	A	335	5% 58% 33% 5%
4	B	335	6% 59% 32% 5%

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
5	BTB	C	201	-	-	-	X
5	BTB	F	202	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7188 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 DNA chain called 5'-D(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	24	Total	C	N	O	P	0	0	0
			494	236	91	144	23			
1	F	24	Total	C	N	O	P	0	0	0
			494	236	91	144	23			

- Molecule 2 is DNA/RNA hybrid called 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			241	116	44	70	11			
2	G	12	Total	C	N	O	P	0	0	0
			241	116	44	70	11			

- Molecule 3 is a DNA chain called 5'-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	12	Total	C	N	O	P	0	0	0
			245	117	45	71	12			
3	H	12	Total	C	N	O	P	0	0	0
			245	117	45	71	12			

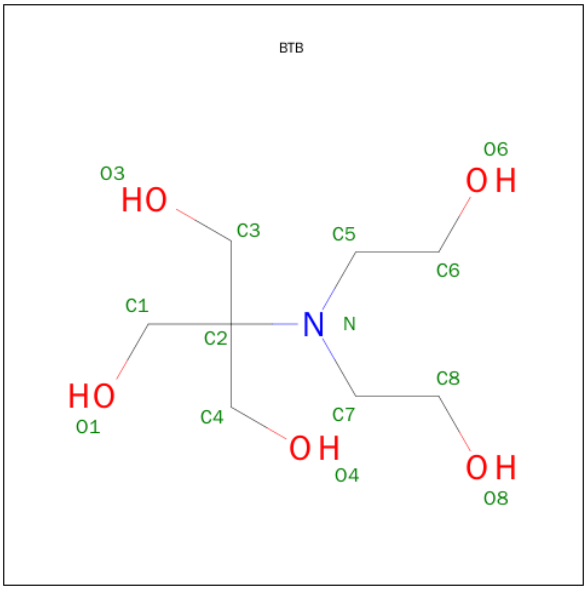
- Molecule 4 is a protein called T4 RNA Ligase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	319	Total	C	N	O	S	0	0	0
			2521	1617	409	482	13			
4	B	319	Total	C	N	O	S	0	0	0
			2521	1617	409	482	13			

There are 4 discrepancies between the modelled and reference sequences:

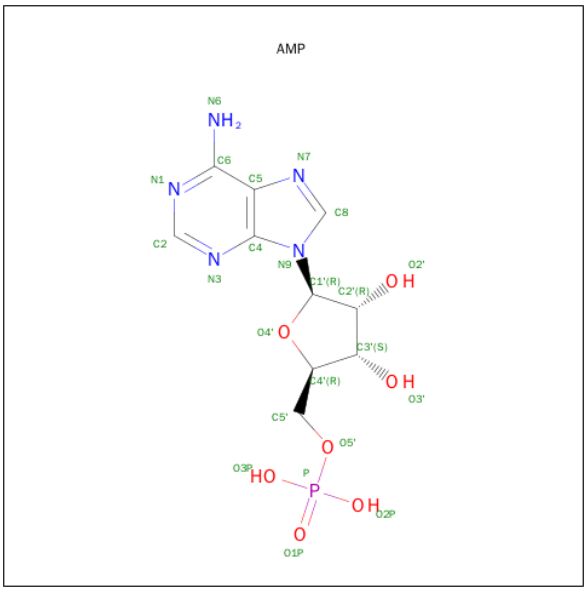
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	UNP P32277
A	112	GLY	CYS	SEE REMARK 999	UNP P32277
B	0	SER	-	CLONING ARTIFACT	UNP P32277
B	112	GLY	CYS	SEE REMARK 999	UNP P32277

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
6	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

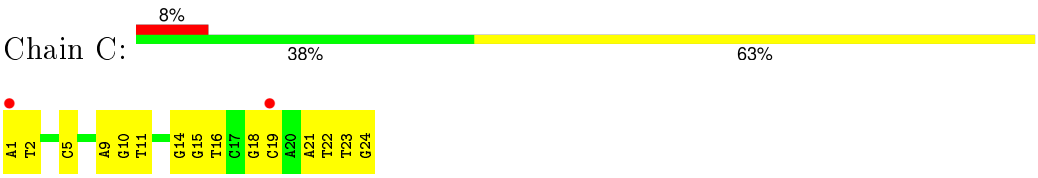
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	O	0	0
			1	1		
7	E	1	Total	O	0	0
			1	1		
7	A	59	Total	O	0	0
			59	59		
7	B	37	Total	O	0	0
			37	37		

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.

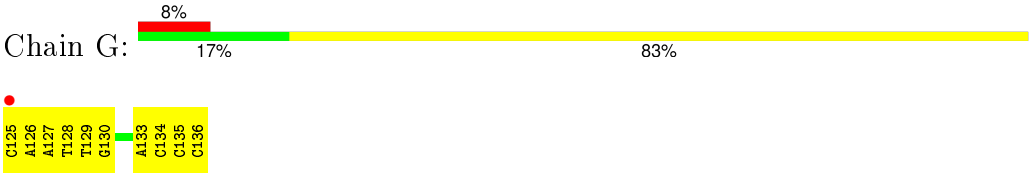
• Molecule 1: 5'-D(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'



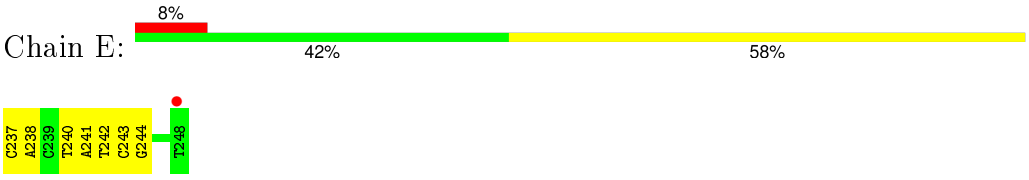
• Molecule 1: 5'-D(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'

• Molecule 2: 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'

• Molecule 2: 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'

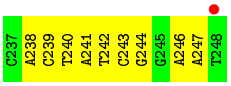


• Molecule 3: 5'-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'



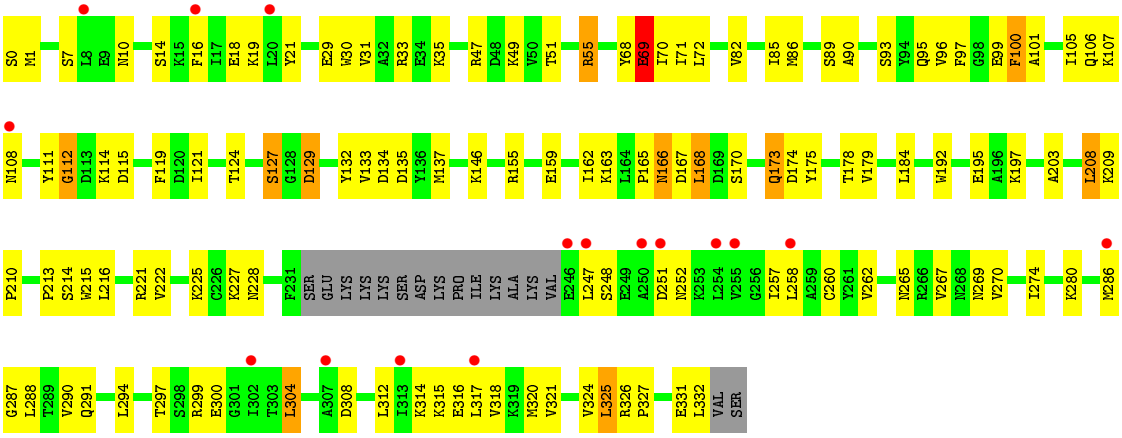
• Molecule 3: 5'-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'

Chain H:



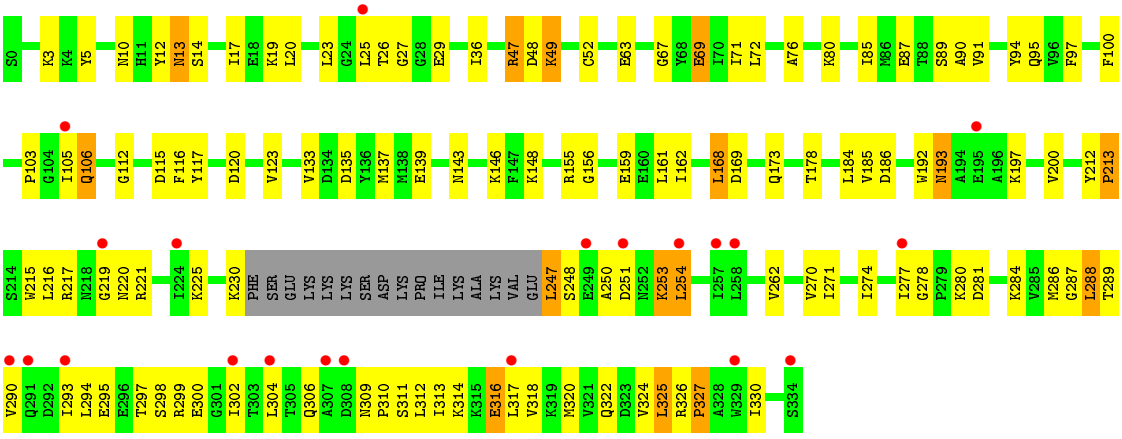
• Molecule 4: T4 RNA Ligase 2

Chain A:



• Molecule 4: T4 RNA Ligase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.42Å 106.74Å 124.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.82 – 2.50 49.81 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.82-2.50) 98.3 (49.81-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.283 0.246 , 0.240	Depositor DCC
R_{free} test set	1924 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	50.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	2 of 38411 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7188	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.20 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.3143e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: OMC, AMP, BTB

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	C	0.29	0/554	0.68	0/855
1	F	0.31	0/554	0.69	0/855
2	D	0.27	0/246	0.64	0/377
2	G	0.36	0/246	0.70	0/377
3	E	0.50	0/274	0.73	0/420
3	H	0.51	0/274	0.69	0/420
4	A	0.42	0/2570	0.61	0/3472
4	B	0.42	0/2570	0.60	0/3471
All	All	0.40	0/7288	0.63	0/10247

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
1	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	15	DG	Sidechain

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	C	494	0	273	21	0
1	F	494	0	273	17	0
2	D	241	0	138	13	0
2	G	241	0	138	9	0
3	E	245	0	136	6	0
3	H	245	0	136	12	0
4	A	2521	0	2511	96	0
4	B	2521	0	2517	90	0
5	A	14	0	19	0	0
5	C	14	0	19	2	0
5	F	14	0	19	1	0
6	E	23	0	12	1	0
6	H	23	0	12	0	0
7	A	59	0	0	4	0
7	B	37	0	0	2	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
All	All	7188	0	6203	258	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 19.

All (258) 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)
3:H:238:DA:H2"	3:H:239:DC:H5"	1.26	1.11
2:G:133:DA:H2"	2:G:134:DC:H5"	1.24	1.09
1:C:9:DA:H2"	1:C:10:DG:H5"	1.27	1.07
3:H:239:DC:H2"	3:H:240:DT:H5'	1.48	0.94
2:D:133:DA:H2"	2:D:134:DC:H5"	1.47	0.94
4:A:133:VAL:HG13	4:A:137:MET:HB3	1.55	0.86
1:C:10:DG:H2"	1:C:11:DT:H5'	1.56	0.85
1:C:9:DA:C2'	1:C:10:DG:H5"	2.06	0.85
4:A:326:ARG:HB3	4:A:327:PRO:HD3	1.59	0.84
2:G:133:DA:C2'	2:G:134:DC:H5"	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:238:DA:C2'	3:H:239:DC:H5"	2.08	0.81
1:F:6:DG:H2"	1:F:7:DA:H5"	1.66	0.78
3:H:241:DA:H2"	3:H:242:DT:H5'	1.63	0.78
1:F:15:DG:H2'	1:F:16:DT:C7	2.13	0.77
4:A:290:VAL:HG13	4:A:317:LEU:HD22	1.64	0.77
1:F:6:DG:H1	3:H:243:DC:H42	1.32	0.76
4:B:133:VAL:CG1	4:B:137:MET:HB3	2.16	0.75
1:F:7:DA:H2"	1:F:8:DT:H5'	1.67	0.74
1:F:15:DG:H2'	1:F:16:DT:H72	1.69	0.74
4:B:106:GLN:HA	4:B:106:GLN:HE21	1.52	0.74
2:D:133:DA:C2'	2:D:134:DC:H5"	2.17	0.74
4:B:133:VAL:HG13	4:B:137:MET:HB3	1.69	0.73
4:A:287:GLY:O	4:A:291:GLN:HG2	1.89	0.71
4:B:304:LEU:HD11	4:B:313:ILE:HG21	1.71	0.70
4:A:248:SER:OG	4:A:251:ASP:HB3	1.91	0.69
4:B:13:ASN:O	4:B:17:ILE:HG13	1.92	0.69
4:B:270:VAL:HG13	4:B:288:LEU:HD22	1.74	0.68
3:H:246:DA:H2"	3:H:247:DA:H5'	1.75	0.68
1:F:8:DT:H2"	1:F:9:DA:C8	2.29	0.67
4:B:3:LYS:O	4:B:97:PHE:HZ	1.77	0.66
2:D:133:DA:H2"	2:D:134:DC:C5'	2.25	0.66
1:C:15:DG:H2'	1:C:16:DT:H72	1.78	0.65
4:A:30:TRP:HE3	4:A:208:LEU:HD22	1.61	0.65
2:D:126:DA:H2"	2:D:127:DA:H5'	1.79	0.64
4:B:156:GLY:H	4:B:161:LEU:HD11	1.61	0.64
4:A:105:ILE:O	4:A:106:GLN:HG2	1.97	0.63
3:H:238:DA:H2"	3:H:239:DC:C5'	2.18	0.63
4:A:10:ASN:CG	4:A:225:LYS:HE3	2.19	0.63
1:C:15:DG:H2'	1:C:16:DT:C7	2.30	0.62
4:B:262:VAL:HG12	4:B:324:VAL:HG21	1.81	0.62
4:A:288:LEU:O	4:A:291:GLN:HB2	2.00	0.62
4:B:294:LEU:HA	4:B:297:THR:HG22	1.82	0.62
1:C:23:DT:H2"	1:C:24:DG:C5'	2.30	0.61
4:B:286:MET:O	4:B:290:VAL:HG23	1.99	0.61
4:B:326:ARG:HB2	4:B:327:PRO:HD3	1.83	0.61
4:A:71:ILE:HD11	4:A:100:PHE:CD1	2.35	0.60
4:A:89:SER:O	4:A:90:ALA:HB3	2.01	0.60
1:C:23:DT:H2"	1:C:24:DG:H5'	1.83	0.60
4:B:94:TYR:CE2	4:B:123:VAL:HG22	2.37	0.59
4:A:315:LYS:O	4:A:318:VAL:HG22	2.02	0.59
4:B:274:ILE:HD11	4:B:288:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:243:DC:H2"	3:E:244:DG:C8	2.38	0.59
2:G:125:DC:H2"	2:G:126:DA:C8	2.37	0.58
4:B:69:GLU:HA	4:B:72:LEU:HD23	1.84	0.58
1:F:18:DG:H2'	1:F:19:DC:C6	2.39	0.58
4:B:52:CYS:SG	4:B:72:LEU:HD21	2.44	0.58
3:H:239:DC:H2'	3:H:240:DT:H72	1.85	0.57
1:C:21:DA:H1'	1:C:22:DT:H5"	1.87	0.56
4:A:69:GLU:CD	4:A:69:GLU:H	2.06	0.56
4:B:295:GLU:O	4:B:299:ARG:HB2	2.05	0.56
4:B:71:ILE:HD11	4:B:100:PHE:CD1	2.41	0.55
4:B:10:ASN:OD1	4:B:225:LYS:HE3	2.07	0.55
2:D:134:DC:H2"	2:D:135:OMC:H6	1.71	0.55
4:B:193:ASN:H	4:B:193:ASN:HD22	1.54	0.55
4:A:159:GLU:O	4:A:163:LYS:HE3	2.07	0.55
4:A:290:VAL:HG22	4:A:321:VAL:HG21	1.89	0.55
4:A:146:LYS:NZ	7:A:356:HOH:O	2.40	0.55
4:B:248:SER:H	4:B:251:ASP:HB3	1.71	0.55
3:H:240:DT:H2"	3:H:241:DA:C8	2.42	0.54
1:F:18:DG:OP1	1:F:18:DG:H4'	2.07	0.54
4:A:215:TRP:O	4:A:216:LEU:HD23	2.06	0.54
4:B:159:GLU:CD	4:B:159:GLU:H	2.09	0.54
4:A:173:GLN:HG2	4:A:174:ASP:N	2.22	0.54
4:B:105:ILE:HG22	4:B:106:GLN:HG2	1.89	0.54
4:B:219:GLY:O	4:B:220:ASN:ND2	2.40	0.54
4:A:82:VAL:O	4:A:85:ILE:HG13	2.08	0.54
4:A:257:ILE:O	4:A:260:CYS:HB2	2.08	0.54
2:G:134:DC:H2"	2:G:135:OMC:H6	1.73	0.54
4:A:132:TYR:O	4:A:213:PRO:HG2	2.08	0.54
4:B:20:LEU:HB3	4:B:26:THR:HG23	1.90	0.54
3:H:239:DC:C2'	3:H:240:DT:H5'	2.32	0.53
4:A:133:VAL:CG1	4:A:137:MET:HB3	2.33	0.53
4:B:284:LYS:O	4:B:288:LEU:HB2	2.09	0.53
1:C:5:DC:H42	3:E:244:DG:H1	1.56	0.53
4:B:139:GLU:HG2	4:B:143:ASN:ND2	2.24	0.53
4:B:271:ILE:HG23	4:B:277:ILE:HD12	1.91	0.53
1:C:1:DA:H5"	4:B:318:VAL:HG11	1.90	0.53
4:B:314:LYS:O	4:B:318:VAL:HG23	2.08	0.52
4:A:247:LEU:HD23	4:A:312:LEU:HD21	1.90	0.52
4:A:265:ASN:ND2	4:A:269:ASN:HD21	2.08	0.52
4:A:286:MET:HG3	4:A:287:GLY:N	2.25	0.52
4:A:7:SER:HA	7:A:349:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:DA:H2"	1:F:10:DG:H5'	1.92	0.52
4:A:304:LEU:N	4:A:304:LEU:HD13	2.25	0.52
1:F:6:DG:C2'	1:F:7:DA:H5"	2.40	0.51
4:A:71:ILE:HD11	4:A:100:PHE:CE1	2.45	0.51
5:C:201:BTB:H82	2:D:135:OMC:HN42	1.75	0.51
4:A:170:SER:HA	4:A:203:ALA:HB2	1.93	0.51
4:B:290:VAL:HG13	4:B:317:LEU:HD12	1.93	0.51
4:B:271:ILE:HG23	4:B:277:ILE:CD1	2.41	0.51
1:F:7:DA:C2'	1:F:8:DT:H5'	2.40	0.51
4:A:294:LEU:HD21	4:A:317:LEU:HD13	1.92	0.51
4:B:168:LEU:HD13	4:B:168:LEU:O	2.11	0.50
1:F:8:DT:H2"	1:F:9:DA:N7	2.25	0.50
1:C:1:DA:H2"	1:C:2:DT:O5'	2.11	0.50
4:B:67:GLY:HA2	4:B:69:GLU:OE1	2.11	0.50
4:A:209:LYS:HD2	4:A:221:ARG:NH2	2.27	0.50
2:G:128:DT:H2"	2:G:129:DT:H5'	1.94	0.50
4:A:30:TRP:CE3	4:A:208:LEU:HD22	2.43	0.50
4:B:286:MET:HG3	4:B:287:GLY:N	2.27	0.50
4:A:294:LEU:O	4:A:297:THR:HG22	2.12	0.50
4:A:262:VAL:HG12	4:A:324:VAL:HG21	1.94	0.50
4:A:195:GLU:OE1	4:A:197:LYS:HE3	2.12	0.50
1:F:15:DG:H2'	1:F:16:DT:H73	1.94	0.49
4:B:95:GLN:NE2	4:B:97:PHE:CZ	2.80	0.49
4:B:290:VAL:O	4:B:294:LEU:HD23	2.13	0.49
4:A:314:LYS:O	4:A:318:VAL:HG13	2.12	0.49
4:B:89:SER:O	4:B:90:ALA:HB3	2.13	0.49
4:A:225:LYS:HD2	4:A:227:LYS:HE2	1.94	0.48
4:A:214:SER:O	4:A:222:VAL:HG23	2.14	0.48
4:A:127:SER:HB2	4:A:129:ASP:OD1	2.13	0.48
4:B:115:ASP:OD1	4:B:148:LYS:HD2	2.13	0.48
4:B:289:THR:O	4:B:293:ILE:HG13	2.13	0.48
4:A:146:LYS:HE2	7:A:356:HOH:O	2.13	0.48
4:B:247:LEU:N	4:B:247:LEU:HD23	2.27	0.48
4:A:316:GLU:O	4:A:320:MET:HG3	2.14	0.48
4:A:165:PRO:HB2	4:A:167:ASP:OD2	2.13	0.48
3:H:243:DC:H2"	3:H:244:DG:C8	2.47	0.48
4:B:254:LEU:HD21	4:B:306:GLN:NE2	2.29	0.48
4:A:178:THR:OG1	4:A:192:TRP:HH2	1.97	0.48
4:B:248:SER:H	4:B:251:ASP:CB	2.26	0.48
4:A:267:VAL:O	4:A:270:VAL:HB	2.13	0.47
4:A:134:ASP:HA	4:A:213:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:55:ARG:NH1	4:A:55:ARG:HG3	2.30	0.47
1:C:2:DT:H5'	4:B:287:GLY:HA3	1.97	0.47
1:C:1:DA:C8	4:B:318:VAL:HG21	2.50	0.47
1:F:11:DT:H1'	1:F:12:DG:H5"	1.95	0.47
4:B:103:PRO:HD3	4:B:112:GLY:O	2.14	0.47
4:B:47:ARG:NH1	4:B:87:GLU:HA	2.30	0.46
4:B:94:TYR:CD2	4:B:123:VAL:HG22	2.50	0.46
4:A:55:ARG:HG3	4:A:55:ARG:HH11	1.80	0.46
4:A:35:LYS:HE3	4:A:227:LYS:HD3	1.97	0.46
4:B:19:LYS:O	4:B:23:LEU:HD13	2.15	0.46
2:D:134:DC:H2"	2:D:135:OMC:C6	2.51	0.46
4:A:299:ARG:HH11	4:A:299:ARG:HG3	1.81	0.46
4:A:68:TYR:O	4:A:70:ILE:N	2.49	0.46
4:A:290:VAL:O	4:A:294:LEU:HD23	2.15	0.46
3:E:240:DT:H2"	3:E:241:DA:C8	2.51	0.46
4:B:248:SER:OG	4:B:251:ASP:HB2	2.16	0.45
4:B:316:GLU:O	4:B:320:MET:HG3	2.16	0.45
2:D:127:DA:H2"	2:D:128:DT:O5'	2.16	0.45
4:A:0:SER:HB2	7:B:368:HOH:O	2.14	0.45
4:A:321:VAL:O	4:A:325:LEU:HB2	2.16	0.45
4:A:33:ARG:HH11	4:A:135:ASP:CG	2.20	0.45
4:A:258:LEU:HD13	4:A:317:LEU:HD12	1.97	0.45
4:A:248:SER:O	4:A:252:ASN:HB2	2.17	0.45
4:A:304:LEU:HD22	4:A:304:LEU:H	1.81	0.45
4:B:313:ILE:HD12	4:B:313:ILE:N	2.32	0.45
1:C:14:DG:H2"	1:C:15:DG:O5'	2.16	0.45
4:B:299:ARG:HH11	4:B:299:ARG:HG3	1.81	0.45
4:B:248:SER:C	4:B:250:ALA:H	2.19	0.45
4:A:1:MET:HE1	4:A:124:THR:HG21	1.99	0.45
4:A:111:TYR:O	4:A:112:GLY:O	2.34	0.45
4:B:72:LEU:O	4:B:76:ALA:HB2	2.17	0.45
4:A:124:THR:HA	4:A:129:ASP:O	2.17	0.45
4:B:250:ALA:HA	4:B:253:LYS:HG2	1.99	0.45
1:F:12:DG:H2"	1:F:13:DG:O5'	2.16	0.45
2:D:130:DG:H2"	2:D:131:DC:O5'	2.17	0.44
4:B:36:ILE:HD13	4:B:117:TYR:CG	2.52	0.44
4:B:309:ASN:C	4:B:311:SER:H	2.20	0.44
4:B:254:LEU:HD21	4:B:306:GLN:HE22	1.82	0.44
2:D:136:DC:H2"	3:E:237:DC:O4'	2.17	0.44
1:F:6:DG:H2"	1:F:7:DA:C5'	2.41	0.44
4:A:101:ALA:O	4:A:114:LYS:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:129:DT:H2"	2:G:130:DG:O5'	2.17	0.44
4:A:135:ASP:OD1	4:A:155:ARG:NH2	2.42	0.44
4:A:86:MET:CE	4:A:93:SER:HA	2.48	0.44
4:A:10:ASN:OD1	4:A:225:LYS:HE3	2.18	0.44
4:A:175:TYR:O	4:A:179:VAL:HG23	2.18	0.44
4:A:159:GLU:N	4:A:159:GLU:OE2	2.47	0.44
4:B:14:SER:HA	4:B:17:ILE:HD12	2.00	0.43
4:B:277:ILE:HG23	4:B:281:ASP:HB2	1.99	0.43
4:B:5:TYR:HB2	4:B:97:PHE:CE2	2.53	0.43
4:A:146:LYS:HA	4:A:184:LEU:CD2	2.48	0.43
4:B:139:GLU:O	4:B:143:ASN:ND2	2.51	0.43
4:B:48:ASP:O	4:B:49:LYS:HB3	2.18	0.43
2:D:129:DT:H2"	2:D:130:DG:OP2	2.18	0.43
4:A:168:LEU:N	4:A:168:LEU:CD1	2.80	0.43
4:B:278:GLY:C	4:B:280:LYS:H	2.21	0.43
4:B:47:ARG:CZ	4:B:87:GLU:HA	2.49	0.43
4:B:85:ILE:C	4:B:85:ILE:HD12	2.39	0.43
4:B:320:MET:O	4:B:324:VAL:HG23	2.18	0.43
4:A:257:ILE:HG22	4:A:258:LEU:N	2.34	0.43
4:B:309:ASN:OD1	4:B:312:LEU:HB3	2.18	0.43
4:B:286:MET:SD	4:B:322:GLN:HG2	2.59	0.43
4:A:99:GLU:OE2	4:A:99:GLU:HA	2.19	0.43
4:B:309:ASN:O	4:B:313:ILE:HD13	2.19	0.42
4:B:286:MET:HB3	4:B:325:LEU:HD12	2.01	0.42
4:A:168:LEU:HD12	4:A:168:LEU:H	1.83	0.42
5:F:202:BTB:H81	2:G:135:OMC:HN42	1.84	0.42
3:E:241:DA:H2"	3:E:242:DT:O5'	2.18	0.42
4:B:215:TRP:CZ3	4:B:221:ARG:HB2	2.55	0.42
1:C:22:DT:H2'	1:C:23:DT:H72	2.01	0.42
4:B:330:ILE:H	4:B:330:ILE:HG13	1.58	0.42
1:F:2:DT:H2"	1:F:3:DT:O5'	2.20	0.42
4:A:86:MET:HE1	4:A:93:SER:HA	2.01	0.42
4:B:169:ASP:HB3	4:B:200:VAL:HG23	2.01	0.42
4:A:49:LYS:HE2	4:A:51:THR:OG1	2.20	0.42
6:E:236:AMP:H2'	4:A:119:PHE:CZ	2.55	0.42
3:E:237:DC:H2'	3:E:238:DA:C8	2.55	0.42
4:A:100:PHE:HE1	4:A:114:LYS:HB3	1.84	0.42
4:B:298:SER:C	4:B:300:GLU:H	2.22	0.42
2:G:135:OMC:HM22	2:G:136:DC:H5'	2.00	0.42
4:B:286:MET:CE	4:B:318:VAL:HG13	2.49	0.42
1:C:23:DT:H2"	1:C:24:DG:H5"	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:33:ARG:NH1	4:A:135:ASP:OD1	2.51	0.42
1:C:18:DG:OP1	1:C:18:DG:H4'	2.20	0.42
4:B:302:ILE:HD12	4:B:302:ILE:H	1.85	0.42
1:C:18:DG:H2"	1:C:19:DC:C5'	2.50	0.42
4:A:146:LYS:HD2	4:A:146:LYS:N	2.35	0.41
1:C:9:DA:C3'	1:C:10:DG:H5"	2.47	0.41
4:A:29:GLU:HG2	4:A:29:GLU:H	1.57	0.41
5:C:201:BTB:C8	2:D:135:OMC:HN42	2.32	0.41
4:A:146:LYS:CE	7:A:356:HOH:O	2.68	0.41
4:A:129:ASP:OD1	4:A:129:ASP:N	2.52	0.41
4:A:331:GLU:O	4:A:332:LEU:HD23	2.20	0.41
2:D:135:OMC:HM22	2:D:136:DC:H5'	2.02	0.41
4:B:71:ILE:HD13	4:B:116:PHE:HB2	2.02	0.41
4:A:251:ASP:CB	4:A:308:ASP:HB3	2.50	0.41
4:A:10:ASN:HA	4:A:225:LYS:HG3	2.02	0.41
4:B:143:ASN:OD1	4:B:185:VAL:HA	2.21	0.41
4:A:95:GLN:HG2	4:A:97:PHE:CE1	2.55	0.41
4:B:12:TYR:O	4:B:14:SER:N	2.53	0.41
3:H:246:DA:C2'	3:H:247:DA:H5'	2.45	0.41
4:B:286:MET:HE3	4:B:318:VAL:HG13	2.03	0.41
4:B:91:VAL:HG13	4:B:123:VAL:HG13	2.03	0.41
4:A:68:TYR:C	4:A:70:ILE:N	2.74	0.41
1:C:18:DG:H2'	1:C:19:DC:C6	2.56	0.41
4:B:212:TYR:HA	4:B:213:PRO:HD2	1.90	0.41
4:B:133:VAL:HG13	4:B:137:MET:CB	2.46	0.41
2:G:127:DA:H2"	2:G:128:DT:OP2	2.21	0.41
4:B:178:THR:OG1	4:B:192:TRP:HH2	2.02	0.41
4:B:216:LEU:HB2	4:B:220:ASN:HB2	2.02	0.41
4:A:214:SER:OG	4:A:222:VAL:HG21	2.21	0.41
4:B:146:LYS:HA	4:B:184:LEU:CD2	2.51	0.40
4:A:326:ARG:HB3	4:A:327:PRO:CD	2.40	0.40
4:A:72:LEU:HD12	4:A:72:LEU:HA	1.86	0.40
4:A:14:SER:O	4:A:18:GLU:HG2	2.21	0.40
4:B:173:GLN:HB2	7:B:344:HOH:O	2.19	0.40
4:B:25:LEU:C	4:B:27:GLY:H	2.25	0.40
1:C:22:DT:C6	1:C:23:DT:H72	2.57	0.40
4:A:31:VAL:HG23	4:A:155:ARG:HG3	2.02	0.40
4:A:166:ASN:OD1	4:A:228:ASN:HA	2.21	0.40
4:A:107:LYS:O	4:A:108:ASN:HB2	2.21	0.40
4:A:30:TRP:CZ2	4:A:210:PRO:HG3	2.57	0.40
4:A:215:TRP:CZ3	4:A:221:ARG:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:96:VAL:HG13	4:A:121:ILE:HG12	2.01	0.40
4:A:16:PHE:HA	4:A:19:LYS:HD3	2.02	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
4	A	315/335 (94%)	283 (90%)	29 (9%)	3 (1%)	19 34
4	B	315/335 (94%)	268 (85%)	40 (13%)	7 (2%)	8 13
All	All	630/670 (94%)	551 (88%)	69 (11%)	10 (2%)	12 21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	197	LYS
4	A	112	GLY
4	A	69	GLU
4	B	13	ASN
4	B	63	GLU
4	A	274	ILE
4	B	213	PRO
4	B	217	ARG
4	B	310	PRO
4	B	327	PRO

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	
4	A	277/293 (94%)	260 (94%)	17 (6%)	23	42
4	B	278/293 (95%)	258 (93%)	20 (7%)	18	33
All	All	555/586 (95%)	518 (93%)	37 (7%)	20	37

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	TYR
4	A	47	ARG
4	A	55	ARG
4	A	69	GLU
4	A	100	PHE
4	A	115	ASP
4	A	127	SER
4	A	129	ASP
4	A	162	ILE
4	A	166	ASN
4	A	168	LEU
4	A	173	GLN
4	A	208	LEU
4	A	280	LYS
4	A	300	GLU
4	A	304	LEU
4	A	325	LEU
4	B	29	GLU
4	B	47	ARG
4	B	49	LYS
4	B	69	GLU
4	B	80	LYS
4	B	106	GLN
4	B	120	ASP
4	B	135	ASP
4	B	155	ARG
4	B	162	ILE
4	B	168	LEU
4	B	186	ASP
4	B	193	ASN
4	B	230	LYS
4	B	247	LEU
4	B	253	LYS

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Mol	Chain	Res	Type
4	B	254	LEU
4	B	288	LEU
4	B	316	GLU
4	B	325	LEU

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

Mol	Chain	Res	Type
4	A	193	ASN
4	A	220	ASN
4	A	228	ASN
4	A	265	ASN
4	A	268	ASN
4	A	322	GLN
4	B	106	GLN
4	B	173	GLN
4	B	193	ASN
4	B	228	ASN
4	B	268	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	OMC	D	135	1,2	13,22,23	0.79	0	20,31,34	1.12	1 (5%)
2	OMC	G	135	1,2	13,22,23	0.85	1 (7%)	20,31,34	1.08	1 (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
2	OMC	D	135	1,2	-	0/5/27/28	0/2/2/2
2	OMC	G	135	1,2	-	0/5/27/28	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	135	OMC	C6-C5	-2.24	1.33	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	135	OMC	C2-N3-C4	3.02	119.88	115.61
2	G	135	OMC	C2-N3-C4	3.11	120.00	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	135	OMC	5	0
2	G	135	OMC	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
5	BTB	A	335	-	12,13,13	1.71	1 (8%)	8,16,16	2.27	2 (25%)
5	BTB	C	201	-	12,13,13	1.77	1 (8%)	8,16,16	2.24	2 (25%)
6	AMP	E	236	3	20,25,25	1.61	3 (15%)	22,38,38	2.57	5 (22%)
5	BTB	F	202	-	12,13,13	1.67	1 (8%)	8,16,16	2.20	2 (25%)
6	AMP	H	236	3	20,25,25	1.71	3 (15%)	22,38,38	2.53	4 (18%)

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
5	BTB	A	335	-	-	0/21/21/21	0/0/0/0
5	BTB	C	201	-	-	0/21/21/21	0/0/0/0
6	AMP	E	236	3	-	0/6/26/26	0/3/3/3
5	BTB	F	202	-	-	0/21/21/21	0/0/0/0
6	AMP	H	236	3	-	0/6/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	236	AMP	C2-N1	3.26	1.40	1.33
6	E	236	AMP	C2-N1	3.47	1.40	1.33
6	E	236	AMP	C4-N3	3.85	1.41	1.35
6	E	236	AMP	C2-N3	3.92	1.39	1.32
6	H	236	AMP	C4-N3	4.16	1.41	1.35
6	H	236	AMP	C2-N3	4.78	1.40	1.32
5	A	335	BTB	C5-N	5.15	1.55	1.48
5	F	202	BTB	C5-N	5.17	1.56	1.48
5	C	201	BTB	C5-N	5.41	1.56	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	236	AMP	N3-C2-N1	-10.82	120.61	128.89
6	H	236	AMP	N3-C2-N1	-10.66	120.73	128.89
5	A	335	BTB	O3-C3-C2	-2.51	105.07	111.12
6	E	236	AMP	C4'-O4'-C1'	-2.39	107.09	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	202	BTB	O3-C3-C2	-2.31	105.54	111.12
5	C	201	BTB	O3-C3-C2	-2.28	105.62	111.12
6	E	236	AMP	C4-C5-N7	-2.20	107.46	109.48
6	H	236	AMP	C4-C5-N7	-2.01	107.63	109.48
6	E	236	AMP	C1'-N9-C4	2.00	129.96	126.94
6	E	236	AMP	O2'-C2'-C3'	2.08	118.60	111.83
6	H	236	AMP	O2'-C2'-C3'	2.21	119.00	111.83
6	H	236	AMP	C1'-N9-C4	2.26	130.34	126.94
5	F	202	BTB	C7-N-C2	4.98	128.25	113.86
5	A	335	BTB	C7-N-C2	5.06	128.49	113.86
5	C	201	BTB	C7-N-C2	5.07	128.51	113.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	201	BTB	2	0
6	E	236	AMP	1	0
5	F	202	BTB	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	C	24/24 (100%)	0.17	2 (8%) 14 15	64, 111, 138, 140	0
1	F	24/24 (100%)	-0.29	0 100 100	56, 85, 140, 157	0
2	D	11/12 (91%)	0.39	0 100 100	50, 118, 134, 141	0
2	G	11/12 (91%)	0.05	1 (9%) 11 12	51, 82, 89, 95	0
3	E	12/12 (100%)	0.04	1 (8%) 14 15	67, 115, 140, 150	0
3	H	12/12 (100%)	-0.25	1 (8%) 14 15	60, 127, 146, 151	0
4	A	319/335 (95%)	0.33	16 (5%) 32 37	22, 53, 107, 129	0
4	B	319/335 (95%)	0.49	21 (6%) 22 24	27, 59, 123, 141	0
All	All	732/766 (95%)	0.35	42 (5%) 27 31	22, 60, 127, 157	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	302	ILE	6.2
4	B	277	ILE	5.9
4	B	25	LEU	5.8
4	A	247	LEU	5.6
4	A	313	ILE	5.5
4	B	308	ASP	5.5
1	C	1	DA	5.0
4	B	249	GLU	4.9
4	A	250	ALA	4.5
4	B	258	LEU	4.3
4	B	317	LEU	4.1
4	B	254	LEU	4.1
4	B	304	LEU	3.9
4	B	307	ALA	3.9
3	E	248	DT	3.4
4	B	290	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
4	B	293	ILE	3.1
2	G	125	DC	2.9
4	B	334	SER	2.9
4	B	224	ILE	2.9
4	B	219	GLY	2.8
4	A	255	VAL	2.8
1	C	19	DC	2.7
4	A	286	MET	2.7
4	A	258	LEU	2.6
4	A	8	LEU	2.5
4	A	246	GLU	2.5
4	B	291	GLN	2.5
4	A	251	ASP	2.4
4	A	302	ILE	2.4
4	B	105	ILE	2.4
4	A	307	ALA	2.4
4	A	108	ASN	2.4
4	A	16	PHE	2.3
4	B	251	ASP	2.3
4	B	257	ILE	2.3
3	H	248	DT	2.3
4	B	329	TRP	2.2
4	A	254	LEU	2.1
4	A	20	LEU	2.1
4	B	195	GLU	2.1
4	A	317	LEU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	OMC	D	135	21/22	0.95	0.14	-	39,46,53,59	0
2	OMC	G	135	21/22	0.94	0.15	-	33,41,49,52	0

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
5	BTB	F	202	14/14	0.72	0.47	11.45	96,108,113,114	0
5	BTB	C	201	14/14	0.68	0.46	7.63	111,116,118,119	0
5	BTB	A	335	14/14	0.82	0.29	1.93	119,124,127,129	0
6	AMP	E	236	23/23	0.97	0.17	-0.12	37,43,63,67	0
6	AMP	H	236	23/23	0.97	0.16	-0.34	26,37,59,63	0

6.5 Other polymers (i)

There are no such residues in this entry.