



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:25 AM UTC

PDB ID : 2HVS / pdb_00002hvs
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

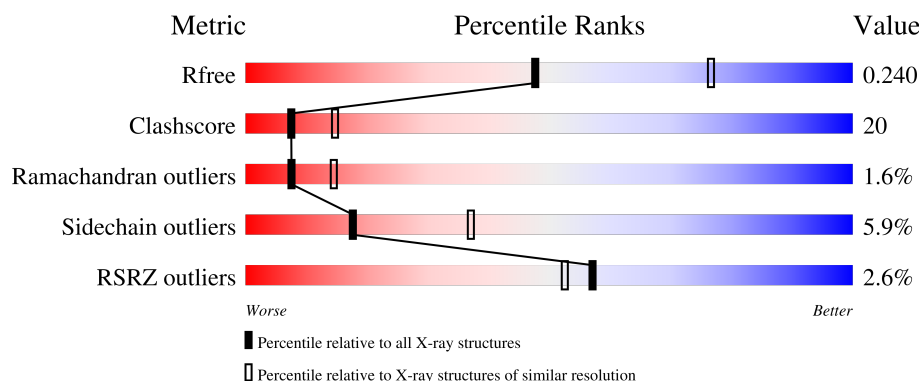
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	24	38% 63%
1	F	24	42% 54% .
2	D	12	17% 83%
2	G	12	17% 83%
3	E	12	42% 58%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	H	12	8% 25% 75%
4	A	335	2% 56% 34% 5%
4	B	335	3% 57% 33% 5% 5%

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*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			

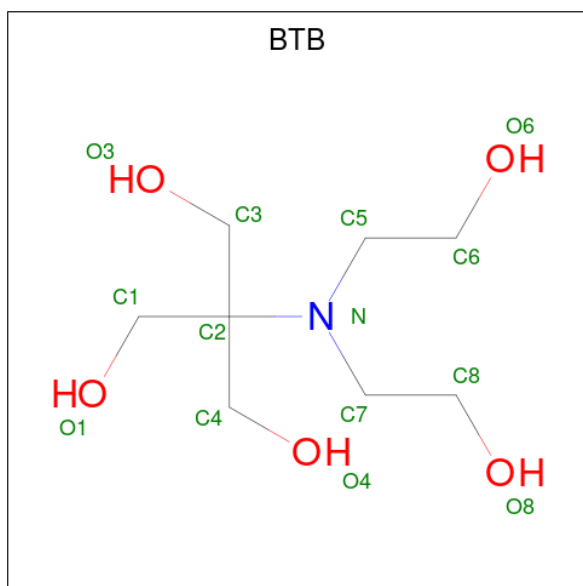
- Molecule 4 is a protein called T4 RNA Ligase 2.

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:

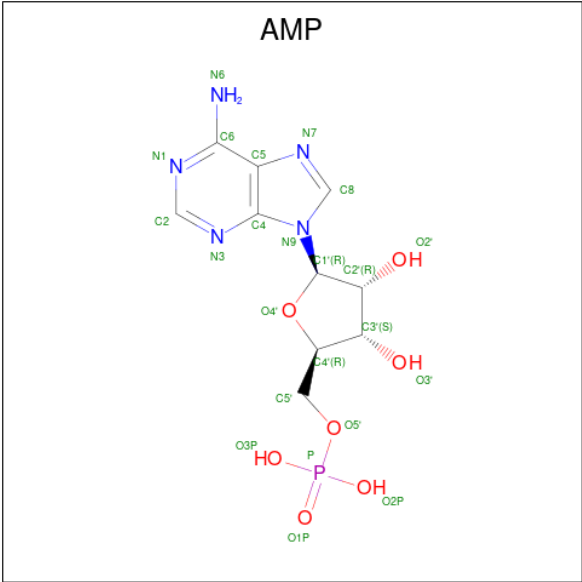
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	cloning artifact	UNP P32277
A	112	GLY	CYS	SEE REMARK 999	UNP P32277
B	0	SER	-	cloning artifact	UNP P32277
B	112	GLY	CYS	SEE REMARK 999	UNP P32277

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (CCD ID: 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 (CCD ID: 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		

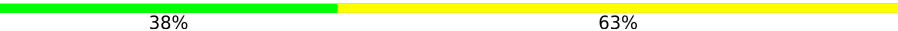
- Molecule 7 is water.

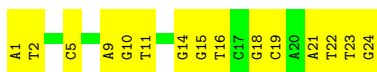
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	O	0	0
			1	1		
7	E	1	Total	O	0	0
			1	1		
7	A	59	Total	O	0	0
			59	59		
7	B	37	Total	O	0	0
			37	37		

3 Residue-property plots

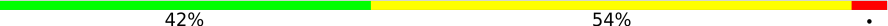
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

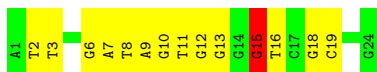
- Molecule 1: 5'-D(*AP*TP*TP*CP*CP*GP*AP*TP*AP*GP*TP*GP*GP*GP*GP*TP*CP*GP*CP*AP*AP*TP*TP*G)-3'

Chain C:  38% 63%



- 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'

Chain F:  42% 54% .



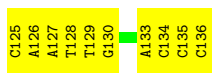
- Molecule 2: 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'

Chain D:  17% 83%

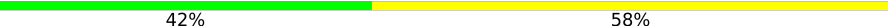


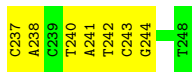
- Molecule 2: 5'-D(*CP*AP*AP*TP*TP*GP*CP*GP*AP*C)-R(P*(OMC)P*C)-3'

Chain G:  17% 83%

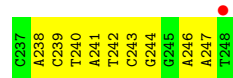


- Molecule 3: 5'-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'

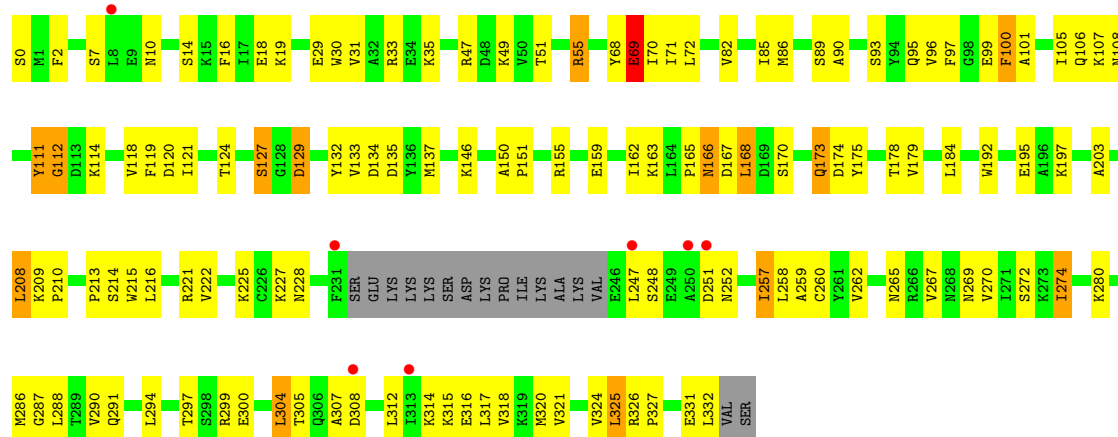
Chain E:  42% 58%



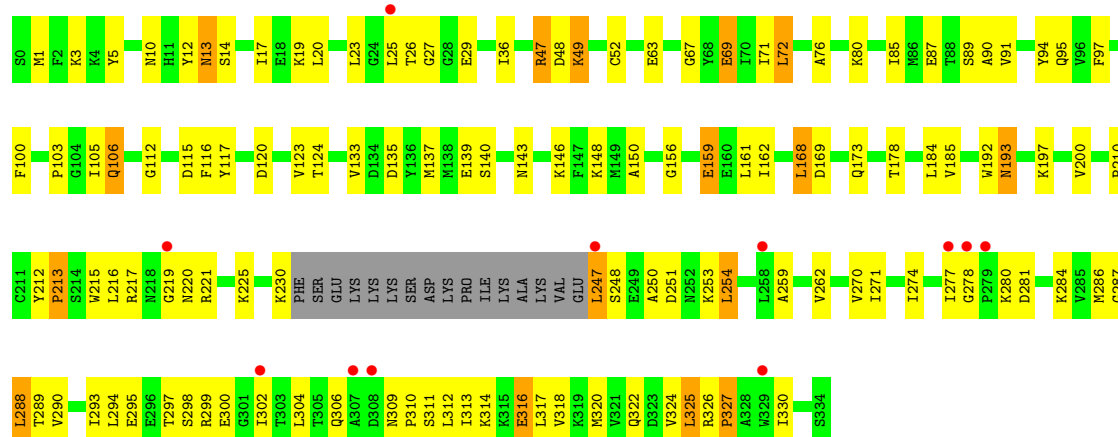
- Molecule 3: 5'-D(P*CP*AP*CP*TP*AP*TP*CP*GP*GP*AP*AP*T)-3'



• Molecule 4: T4 RNA Ligase 2



• Molecule 4: T4 RNA Ligase 2



4 Data and refinement statistics

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 19.82 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.82-2.50) 98.1 (19.82-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.283 0.246 , 0.240	Depositor DCC
R_{free} test set	1926 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7188	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: BTB, AMP, OMC

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	0.67	0/855
1	F	0.29	0/554	0.67	1/855 (0.1%)
2	D	0.27	0/246	0.55	0/377
2	G	0.31	0/246	0.70	0/377
3	E	0.33	0/274	0.65	0/420
3	H	0.34	0/274	0.58	0/420
4	A	0.49	0/2570	0.91	3/3472 (0.1%)
4	B	0.47	0/2570	0.90	2/3471 (0.1%)
All	All	0.44	0/7288	0.83	6/10247 (0.1%)

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.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	111	TYR	N-CA-C	-7.09	100.31	110.59
4	B	72	LEU	N-CA-C	-7.05	103.65	111.82
4	B	150	ALA	N-CA-C	-5.41	99.65	109.44
4	A	118	VAL	N-CA-C	5.29	115.91	109.30
4	A	100	PHE	N-CA-C	-5.21	101.28	109.25
1	F	15	DG	N9-C1'-C2'	-5.13	105.80	113.50

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

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	103	0
4	B	2521	0	2517	96	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	270	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 20.

All (270) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:86:MET:HE1	4:A:93:SER:HA	1.70	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
1:C:22:DT:H2'	1:C:23:DT:H71	1.70	0.73
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:A:10:ASN:CG	4:A:225:LYS:HE3	2.19	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
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
4:A:69:GLU:CD	4:A:69:GLU:H	2.06	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:E:243:DC:H2''	3:E:244:DG:C8	2.38	0.59
4:B:1:MET:HE2	4:B:124:THR:HG21	1.85	0.59
4:B:159:GLU:H	4:B:159:GLU:CD	2.09	0.59
2:G:125:DC:H2''	2:G:126:DA:C8	2.37	0.58
1:F:18:DG:H2'	1:F:19:DC:C6	2.39	0.58
4:B:69:GLU:HA	4:B:72:LEU:HD23	1.84	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: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:A:159:GLU:O	4:A:163:LYS:HE3	2.07	0.55
4:B:193:ASN:H	4:B:193:ASN:HD22	1.54	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
1:F:18:DG:H4'	1:F:18:DG:OP1	2.07	0.54
3:H:240:DT:H2''	3:H:241:DA:C8	2.42	0.54
4:A:215:TRP:O	4:A:216:LEU:HD23	2.06	0.54
4:A:82:VAL:O	4:A:85:ILE:HG13	2.08	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:173:GLN:HG2	4:A:174:ASP:N	2.22	0.53
4:A:286:MET:HE1	4:A:318:VAL:HB	1.91	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
1:F:9:DA:H2''	1:F:10:DG:H5'	1.92	0.52
4:A:304:LEU:HD13	4:A:304:LEU:N	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:271:ILE:HG23	4:B:277:ILE:CD1	2.41	0.51
4:B:290:VAL:HG13	4:B:317:LEU:HD12	1.93	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
2:G:128:DT:H2''	2:G:129:DT:H5'	1.94	0.50
4:A:209:LYS:HD2	4:A:221:ARG:NH2	2.27	0.50
4:B:67:GLY:HA2	4:B:69:GLU:OE1	2.11	0.50
4:A:33:ARG:HH11	4:A:135:ASP:CG	2.20	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:195:GLU:OE1	4:A:197:LYS:HE3	2.12	0.50
4:A:262:VAL:HG12	4:A:324:VAL:HG21	1.94	0.50
4:A:294:LEU:O	4:A:297:THR:HG22	2.12	0.50
4:B:248:SER:C	4:B:250:ALA:H	2.19	0.49
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:309:ASN:C	4:B:311:SER:H	2.20	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:B:290:VAL:O	4:B:294:LEU:HD23	2.13	0.49
4:A:127:SER:HB2	4:A:129:ASP:OD1	2.13	0.48
4:A:214:SER:O	4:A:222:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:225:LYS:HD2	4:A:227:LYS:HE2	1.94	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:A:316:GLU:O	4:A:320:MET:HG3	2.14	0.48
4:B:247:LEU:N	4:B:247:LEU:HD23	2.27	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:85:ILE:HD12	4:B:85:ILE:C	2.39	0.48
4:B:248:SER:H	4:B:251:ASP:CB	2.26	0.48
4:B:278:GLY:C	4:B:280:LYS:H	2.21	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
4:A:55:ARG:NH1	4:A:55:ARG:HG3	2.30	0.47
1:C:1:DA:C8	4:B:318:VAL:HG21	2.50	0.47
1:C:2:DT:H5'	4:B:287:GLY:HA3	1.97	0.47
1:F:11:DT:H1'	1:F:12:DG:H5''	1.95	0.47
4:B:298:SER:C	4:B:300:GLU:H	2.22	0.47
1:C:1:DA:O4'	4:B:286:MET:HE2	2.15	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:68:TYR:O	4:A:70:ILE:N	2.49	0.46
4:A:299:ARG:HG3	4:A:299:ARG:HH11	1.81	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:68:TYR:C	4:A:70:ILE:N	2.74	0.45
4:A:321:VAL:O	4:A:325:LEU:HB2	2.16	0.45
4:B:25:LEU:C	4:B:27:GLY:H	2.25	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:304:LEU:H	4:A:304:LEU:HD22	1.81	0.45
1:C:14:DG:H2''	1:C:15:DG:O5'	2.16	0.45
4:A:111:TYR:O	4:A:112:GLY:O	2.34	0.45
4:B:259:ALA:HB1	4:B:320:MET:HE1	1.97	0.45
4:B:299:ARG:HH11	4:B:299:ARG:HG3	1.81	0.45
4:B:313:ILE:N	4:B:313:ILE:HD12	2.32	0.45
4:A:124:THR:HA	4:A:129:ASP:O	2.17	0.45
4:B:72:LEU:O	4:B:76:ALA:HB2	2.17	0.45
1:F:12:DG:H2''	1:F:13:DG:O5'	2.16	0.45
4:B:192:TRP:H	4:B:192:TRP:CD1	2.34	0.45
4:B:250:ALA:HA	4:B:253:LYS:HG2	1.99	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: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
2:G:129:DT:H2''	2:G:130:DG:O5'	2.17	0.44
4:A:101:ALA:O	4:A:114:LYS:HA	2.18	0.44
4:A:135:ASP:OD1	4:A:155:ARG:NH2	2.42	0.44
4:A:175:TYR:O	4:A:179:VAL:HG23	2.18	0.44
4:A:2:PHE:CD2	4:A:2:PHE:C	2.96	0.44
4:A:159:GLU:OE2	4:A:159:GLU:N	2.47	0.44
4:A:120:ASP:CG	4:A:221:ARG:HH12	2.25	0.43
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:A:146:LYS:HA	4:A:184:LEU:CD2	2.48	0.43
4:B:5:TYR:HB2	4:B:97:PHE:CE2	2.53	0.43
4:B:48:ASP:O	4:B:49:LYS:HB3	2.18	0.43
4:B:139:GLU:O	4:B:143:ASN:ND2	2.51	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:47:ARG:CZ	4:B:87:GLU:HA	2.49	0.43
4:A:68:TYR:O	4:A:69:GLU:C	2.61	0.43
4:B:210:PRO:C	4:B:212:TYR:N	2.75	0.43
4:B:320:MET:O	4:B:324:VAL:HG23	2.18	0.43
4:A:99:GLU:OE2	4:A:99:GLU:HA	2.19	0.43
4:A:257:ILE:HG22	4:A:258:LEU:N	2.34	0.43
4:B:286:MET:SD	4:B:322:GLN:HG2	2.59	0.43
4:B:309:ASN:OD1	4:B:312:LEU:HB3	2.18	0.43
4:A:305:THR:C	4:A:307:ALA:H	2.27	0.43
4:B:137:MET:HE3	4:B:140:SER:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:286:MET:HB3	4:B:325:LEU:HD12	2.01	0.42
4:B:309:ASN:O	4:B:313:ILE:HD13	2.19	0.42
4:A:168:LEU:HD12	4:A:168:LEU:H	1.83	0.42
3:E:241:DA:H2''	3:E:242:DT:O5'	2.18	0.42
5:F:202:BTB:H81	2:G:135:OMC:HN42	1.84	0.42
4:B:215:TRP:CZ3	4:B:221:ARG:HB2	2.55	0.42
1:F:2:DT:H2''	1:F:3:DT:O5'	2.20	0.42
4:A:150:ALA:O	4:A:151:PRO:C	2.62	0.42
4:B:330:ILE:H	4:B:330:ILE:HG13	1.58	0.42
4:B:169:ASP:HB3	4:B:200:VAL:HG23	2.01	0.42
6:E:236:AMP:H2'	4:A:119:PHE:CZ	2.55	0.42
4:A:49:LYS:HE2	4:A:51:THR:OG1	2.20	0.42
4:A:272:SER:C	4:A:274:ILE:H	2.27	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
1:C:18:DG:OP1	1:C:18:DG:H4'	2.20	0.42
1:C:23:DT:H2''	1:C:24:DG:H5''	2.02	0.42
2:G:135:OMC:HM22	2:G:136:DC:H5'	2.00	0.42
4:A:10:ASN:OD1	4:A:225:LYS:HE3	2.18	0.42
4:A:33:ARG:NH1	4:A:135:ASP:OD1	2.51	0.42
4:B:286:MET:CE	4:B:318:VAL:HG13	2.49	0.42
4:B:286:MET:HE1	4:B:318:VAL:HG13	2.02	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:N	4:A:146:LYS:HD2	2.35	0.41
1:C:9:DA:C3'	1:C:10:DG:H5''	2.47	0.41
4:A:29:GLU:H	4:A:29:GLU:HG2	1.57	0.41
5:C:201:BTB:C8	2:D:135:OMC:HN42	2.32	0.41
4:A:129:ASP:OD1	4:A:129:ASP:N	2.52	0.41
4:A:146:LYS:CE	7:A:356:HOH:O	2.68	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:A:105:ILE:C	4:A:106:GLN:HG2	2.44	0.41
4:B:71:ILE:HD13	4:B:116:PHE:HB2	2.02	0.41
4:A:10:ASN:HA	4:A:225:LYS:HG3	2.02	0.41
4:A:95:GLN:HG2	4:A:97:PHE:CE1	2.55	0.41
4:A:251:ASP:CB	4:A:308:ASP:HB3	2.50	0.41
4:B:143:ASN:OD1	4:B:185:VAL:HA	2.21	0.41
4:A:259:ALA:CB	4:A:320:MET:HE1	2.50	0.41
4:B:12:TYR:O	4:B:14:SER:N	2.53	0.41
1:C:18:DG:H2'	1:C:19:DC:C6	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:246:DA:C2'	3:H:247:DA:H5'	2.45	0.41
4:B:91:VAL:HG13	4:B:123:VAL:HG13	2.03	0.41
4:B:212:TYR:HA	4:B:213:PRO:HD2	1.90	0.41
2:G:127:DA:H2''	2:G:128:DT:OP2	2.21	0.41
4:B:133:VAL:HG13	4:B:137:MET:CB	2.46	0.41
4:B:178:THR:OG1	4:B:192:TRP:HH2	2.02	0.41
4:A:214:SER:OG	4:A:222:VAL:HG21	2.21	0.41
4:B:216:LEU:HB2	4:B:220:ASN:HB2	2.02	0.41
4:B:146:LYS:HA	4:B:184:LEU:CD2	2.51	0.40
4:A:14:SER:O	4:A:18:GLU:HG2	2.21	0.40
4:A:72:LEU:HD12	4:A:72:LEU:HA	1.86	0.40
4:A:326:ARG:HB3	4:A:327:PRO:CD	2.40	0.40
4:B:173:GLN:HB2	7:B:344:HOH:O	2.19	0.40
4:A:31:VAL:HG23	4:A:155:ARG:HG3	2.02	0.40
4:A:107:LYS:O	4:A:108:ASN:HB2	2.21	0.40
4:A:166:ASN:OD1	4:A:228:ASN:HA	2.21	0.40
4:A:30:TRP:CZ2	4:A:210:PRO:HG3	2.57	0.40
4:A:96:VAL:HG13	4:A:121:ILE:HG12	2.01	0.40
4:A:215:TRP:CZ3	4:A:221:ARG:HB2	2.56	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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	315/335 (94%)	283 (90%)	29 (9%)	3 (1%)	12 24
4	B	315/335 (94%)	268 (85%)	40 (13%)	7 (2%)	5 9
All	All	630/670 (94%)	551 (88%)	69 (11%)	10 (2%)	7 14

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 ⓘ

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%)	262 (95%)	15 (5%)	20	41
4	B	278/293 (95%)	260 (94%)	18 (6%)	15	32
All	All	555/586 (95%)	522 (94%)	33 (6%)	18	37

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	47	ARG
4	A	55	ARG
4	A	69	GLU
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	257	ILE
4	A	280	LYS
4	A	300	GLU
4	A	304	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	159	GLU
4	B	162	ILE
4	B	168	LEU
4	B	193	ASN
4	B	230	LYS
4	B	247	LEU
4	B	254	LEU
4	B	288	LEU
4	B	316	GLU
4	B	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	40	ASN
4	A	220	ASN
4	A	228	ASN
4	A	265	ASN
4	A	268	ASN
4	A	269	ASN
4	A	306	GLN
4	A	322	GLN
4	B	106	GLN
4	B	143	ASN
4	B	173	GLN
4	B	181	HIS
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	G	135	1,2	19,22,23	0.65	0	25,31,34	0.71	0
2	OMC	D	135	1,2	19,22,23	0.61	0	25,31,34	0.80	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
2	OMC	G	135	1,2	-	0/9/27/28	0/2/2/2
2	OMC	D	135	1,2	-	1/9/27/28	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	135	OMC	C3'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 8 short contacts:

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

Continued on next page...

Continued from previous page...

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	C	201	-	13,13,13	2.43	3 (23%)	7,16,16	1.92	3 (42%)
6	AMP	E	236	3	25,25,25	1.45	3 (12%)	37,38,38	1.94	9 (24%)
5	BTB	F	202	-	13,13,13	2.26	2 (15%)	7,16,16	1.87	3 (42%)
5	BTB	A	335	-	13,13,13	2.36	2 (15%)	7,16,16	1.90	3 (42%)
6	AMP	H	236	3	25,25,25	1.53	3 (12%)	37,38,38	1.96	9 (24%)

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	C	201	-	-	5/21/21/21	-
6	AMP	E	236	3	-	0/10/26/26	0/3/3/3
5	BTB	F	202	-	-	6/21/21/21	-
5	BTB	A	335	-	-	7/21/21/21	-
6	AMP	H	236	3	-	1/10/26/26	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	201	BTB	C5-N	5.92	1.56	1.48
5	F	202	BTB	C5-N	5.66	1.56	1.48
5	C	201	BTB	C2-N	5.66	1.59	1.48
5	A	335	BTB	C5-N	5.65	1.55	1.48
5	A	335	BTB	C2-N	5.48	1.59	1.48
5	F	202	BTB	C2-N	5.11	1.58	1.48
6	H	236	AMP	C4-N3	3.93	1.41	1.34
6	H	236	AMP	C2-N3	3.78	1.40	1.33
6	E	236	AMP	C2-N1	3.69	1.40	1.33
6	E	236	AMP	C4-N3	3.68	1.41	1.34
6	H	236	AMP	C2-N1	3.47	1.40	1.33
6	E	236	AMP	C2-N3	2.92	1.39	1.33
5	C	201	BTB	C7-N	2.01	1.50	1.48

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	236	AMP	C5-C4-N3	-5.35	119.34	126.72
6	E	236	AMP	C5-C4-N3	-5.31	119.41	126.72
6	E	236	AMP	N3-C2-N1	-5.27	120.61	128.58
6	H	236	AMP	N3-C2-N1	-5.19	120.73	128.58
6	E	236	AMP	N3-C4-N9	3.75	133.54	127.17
6	H	236	AMP	N3-C4-N9	3.73	133.50	127.17
6	E	236	AMP	C2-N3-C4	3.54	120.47	111.83
6	H	236	AMP	C2-N3-C4	3.48	120.32	111.83
6	H	236	AMP	C5-N7-C8	3.44	108.86	103.45
6	E	236	AMP	C5-N7-C8	3.26	108.58	103.45
6	H	236	AMP	N9-C8-N7	-3.20	109.40	113.94
5	C	201	BTB	C8-C7-N	2.81	122.54	111.59
6	E	236	AMP	N9-C8-N7	-2.74	110.04	113.94
6	E	236	AMP	C4-C5-N7	-2.73	107.46	110.58
5	A	335	BTB	O3-C3-C2	-2.69	105.07	111.40
5	A	335	BTB	C8-C7-N	2.66	121.95	111.59
5	F	202	BTB	C8-C7-N	2.60	121.73	111.59
6	H	236	AMP	C4-C5-N7	-2.59	107.63	110.58
5	F	202	BTB	O3-C3-C2	-2.49	105.54	111.40
5	C	201	BTB	O3-C3-C2	-2.46	105.62	111.40
5	C	201	BTB	C6-C5-N	2.38	120.87	111.59
5	F	202	BTB	C6-C5-N	2.33	120.68	111.59
6	H	236	AMP	O2'-C2'-C3'	2.24	119.00	111.82
5	A	335	BTB	C6-C5-N	2.14	119.94	111.59
6	E	236	AMP	O2'-C2'-C3'	2.12	118.60	111.82
6	H	236	AMP	C6-C5-C4	2.05	119.97	117.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	E	236	AMP	C6-C5-C4	2.03	119.95	117.18

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	201	BTB	C1-C2-N-C7
5	C	201	BTB	C3-C2-N-C7
5	C	201	BTB	C4-C2-N-C7
5	F	202	BTB	O1-C1-C2-C4
5	F	202	BTB	C1-C2-N-C7
5	F	202	BTB	C3-C2-N-C7
5	F	202	BTB	C4-C2-N-C7
5	A	335	BTB	O1-C1-C2-C3
5	A	335	BTB	O1-C1-C2-C4
5	A	335	BTB	O1-C1-C2-N
5	A	335	BTB	C1-C2-N-C7
5	A	335	BTB	C3-C2-N-C7
5	A	335	BTB	C4-C2-N-C7
5	A	335	BTB	N-C5-C6-O6
5	C	201	BTB	N-C7-C8-O8
5	C	201	BTB	N-C5-C6-O6
5	F	202	BTB	O1-C1-C2-C3
5	F	202	BTB	O1-C1-C2-N
6	H	236	AMP	O4'-C1'-N9-C8

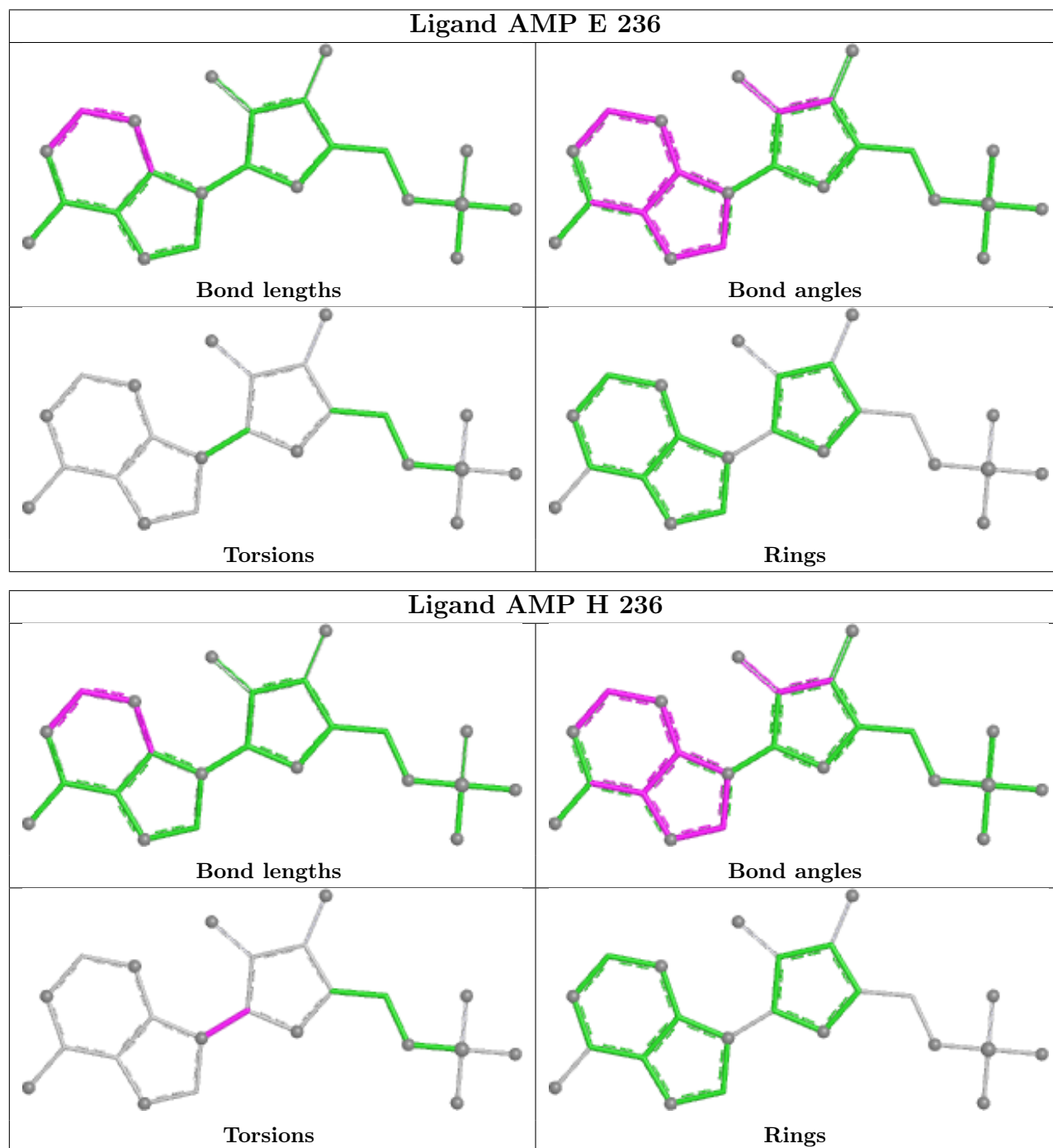
There are no ring outliers.

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	C	24/24 (100%)	0.46	0	100	100	64, 111, 138, 140	0
1	F	24/24 (100%)	0.11	0	100	100	56, 85, 140, 157	0
2	D	11/12 (91%)	0.27	0	100	100	50, 118, 134, 141	0
2	G	11/12 (91%)	-0.05	0	100	100	51, 82, 89, 94	0
3	E	12/12 (100%)	0.32	0	100	100	67, 115, 140, 150	0
3	H	12/12 (100%)	0.44	1 (8%)	17	15	60, 127, 146, 151	0
4	A	319/335 (95%)	-0.12	7 (2%)	62	58	22, 53, 107, 129	0
4	B	319/335 (95%)	0.01	11 (3%)	48	43	27, 59, 123, 141	0
All	All	732/766 (95%)	-0.01	19 (2%)	57	52	22, 60, 127, 157	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	247	LEU	4.0
4	A	313	ILE	3.2
4	B	277	ILE	3.0
4	B	25	LEU	3.0
4	B	278	GLY	2.8
4	B	219	GLY	2.6
4	B	258	LEU	2.5
4	A	251	ASP	2.5
4	A	250	ALA	2.4
4	B	279	PRO	2.4
4	A	231	PHE	2.3
4	B	308	ASP	2.3
4	A	247	LEU	2.2
4	B	329	TRP	2.2
4	A	8	LEU	2.2
4	B	307	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	248	DT	2.1
4	A	308	ASP	2.1
4	B	302	ILE	2.0

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OMC	D	135	21/22	0.93	0.08	39,46,53,59	0
2	OMC	G	135	21/22	0.95	0.08	33,41,49,52	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

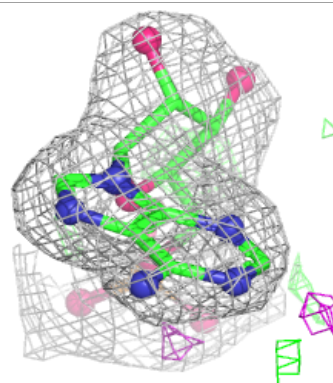
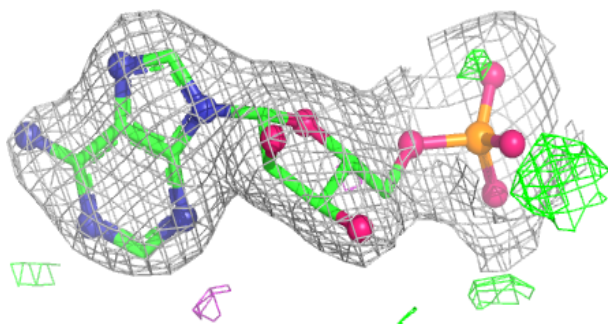
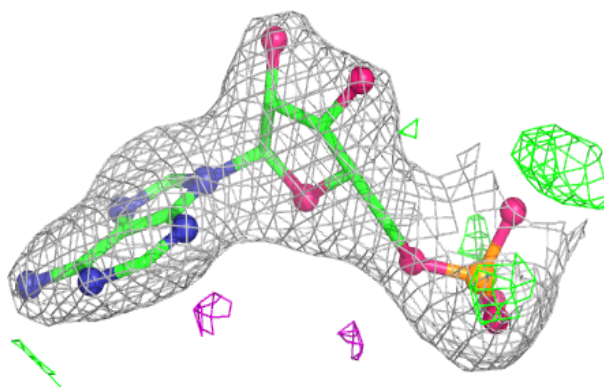
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BTB	F	202	14/14	0.73	0.33	96,108,113,114	0
5	BTB	A	335	14/14	0.78	0.15	119,124,127,129	0
5	BTB	C	201	14/14	0.79	0.23	111,116,118,119	0
6	AMP	E	236	23/23	0.95	0.08	37,43,63,67	0
6	AMP	H	236	23/23	0.95	0.07	26,37,59,63	0

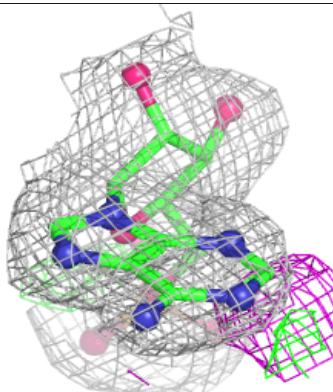
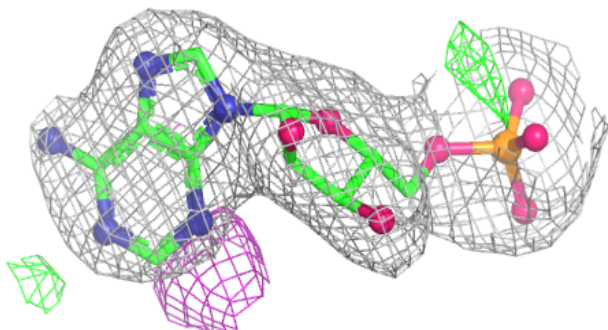
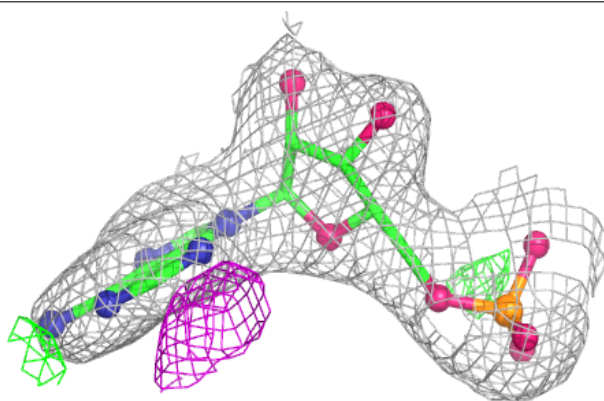
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around AMP E 236:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AMP H 236:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.