Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 10:31 AM EDT

PDB ID	:	1ZBH
Title	:	3'-end specific recognition of histone mRNA stem-loop by 3'-exonuclease
Authors	:	Cheng, Y.; Patel, D.J.
Deposited on	:	2005-04-08
Resolution	:	3.00 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 (i) symbol.

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

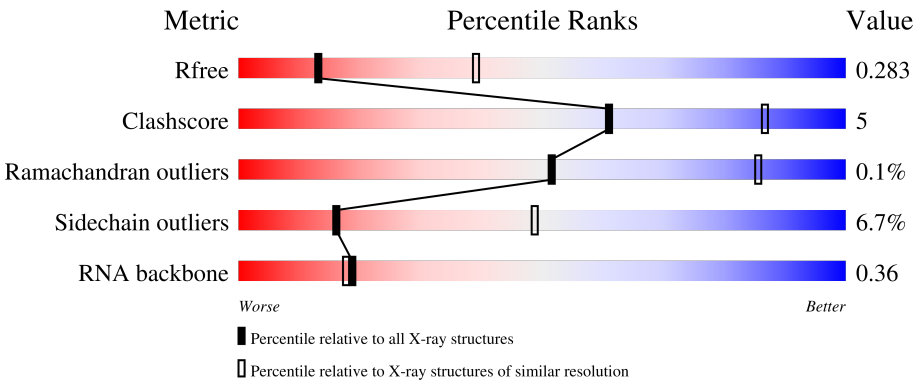
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 <=5%

Mol	Chain	Length	Quality of chain
1	E	20	35% 40% 5% 20%
1	F	20	35% 30% 15% 20%
2	A	299	82% 13% • •
2	B	299	64% 10% • 25%
2	C	299	67% 7% • 25%
2	D	299	79% 15% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9138 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 RNA chain called 5'-R(*CP*CP*GP*GP*CP*UP*CP*UP*UP*UP*UP*CP *AP*GP*AP*GP*CP*CP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	F	16	333	150	55	113	15	0	0	0
1	E	16	333	150	55	113	15	0	0	0

- Molecule 2 is a protein called 3'-5' exonuclease ERI1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	289	2354	1503	395	439	17	0	0	0
2	B	225	1823	1164	302	343	14	0	0	0
2	C	225	1823	1164	302	343	14	0	0	0
2	D	289	2354	1503	395	439	17	0	0	0

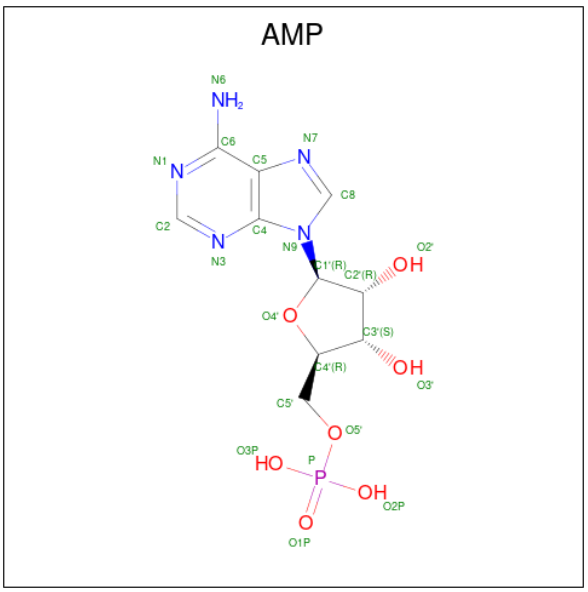
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	LEU	TRP	engineered mutation	UNP Q8IV48
A	293	ASN	HIS	engineered mutation	UNP Q8IV48
B	213	LEU	TRP	engineered mutation	UNP Q8IV48
B	293	ASN	HIS	engineered mutation	UNP Q8IV48
C	213	LEU	TRP	engineered mutation	UNP Q8IV48
C	293	ASN	HIS	engineered mutation	UNP Q8IV48
D	213	LEU	TRP	engineered mutation	UNP Q8IV48
D	293	ASN	HIS	engineered mutation	UNP Q8IV48

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
			Total	Mg		
3	B	2	2	2	0	0
			Total	Mg		
3	C	2	2	2	0	0
			Total	Mg		
3	D	2	2	2	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
4	B	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
4	C	1	23	10	5	7	1	0	0
			Total	C	N	O	P		
4	D	1	23	10	5	7	1	0	0

- Molecule 5 is water.

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

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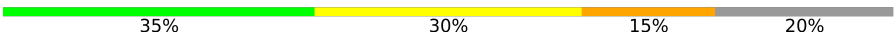
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	5	5	5	0	0
			Total	O		
5	C	2	2	2	0	0
			Total	O		
5	D	2	2	2	0	0

3 Residue-property plots (i)

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. 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. 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.

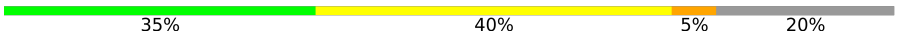
• Molecule 1: 5'-R(*CP*CP*GP*GP*CP*UP*CP*UP*UP*UP*UP*CP*AP*GP*AP*GP*CP*CP*GP*G)-3'

Chain F:



• Molecule 1: 5'-R(*CP*CP*GP*GP*CP*UP*CP*UP*UP*UP*UP*CP*AP*GP*AP*GP*CP*CP*GP*G)-3'

Chain E:

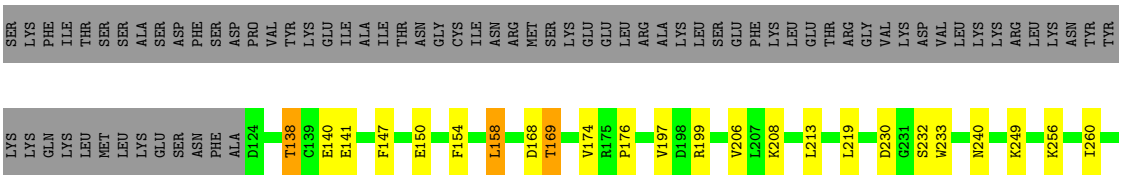


• Molecule 2: 3'-5' exonuclease ERI1

Chain A:

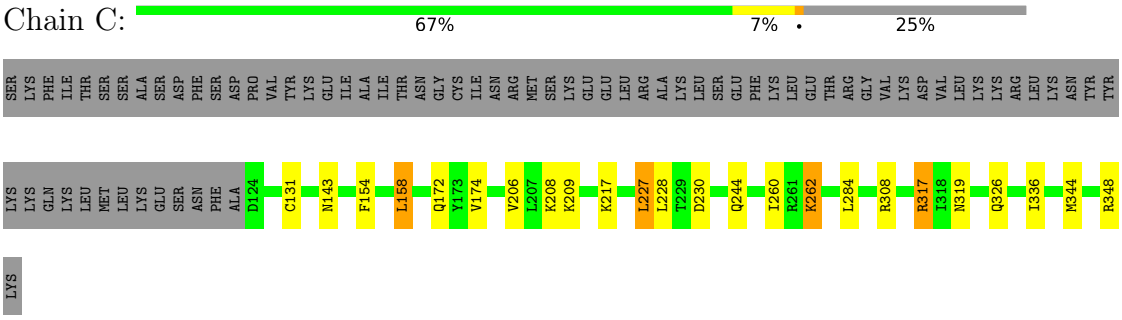
• Molecule 2: 3'-5' exonuclease ERI1

Chain B:



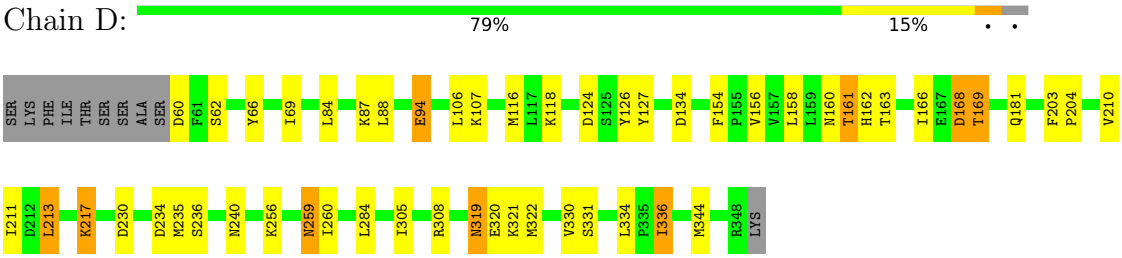
• Molecule 2: 3'-5' exonuclease ERI1

Chain C:



• Molecule 2: 3'-5' exonuclease ERI1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.39Å 195.15Å 87.97Å 90.00° 92.13° 90.00°	Depositor
Resolution (Å)	19.92 – 3.00 19.91 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (19.92-3.00) 95.7 (19.91-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.36 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.209 , 0.260 0.264 , 0.283	Depositor DCC
R_{free} test set	3372 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 5.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	9138	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AMP

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	E	0.66	0/370	1.27	3/574 (0.5%)
1	F	0.65	0/370	1.32	3/574 (0.5%)
2	A	0.33	0/2402	0.49	0/3235
2	B	0.33	0/1864	0.49	0/2521
2	C	0.33	0/1864	0.48	0/2521
2	D	0.35	0/2402	0.49	0/3235
All	All	0.37	0/9272	0.61	6/12660 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	7	G	O3'-P-O5'	-11.54	82.08	104.00
1	E	7	G	O3'-P-O5'	-11.16	82.80	104.00
1	F	7	G	OP1-P-O3'	-9.85	83.52	105.20
1	E	7	G	OP1-P-O3'	-8.45	86.60	105.20
1	E	7	G	OP2-P-O3'	-8.43	86.65	105.20
1	F	8	C	O5'-P-OP1	6.87	118.94	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	333	0	173	0	0
1	F	333	0	173	3	0
2	A	2354	0	2381	21	0
2	B	1823	0	1817	13	0
2	C	1823	0	1817	17	0
2	D	2354	0	2381	31	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	23	0	12	0	0
4	B	23	0	12	0	0
4	C	23	0	12	0	0
4	D	23	0	12	0	0
5	A	8	0	0	0	0
5	B	5	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
5	F	1	0	0	0	0
All	All	9138	0	8790	81	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 5.

All (81) 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:C:317:ARG:HH11	2:C:317:ARG:HG3	1.18	1.03
2:D:259:ASN:H	2:D:319:ASN:HD21	1.13	0.93
2:D:127:TYR:O	2:D:161:THR:HG21	1.82	0.80
2:D:160:ASN:ND2	2:D:163:THR:H	1.81	0.78
2:C:317:ARG:HG3	2:C:317:ARG:NH1	1.97	0.72
2:C:317:ARG:HH12	2:C:336:ILE:HG13	1.55	0.72
2:B:308:ARG:HA	2:B:311:GLN:HE21	1.56	0.71
2:C:208:LYS:HD2	2:C:344:MET:HG3	1.75	0.68
2:D:259:ASN:H	2:D:319:ASN:ND2	1.88	0.68
2:D:160:ASN:HD22	2:D:163:THR:H	1.41	0.67
2:D:259:ASN:N	2:D:319:ASN:HD21	1.90	0.67
2:C:228:LEU:HD21	2:C:260:ILE:HB	1.79	0.65
2:B:176:PRO:HD2	2:B:197:VAL:HG13	1.78	0.65
2:A:326:GLN:HE21	2:A:326:GLN:HA	1.62	0.64
2:A:120:SER:HA	2:A:123:ALA:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:THR:HG23	2:B:296:LEU:HD11	1.81	0.61
2:B:208:LYS:HG2	2:B:344:MET:HG3	1.83	0.61
2:A:151:ILE:H	2:A:242:GLN:HE21	1.50	0.60
2:D:168:ASP:OD2	2:D:217:LYS:HE3	2.05	0.57
2:B:140:GLU:HG2	2:B:147:PHE:CE1	2.39	0.57
1:F:13:U:O4'	2:D:66:TYR:HB3	2.05	0.56
2:C:317:ARG:HH11	2:C:317:ARG:CG	2.03	0.56
2:A:134:ASP:HA	2:A:234:ASP:OD1	2.06	0.56
2:B:176:PRO:HD2	2:B:197:VAL:CG1	2.37	0.55
2:B:138:THR:HG22	2:B:150:GLU:H	1.73	0.53
2:B:232:SER:HB3	2:B:320:GLU:OE2	2.08	0.53
2:B:158:LEU:HD11	2:B:219:LEU:HD11	1.91	0.52
2:C:317:ARG:NH1	2:C:336:ILE:HG13	2.24	0.52
2:D:230:ASP:HA	2:D:260:ILE:HG22	1.93	0.51
2:C:131:CYS:HB2	2:C:227:LEU:HD12	1.92	0.50
2:A:235:MET:HG3	2:A:250:TYR:OH	2.13	0.49
2:A:88:LEU:HD21	2:A:105:ARG:HD2	1.94	0.49
2:D:331:SER:HB3	2:D:334:LEU:HG	1.95	0.49
2:D:84:LEU:O	2:D:88:LEU:HB2	2.13	0.49
2:D:284:LEU:HD11	2:D:305:ILE:HG23	1.95	0.48
2:A:271:PRO:HD2	2:A:274:GLN:HG3	1.97	0.47
2:D:168:ASP:OD1	2:D:213:LEU:HD21	2.14	0.47
2:D:284:LEU:HD22	2:D:308:ARG:HG2	1.97	0.47
2:A:160:ASN:HD21	2:A:162:HIS:HB2	1.80	0.47
2:C:158:LEU:HD12	2:C:217:LYS:HE2	1.98	0.46
2:D:259:ASN:C	2:D:259:ASN:HD22	2.19	0.46
2:A:127:TYR:HA	2:A:224:LYS:HB3	1.98	0.46
2:A:133:ILE:O	2:A:229:THR:HG22	2.16	0.46
2:A:160:ASN:ND2	2:A:163:THR:H	2.14	0.46
2:A:308:ARG:HH12	2:D:94:GLU:HG3	1.79	0.46
2:C:317:ARG:HH12	2:C:336:ILE:CG1	2.26	0.45
2:D:336:ILE:H	2:D:336:ILE:HG13	1.44	0.45
2:B:339:THR:HG22	2:B:340:PRO:HD2	1.99	0.45
2:C:262:LYS:HE2	2:C:319:ASN:HB2	2.00	0.44
2:D:156:VAL:HG21	2:D:210:VAL:HG13	1.99	0.44
2:D:166:ILE:HG21	2:D:169:THR:HG22	1.99	0.44
2:C:230:ASP:HA	2:C:260:ILE:HG22	2.00	0.44
2:D:60:ASP:C	2:D:62:SER:H	2.22	0.44
2:A:326:GLN:HE21	2:A:326:GLN:CA	2.30	0.43
2:A:336:ILE:H	2:A:336:ILE:HG13	1.72	0.43
2:A:88:LEU:HD23	2:A:95:THR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:151:ILE:H	2:A:242:GLN:NE2	2.15	0.43
2:A:308:ARG:NH1	2:D:94:GLU:HG3	2.34	0.42
2:D:319:ASN:HD22	2:D:320:GLU:N	2.16	0.42
2:D:160:ASN:ND2	2:D:162:HIS:H	2.17	0.42
2:C:284:LEU:HD13	2:C:308:ARG:HG2	2.01	0.42
2:D:321:LYS:HD2	2:D:330:VAL:HG22	2.01	0.42
2:C:244:GLN:HA	2:C:348:ARG:HH21	1.85	0.42
2:B:230:ASP:HA	2:B:260:ILE:HG22	2.01	0.42
2:A:63:ASP:CG	2:A:64:PRO:HD2	2.41	0.41
2:B:174:VAL:HG22	2:B:206:VAL:HG21	2.02	0.41
2:A:291:ARG:O	2:A:294:CYS:HB3	2.19	0.41
2:B:296:LEU:HG	2:B:300:LYS:HE3	2.01	0.41
2:C:336:ILE:HD12	2:C:336:ILE:H	1.85	0.41
2:C:174:VAL:HG22	2:C:206:VAL:HG21	2.03	0.41
2:D:66:TYR:HA	2:D:69:ILE:HD12	2.01	0.41
2:D:211:ILE:HD13	2:D:344:MET:HA	2.03	0.41
2:D:134:ASP:HA	2:D:234:ASP:OD1	2.20	0.41
2:D:158:LEU:HB3	2:D:168:ASP:HB2	2.03	0.41
1:F:9:U:H2'	1:F:10:C:C6	2.55	0.41
1:F:17:G:OP1	2:D:107:LYS:HE3	2.21	0.41
2:A:172:GLN:HE21	2:A:206:VAL:HG22	1.86	0.41
2:D:203:PHE:N	2:D:204:PRO:HD2	2.36	0.41
2:D:236:SER:HA	2:D:322:MET:SD	2.61	0.41
2:A:284:LEU:HD22	2:A:308:ARG:HG2	2.03	0.40
2:C:172:GLN:HE22	2:C:209:LYS:HD2	1.87	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
2	A	287/299 (96%)	276 (96%)	10 (4%)	1 (0%)	41 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	223/299 (75%)	218 (98%)	5 (2%)	0	100	100
2	C	223/299 (75%)	217 (97%)	6 (3%)	0	100	100
2	D	287/299 (96%)	277 (96%)	10 (4%)	0	100	100
All	All	1020/1196 (85%)	988 (97%)	31 (3%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	99	LYS

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	
2	A	267/276 (97%)	247 (92%)	20 (8%)	13	43
2	B	208/276 (75%)	191 (92%)	17 (8%)	11	39
2	C	208/276 (75%)	201 (97%)	7 (3%)	37	72
2	D	267/276 (97%)	247 (92%)	20 (8%)	13	43
All	All	950/1104 (86%)	886 (93%)	64 (7%)	16	49

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	87	LYS
2	A	106	LEU
2	A	133	ILE
2	A	140	GLU
2	A	141	GLU
2	A	154	PHE
2	A	160	ASN
2	A	168	ASP
2	A	213	LEU
2	A	234	ASP

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Mol	Chain	Res	Type
2	A	235	MET
2	A	240	ASN
2	A	256	LYS
2	A	276	LYS
2	A	294	CYS
2	A	326	GLN
2	A	327	LEU
2	A	329	SER
2	A	339	THR
2	A	348	ARG
2	B	138	THR
2	B	141	GLU
2	B	154	PHE
2	B	158	LEU
2	B	168	ASP
2	B	169	THR
2	B	199	ARG
2	B	213	LEU
2	B	233	TRP
2	B	240	ASN
2	B	249	LYS
2	B	256	LYS
2	B	276	LYS
2	B	294	CYS
2	B	318	ILE
2	B	339	THR
2	B	344	MET
2	C	143	ASN
2	C	154	PHE
2	C	158	LEU
2	C	227	LEU
2	C	262	LYS
2	C	317	ARG
2	C	326	GLN
2	D	87	LYS
2	D	94	GLU
2	D	106	LEU
2	D	116	MET
2	D	118	LYS
2	D	124	ASP
2	D	126	TYR
2	D	154	PHE

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Mol	Chain	Res	Type
2	D	161	THR
2	D	168	ASP
2	D	169	THR
2	D	181	GLN
2	D	213	LEU
2	D	217	LYS
2	D	235	MET
2	D	240	ASN
2	D	256	LYS
2	D	259	ASN
2	D	319	ASN
2	D	336	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	160	ASN
2	A	172	GLN
2	A	240	ASN
2	A	242	GLN
2	A	326	GLN
2	B	240	ASN
2	B	311	GLN
2	B	343	GLN
2	C	143	ASN
2	C	172	GLN
2	C	205	GLN
2	C	343	GLN
2	D	149	HIS
2	D	160	ASN
2	D	172	GLN
2	D	181	GLN
2	D	240	ASN
2	D	259	ASN
2	D	319	ASN
2	D	326	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	15/20 (75%)	8 (53%)	1 (6%)
1	F	15/20 (75%)	6 (40%)	0
All	All	30/40 (75%)	14 (46%)	1 (3%)

All (14) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	F	8	C
1	F	9	U
1	F	12	U
1	F	13	U
1	F	15	C
1	F	21	C
1	E	7	G
1	E	8	C
1	E	9	U
1	E	10	C
1	E	12	U
1	E	13	U
1	E	15	C
1	E	19	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	14	U

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AMP	B	2002	3	22,25,25	1.03	1 (4%)	25,38,38	1.31	3 (12%)
4	AMP	D	4002	3	22,25,25	1.07	2 (9%)	25,38,38	1.27	3 (12%)
4	AMP	A	1002	3	22,25,25	1.07	2 (9%)	25,38,38	1.29	3 (12%)
4	AMP	C	3002	3	22,25,25	1.02	1 (4%)	25,38,38	1.26	2 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AMP	B	2002	3	-	2/6/26/26	0/3/3/3
4	AMP	D	4002	3	-	1/6/26/26	0/3/3/3
4	AMP	A	1002	3	-	2/6/26/26	0/3/3/3
4	AMP	C	3002	3	-	1/6/26/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4002	AMP	C5-C4	2.68	1.48	1.40
4	A	1002	AMP	C5-C4	2.61	1.47	1.40
4	B	2002	AMP	C5-C4	2.50	1.47	1.40
4	C	3002	AMP	C5-C4	2.50	1.47	1.40
4	A	1002	AMP	C2-N3	2.15	1.35	1.32
4	D	4002	AMP	C2-N3	2.05	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	2002	AMP	N3-C2-N1	-3.52	123.17	128.68
4	A	1002	AMP	N3-C2-N1	-3.46	123.28	128.68
4	C	3002	AMP	N3-C2-N1	-3.44	123.30	128.68
4	D	4002	AMP	N3-C2-N1	-3.36	123.42	128.68
4	B	2002	AMP	C4-C5-N7	-2.61	106.68	109.40
4	C	3002	AMP	C4-C5-N7	-2.56	106.73	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4002	AMP	C4-C5-N7	-2.50	106.80	109.40
4	A	1002	AMP	C3'-C2'-C1'	2.19	104.27	100.98
4	D	4002	AMP	C3'-C2'-C1'	2.18	104.25	100.98
4	A	1002	AMP	C4-C5-N7	-2.13	107.18	109.40
4	B	2002	AMP	O3P-P-O2P	2.00	115.29	107.64

There are no chirality outliers.

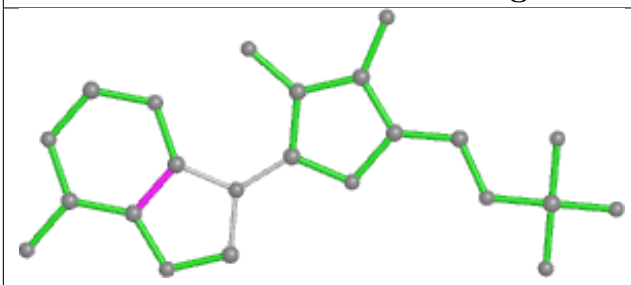
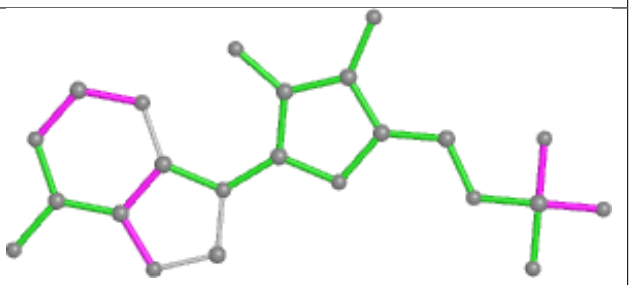
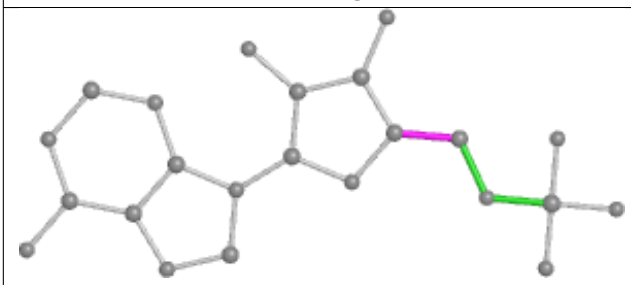
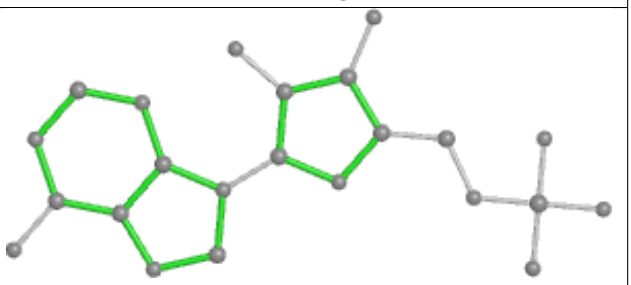
All (6) torsion outliers are listed below:

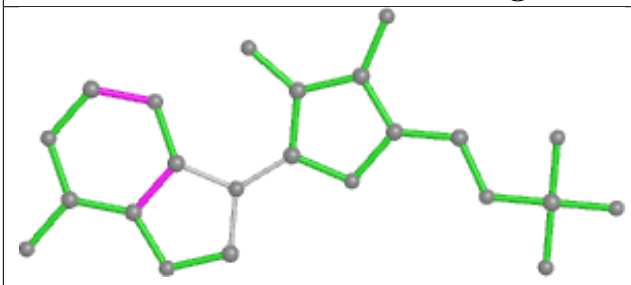
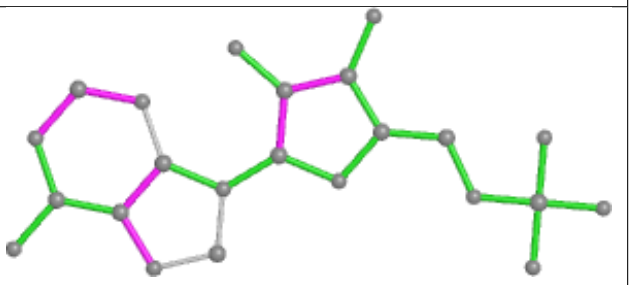
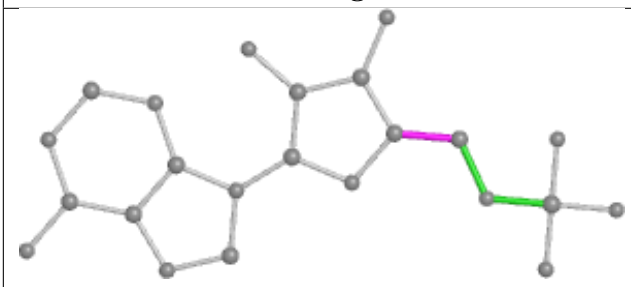
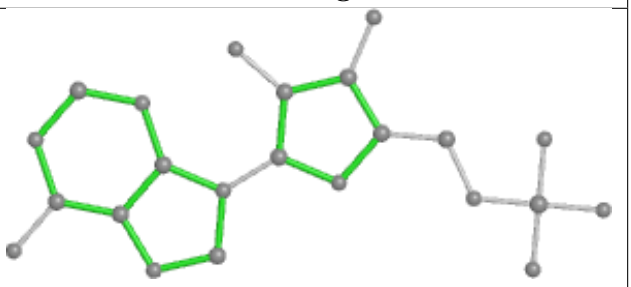
Mol	Chain	Res	Type	Atoms
4	A	1002	AMP	O4'-C4'-C5'-O5'
4	A	1002	AMP	C3'-C4'-C5'-O5'
4	B	2002	AMP	O4'-C4'-C5'-O5'
4	B	2002	AMP	C3'-C4'-C5'-O5'
4	D	4002	AMP	O4'-C4'-C5'-O5'
4	C	3002	AMP	C5'-O5'-P-O2P

There are no ring outliers.

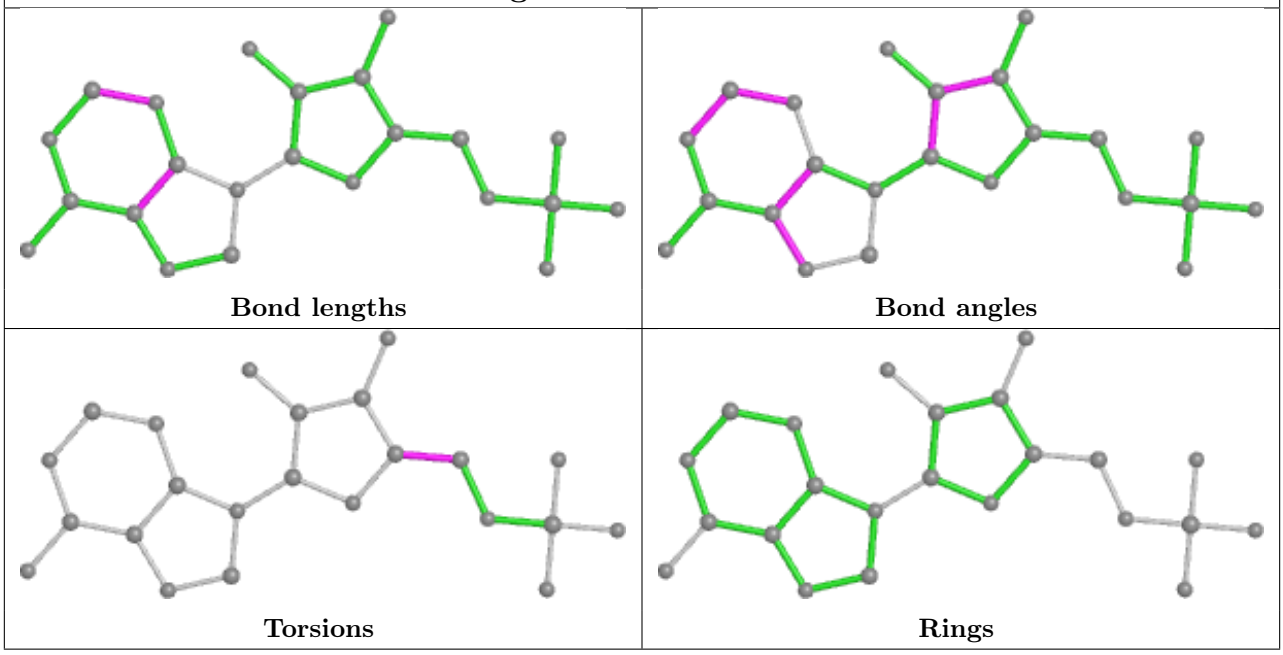
No monomer is involved in short contacts.

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 then 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.

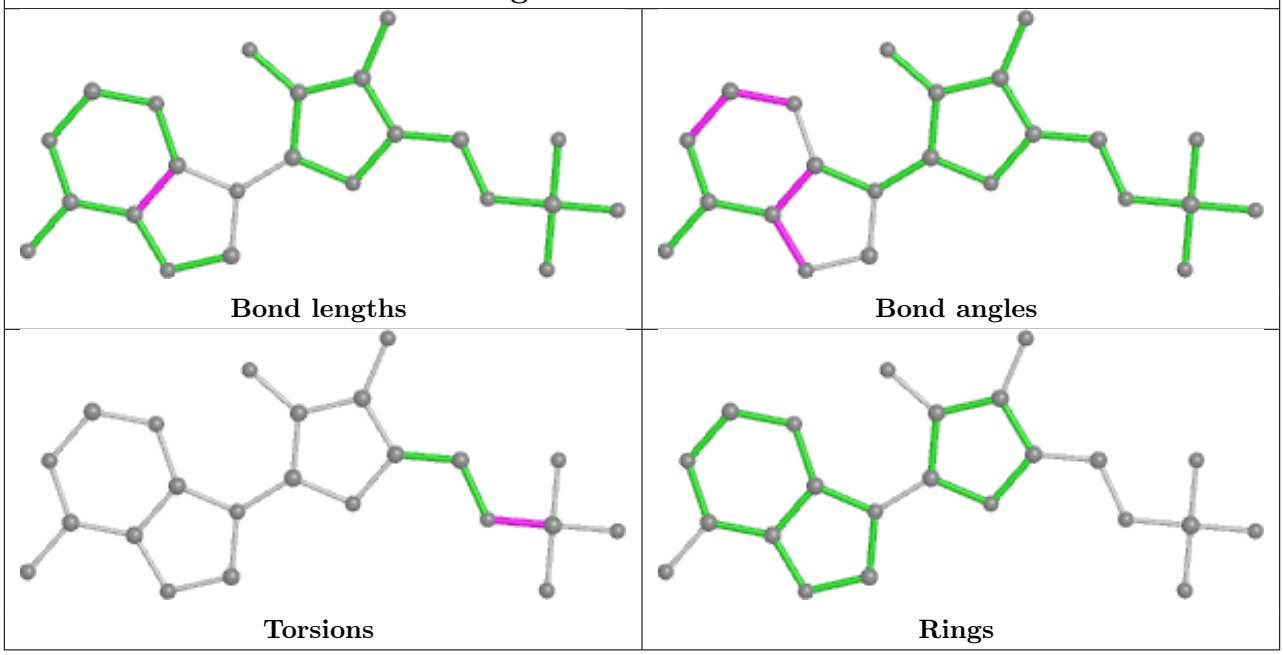
Ligand AMP B 2002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP D 4002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP A 1002



Ligand AMP C 3002



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 (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

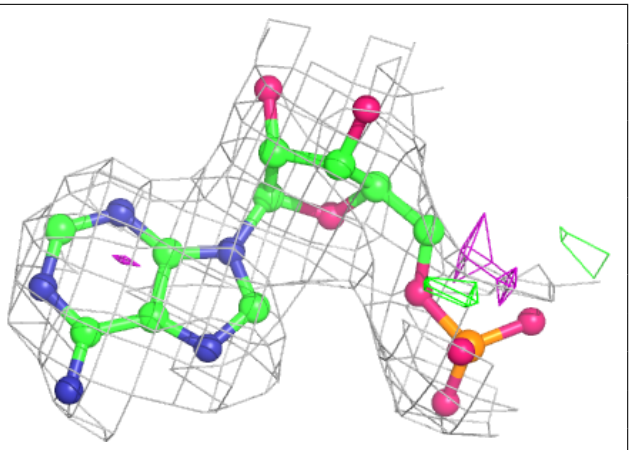
6.4 Ligands (i)

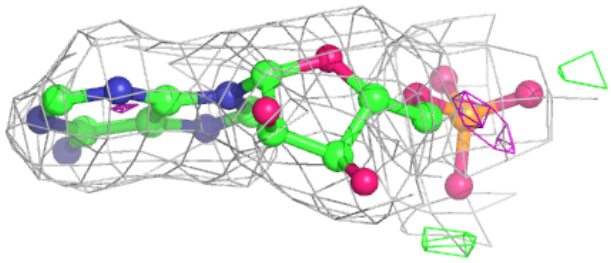
Unable to reproduce the depositors R factor - this section is therefore empty.

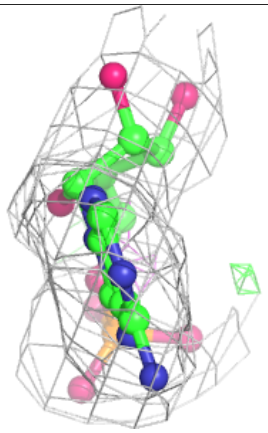
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP A 1002:

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

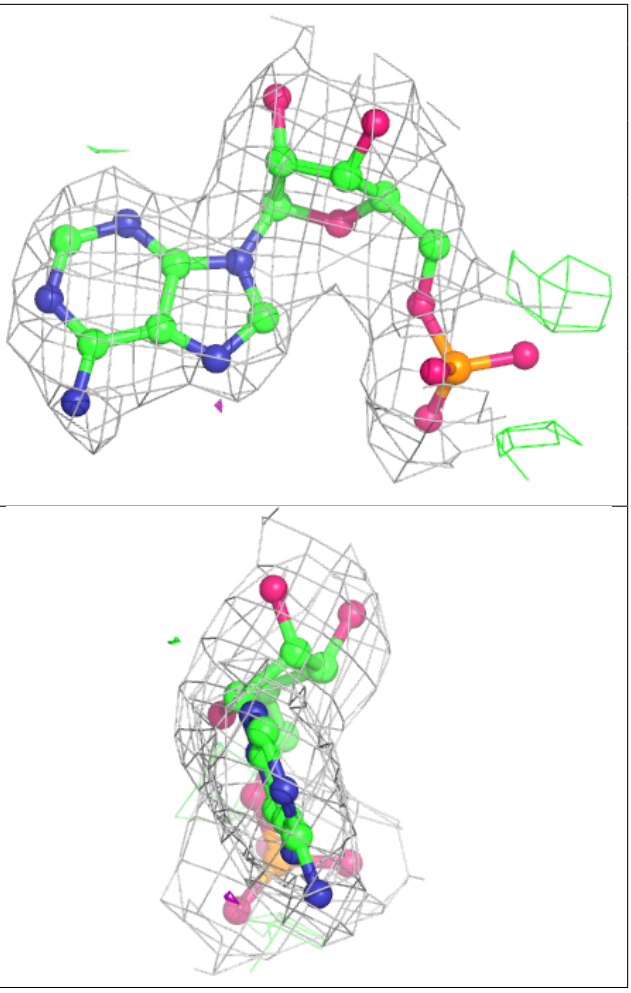






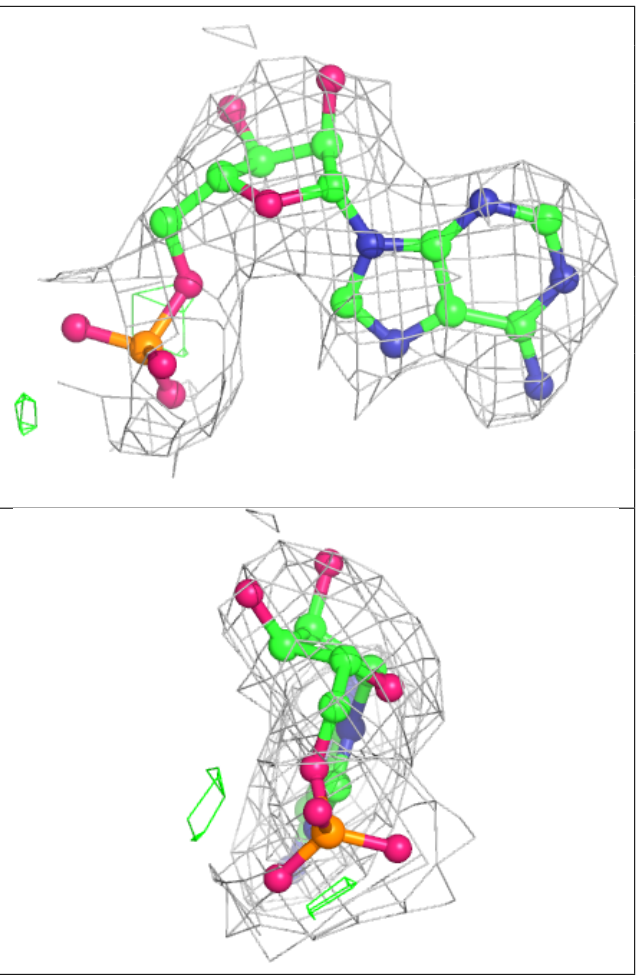
Electron density around AMP B 2002:

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



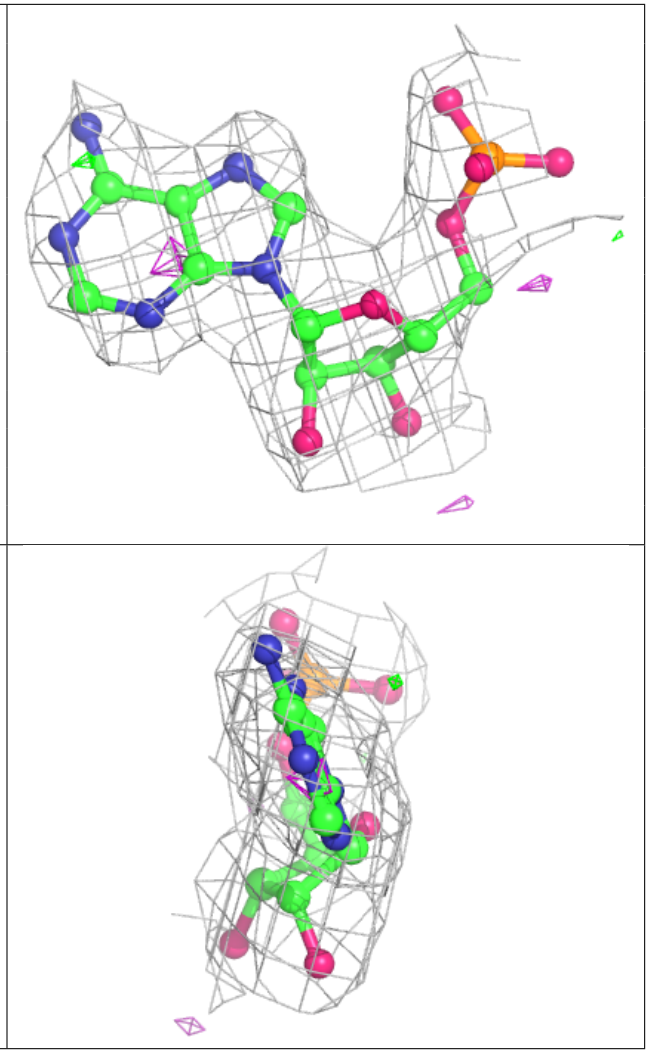
Electron density around AMP C 3002:

$2mF_o$-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 D 4002:

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)

Unable to reproduce the depositors R factor - this section is therefore empty.