



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:38 PM UTC

PDB ID : 6NBJ / pdb_00006nbj
Title : Qri7
Authors : Stec, B.
Deposited on : 2018-12-07
Resolution : 2.94 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

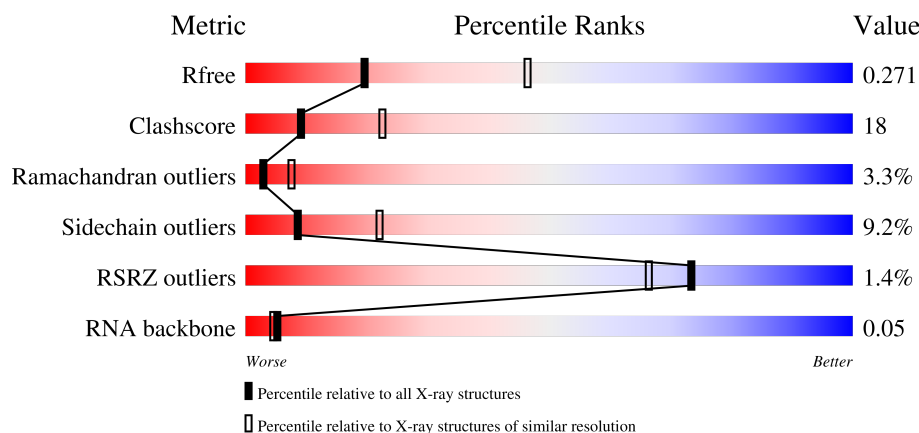
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)
RNA backbone	3983	1018 (3.14-2.74)

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	A	383	2% 61% 32% . .
1	B	383	2% 64% 29% 5% . .
2	C	4	25% 25% 50%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6084 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called tRNA N6-adenosine threonylcarbamoyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2949	1865	513	554	17			
1	B	378	Total	C	N	O	S	0	0	0
			2949	1865	513	554	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	GLY	-	expression tag	UNP P43122
A	26	PRO	-	expression tag	UNP P43122
A	27	LEU	-	expression tag	UNP P43122
A	28	HIS	-	expression tag	UNP P43122
A	29	MET	-	expression tag	UNP P43122
B	25	GLY	-	expression tag	UNP P43122
B	26	PRO	-	expression tag	UNP P43122
B	27	LEU	-	expression tag	UNP P43122
B	28	HIS	-	expression tag	UNP P43122
B	29	MET	-	expression tag	UNP P43122

- Molecule 2 is a RNA chain called RNA (5'-R(P*CP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	P	0	0	0
			64	27	9	24	4			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

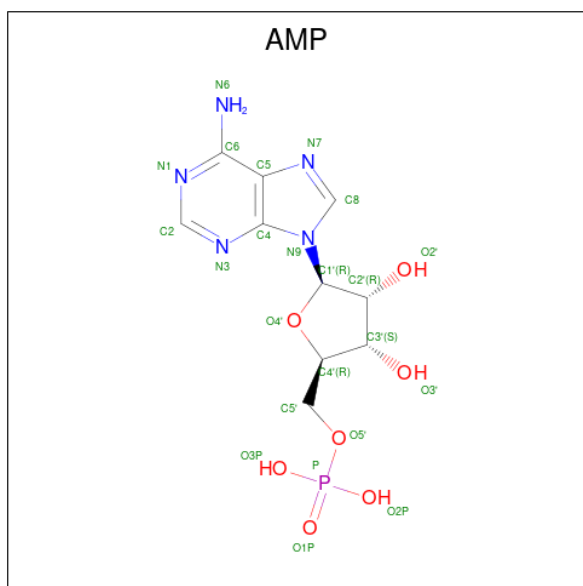
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

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



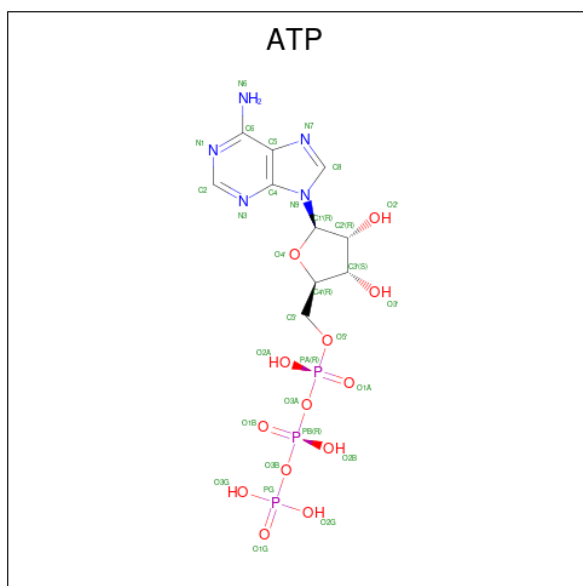
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



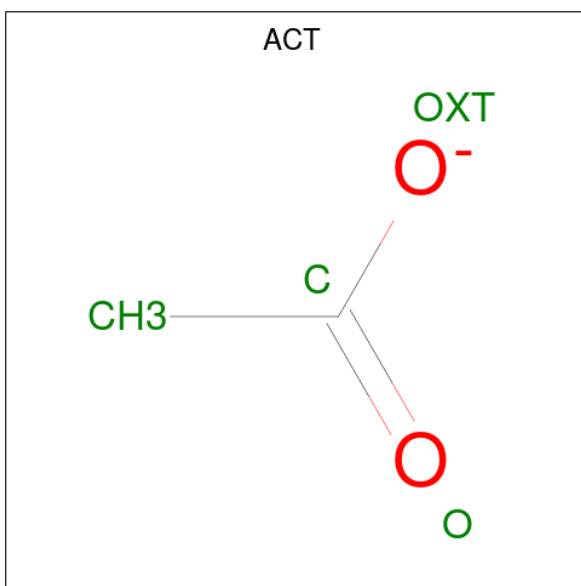
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

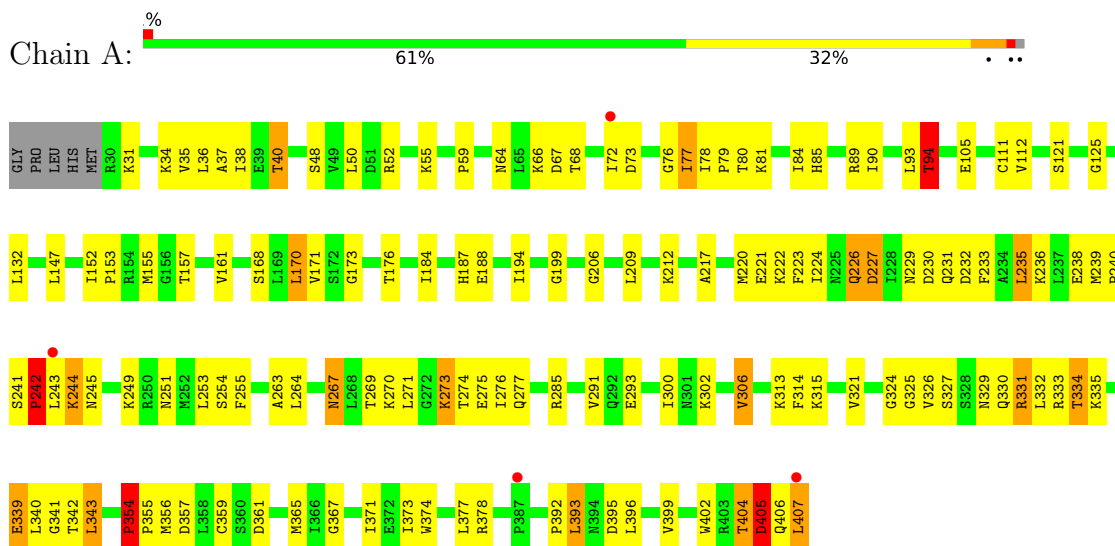
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	9	Total 9	O 9	0	0
9	B	15	Total 15	O 15	0	0

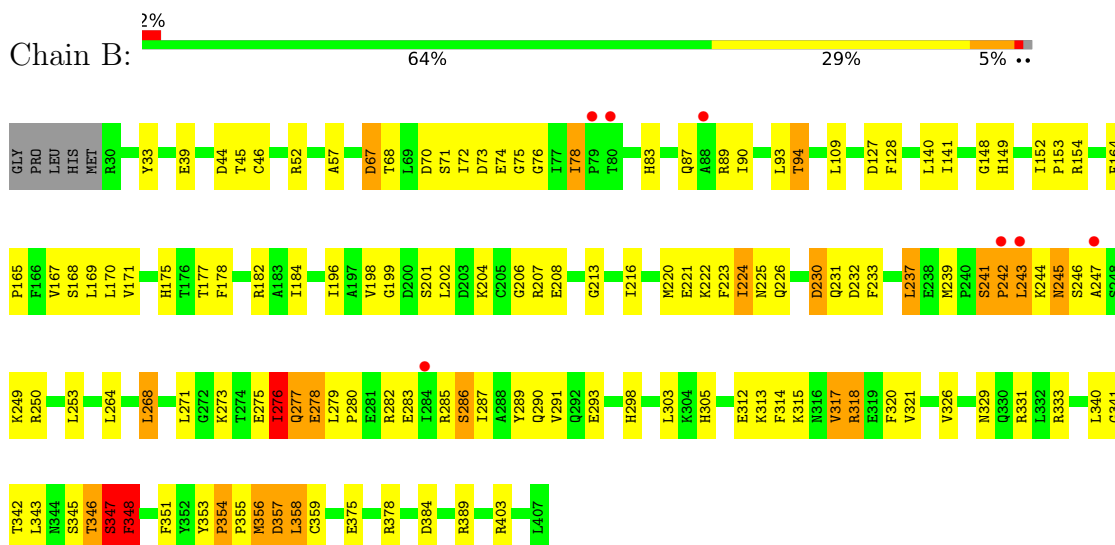
3 Residue-property plots

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.

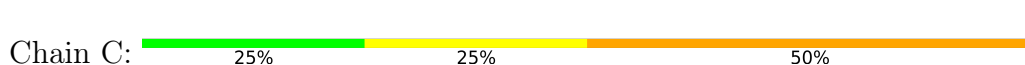
- Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase, mitochondrial



- Molecule 1: tRNA N6-adenosine threonylcarbamoyltransferase, mitochondrial



- Molecule 2: RNA (5'-R(P*CP*CP*CP*C)-3')





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	180.31 Å 180.31 Å 180.31 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.06 – 2.94 50.06 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.06-2.94) 99.2 (50.06-2.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.80 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.196 , 0.270 0.203 , 0.271	Depositor DCC
R_{free} test set	1121 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6084	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SO4, ACT, ATP, PGE, ZN, 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	A	0.90	3/3006 (0.1%)	1.20	15/4063 (0.4%)
1	B	0.89	1/3006 (0.0%)	1.24	9/4063 (0.2%)
2	C	0.61	0/69	1.29	0/105
All	All	0.89	4/6081 (0.1%)	1.22	24/8231 (0.3%)

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	A	0	1
1	B	0	6
All	All	0	7

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	357	ASP	CA-C	8.64	1.64	1.52
1	A	402	TRP	C-O	-5.67	1.16	1.23
1	A	66	LYS	C-O	-5.50	1.17	1.23
1	A	64	ASN	C-O	-5.33	1.17	1.23

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	356	MET	N-CA-C	-9.07	100.85	113.37
1	B	358	LEU	N-CA-C	8.27	123.59	113.17
1	B	358	LEU	N-CA-CB	-8.11	98.50	110.49
1	A	341	GLY	N-CA-C	-7.75	102.84	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	PRO	N-CA-C	7.41	119.73	110.70
1	A	94	THR	CB-CA-C	6.83	123.19	110.70
1	A	343	LEU	N-CA-CB	-6.59	100.61	110.90
1	A	68	THR	CA-CB-OG1	-6.38	100.03	109.60
1	A	241	SER	CA-C-N	6.23	127.62	119.84
1	A	241	SER	C-N-CA	6.23	127.62	119.84
1	A	242	PRO	N-CA-CB	-6.12	96.82	103.25
1	B	348	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	405	ASP	N-CA-C	-5.89	98.24	110.80
1	B	241	SER	CA-C-N	5.81	127.11	119.84
1	B	241	SER	C-N-CA	5.81	127.11	119.84
1	B	286	SER	N-CA-C	-5.72	106.22	113.43
1	B	384	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	242	PRO	CA-N-CD	-5.67	104.07	112.00
1	A	94	THR	CA-CB-OG1	5.58	117.97	109.60
1	A	229	ASN	N-CA-C	5.43	118.37	111.69
1	B	357	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	361	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	405	ASP	CA-C-N	-5.06	115.45	123.24
1	A	405	ASP	C-N-CA	-5.06	115.45	123.24

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	ARG	Sidechain
1	B	182	ARG	Sidechain
1	B	207	ARG	Sidechain
1	B	250	ARG	Sidechain
1	B	331	ARG	Sidechain
1	B	378	ARG	Sidechain
1	B	403	ARG	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	A	2949	0	2972	108	1
1	B	2949	0	2972	109	1
2	C	64	0	33	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	23	0	12	3	0
4	B	23	0	12	0	0
5	A	10	0	14	4	0
6	A	31	0	12	0	0
7	B	5	0	0	0	0
8	B	4	0	3	0	0
9	A	9	0	0	1	0
9	B	15	0	0	3	0
All	All	6084	0	6030	221	1

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 18.

All (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ILE:HG22	1:A:285:ARG:HG3	1.27	1.10
1:A:239:MET:HE1	1:A:264:LEU:N	1.74	1.02
1:B:315:LYS:HE3	9:B:614:HOH:O	1.70	0.91
1:A:78:ILE:HB	1:A:79:PRO:HD2	1.55	0.89
1:A:271:LEU:HD12	1:A:271:LEU:O	1.72	0.88
1:B:72:ILE:HG21	1:B:89:ARG:HH22	1.38	0.87
1:A:36:LEU:HD23	1:A:132:LEU:HD13	1.58	0.84
1:B:320:PHE:HD2	1:B:351:PHE:CD2	1.96	0.83
1:B:245:ASN:O	1:B:249:LYS:HE2	1.79	0.83
1:B:356:MET:HA	1:B:359:CYS:HB2	1.61	0.83
1:A:242:PRO:O	1:A:244:LYS:HD2	1.78	0.82
1:A:404:THR:HG23	1:A:405:ASP:O	1.80	0.81
1:B:44:ASP:CG	1:B:68:THR:HG22	2.05	0.81
1:A:90:ILE:O	1:A:94:THR:HG23	1.80	0.80
1:B:127:ASP:OD2	9:B:601:HOH:O	2.01	0.79
1:B:320:PHE:CD2	1:B:351:PHE:CE2	2.71	0.78
1:B:320:PHE:CD2	1:B:351:PHE:CD2	2.72	0.77
1:A:342:THR:HG23	1:A:343:LEU:H	1.51	0.75
1:B:318:ARG:HG2	1:B:318:ARG:HH21	1.50	0.74
1:B:72:ILE:CD1	1:B:89:ARG:HH12	2.00	0.74
1:B:273:LYS:O	1:B:276:ILE:HG23	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:GLN:O	1:A:227:ASP:HB2	1.90	0.72
1:B:167:VAL:HG23	1:B:320:PHE:HD1	1.55	0.72
1:B:243:LEU:O	1:B:246:SER:HB3	1.90	0.71
1:A:224:ILE:CG2	1:A:285:ARG:HG3	2.15	0.70
1:B:83:HIS:O	1:B:87:GLN:HG3	1.92	0.69
1:A:36:LEU:CD2	1:A:132:LEU:HD13	2.24	0.68
1:A:239:MET:HE1	1:A:264:LEU:CA	2.22	0.68
1:A:40:THR:HG21	1:A:125:GLY:H	1.60	0.66
1:A:407:LEU:HD22	1:A:407:LEU:O	1.94	0.66
1:A:78:ILE:HB	1:A:79:PRO:CD	2.24	0.66
1:A:224:ILE:HA	1:A:285:ARG:HD3	1.78	0.66
1:A:342:THR:CG2	1:A:343:LEU:H	2.09	0.65
1:B:153:PRO:HG3	1:B:354:PRO:HG3	1.79	0.64
1:A:40:THR:HG23	1:A:40:THR:O	1.97	0.64
1:A:335:LYS:O	1:A:339:GLU:HG3	1.98	0.64
1:B:222:LYS:C	1:B:226:GLN:HE21	2.06	0.64
1:A:239:MET:HE1	1:A:263:ALA:C	2.24	0.63
1:B:280:PRO:C	1:B:282:ARG:H	2.06	0.62
2:C:2:C:H2'	2:C:3:C:H5'	1.81	0.62
1:A:342:THR:HG23	1:A:343:LEU:N	2.14	0.62
1:A:325:GLY:N	4:A:502:AMP:O2P	2.33	0.62
1:A:242:PRO:O	1:A:244:LYS:CD	2.48	0.62
1:A:253:LEU:HD12	1:A:306:VAL:HG12	1.80	0.61
1:A:85:HIS:CE1	1:A:89:ARG:HG3	2.36	0.61
1:B:246:SER:HB2	1:B:305:HIS:CE1	2.36	0.61
1:B:275:GLU:O	1:B:277:GLN:N	2.34	0.61
2:C:3:C:O5'	2:C:4:C:OP2	2.18	0.60
1:B:241:SER:O	1:B:241:SER:OG	2.14	0.60
1:B:72:ILE:HG21	1:B:89:ARG:NH2	2.12	0.60
1:B:90:ILE:O	1:B:94:THR:HG23	2.01	0.60
2:C:2:C:C2'	2:C:3:C:H5'	2.30	0.60
1:A:226:GLN:O	1:A:227:ASP:CB	2.50	0.59
1:A:271:LEU:O	1:A:271:LEU:CD1	2.49	0.59
1:B:246:SER:OG	1:B:246:SER:O	2.19	0.59
1:A:40:THR:HG22	9:A:605:HOH:O	2.03	0.59
1:B:231:GLN:CD	1:B:285:ARG:O	2.46	0.58
1:A:84:ILE:HD11	2:C:2:C:N4	2.19	0.58
1:B:239:MET:HE3	1:B:291:VAL:HG22	1.85	0.58
1:B:231:GLN:O	1:B:233:PHE:CD1	2.56	0.58
1:A:55:LYS:NZ	5:A:503:PGE:H52	2.19	0.58
1:B:206:GLY:CA	1:B:220:MET:HE2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:O	1:B:315:LYS:C	2.47	0.58
1:B:220:MET:O	1:B:224:ILE:HG22	2.03	0.58
1:B:72:ILE:HG22	1:B:78:ILE:HD11	1.86	0.57
1:A:406:GLN:O	1:A:407:LEU:OXT	2.22	0.57
1:B:153:PRO:HG3	1:B:354:PRO:CG	2.35	0.57
1:B:171:VAL:HG23	1:B:171:VAL:O	2.05	0.56
1:B:355:PRO:HG2	1:B:358:LEU:HD12	1.88	0.56
1:A:37:ALA:HA	1:A:111:CYS:O	2.04	0.56
1:B:329:ASN:O	1:B:333:ARG:HG3	2.05	0.56
1:A:378:ARG:HG3	1:A:407:LEU:HA	1.88	0.56
1:B:312:GLU:HG2	1:B:313:LYS:N	2.20	0.55
1:A:187:HIS:HB2	1:A:393:LEU:HG	1.88	0.55
1:A:224:ILE:HG22	1:A:285:ARG:CG	2.19	0.55
1:A:40:THR:HG23	1:A:121:SER:O	2.05	0.54
1:A:206:GLY:CA	1:A:220:MET:HE2	2.37	0.54
1:B:245:ASN:OD1	1:B:253:LEU:HD23	2.07	0.54
1:B:109:LEU:HD21	1:B:141:ILE:HD12	1.89	0.54
1:B:245:ASN:O	1:B:249:LYS:CE	2.53	0.54
1:B:178:PHE:CE1	1:B:320:PHE:HE1	2.25	0.54
1:B:178:PHE:HE1	1:B:320:PHE:HE1	1.55	0.54
1:A:152:ILE:HD13	1:A:365:MET:HA	1.88	0.54
1:B:355:PRO:C	1:B:357:ASP:H	2.14	0.54
1:A:374:TRP:CZ3	5:A:503:PGE:H4	2.43	0.53
1:B:167:VAL:HG23	1:B:320:PHE:CD1	2.41	0.52
1:A:227:ASP:OD1	1:A:230:ASP:CB	2.58	0.52
1:B:283:GLU:O	1:B:286:SER:N	2.40	0.52
1:B:275:GLU:O	1:B:276:ILE:C	2.52	0.52
1:A:355:PRO:HB2	1:A:357:ASP:OD1	2.10	0.52
1:B:52:ARG:NH1	1:B:57:ALA:O	2.42	0.52
1:A:157:THR:HG21	1:A:161:VAL:HB	1.90	0.52
1:A:253:LEU:CD1	1:A:306:VAL:HG12	2.41	0.51
1:B:68:THR:OG1	1:B:71:SER:HB3	2.10	0.51
1:A:329:ASN:HB2	4:A:502:AMP:N1	2.26	0.51
1:A:194:ILE:HG23	1:A:254:SER:HB3	1.93	0.51
1:B:355:PRO:C	1:B:357:ASP:N	2.67	0.51
1:A:59:PRO:HG2	1:A:155:MET:HE3	1.93	0.51
1:A:326:VAL:HG12	1:A:326:VAL:O	2.10	0.51
1:B:264:LEU:HD11	1:B:287:ILE:CG2	2.40	0.51
1:A:34:LYS:HA	1:A:50:LEU:O	2.11	0.50
1:A:170:LEU:O	1:A:176:THR:HA	2.10	0.50
1:A:374:TRP:CE3	5:A:503:PGE:H4	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PRO:HG2	1:B:317:VAL:HG12	1.92	0.50
1:B:208:GLU:O	1:B:208:GLU:HG3	2.09	0.50
1:B:237:LEU:HD22	1:B:239:MET:HE2	1.93	0.50
1:B:346:THR:O	1:B:346:THR:HG22	2.12	0.49
1:A:342:THR:CG2	1:A:343:LEU:N	2.75	0.49
1:B:268:LEU:HB3	1:B:273:LYS:HB3	1.93	0.49
1:A:217:ALA:HB3	4:A:502:AMP:O2'	2.11	0.49
1:A:330:GLN:O	1:A:330:GLN:NE2	2.45	0.49
1:A:221:GLU:O	1:A:224:ILE:HG13	2.13	0.49
1:B:94:THR:HG21	1:B:128:PHE:CE2	2.48	0.49
1:A:377:LEU:O	1:A:378:ARG:C	2.55	0.48
1:B:74:GLU:OE2	1:B:75:GLY:N	2.46	0.48
1:A:67:ASP:OD2	1:A:89:ARG:HD2	2.13	0.48
1:A:314:PHE:O	1:A:315:LYS:C	2.55	0.48
1:B:221:GLU:O	1:B:224:ILE:HG23	2.13	0.48
1:A:227:ASP:OD1	1:A:230:ASP:HB3	2.13	0.48
1:A:73:ASP:OD1	1:A:80:THR:HB	2.14	0.48
1:B:264:LEU:HD11	1:B:287:ILE:HG21	1.95	0.48
1:A:302:LYS:O	1:A:306:VAL:HG13	2.14	0.48
1:B:320:PHE:HD2	1:B:351:PHE:HD2	1.55	0.48
1:B:169:LEU:HD22	1:B:303:LEU:HD11	1.95	0.48
1:B:72:ILE:CG2	1:B:89:ARG:HH22	2.20	0.48
1:B:318:ARG:HG2	1:B:318:ARG:NH2	2.24	0.48
1:A:274:THR:O	1:A:275:GLU:C	2.56	0.47
1:B:244:LYS:C	1:B:246:SER:H	2.23	0.47
1:B:347:SER:C	1:B:348:PHE:O	2.56	0.47
2:C:2:C:O2'	2:C:3:C:H5'	2.13	0.47
1:B:246:SER:HB2	1:B:305:HIS:NE2	2.29	0.47
1:A:55:LYS:NZ	5:A:503:PGE:C5	2.77	0.47
1:B:152:ILE:CG2	1:B:153:PRO:HD3	2.45	0.47
1:B:33:TYR:OH	1:B:375:GLU:OE2	2.27	0.47
1:A:406:GLN:C	1:A:407:LEU:OXT	2.58	0.47
1:B:72:ILE:HD12	1:B:89:ARG:HH12	1.78	0.47
1:B:196:ILE:HD11	1:B:201:SER:HB3	1.97	0.47
1:B:67:ASP:OD1	1:B:67:ASP:C	2.57	0.46
1:B:206:GLY:HA2	1:B:220:MET:HE2	1.96	0.46
1:B:289:TYR:O	1:B:293:GLU:HB2	2.16	0.46
1:A:231:GLN:O	1:A:233:PHE:N	2.49	0.46
1:A:324:GLY:O	1:A:327:SER:OG	2.32	0.46
1:B:333:ARG:HG2	1:B:353:TYR:CE2	2.51	0.46
1:B:39:GLU:HB3	1:B:46:CYS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLU:HB3	1:A:267:ASN:HD21	1.80	0.46
1:A:35:VAL:HG21	1:A:371:ILE:HD11	1.99	0.45
1:A:239:MET:HE1	1:A:264:LEU:HA	1.97	0.45
1:A:293:GLU:OE1	1:A:331:ARG:HD3	2.15	0.45
1:A:67:ASP:OD2	1:A:89:ARG:CD	2.65	0.45
1:A:184:ILE:O	1:A:187:HIS:NE2	2.41	0.45
1:A:153:PRO:HG2	1:A:321:VAL:HG11	1.98	0.45
1:A:239:MET:HE2	1:A:263:ALA:HB1	1.99	0.45
1:A:332:LEU:O	1:A:333:ARG:C	2.59	0.45
1:B:356:MET:HA	1:B:359:CYS:CB	2.41	0.45
1:B:243:LEU:O	1:B:246:SER:N	2.42	0.45
1:A:152:ILE:CG2	1:A:153:PRO:HD3	2.47	0.44
1:A:227:ASP:OD1	1:A:230:ASP:HB2	2.17	0.44
1:A:188:GLU:OE2	1:A:313:LYS:CE	2.65	0.44
1:B:280:PRO:C	1:B:282:ARG:N	2.75	0.44
1:A:392:PRO:O	1:A:395:ASP:N	2.47	0.44
1:B:152:ILE:N	1:B:153:PRO:CD	2.80	0.44
1:A:152:ILE:HG22	1:A:153:PRO:HD3	2.00	0.44
1:B:165:PRO:CG	1:B:317:VAL:HG12	2.48	0.44
1:A:89:ARG:O	1:A:93:LEU:HB2	2.18	0.43
1:A:330:GLN:HE22	1:A:334:THR:HG23	1.83	0.43
1:A:395:ASP:O	1:A:396:LEU:C	2.61	0.43
1:B:222:LYS:C	1:B:226:GLN:NE2	2.76	0.43
1:A:153:PRO:HG3	1:A:354:PRO:CG	2.49	0.43
1:B:355:PRO:CG	1:B:358:LEU:HD12	2.48	0.43
1:B:245:ASN:HD22	1:B:245:ASN:HA	1.55	0.43
1:B:178:PHE:HE1	1:B:320:PHE:CE1	2.34	0.43
1:B:244:LYS:C	1:B:246:SER:N	2.75	0.43
1:B:340:LEU:C	1:B:342:THR:H	2.27	0.43
1:B:268:LEU:HB3	1:B:273:LYS:CB	2.49	0.43
1:B:326:VAL:O	1:B:326:VAL:HG12	2.18	0.43
1:A:239:MET:CE	1:A:263:ALA:C	2.91	0.43
1:A:171:VAL:HG12	1:A:176:THR:HG23	2.01	0.43
1:A:194:ILE:HG12	1:A:255:PHE:O	2.19	0.43
1:B:231:GLN:NE2	1:B:285:ARG:O	2.52	0.42
1:A:222:LYS:O	1:A:223:PHE:C	2.62	0.42
1:A:242:PRO:O	1:A:244:LYS:N	2.52	0.42
1:B:318:ARG:NH2	1:B:318:ARG:CG	2.82	0.42
1:B:317:VAL:O	1:B:317:VAL:CG2	2.67	0.42
1:A:147:LEU:HD23	1:A:373:ILE:HD11	2.01	0.42
1:A:38:ILE:CG2	1:A:112:VAL:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:CG2	1:B:320:PHE:HD1	2.28	0.42
1:B:275:GLU:C	1:B:277:GLN:N	2.77	0.42
1:A:168:SER:HA	1:A:321:VAL:O	2.19	0.42
1:A:300:ILE:HG21	1:A:339:GLU:HB2	2.02	0.42
1:A:339:GLU:O	1:A:340:LEU:HD23	2.20	0.42
1:B:68:THR:OG1	1:B:71:SER:CB	2.67	0.42
1:B:152:ILE:O	1:B:154:ARG:N	2.53	0.42
1:A:38:ILE:HG22	1:A:112:VAL:HG23	2.01	0.42
1:A:173:GLY:HA2	1:A:199:GLY:HA3	2.02	0.42
1:A:324:GLY:C	1:A:359:CYS:HB3	2.45	0.41
1:B:222:LYS:HA	1:B:225:ASN:HD22	1.85	0.41
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.91	0.41
1:B:169:LEU:HG	1:B:171:VAL:HG13	2.01	0.41
1:B:243:LEU:H	1:B:243:LEU:HG	1.51	0.41
1:B:237:LEU:HD11	1:B:290:GLN:HB3	2.03	0.41
1:B:148:GLY:O	1:B:149:HIS:C	2.63	0.41
1:B:278:GLU:H	1:B:278:GLU:CD	2.29	0.41
1:A:40:THR:HG21	1:A:125:GLY:N	2.32	0.41
1:A:153:PRO:HG3	1:A:354:PRO:HG3	2.03	0.41
1:A:274:THR:O	1:A:277:GLN:N	2.52	0.41
1:A:378:ARG:CG	1:A:407:LEU:HD23	2.51	0.41
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.88	0.41
1:B:223:PHE:O	1:B:285:ARG:HD3	2.21	0.41
1:A:235:LEU:O	1:A:236:LYS:C	2.63	0.41
1:A:324:GLY:O	1:A:325:GLY:C	2.64	0.41
1:B:321:VAL:HG11	9:B:603:HOH:O	2.21	0.41
1:B:245:ASN:OD1	1:B:253:LEU:CD2	2.69	0.40
1:B:340:LEU:O	1:B:342:THR:N	2.54	0.40
1:A:367:GLY:O	1:A:371:ILE:HG12	2.20	0.40
1:B:164:PHE:CE2	1:B:184:ILE:HG13	2.56	0.40
1:A:36:LEU:HD12	1:A:48:SER:O	2.21	0.40
1:B:320:PHE:CE2	1:B:351:PHE:HE2	2.39	0.40
1:B:198:VAL:HG13	1:B:199:GLY:N	2.36	0.40
1:A:152:ILE:N	1:A:153:PRO:CD	2.85	0.40
1:A:242:PRO:C	1:A:244:LYS:HD2	2.46	0.40
1:A:269:THR:O	1:A:271:LEU:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:ASP:OD1	1:B:313:LYS:NZ[23_654]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	376/383 (98%)	316 (84%)	46 (12%)	14 (4%)	2	6
1	B	376/383 (98%)	323 (86%)	42 (11%)	11 (3%)	3	9
All	All	752/766 (98%)	639 (85%)	88 (12%)	25 (3%)	3	7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	ASP
1	A	242	PRO
1	A	273	LYS
1	A	399	VAL
1	B	242	PRO
1	B	276	ILE
1	B	348	PHE
1	A	77	ILE
1	A	226	GLN
1	A	243	LEU
1	A	270	LYS
1	B	232	ASP
1	A	232	ASP
1	A	240	PRO
1	A	354	PRO
1	A	405	ASP
1	B	76	GLY
1	B	230	ASP
1	B	247	ALA
1	A	276	ILE

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Mol	Chain	Res	Type
1	B	341	GLY
1	B	347	SER
1	B	354	PRO
1	A	76	GLY
1	B	213	GLY

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	
1	A	330/334 (99%)	303 (92%)	27 (8%)	10	26
1	B	330/334 (99%)	296 (90%)	34 (10%)	7	18
All	All	660/668 (99%)	599 (91%)	61 (9%)	8	22

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	40	THR
1	A	72	ILE
1	A	77	ILE
1	A	81	LYS
1	A	94	THR
1	A	105	GLU
1	A	170	LEU
1	A	209	LEU
1	A	212	LYS
1	A	235	LEU
1	A	242	PRO
1	A	244	LYS
1	A	245	ASN
1	A	249	LYS
1	A	251	ASN
1	A	267	ASN
1	A	273	LYS

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Mol	Chain	Res	Type
1	A	291	VAL
1	A	306	VAL
1	A	331	ARG
1	A	334	THR
1	A	339	GLU
1	A	356	MET
1	A	393	LEU
1	A	404	THR
1	A	407	LEU
1	B	45	THR
1	B	67	ASP
1	B	70	ASP
1	B	73	ASP
1	B	78	ILE
1	B	94	THR
1	B	140	LEU
1	B	168	SER
1	B	170	LEU
1	B	175	HIS
1	B	177	THR
1	B	204	LYS
1	B	216	ILE
1	B	224	ILE
1	B	230	ASP
1	B	237	LEU
1	B	242	PRO
1	B	243	LEU
1	B	245	ASN
1	B	268	LEU
1	B	271	LEU
1	B	276	ILE
1	B	277	GLN
1	B	278	GLU
1	B	279	LEU
1	B	298	HIS
1	B	317	VAL
1	B	318	ARG
1	B	343	LEU
1	B	345	SER
1	B	346	THR
1	B	347	SER
1	B	348	PHE

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Mol	Chain	Res	Type
1	B	389	ARG

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

Mol	Chain	Res	Type
1	A	60	ASN
1	A	83	HIS
1	A	85	HIS
1	A	175	HIS
1	A	229	ASN
1	A	245	ASN
1	A	305	HIS
1	A	330	GLN
1	A	344	ASN
1	A	390	GLN
1	B	87	GLN
1	B	226	GLN
1	B	251	ASN
1	B	267	ASN
1	B	301	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	2/4 (50%)	1 (50%)	2 (100%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	2	C
2	C	3	C

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
7	SO4	B	503	-	4,4,4	0.49	0	6,6,6	0.21	0
6	ATP	A	504	-	32,33,33	2.38	7 (21%)	48,52,52	2.20	15 (31%)
4	AMP	A	502	-	25,25,25	1.80	5 (20%)	37,38,38	2.72	14 (37%)
8	ACT	B	504	-	3,3,3	0.78	0	3,3,3	0.80	0
5	PGE	A	503	-	9,9,9	0.80	0	8,8,8	1.09	0
4	AMP	B	502	-	25,25,25	1.67	5 (20%)	37,38,38	2.02	12 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	A	504	-	-	5/22/38/38	0/3/3/3
5	PGE	A	503	-	-	4/7/7/7	-
4	AMP	A	502	-	-	4/10/26/26	0/3/3/3
4	AMP	B	502	-	-	2/10/26/26	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	504	ATP	PB-O3B	8.76	1.69	1.59
4	A	502	AMP	C5-C4	5.31	1.48	1.39
4	B	502	AMP	C5-C4	5.09	1.48	1.39
6	A	504	ATP	PB-O3A	4.87	1.64	1.59
6	A	504	ATP	C5-C4	4.78	1.47	1.39
6	A	504	ATP	PA-O3A	4.61	1.64	1.59
4	A	502	AMP	C5-C6	4.05	1.52	1.41
4	B	502	AMP	C5-C6	3.27	1.50	1.41
6	A	504	ATP	C5-N7	-3.05	1.33	1.39
4	B	502	AMP	C4-N9	-2.91	1.31	1.37
4	B	502	AMP	C8-N7	2.77	1.37	1.31
4	A	502	AMP	C5-N7	-2.48	1.34	1.39
4	B	502	AMP	C5-N7	-2.37	1.34	1.39
6	A	504	ATP	C8-N7	2.30	1.36	1.31
6	A	504	ATP	C1'-N9	2.20	1.52	1.46
4	A	502	AMP	C2-N3	2.18	1.37	1.33
4	A	502	AMP	C8-N7	2.16	1.35	1.31

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	AMP	C5-C4-N3	-8.44	115.10	126.72
6	A	504	ATP	C5-C4-N3	-6.78	117.39	126.72
4	A	502	AMP	N3-C4-N9	5.89	137.18	127.17
6	A	504	ATP	N3-C4-N9	5.73	136.92	127.17
4	A	502	AMP	C4-C5-N7	-5.55	104.23	110.58
4	B	502	AMP	O3P-P-O5'	-4.90	93.89	106.67
4	A	502	AMP	C2-N3-C4	4.61	123.08	111.83
6	A	504	ATP	N3-C2-N1	-4.57	121.66	128.58
4	B	502	AMP	C5-C4-N3	-4.53	120.48	126.72
6	A	504	ATP	C2-N3-C4	4.32	122.39	111.83
4	A	502	AMP	C5-N7-C8	4.13	109.94	103.45
4	B	502	AMP	C4-C5-N7	-4.05	105.95	110.58
6	A	504	ATP	C2'-C1'-N9	3.79	122.72	113.30
4	A	502	AMP	O4'-C1'-C2'	-3.43	99.28	106.62
4	A	502	AMP	O4'-C1'-N9	3.37	114.57	108.09
4	B	502	AMP	C4-N9-C8	3.34	109.24	105.74
4	B	502	AMP	N3-C4-N9	3.27	132.74	127.17
4	B	502	AMP	C2-N3-C4	3.17	119.56	111.83
6	A	504	ATP	C1'-N9-C8	-3.16	120.09	127.09
6	A	504	ATP	C3'-C2'-C1'	3.13	107.39	101.46
4	B	502	AMP	N3-C2-N1	-3.04	123.97	128.58
6	A	504	ATP	O3G-PG-O1G	2.89	122.09	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	AMP	O3P-P-O1P	2.77	121.64	110.83
4	B	502	AMP	O3P-P-O2P	2.77	118.18	107.80
4	A	502	AMP	C4'-O4'-C1'	-2.69	103.53	109.47
4	B	502	AMP	C5-N7-C8	2.67	107.65	103.45
4	A	502	AMP	N3-C2-N1	-2.66	124.55	128.58
4	B	502	AMP	C6-C5-N7	2.65	137.19	132.09
6	A	504	ATP	C4-N9-C1'	2.54	132.56	126.63
4	B	502	AMP	N9-C8-N7	-2.51	110.38	113.94
4	A	502	AMP	O2'-C2'-C1'	2.44	118.49	110.10
4	A	502	AMP	O3P-P-O5'	-2.35	100.55	106.67
6	A	504	ATP	C4-C5-N7	-2.32	107.93	110.58
6	A	504	ATP	O3'-C3'-C2'	2.27	119.09	111.82
4	B	502	AMP	C2-N1-C6	2.24	122.41	118.73
6	A	504	ATP	C5-N7-C8	2.21	106.93	103.45
6	A	504	ATP	C2-N1-C6	2.20	122.34	118.73
4	A	502	AMP	O4'-C4'-C5'	2.19	116.35	109.33
6	A	504	ATP	N6-C6-N1	2.09	123.03	118.38
6	A	504	ATP	C2'-C3'-C4'	-2.09	98.57	102.61
4	A	502	AMP	O5'-P-O1P	-2.04	100.93	106.44

There are no chirality outliers.

All (15) torsion outliers are listed below:

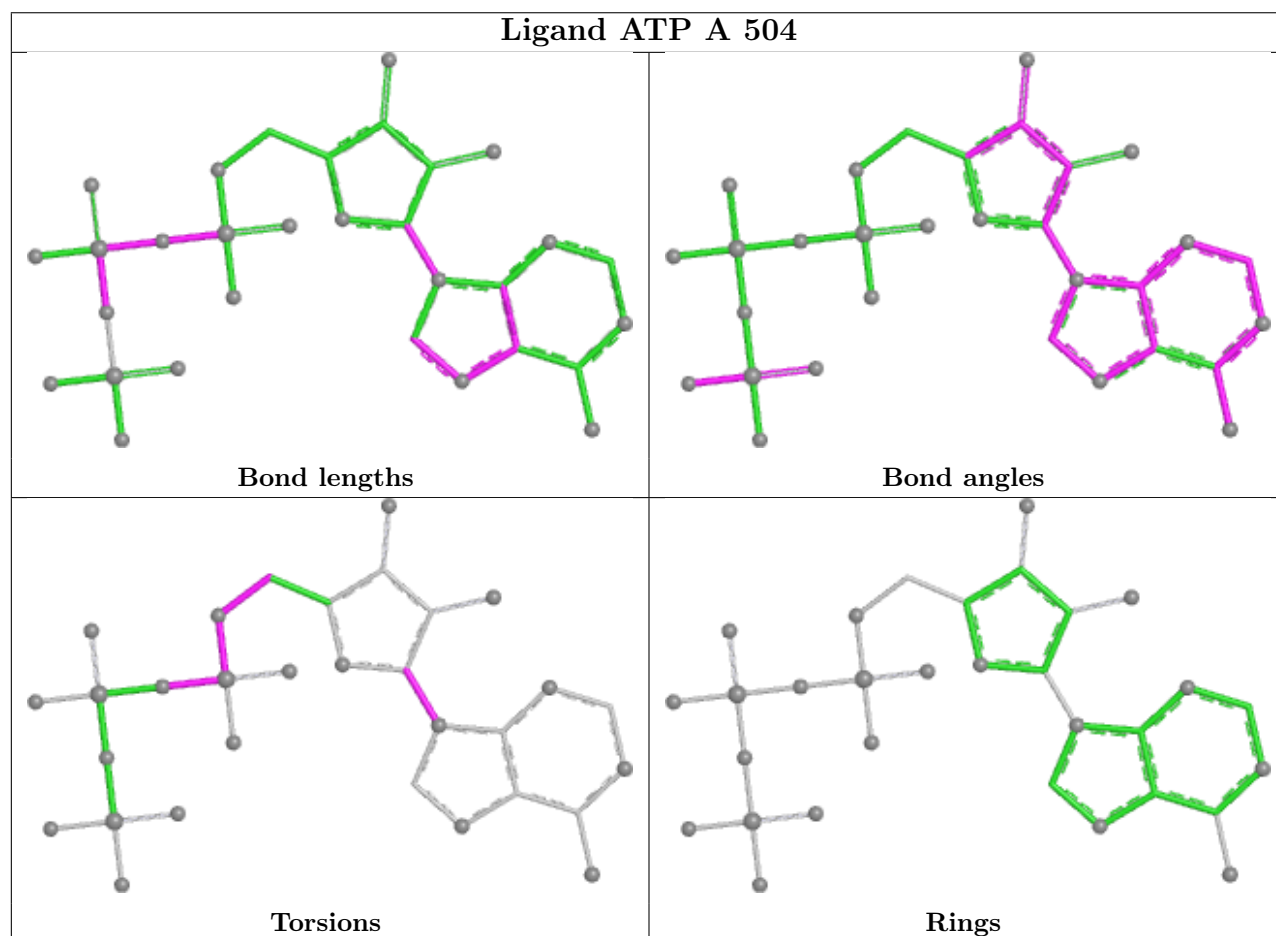
Mol	Chain	Res	Type	Atoms
4	A	502	AMP	C5'-O5'-P-O2P
4	A	502	AMP	C5'-O5'-P-O3P
4	B	502	AMP	O4'-C4'-C5'-O5'
4	B	502	AMP	C3'-C4'-C5'-O5'
5	A	503	PGE	O2-C3-C4-O3
5	A	503	PGE	O1-C1-C2-O2
6	A	504	ATP	C2'-C1'-N9-C4
6	A	504	ATP	C4'-C5'-O5'-PA
4	A	502	AMP	C5'-O5'-P-O1P
6	A	504	ATP	C2'-C1'-N9-C8
5	A	503	PGE	O3-C5-C6-O4
6	A	504	ATP	C5'-O5'-PA-O3A
5	A	503	PGE	C1-C2-O2-C3
4	A	502	AMP	C3'-C4'-C5'-O5'
6	A	504	ATP	PB-O3A-PA-O2A

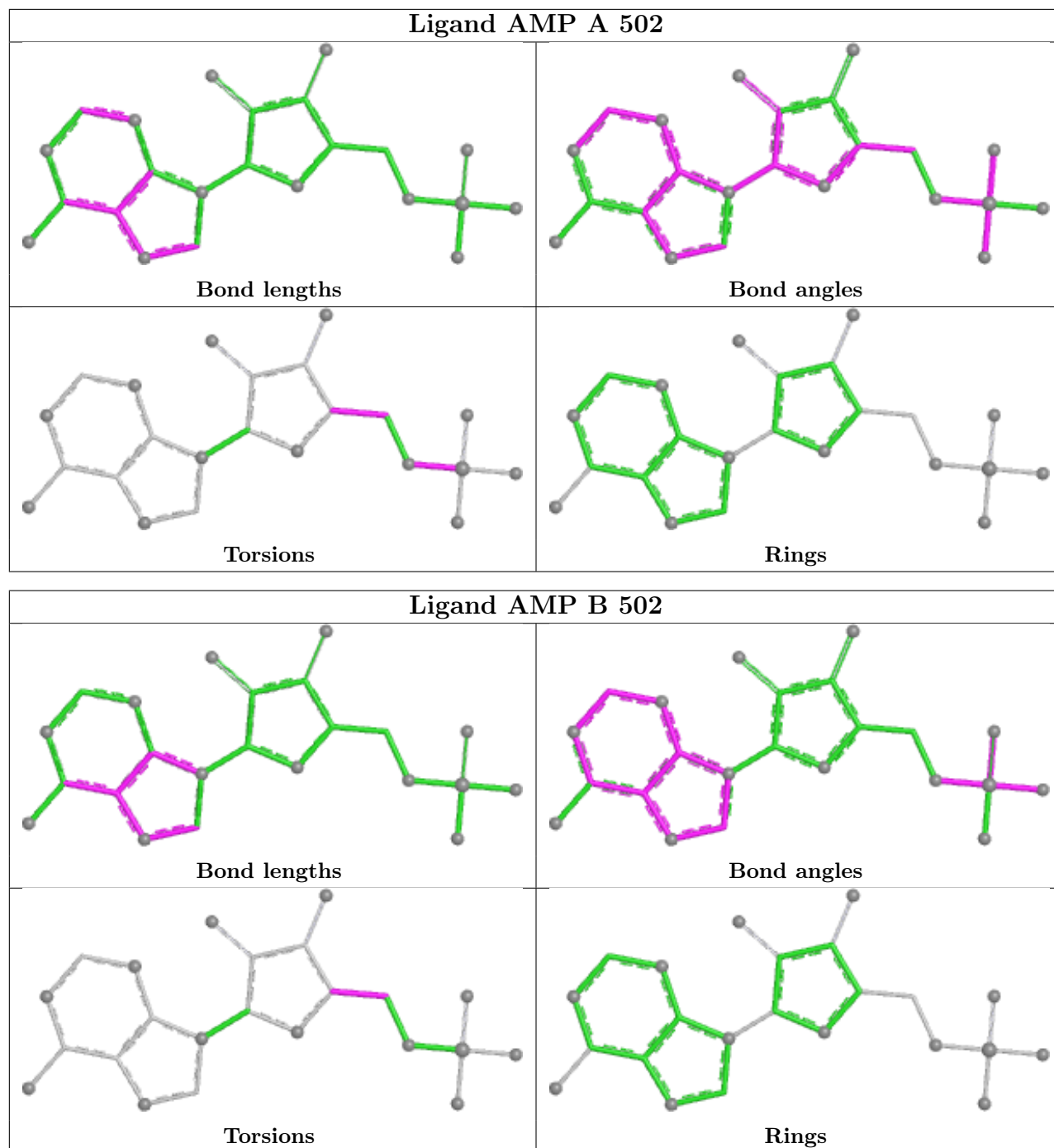
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	AMP	3	0
5	A	503	PGE	4	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 [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](#)

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	A	378/383 (98%)	-0.26	4 (1%) 78 72	52, 92, 187, 247	0
1	B	378/383 (98%)	-0.12	7 (1%) 66 58	57, 92, 185, 291	0
2	C	4/4 (100%)	-0.11	0 100 100	148, 170, 193, 224	0
All	All	760/770 (98%)	-0.19	11 (1%) 73 66	52, 92, 188, 291	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	80	THR	5.2
1	B	242	PRO	3.7
1	B	247	ALA	3.1
1	A	407	LEU	2.7
1	B	88	ALA	2.6
1	A	387	PRO	2.5
1	B	79	PRO	2.5
1	B	243	LEU	2.5
1	A	72	ILE	2.3
1	A	243	LEU	2.2
1	B	284	ILE	2.1

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

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

6.3 Carbohydrates [i](#)

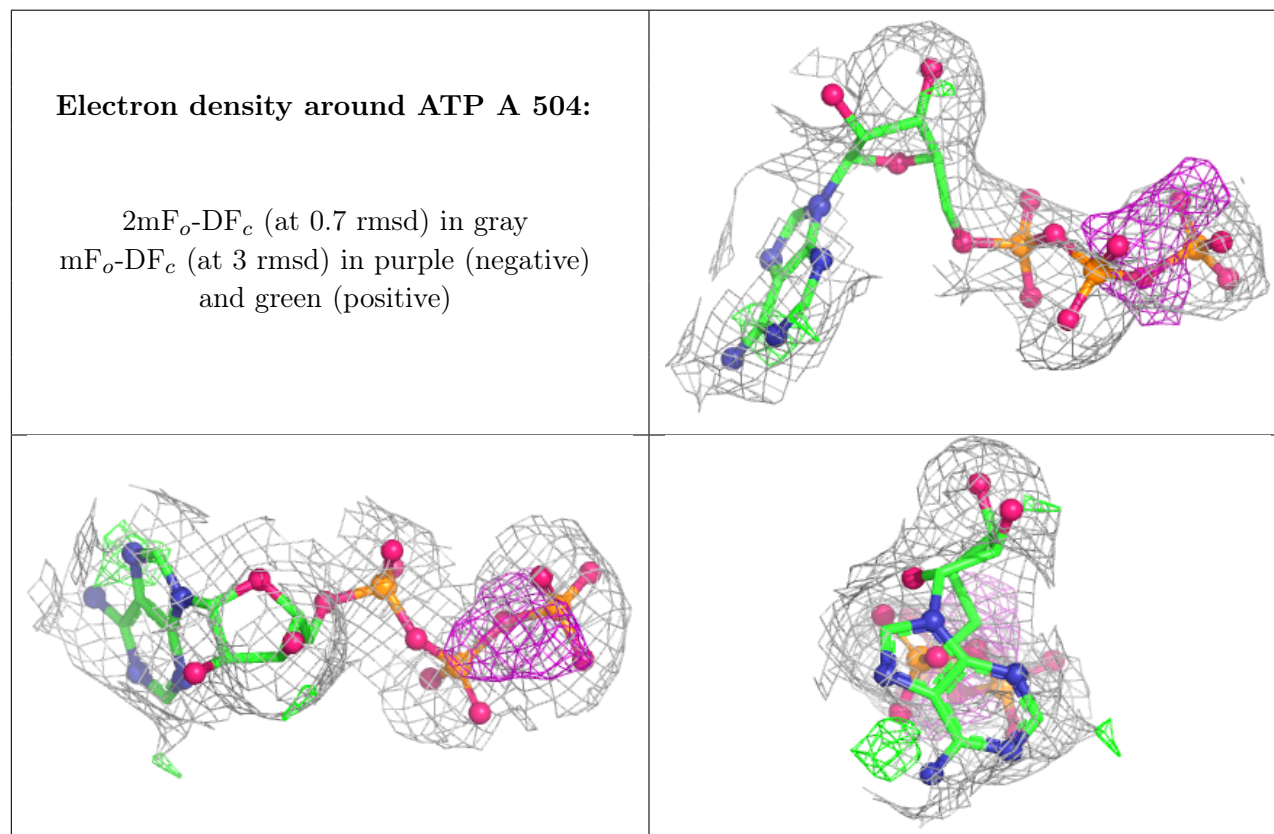
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

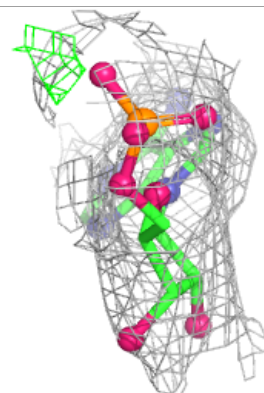
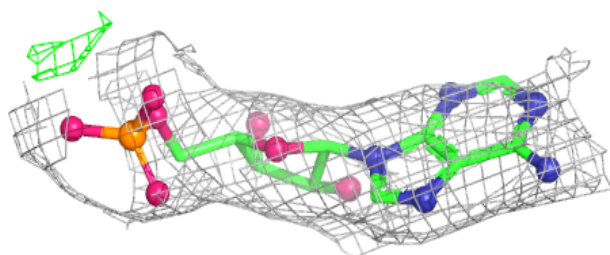
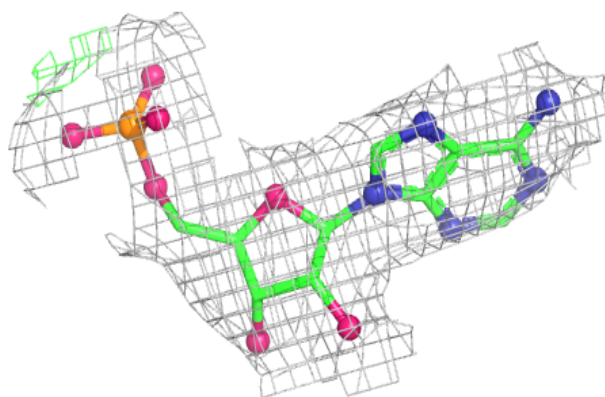
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	ATP	A	504	31/31	0.61	0.13	83,152,223,264	0
7	SO4	B	503	5/5	0.70	0.07	130,156,170,175	0
8	ACT	B	504	4/4	0.78	0.09	95,108,116,121	0
5	PGE	A	503	10/10	0.91	0.10	75,85,102,102	0
4	AMP	A	502	23/23	0.92	0.08	89,102,114,118	0
4	AMP	B	502	23/23	0.93	0.08	88,107,116,120	0
3	ZN	A	501	1/1	0.99	0.04	99,99,99,99	0
3	ZN	B	501	1/1	1.00	0.03	93,93,93,93	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.

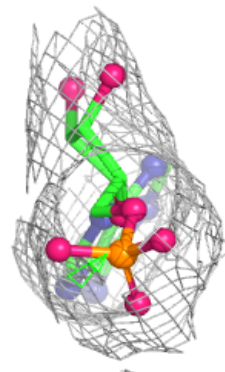
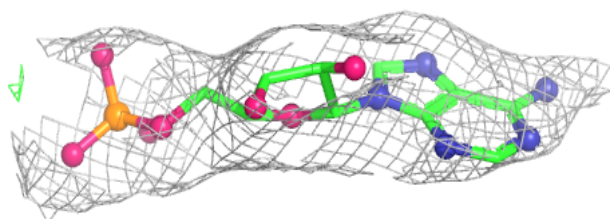
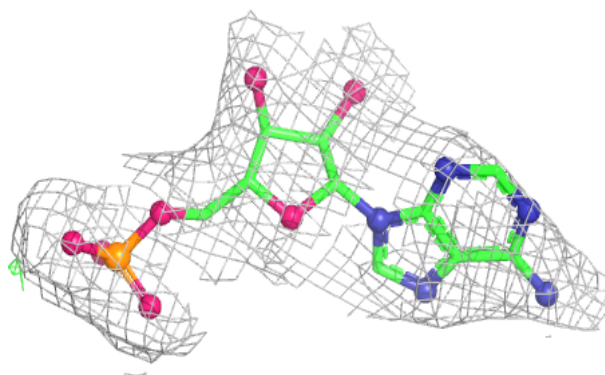


Electron density around AMP A 502:

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

**Electron density around AMP B 502:**

$2mF_o-DF_c$ (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.