Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 01:48 PM JST

PDB ID	:	5F1C
Title	:	Crystal structure of an invertebrate P2X receptor from the Gulf Coast tick in the presence of ATP and Zn2+ ion at 2.9 Angstroms
Authors	:	Kasuya, G.; Hattori, M.; Ishitani, R.; Nureki, O.
Deposited on	:	2015-11-30
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

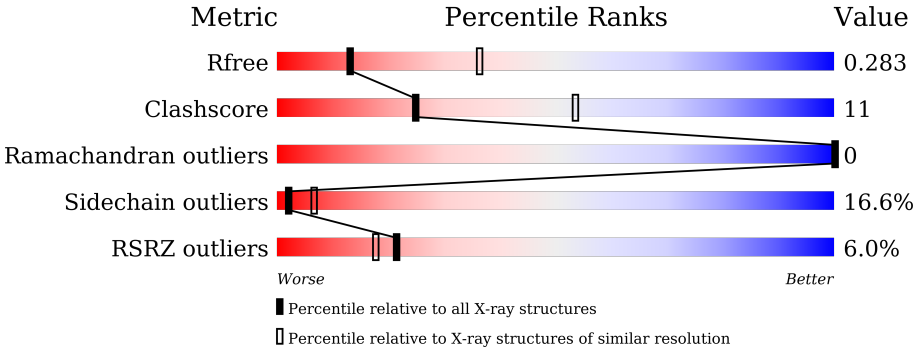
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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% 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	358	5% 66% 25% 5% •
1	B	358	3% 66% 28% 5% •
1	C	358	9% 65% 27% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8095 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 Putative uncharacterized protein.

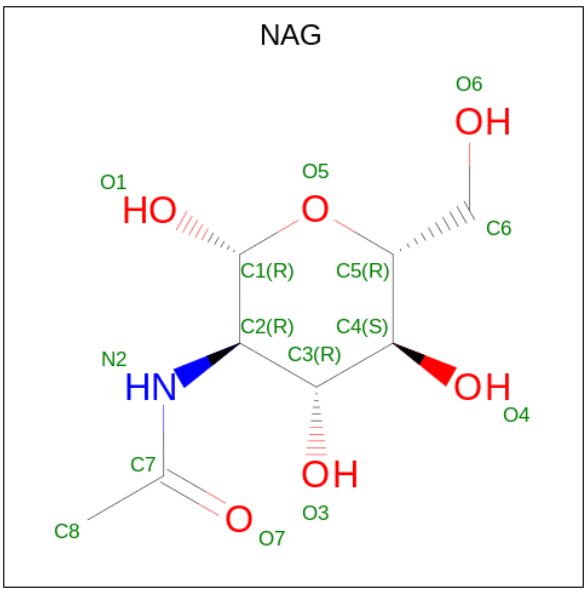
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2569	1646	426	482	15	0	0	0
1	B	355	2669	1709	442	504	14	0	0	0
1	C	344	2562	1641	425	482	14	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP G3MM57
A	20	SER	-	expression tag	UNP G3MM57
A	21	ARG	-	expression tag	UNP G3MM57
A	22	GLU	-	expression tag	UNP G3MM57
A	23	PHE	-	expression tag	UNP G3MM57
A	171	GLN	ASN	engineered mutation	UNP G3MM57
A	374	LEU	CYS	engineered mutation	UNP G3MM57
B	19	GLY	-	expression tag	UNP G3MM57
B	20	SER	-	expression tag	UNP G3MM57
B	21	ARG	-	expression tag	UNP G3MM57
B	22	GLU	-	expression tag	UNP G3MM57
B	23	PHE	-	expression tag	UNP G3MM57
B	171	GLN	ASN	engineered mutation	UNP G3MM57
B	374	LEU	CYS	engineered mutation	UNP G3MM57
C	19	GLY	-	expression tag	UNP G3MM57
C	20	SER	-	expression tag	UNP G3MM57
C	21	ARG	-	expression tag	UNP G3MM57
C	22	GLU	-	expression tag	UNP G3MM57
C	23	PHE	-	expression tag	UNP G3MM57
C	171	GLN	ASN	engineered mutation	UNP G3MM57
C	374	LEU	CYS	engineered mutation	UNP G3MM57

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).

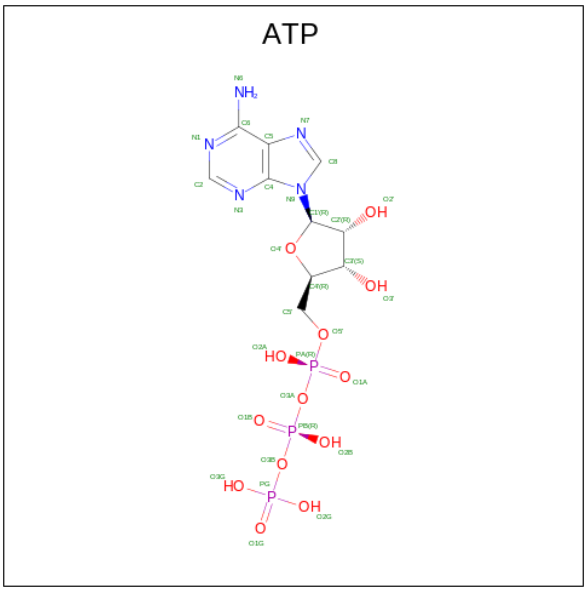


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
			Total	C	N	O		
2	B	1	14	8	1	5	0	0
			Total	C	N	O		
2	C	1	14	8	1	5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	6	6	6	0	0
			Total	Zn		
3	B	4	4	4	0	0
			Total	Zn		
3	C	3	3	3	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 5 is water.

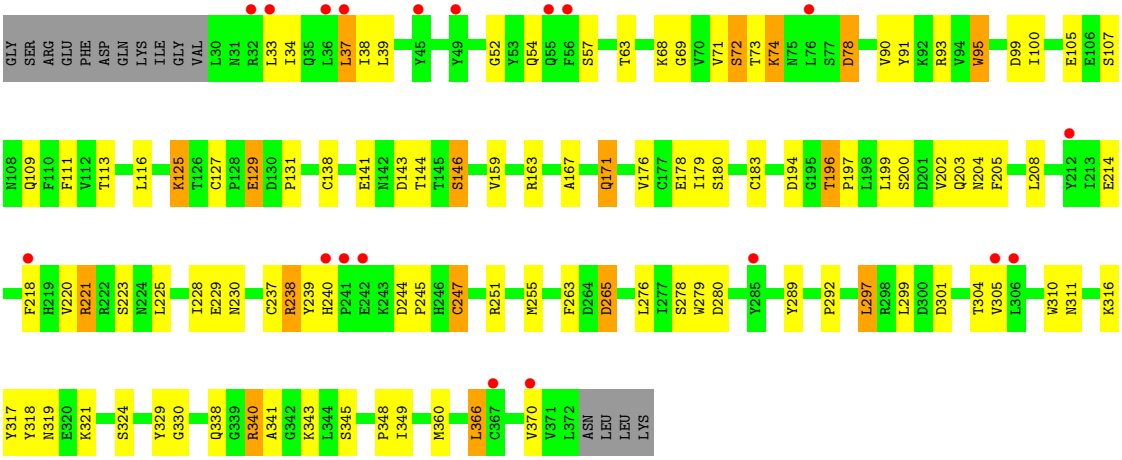
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	50	Total	O	0	0
			50	50		
5	C	31	Total	O	0	0
			31	31		

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 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.

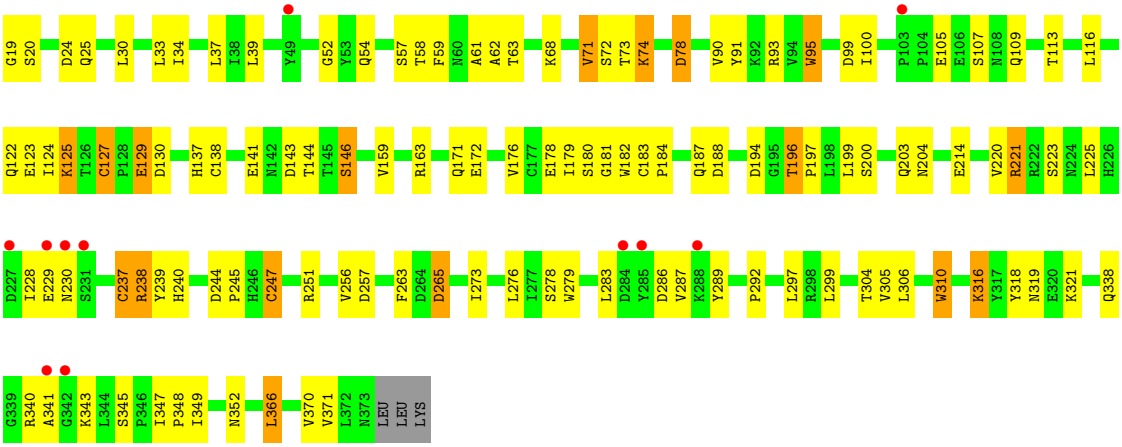
• Molecule 1: Putative uncharacterized protein

Chain A:



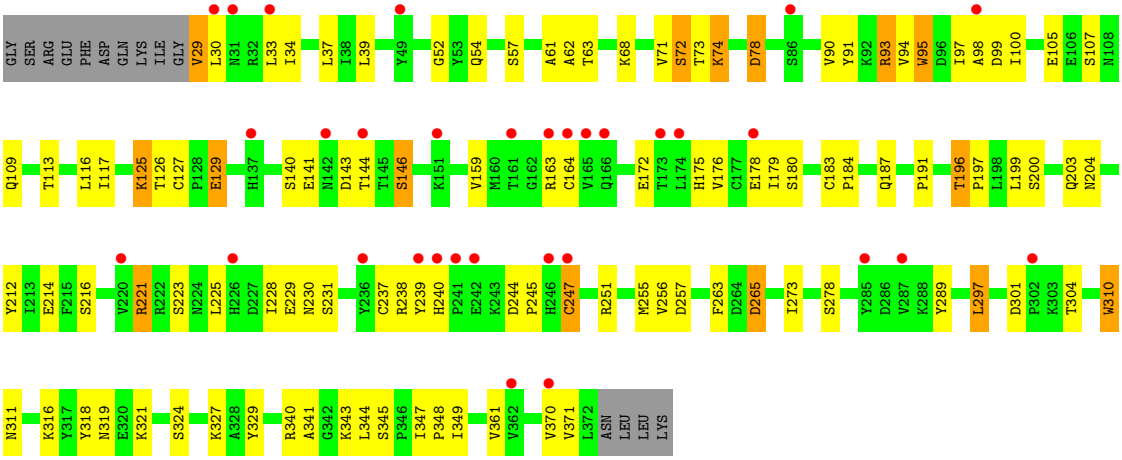
• Molecule 1: Putative uncharacterized protein

Chain B:



• Molecule 1: Putative uncharacterized protein

Chain C:


GLY SER ARG GLU PHE ASP GLN LYS ILE GLY V29 L30 N31 R32 L33 I34 L37 I38 L39 Y49 G52 Y53 Q54 S57 A61 A62 T63 K68 V71 S72 T73 K74 D78 S86 V90 Y91 K92 R93 V94 W95 D96 I97 A98 D99 I100 E105 E106 S107 N108
Q109 T113 L116 I117 K125 T126 C127 P128 E129 H137 S140 E141 N142 D143 T144 T145 S146 K151 V159 M160 T161 G162 R163 C164 V165 Q166 E172 T173 L174 H175 V176 C177 E178 I179 S180 C183 P184 Q187 P191 T196 P197 L198 L199 S200 Q203 N204
Y212 I213 E214 F215 S216 V220 R221 R222 S223 N224 L225 H226 D227 I228 E229 N230 S231 Y236 C237 R238 Y239 H240 P241 E242 K243 D244 P245 H246 C247 R251 M255 V256 D257 F263 D264 D265 I273 S278 Y285 D286 V287 K288 Y289 L297 D301 P302 K303 T304 W310
N311 K316 Y317 Y318 N319 E320 K321 S324 K327 A328 Y329 R340 A341 G342 K343 L344 S345 P346 I347 P348 I349 V361 V362 V370 V371 L372 ASN LEU LEU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.46Å 139.90Å 202.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.07 – 2.90 43.07 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.07-2.90) 99.1 (43.07-2.89)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.255 , 0.289 0.250 , 0.283	Depositor DCC
R_{free} test set	2000 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: ZN, ATP, NAG

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	0.68	3/2628 (0.1%)	0.77	0/3592
1	B	0.68	3/2729 (0.1%)	0.77	0/3729
1	C	0.65	0/2620	0.80	2/3586 (0.1%)
All	All	0.67	6/7977 (0.1%)	0.78	2/10907 (0.0%)

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	2
1	C	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	CYS	CB-SG	-8.18	1.68	1.82
1	B	138	CYS	CB-SG	-7.04	1.70	1.82
1	A	141	GLU	CG-CD	5.87	1.60	1.51
1	B	141	GLU	CG-CD	5.78	1.60	1.51
1	B	127	CYS	CB-SG	-5.69	1.72	1.81
1	A	138	CYS	CB-SG	-5.17	1.73	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	344	LEU	CA-CB-CG	5.09	127.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	29	VAL	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	TYR	Peptide
1	B	289	TYR	Peptide
1	B	371	VAL	Peptide
1	C	289	TYR	Peptide
1	C	371	VAL	Mainchain

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	A	2569	0	2416	60	0
1	B	2669	0	2524	64	0
1	C	2562	0	2399	55	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
2	C	14	0	13	0	0
3	A	6	0	0	0	0
3	B	4	0	0	0	0
3	C	3	0	0	0	0
4	A	31	0	12	2	0
4	B	31	0	12	2	0
4	C	31	0	12	3	0
5	A	38	0	0	2	0
5	B	50	0	0	6	0
5	C	31	0	0	5	0
All	All	8095	0	7440	167	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 11.

All (167) 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:B:19:GLY:N	1:B:24:ASP:OD2	2.06	0.87
1:B:34:ILE:HD13	1:B:366:LEU:HD13	1.63	0.80
1:B:214:GLU:OE2	5:B:501:HOH:O	2.02	0.75
1:A:34:ILE:HD13	1:A:366:LEU:HD13	1.68	0.75
1:B:214:GLU:HG3	1:B:221:ARG:HG2	1.69	0.74
1:B:194:ASP:O	5:B:502:HOH:O	2.06	0.74
1:C:214:GLU:HG3	1:C:221:ARG:HG2	1.71	0.72
1:A:125:LYS:HG3	1:A:183:CYS:HB2	1.72	0.72
1:A:71:VAL:HG22	1:A:95:TRP:HB2	1.72	0.71
1:A:214:GLU:HG3	1:A:221:ARG:HG2	1.70	0.71
1:A:73:THR:HG1	1:A:95:TRP:HZ3	1.39	0.70
1:C:318:TYR:O	5:C:501:HOH:O	2.09	0.69
1:C:71:VAL:HG22	1:C:95:TRP:HB2	1.75	0.69
1:B:125:LYS:HG3	1:B:183:CYS:HB2	1.73	0.69
1:B:306:LEU:HD11	1:C:231:SER:HA	1.75	0.68
1:A:69:GLY:N	5:A:501:HOH:O	2.19	0.67
1:C:125:LYS:HG3	1:C:183:CYS:HB2	1.78	0.66
1:B:71:VAL:HG22	1:B:95:TRP:HB2	1.76	0.66
1:B:137:HIS:HE1	5:B:536:HOH:O	1.79	0.65
4:B:407:ATP:C6	1:C:68:LYS:HD3	2.33	0.64
1:C:73:THR:OG1	1:C:95:TRP:HZ3	1.80	0.64
1:C:129:GLU:HG2	1:C:179:ILE:HG12	1.80	0.64
1:A:73:THR:OG1	1:A:95:TRP:HZ3	1.81	0.63
1:A:71:VAL:HG21	1:A:199:LEU:HD22	1.81	0.63
1:B:73:THR:OG1	1:B:95:TRP:HZ3	1.82	0.62
1:A:129:GLU:HG2	1:A:179:ILE:HG12	1.83	0.61
1:B:265:ASP:OD1	1:B:265:ASP:N	2.34	0.59
1:C:73:THR:HG1	1:C:95:TRP:HZ3	1.50	0.59
1:A:299:LEU:HB3	1:B:62:ALA:HB2	1.84	0.58
1:A:95:TRP:HD1	1:A:99:ASP:HB3	1.68	0.58
1:B:129:GLU:HG2	1:B:179:ILE:HG12	1.86	0.57
1:B:52:GLY:O	1:B:348:PRO:HB2	2.05	0.57
1:B:163:ARG:HD3	1:B:178:GLU:OE2	2.05	0.57
1:A:163:ARG:HD3	1:A:178:GLU:OE2	2.04	0.57
1:A:68:LYS:HD3	4:C:401:ATP:C6	2.40	0.56
1:A:78:ASP:OD1	1:A:78:ASP:N	2.37	0.56
1:C:71:VAL:HG21	1:C:199:LEU:HD22	1.88	0.56
1:A:265:ASP:N	1:A:265:ASP:OD1	2.38	0.56
1:C:78:ASP:N	1:C:78:ASP:OD1	2.39	0.55
1:C:265:ASP:OD1	1:C:265:ASP:N	2.38	0.55
4:B:407:ATP:C5	1:C:68:LYS:HD3	2.42	0.55
1:B:73:THR:HG1	1:B:95:TRP:HZ3	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASP:N	1:B:78:ASP:OD1	2.39	0.54
1:C:163:ARG:HD3	1:C:178:GLU:OE2	2.06	0.54
1:C:212:TYR:HE2	5:C:520:HOH:O	1.90	0.54
1:A:34:ILE:HG21	1:A:366:LEU:HD22	1.89	0.54
1:B:220:VAL:HG11	1:B:283:LEU:HD21	1.90	0.54
4:A:409:ATP:C5	1:B:68:LYS:HD3	2.43	0.53
1:B:310:TRP:HH2	1:C:105:GLU:HG3	1.73	0.53
1:C:143:ASP:OD2	1:C:146:SER:OG	2.27	0.53
4:A:409:ATP:C6	1:B:68:LYS:HD3	2.44	0.53
1:A:52:GLY:O	1:A:348:PRO:HB2	2.09	0.53
1:A:100:ILE:CD1	1:A:199:LEU:HD13	2.39	0.53
1:B:143:ASP:OD2	1:B:146:SER:OG	2.27	0.52
1:C:54:GLN:HG2	1:C:343:LYS:C	2.29	0.52
1:A:167:ALA:HB3	1:A:171:GLN:O	2.10	0.52
1:A:239:TYR:HB2	1:A:247:CYS:O	2.09	0.52
1:B:204:ASN:OD1	1:B:251:ARG:NH1	2.43	0.52
1:C:52:GLY:O	1:C:348:PRO:HB2	2.09	0.52
1:B:276:LEU:HD11	1:B:338:GLN:HG2	1.92	0.51
1:C:95:TRP:HD1	1:C:99:ASP:HB3	1.74	0.51
1:C:73:THR:OG1	1:C:91:TYR:O	2.26	0.51
1:A:54:GLN:HG2	1:A:343:LYS:C	2.31	0.51
1:B:95:TRP:HD1	1:B:99:ASP:HB3	1.76	0.51
1:B:237:CYS:O	1:B:238:ARG:NH1	2.45	0.50
1:A:38:ILE:HG21	1:A:360:MET:HG3	1.94	0.50
1:B:54:GLN:HG2	1:B:343:LYS:C	2.32	0.50
1:B:100:ILE:CD1	1:B:199:LEU:HD13	2.42	0.50
1:A:203:GLN:HB3	1:A:263:PHE:CZ	2.47	0.49
1:A:318:TYR:CG	1:C:319:ASN:HA	2.48	0.49
1:B:239:TYR:HB2	1:B:247:CYS:O	2.13	0.49
1:A:297:LEU:HD23	5:A:521:HOH:O	2.12	0.48
1:C:204:ASN:OD1	1:C:251:ARG:NH1	2.46	0.48
1:A:73:THR:OG1	1:A:91:TYR:O	2.32	0.48
1:B:123:GLU:HG3	1:B:125:LYS:HE3	1.94	0.48
1:B:130:ASP:OD1	5:B:503:HOH:O	2.20	0.48
1:B:196:THR:HG22	1:B:197:PRO:HD2	1.95	0.48
1:C:256:VAL:HG22	1:C:273:ILE:HD12	1.96	0.47
1:C:297:LEU:HD23	5:C:516:HOH:O	2.13	0.47
1:B:116:LEU:HD12	1:B:116:LEU:HA	1.64	0.47
1:B:214:GLU:HB3	5:B:501:HOH:O	2.14	0.47
1:A:228:ILE:HA	1:A:229:GLU:HA	1.59	0.47
1:B:34:ILE:HG21	1:B:366:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HD12	1:C:98:ALA:N	2.30	0.47
1:C:116:LEU:HD12	1:C:116:LEU:HA	1.57	0.47
1:C:117:ILE:HB	1:C:327:LYS:HB3	1.97	0.47
1:C:72:SER:OG	1:C:74:LYS:HG3	2.15	0.47
1:C:140:SER:HA	1:C:175:HIS:CG	2.50	0.47
1:C:228:ILE:HA	1:C:229:GLU:HA	1.60	0.46
1:A:299:LEU:HD13	1:B:61:ALA:O	2.15	0.46
1:B:71:VAL:HG21	1:B:199:LEU:HD22	1.96	0.46
1:C:191:PRO:HD2	5:C:507:HOH:O	2.15	0.46
1:C:127:CYS:SG	1:C:184:PRO:HA	2.56	0.46
1:A:204:ASN:OD1	1:A:251:ARG:NH1	2.45	0.46
1:B:299:LEU:HB3	1:C:62:ALA:HB2	1.97	0.46
1:C:196:THR:HG22	1:C:197:PRO:HD2	1.97	0.46
1:A:317:TYR:CD1	1:B:316:LYS:HE3	2.51	0.45
1:C:311:ASN:HB3	1:C:329:TYR:CD2	2.52	0.45
1:A:319:ASN:HA	1:B:318:TYR:CG	2.51	0.45
1:B:182:TRP:HB2	5:C:513:HOH:O	2.16	0.45
1:C:73:THR:OG1	1:C:95:TRP:CZ3	2.66	0.45
1:B:122:GLN:NE2	5:B:507:HOH:O	2.43	0.45
1:A:95:TRP:HD1	1:A:99:ASP:CB	2.29	0.45
1:B:113:THR:HG21	1:B:116:LEU:HD13	1.99	0.45
1:A:196:THR:HG22	1:A:197:PRO:HD2	1.98	0.45
1:B:256:VAL:HG22	1:B:273:ILE:HD12	1.99	0.45
1:A:218:PHE:HB2	1:A:220:VAL:HG12	1.98	0.45
1:B:345:SER:O	1:B:349:ILE:HG13	2.17	0.45
1:C:164:CYS:SG	1:C:175:HIS:HB3	2.57	0.45
1:B:228:ILE:HA	1:B:229:GLU:HA	1.57	0.45
1:C:125:LYS:HG3	1:C:183:CYS:CB	2.47	0.44
1:A:143:ASP:OD2	1:A:146:SER:OG	2.36	0.44
1:A:208:LEU:HD22	4:C:401:ATP:C8	2.53	0.44
1:A:57:SER:H	1:A:341:ALA:HB3	1.83	0.44
1:C:239:TYR:HB2	1:C:247:CYS:O	2.17	0.44
1:C:100:ILE:CD1	1:C:199:LEU:HD13	2.48	0.44
1:A:279:TRP:CE2	1:A:292:PRO:HB3	2.52	0.44
1:A:255:MET:HB2	1:A:255:MET:HE3	1.73	0.44
1:A:72:SER:OG	1:A:74:LYS:HG3	2.17	0.43
1:A:202:VAL:HA	1:A:205:PHE:CD1	2.53	0.43
1:C:239:TYR:CE1	1:C:245:PRO:HA	2.52	0.43
1:B:124:ILE:HA	1:B:181:GLY:O	2.18	0.43
1:B:347:ILE:H	1:B:347:ILE:HG13	1.53	0.43
1:A:311:ASN:HB3	1:A:329:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:SER:OG	1:B:74:LYS:HG3	2.18	0.43
1:A:310:TRP:HH2	1:B:105:GLU:HG3	1.83	0.43
1:C:141:GLU:OE1	1:C:175:HIS:NE2	2.52	0.43
1:B:239:TYR:CE1	1:B:245:PRO:HA	2.54	0.43
1:A:276:LEU:HD11	1:A:338:GLN:HG2	2.01	0.43
1:B:240:HIS:O	1:B:244:ASP:N	2.51	0.43
1:C:93:ARG:NH1	1:C:94:VAL:O	2.36	0.43
1:C:203:GLN:HB3	1:C:263:PHE:CZ	2.53	0.43
1:B:279:TRP:CZ3	1:B:292:PRO:HD3	2.53	0.43
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.65	0.42
1:B:95:TRP:HD1	1:B:99:ASP:CB	2.32	0.42
1:A:240:HIS:O	1:A:244:ASP:N	2.52	0.42
1:B:319:ASN:HA	1:C:318:TYR:CG	2.54	0.42
1:A:111:PHE:CZ	1:A:330:GLY:HA3	2.54	0.42
1:B:57:SER:H	1:B:341:ALA:HB3	1.83	0.42
1:A:34:ILE:HA	1:A:37:LEU:HB2	2.02	0.42
1:B:58:THR:OG1	1:B:59:PHE:N	2.53	0.42
1:C:345:SER:O	1:C:349:ILE:HG13	2.20	0.42
1:A:105:GLU:HG3	1:C:310:TRP:HH2	1.85	0.42
1:C:255:MET:HB2	1:C:255:MET:HE3	1.79	0.42
1:C:126:THR:HA	1:C:179:ILE:O	2.19	0.42
1:A:279:TRP:CD2	1:A:292:PRO:HB3	2.54	0.42
1:A:345:SER:O	1:A:349:ILE:HG13	2.20	0.42
1:A:237:CYS:O	1:A:238:ARG:NH1	2.52	0.42
1:B:286:ASP:OD1	1:B:287:VAL:N	2.52	0.42
1:A:194:ASP:O	1:A:196:THR:OG1	2.38	0.42
1:B:73:THR:OG1	1:B:91:TYR:O	2.35	0.42
1:C:240:HIS:O	1:C:244:ASP:N	2.52	0.42
1:B:299:LEU:HD13	1:C:61:ALA:O	2.20	0.41
1:C:113:THR:HG21	1:C:116:LEU:HD13	2.01	0.41
1:B:203:GLN:HB3	1:B:263:PHE:CZ	2.54	0.41
1:A:239:TYR:CE1	1:A:245:PRO:HA	2.55	0.41
1:C:57:SER:H	1:C:341:ALA:HB3	1.85	0.41
1:A:280:ASP:OD1	1:A:340:ARG:NH1	2.54	0.41
1:C:347:ILE:H	1:C:347:ILE:HG13	1.58	0.41
1:A:113:THR:HG21	1:A:116:LEU:HD13	2.03	0.41
1:A:238:ARG:HD3	1:A:238:ARG:HA	1.90	0.40
1:A:73:THR:OG1	1:A:95:TRP:CZ3	2.68	0.40
1:B:129:GLU:OE1	1:B:130:ASP:N	2.37	0.40
1:A:68:LYS:HD3	4:C:401:ATP:C5	2.56	0.40
1:B:19:GLY:HA2	1:B:20:SER:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:CYS:SG	1:B:184:PRO:HA	2.61	0.40
1:A:131:PRO:HG2	1:A:171:GLN:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/358 (95%)	327 (96%)	14 (4%)	0	100	100
1	B	353/358 (99%)	339 (96%)	14 (4%)	0	100	100
1	C	342/358 (96%)	328 (96%)	14 (4%)	0	100	100
All	All	1036/1074 (96%)	994 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/317 (84%)	225 (85%)	40 (15%)	3	9
1	B	278/317 (88%)	231 (83%)	47 (17%)	2	6
1	C	262/317 (83%)	215 (82%)	47 (18%)	2	5
All	All	805/951 (85%)	671 (83%)	134 (17%)	2	7

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	37	LEU
1	A	39	LEU
1	A	63	THR
1	A	72	SER
1	A	74	LYS
1	A	78	ASP
1	A	90	VAL
1	A	93	ARG
1	A	95	TRP
1	A	107	SER
1	A	109	GLN
1	A	125	LYS
1	A	129	GLU
1	A	144	THR
1	A	146	SER
1	A	159	VAL
1	A	171	GLN
1	A	176	VAL
1	A	180	SER
1	A	196	THR
1	A	200	SER
1	A	221	ARG
1	A	223	SER
1	A	225	LEU
1	A	230	ASN
1	A	238	ARG
1	A	247	CYS
1	A	265	ASP
1	A	278	SER
1	A	297	LEU
1	A	301	ASP
1	A	304	THR
1	A	305	VAL
1	A	316	LYS
1	A	321	LYS
1	A	324	SER
1	A	340	ARG
1	A	366	LEU
1	A	370	VAL
1	B	25	GLN
1	B	30	LEU

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Mol	Chain	Res	Type
1	B	33	LEU
1	B	37	LEU
1	B	39	LEU
1	B	63	THR
1	B	71	VAL
1	B	74	LYS
1	B	78	ASP
1	B	90	VAL
1	B	93	ARG
1	B	95	TRP
1	B	107	SER
1	B	109	GLN
1	B	125	LYS
1	B	129	GLU
1	B	144	THR
1	B	146	SER
1	B	159	VAL
1	B	171	GLN
1	B	172	GLU
1	B	176	VAL
1	B	180	SER
1	B	187	GLN
1	B	188	ASP
1	B	196	THR
1	B	200	SER
1	B	221	ARG
1	B	223	SER
1	B	225	LEU
1	B	230	ASN
1	B	237	CYS
1	B	238	ARG
1	B	247	CYS
1	B	257	ASP
1	B	265	ASP
1	B	278	SER
1	B	297	LEU
1	B	304	THR
1	B	305	VAL
1	B	310	TRP
1	B	316	LYS
1	B	321	LYS
1	B	340	ARG

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Mol	Chain	Res	Type
1	B	352	ASN
1	B	366	LEU
1	B	370	VAL
1	C	29	VAL
1	C	30	LEU
1	C	33	LEU
1	C	34	ILE
1	C	37	LEU
1	C	39	LEU
1	C	63	THR
1	C	72	SER
1	C	74	LYS
1	C	78	ASP
1	C	90	VAL
1	C	93	ARG
1	C	95	TRP
1	C	107	SER
1	C	109	GLN
1	C	125	LYS
1	C	129	GLU
1	C	144	THR
1	C	146	SER
1	C	159	VAL
1	C	172	GLU
1	C	176	VAL
1	C	180	SER
1	C	187	GLN
1	C	196	THR
1	C	200	SER
1	C	216	SER
1	C	221	ARG
1	C	223	SER
1	C	225	LEU
1	C	230	ASN
1	C	237	CYS
1	C	238	ARG
1	C	247	CYS
1	C	257	ASP
1	C	265	ASP
1	C	278	SER
1	C	297	LEU
1	C	301	ASP

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Mol	Chain	Res	Type
1	C	304	THR
1	C	310	TRP
1	C	316	LYS
1	C	321	LYS
1	C	324	SER
1	C	340	ARG
1	C	361	VAL
1	C	370	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	166	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 21 ligands modelled in this entry, 13 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
2	NAG	A	401	1	14,14,15	0.66	0	17,19,21	2.74	7 (41%)
4	ATP	A	409	3	26,33,33	1.09	2 (7%)	31,52,52	1.56	7 (22%)
2	NAG	C	402	1	14,14,15	0.58	0	17,19,21	1.45	2 (11%)
4	ATP	B	407	3	26,33,33	1.11	2 (7%)	31,52,52	1.50	6 (19%)
4	ATP	C	401	3	26,33,33	1.17	4 (15%)	31,52,52	1.48	5 (16%)
2	NAG	A	402	1	14,14,15	0.75	0	17,19,21	1.42	2 (11%)
2	NAG	B	401	1	14,14,15	0.71	1 (7%)	17,19,21	1.49	3 (17%)
2	NAG	B	402	1	14,14,15	1.03	2 (14%)	17,19,21	1.67	4 (23%)

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	NAG	A	401	1	-	4/6/23/26	0/1/1/1
4	ATP	A	409	3	-	1/18/38/38	0/3/3/3
2	NAG	C	402	1	-	2/6/23/26	0/1/1/1
4	ATP	B	407	3	-	5/18/38/38	0/3/3/3
4	ATP	C	401	3	-	6/18/38/38	0/3/3/3
2	NAG	A	402	1	-	4/6/23/26	0/1/1/1
2	NAG	B	401	1	-	4/6/23/26	0/1/1/1
2	NAG	B	402	1	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	ATP	C5-C4	3.03	1.49	1.40
4	B	407	ATP	C5-C4	2.94	1.48	1.40
4	A	409	ATP	C5-C4	2.90	1.48	1.40
4	B	407	ATP	C2-N3	2.33	1.35	1.32
4	A	409	ATP	C8-N7	2.28	1.38	1.34
2	B	402	NAG	C1-C2	2.25	1.55	1.52
4	C	401	ATP	C2'-C1'	-2.25	1.50	1.53
2	B	402	NAG	C3-C2	2.15	1.57	1.52
4	C	401	ATP	O4'-C4'	-2.06	1.40	1.45
2	B	401	NAG	C2-N2	-2.05	1.42	1.46
4	C	401	ATP	C2-N3	2.00	1.35	1.32

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NAG	C2-N2-C7	-6.41	113.77	122.90
2	A	401	NAG	C1-O5-C5	5.69	119.90	112.19
2	A	401	NAG	O5-C1-C2	4.61	118.57	111.29
4	C	401	ATP	PB-O3B-PG	-3.54	120.67	132.83
2	B	402	NAG	C4-C3-C2	3.51	116.16	111.02
4	B	407	ATP	N3-C2-N1	-3.18	123.70	128.68
4	A	409	ATP	C5-C6-N6	3.08	125.03	120.35
4	B	407	ATP	O3'-C3'-C2'	-2.99	102.14	111.82
2	C	402	NAG	O5-C5-C6	2.92	111.78	107.20
4	C	401	ATP	C2'-C3'-C4'	2.87	108.21	102.64
4	C	401	ATP	N3-C2-N1	-2.84	124.23	128.68
2	B	401	NAG	C1-C2-N2	-2.83	105.65	110.49
2	B	402	NAG	O5-C1-C2	-2.81	106.84	111.29
2	A	402	NAG	C1-O5-C5	2.78	115.96	112.19
4	A	409	ATP	O3'-C3'-C4'	-2.76	103.06	111.05
2	B	401	NAG	C4-C3-C2	-2.75	106.98	111.02
2	B	401	NAG	C1-O5-C5	2.74	115.90	112.19
4	B	407	ATP	C2-N1-C6	2.73	123.42	118.75
4	A	409	ATP	C4-C5-N7	-2.73	106.56	109.40
4	B	407	ATP	PB-O3B-PG	-2.71	123.52	132.83
2	A	401	NAG	C6-C5-C4	-2.58	106.97	113.00
4	A	409	ATP	N3-C2-N1	-2.57	124.66	128.68
2	C	402	NAG	C1-O5-C5	2.56	115.66	112.19
4	A	409	ATP	PB-O3B-PG	-2.50	124.26	132.83
2	A	401	NAG	O5-C5-C6	2.44	111.03	107.20
2	A	402	NAG	C1-C2-N2	2.37	114.54	110.49
4	A	409	ATP	O3G-PG-O2G	2.35	116.63	107.64
4	B	407	ATP	N6-C6-N1	2.31	123.38	118.57
2	B	402	NAG	O5-C5-C6	2.24	110.71	107.20
2	B	402	NAG	O7-C7-C8	-2.22	117.94	122.06
4	A	409	ATP	C2'-C3'-C4'	2.17	106.86	102.64
4	B	407	ATP	C2'-C3'-C4'	2.15	106.82	102.64
2	A	401	NAG	O3-C3-C4	-2.13	105.44	110.35
2	A	401	NAG	O3-C3-C2	2.10	113.81	109.47
4	C	401	ATP	C2-N1-C6	2.09	122.33	118.75
4	C	401	ATP	O3B-PG-O1G	-2.04	99.86	111.19

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	ATP	PB-O3B-PG-O2G
2	A	402	NAG	O5-C5-C6-O6
2	B	401	NAG	O5-C5-C6-O6
2	C	402	NAG	O5-C5-C6-O6
2	A	401	NAG	C8-C7-N2-C2
2	A	402	NAG	C4-C5-C6-O6
2	B	401	NAG	C4-C5-C6-O6
2	C	402	NAG	C4-C5-C6-O6
2	A	401	NAG	O7-C7-N2-C2
2	B	401	NAG	C8-C7-N2-C2
2	A	401	NAG	O5-C5-C6-O6
2	B	401	NAG	O7-C7-N2-C2
4	C	401	ATP	O4'-C4'-C5'-O5'
4	C	401	ATP	C3'-C4'-C5'-O5'
4	B	407	ATP	PB-O3B-PG-O1G
4	C	401	ATP	C4'-C5'-O5'-PA
2	A	402	NAG	C8-C7-N2-C2
4	B	407	ATP	PB-O3A-PA-O1A
4	B	407	ATP	PB-O3A-PA-O2A
2	A	402	NAG	O7-C7-N2-C2
4	C	401	ATP	PB-O3B-PG-O1G
4	B	407	ATP	PB-O3B-PG-O2G
4	B	407	ATP	PB-O3B-PG-O3G
4	C	401	ATP	PB-O3B-PG-O3G
2	A	401	NAG	C4-C5-C6-O6
4	A	409	ATP	PB-O3A-PA-O2A
2	B	402	NAG	C8-C7-N2-C2

There are no ring outliers.

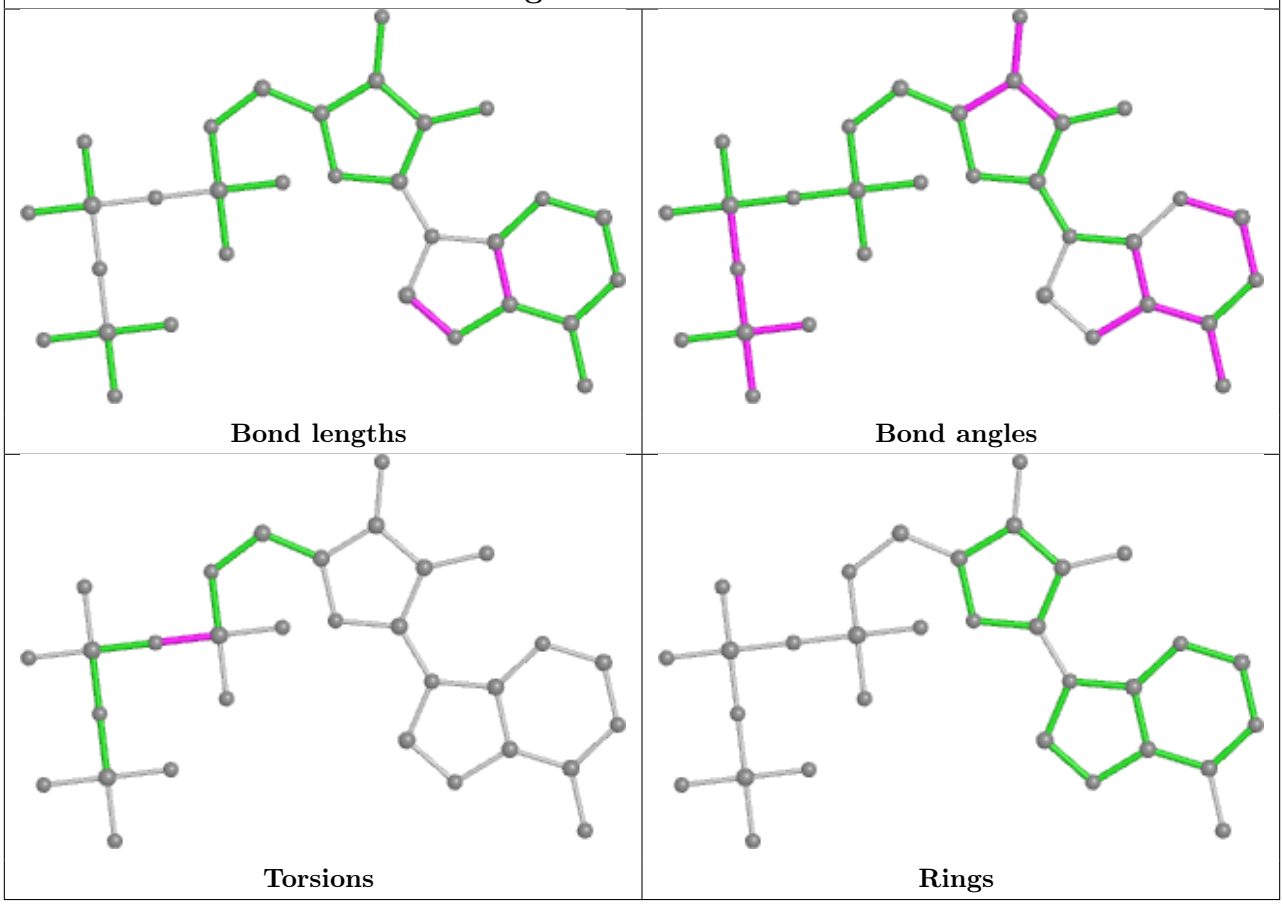
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	409	ATP	2	0
4	B	407	ATP	2	0
4	C	401	ATP	3	0

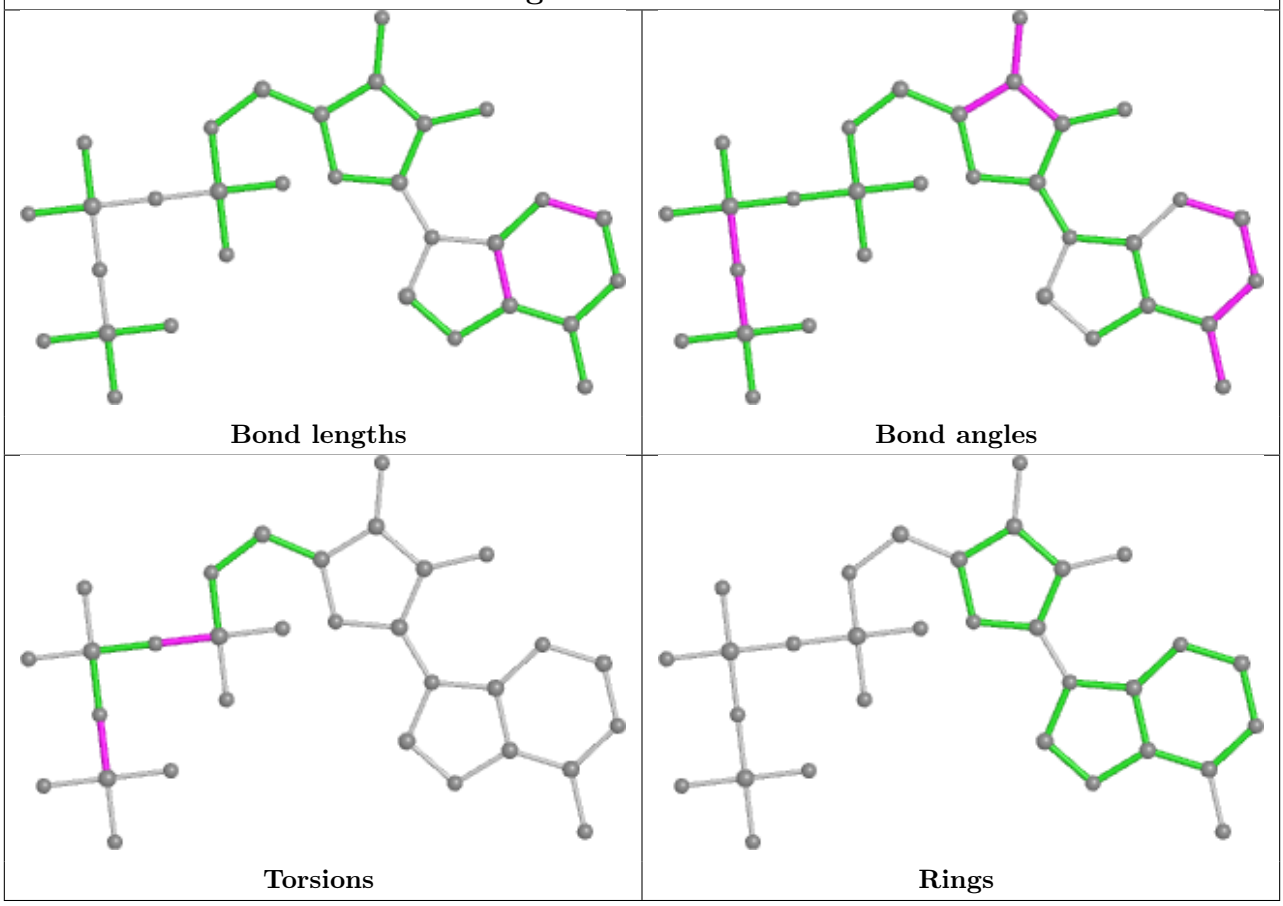
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

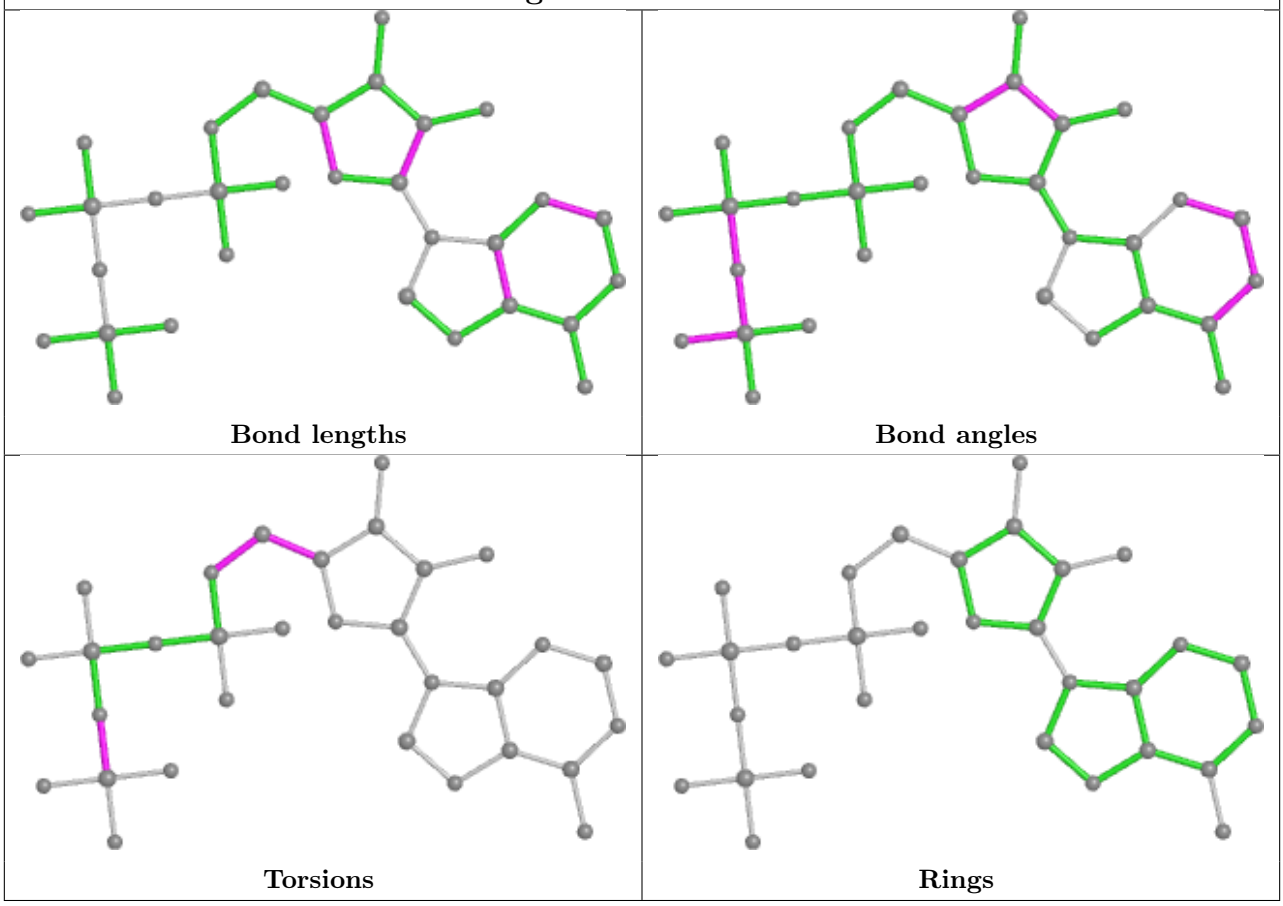
Ligand ATP A 409



Ligand ATP B 407



Ligand ATP C 401



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	343/358 (95%)	0.03	19 (5%)	25	21	30, 61, 111, 145	0
1	B	355/358 (99%)	0.09	11 (3%)	49	44	29, 60, 108, 143	0
1	C	344/358 (96%)	0.34	32 (9%)	8	6	32, 64, 110, 144	0
All	All	1042/1074 (97%)	0.15	62 (5%)	21	18	29, 61, 110, 145	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	PRO	5.4
1	A	36	LEU	4.9
1	B	231	SER	4.5
1	C	246	HIS	4.3
1	A	32	ARG	4.0
1	C	239	TYR	4.0
1	B	230	ASN	3.8
1	A	33	LEU	3.7
1	C	163	ARG	3.7
1	C	362	VAL	3.6
1	C	173	THR	3.5
1	C	49	TYR	3.4
1	B	342	GLY	3.4
1	A	49	TYR	3.3
1	C	31	ASN	3.2
1	A	242	GLU	3.1
1	A	367	CYS	3.1
1	B	227	ASP	3.0
1	C	242	GLU	3.0
1	C	144	THR	2.9
1	C	240	HIS	2.9
1	C	137	HIS	2.7
1	C	161	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	37	LEU	2.6
1	C	30	LEU	2.6
1	C	165	VAL	2.5
1	B	285	TYR	2.5
1	C	174	LEU	2.5
1	C	178	GLU	2.4
1	A	76	LEU	2.4
1	C	220	VAL	2.4
1	C	370	VAL	2.4
1	B	341	ALA	2.4
1	A	240	HIS	2.3
1	C	287	VAL	2.3
1	C	302	PRO	2.3
1	B	229	GLU	2.3
1	C	226	HIS	2.3
1	A	370	VAL	2.2
1	B	103	PRO	2.2
1	B	49	TYR	2.2
1	C	164	CYS	2.2
1	A	55	GLN	2.2
1	B	288	LYS	2.2
1	C	151	LYS	2.2
1	C	247	CYS	2.2
1	C	86	SER	2.2
1	C	241	PRO	2.2
1	A	45	TYR	2.1
1	A	218	PHE	2.1
1	C	236	TYR	2.1
1	A	212	TYR	2.1
1	C	142	ASN	2.1
1	A	305	VAL	2.1
1	C	285	TYR	2.1
1	C	33	LEU	2.1
1	A	56	PHE	2.1
1	B	284	ASP	2.1
1	C	98	ALA	2.1
1	A	306	LEU	2.0
1	C	166	GLN	2.0
1	A	285	TYR	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

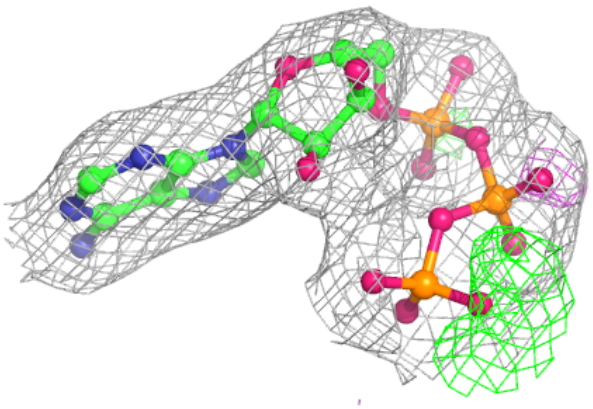
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

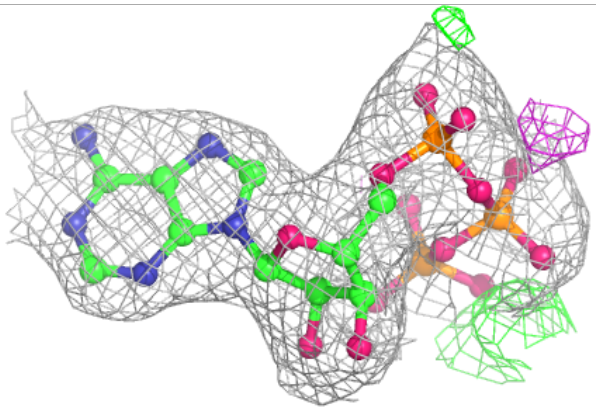
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	A	402	14/15	0.73	0.36	65,98,122,123	0
3	ZN	C	404	1/1	0.89	0.07	105,105,105,105	0
3	ZN	B	405	1/1	0.91	0.06	126,126,126,126	0
3	ZN	A	408	1/1	0.93	0.05	125,125,125,125	0
2	NAG	A	401	14/15	0.93	0.20	45,87,112,133	0
2	NAG	B	402	14/15	0.93	0.28	38,60,82,87	0
2	NAG	C	402	14/15	0.95	0.24	42,55,65,69	0
2	NAG	B	401	14/15	0.96	0.15	28,45,60,72	0
3	ZN	C	405	1/1	0.96	0.06	115,115,115,115	0
3	ZN	A	407	1/1	0.97	0.21	66,66,66,66	0
4	ATP	A	409	31/31	0.97	0.15	27,34,44,54	0
4	ATP	C	401	31/31	0.97	0.15	30,55,65,80	0
3	ZN	A	403	1/1	0.98	0.21	52,52,52,52	0
3	ZN	C	403	1/1	0.98	0.21	65,65,65,65	0
4	ATP	B	407	31/31	0.98	0.14	27,36,44,52	0
3	ZN	B	404	1/1	0.98	0.21	66,66,66,66	0
3	ZN	A	406	1/1	0.99	0.24	70,70,70,70	0
3	ZN	B	406	1/1	0.99	0.15	58,58,58,58	0
3	ZN	B	403	1/1	0.99	0.18	50,50,50,50	0
3	ZN	A	405	1/1	0.99	0.17	38,38,38,38	0
3	ZN	A	404	1/1	1.00	0.10	38,38,38,38	0

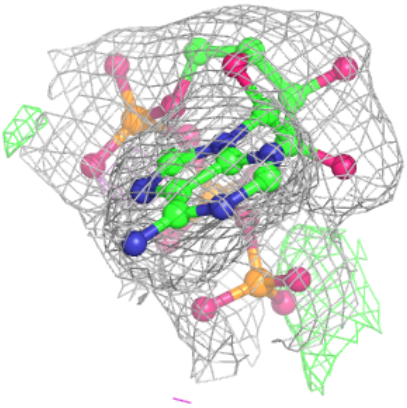
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP A 409:

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

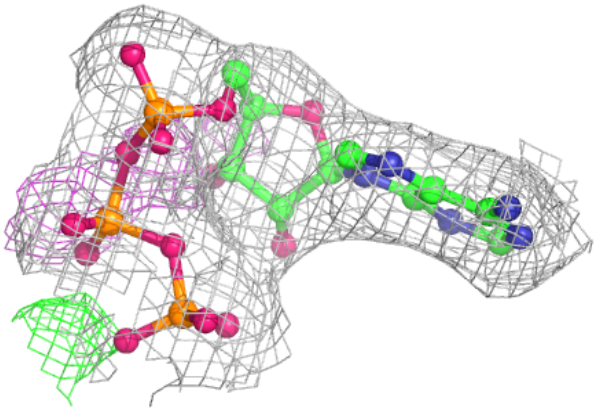


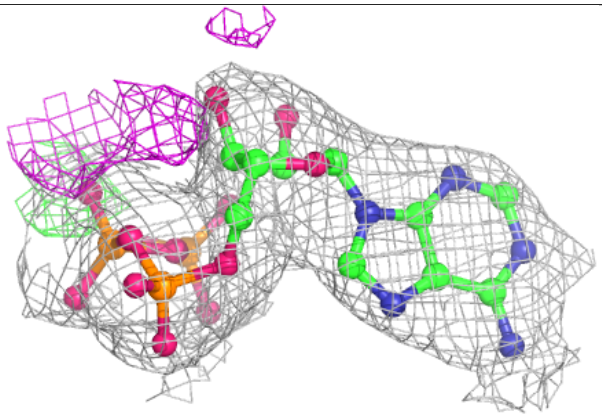


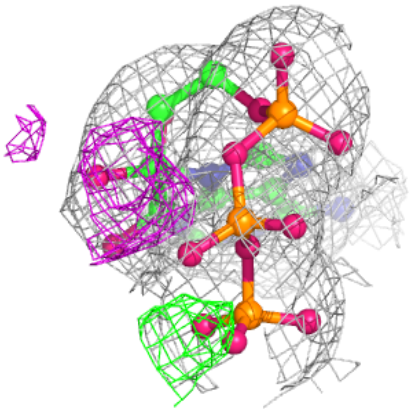


Electron density around ATP C 401:

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

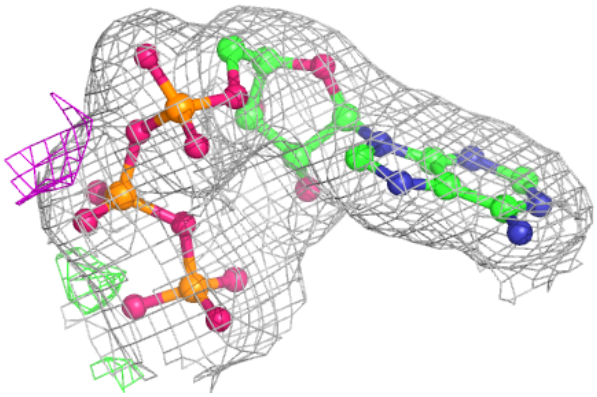


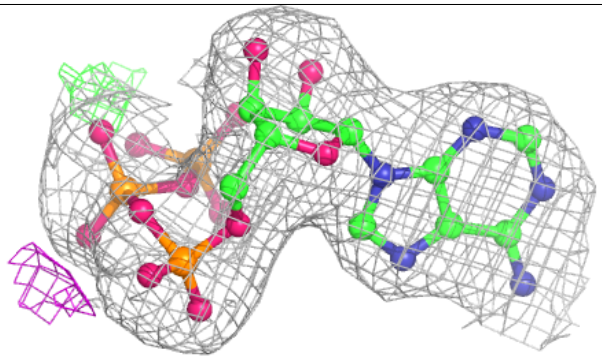


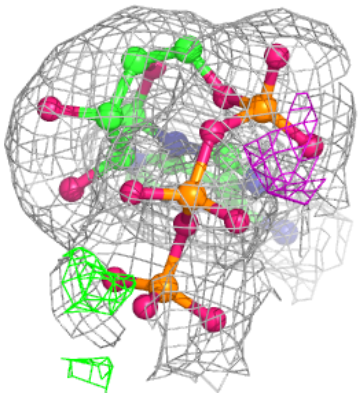


Electron density around ATP B 407:

$2mF_o$-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.