Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2022 – 10:13 am BST

PDB ID	:	7PVN
Title	:	Crystal Structure of Human UBA6 in Complex with ATP
Authors	:	Truongvan, N.; Li, S.; Schindelin, H.
Deposited on	:	2021-10-05
Resolution	:	2.71 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:

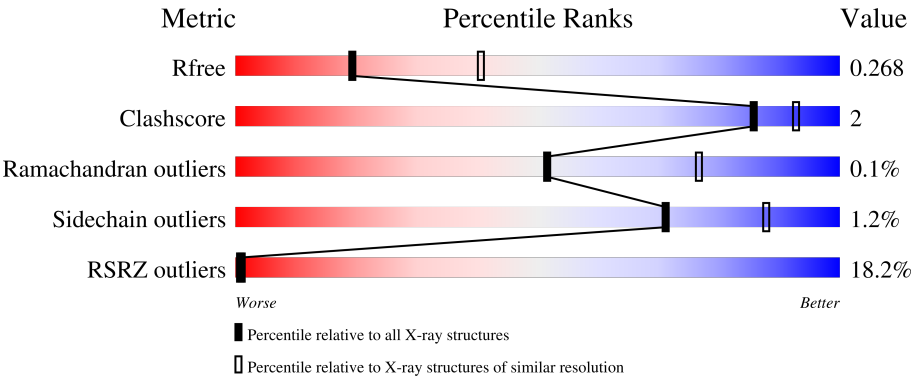
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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% 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	1052	13% 88% 6% 5%
1	B	1052	21% 88% 6% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32030 atoms, of which 15920 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.

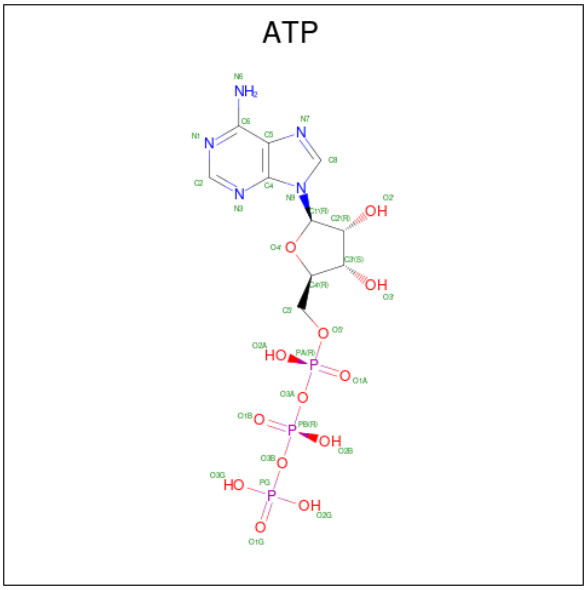
- Molecule 1 is a protein called Ubiquitin-like modifier-activating enzyme 6.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	998	Total	As	C	H	N	O	S	0	0	0
			15875	8	5076	7944	1325	1485	37			
1	B	990	Total	As	C	H	N	O	S	0	0	0
			15749	8	5038	7882	1311	1473	37			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	625	ALA	CYS	engineered mutation	UNP A0AVT1
B	625	ALA	CYS	engineered mutation	UNP A0AVT1

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			46	10	15	5	13	3		

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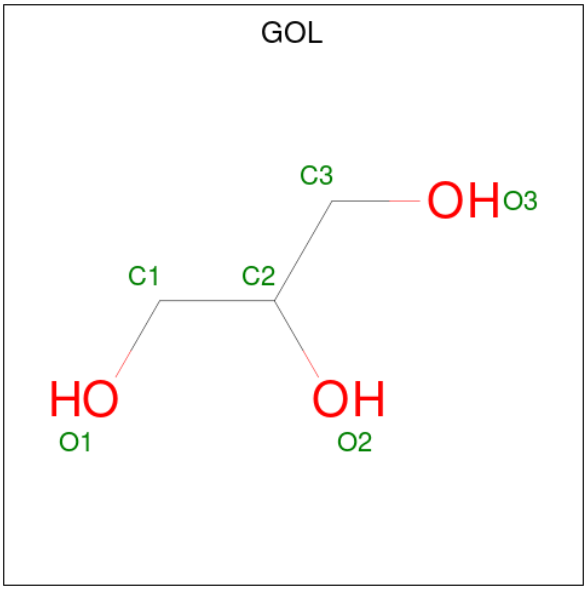
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	H	N	O	P	0	0
			46	10	15	5	13	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

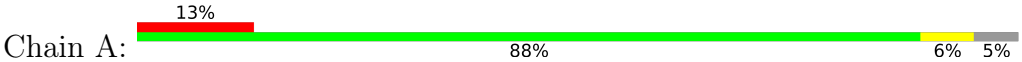
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	134	Total O 134 134	0	0
7	B	62	Total O 62 62	0	0

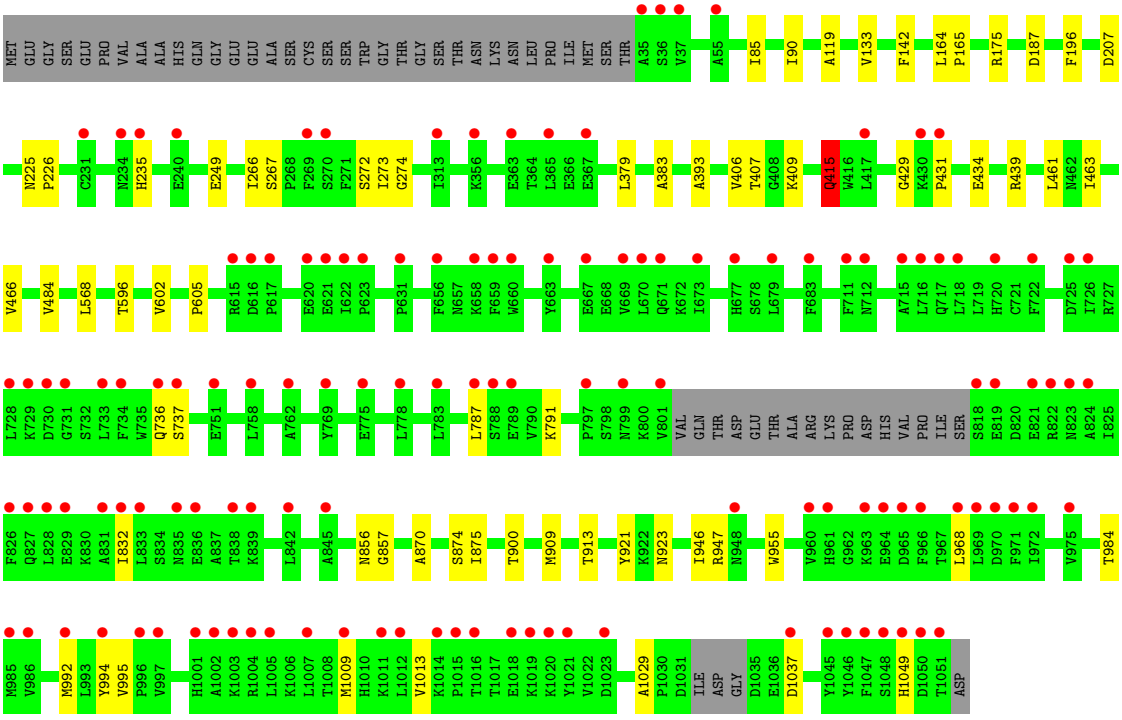
3 Residue-property plots (i)

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 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: Ubiquitin-like modifier-activating enzyme 6

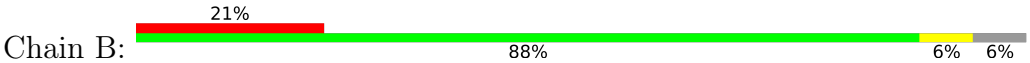
Chain A:

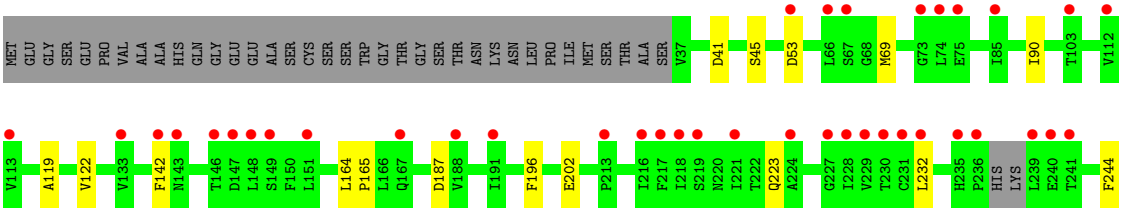


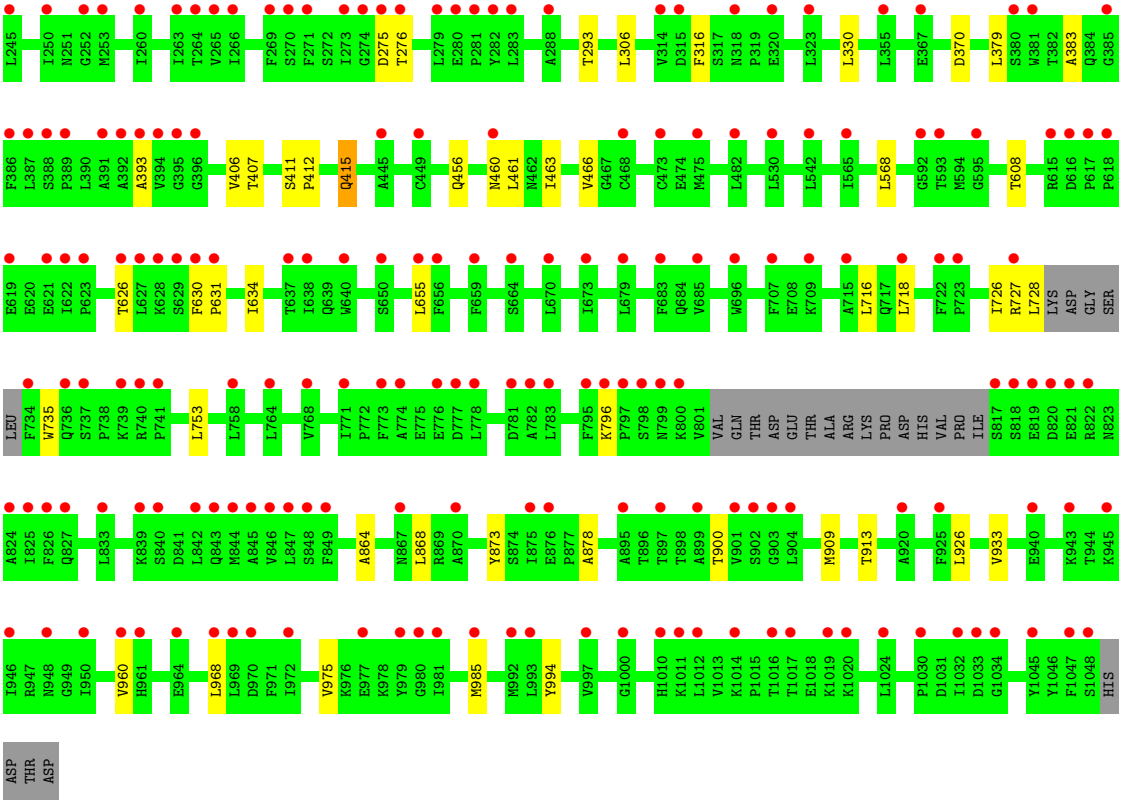


• Molecule 1: Ubiquitin-like modifier-activating enzyme 6

Chain B:






L245 I250 N251 G252 M253 I260 I263 T264 V265 I266 F269 S270 F271 S272 I273 G274 D275 T276 L279 E280 P281 Y282 L283 A288 T293 L306 V314 D315 F316 S317 N318 P319 E320 L323 L330 L355 E367 D370 L379 S380 W381 T382 A383 Q384 G385
F386 L387 S388 P389 L390 A391 A392 A393 V394 G395 G396 V406 T407 S411 P412 Q415 A445 C449 Q456 N460 L461 N462 I463 V466 G467 C468 C473 E474 M475 L482 L530 L542 I565 L568 G592 T593 M594 G596 T608 R615 D616 P617 P618
E619 E620 E621 I622 P623 T626 L627 K628 S629 F630 P631 I634 T637 I638 Q639 W640 S650 L655 F656 F659 S664 L670 I673 L679 F683 Q684 V685 W696 F707 E708 K709 A715 L716 Q717 L718 F722 P723 I726 R727 L728 LYS ASP GLY SER
LEU F734 W735 Q736 S737 P738 K739 R740 P741 L753 L758 L764 V768 I771 P772 F773 A774 E775 E776 D777 L778 D781 A782 L783 F795 K796 P797 S798 N799 K800 V801 VAL GLN THR ASP GLU THR ALA ARG LYS PRO ASP HIS VAL PRO ILE S817 S818 E819 D820 E821 R822 N823
A824 I825 F826 Q827 L833 K839 S840 D841 L842 Q843 M844 A845 V846 L847 S848 F849 A864 M867 L868 R869 A870 Y873 S874 I875 E876 P877 A878 A895 T896 T897 T898 A899 T900 V901 S902 G903 L904 M909 T913 A920 F925 L926 V933 E940 K943 T944 K945
I946 R947 N948 G949 I950 V960 H961 E964 L968 L969 D970 F971 I972 V975 K976 E977 K978 Y979 G980 I981 M985 M992 L993 Y994 V997 G1000 H1010 K1011 L1012 V1013 K1014 P1015 T1016 T1017 E1018 K1019 K1020 L1024 P1030 D1031 I1032 D1033 G1034 Y1045 Y1046 F1047 S1048 HIS
ASP THR ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	123.95Å 113.75Å 183.54Å 90.00° 96.49° 90.00°	Depositor
Resolution (Å)	19.98 – 2.71 48.26 – 2.71	Depositor EDS
% Data completeness (in resolution range)	71.8 (19.98-2.71) 71.6 (48.26-2.71)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.233 , 0.262 0.239 , 0.268	Depositor DCC
R_{free} test set	2502 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	32030	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.42% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, ATP, CL, MG, CAS

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	0.32	0/8030	0.51	0/10872
1	B	0.31	0/7963	0.49	0/10781
All	All	0.32	0/15993	0.50	0/21653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7931	7944	7892	35	0
1	B	7867	7882	7831	34	1
2	A	31	15	12	0	0
2	B	31	15	12	0	0
3	A	24	32	32	1	0
3	B	24	32	32	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	134	0	0	1	0
7	B	62	0	0	0	0
All	All	16110	15920	15811	69	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 2.

All (69) 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:716:LEU:HD13	1:B:796:LYS:HD3	1.58	0.85
1:A:596:THR:HG1	3:A:1104:GOL:HO2	1.24	0.83
1:B:630:PHE:CZ	1:B:718:LEU:HD22	2.14	0.83
1:B:461:LEU:HD11	1:B:913:THR:HG21	1.62	0.82
1:B:753:LEU:HD12	1:B:868:LEU:HD12	1.73	0.70
1:A:461:LEU:HD11	1:A:913:THR:HG21	1.72	0.69
1:A:90:ILE:HG22	1:A:119:ALA:HB1	1.76	0.67
1:B:461:LEU:HD11	1:B:913:THR:CG2	2.28	0.62
1:B:716:LEU:HD22	1:B:796:LYS:HE2	1.81	0.61
1:B:630:PHE:CE1	1:B:718:LEU:HD22	2.36	0.60
1:A:968:LEU:HD21	1:A:994:TYR:HB2	1.84	0.58
1:B:461:LEU:HD13	1:B:463:ILE:HD11	1.86	0.57
1:B:864:ALA:O	1:B:868:LEU:HD13	2.04	0.57
1:B:69:MET:SD	1:B:90:ILE:HG23	2.45	0.57
1:A:909:MET:O	1:A:913:THR:HG23	2.04	0.56
1:A:379:LEU:O	1:A:383:ALA:HB2	2.07	0.55
1:A:461:LEU:HD11	1:A:913:THR:CG2	2.37	0.55
1:B:223:GLN:HA	1:B:276:THR:OG1	2.08	0.53
1:B:634:ILE:HG12	1:B:878:ALA:HB2	1.91	0.52
1:B:244:PHE:HD2	1:B:293:THR:HG21	1.75	0.51
1:B:90:ILE:HG22	1:B:119:ALA:HB1	1.92	0.51
1:B:630:PHE:CE1	1:B:735:TRP:CZ3	3.00	0.50
1:A:870:ALA:O	1:A:874:SER:N	2.45	0.50
1:B:406:VAL:HG23	1:B:407:THR:HG23	1.95	0.49
1:A:602:VAL:HG11	1:A:921:TYR:HB3	1.95	0.49
1:B:630:PHE:CE1	1:B:735:TRP:CH2	3.00	0.49
1:B:306:LEU:HD22	1:B:330:LEU:HD21	1.94	0.49
1:A:466:VAL:HG12	1:A:568:LEU:HD21	1.94	0.48
1:A:406:VAL:HG23	1:A:407:THR:HG23	1.94	0.48
1:A:164:LEU:N	1:A:165:PRO:HD2	2.28	0.48
1:A:226:PRO:HB2	1:A:272:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:GLN:HG3	1:A:737:SER:H	1.81	0.46
1:A:207:ASP:O	1:A:409:LYS:O	2.34	0.46
1:B:379:LEU:O	1:B:383:ALA:HB2	2.15	0.46
1:B:968:LEU:HD21	1:B:994:TYR:HB2	1.98	0.45
1:B:393:ALA:HA	1:B:900:THR:HA	1.98	0.45
1:B:53:ASP:OD1	1:B:53:ASP:N	2.47	0.45
1:A:273:ILE:HG13	1:A:274:GLY:N	2.32	0.44
1:B:466:VAL:HG12	1:B:568:LEU:HD21	1.99	0.44
1:A:787:LEU:O	1:A:791:LYS:HB2	2.18	0.44
1:A:393:ALA:HA	1:A:900:THR:HA	1.99	0.44
1:A:429:GLY:O	1:A:431:PRO:HD3	2.19	0.43
1:B:726:ILE:O	1:B:726:ILE:HG23	2.19	0.43
1:B:631:PRO:HD2	1:B:873:TYR:CZ	2.54	0.43
1:A:856:ASN:OD1	1:A:857:GLY:N	2.52	0.42
1:B:909:MET:O	1:B:913:THR:HG23	2.19	0.42
1:A:196:PHE:HA	1:A:415:GLN:O	2.19	0.42
1:A:870:ALA:HB1	1:A:875:ILE:HG23	2.00	0.42
1:A:434:GLU:O	1:A:439:ARG:NH2	2.52	0.42
1:B:960:VAL:HG11	1:B:975:VAL:HG22	2.00	0.42
1:A:461:LEU:HD13	1:A:463:ILE:HD11	2.02	0.42
1:A:602:VAL:HG12	1:A:923:ASN:OD1	2.20	0.42
1:A:984:THR:HG21	1:A:1029:ALA:HB2	2.02	0.42
1:A:85:ILE:O	1:A:133:VAL:HG22	2.19	0.42
1:A:175:ARG:O	7:A:1201:HOH:O	2.21	0.41
1:A:1009:MET:O	1:A:1013:VAL:HG22	2.20	0.41
1:A:605:PRO:HA	1:A:955:TRP:CE2	2.55	0.41
1:B:196:PHE:HA	1:B:415:GLN:O	2.20	0.41
1:B:122:VAL:O	1:B:122:VAL:HG12	2.20	0.41
1:B:926:LEU:HD23	1:B:933:VAL:HG22	2.02	0.41
1:B:41:ASP:O	1:B:45:SER:HB2	2.21	0.41
1:A:463:ILE:HD12	1:A:484:VAL:HG11	2.02	0.41
1:A:266:ILE:HD11	1:A:272:SER:HB2	2.02	0.41
1:A:946:ILE:O	1:A:947:ARG:C	2.57	0.41
1:A:992:MET:SD	1:A:995:VAL:HG23	2.60	0.41
1:B:727:ARG:O	1:B:728:LEU:C	2.59	0.41
1:B:164:LEU:N	1:B:165:PRO:HD2	2.36	0.41
1:B:411:SER:HA	1:B:412:PRO:HD3	1.96	0.40
1:A:225:ASN:HA	1:A:226:PRO:HA	1.97	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:B:202:GLU:OE2	1:B:456:GLN:NE2[4_555]	2.15	0.05

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	984/1052 (94%)	958 (97%)	25 (2%)	1 (0%)	51 77
1	B	974/1052 (93%)	953 (98%)	21 (2%)	0	100 100
All	All	1958/2104 (93%)	1911 (98%)	46 (2%)	1 (0%)	51 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	GLN

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	872/917 (95%)	863 (99%)	9 (1%)	76 90
1	B	865/917 (94%)	853 (99%)	12 (1%)	67 85
All	All	1737/1834 (95%)	1716 (99%)	21 (1%)	71 88

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	PHE
1	A	187	ASP
1	A	235	HIS
1	A	249	GLU
1	A	267	SER
1	A	415	GLN
1	A	832	ILE
1	A	1037	ASP
1	A	1049	HIS
1	B	142	PHE
1	B	187	ASP
1	B	232	LEU
1	B	275	ASP
1	B	316	PHE
1	B	370	ASP
1	B	415	GLN
1	B	460	ASN
1	B	608	THR
1	B	626	THR
1	B	655	LEU
1	B	985	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	47	GLN
1	B	507	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CAS	A	433	1	5,8,9	0.61	0	1,9,11	0.53	0
1	CAS	A	770	1	5,8,9	0.75	0	1,9,11	1.91	0
1	CAS	A	414	1	5,8,9	0.76	0	1,9,11	1.75	0
1	CAS	B	347	1	5,8,9	0.73	0	1,9,11	1.06	0
1	CAS	B	311	1	5,8,9	0.83	0	1,9,11	0.57	0
1	CAS	A	178	1	5,8,9	0.61	0	1,9,11	1.97	0
1	CAS	B	770	1	5,8,9	0.65	0	1,9,11	0.74	0
1	CAS	A	682	1	5,8,9	0.49	0	1,9,11	0.42	0
1	CAS	A	311	1	5,8,9	0.61	0	1,9,11	0.27	0
1	CAS	A	721	1	5,8,9	0.60	0	1,9,11	0.54	0
1	CAS	B	414	1	5,8,9	0.76	0	1,9,11	1.29	0
1	CAS	B	433	1	5,8,9	0.56	0	1,9,11	1.13	0
1	CAS	A	347	1	5,8,9	0.58	0	1,9,11	0.73	0
1	CAS	B	178	1	5,8,9	0.51	0	1,9,11	0.82	0
1	CAS	B	721	1	5,8,9	0.49	0	1,9,11	0.42	0
1	CAS	B	682	1	5,8,9	0.59	0	1,9,11	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAS	A	433	1	-	0/0/7/9	-
1	CAS	A	770	1	-	0/0/7/9	-
1	CAS	A	414	1	-	0/0/7/9	-
1	CAS	B	347	1	-	0/0/7/9	-
1	CAS	B	311	1	-	0/0/7/9	-
1	CAS	A	178	1	-	0/0/7/9	-
1	CAS	B	770	1	-	0/0/7/9	-
1	CAS	A	682	1	-	0/0/7/9	-
1	CAS	A	311	1	-	0/0/7/9	-
1	CAS	A	721	1	-	0/0/7/9	-
1	CAS	B	414	1	-	0/0/7/9	-
1	CAS	B	433	1	-	0/0/7/9	-
1	CAS	A	347	1	-	0/0/7/9	-
1	CAS	B	178	1	-	0/0/7/9	-
1	CAS	B	721	1	-	0/0/7/9	-
1	CAS	B	682	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
3	GOL	A	1103	-	5,5,5	0.97	0	5,5,5	1.04	0
3	GOL	B	1103	-	5,5,5	1.01	0	5,5,5	0.99	0
2	ATP	B	1101	4	26,33,33	0.75	1 (3%)	31,52,52	0.66	0
3	GOL	B	1102	-	5,5,5	0.99	0	5,5,5	0.85	0
3	GOL	A	1105	-	5,5,5	0.92	0	5,5,5	0.86	0
2	ATP	A	1101	4	26,33,33	0.66	1 (3%)	31,52,52	0.85	2 (6%)
3	GOL	A	1104	-	5,5,5	0.93	0	5,5,5	0.86	0
3	GOL	B	1105	-	5,5,5	0.98	0	5,5,5	0.96	0
3	GOL	A	1102	-	5,5,5	0.98	0	5,5,5	1.03	0
3	GOL	B	1104	-	5,5,5	1.02	0	5,5,5	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1103	-	-	2/4/4/4	-
3	GOL	B	1103	-	-	2/4/4/4	-
2	ATP	B	1101	4	-	2/18/38/38	0/3/3/3
3	GOL	B	1102	-	-	1/4/4/4	-
3	GOL	A	1105	-	-	2/4/4/4	-
2	ATP	A	1101	4	-	2/18/38/38	0/3/3/3
3	GOL	A	1104	-	-	0/4/4/4	-
3	GOL	B	1105	-	-	0/4/4/4	-
3	GOL	A	1102	-	-	2/4/4/4	-
3	GOL	B	1104	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	ATP	C8-N7	-2.94	1.29	1.34
2	A	1101	ATP	C8-N7	-2.23	1.30	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1101	ATP	PA-O3A-PB	-2.50	124.25	132.83
2	A	1101	ATP	C5-C6-N6	2.14	123.60	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1103	GOL	O1-C1-C2-C3
3	B	1103	GOL	C1-C2-C3-O3
3	A	1105	GOL	C1-C2-C3-O3
3	A	1103	GOL	O1-C1-C2-O2
3	B	1103	GOL	O2-C2-C3-O3
3	A	1102	GOL	C1-C2-C3-O3
3	B	1102	GOL	C1-C2-C3-O3
3	A	1102	GOL	O2-C2-C3-O3
3	A	1105	GOL	O2-C2-C3-O3
2	A	1101	ATP	C5'-O5'-PA-O1A
2	B	1101	ATP	C5'-O5'-PA-O1A
2	A	1101	ATP	O4'-C4'-C5'-O5'
2	B	1101	ATP	O4'-C4'-C5'-O5'

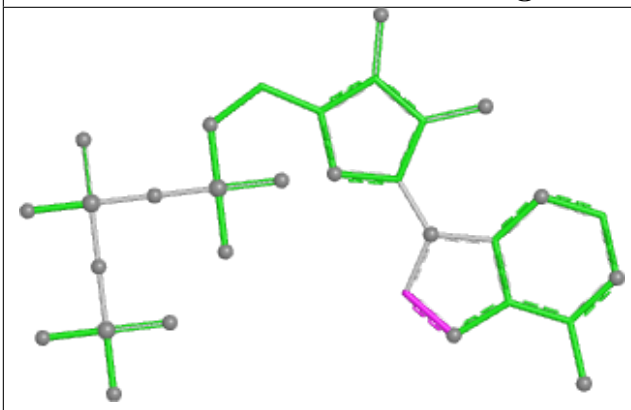
There are no ring outliers.

1 monomer is involved in 1 short contact:

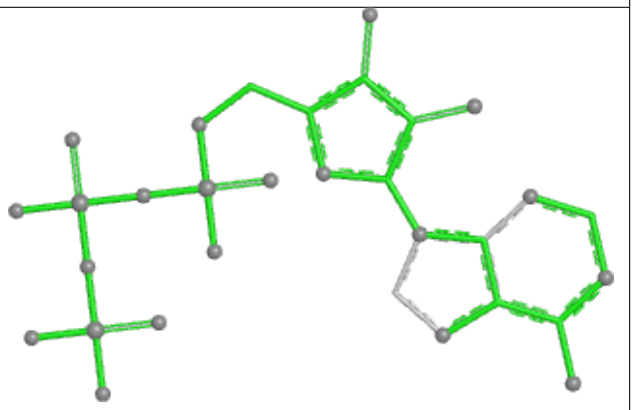
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1104	GOL	1	0

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

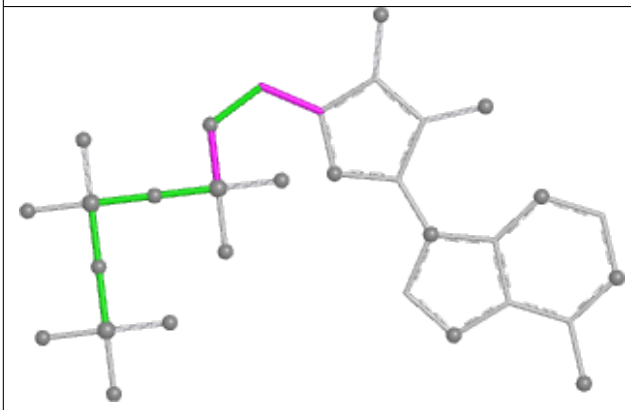
Ligand ATP B 1101



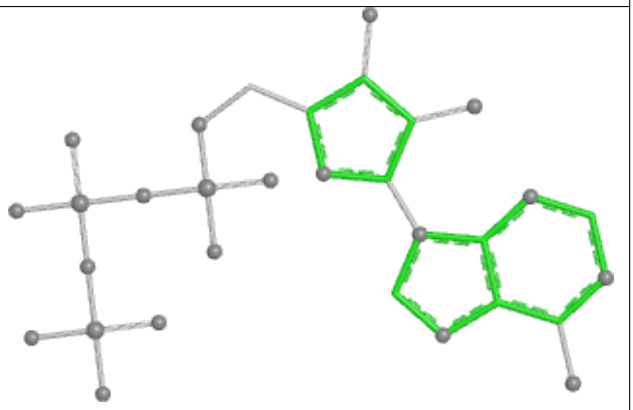
Bond lengths



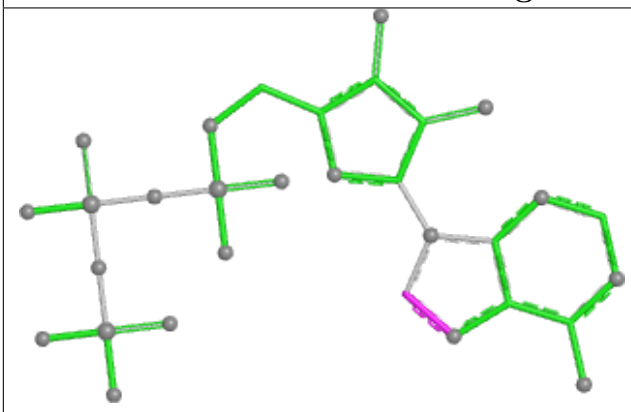
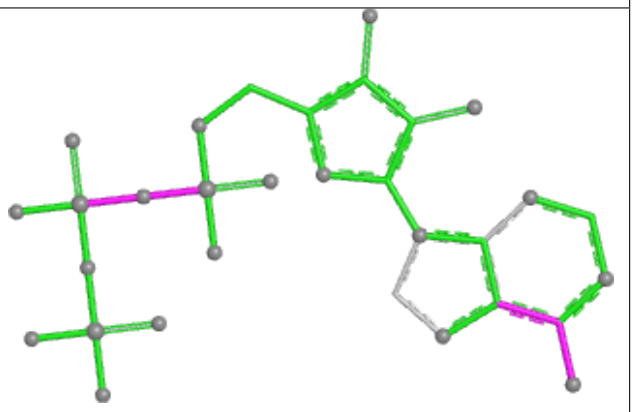
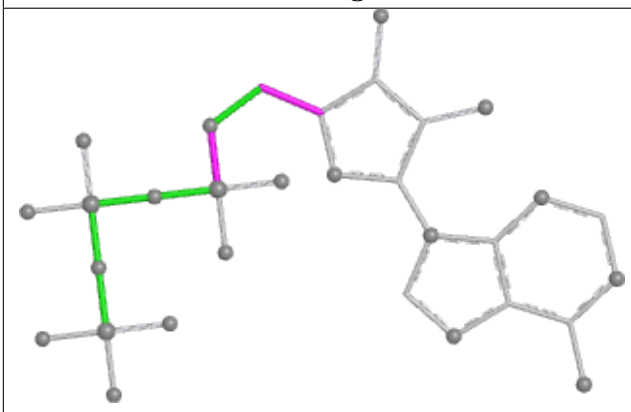
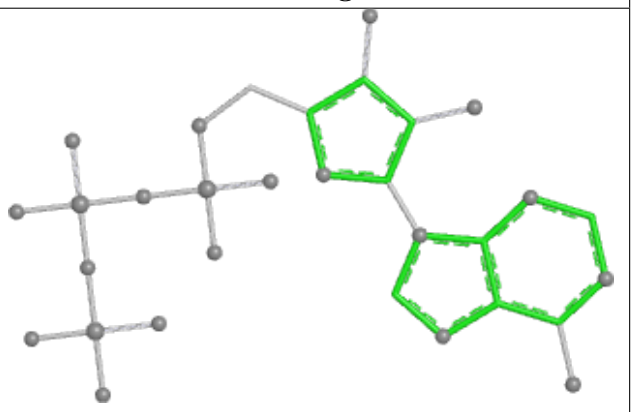
Bond angles



Torsions



Rings

Ligand ATP A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	990/1052 (94%)	0.96	133 (13%)	3	2	19, 55, 138, 193	0
1	B	982/1052 (93%)	1.35	225 (22%)	0	0	44, 84, 140, 189	0
All	All	1972/2104 (93%)	1.16	358 (18%)	1	1	19, 73, 139, 193	0

All (358) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	ILE	8.8
1	B	239	LEU	8.4
1	B	737	SER	8.2
1	B	946	ILE	7.3
1	B	818	SER	7.3
1	B	229	VAL	6.9
1	B	252	GLY	6.9
1	B	269	PHE	6.8
1	A	234	ASN	6.5
1	A	729	LYS	6.5
1	A	1047	PHE	6.3
1	B	981	ILE	6.2
1	A	730	ASP	6.2
1	A	737	SER	6.1
1	B	271	PHE	6.0
1	B	615	ARG	6.0
1	A	968	LEU	5.8
1	B	1020	LYS	5.7
1	B	276	THR	5.6
1	B	997	VAL	5.5
1	B	228	ILE	5.5
1	B	972	ILE	5.5
1	B	718	LEU	5.3
1	A	836	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	787	LEU	5.2
1	A	736	GLN	5.2
1	A	964	GLU	5.1
1	A	1003	LYS	5.0
1	B	799	ASN	5.0
1	A	430	LYS	5.0
1	B	875	ILE	4.9
1	A	788	SER	4.9
1	A	827	GLN	4.8
1	A	1051	THR	4.8
1	B	221	ILE	4.8
1	A	1014	LYS	4.7
1	B	236	PRO	4.6
1	A	789	GLU	4.6
1	B	626	THR	4.6
1	B	631	PRO	4.5
1	B	227	GLY	4.5
1	B	231	CYS	4.5
1	B	217	PHE	4.5
1	B	1047	PHE	4.4
1	A	801	VAL	4.4
1	A	1037	ASP	4.3
1	A	679	LEU	4.3
1	B	824	ALA	4.3
1	B	253	MET	4.3
1	B	1016	THR	4.3
1	A	997	VAL	4.3
1	B	825	ILE	4.2
1	B	530	LEU	4.2
1	B	265	VAL	4.2
1	A	717	GLN	4.2
1	B	149	SER	4.2
1	B	1032	ILE	4.2
1	B	592	GLY	4.1
1	A	1020	LYS	4.1
1	B	235	HIS	4.0
1	B	630	PHE	4.0
1	B	797	PRO	4.0
1	A	828	LEU	4.0
1	A	671	GLN	4.0
1	A	1045	TYR	4.0
1	B	961	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	615	ARG	4.0
1	A	667	GLU	4.0
1	B	274	GLY	3.9
1	B	727	ARG	3.9
1	A	725	ASP	3.9
1	A	758	LEU	3.9
1	B	1048	SER	3.9
1	A	799	ASN	3.9
1	A	996	PRO	3.9
1	A	1011	LYS	3.9
1	B	722	PHE	3.9
1	B	776	GLU	3.8
1	B	800	LYS	3.8
1	A	1048	SER	3.8
1	B	240	GLU	3.8
1	B	627	LEU	3.8
1	B	147	ASP	3.8
1	A	1012	LEU	3.8
1	A	823	ASN	3.8
1	B	940	GLU	3.7
1	B	1045	TYR	3.7
1	A	972	ILE	3.7
1	B	218	ILE	3.7
1	B	826	PHE	3.7
1	B	283	LEU	3.7
1	A	826	PHE	3.7
1	B	232	LEU	3.7
1	A	961	HIS	3.6
1	B	796	LYS	3.6
1	A	1021	TYR	3.6
1	A	842	LEU	3.6
1	B	1012	LEU	3.6
1	B	66	LEU	3.6
1	B	219	SER	3.6
1	B	768	VAL	3.6
1	A	35	ALA	3.5
1	B	848	SER	3.5
1	B	1011	LYS	3.5
1	B	821	GLU	3.5
1	B	664	SER	3.5
1	A	620	GLU	3.5
1	B	389	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	740	ARG	3.5
1	B	817	SER	3.5
1	B	266	ILE	3.4
1	B	945	LYS	3.4
1	A	673	ILE	3.4
1	B	282	TYR	3.4
1	A	751	GLU	3.4
1	B	619	GLU	3.4
1	A	1049	HIS	3.3
1	A	970	ASP	3.3
1	A	832	ILE	3.3
1	B	833	LEU	3.3
1	B	707	PHE	3.3
1	A	829	GLU	3.3
1	B	977	GLU	3.3
1	A	778	LEU	3.3
1	A	985	MET	3.3
1	B	741	PRO	3.2
1	B	783	LEU	3.2
1	B	764	LEU	3.2
1	A	819	GLU	3.2
1	A	1002	ALA	3.2
1	A	660	TRP	3.2
1	A	1015	PRO	3.2
1	B	270	SER	3.2
1	B	241	THR	3.1
1	B	822	ARG	3.1
1	B	849	PHE	3.1
1	B	778	LEU	3.1
1	B	985	MET	3.1
1	A	731	GLY	3.1
1	A	824	ALA	3.1
1	B	683	PHE	3.1
1	A	971	PHE	3.1
1	B	1019	LYS	3.1
1	A	1050	ASP	3.1
1	B	819	GLU	3.1
1	B	224	ALA	3.0
1	B	445	ALA	3.0
1	A	1018	GLU	3.0
1	A	965	ASP	3.0
1	A	734	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	656	PHE	3.0
1	B	616	ASP	3.0
1	B	263	ILE	3.0
1	A	669	VAL	3.0
1	B	320	GLU	3.0
1	B	395	GLY	3.0
1	A	617	PRO	3.0
1	B	709	LYS	2.9
1	A	722	PHE	2.9
1	A	718	LEU	2.9
1	B	845	ALA	2.9
1	B	67	SER	2.9
1	A	833	LEU	2.9
1	B	650	SER	2.9
1	B	781	ASP	2.9
1	B	992	MET	2.9
1	B	617	PRO	2.9
1	B	968	LEU	2.9
1	B	618	PRO	2.9
1	B	1033	ASP	2.8
1	A	960	VAL	2.8
1	B	245	LEU	2.8
1	B	628	LYS	2.8
1	B	839	LYS	2.8
1	B	593	THR	2.8
1	A	720	HIS	2.8
1	B	392	ALA	2.8
1	B	396	GLY	2.8
1	A	992	MET	2.7
1	B	774	ALA	2.7
1	B	670	LEU	2.7
1	B	279	LEU	2.7
1	B	979	TYR	2.7
1	A	783	LEU	2.7
1	B	250	ILE	2.7
1	B	870	ALA	2.7
1	A	986	VAL	2.7
1	A	356	LYS	2.7
1	B	950	ILE	2.7
1	A	36	SER	2.7
1	A	1001	HIS	2.7
1	A	231	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	683	PHE	2.7
1	B	773	PHE	2.7
1	B	902	SER	2.7
1	B	782	ALA	2.7
1	B	920	ALA	2.7
1	A	969	LEU	2.7
1	B	659	PHE	2.7
1	A	726	ILE	2.7
1	B	715	ALA	2.6
1	B	53	ASP	2.6
1	B	388	SER	2.6
1	B	393	ALA	2.6
1	B	148	LEU	2.6
1	B	655	LEU	2.6
1	B	629	SER	2.6
1	B	960	VAL	2.6
1	B	216	ILE	2.6
1	B	736	GLN	2.6
1	B	75	GLU	2.6
1	B	1014	LYS	2.6
1	B	264	THR	2.6
1	B	113	VAL	2.6
1	A	728	LEU	2.6
1	B	840	SER	2.6
1	B	191	ILE	2.6
1	B	638	ILE	2.6
1	B	895	ALA	2.6
1	A	269	PHE	2.6
1	A	948	ASN	2.5
1	A	963	LYS	2.5
1	B	623	PRO	2.5
1	B	739	LYS	2.5
1	B	696	TRP	2.5
1	B	827	GLN	2.5
1	B	843	GLN	2.5
1	B	897	THR	2.5
1	A	835	ASN	2.5
1	B	260	ILE	2.5
1	B	673	ILE	2.5
1	A	733	LEU	2.5
1	A	659	PHE	2.5
1	B	899	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	685	VAL	2.5
1	A	966	PHE	2.5
1	B	355	LEU	2.5
1	A	775	GLU	2.5
1	A	839	LYS	2.5
1	A	769	TYR	2.5
1	B	798	SER	2.5
1	B	734	PHE	2.5
1	B	394	VAL	2.5
1	B	1034	GLY	2.4
1	B	85	ILE	2.4
1	B	622	ILE	2.4
1	B	318	ASN	2.4
1	B	73	GLY	2.4
1	B	943	LYS	2.4
1	B	1017	THR	2.4
1	A	663	TYR	2.4
1	A	622	ILE	2.4
1	A	677	HIS	2.4
1	A	821	GLU	2.4
1	A	270	SER	2.4
1	B	314	VAL	2.4
1	B	820	ASP	2.4
1	A	762	ALA	2.4
1	A	1019	LYS	2.4
1	B	1000	GLY	2.4
1	A	365	LEU	2.4
1	B	640	TRP	2.4
1	A	1009	MET	2.4
1	B	151	LEU	2.4
1	B	288	ALA	2.4
1	B	275	ASP	2.4
1	A	623	PRO	2.3
1	B	904	LEU	2.3
1	A	658	LYS	2.3
1	B	771	ILE	2.3
1	A	37	VAL	2.3
1	B	993	LEU	2.3
1	B	146	THR	2.3
1	B	230	THR	2.3
1	B	133	VAL	2.3
1	A	1046	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	842	LEU	2.3
1	B	903	GLY	2.3
1	A	838	THR	2.3
1	B	315	ASP	2.3
1	B	449	CYS	2.3
1	B	112	VAL	2.3
1	B	143	ASN	2.3
1	B	565	ILE	2.3
1	B	925	PHE	2.3
1	B	385	GLY	2.2
1	B	758	LEU	2.2
1	B	948	ASN	2.2
1	B	281	PRO	2.2
1	B	380	SER	2.2
1	A	1007	LEU	2.2
1	B	460	ASN	2.2
1	B	844	MET	2.2
1	B	473	CYS	2.2
1	B	901	VAL	2.2
1	B	213	PRO	2.2
1	A	831	ALA	2.2
1	A	313	ILE	2.2
1	A	822	ARG	2.2
1	B	280	GLU	2.2
1	B	980	GLY	2.2
1	A	431	PRO	2.2
1	B	1010	HIS	2.2
1	B	1030	PRO	2.2
1	B	964	GLU	2.2
1	B	656	PHE	2.2
1	A	417	LEU	2.2
1	B	542	LEU	2.2
1	B	969	LEU	2.2
1	A	1016	THR	2.2
1	A	797	PRO	2.2
1	B	74	LEU	2.2
1	B	876	GLU	2.2
1	A	715	ALA	2.2
1	B	103	THR	2.2
1	B	1024	LEU	2.1
1	A	55	ALA	2.1
1	B	391	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	188	VAL	2.1
1	A	716	LEU	2.1
1	B	323	LEU	2.1
1	B	475	MET	2.1
1	B	867	ASN	2.1
1	B	387	LEU	2.1
1	B	777	ASP	2.1
1	B	381	TRP	2.1
1	B	637	THR	2.1
1	B	468	CYS	2.1
1	B	367	GLU	2.1
1	A	818	SER	2.1
1	B	679	LEU	2.1
1	B	723	PRO	2.1
1	A	975	VAL	2.1
1	A	1005	LEU	2.1
1	B	846	VAL	2.1
1	B	167	GLN	2.1
1	A	712	ASN	2.1
1	A	1004	ARG	2.1
1	B	386	PHE	2.1
1	A	240	GLU	2.1
1	A	363	GLU	2.1
1	A	235	HIS	2.1
1	A	616	ASP	2.1
1	A	670	LEU	2.0
1	A	1023	ASP	2.0
1	B	970	ASP	2.0
1	B	142	PHE	2.0
1	B	847	LEU	2.0
1	A	367	GLU	2.0
1	A	994	TYR	2.0
1	A	711	PHE	2.0
1	B	795	PHE	2.0
1	A	631	PRO	2.0
1	A	845	ALA	2.0
1	B	595	GLY	2.0
1	A	621	GLU	2.0
1	B	482	LEU	2.0
1	B	621	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CAS	B	721	9/10	0.79	0.24	138,163,195,195	0
1	CAS	A	721	9/10	0.85	0.28	133,158,189,189	0
1	CAS	B	414	9/10	0.86	0.19	78,104,148,148	0
1	CAS	A	347	9/10	0.90	0.17	70,88,141,141	0
1	CAS	B	347	9/10	0.90	0.20	106,129,182,182	0
1	CAS	B	770	9/10	0.90	0.23	68,105,150,150	0
1	CAS	B	682	9/10	0.91	0.29	89,112,154,154	0
1	CAS	B	178	9/10	0.91	0.24	103,119,136,136	0
1	CAS	B	311	9/10	0.91	0.18	88,110,168,168	0
1	CAS	A	414	9/10	0.92	0.21	34,66,110,110	0
1	CAS	A	770	9/10	0.92	0.20	82,104,174,174	0
1	CAS	A	682	9/10	0.92	0.25	97,124,152,152	0
1	CAS	A	311	9/10	0.93	0.22	64,84,104,104	0
1	CAS	B	433	9/10	0.94	0.22	89,109,151,151	0
1	CAS	A	433	9/10	0.95	0.18	60,73,115,115	0
1	CAS	A	178	9/10	0.97	0.17	47,62,81,81	0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1102	6/6	0.74	0.32	76,91,102,103	0
3	GOL	B	1104	6/6	0.78	0.29	78,94,95,95	0
3	GOL	B	1105	6/6	0.85	0.24	84,102,106,108	0
3	GOL	A	1103	6/6	0.88	0.20	52,63,68,68	0
3	GOL	A	1105	6/6	0.89	0.20	50,60,65,65	0
3	GOL	A	1104	6/6	0.89	0.22	44,54,60,60	0

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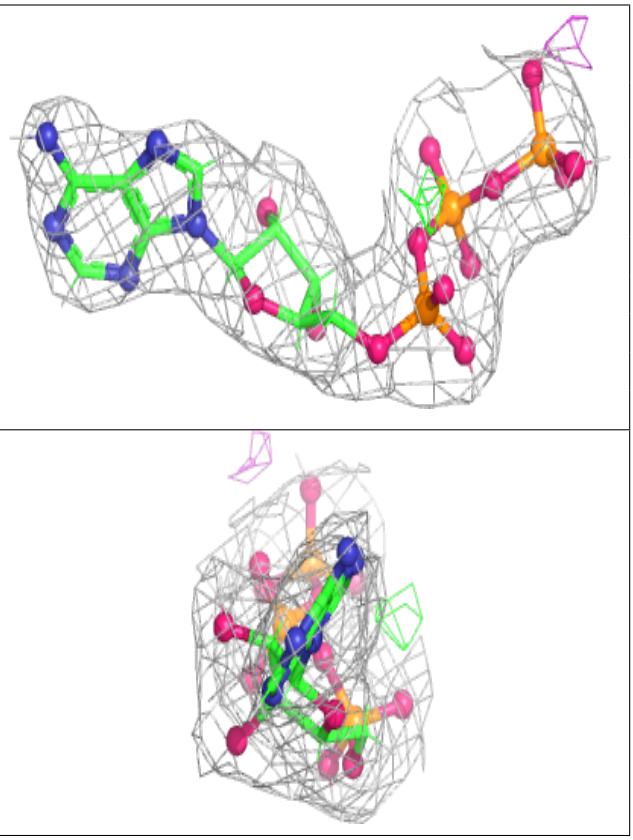
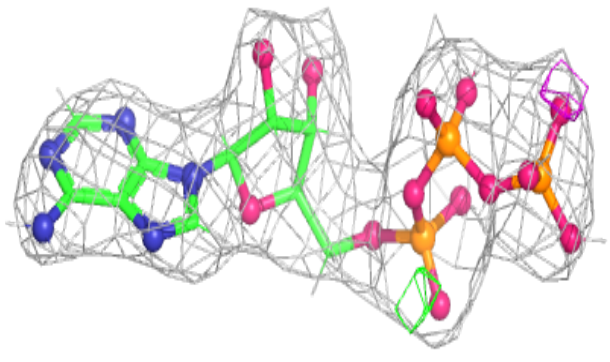
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	B	1103	6/6	0.91	0.18	54,65,70,70	0
3	GOL	A	1102	6/6	0.93	0.25	51,62,70,71	0
2	ATP	B	1101	31/31	0.93	0.22	56,70,85,101	0
4	MG	A	1106	1/1	0.93	0.18	11,11,11,11	0
5	CA	A	1107	1/1	0.94	0.21	89,89,89,89	0
2	ATP	A	1101	31/31	0.96	0.21	24,33,43,71	0
5	CA	B	1107	1/1	0.97	0.22	65,65,65,65	0
5	CA	A	1108	1/1	0.98	0.24	49,49,49,49	0
4	MG	B	1106	1/1	0.98	0.26	38,38,38,38	0
6	CL	A	1109	1/1	0.98	0.06	62,62,62,62	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 B 1101:

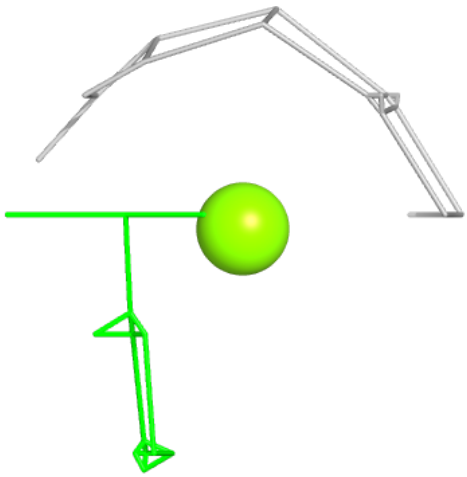
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

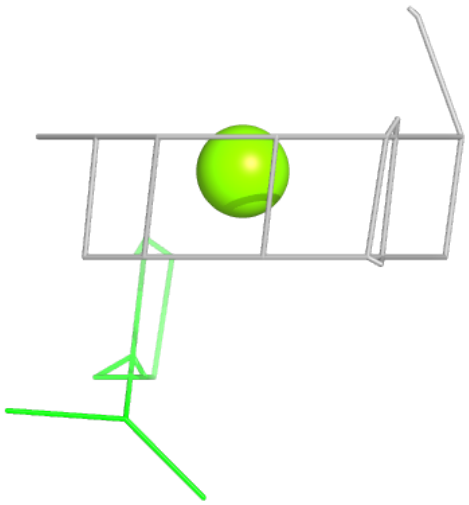


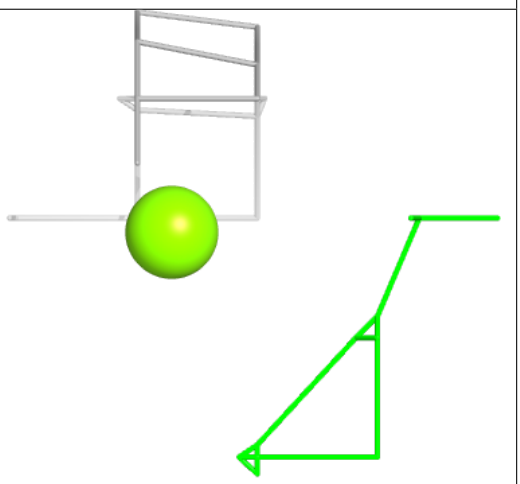


Electron density around MG A 1106:

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

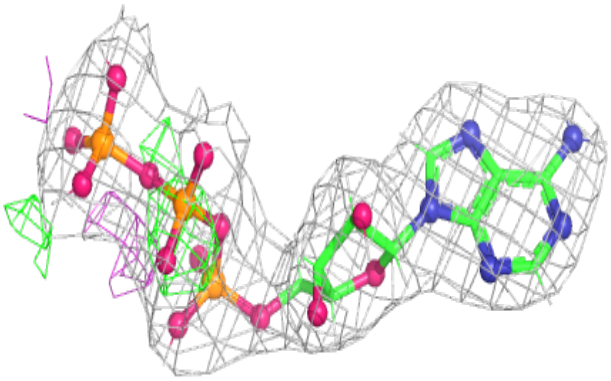


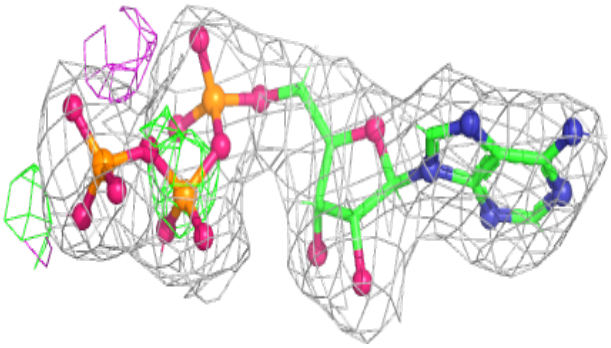


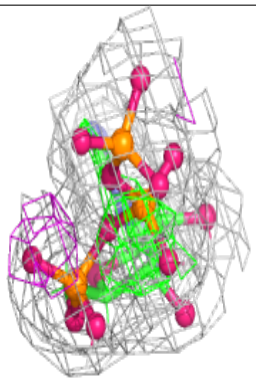


Electron density around ATP A 1101:

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

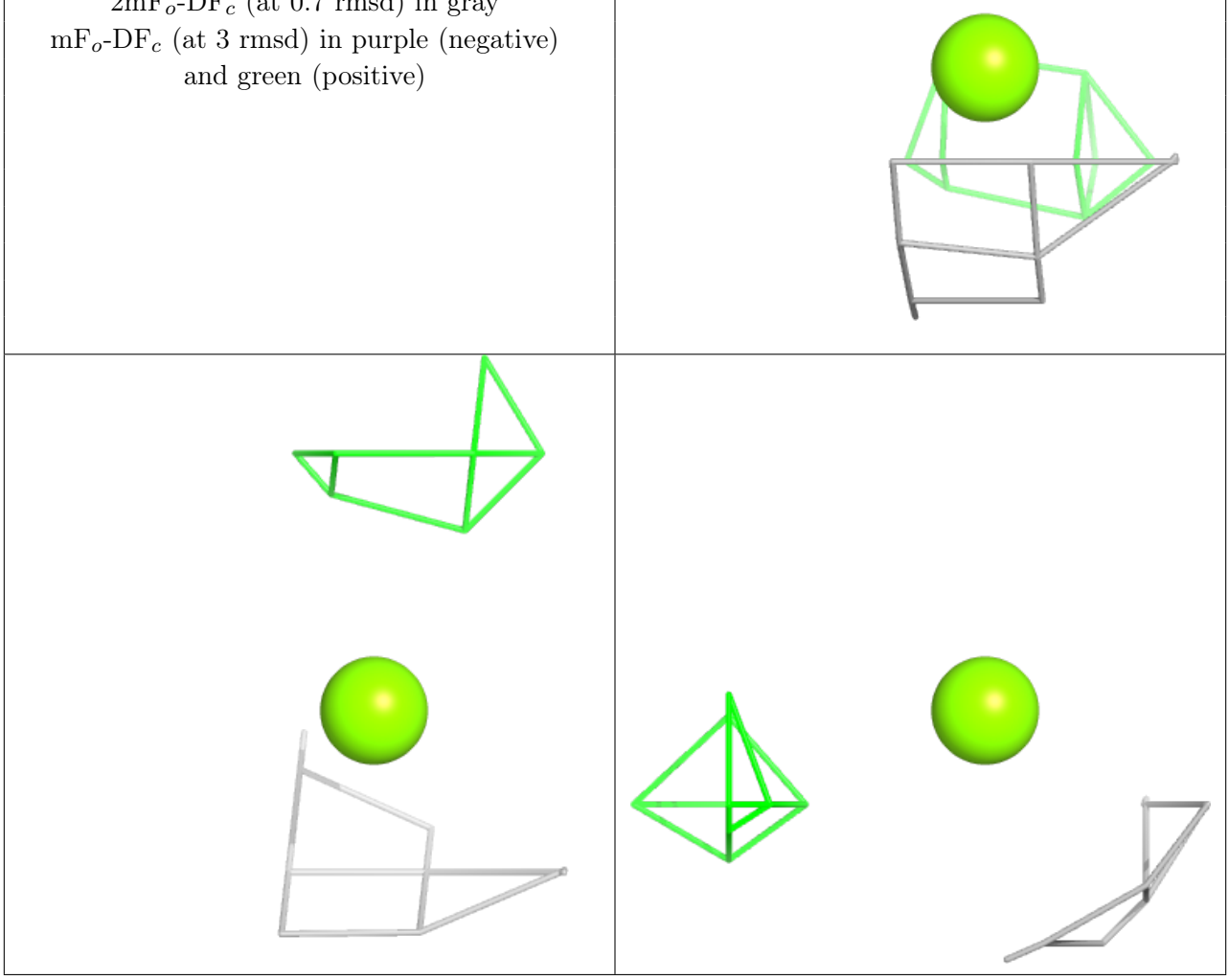






Electron density around MG B 1106:

$2mF_o$-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

There are no such residues in this entry.