



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:00 AM UTC

PDB ID : 7PVN / pdb_00007pvn
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 ⓘ 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

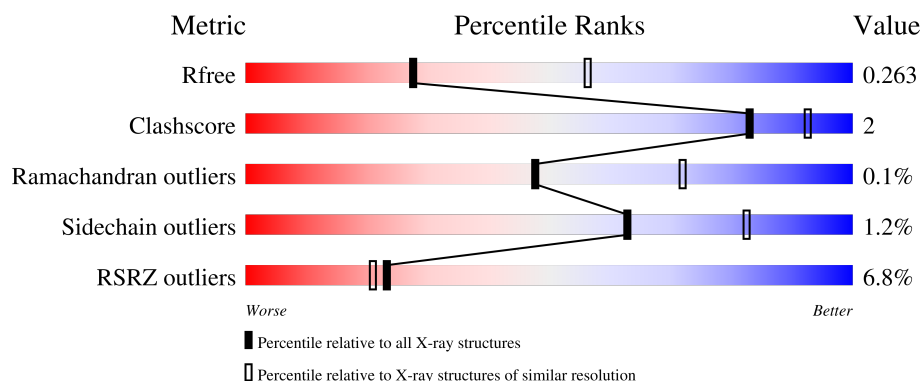
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (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 $\leq 5\%$. 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	1052	4% 88% 7% 5%
1	B	1052	8% 88% 6% 6%

2 Entry composition [i](#)

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.

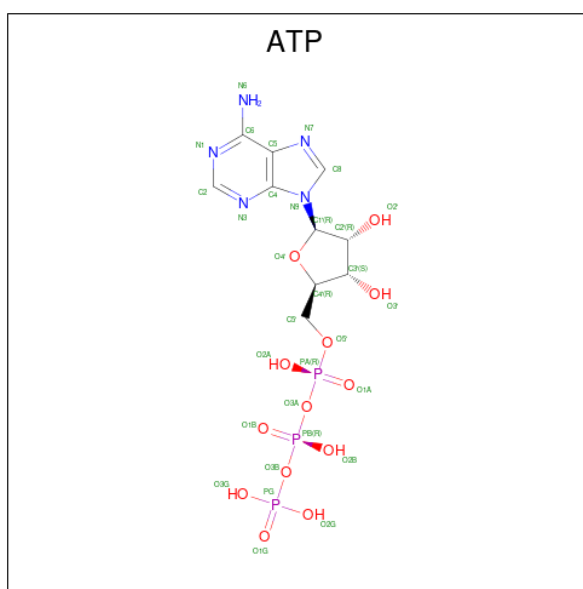
- Molecule 1 is a protein called Ubiquitin-like modifier-activating enzyme 6.

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 (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Continued from previous page...

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: 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 (CCD ID: 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 (CCD ID: CL) (formula: Cl).

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

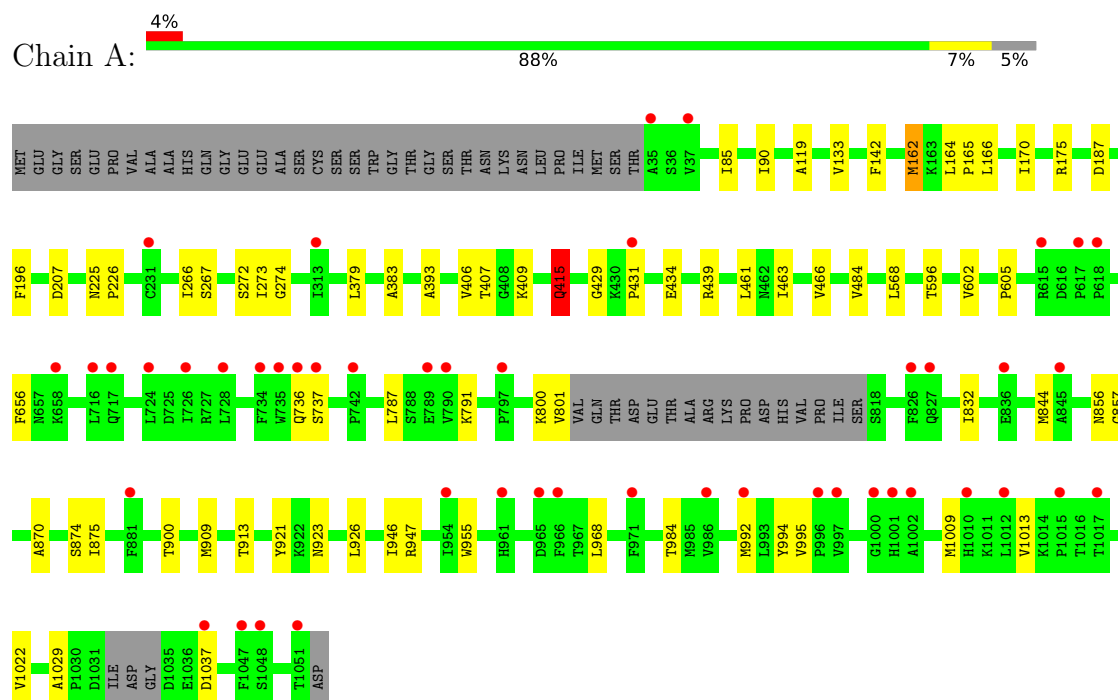
- Molecule 7 is water.

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

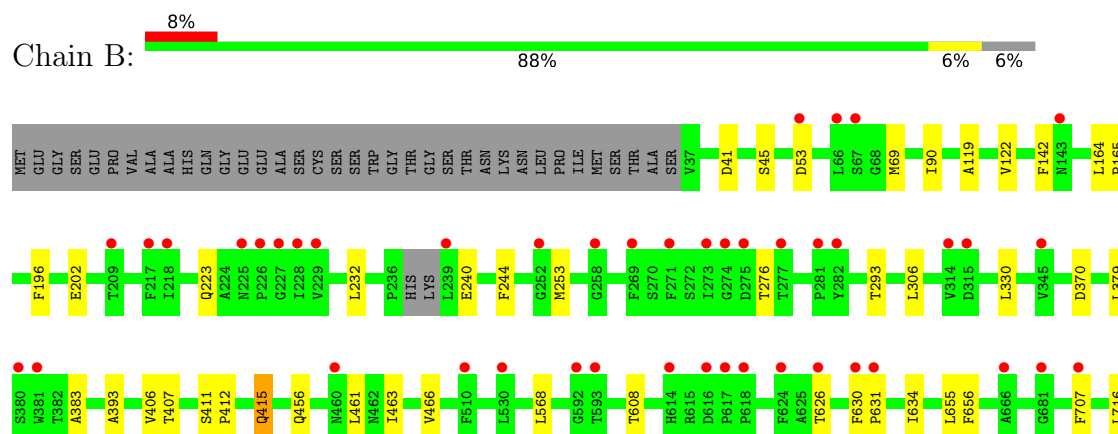
3 Residue-property plots

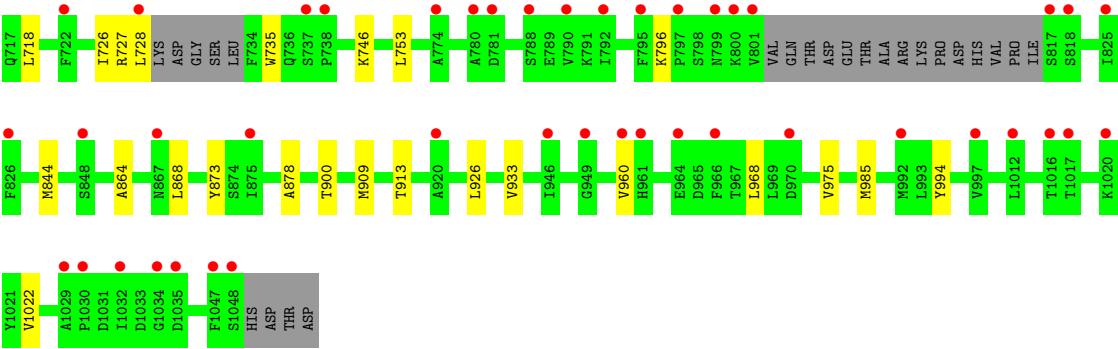
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



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





4 Data and refinement statistics

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 19.98 – 2.71	Depositor EDS
% Data completeness (in resolution range)	71.8 (19.98-2.71) 71.4 (19.98-2.71)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.233 , 0.262 0.234 , 0.263	Depositor DCC
R_{free} test set	2502 reflections (3.64%)	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)	0.37 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

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: ATP, MG, CAS, GOL, CL, CA

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	0.25	0/8030	0.47	0/10872
1	B	0.24	0/7963	0.45	0/10781
All	All	0.24	0/15993	0.46	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	7893	40	0
1	B	7867	7882	7831	36	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

Continued on next page...

Continued from previous page...

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	15812	76	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 (76) 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: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:596:THR:HG1	3:A:1104:GOL:HO2	1.32	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:656:PHE:CG	1:A:844:MET:HE3	2.38	0.59
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:162:MET:HE1	1:A:170:ILE:HD12	1.86	0.56
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:A:162:MET:HE3	1:A:166:LEU:HB3	1.93	0.51
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:656:PHE:CG	1:B:844:MET:HE3	2.46	0.50
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:946:ILE:O	1:A:947:ARG:C	2.57	0.46
1:B:968:LEU:HD21	1:B:994:TYR:HB2	1.98	0.45
1:B:727:ARG:O	1:B:728:LEU:C	2.59	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:656:PHE:CD2	1:A:844:MET:HE3	2.55	0.41
1:A:992:MET:SD	1:A:995:VAL:HG23	2.60	0.41
1:B:164:LEU:N	1:B:165:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:LYS:O	1:A:801:VAL:C	2.64	0.40
1:B:411:SER:HA	1:B:412:PRO:HD3	1.96	0.40
1:B:707:PHE:CD1	1:B:707:PHE:C	3.00	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%)	48	72
1	B	974/1052 (93%)	953 (98%)	21 (2%)	0	100	100
All	All	1958/2104 (93%)	1911 (98%)	46 (2%)	1 (0%)	48	72

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%)	68	85
1	B	865/917 (94%)	853 (99%)	12 (1%)	59	80
All	All	1737/1834 (95%)	1716 (99%)	21 (1%)	63	82

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

Mol	Chain	Res	Type
1	A	142	PHE
1	A	162	MET
1	A	187	ASP
1	A	267	SER
1	A	415	GLN
1	A	832	ILE
1	A	926	LEU
1	A	1022	VAL
1	A	1037	ASP
1	B	142	PHE
1	B	232	LEU
1	B	240	GLU
1	B	253	MET
1	B	370	ASP
1	B	415	GLN
1	B	608	THR
1	B	626	THR
1	B	655	LEU
1	B	746	LYS
1	B	985	MET
1	B	1022	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	177	GLN
1	A	235	HIS
1	A	290	GLN
1	A	541	HIS
1	A	543	ASN
1	A	606	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	695	ASN
1	A	698	GLN
1	A	717	GLN
1	A	736	GLN
1	A	785	ASN
1	B	47	GLN
1	B	177	GLN
1	B	235	HIS
1	B	541	HIS
1	B	639	GLN
1	B	712	ASN
1	B	720	HIS
1	B	785	ASN
1	B	793	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	414	1	5,8,9	0.77	0	1,9,11	0.19	0
1	CAS	B	433	1	5,8,9	0.56	0	1,9,11	0.68	0
1	CAS	B	770	1	5,8,9	0.65	0	1,9,11	0.59	0
1	CAS	A	178	1	5,8,9	0.61	0	1,9,11	0.71	0
1	CAS	B	721	1	5,8,9	0.49	0	1,9,11	0.96	0
1	CAS	B	682	1	5,8,9	0.59	0	1,9,11	0.42	0
1	CAS	A	311	1	5,8,9	0.61	0	1,9,11	1.27	0
1	CAS	A	682	1	5,8,9	0.49	0	1,9,11	0.89	0
1	CAS	A	433	1	5,8,9	0.62	0	1,9,11	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CAS	A	721	1	5,8,9	0.60	0	1,9,11	1.15	0
1	CAS	B	178	1	5,8,9	0.51	0	1,9,11	0.27	0
1	CAS	A	347	1	5,8,9	0.58	0	1,9,11	0.52	0
1	CAS	B	414	1	5,8,9	0.77	0	1,9,11	0.08	0
1	CAS	B	347	1	5,8,9	0.74	0	1,9,11	0.51	0
1	CAS	A	770	1	5,8,9	0.75	0	1,9,11	0.52	0
1	CAS	B	311	1	5,8,9	0.83	0	1,9,11	0.68	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	414	1	-	0/0/7/9	-
1	CAS	B	433	1	-	0/0/7/9	-
1	CAS	B	770	1	-	0/0/7/9	-
1	CAS	A	178	1	-	0/0/7/9	-
1	CAS	B	721	1	-	0/0/7/9	-
1	CAS	B	682	1	-	0/0/7/9	-
1	CAS	A	311	1	-	0/0/7/9	-
1	CAS	A	682	1	-	0/0/7/9	-
1	CAS	A	433	1	-	0/0/7/9	-
1	CAS	A	721	1	-	0/0/7/9	-
1	CAS	B	178	1	-	0/0/7/9	-
1	CAS	A	347	1	-	0/0/7/9	-
1	CAS	B	414	1	-	0/0/7/9	-
1	CAS	B	347	1	-	0/0/7/9	-
1	CAS	A	770	1	-	0/0/7/9	-
1	CAS	B	311	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 oligosaccharides 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	1105	-	5,5,5	0.97	0	5,5,5	0.92	0
3	GOL	B	1103	-	5,5,5	1.05	0	5,5,5	1.07	0
3	GOL	A	1102	-	5,5,5	1.03	0	5,5,5	1.11	1 (20%)
2	ATP	A	1101	4	32,33,33	0.31	0	48,52,52	0.57	0
3	GOL	B	1104	-	5,5,5	1.07	0	5,5,5	0.98	0
3	GOL	A	1104	-	5,5,5	0.97	0	5,5,5	0.93	0
3	GOL	B	1102	-	5,5,5	1.04	0	5,5,5	0.91	0
2	ATP	B	1101	4	32,33,33	0.42	0	48,52,52	0.59	0
3	GOL	B	1105	-	5,5,5	1.02	0	5,5,5	1.04	0
3	GOL	A	1103	-	5,5,5	1.02	0	5,5,5	1.12	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	1105	-	-	2/4/4/4	-
3	GOL	B	1103	-	-	2/4/4/4	-
3	GOL	A	1102	-	-	2/4/4/4	-
2	ATP	A	1101	4	-	1/22/38/38	0/3/3/3
3	GOL	B	1104	-	-	0/4/4/4	-
3	GOL	A	1104	-	-	0/4/4/4	-
3	GOL	B	1102	-	-	0/4/4/4	-
2	ATP	B	1101	4	-	1/22/38/38	0/3/3/3
3	GOL	B	1105	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1103	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1102	GOL	C3-C2-C1	-2.06	104.25	111.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

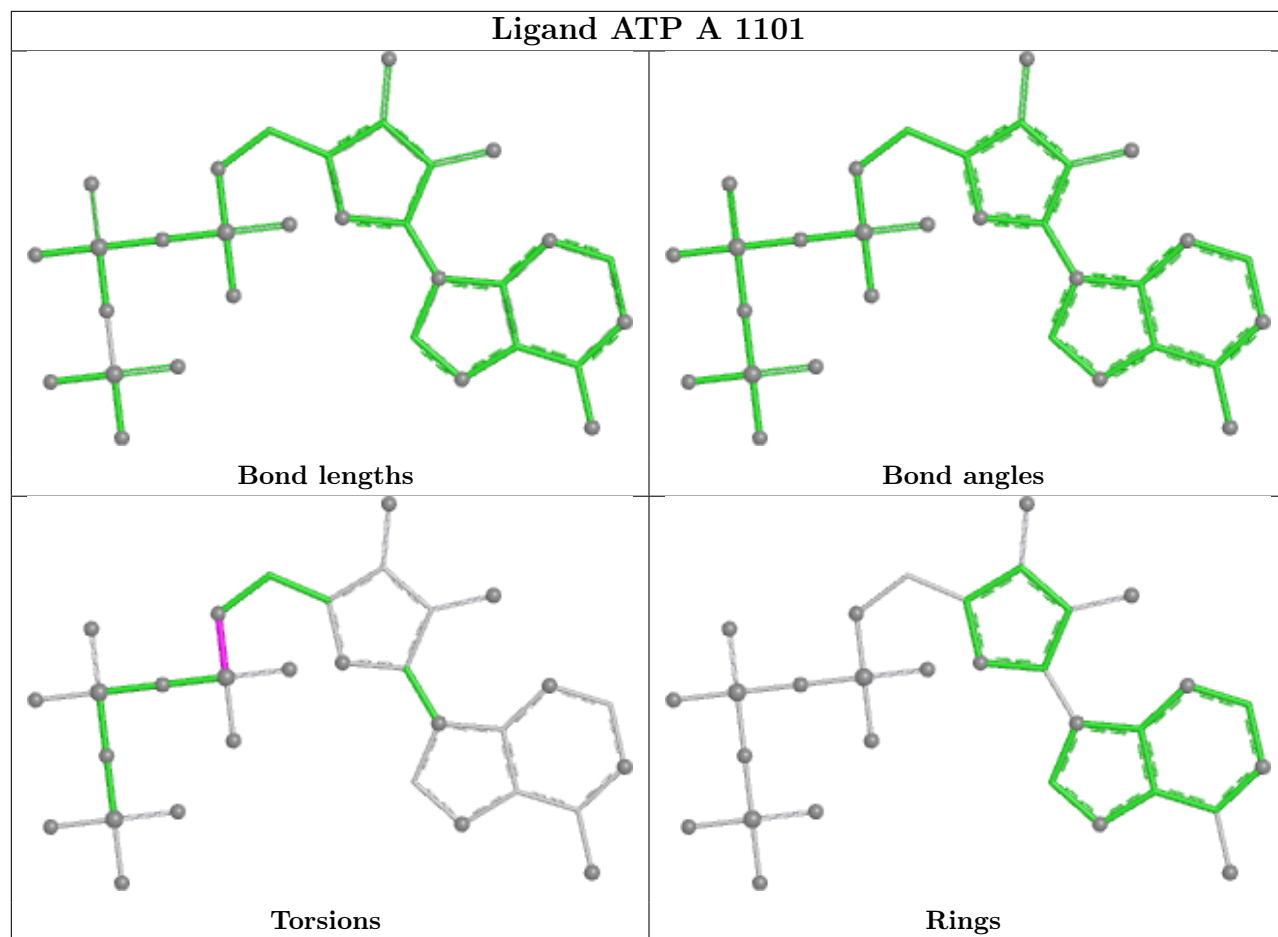
Mol	Chain	Res	Type	Atoms
3	A	1103	GOL	O1-C1-C2-C3
3	B	1103	GOL	C1-C2-C3-O3
3	A	1105	GOL	C1-C2-C3-O3
3	A	1103	GOL	O1-C1-C2-O2
3	B	1103	GOL	O2-C2-C3-O3
2	A	1101	ATP	C5'-O5'-PA-O1A
2	B	1101	ATP	C5'-O5'-PA-O1A
3	A	1102	GOL	O2-C2-C3-O3
3	A	1105	GOL	O2-C2-C3-O3
3	A	1102	GOL	C1-C2-C3-O3

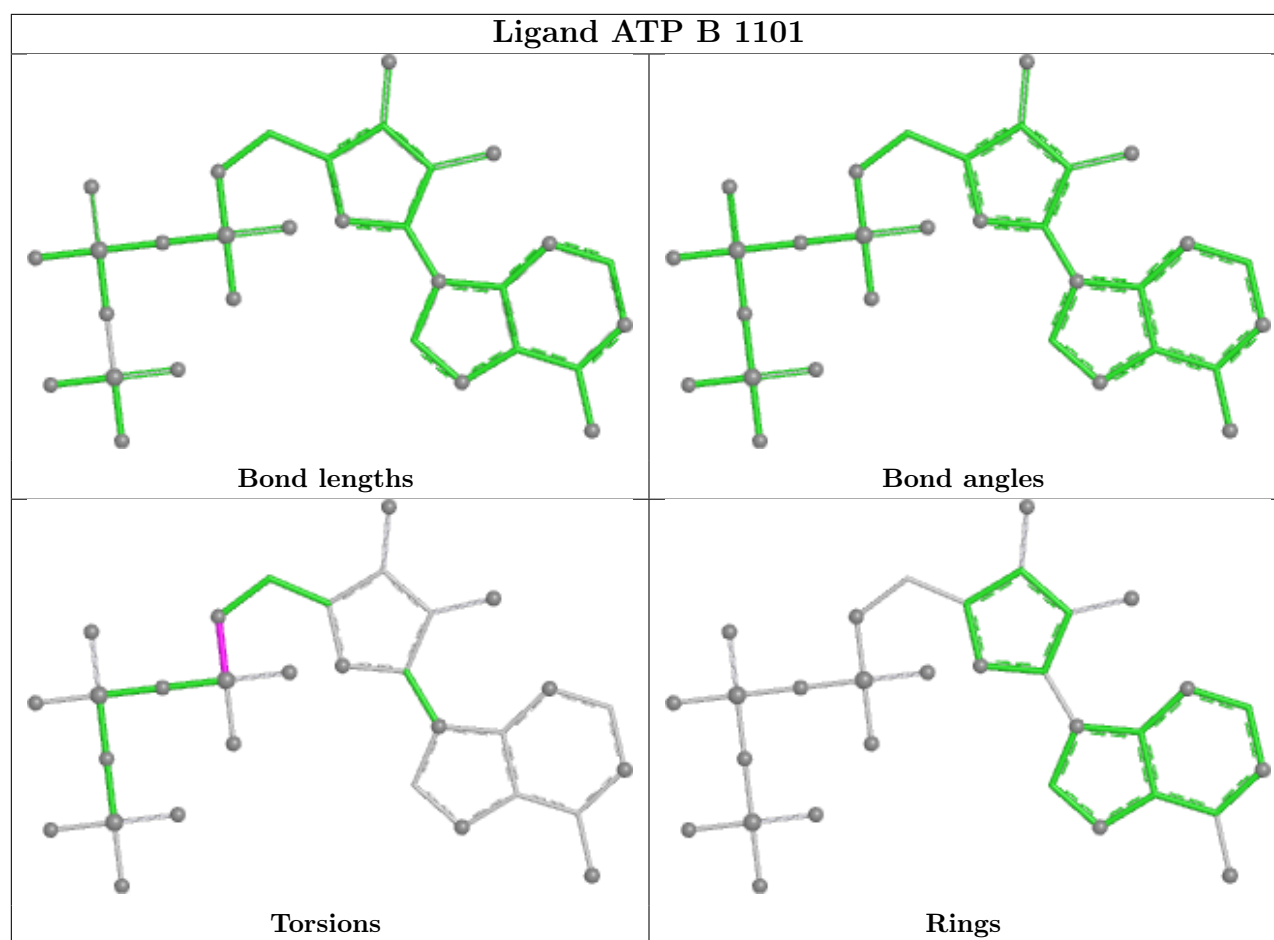
There are no ring outliers.

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 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	990/1052 (94%)	0.28	47 (4%)	36 33	20, 60, 151, 213	0
1	B	982/1052 (93%)	0.79	87 (8%)	15 13	47, 92, 153, 206	0
All	All	1972/2104 (93%)	0.54	134 (6%)	23 21	20, 80, 152, 213	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	737	SER	6.1
1	B	274	GLY	5.6
1	B	273	ILE	4.9
1	B	1032	ILE	4.9
1	A	35	ALA	3.9
1	B	66	LEU	3.9
1	B	460	ASN	3.9
1	B	630	PHE	3.8
1	B	738	PRO	3.7
1	B	997	VAL	3.5
1	B	1012	LEU	3.5
1	B	875	ILE	3.5
1	A	1047	PHE	3.5
1	B	271	PHE	3.4
1	B	617	PRO	3.4
1	B	530	LEU	3.4
1	A	1000	GLY	3.2
1	B	728	LEU	3.2
1	A	790	VAL	3.2
1	B	252	GLY	3.1
1	A	734	PHE	3.1
1	B	1048	SER	3.1
1	B	277	THR	3.1
1	B	229	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	867	ASN	3.1
1	B	681	GLY	3.0
1	A	826	PHE	3.0
1	B	960	VAL	3.0
1	A	836	GLU	3.0
1	B	239	LEU	2.9
1	B	592	GLY	2.9
1	A	716	LEU	2.9
1	B	790	VAL	2.9
1	A	996	PRO	2.8
1	B	67	SER	2.8
1	B	1035	ASP	2.8
1	B	826	PHE	2.8
1	A	615	ARG	2.8
1	B	209	THR	2.8
1	A	1002	ALA	2.7
1	A	1015	PRO	2.7
1	A	971	PHE	2.7
1	A	1048	SER	2.7
1	B	1034	GLY	2.7
1	A	728	LEU	2.7
1	B	946	ILE	2.6
1	B	964	GLU	2.6
1	B	795	PHE	2.6
1	B	228	ILE	2.6
1	B	792	ILE	2.6
1	B	797	PRO	2.6
1	B	315	ASP	2.6
1	B	380	SER	2.5
1	B	970	ASP	2.5
1	A	724	LEU	2.5
1	B	227	GLY	2.5
1	B	281	PRO	2.5
1	A	992	MET	2.5
1	B	818	SER	2.5
1	A	789	GLU	2.5
1	B	226	PRO	2.5
1	A	231	CYS	2.5
1	A	737	SER	2.5
1	B	788	SER	2.5
1	B	282	TYR	2.5
1	A	966	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	510	PHE	2.5
1	B	593	THR	2.5
1	B	269	PHE	2.5
1	A	961	HIS	2.4
1	B	53	ASP	2.4
1	A	617	PRO	2.4
1	A	1012	LEU	2.4
1	B	275	ASP	2.4
1	B	381	TRP	2.4
1	B	992	MET	2.4
1	B	618	PRO	2.4
1	B	961	HIS	2.4
1	B	616	ASP	2.4
1	A	717	GLN	2.4
1	B	800	LYS	2.4
1	A	797	PRO	2.4
1	B	949	GLY	2.4
1	A	1051	THR	2.3
1	B	1020	LYS	2.3
1	B	624	PHE	2.3
1	B	1047	PHE	2.3
1	B	225	ASN	2.3
1	A	431	PRO	2.3
1	B	1030	PRO	2.3
1	A	726	ILE	2.3
1	B	920	ALA	2.3
1	A	618	PRO	2.3
1	A	827	GLN	2.3
1	A	735	TRP	2.3
1	B	258	GLY	2.3
1	B	801	VAL	2.3
1	B	666	ALA	2.2
1	B	780	ALA	2.2
1	B	631	PRO	2.2
1	A	997	VAL	2.2
1	A	881	PHE	2.2
1	B	217	PHE	2.2
1	B	1017	THR	2.2
1	A	1010	HIS	2.2
1	B	825	ILE	2.2
1	A	1017	THR	2.2
1	B	626	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	658	LYS	2.2
1	A	313	ILE	2.2
1	A	954	ILE	2.2
1	B	218	ILE	2.2
1	B	707	PHE	2.2
1	A	742	PRO	2.1
1	B	143	ASN	2.1
1	A	37	VAL	2.1
1	B	966	PHE	2.1
1	A	845	ALA	2.1
1	B	774	ALA	2.1
1	B	1016	THR	2.1
1	B	614	HIS	2.1
1	A	986	VAL	2.1
1	B	345	VAL	2.1
1	B	781	ASP	2.1
1	B	817	SER	2.1
1	B	1029	ALA	2.1
1	A	736	GLN	2.1
1	B	799	ASN	2.1
1	A	1001	HIS	2.1
1	B	848	SER	2.0
1	B	314	VAL	2.0
1	B	722	PHE	2.0
1	A	965	ASP	2.0
1	A	1037	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CAS	B	721	9/10	0.73	0.15	138,163,195,195	0
1	CAS	A	721	9/10	0.81	0.14	133,158,189,189	0
1	CAS	B	414	9/10	0.84	0.15	78,104,148,148	0
1	CAS	A	347	9/10	0.86	0.16	70,88,141,141	0
1	CAS	B	347	9/10	0.87	0.15	106,129,182,182	0
1	CAS	B	682	9/10	0.89	0.14	89,112,154,154	0
1	CAS	B	311	9/10	0.90	0.13	88,110,168,168	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CAS	B	770	9/10	0.90	0.14	68,105,150,150	0
1	CAS	A	682	9/10	0.91	0.11	97,124,152,152	0
1	CAS	A	770	9/10	0.91	0.12	82,104,174,174	0
1	CAS	B	178	9/10	0.91	0.17	103,119,136,136	0
1	CAS	A	414	9/10	0.92	0.12	34,66,110,110	0
1	CAS	A	311	9/10	0.92	0.14	64,84,104,104	0
1	CAS	B	433	9/10	0.92	0.11	89,109,151,151	0
1	CAS	A	433	9/10	0.93	0.10	60,73,115,115	0
1	CAS	A	178	9/10	0.97	0.09	47,62,81,81	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

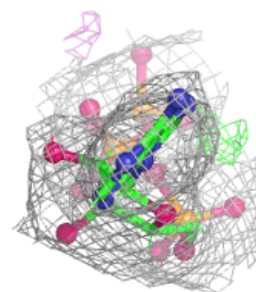
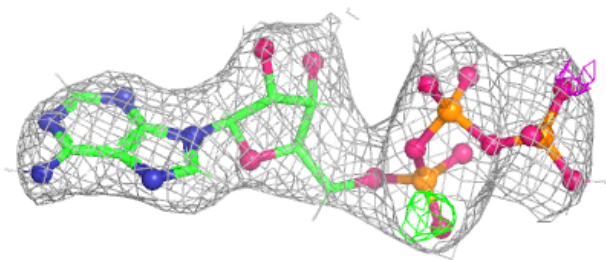
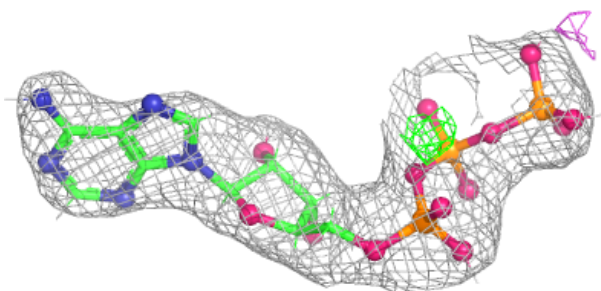
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	1104	6/6	0.67	0.11	78,94,95,95	0
3	GOL	B	1105	6/6	0.76	0.15	84,102,106,108	0
3	GOL	B	1102	6/6	0.79	0.17	76,91,102,103	0
3	GOL	B	1103	6/6	0.85	0.12	54,65,70,70	0
3	GOL	A	1105	6/6	0.86	0.12	50,60,65,65	0
5	CA	A	1107	1/1	0.86	0.11	89,89,89,89	0
2	ATP	B	1101	31/31	0.87	0.11	56,70,85,101	0
3	GOL	A	1102	6/6	0.88	0.10	51,62,70,71	0
3	GOL	A	1103	6/6	0.88	0.09	52,63,68,68	0
3	GOL	A	1104	6/6	0.89	0.12	44,54,60,60	0
2	ATP	A	1101	31/31	0.94	0.09	24,33,43,71	0
5	CA	A	1108	1/1	0.95	0.13	49,49,49,49	0
4	MG	A	1106	1/1	0.96	0.07	11,11,11,11	0
4	MG	B	1106	1/1	0.96	0.14	38,38,38,38	0
6	CL	A	1109	1/1	0.96	0.04	62,62,62,62	0
5	CA	B	1107	1/1	0.98	0.08	65,65,65,65	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.

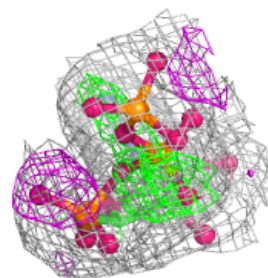
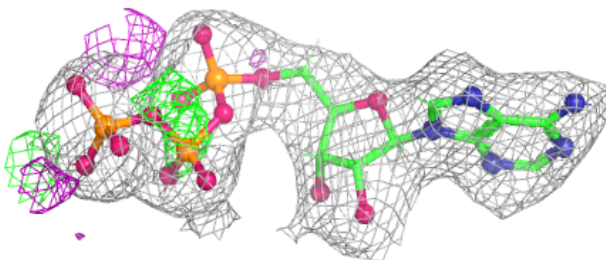
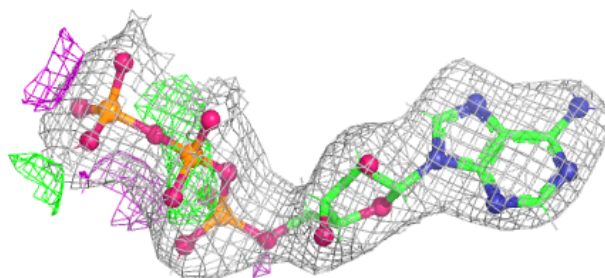
Electron density around ATP B 1101:

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



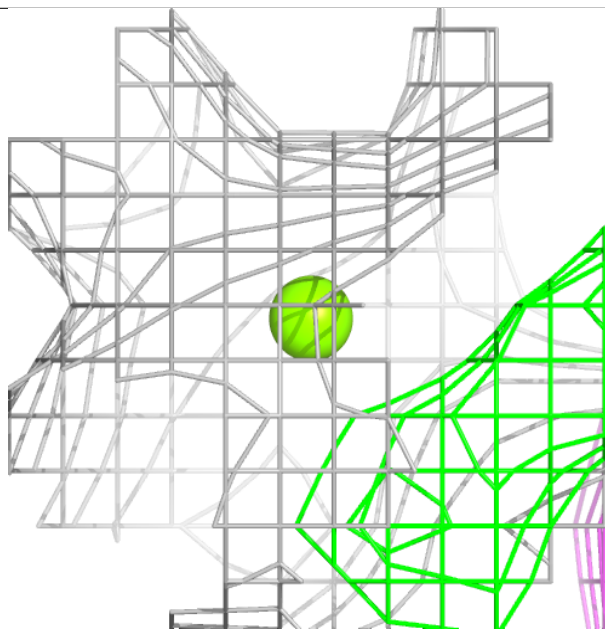
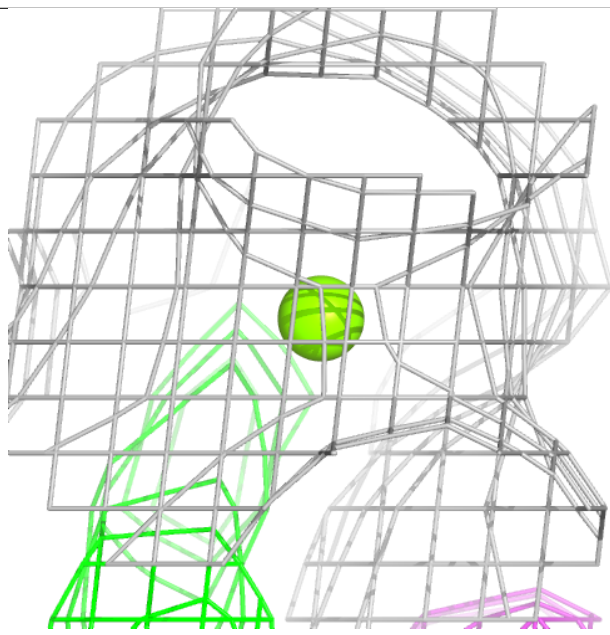
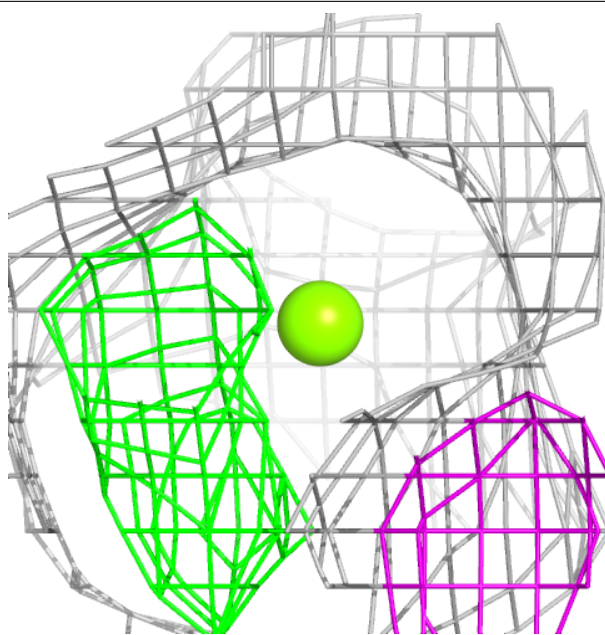
Electron density around ATP A 1101:

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



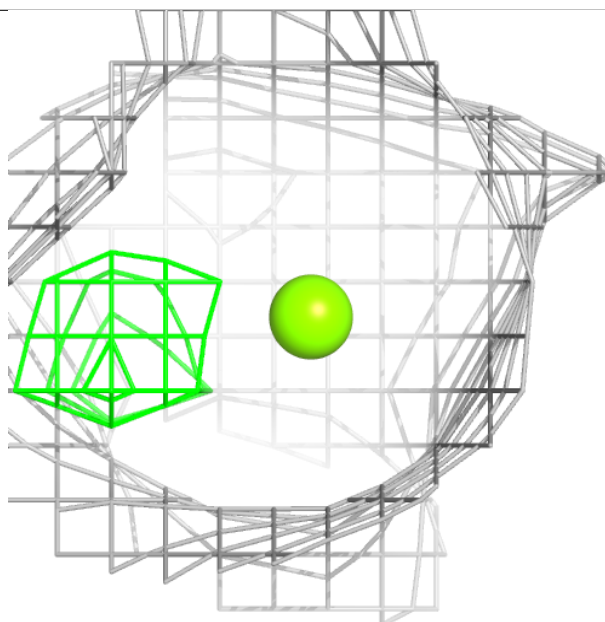
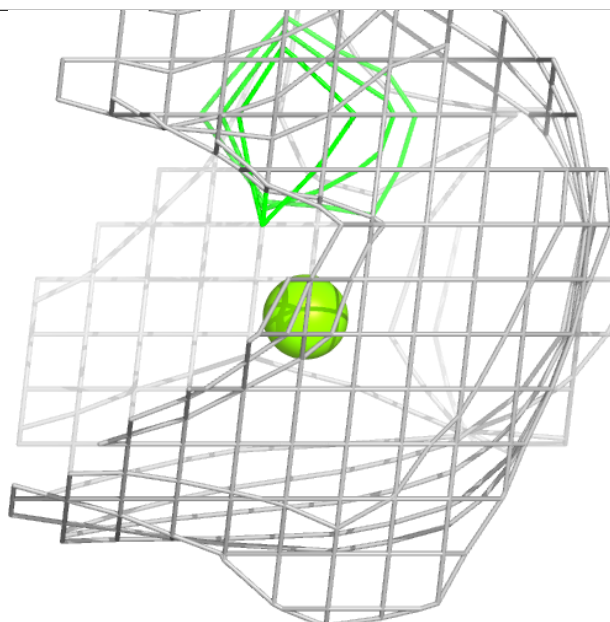
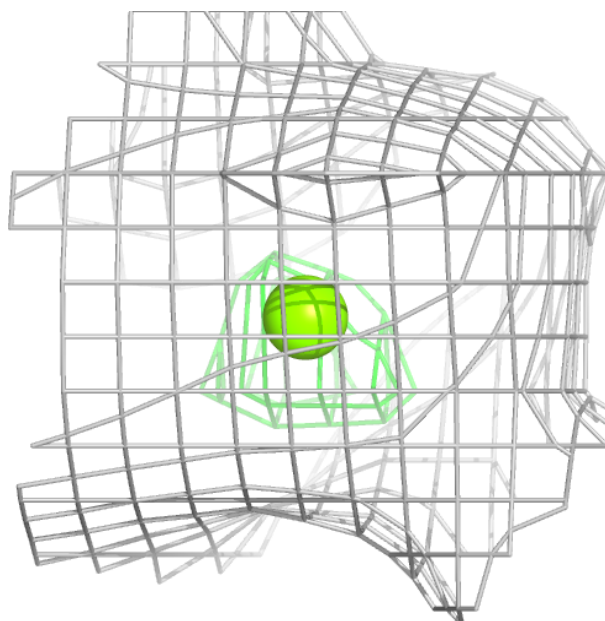
Electron density around MG A 1106:

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



Electron density around 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.