



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:44 PM UTC

PDB ID : 7SOL / pdb_00007sol
Title : Crystal Structures of the bispecific ubiquitin/FAT10 activating enzyme, Uba6
Authors : Olsen, S.K.; Gao, F.; Lv, Z.
Deposited on : 2021-10-31
Resolution : 2.25 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

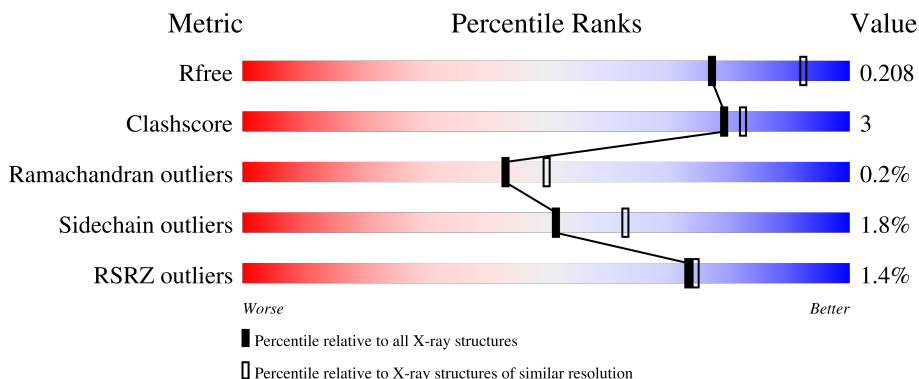
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	1020	 91% 8%
1	C	1020	 88% 6% 5%
2	B	83	 95% 5%
2	D	83	 86% 11%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 17964 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 Ubiquitin-like modifier-activating enzyme 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1011	Total 8021	C 5131	N 1346	O 1507	S 37	0	1	0
1	C	970	Total 7682	C 4923	N 1284	O 1439	S 36	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP A0AVT1
A	34	ALA	-	expression tag	UNP A0AVT1
A	35	MET	-	expression tag	UNP A0AVT1
A	36	GLY	-	expression tag	UNP A0AVT1
A	625	ALA	CYS	engineered mutation	UNP A0AVT1
C	33	GLY	-	expression tag	UNP A0AVT1
C	34	ALA	-	expression tag	UNP A0AVT1
C	35	MET	-	expression tag	UNP A0AVT1
C	36	GLY	-	expression tag	UNP A0AVT1
C	625	ALA	CYS	engineered mutation	UNP A0AVT1

- Molecule 2 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	83	Total 680	C 416	N 138	O 124	S 2	0	0	0
2	D	80	Total 652	C 399	N 131	O 121	S 1	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

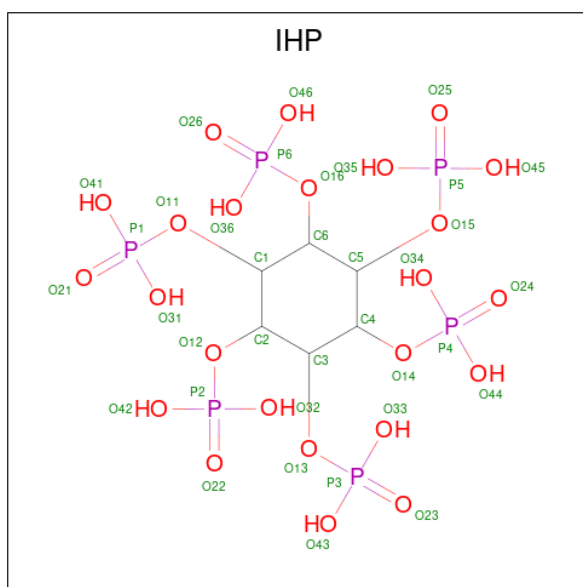
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	expression tag	UNP P69326
B	-5	HIS	-	expression tag	UNP P69326

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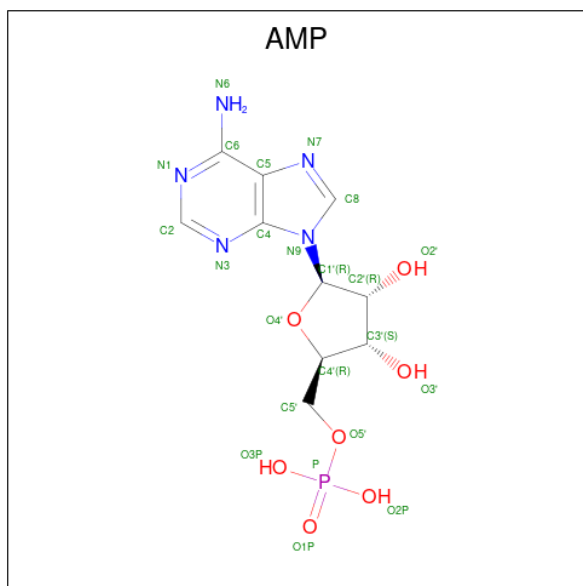
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P69326
B	-3	HIS	-	expression tag	UNP P69326
B	-2	HIS	-	expression tag	UNP P69326
B	-1	HIS	-	expression tag	UNP P69326
B	0	HIS	-	expression tag	UNP P69326
B	6	ARG	LYS	engineered mutation	UNP P69326
B	11	ARG	LYS	engineered mutation	UNP P69326
B	27	ARG	LYS	engineered mutation	UNP P69326
B	29	ARG	LYS	engineered mutation	UNP P69326
B	33	ARG	LYS	engineered mutation	UNP P69326
B	48	ARG	LYS	engineered mutation	UNP P69326
B	63	ARG	LYS	engineered mutation	UNP P69326
D	-6	MET	-	expression tag	UNP P69326
D	-5	HIS	-	expression tag	UNP P69326
D	-4	HIS	-	expression tag	UNP P69326
D	-3	HIS	-	expression tag	UNP P69326
D	-2	HIS	-	expression tag	UNP P69326
D	-1	HIS	-	expression tag	UNP P69326
D	0	HIS	-	expression tag	UNP P69326
D	6	ARG	LYS	engineered mutation	UNP P69326
D	11	ARG	LYS	engineered mutation	UNP P69326
D	27	ARG	LYS	engineered mutation	UNP P69326
D	29	ARG	LYS	engineered mutation	UNP P69326
D	33	ARG	LYS	engineered mutation	UNP P69326
D	48	ARG	LYS	engineered mutation	UNP P69326
D	63	ARG	LYS	engineered mutation	UNP P69326

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	36	6	24	6	0	0

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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

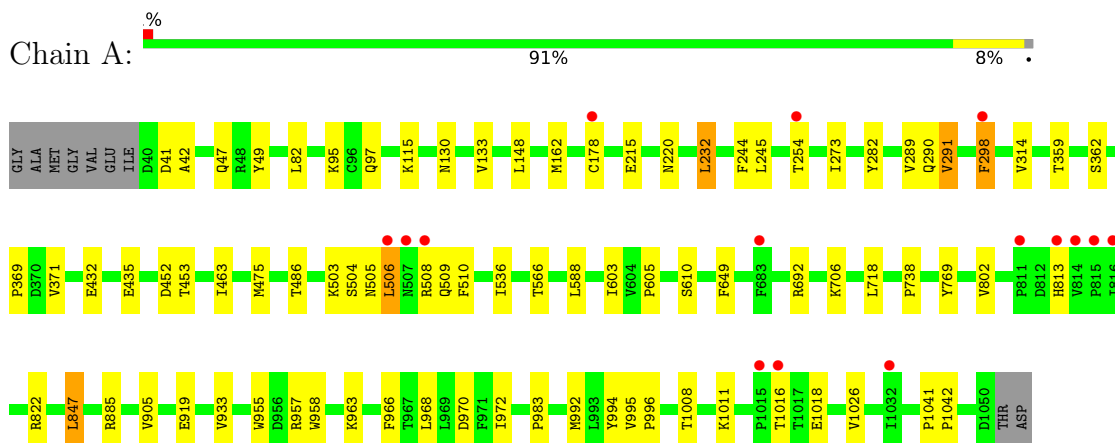
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total 354	O 354	0	0
5	B	62	Total 62	O 62	0	0
5	C	389	Total 389	O 389	0	0
5	D	42	Total 42	O 42	0	0

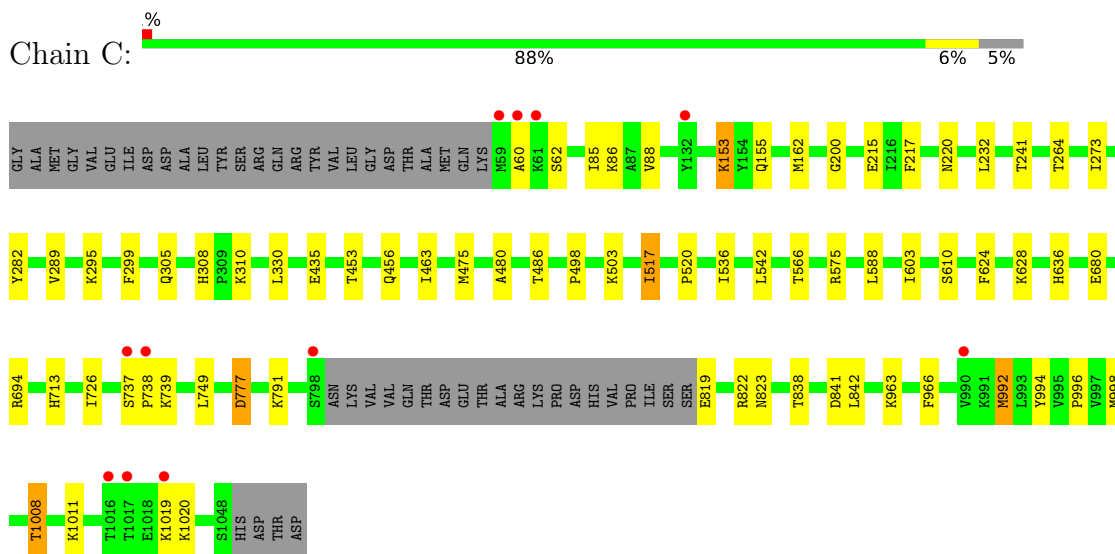
3 Residue-property plots [i](#)

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

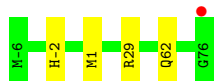


- Molecule 1: Ubiquitin-like modifier-activating enzyme 6

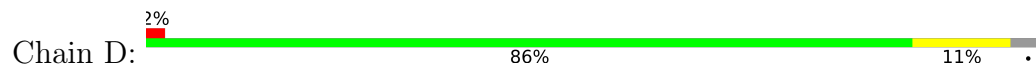


- Molecule 2: Ubiquitin





- Molecule 2: Ubiquitin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.57Å 101.32Å 122.92Å 90.00° 118.00° 90.00°	Depositor
Resolution (Å)	45.90 – 2.25 45.90 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.90-2.25) 93.7 (45.90-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.166 , 0.206 0.168 , 0.208	Depositor DCC
R_{free} test set	2000 reflections (1.56%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtrriage
Anisotropy	0.210	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17964	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: AMP, IHP

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	0.19	0/8206	0.40	0/11128
1	C	0.20	0/7859	0.41	0/10656
2	B	0.21	0/691	0.44	0/931
2	D	0.23	0/661	0.48	0/891
All	All	0.20	0/17417	0.41	0/23606

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	CYS	Peptide

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	8021	0	8011	47	0
1	C	7682	0	7686	38	0
2	B	680	0	676	2	0
2	D	652	0	653	6	0
3	A	36	0	6	1	0
4	B	23	0	12	0	0
4	D	23	0	12	0	0
5	A	354	0	0	8	0
5	B	62	0	0	1	0
5	C	389	0	0	3	0
5	D	42	0	0	1	0
All	All	17964	0	17056	93	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 3.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:919:GLU:OE1	5:A:1201:HOH:O	1.92	0.87
2:D:63:ARG:HG2	2:D:64:GLU:HG2	1.63	0.80
1:A:649:PHE:HB3	1:A:847:LEU:HD22	1.63	0.79
1:C:85:ILE:HD11	1:C:88:VAL:HG22	1.66	0.77
1:C:217:PHE:HB2	1:C:232:LEU:HD22	1.71	0.73
1:A:919:GLU:OE2	5:A:1202:HOH:O	2.10	0.68
1:A:362:SER:OG	1:A:369:PRO:O	2.12	0.67
1:A:992:MET:HE3	1:A:995:VAL:HG21	1.77	0.67
1:C:456:GLN:NE2	5:C:1103:HOH:O	2.27	0.66
1:A:215:GLU:OE1	5:A:1203:HOH:O	2.13	0.65
1:A:885:ARG:NH1	5:A:1207:HOH:O	2.32	0.63
1:A:298[A]:PHE:H	1:A:298[A]:PHE:HD1	1.48	0.62
1:C:520:PRO:HB3	1:C:542:LEU:HD21	1.83	0.61
1:C:435:GLU:OE2	1:C:453:THR:OG1	2.17	0.61
1:A:41:ASP:OD1	1:A:42:ALA:N	2.35	0.60
1:C:566:THR:HG23	1:C:588:LEU:HD11	1.84	0.60
1:C:503:LYS:HB3	1:C:517:ILE:HD11	1.83	0.59
1:C:503:LYS:H	1:C:517:ILE:HD11	1.69	0.58
1:C:503:LYS:N	1:C:517:ILE:HD11	2.19	0.57
1:A:983:PRO:HB3	1:A:1026:VAL:HG13	1.87	0.57
1:A:566:THR:HG23	1:A:588:LEU:HD11	1.87	0.57
1:C:241:THR:HG23	1:C:264:THR:HA	1.88	0.56
1:A:232:LEU:HD21	1:A:738:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:MET:HE1	1:A:905:VAL:HB	1.89	0.55
1:C:215:GLU:HG2	1:C:289:VAL:HG22	1.88	0.55
1:A:958:TRP:CE2	1:A:1041:PRO:HG2	2.43	0.54
1:C:777:ASP:OD1	1:C:777:ASP:N	2.33	0.54
1:C:575:ARG:NH1	5:C:1104:HOH:O	2.28	0.53
1:A:432:GLU:OE2	5:A:1204:HOH:O	2.19	0.53
1:A:822:ARG:NH1	5:A:1213:HOH:O	2.42	0.53
1:A:82:LEU:HD11	1:A:510:PHE:HB3	1.91	0.53
1:A:435:GLU:OE2	1:A:453:THR:OG1	2.26	0.52
1:C:200:GLY:O	1:C:299:PHE:HB2	2.11	0.50
2:D:63:ARG:NH1	5:D:2201:HOH:O	2.37	0.50
1:C:1008:THR:CG2	1:C:1011:LYS:H	2.25	0.49
1:C:994:TYR:CE2	1:C:996:PRO:HG3	2.48	0.49
1:A:994:TYR:CZ	1:A:996:PRO:HG3	2.47	0.48
1:A:314:VAL:HG12	1:A:933:VAL:HB	1.95	0.48
1:A:603:ILE:HG12	1:A:610:SER:HA	1.96	0.47
1:C:694:ARG:NH1	1:C:841:ASP:OD1	2.46	0.47
1:A:963:LYS:H	1:A:966:PHE:HB2	1.80	0.47
1:C:603:ILE:HG12	1:C:610:SER:HA	1.97	0.47
1:A:506:LEU:HD22	1:A:506:LEU:H	1.79	0.46
1:C:305:GLN:NE2	1:C:310:LYS:HE2	2.29	0.46
1:C:517:ILE:HA	1:C:517:ILE:HD13	1.54	0.46
1:A:215:GLU:HG2	1:A:289:VAL:HG22	1.96	0.46
1:C:60:ALA:O	1:C:155:GLN:HB2	2.16	0.46
1:C:1008:THR:HG22	1:C:1011:LYS:HG2	1.97	0.46
1:A:503:LYS:HD3	1:A:506:LEU:HD23	1.98	0.45
1:A:505:ASN:HB3	1:A:509:GLN:OE1	2.17	0.45
1:A:95:LYS:HD2	1:A:115:LYS:O	2.15	0.45
1:C:498:PRO:O	1:C:739:LYS:HD3	2.17	0.45
2:D:0:HIS:NE2	2:D:16:GLU:HB3	2.32	0.45
2:B:1:MET:HE1	2:B:62:GLN:HA	1.99	0.45
1:A:1008:THR:CG2	1:A:1011:LYS:H	2.30	0.44
1:C:628:LYS:HD2	1:C:636:HIS:CG	2.51	0.44
1:C:62:SER:HB3	1:C:86:LYS:HB3	1.99	0.44
1:A:966:PHE:CE1	1:A:970:ASP:HB3	2.53	0.44
1:A:49:TYR:CE1	1:A:885:ARG:HB2	2.53	0.44
1:C:713:HIS:HE1	5:C:1108:HOH:O	1.99	0.44
1:A:706:LYS:NZ	3:A:1101:IHP:O32	2.42	0.44
1:C:153:LYS:HB2	1:C:153:LYS:HE3	1.82	0.44
1:C:220:ASN:HA	1:C:282:TYR:CE2	2.53	0.44
1:A:359:THR:HA	1:A:371:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:LEU:O	1:A:972:ILE:HG12	2.18	0.44
1:C:162:MET:HE3	1:C:162:MET:HB2	1.83	0.44
2:D:0:HIS:CE1	2:D:16:GLU:HB3	2.52	0.44
1:A:244:PHE:O	1:A:291:VAL:HG13	2.18	0.44
1:A:486:THR:HG22	1:A:536:ILE:HA	2.00	0.44
1:C:819:GLU:HA	1:C:822:ARG:HD2	1.99	0.43
1:A:162:MET:HE3	1:A:162:MET:HB2	1.95	0.43
1:A:435:GLU:HG2	1:A:452:ASP:H	1.84	0.43
1:A:605:PRO:HA	1:A:955:TRP:CE2	2.54	0.43
1:A:957:ARG:HG3	1:A:1042:PRO:HG2	2.00	0.42
1:C:726:ILE:HD12	1:C:726:ILE:HA	1.93	0.42
1:A:97:GLN:HG2	5:A:1312:HOH:O	2.20	0.42
1:C:992:MET:HB2	1:C:992:MET:HE2	1.64	0.42
1:C:295:LYS:HE2	1:C:295:LYS:HB3	1.85	0.42
1:A:692:ARG:HG3	1:A:769:TYR:CD1	2.55	0.42
1:C:838:THR:O	1:C:842:LEU:HG	2.20	0.41
1:C:963:LYS:H	1:C:966:PHE:HB2	1.85	0.41
1:C:480:ALA:HA	1:C:536:ILE:HD12	2.02	0.41
2:D:0:HIS:HE2	2:D:16:GLU:HB3	1.84	0.41
1:A:245:LEU:HD23	1:A:290:GLN:HA	2.03	0.41
1:A:254:THR:HA	5:A:1447:HOH:O	2.20	0.41
1:C:749:LEU:HA	1:C:749:LEU:HD12	1.84	0.41
1:C:486:THR:HG22	1:C:536:ILE:HA	2.03	0.41
2:D:17:VAL:HG12	2:D:29:ARG:HD2	2.02	0.41
1:A:130:ASN:HD21	1:A:133:VAL:HG23	1.86	0.40
2:B:29:ARG:HD3	5:B:1243:HOH:O	2.20	0.40
1:A:1008:THR:HG23	1:A:1011:LYS:H	1.85	0.40
1:A:220:ASN:HA	1:A:282:TYR:CE2	2.57	0.40
1:A:475:MET:HE1	1:A:905:VAL:CB	2.51	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	1010/1020 (99%)	976 (97%)	32 (3%)	2 (0%)	43	50
1	C	966/1020 (95%)	937 (97%)	26 (3%)	3 (0%)	36	40
2	B	81/83 (98%)	81 (100%)	0	0	100	100
2	D	78/83 (94%)	78 (100%)	0	0	100	100
All	All	2135/2206 (97%)	2072 (97%)	58 (3%)	5 (0%)	43	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	SER
1	C	737	SER
1	C	738	PRO
1	A	273	ILE
1	C	273	ILE

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	893/898 (99%)	878 (98%)	15 (2%)	53	65
1	C	855/898 (95%)	839 (98%)	16 (2%)	50	61
2	B	74/74 (100%)	73 (99%)	1 (1%)	59	70
2	D	71/74 (96%)	68 (96%)	3 (4%)	26	31
All	All	1893/1944 (97%)	1858 (98%)	35 (2%)	51	63

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	148	LEU
1	A	232	LEU
1	A	291	VAL
1	A	298[A]	PHE
1	A	298[B]	PHE

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Mol	Chain	Res	Type
1	A	463	ILE
1	A	506	LEU
1	A	508	ARG
1	A	718	LEU
1	A	802	VAL
1	A	813	HIS
1	A	847	LEU
1	A	1016	THR
1	A	1018	GLU
2	B	-2	HIS
1	C	153	LYS
1	C	308	HIS
1	C	330	LEU
1	C	463	ILE
1	C	475	MET
1	C	517	ILE
1	C	624	PHE
1	C	680	GLU
1	C	777	ASP
1	C	791	LYS
1	C	823	ASN
1	C	992	MET
1	C	998	MET
1	C	1008	THR
1	C	1019	LYS
1	C	1020	LYS
2	D	-2	HIS
2	D	71	LEU
2	D	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	251	ASN
1	A	308	HIS
1	A	614	HIS
1	A	671	GLN
1	A	793	GLN
2	B	60	ASN
1	C	134	HIS
1	C	177	GLN

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Mol	Chain	Res	Type
1	C	223	GLN
1	C	606	HIS
1	C	717	GLN
1	C	736	GLN
1	C	760	ASN
1	C	835	ASN
1	C	1010	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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
4	AMP	B	1101	2	25,25,25	0.94	2 (8%)	37,38,38	1.94	9 (24%)
4	AMP	D	2101	2	25,25,25	0.92	1 (4%)	37,38,38	1.94	9 (24%)
3	IHP	A	1101	-	36,36,36	1.18	0	60,60,60	0.61	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
4	AMP	B	1101	2	-	2/10/26/26	0/3/3/3
4	AMP	D	2101	2	-	1/10/26/26	0/3/3/3
3	IHP	A	1101	-	-	6/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	AMP	C8-N7	2.42	1.36	1.31
4	D	2101	AMP	C8-N7	2.25	1.36	1.31
4	B	1101	AMP	C5-N7	-2.01	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1101	AMP	C5-C4-N3	-5.35	119.35	126.72
4	D	2101	AMP	C5-C4-N3	-5.01	119.83	126.72
4	D	2101	AMP	N3-C2-N1	-4.94	121.10	128.58
4	B	1101	AMP	N3-C2-N1	-4.57	121.66	128.58
4	D	2101	AMP	N9-C8-N7	-3.72	108.66	113.94
4	D	2101	AMP	C2-N3-C4	3.44	120.23	111.83
4	B	1101	AMP	C2-N3-C4	3.38	120.08	111.83
4	B	1101	AMP	N9-C8-N7	-3.35	109.19	113.94
4	B	1101	AMP	N3-C4-N9	3.29	132.76	127.17
4	D	2101	AMP	N3-C4-N9	3.15	132.53	127.17
4	B	1101	AMP	C4-C5-N7	-2.95	107.21	110.58
4	B	1101	AMP	O2P-P-O5'	2.82	114.03	106.67
4	D	2101	AMP	C4-C5-N7	-2.81	107.37	110.58
4	D	2101	AMP	C4-N9-C8	2.77	108.65	105.74
4	B	1101	AMP	C5-N7-C8	2.69	107.67	103.45
4	D	2101	AMP	C5-N7-C8	2.68	107.67	103.45
4	D	2101	AMP	O2P-P-O5'	2.56	113.35	106.67
4	B	1101	AMP	C4-N9-C8	2.18	108.03	105.74

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1101	AMP	O4'-C4'-C5'-O5'
4	B	1101	AMP	C3'-C4'-C5'-O5'

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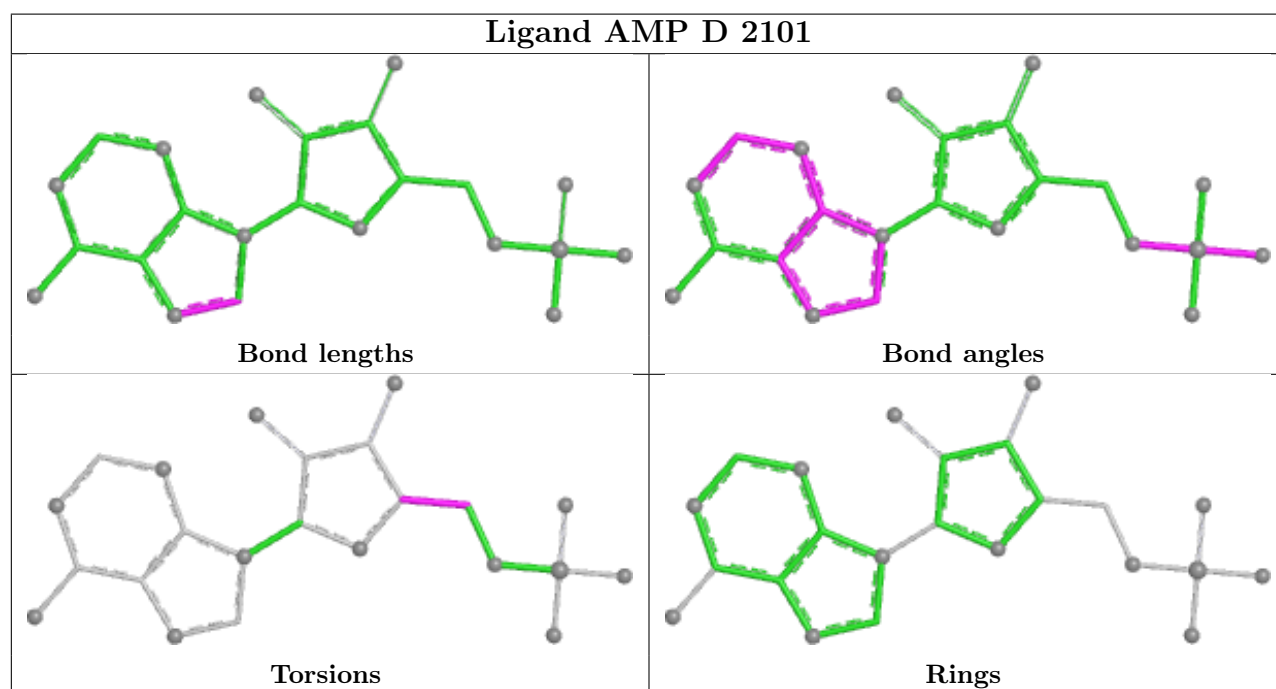
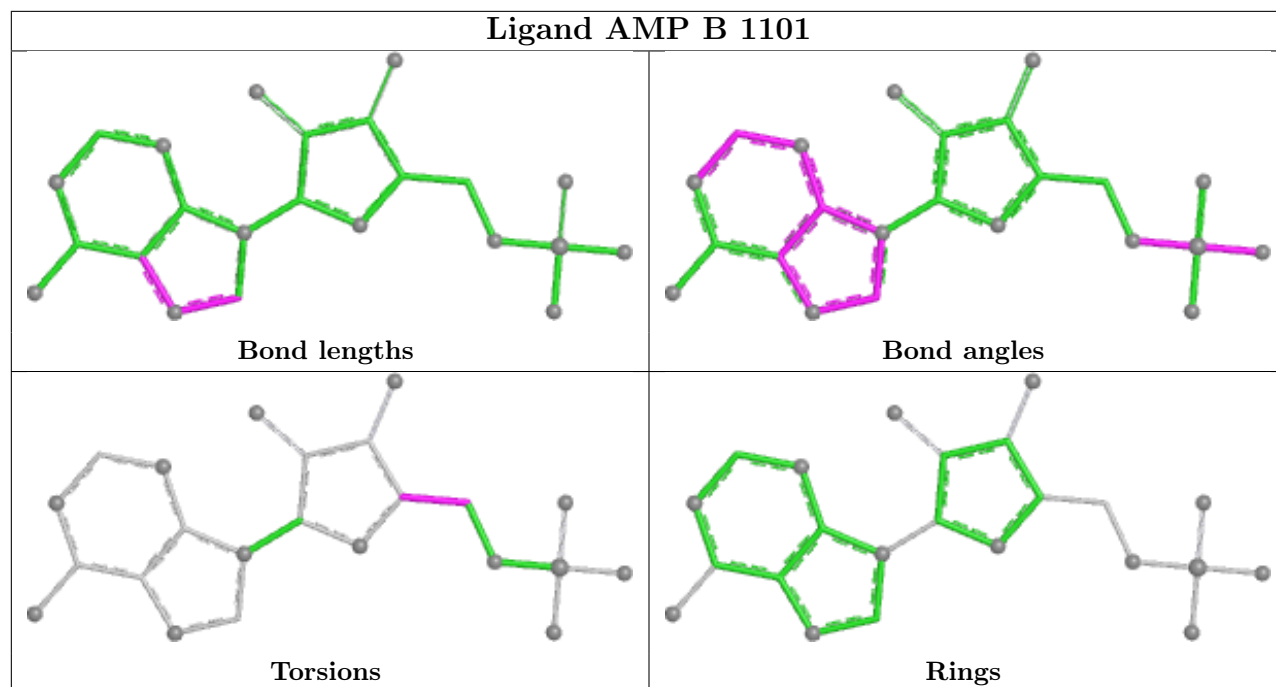
Mol	Chain	Res	Type	Atoms
3	A	1101	IHP	C5-O15-P5-O45
4	D	2101	AMP	O4'-C4'-C5'-O5'
3	A	1101	IHP	C3-O13-P3-O23
3	A	1101	IHP	C3-O13-P3-O33
3	A	1101	IHP	C3-O13-P3-O43
3	A	1101	IHP	C4-O14-P4-O44
3	A	1101	IHP	C6-O16-P6-O26

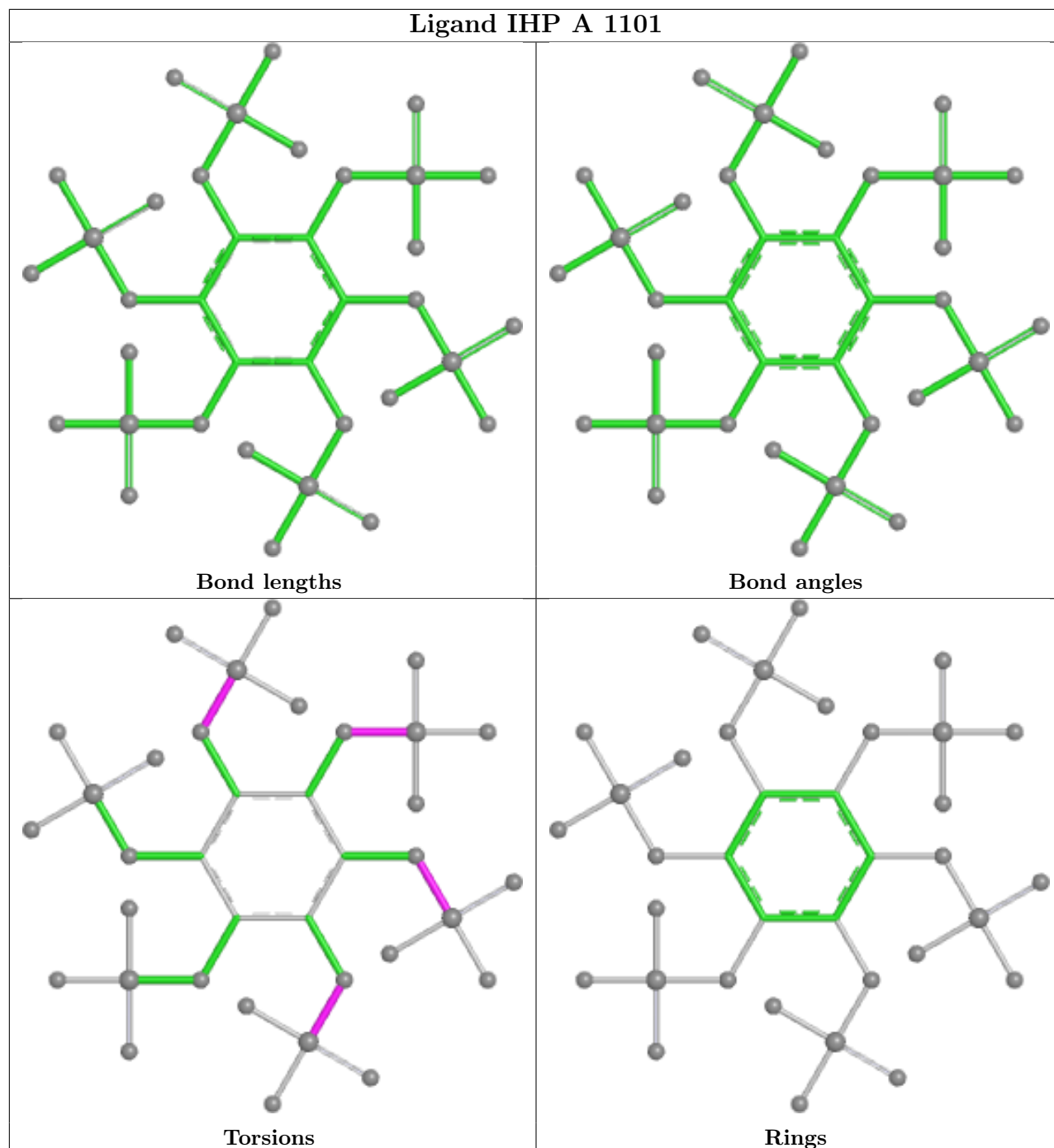
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	IHP	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	1011/1020 (99%)	-0.28	15 (1%) 72 73	24, 48, 105, 149	1 (0%)
1	C	970/1020 (95%)	-0.30	11 (1%) 78 79	25, 45, 110, 163	0
2	B	83/83 (100%)	-0.44	1 (1%) 76 77	27, 45, 74, 109	0
2	D	80/83 (96%)	-0.41	2 (2%) 58 59	28, 45, 75, 149	0
All	All	2144/2206 (97%)	-0.30	29 (1%) 73 74	24, 47, 106, 163	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	298[A]	PHE	4.7
1	A	254	THR	4.4
1	A	507	ASN	4.2
1	A	814	VAL	4.1
1	C	59	MET	3.7
1	C	738	PRO	3.7
1	A	816	ILE	3.2
1	A	178	CYS	3.1
1	C	1019	LYS	3.0
1	A	1015	PRO	2.9
1	A	813	HIS	2.9
1	C	61	LYS	2.8
1	C	737	SER	2.8
1	C	60	ALA	2.8
1	A	811	PRO	2.7
1	A	508	ARG	2.7
1	C	990	VAL	2.6
1	A	1032	ILE	2.6
1	C	1017	THR	2.6
2	B	76	GLY	2.5
1	C	1016	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	683	PHE	2.5
2	D	-3	HIS	2.4
1	A	1016	THR	2.3
1	C	798	SER	2.3
2	D	76	GLY	2.3
1	A	815	PRO	2.2
1	C	132	TYR	2.1
1	A	506	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

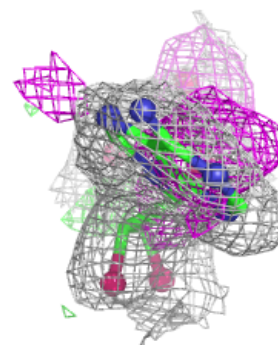
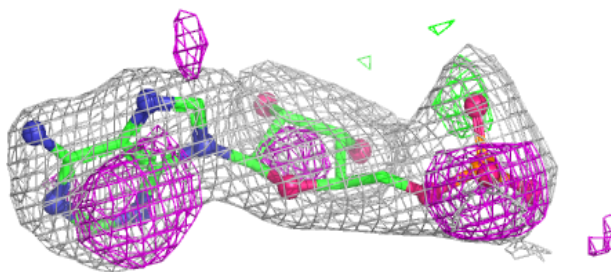
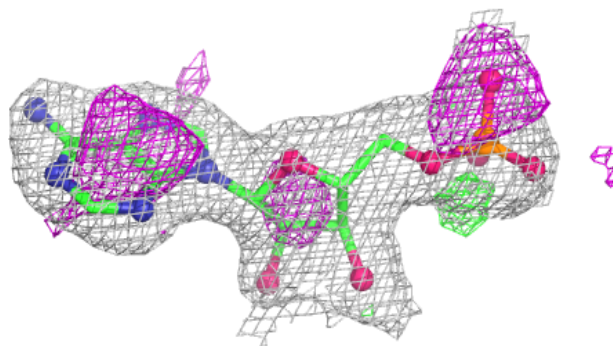
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q < 0.9
4	AMP	B	1101	23/23	0.89	0.09	33,47,58,63	0
3	IHP	A	1101	36/36	0.97	0.05	40,52,66,74	0
4	AMP	D	2101	23/23	0.97	0.05	30,37,49,54	0

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

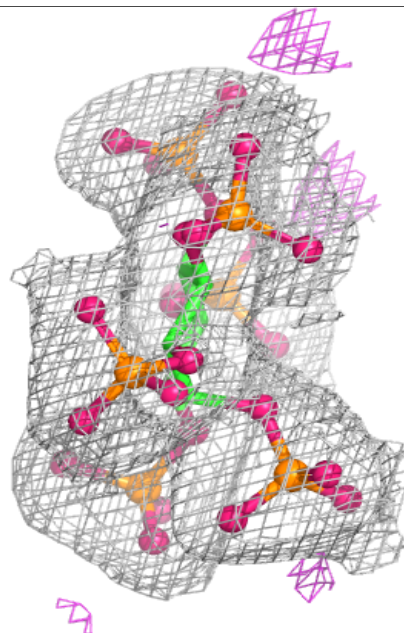
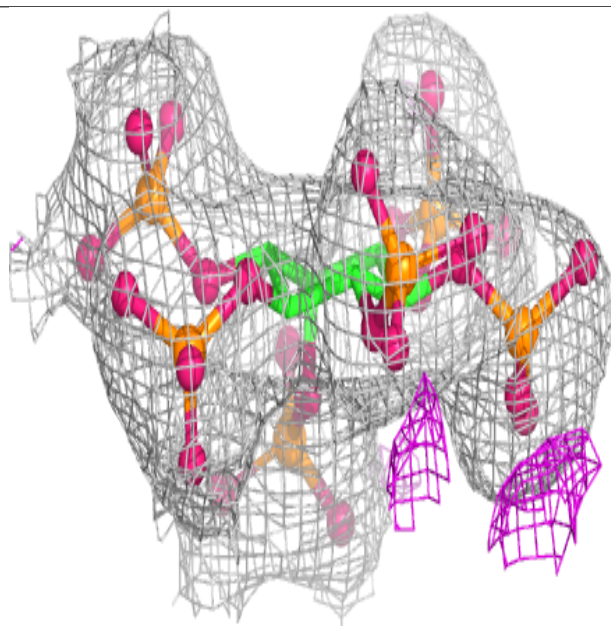
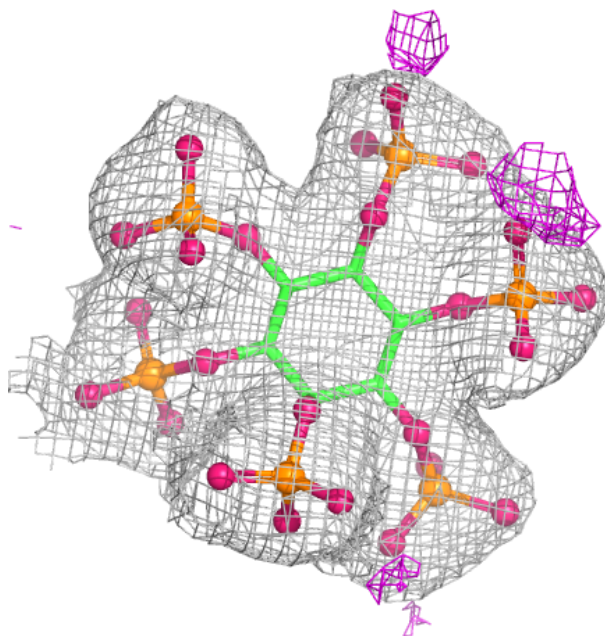
Electron density around AMP B 1101:

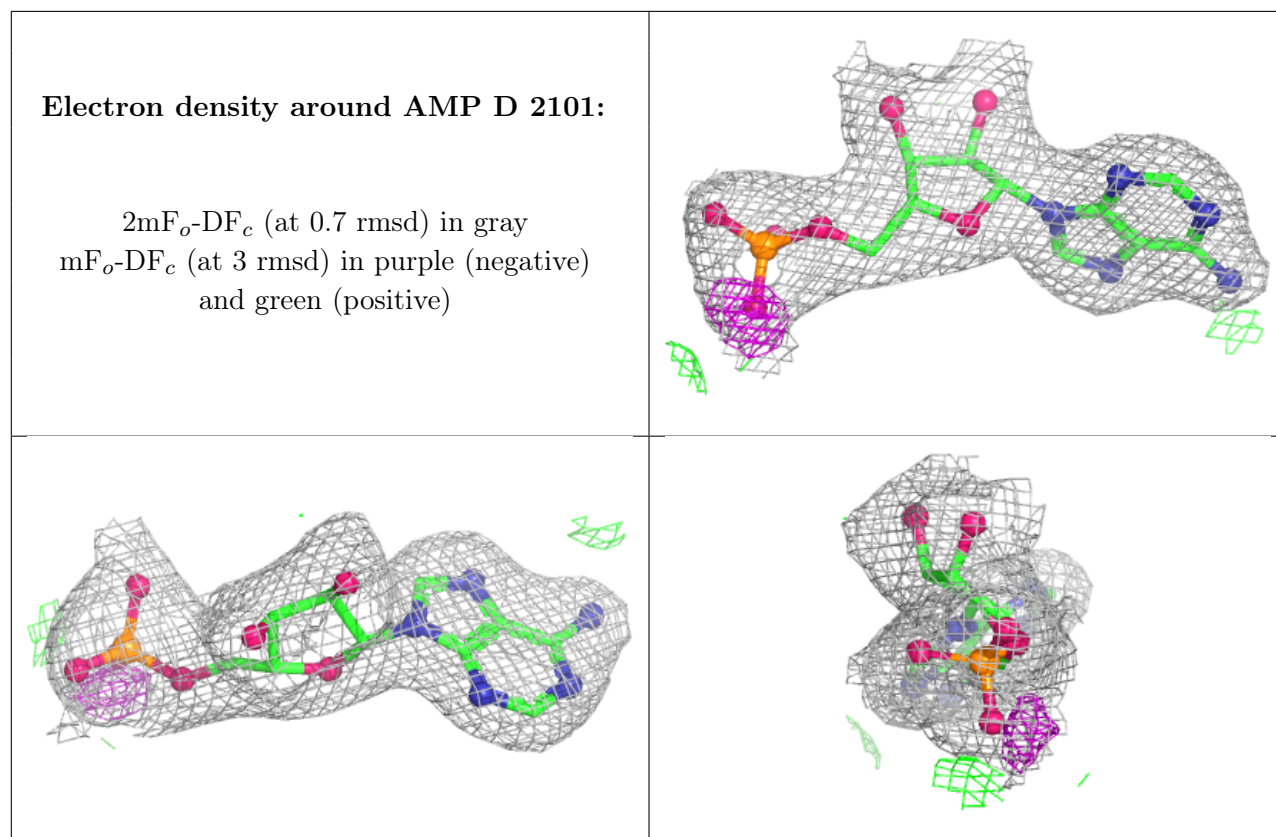
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around IHP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.