



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2022 – 05:34 PM EDT

PDB ID : 7SOL  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

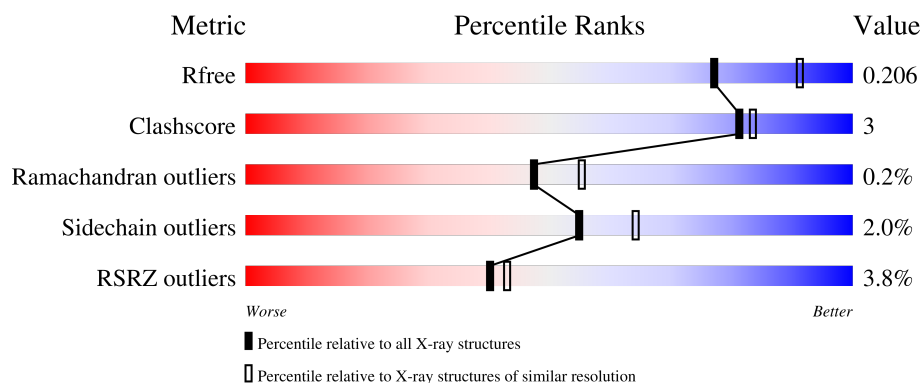
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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  $\geq 3$ , 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	<div> <div>2%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	C	1020	<div> <div>5%</div> <div>88%</div> <div>6%</div> <div>5%</div> <div>.</div> </div>
2	B	83	<div> <div>96%</div> <div>.</div> </div>
2	D	83	<div> <div>2%</div> <div>84%</div> <div>12%</div> <div>.</div> </div>

## 2 Entry composition

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
1	A	1011	Total	C	N	O	S	0	1	0
			8021	5131	1346	1507	37			
1	C	970	Total	C	N	O	S	0	0	0
			7682	4923	1284	1439	36			

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
2	B	83	Total	C	N	O	S	0	0	0
			680	416	138	124	2			
2	D	80	Total	C	N	O	S	0	0	0
			652	399	131	121	1			

There are 28 discrepancies between the modelled and reference sequences:

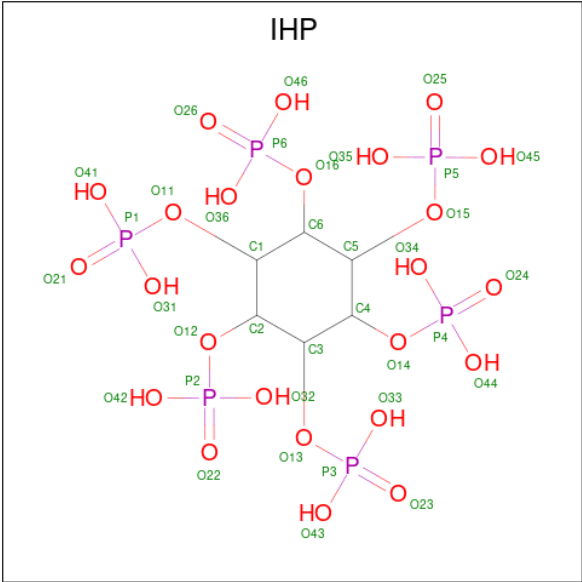
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	MET	-	expression tag	UNP P69326
B	-5	HIS	-	expression tag	UNP P69326

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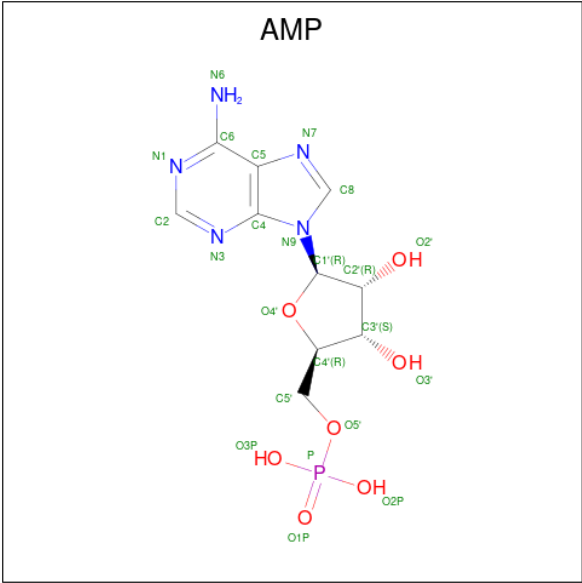
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P69326
B	-3	HIS	-	expression tag	UNP P69326
B	-2	HIS	-	expression tag	UNP P69326
B	-1	HIS	-	expression tag	UNP P69326
B	0	HIS	-	expression tag	UNP P69326
B	6	ARG	LYS	engineered mutation	UNP P69326
B	11	ARG	LYS	engineered mutation	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 (three-letter code: IHP) (formula:  $C_6H_{18}O_{24}P_6$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P) (labeled as "Ligand of Interest" by depositor).



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

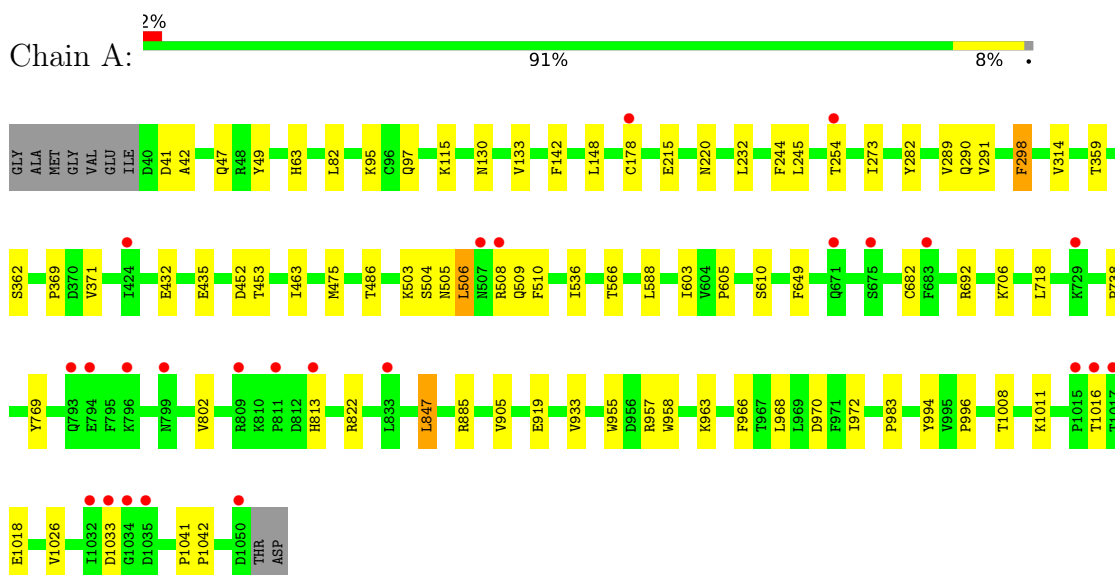
- Molecule 5 is water.

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

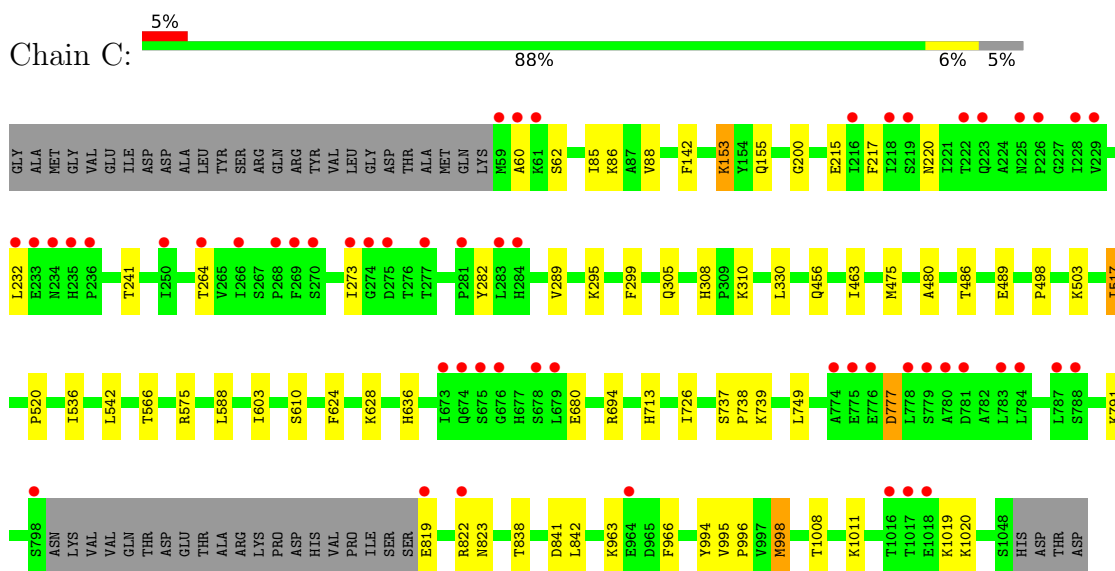
### 3 Residue-property plots

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

Chain B: 

96%

•



• Molecule 2: Ubiquitin

Chain D: 

2%

84%

12%

•





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	248.57Å 101.32Å 122.92Å 90.00° 118.00° 90.00°	Depositor
Resolution (Å)	45.90 – 2.25 45.99 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.0 (45.90-2.25) 92.5 (45.99-2.24)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.166 , 0.206 0.166 , 0.206	Depositor DCC
$R_{free}$ test set	2000 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.3	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17964	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, AMP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.29	0/8206	0.47	0/11128
1	C	0.30	0/7859	0.48	0/10656
2	B	0.28	0/691	0.52	0/931
2	D	0.29	0/661	0.57	0/891
All	All	0.29	0/17417	0.48	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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8021	0	8011	44	0
1	C	7682	0	7686	36	0
2	B	680	0	676	1	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	87	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 (87) 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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:475:MET:HE1	1:A:905:VAL:HB	1.95	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:C:995:VAL:HB	1:C:998:MET:HE2	1.98	0.45
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
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: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
1:A:968:LEU:O	1:A:972:ILE:HG12	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:819:GLU:HA	1:C:822:ARG:HD2	1.99	0.43
1:A:435:GLU:HG2	1:A:452:ASP:H	1.84	0.43
1:A:435:GLU:OE2	1:A:453:THR:OG1	2.26	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: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:A:706:LYS:NZ	3:A:1101:IHP:O32	2.42	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

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%)	47 55
1	C	966/1020 (95%)	937 (97%)	26 (3%)	3 (0%)	41 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	47	55

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 ⓘ

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%)	876 (98%)	17 (2%)	57	66
1	C	855/898 (95%)	839 (98%)	16 (2%)	57	66
2	B	74/74 (100%)	72 (97%)	2 (3%)	44	54
2	D	71/74 (96%)	67 (94%)	4 (6%)	21	21
All	All	1893/1944 (97%)	1854 (98%)	39 (2%)	55	62

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	63	HIS
1	A	142	PHE
1	A	148	LEU
1	A	298[A]	PHE
1	A	298[B]	PHE
1	A	463	ILE

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Mol	Chain	Res	Type
1	A	506	LEU
1	A	508	ARG
1	A	682	CYS
1	A	718	LEU
1	A	802	VAL
1	A	813	HIS
1	A	847	LEU
1	A	1016	THR
1	A	1018	GLU
1	A	1033	ASP
2	B	-2	HIS
2	B	24	ASP
1	C	142	PHE
1	C	153	LYS
1	C	308	HIS
1	C	330	LEU
1	C	463	ILE
1	C	475	MET
1	C	489	GLU
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	998	MET
1	C	1019	LYS
1	C	1020	LYS
2	D	-2	HIS
2	D	24	ASP
2	D	71	LEU
2	D	74	ARG

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

Mol	Chain	Res	Type
1	A	614	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	22,25,25	0.80	0	25,38,38	1.47	4 (16%)
3	IHP	A	1101	-	36,36,36	1.15	0	54,60,60	0.55	0
4	AMP	D	2101	2	22,25,25	0.87	0	25,38,38	1.43	2 (8%)

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	-	2/6/26/26	0/3/3/3
3	IHP	A	1101	-	-	5/30/54/54	0/1/1/1
4	AMP	D	2101	2	-	2/6/26/26	0/3/3/3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2101	AMP	N3-C2-N1	-4.85	121.09	128.68
4	B	1101	AMP	N3-C2-N1	-4.49	121.66	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1101	AMP	O2P-P-O5'	2.74	114.03	106.73
4	D	2101	AMP	O5'-P-O1P	2.45	113.35	106.47
4	B	1101	AMP	C3'-C2'-C1'	2.23	104.34	100.98
4	B	1101	AMP	C4-C5-N7	-2.10	107.21	109.40

There are no chirality outliers.

All (9) torsion outliers are listed below:

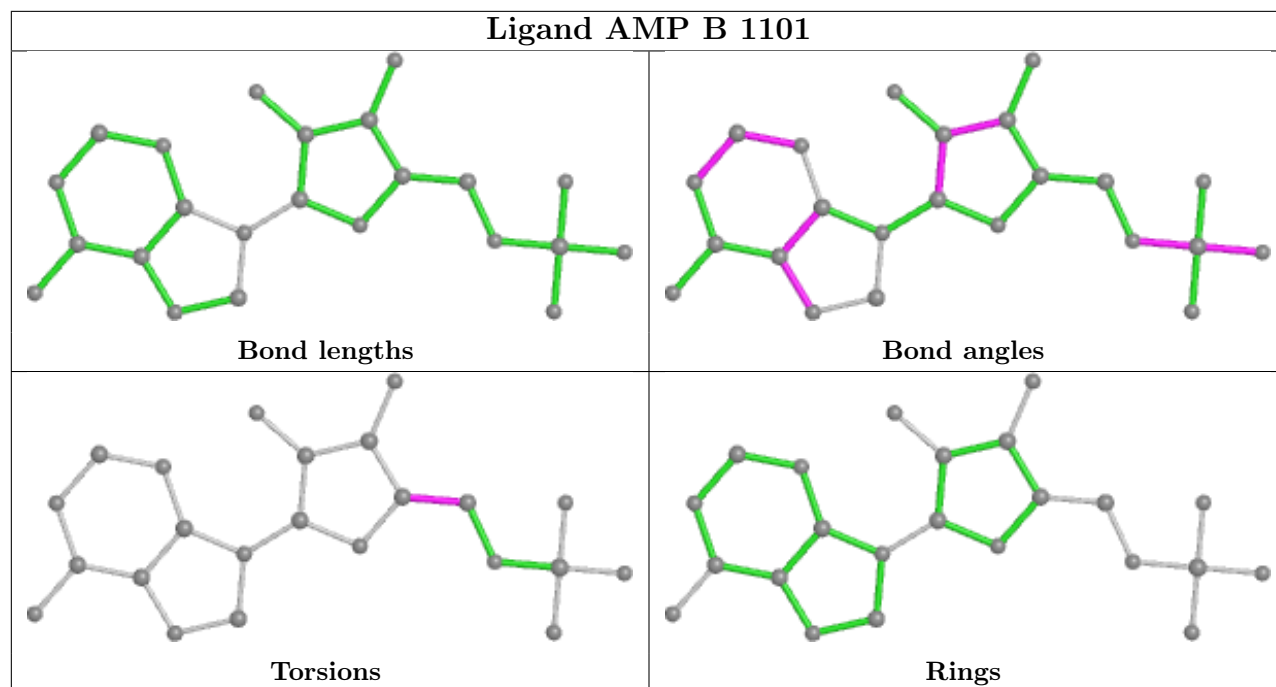
Mol	Chain	Res	Type	Atoms
3	A	1101	IHP	C5-O15-P5-O45
4	B	1101	AMP	O4'-C4'-C5'-O5'
4	B	1101	AMP	C3'-C4'-C5'-O5'
4	D	2101	AMP	O4'-C4'-C5'-O5'
3	A	1101	IHP	C4-O14-P4-O44
3	A	1101	IHP	C3-O13-P3-O23
3	A	1101	IHP	C3-O13-P3-O33
3	A	1101	IHP	C3-O13-P3-O43
4	D	2101	AMP	C3'-C4'-C5'-O5'

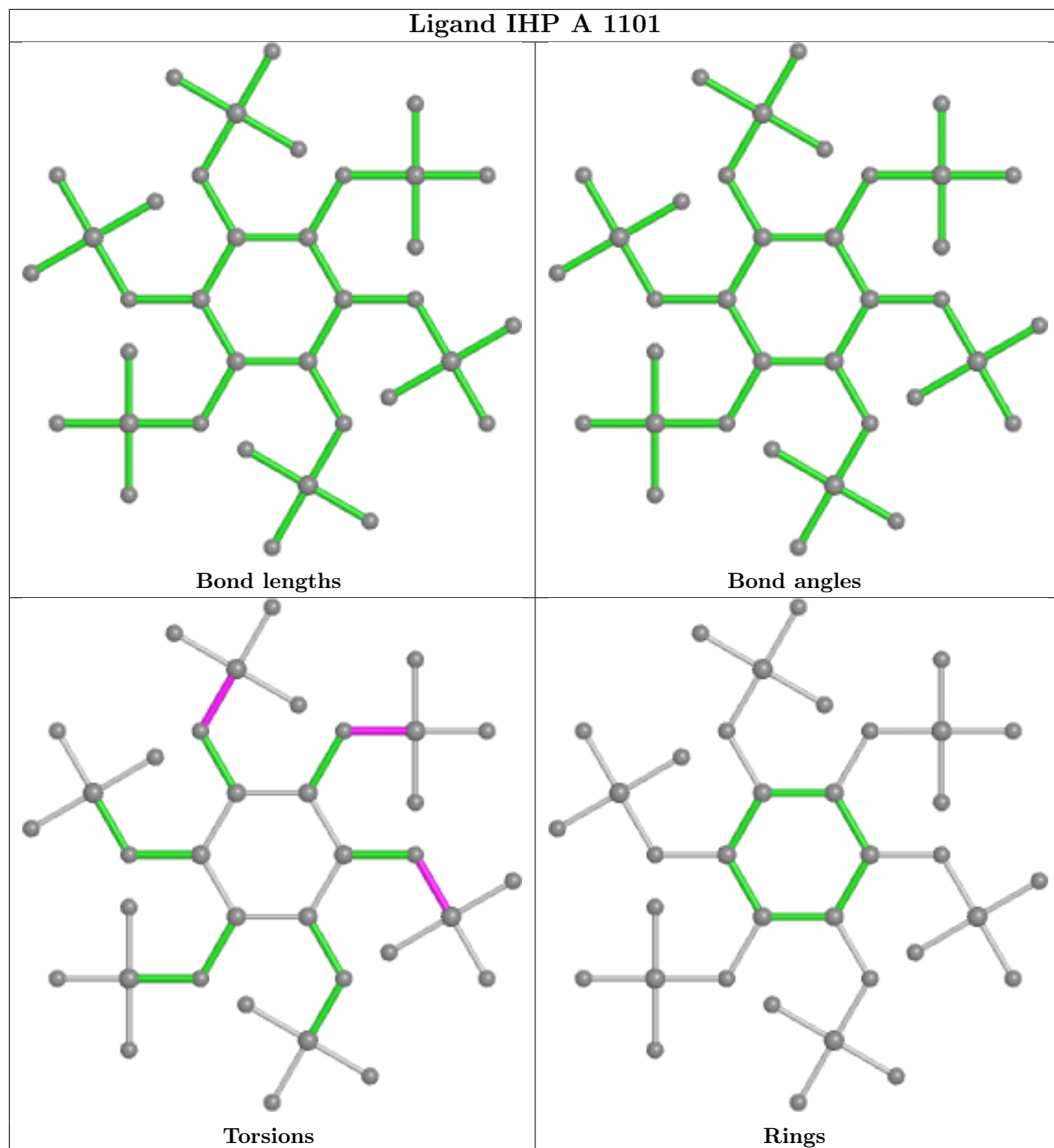
There are no ring outliers.

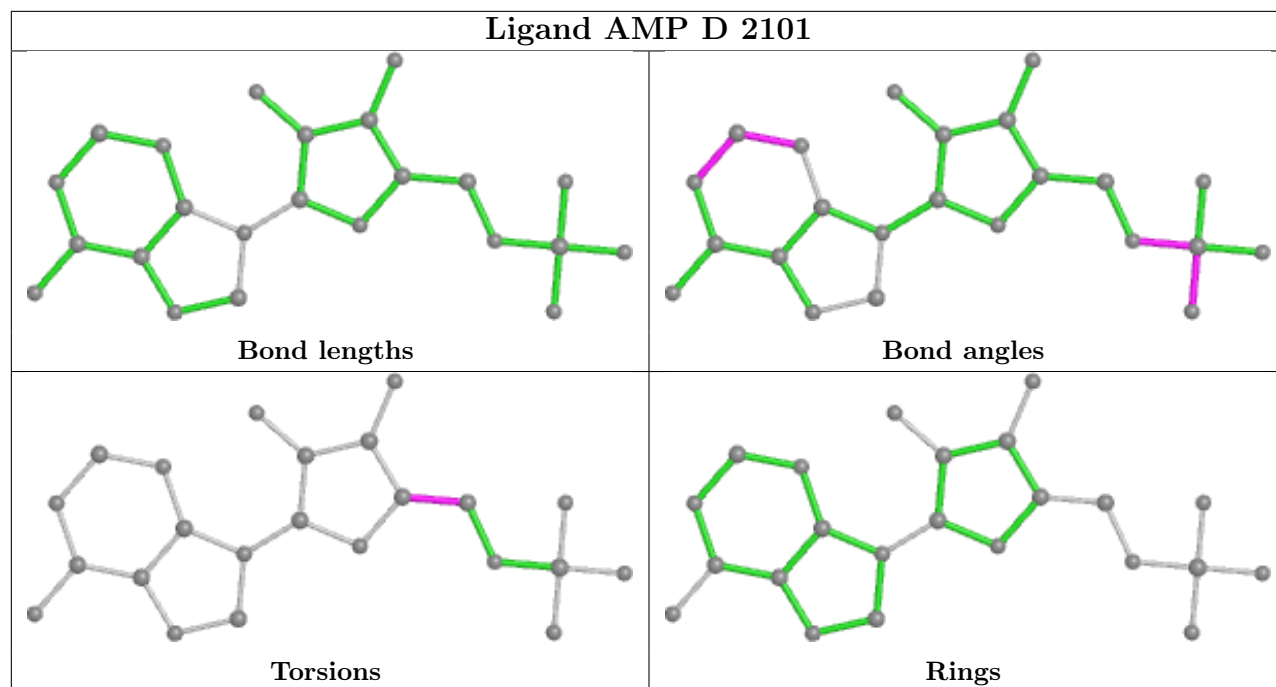
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1011/1020 (99%)	-0.14	25 (2%) 57 60	24, 48, 105, 149	0
1	C	970/1020 (95%)	-0.01	54 (5%) 24 26	25, 45, 110, 163	0
2	B	83/83 (100%)	-0.39	0 100 100	27, 45, 74, 109	0
2	D	80/83 (96%)	-0.40	2 (2%) 57 60	28, 45, 75, 149	0
All	All	2144/2206 (97%)	-0.10	81 (3%) 40 43	24, 47, 106, 163	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1032	ILE	7.7
1	C	234	ASN	5.9
1	C	59	MET	5.3
1	C	774	ALA	4.9
1	C	281	PRO	4.7
1	C	678	SER	4.7
1	C	269	PHE	4.5
1	C	673	ILE	4.4
1	A	1017	THR	4.3
1	C	776	GLU	4.0
1	C	233	GLU	3.9
1	C	232	LEU	3.9
1	C	819	GLU	3.9
1	C	226	PRO	3.9
1	C	60	ALA	3.8
1	C	283	LEU	3.6
1	C	676	GLY	3.5
1	C	1017	THR	3.5
1	A	799	ASN	3.4
1	C	778	LEU	3.4
1	C	779	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	277	THR	3.4
1	A	811	PRO	3.3
1	A	1035	ASP	3.3
1	A	833	LEU	3.2
1	A	793	GLN	3.2
1	C	1018	GLU	3.1
1	C	675	SER	3.1
1	A	178	CYS	3.1
1	C	275	ASP	3.0
1	C	222	THR	2.9
1	C	250	ILE	2.9
1	C	781	ASP	2.9
1	A	1034	GLY	2.9
1	C	964	GLU	2.9
1	C	266	ILE	2.8
1	A	1033	ASP	2.8
1	C	679	LEU	2.8
1	A	729	LYS	2.8
1	C	218	ILE	2.8
1	C	228	ILE	2.8
1	C	273	ILE	2.8
1	A	1016	THR	2.7
1	C	235	HIS	2.7
1	C	788	SER	2.7
1	C	822	ARG	2.7
1	A	1050	ASP	2.6
1	C	787	LEU	2.6
1	C	216	ILE	2.6
1	C	264	THR	2.6
1	C	219	SER	2.6
1	A	507	ASN	2.6
1	C	229	VAL	2.5
1	C	784	LEU	2.5
1	C	225	ASN	2.5
1	C	775	GLU	2.5
1	A	796	LYS	2.4
1	C	798	SER	2.4
1	C	783	LEU	2.4
1	A	813	HIS	2.4
1	C	1016	THR	2.4
1	C	674	GLN	2.4
2	D	-2	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	76	GLY	2.3
1	C	236	PRO	2.3
1	C	61	LYS	2.3
1	A	794	GLU	2.2
1	A	809	ARG	2.2
1	C	274	GLY	2.2
1	A	675	SER	2.2
1	C	780	ALA	2.2
1	C	223	GLN	2.2
1	C	268	PRO	2.1
1	A	254	THR	2.1
1	A	1015	PRO	2.1
1	A	683	PHE	2.1
1	C	284	HIS	2.1
1	C	270	SER	2.1
1	A	671	GLN	2.0
1	A	424	ILE	2.0
1	A	508	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

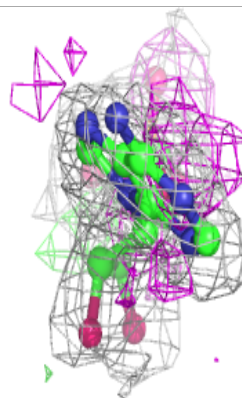
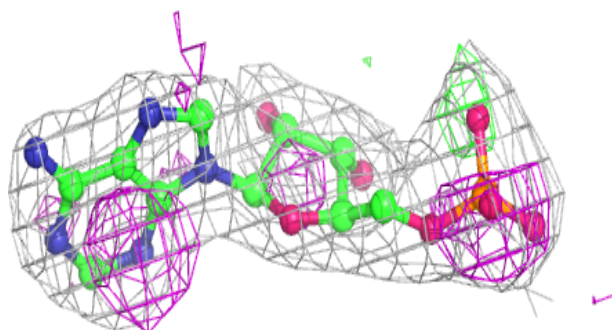
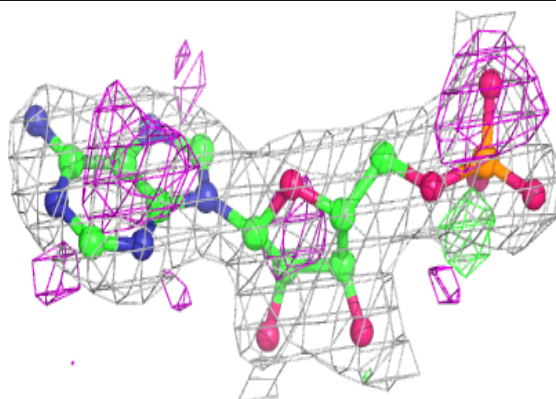
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	AMP	B	1101	23/23	0.90	0.14	33,47,58,63	0
4	AMP	D	2101	23/23	0.97	0.10	30,37,49,54	0
3	IHP	A	1101	36/36	0.98	0.08	40,52,66,74	0

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:**

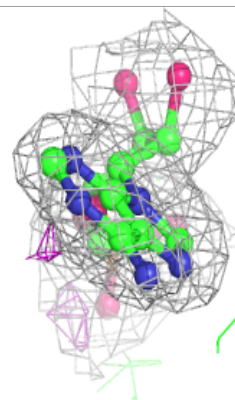
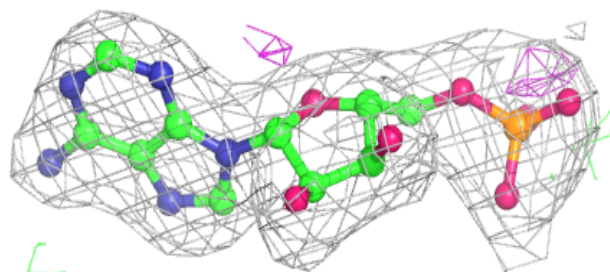
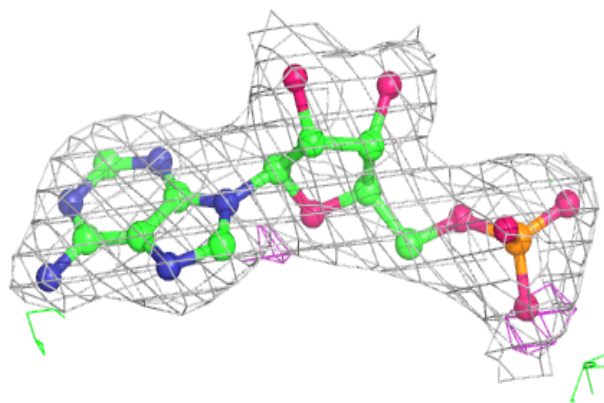
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





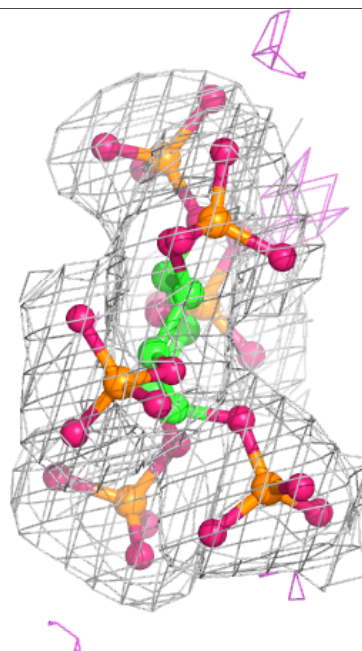
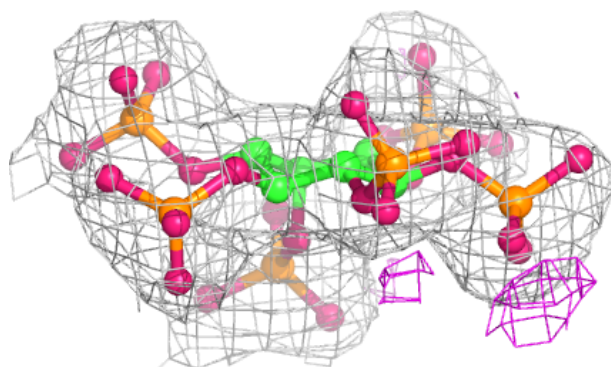
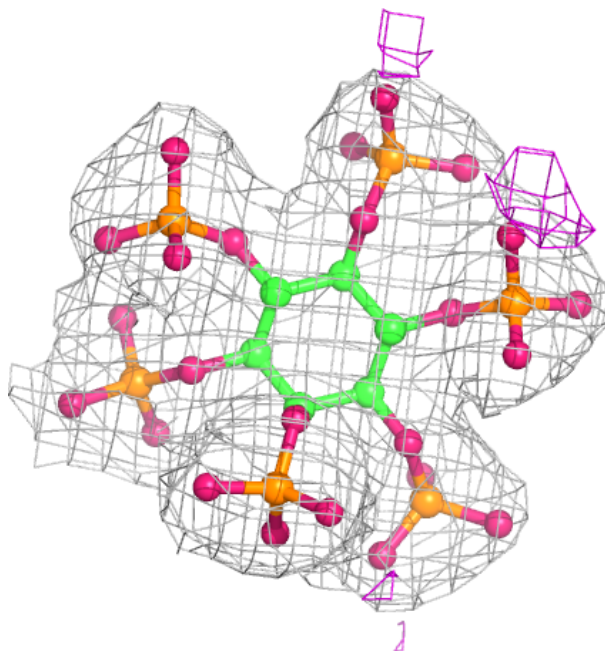
**Electron density around AMP D 2101:**

$2mF_o-DF_c$  (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.