



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 16, 2024 – 07:24 AM EST

PDB ID : 7K5J
Title : Structure of an E1-E2-ubiquitin thioester mimetic
Authors : Yuan, L.; Lv, Z.; Olsen, S.K.
Deposited on : 2020-09-16
Resolution : 3.42 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

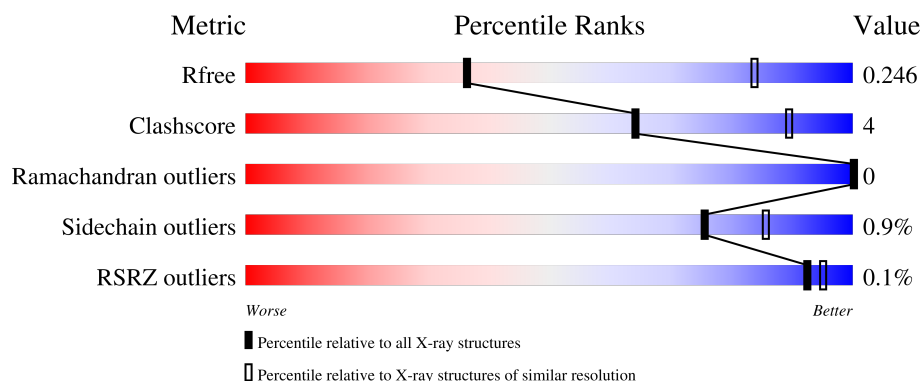
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.42 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}	164625	1112 (3.48-3.36)
Clashscore	180529	1144 (3.48-3.36)
Ramachandran outliers	177936	1146 (3.48-3.36)
Sidechain outliers	177891	1146 (3.48-3.36)
RSRZ outliers	164620	1112 (3.48-3.36)

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	M	83	
1	N	83	
1	O	83	
1	P	83	
1	Q	83	

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Mol	Chain	Length	Quality of chain
1	R	83	
1	W	83	
1	X	83	
2	A	1017	
2	C	1017	
2	D	1017	
2	G	1017	
2	I	1017	
2	K	1017	
2	S	1017	
2	U	1017	
3	B	197	
3	E	197	
3	F	197	
3	H	197	
3	J	197	
3	L	197	
3	T	197	
3	V	197	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 76643 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	80	Total	C	N	O	S	0	0	0
			652	399	131	121	1			
1	M	77	Total	C	N	O	S	0	0	0
			622	381	122	118	1			
1	O	73	Total	C	N	O	S	0	0	0
			593	365	113	114	1			
1	P	80	Total	C	N	O	S	0	0	0
			652	399	131	121	1			
1	Q	76	Total	C	N	O	S	0	0	0
			612	375	119	117	1			
1	R	76	Total	C	N	O	S	0	0	0
			623	383	122	117	1			
1	W	70	Total	C	N	O	S	0	0	0
			566	347	107	111	1			
1	X	73	Total	C	N	O	S	0	0	0
			596	365	116	114	1			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	-6	MET	-	initiating methionine	UNP P69326
N	-5	HIS	-	expression tag	UNP P69326
N	-4	HIS	-	expression tag	UNP P69326
N	-3	HIS	-	expression tag	UNP P69326
N	-2	HIS	-	expression tag	UNP P69326
N	-1	HIS	-	expression tag	UNP P69326
N	0	HIS	-	expression tag	UNP P69326
N	6	ARG	LYS	conflict	UNP P69326
N	11	ARG	LYS	conflict	UNP P69326
N	27	ARG	LYS	conflict	UNP P69326
N	29	ARG	LYS	conflict	UNP P69326
N	33	ARG	LYS	conflict	UNP P69326
N	48	ARG	LYS	conflict	UNP P69326

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Chain	Residue	Modelled	Actual	Comment	Reference
N	63	ARG	LYS	conflict	UNP P69326
M	-6	MET	-	initiating methionine	UNP P69326
M	-5	HIS	-	expression tag	UNP P69326
M	-4	HIS	-	expression tag	UNP P69326
M	-3	HIS	-	expression tag	UNP P69326
M	-2	HIS	-	expression tag	UNP P69326
M	-1	HIS	-	expression tag	UNP P69326
M	0	HIS	-	expression tag	UNP P69326
M	6	ARG	LYS	conflict	UNP P69326
M	11	ARG	LYS	conflict	UNP P69326
M	27	ARG	LYS	conflict	UNP P69326
M	29	ARG	LYS	conflict	UNP P69326
M	33	ARG	LYS	conflict	UNP P69326
M	48	ARG	LYS	conflict	UNP P69326
M	63	ARG	LYS	conflict	UNP P69326
O	-6	MET	-	initiating methionine	UNP P69326
O	-5	HIS	-	expression tag	UNP P69326
O	-4	HIS	-	expression tag	UNP P69326
O	-3	HIS	-	expression tag	UNP P69326
O	-2	HIS	-	expression tag	UNP P69326
O	-1	HIS	-	expression tag	UNP P69326
O	0	HIS	-	expression tag	UNP P69326
O	6	ARG	LYS	conflict	UNP P69326
O	11	ARG	LYS	conflict	UNP P69326
O	27	ARG	LYS	conflict	UNP P69326
O	29	ARG	LYS	conflict	UNP P69326
O	33	ARG	LYS	conflict	UNP P69326
O	48	ARG	LYS	conflict	UNP P69326
O	63	ARG	LYS	conflict	UNP P69326
P	-6	MET	-	initiating methionine	UNP P69326
P	-5	HIS	-	expression tag	UNP P69326
P	-4	HIS	-	expression tag	UNP P69326
P	-3	HIS	-	expression tag	UNP P69326
P	-2	HIS	-	expression tag	UNP P69326
P	-1	HIS	-	expression tag	UNP P69326
P	0	HIS	-	expression tag	UNP P69326
P	6	ARG	LYS	conflict	UNP P69326
P	11	ARG	LYS	conflict	UNP P69326
P	27	ARG	LYS	conflict	UNP P69326
P	29	ARG	LYS	conflict	UNP P69326
P	33	ARG	LYS	conflict	UNP P69326
P	48	ARG	LYS	conflict	UNP P69326

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Chain	Residue	Modelled	Actual	Comment	Reference
P	63	ARG	LYS	conflict	UNP P69326
Q	-6	MET	-	initiating methionine	UNP P69326
Q	-5	HIS	-	expression tag	UNP P69326
Q	-4	HIS	-	expression tag	UNP P69326
Q	-3	HIS	-	expression tag	UNP P69326
Q	-2	HIS	-	expression tag	UNP P69326
Q	-1	HIS	-	expression tag	UNP P69326
Q	0	HIS	-	expression tag	UNP P69326
Q	6	ARG	LYS	conflict	UNP P69326
Q	11	ARG	LYS	conflict	UNP P69326
Q	27	ARG	LYS	conflict	UNP P69326
Q	29	ARG	LYS	conflict	UNP P69326
Q	33	ARG	LYS	conflict	UNP P69326
Q	48	ARG	LYS	conflict	UNP P69326
Q	63	ARG	LYS	conflict	UNP P69326
R	-6	MET	-	initiating methionine	UNP P69326
R	-5	HIS	-	expression tag	UNP P69326
R	-4	HIS	-	expression tag	UNP P69326
R	-3	HIS	-	expression tag	UNP P69326
R	-2	HIS	-	expression tag	UNP P69326
R	-1	HIS	-	expression tag	UNP P69326
R	0	HIS	-	expression tag	UNP P69326
R	6	ARG	LYS	conflict	UNP P69326
R	11	ARG	LYS	conflict	UNP P69326
R	27	ARG	LYS	conflict	UNP P69326
R	29	ARG	LYS	conflict	UNP P69326
R	33	ARG	LYS	conflict	UNP P69326
R	48	ARG	LYS	conflict	UNP P69326
R	63	ARG	LYS	conflict	UNP P69326
W	-6	MET	-	initiating methionine	UNP P69326
W	-5	HIS	-	expression tag	UNP P69326
W	-4	HIS	-	expression tag	UNP P69326
W	-3	HIS	-	expression tag	UNP P69326
W	-2	HIS	-	expression tag	UNP P69326
W	-1	HIS	-	expression tag	UNP P69326
W	0	HIS	-	expression tag	UNP P69326
W	6	ARG	LYS	conflict	UNP P69326
W	11	ARG	LYS	conflict	UNP P69326
W	27	ARG	LYS	conflict	UNP P69326
W	29	ARG	LYS	conflict	UNP P69326
W	33	ARG	LYS	conflict	UNP P69326
W	48	ARG	LYS	conflict	UNP P69326

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Chain	Residue	Modelled	Actual	Comment	Reference
W	63	ARG	LYS	conflict	UNP P69326
X	-6	MET	-	initiating methionine	UNP P69326
X	-5	HIS	-	expression tag	UNP P69326
X	-4	HIS	-	expression tag	UNP P69326
X	-3	HIS	-	expression tag	UNP P69326
X	-2	HIS	-	expression tag	UNP P69326
X	-1	HIS	-	expression tag	UNP P69326
X	0	HIS	-	expression tag	UNP P69326
X	6	ARG	LYS	conflict	UNP P69326
X	11	ARG	LYS	conflict	UNP P69326
X	27	ARG	LYS	conflict	UNP P69326
X	29	ARG	LYS	conflict	UNP P69326
X	33	ARG	LYS	conflict	UNP P69326
X	48	ARG	LYS	conflict	UNP P69326
X	63	ARG	LYS	conflict	UNP P69326

- Molecule 2 is a protein called Ubiquitin-activating enzyme E1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	972	Total	C	N	O	S	0	0	0
			7693	4914	1271	1485	23			
2	A	971	Total	C	N	O	S	0	0	0
			7683	4909	1269	1482	23			
2	C	972	Total	C	N	O	S	0	0	0
			7692	4912	1270	1487	23			
2	G	973	Total	C	N	O	S	0	0	0
			7701	4918	1272	1488	23			
2	I	979	Total	C	N	O	S	0	0	0
			7743	4941	1279	1500	23			
2	K	979	Total	C	N	O	S	0	0	0
			7739	4940	1276	1500	23			
2	S	971	Total	C	N	O	S	0	0	0
			7679	4908	1266	1482	23			
2	U	973	Total	C	N	O	S	0	0	0
			7701	4920	1272	1486	23			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLY	-	expression tag	UNP P22515
D	9	ALA	-	expression tag	UNP P22515
D	10	MET	-	expression tag	UNP P22515

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Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	-	expression tag	UNP P22515
A	9	ALA	-	expression tag	UNP P22515
A	10	MET	-	expression tag	UNP P22515
C	8	GLY	-	expression tag	UNP P22515
C	9	ALA	-	expression tag	UNP P22515
C	10	MET	-	expression tag	UNP P22515
G	8	GLY	-	expression tag	UNP P22515
G	9	ALA	-	expression tag	UNP P22515
G	10	MET	-	expression tag	UNP P22515
I	8	GLY	-	expression tag	UNP P22515
I	9	ALA	-	expression tag	UNP P22515
I	10	MET	-	expression tag	UNP P22515
K	8	GLY	-	expression tag	UNP P22515
K	9	ALA	-	expression tag	UNP P22515
K	10	MET	-	expression tag	UNP P22515
S	8	GLY	-	expression tag	UNP P22515
S	9	ALA	-	expression tag	UNP P22515
S	10	MET	-	expression tag	UNP P22515
U	8	GLY	-	expression tag	UNP P22515
U	9	ALA	-	expression tag	UNP P22515
U	10	MET	-	expression tag	UNP P22515

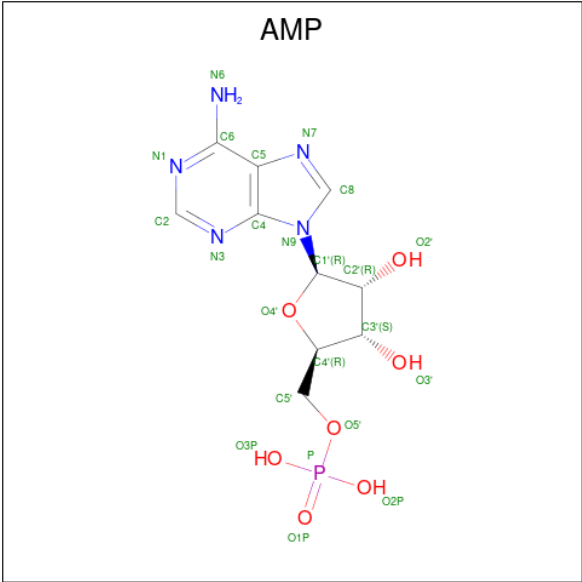
- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2-34 kDa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	152	Total	C	N	O	S	0	0	0
			1240	796	210	229	5			
3	B	153	Total	C	N	O	S	0	0	0
			1246	799	211	231	5			
3	E	151	Total	C	N	O	S	0	0	0
			1234	793	209	228	4			
3	H	152	Total	C	N	O	S	0	0	0
			1241	797	210	229	5			
3	J	156	Total	C	N	O	S	0	0	0
			1269	813	214	237	5			
3	L	155	Total	C	N	O	S	0	0	0
			1263	810	213	235	5			
3	T	153	Total	C	N	O	S	0	0	0
			1249	801	211	232	5			
3	V	146	Total	C	N	O	S	0	0	0
			1193	768	198	223	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	GLY	-	expression tag	UNP P14682
F	0	ALA	-	expression tag	UNP P14682
F	1	MET	-	expression tag	UNP P14682
F	2	ALA	-	expression tag	UNP P14682
F	141	LYS	ALA	engineered mutation	UNP P14682
B	-1	GLY	-	expression tag	UNP P14682
B	0	ALA	-	expression tag	UNP P14682
B	1	MET	-	expression tag	UNP P14682
B	2	ALA	-	expression tag	UNP P14682
B	141	LYS	ALA	engineered mutation	UNP P14682
E	-1	GLY	-	expression tag	UNP P14682
E	0	ALA	-	expression tag	UNP P14682
E	1	MET	-	expression tag	UNP P14682
E	2	ALA	-	expression tag	UNP P14682
E	141	LYS	ALA	engineered mutation	UNP P14682
H	-1	GLY	-	expression tag	UNP P14682
H	0	ALA	-	expression tag	UNP P14682
H	1	MET	-	expression tag	UNP P14682
H	2	ALA	-	expression tag	UNP P14682
H	141	LYS	ALA	engineered mutation	UNP P14682
J	-1	GLY	-	expression tag	UNP P14682
J	0	ALA	-	expression tag	UNP P14682
J	1	MET	-	expression tag	UNP P14682
J	2	ALA	-	expression tag	UNP P14682
J	141	LYS	ALA	engineered mutation	UNP P14682
L	-1	GLY	-	expression tag	UNP P14682
L	0	ALA	-	expression tag	UNP P14682
L	1	MET	-	expression tag	UNP P14682
L	2	ALA	-	expression tag	UNP P14682
L	141	LYS	ALA	engineered mutation	UNP P14682
T	-1	GLY	-	expression tag	UNP P14682
T	0	ALA	-	expression tag	UNP P14682
T	1	MET	-	expression tag	UNP P14682
T	2	ALA	-	expression tag	UNP P14682
T	141	LYS	ALA	engineered mutation	UNP P14682
V	-1	GLY	-	expression tag	UNP P14682
V	0	ALA	-	expression tag	UNP P14682
V	1	MET	-	expression tag	UNP P14682
V	2	ALA	-	expression tag	UNP P14682
V	141	LYS	ALA	engineered mutation	UNP P14682

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C₁₀H₁₄N₅O₇P).




Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	I	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	K	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

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

Chain N: 



- Molecule 1: Ubiquitin

Chain M: 



- Molecule 1: Ubiquitin

Chain O: 



- Molecule 1: Ubiquitin

Chain P: 

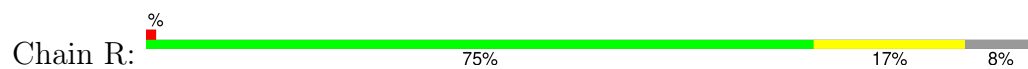


- Molecule 1: Ubiquitin

Chain Q: 



- Molecule 1: Ubiquitin



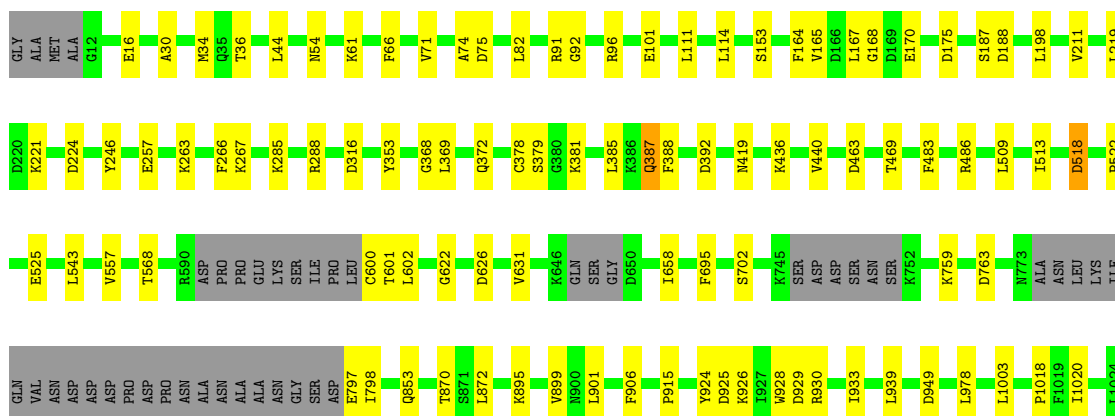
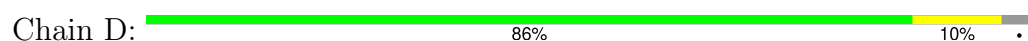
- Molecule 1: Ubiquitin



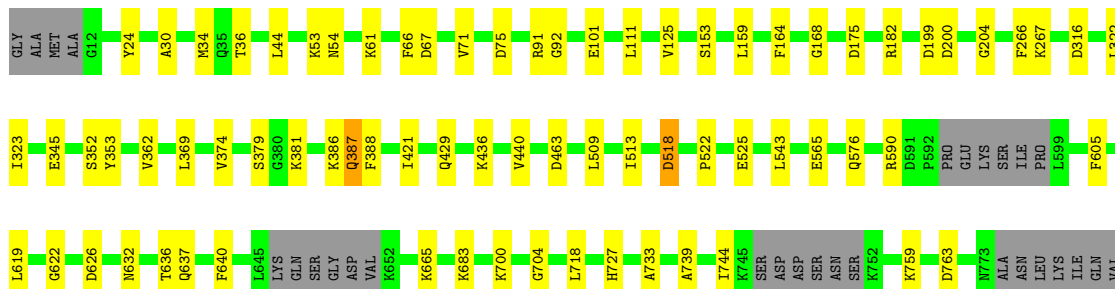
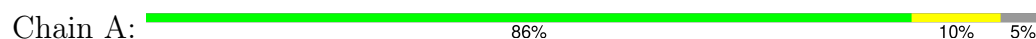
- Molecule 1: Ubiquitin



- Molecule 2: Ubiquitin-activating enzyme E1 1



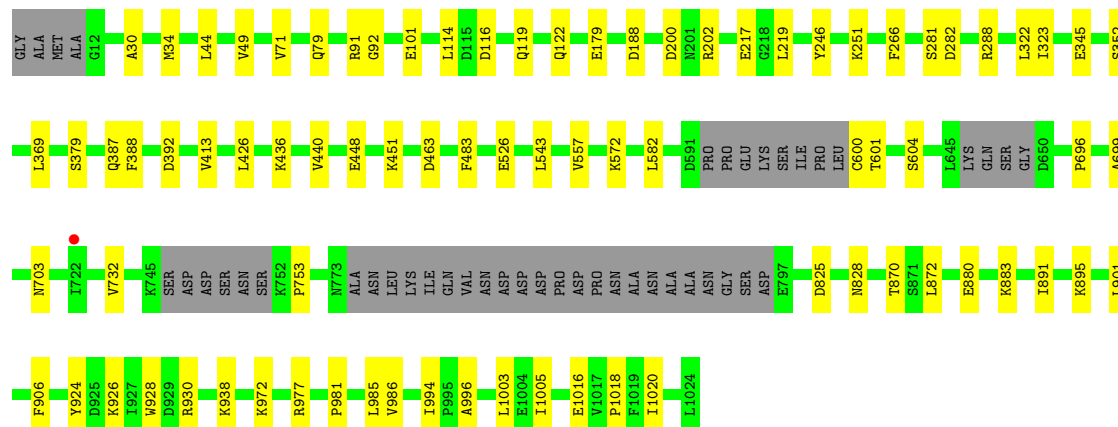
- Molecule 2: Ubiquitin-activating enzyme E1 1

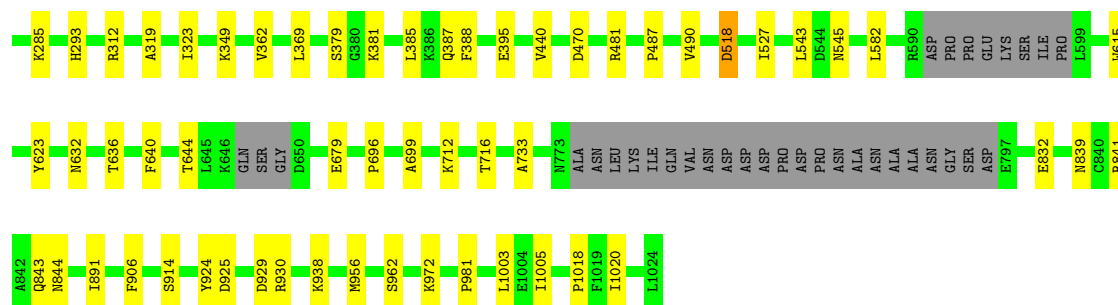




• Molecule 2: Ubiquitin-activating enzyme E1 1

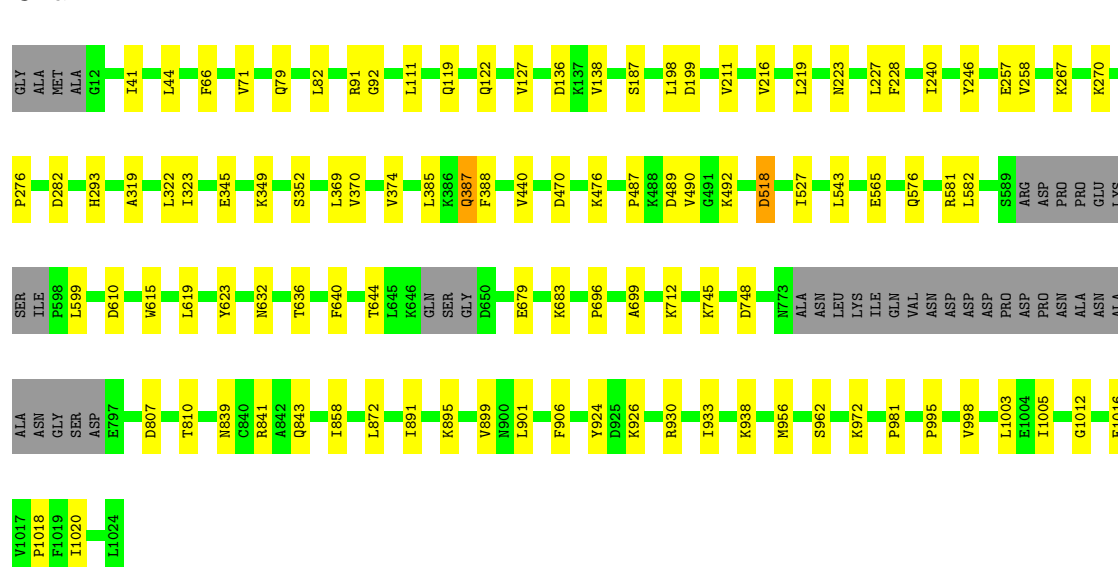
Chain C: 88% 8% .





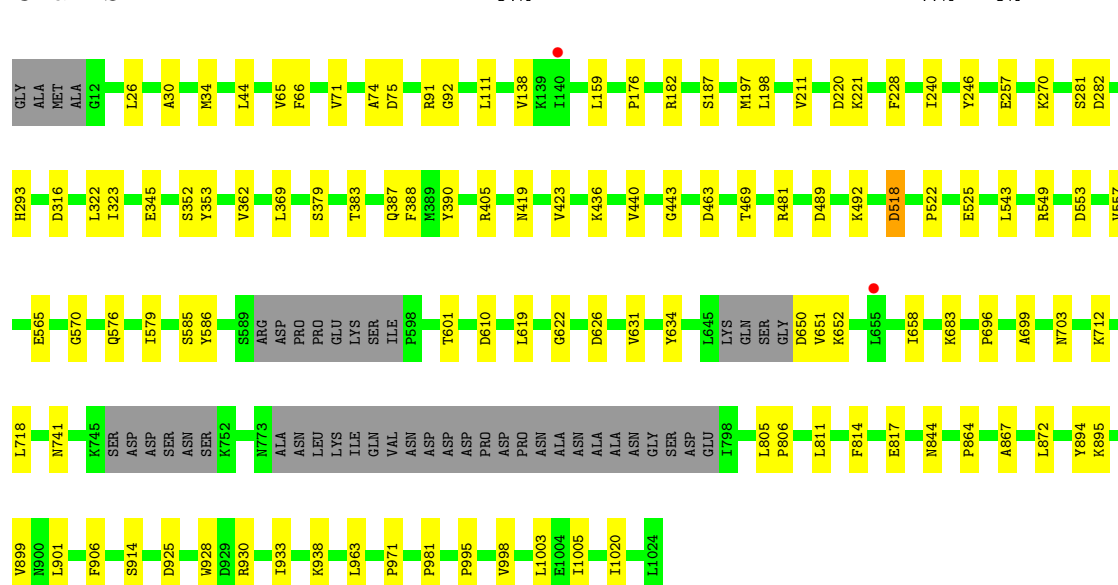
• Molecule 2: Ubiquitin-activating enzyme E1 1

Chain K:

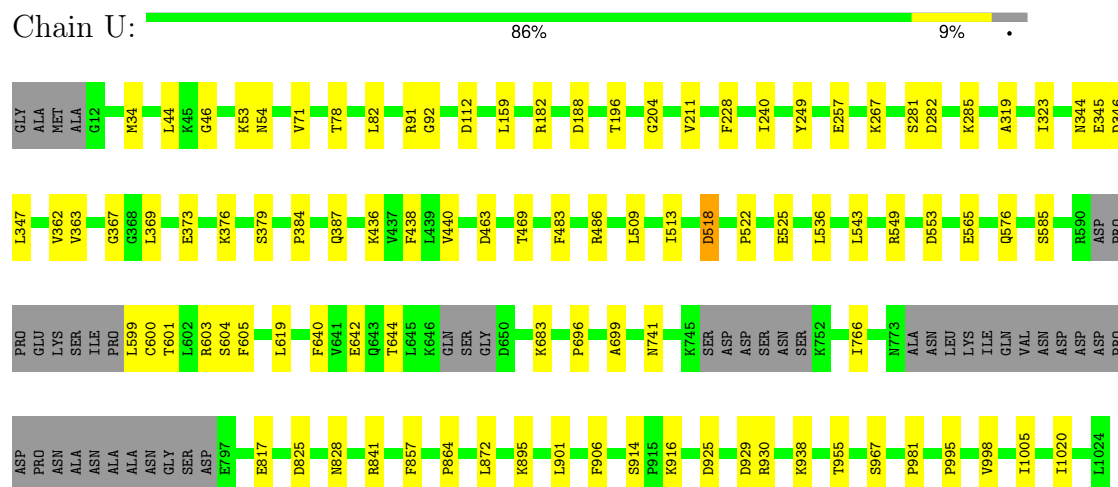


• Molecule 2: Ubiquitin-activating enzyme E1 1

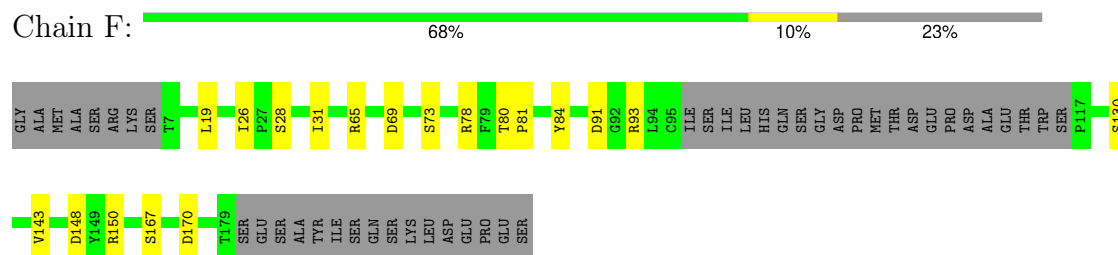
Chain S:



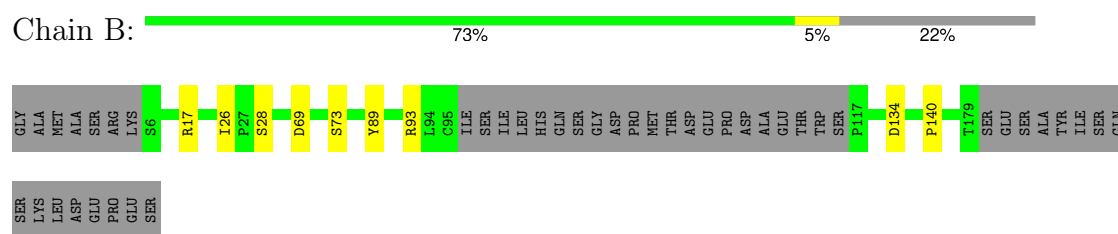
- Molecule 2: Ubiquitin-activating enzyme E1 1



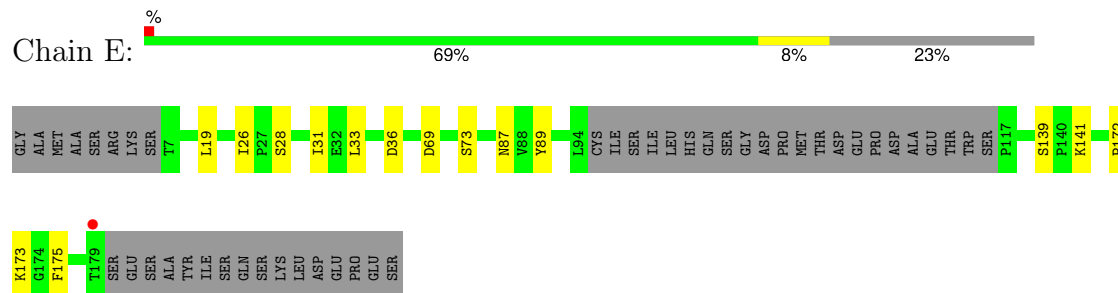
- Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa



- Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa

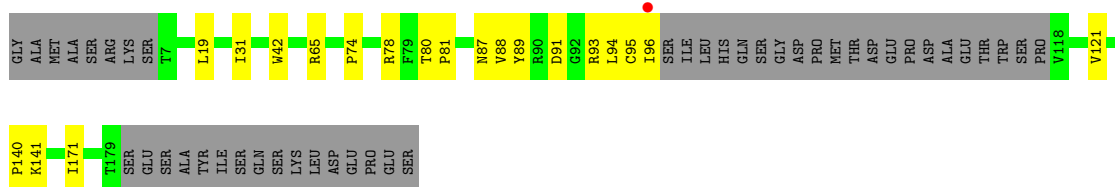


- Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa

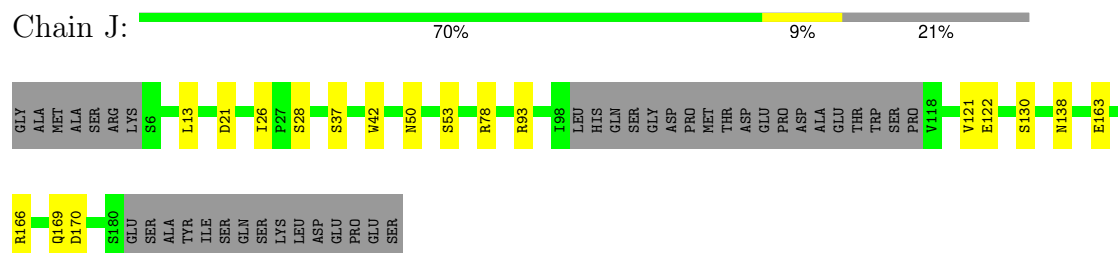


- Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa

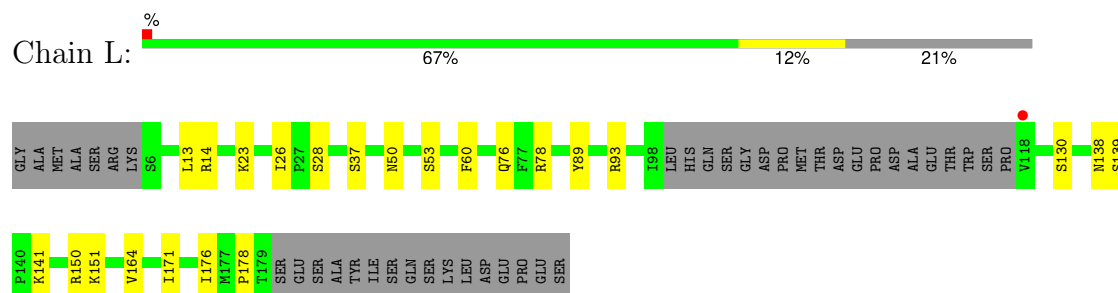




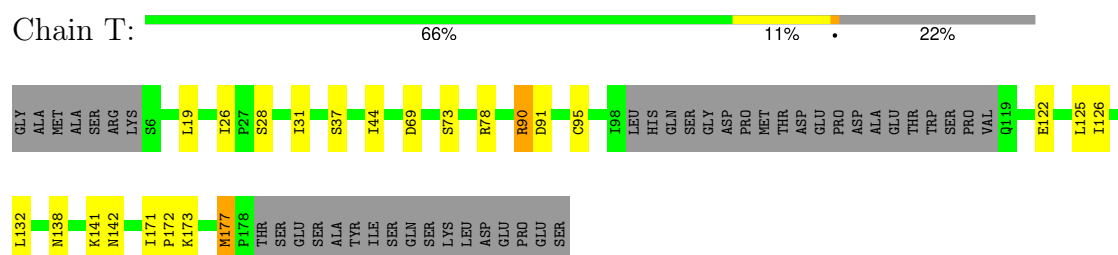
• Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa



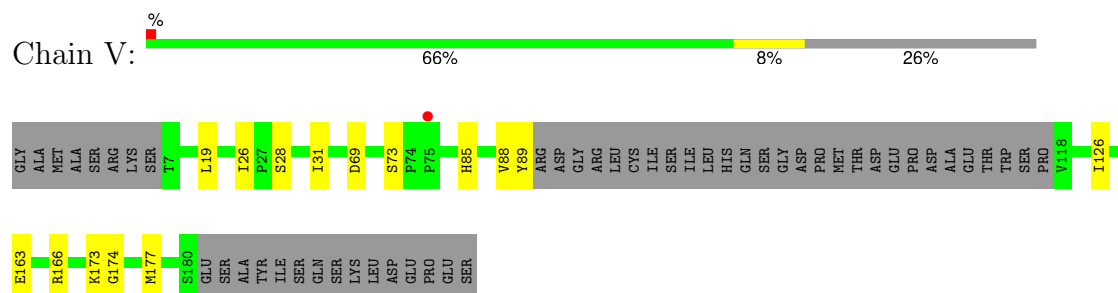
• Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa



• Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa



• Molecule 3: Ubiquitin-conjugating enzyme E2-34 kDa



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.18Å 272.92Å 258.34Å 90.00° 94.59° 90.00°	Depositor
Resolution (Å)	136.46 – 3.42 136.46 – 3.42	Depositor EDS
% Data completeness (in resolution range)	99.2 (136.46-3.42) 89.2 (136.46-3.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.29	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.246 0.204 , 0.246	Depositor DCC
R_{free} test set	173051 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 100.1	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	0.95	EDS
Total number of atoms	76643	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5160e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	M	0.23	0/628	0.47	0/846
1	N	0.22	0/661	0.47	0/891
1	O	0.23	0/598	0.47	0/807
1	P	0.41	1/661 (0.2%)	0.60	1/891 (0.1%)
1	Q	0.23	0/617	0.50	0/831
1	R	0.23	0/631	0.48	0/852
1	W	0.22	0/571	0.44	0/771
1	X	0.23	0/604	0.45	0/816
2	A	0.26	0/7841	0.41	0/10603
2	C	0.26	0/7849	0.42	0/10613
2	D	0.25	0/7850	0.41	0/10613
2	G	0.26	0/7858	0.42	0/10624
2	I	0.26	0/7901	0.42	0/10684
2	K	0.26	0/7898	0.43	0/10681
2	S	0.24	0/7837	0.40	0/10598
2	U	0.24	0/7858	0.40	0/10624
3	B	0.25	0/1279	0.40	0/1733
3	E	0.25	0/1267	0.40	0/1717
3	F	0.25	0/1273	0.39	0/1725
3	H	0.24	0/1273	0.40	0/1725
3	J	0.25	0/1301	0.41	0/1763
3	L	0.25	0/1295	0.42	0/1755
3	T	0.24	0/1281	0.39	0/1735
3	V	0.24	0/1225	0.40	0/1662
All	All	0.25	1/78057 (0.0%)	0.42	1/105560 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	76	GLY	C-O	6.60	1.34	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	76	GLY	CA-C-O	-8.77	104.81	120.60

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	M	622	0	632	13	0
1	N	652	0	653	10	0
1	O	593	0	606	10	0
1	P	652	0	653	25	0
1	Q	612	0	625	6	0
1	R	623	0	627	8	0
1	W	566	0	571	8	0
1	X	596	0	592	9	0
2	A	7683	0	7608	54	0
2	C	7692	0	7610	46	1
2	D	7693	0	7618	58	0
2	G	7701	0	7622	59	0
2	I	7743	0	7659	46	1
2	K	7739	0	7654	62	0
2	S	7679	0	7604	64	0
2	U	7701	0	7630	55	0
3	B	1246	0	1220	5	0
3	E	1234	0	1213	8	0
3	F	1240	0	1215	12	0
3	H	1241	0	1220	13	0
3	J	1269	0	1248	13	0
3	L	1263	0	1244	20	0
3	T	1249	0	1231	16	0
3	V	1193	0	1171	10	0
4	A	23	0	12	0	0
4	C	23	0	12	0	0
4	D	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	23	0	12	0	0
4	I	23	0	12	1	0
4	K	23	0	12	2	0
4	S	23	0	12	1	0
All	All	76643	0	75810	585	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 4.

The worst 5 of 585 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:P:39:ASP:O	1:P:72:ARG:NH2	1.72	1.22
3:L:141:LYS:CE	1:P:76:GLY:C	2.37	0.94
3:L:141:LYS:HZ3	1:P:76:GLY:C	1.76	0.89
2:S:44:LEU:HD11	2:S:65:VAL:HB	1.63	0.79
2:G:282:ASP:OD2	2:G:895:LYS:NZ	2.18	0.76

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)
2:C:101:GLU:OE2	2:I:312:ARG:NH1[1_655]	2.03	0.17

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	M	75/83 (90%)	73 (97%)	2 (3%)	0	100	100
1	N	78/83 (94%)	73 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	71/83 (86%)	71 (100%)	0	0	100	100
1	P	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
1	Q	74/83 (89%)	72 (97%)	2 (3%)	0	100	100
1	R	74/83 (89%)	74 (100%)	0	0	100	100
1	W	68/83 (82%)	66 (97%)	2 (3%)	0	100	100
1	X	71/83 (86%)	71 (100%)	0	0	100	100
2	A	961/1017 (94%)	943 (98%)	18 (2%)	0	100	100
2	C	962/1017 (95%)	943 (98%)	19 (2%)	0	100	100
2	D	962/1017 (95%)	945 (98%)	17 (2%)	0	100	100
2	G	963/1017 (95%)	944 (98%)	19 (2%)	0	100	100
2	I	971/1017 (96%)	953 (98%)	18 (2%)	0	100	100
2	K	971/1017 (96%)	948 (98%)	23 (2%)	0	100	100
2	S	961/1017 (94%)	943 (98%)	18 (2%)	0	100	100
2	U	963/1017 (95%)	944 (98%)	19 (2%)	0	100	100
3	B	149/197 (76%)	144 (97%)	5 (3%)	0	100	100
3	E	147/197 (75%)	140 (95%)	7 (5%)	0	100	100
3	F	148/197 (75%)	143 (97%)	5 (3%)	0	100	100
3	H	148/197 (75%)	144 (97%)	4 (3%)	0	100	100
3	J	152/197 (77%)	146 (96%)	6 (4%)	0	100	100
3	L	151/197 (77%)	147 (97%)	4 (3%)	0	100	100
3	T	149/197 (76%)	143 (96%)	6 (4%)	0	100	100
3	V	142/197 (72%)	131 (92%)	11 (8%)	0	100	100
All	All	9489/10376 (92%)	9274 (98%)	215 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	M	68/74 (92%)	68 (100%)	0	100	100
1	N	71/74 (96%)	71 (100%)	0	100	100
1	O	66/74 (89%)	65 (98%)	1 (2%)	60	76
1	P	71/74 (96%)	68 (96%)	3 (4%)	25	51
1	Q	67/74 (90%)	66 (98%)	1 (2%)	60	76
1	R	69/74 (93%)	68 (99%)	1 (1%)	62	77
1	W	63/74 (85%)	61 (97%)	2 (3%)	34	59
1	X	66/74 (89%)	64 (97%)	2 (3%)	36	61
2	A	856/893 (96%)	849 (99%)	7 (1%)	79	87
2	C	857/893 (96%)	853 (100%)	4 (0%)	86	92
2	D	857/893 (96%)	850 (99%)	7 (1%)	79	87
2	G	858/893 (96%)	851 (99%)	7 (1%)	79	87
2	I	864/893 (97%)	858 (99%)	6 (1%)	81	89
2	K	864/893 (97%)	856 (99%)	8 (1%)	75	86
2	S	856/893 (96%)	849 (99%)	7 (1%)	79	87
2	U	858/893 (96%)	854 (100%)	4 (0%)	86	92
3	B	141/180 (78%)	140 (99%)	1 (1%)	81	89
3	E	139/180 (77%)	138 (99%)	1 (1%)	81	89
3	F	140/180 (78%)	138 (99%)	2 (1%)	62	77
3	H	140/180 (78%)	139 (99%)	1 (1%)	81	89
3	J	145/180 (81%)	143 (99%)	2 (1%)	62	77
3	L	144/180 (80%)	142 (99%)	2 (1%)	62	77
3	T	142/180 (79%)	139 (98%)	3 (2%)	48	69
3	V	136/180 (76%)	135 (99%)	1 (1%)	81	89
All	All	8538/9176 (93%)	8465 (99%)	73 (1%)	75	86

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	S	518	ASP
1	X	6	ARG
2	S	703	ASN
2	U	518	ASP
2	G	388	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	62	GLN
1	O	68	HIS
1	R	62	GLN
3	E	87	ASN
3	B	136	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	C	1101	-	21,25,25	0.79	0	23,38,38	1.24	2 (8%)
4	AMP	A	1101	-	21,25,25	0.77	0	23,38,38	1.26	3 (13%)
4	AMP	D	1101	-	21,25,25	0.77	0	23,38,38	1.24	2 (8%)
4	AMP	G	1101	-	21,25,25	0.77	0	23,38,38	1.25	2 (8%)
4	AMP	K	1101	-	21,25,25	0.80	0	23,38,38	1.25	2 (8%)
4	AMP	S	1101	-	21,25,25	0.79	0	23,38,38	1.27	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	I	1101	-	21,25,25	0.79	0	23,38,38	1.27	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	C	1101	-	-	2/6/26/26	0/3/3/3
4	AMP	A	1101	-	-	2/6/26/26	0/3/3/3
4	AMP	D	1101	-	-	3/6/26/26	0/3/3/3
4	AMP	G	1101	-	-	2/6/26/26	0/3/3/3
4	AMP	K	1101	-	-	3/6/26/26	0/3/3/3
4	AMP	S	1101	-	-	6/6/26/26	0/3/3/3
4	AMP	I	1101	-	-	2/6/26/26	0/3/3/3

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1101	AMP	N3-C2-N1	-3.74	123.60	128.67
4	A	1101	AMP	N3-C2-N1	-3.73	123.60	128.67
4	S	1101	AMP	N3-C2-N1	-3.72	123.62	128.67
4	G	1101	AMP	N3-C2-N1	-3.66	123.71	128.67
4	I	1101	AMP	N3-C2-N1	-3.60	123.78	128.67

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

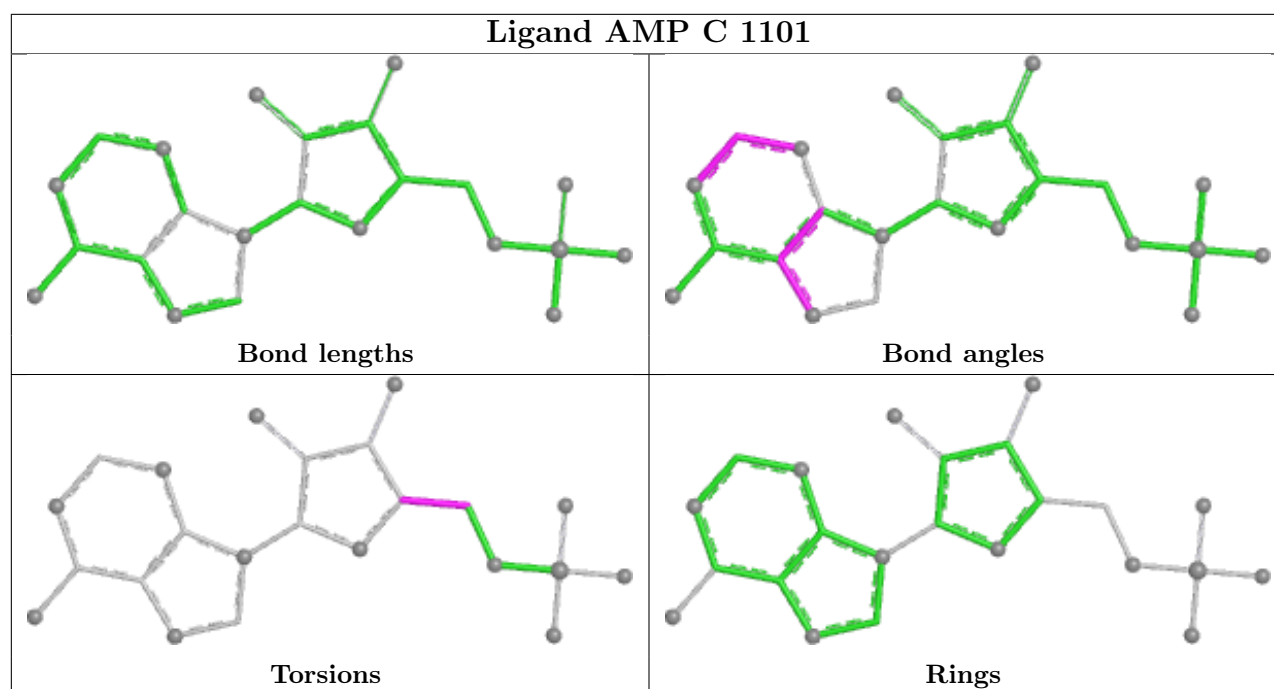
Mol	Chain	Res	Type	Atoms
4	I	1101	AMP	O4'-C4'-C5'-O5'
4	K	1101	AMP	O4'-C4'-C5'-O5'
4	S	1101	AMP	C5'-O5'-P-O2P
4	S	1101	AMP	C5'-O5'-P-O3P
4	A	1101	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

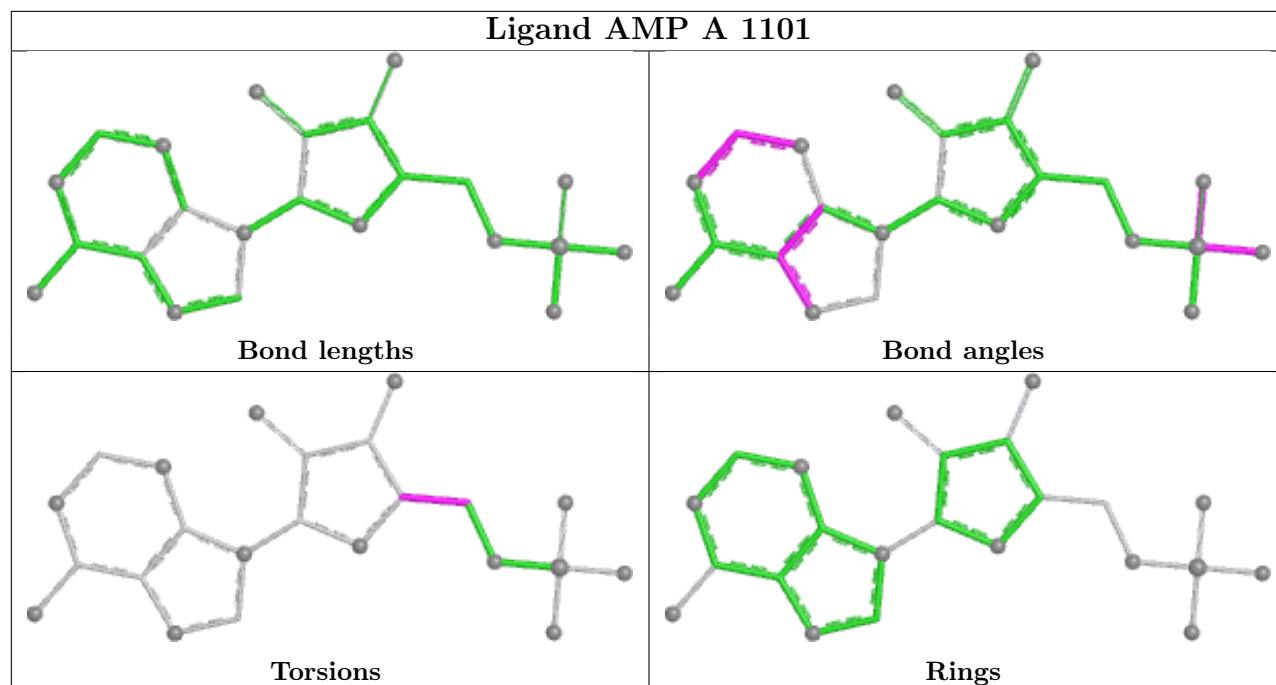
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1101	AMP	2	0
4	S	1101	AMP	1	0
4	I	1101	AMP	1	0

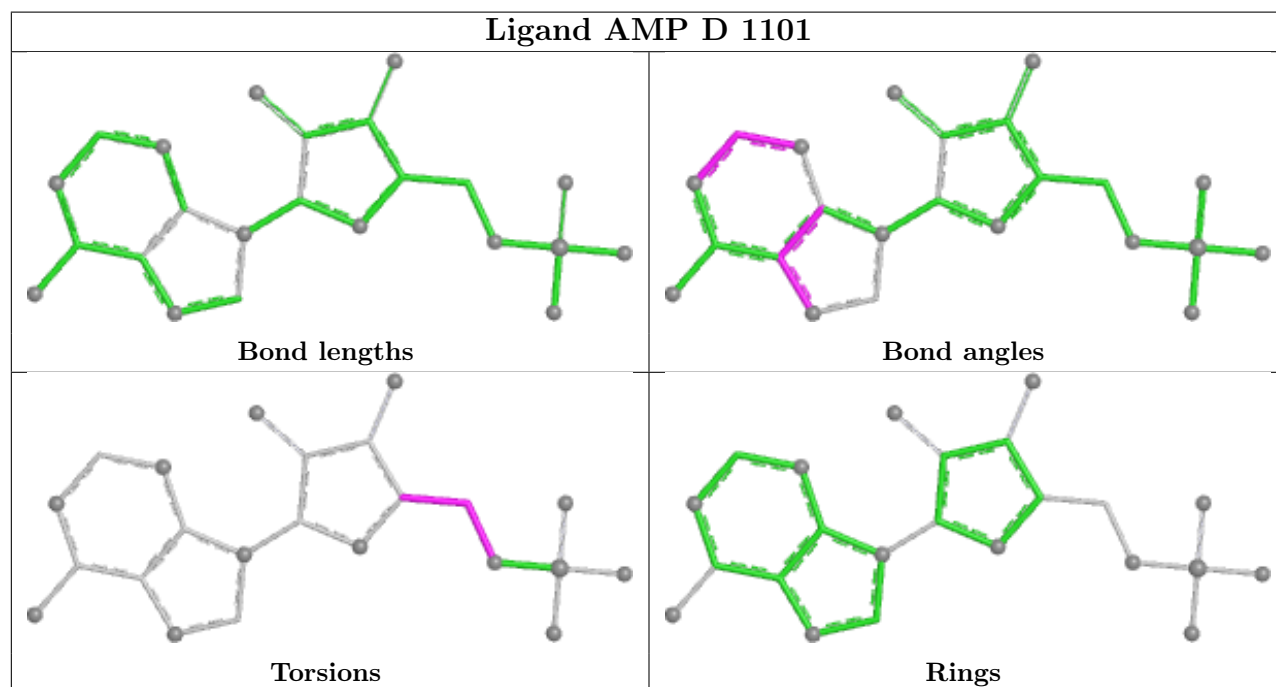
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



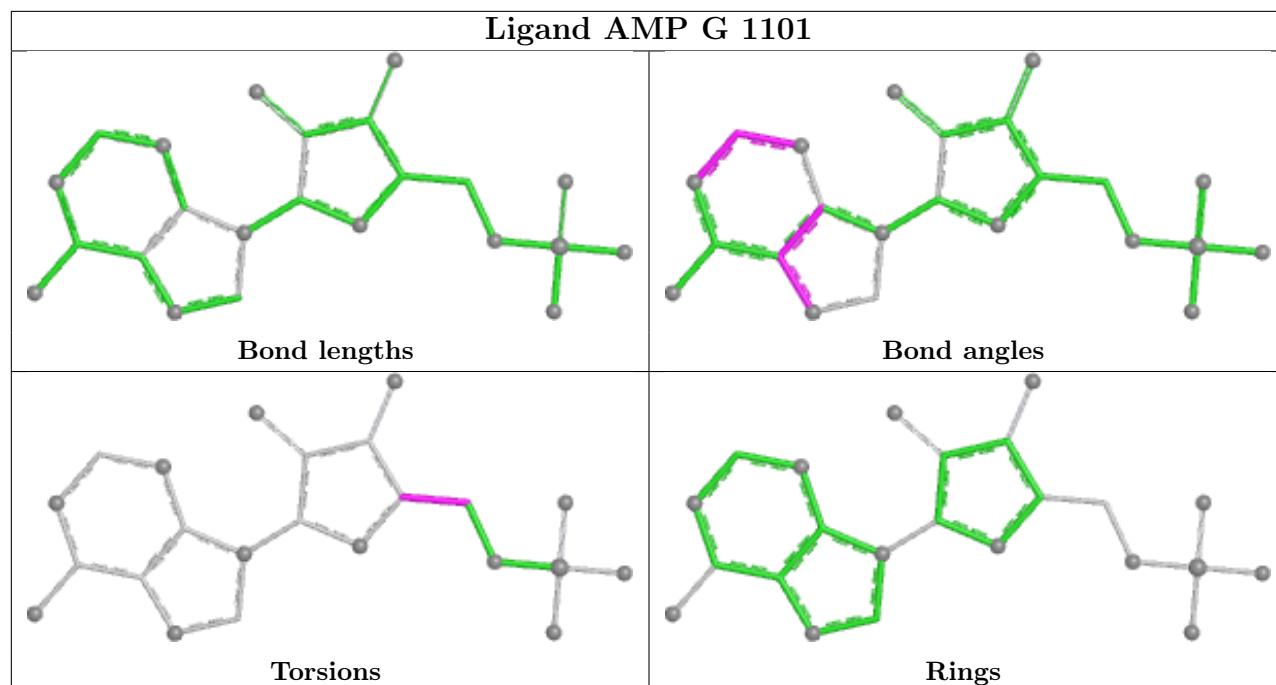
Ligand AMP A 1101



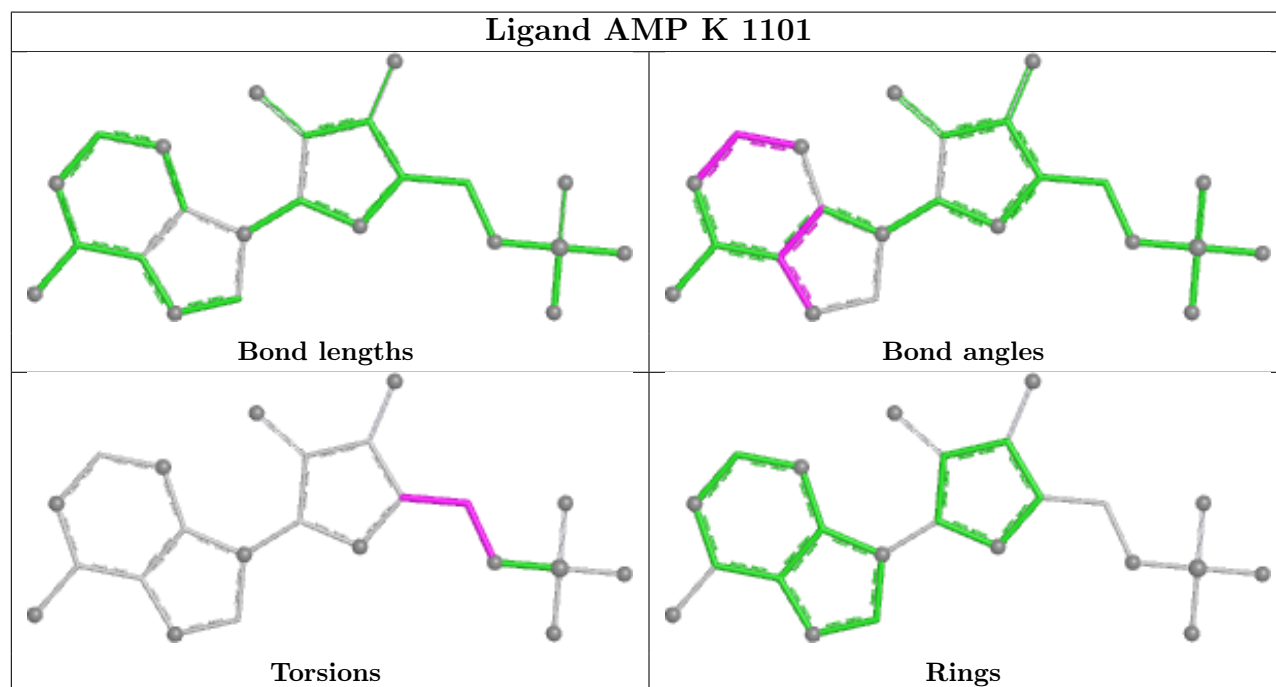
Ligand AMP D 1101

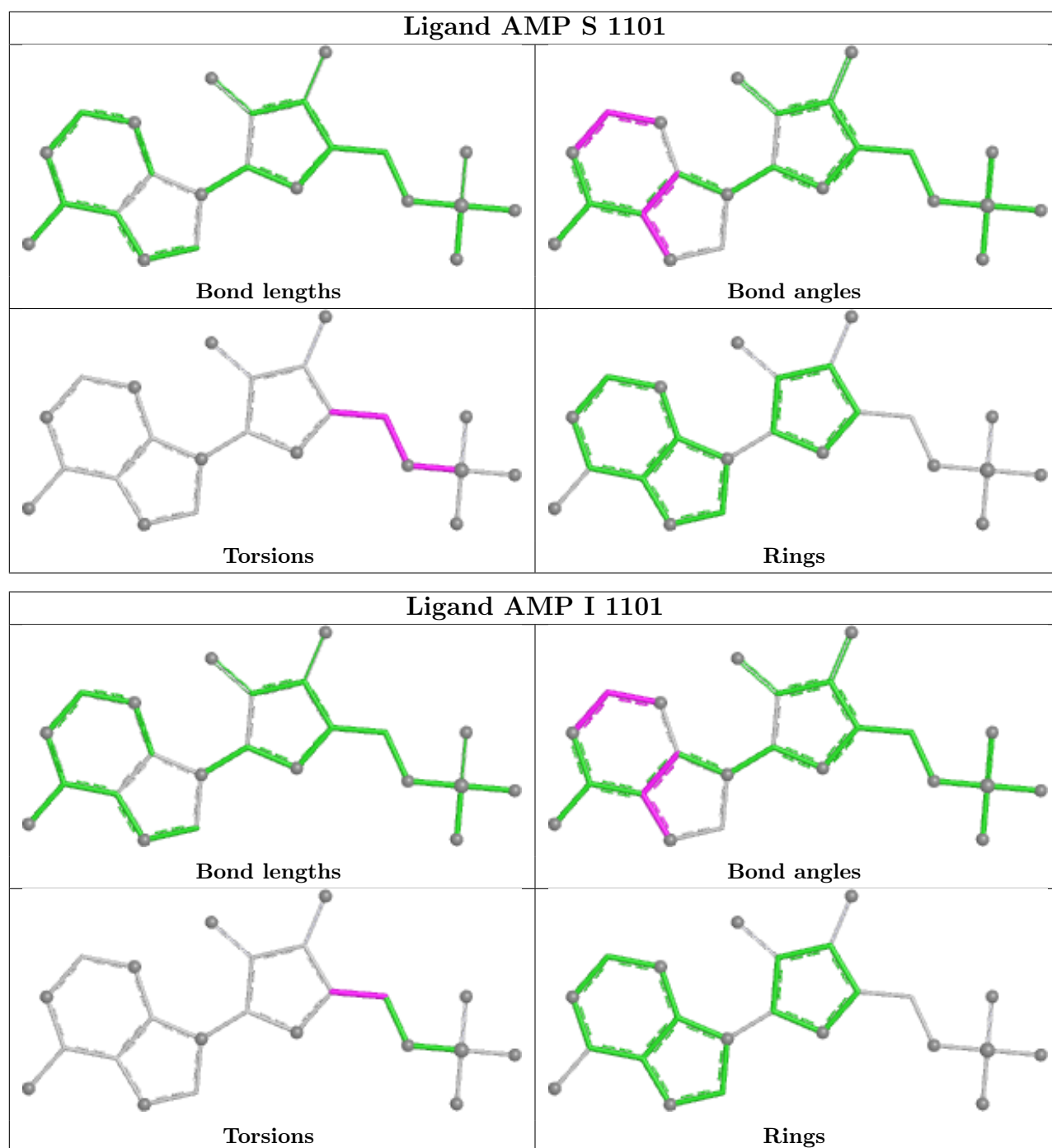


Ligand AMP G 1101



Ligand AMP K 1101





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, 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	M	77/83 (92%)	-0.54	0 100 100	134, 183, 238, 248	0
1	N	80/83 (96%)	-0.46	0 100 100	119, 167, 214, 219	0
1	O	73/83 (87%)	-0.60	0 100 100	133, 177, 236, 244	0
1	P	80/83 (96%)	-0.56	1 (1%) 74 66	93, 147, 183, 217	0
1	Q	76/83 (91%)	-0.68	0 100 100	129, 176, 205, 230	0
1	R	76/83 (91%)	-0.70	1 (1%) 74 66	124, 157, 209, 231	0
1	W	70/83 (84%)	-0.46	0 100 100	155, 233, 268, 290	0
1	X	73/83 (87%)	-0.54	0 100 100	177, 228, 270, 286	0
2	A	971/1017 (95%)	-0.72	1 (0%) 92 95	77, 126, 219, 269	0
2	C	972/1017 (95%)	-0.77	1 (0%) 92 95	61, 112, 206, 242	0
2	D	972/1017 (95%)	-0.76	0 100 100	72, 123, 207, 266	0
2	G	973/1017 (95%)	-0.77	0 100 100	52, 112, 209, 251	0
2	I	979/1017 (96%)	-0.79	0 100 100	66, 104, 165, 213	0
2	K	979/1017 (96%)	-0.83	0 100 100	51, 92, 152, 194	0
2	S	971/1017 (95%)	-0.74	2 (0%) 92 92	98, 178, 248, 279	0
2	U	973/1017 (95%)	-0.70	0 100 100	94, 180, 249, 276	0
3	B	153/197 (77%)	-0.69	0 100 100	114, 171, 211, 253	0
3	E	151/197 (76%)	-0.58	1 (0%) 84 78	135, 191, 225, 247	0
3	F	152/197 (77%)	-0.69	0 100 100	110, 168, 212, 257	0
3	H	152/197 (77%)	-0.53	1 (0%) 84 78	157, 201, 238, 280	0
3	J	156/197 (79%)	-0.60	0 100 100	101, 140, 196, 217	0
3	L	155/197 (78%)	-0.63	1 (0%) 85 80	83, 121, 177, 193	0
3	T	153/197 (77%)	-0.67	0 100 100	155, 208, 241, 258	0
3	V	146/197 (74%)	-0.54	1 (0%) 84 78	161, 217, 246, 281	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	9613/10376 (92%)	-0.73	10 (0%) 92 95	51, 138, 230, 290	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	8	LEU	2.6
3	L	118	VAL	2.6
3	H	96	ILE	2.5
2	S	655	LEU	2.4
2	S	140	ILE	2.2

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

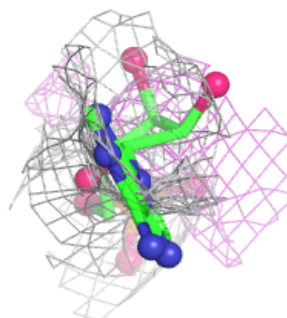
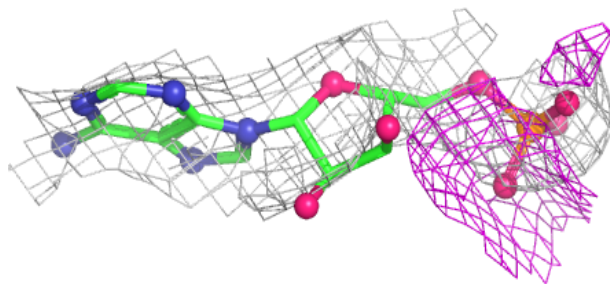
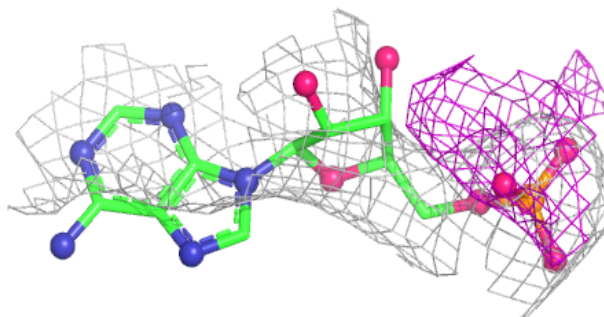
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	S	1101	23/23	0.66	0.11	153,220,239,242	0
4	AMP	A	1101	23/23	0.89	0.06	143,162,175,181	0
4	AMP	D	1101	23/23	0.89	0.06	119,135,151,169	0
4	AMP	I	1101	23/23	0.94	0.06	60,85,118,137	0
4	AMP	C	1101	23/23	0.94	0.05	86,103,133,137	0
4	AMP	G	1101	23/23	0.95	0.05	84,101,130,140	0
4	AMP	K	1101	23/23	0.96	0.05	62,73,102,141	0

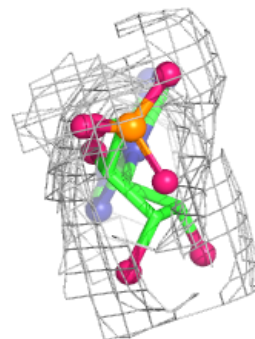
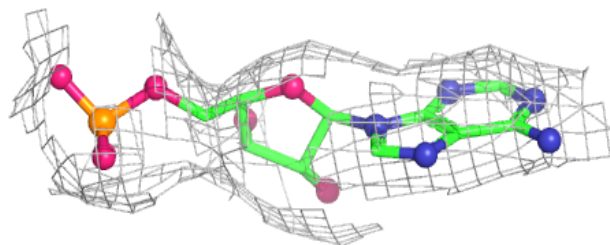
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP S 1101:

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

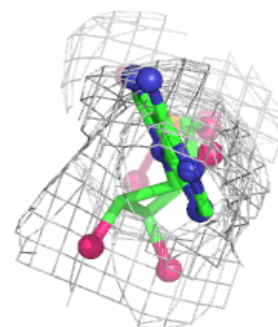
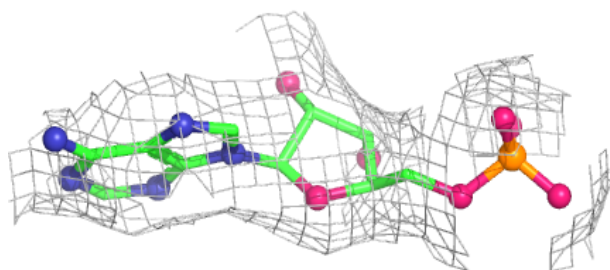
**Electron density around AMP A 1101:**

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

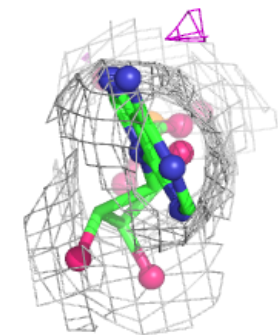
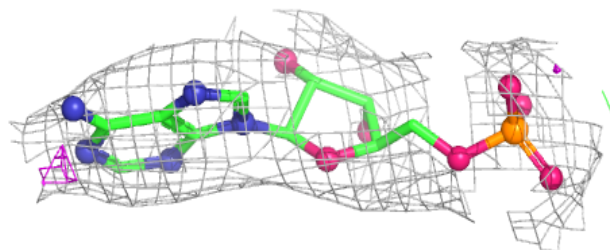
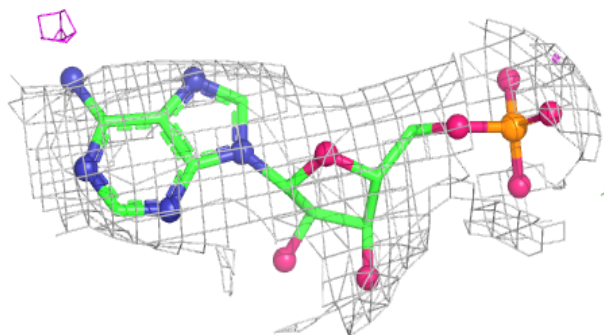


Electron density around AMP D 1101:

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

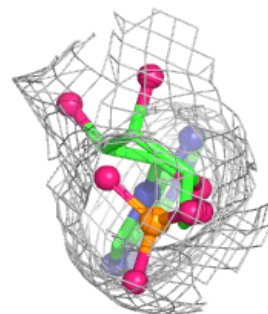
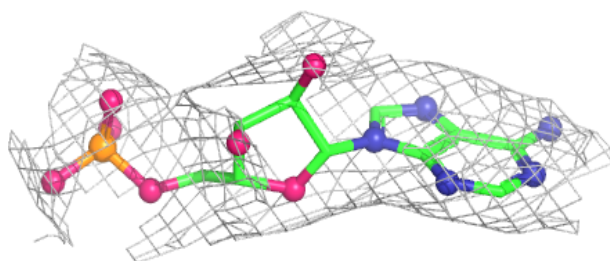
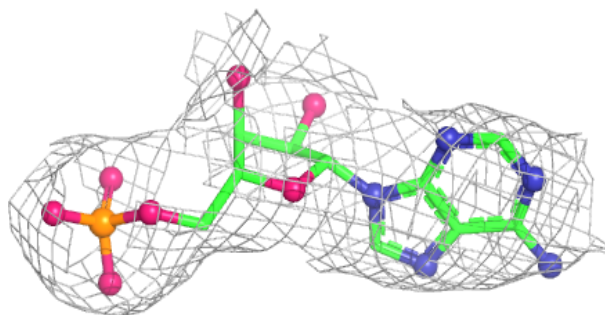
**Electron density around AMP I 1101:**

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

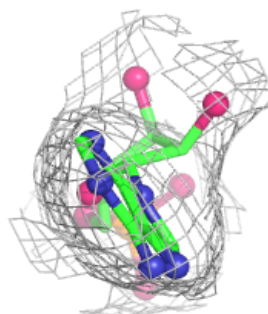
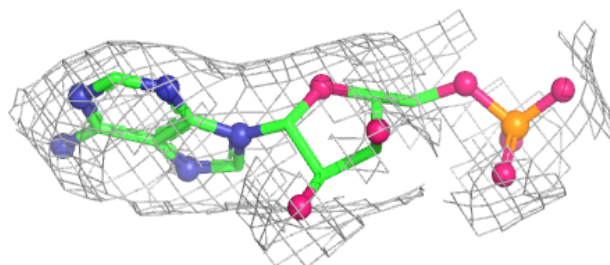
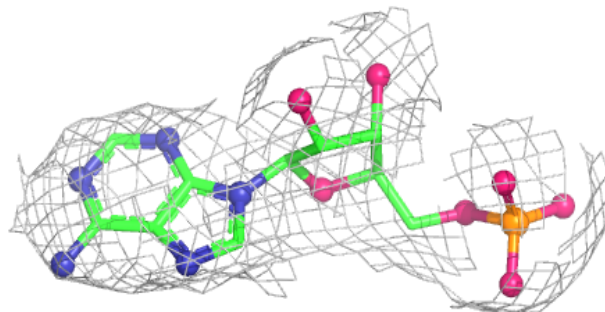


Electron density around AMP C 1101:

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

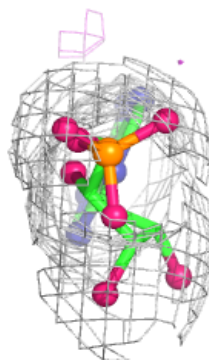
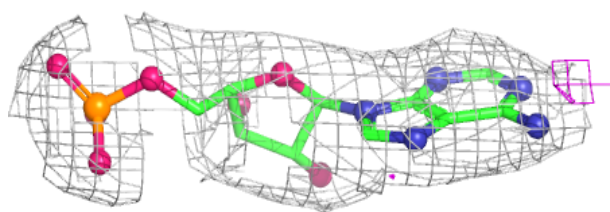
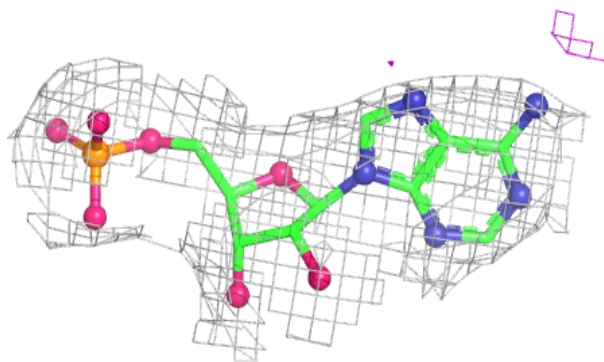
**Electron density around AMP G 1101:**

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



Electron density around AMP K 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.