



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:46 AM UTC

PDB ID : 6L5M / pdb_00006l5m
Title : Crystal structure of human DEAD-box RNA helicase DDX21 in complex with AMP
Authors : Chen, Z.J.; Hu, X.J.; Zhou, Z.; Li, J.X.
Deposited on : 2019-10-24
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

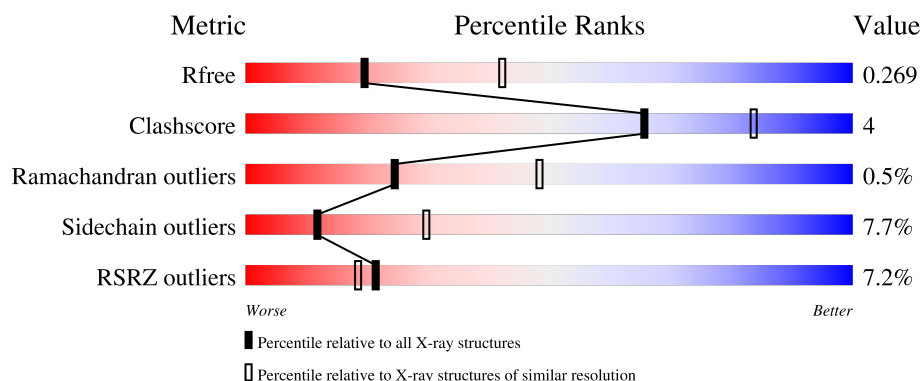
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	377	 7% 81% 13% . .
1	B	377	 6% 81% 14% . .
1	C	377	 5% 80% 15% . .
1	D	377	 9% 79% 16% . .
1	E	377	 7% 82% 13% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14643 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.

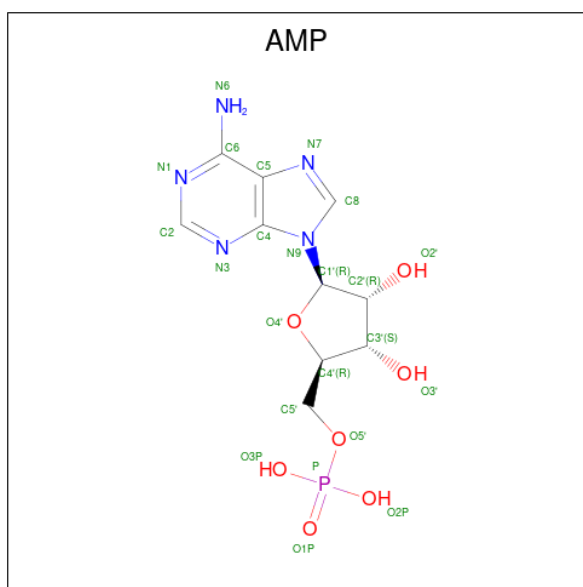
- Molecule 1 is a protein called Nucleolar RNA helicase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2894	1835	515	534	10			
1	B	366	Total	C	N	O	S	0	0	0
			2894	1835	515	534	10			
1	C	366	Total	C	N	O	S	0	0	0
			2894	1835	515	534	10			
1	D	366	Total	C	N	O	S	0	0	0
			2894	1835	515	534	10			
1	E	366	Total	C	N	O	S	0	0	0
			2894	1835	515	534	10			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	SER	-	expression tag	UNP Q9NR30
B	187	SER	-	expression tag	UNP Q9NR30
C	187	SER	-	expression tag	UNP Q9NR30
D	187	SER	-	expression tag	UNP Q9NR30
E	187	SER	-	expression tag	UNP Q9NR30

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P) (labeled as "Ligand of Interest" by depositor).



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

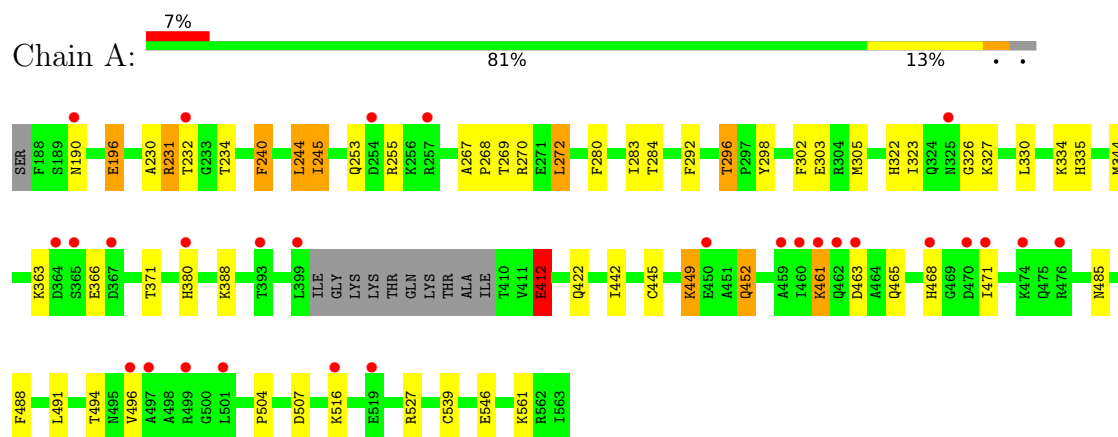
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	13	Total	O	0	0
			13	13		
3	C	11	Total	O	0	0
			11	11		
3	D	10	Total	O	0	0
			10	10		
3	E	9	Total	O	0	0
			9	9		

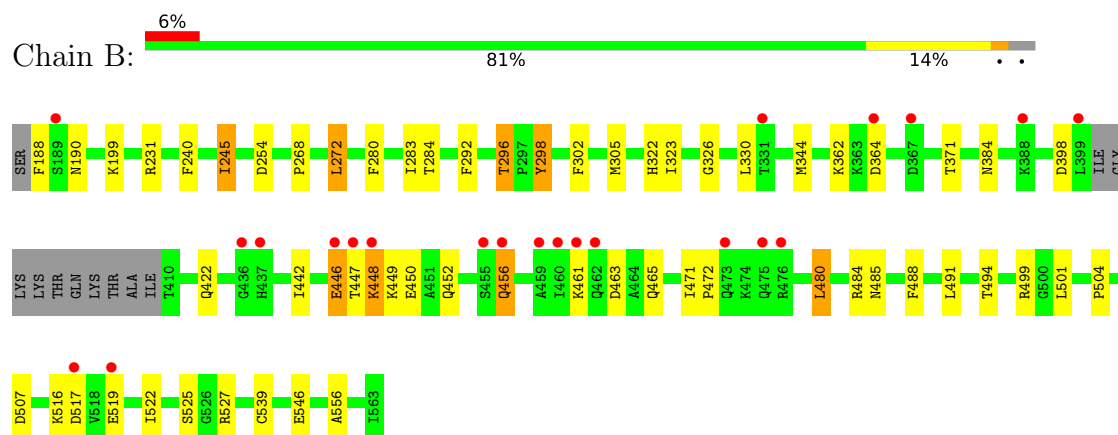
3 Residue-property plots [i](#)

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.

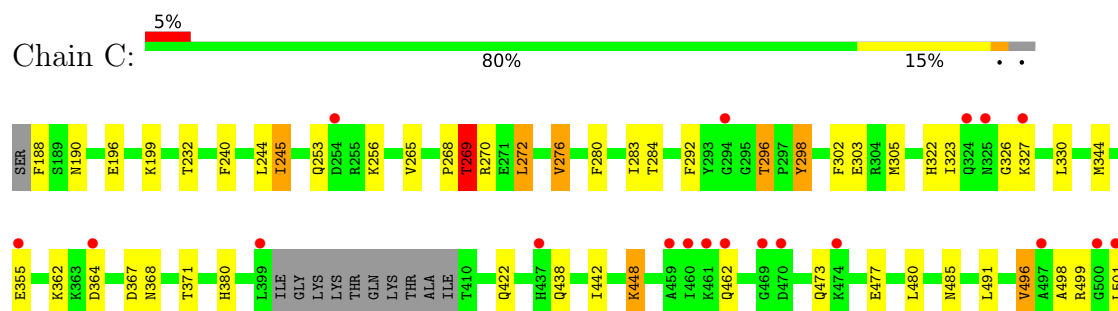
• Molecule 1: Nucleolar RNA helicase 2



• Molecule 1: Nucleolar RNA helicase 2

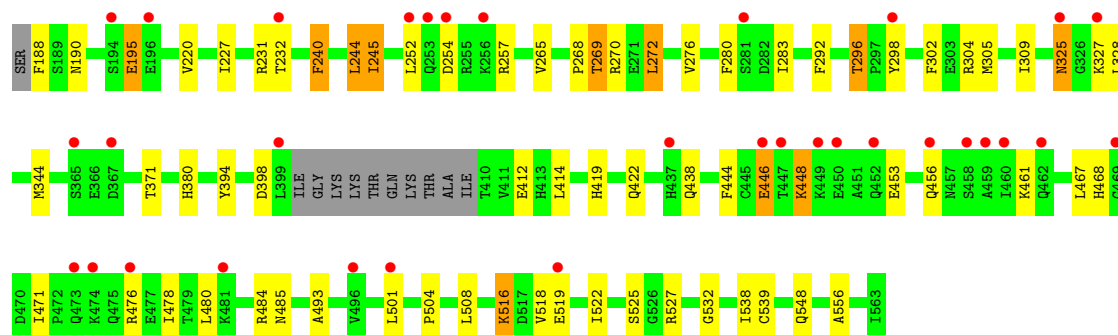
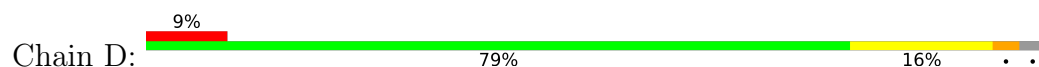


• Molecule 1: Nucleolar RNA helicase 2

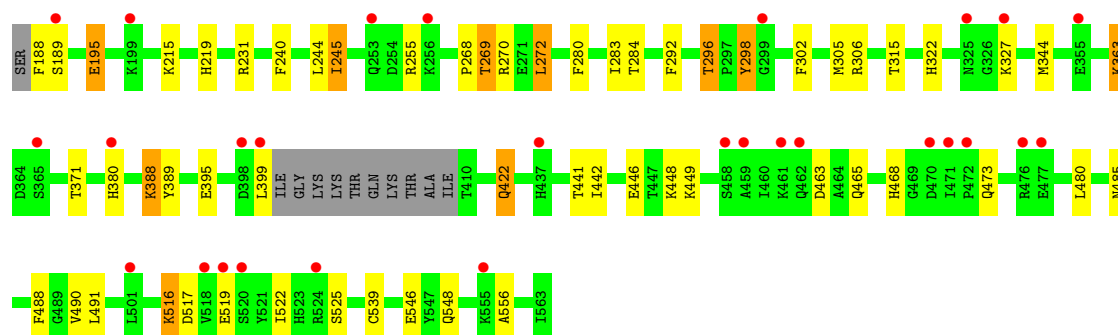
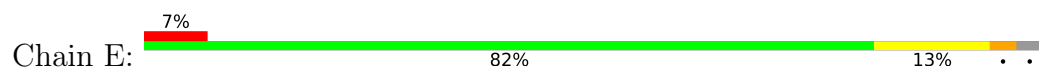




● Molecule 1: Nucleolar RNA helicase 2



● Molecule 1: Nucleolar RNA helicase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.39Å 219.07Å 126.39Å 90.00° 90.79° 90.00°	Depositor
Resolution (Å)	36.51 – 2.70 36.51 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (36.51-2.70) 95.8 (36.51-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.68Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.207 , 0.257 0.221 , 0.269	Depositor DCC
R_{free} test set	2580 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.032 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14643	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 32.59 % 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 9.1762e-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

5.1 Standard geometry

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	A	0.85	0/2949	1.37	15/3972 (0.4%)
1	B	0.87	0/2949	1.38	20/3972 (0.5%)
1	C	0.86	0/2949	1.40	21/3972 (0.5%)
1	D	0.85	0/2949	1.37	14/3972 (0.4%)
1	E	0.86	0/2949	1.40	18/3972 (0.5%)
All	All	0.86	0/14745	1.38	88/19860 (0.4%)

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	412	GLU	CB-CG-CD	6.54	123.72	112.60
1	A	412	GLU	CB-CG-CD	6.49	123.63	112.60
1	B	447	THR	CA-C-N	6.40	129.49	120.28
1	B	447	THR	C-N-CA	6.40	129.49	120.28
1	E	485	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	196	GLU	CB-CG-CD	6.26	123.24	112.60
1	C	269	THR	CA-C-N	6.25	128.95	120.38
1	C	269	THR	C-N-CA	6.25	128.95	120.38
1	B	485	ASN	CA-CB-CG	6.21	118.81	112.60
1	C	485	ASN	CA-CB-CG	6.19	118.79	112.60
1	A	190	ASN	CA-CB-CG	6.19	118.79	112.60
1	C	276	VAL	CA-C-N	6.11	128.38	120.44
1	C	276	VAL	C-N-CA	6.11	128.38	120.44
1	B	472	PRO	CA-C-N	6.09	128.76	120.54
1	B	472	PRO	C-N-CA	6.09	128.76	120.54
1	A	240	PHE	CA-CB-CG	6.04	119.84	113.80
1	A	485	ASN	CA-CB-CG	6.01	118.61	112.60
1	C	240	PHE	CA-CB-CG	5.98	119.78	113.80
1	C	477	GLU	CA-C-N	5.96	128.07	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	477	GLU	C-N-CA	5.96	128.07	120.56
1	A	269	THR	CA-C-N	5.92	128.13	120.44
1	A	269	THR	C-N-CA	5.92	128.13	120.44
1	E	240	PHE	CA-CB-CG	5.85	119.65	113.80
1	E	449	LYS	CA-C-N	5.83	128.34	120.65
1	E	449	LYS	C-N-CA	5.83	128.34	120.65
1	D	240	PHE	CA-CB-CG	5.81	119.61	113.80
1	A	326	GLY	CA-C-N	5.79	128.31	120.38
1	A	326	GLY	C-N-CA	5.79	128.31	120.38
1	A	292	PHE	CA-CB-CG	5.66	119.46	113.80
1	B	298	TYR	CA-C-N	5.62	126.34	119.99
1	B	298	TYR	C-N-CA	5.62	126.34	119.99
1	C	298	TYR	CA-C-N	5.60	126.31	119.99
1	C	298	TYR	C-N-CA	5.60	126.31	119.99
1	E	298	TYR	CA-C-N	5.58	126.30	119.99
1	E	298	TYR	C-N-CA	5.58	126.30	119.99
1	E	188	PHE	CA-C-N	5.56	132.16	121.54
1	E	188	PHE	C-N-CA	5.56	132.16	121.54
1	B	292	PHE	CA-CB-CG	5.50	119.30	113.80
1	E	270	ARG	CA-C-N	5.46	127.54	120.44
1	E	270	ARG	C-N-CA	5.46	127.54	120.44
1	D	518	VAL	CA-C-N	5.44	127.56	120.28
1	D	518	VAL	C-N-CA	5.44	127.56	120.28
1	D	485	ASN	CA-CB-CG	5.42	118.02	112.60
1	C	292	PHE	CA-CB-CG	5.42	119.22	113.80
1	B	494	THR	N-CA-C	-5.36	101.55	110.17
1	C	364	ASP	CA-CB-CG	5.35	117.95	112.60
1	C	296	THR	CB-CA-C	5.32	117.16	109.92
1	B	449	LYS	CA-C-N	5.30	127.70	120.54
1	B	449	LYS	C-N-CA	5.30	127.70	120.54
1	A	449	LYS	CA-C-N	5.30	127.33	120.44
1	A	449	LYS	C-N-CA	5.30	127.33	120.44
1	B	188	PHE	CA-CB-CG	5.27	119.07	113.80
1	D	292	PHE	CA-CB-CG	5.27	119.07	113.80
1	D	269	THR	CA-C-N	5.22	127.59	120.54
1	D	269	THR	C-N-CA	5.22	127.59	120.54
1	B	296	THR	CB-CA-C	5.21	117.73	109.55
1	C	188	PHE	CA-CB-CG	5.21	119.01	113.80
1	E	296	THR	CB-CA-C	5.20	117.71	109.55
1	C	253	GLN	CA-C-N	5.16	128.43	121.05
1	C	253	GLN	C-N-CA	5.16	128.43	121.05
1	C	422	GLN	CA-C-N	5.16	127.50	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	422	GLN	C-N-CA	5.16	127.50	120.54
1	E	422	GLN	CA-C-N	5.15	127.50	120.54
1	E	422	GLN	C-N-CA	5.15	127.50	120.54
1	E	517	ASP	CA-CB-CG	5.15	117.75	112.60
1	D	516	LYS	N-CA-C	-5.14	105.13	111.40
1	D	325	ASN	CA-CB-CG	5.13	117.73	112.60
1	E	292	PHE	CA-CB-CG	5.12	118.92	113.80
1	E	195	GLU	CA-C-N	5.12	127.09	120.44
1	E	195	GLU	C-N-CA	5.12	127.09	120.44
1	B	516	LYS	N-CA-C	-5.11	105.16	111.40
1	B	452	GLN	CA-C-N	5.11	127.43	120.54
1	B	452	GLN	C-N-CA	5.11	127.43	120.54
1	B	240	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	516	LYS	N-CA-C	-5.09	105.19	111.40
1	D	188	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	517	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	296	THR	CB-CA-C	5.02	117.44	109.55
1	B	507	ASP	N-CA-C	-5.02	107.28	113.41
1	A	507	ASP	N-CA-C	-5.02	107.28	113.41
1	C	516	LYS	N-CA-C	-5.02	105.28	111.40
1	D	195	GLU	CA-C-N	5.02	126.96	120.44
1	D	195	GLU	C-N-CA	5.02	126.96	120.44
1	D	296	THR	CB-CA-C	5.01	117.41	109.55
1	E	516	LYS	N-CA-C	-5.01	105.29	111.40
1	C	498	ALA	CA-C-N	5.00	127.69	120.38
1	C	498	ALA	C-N-CA	5.00	127.69	120.38
1	B	471	ILE	CB-CA-C	5.00	114.98	110.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2894	0	2926	24	0
1	B	2894	0	2926	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2894	0	2926	23	0
1	D	2894	0	2926	28	0
1	E	2894	0	2926	19	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0
2	D	23	0	12	0	0
2	E	23	0	12	0	0
3	A	15	0	0	0	0
3	B	13	0	0	0	0
3	C	11	0	0	0	0
3	D	10	0	0	0	0
3	E	9	0	0	0	0
All	All	14643	0	14690	111	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 4.

All (111) 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:230:ALA:HB1	1:A:234:THR:HG21	1.57	0.85
1:D:476:ARG:HE	1:D:501:LEU:HD21	1.55	0.71
1:B:480:LEU:HD21	1:B:501:LEU:HD23	1.81	0.63
1:E:269:THR:HG22	1:E:272:LEU:HB2	1.80	0.63
1:C:509:VAL:HG23	1:C:528:THR:HG21	1.79	0.63
1:C:362:LYS:H	1:C:368:ASN:HD21	1.48	0.61
1:C:448:LYS:H	1:C:448:LYS:HE2	1.64	0.60
1:C:505:GLU:HG3	1:C:527:ARG:HH21	1.65	0.60
1:D:446:GLU:HG3	1:D:516:LYS:HE2	1.83	0.60
1:B:448:LYS:HE3	1:B:448:LYS:H	1.65	0.59
1:E:269:THR:HG22	1:E:272:LEU:H	1.67	0.59
1:D:480:LEU:O	1:D:484:ARG:HG3	2.03	0.58
1:E:268:PRO:HB3	1:E:344:MET:HG2	1.83	0.58
1:C:268:PRO:HB3	1:C:344:MET:HG2	1.85	0.58
1:A:302:PHE:CE1	1:A:327:LYS:HG3	2.40	0.57
1:D:268:PRO:HB3	1:D:344:MET:HG2	1.86	0.56
1:A:268:PRO:HB3	1:A:344:MET:HG2	1.87	0.56
1:B:268:PRO:HD2	1:B:272:LEU:HD12	1.86	0.56
1:C:302:PHE:CE1	1:C:327:LYS:HG3	2.41	0.55
1:B:268:PRO:HB3	1:B:344:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:O	1:A:234:THR:HG22	2.07	0.55
1:B:442:ILE:HD12	1:B:491:LEU:HD23	1.89	0.54
1:D:304:ARG:HB3	1:D:309:ILE:HD11	1.89	0.54
1:D:444:PHE:HA	1:D:493:ALA:O	2.08	0.54
1:D:522:ILE:HD11	1:D:556:ALA:HB1	1.90	0.53
1:C:480:LEU:HD11	1:C:501:LEU:HD23	1.91	0.53
1:E:441:THR:CG2	1:E:490:VAL:HG22	2.38	0.52
1:E:442:ILE:HD12	1:E:491:LEU:HD23	1.90	0.52
1:B:323:ILE:HD11	1:B:330:LEU:HD12	1.92	0.52
1:A:442:ILE:HD12	1:A:491:LEU:HD23	1.90	0.52
1:A:323:ILE:HD11	1:A:330:LEU:HD12	1.91	0.52
1:C:323:ILE:HD11	1:C:330:LEU:HD12	1.92	0.51
1:B:522:ILE:HD11	1:B:556:ALA:HB1	1.93	0.50
1:C:522:ILE:HD11	1:C:556:ALA:HB1	1.94	0.50
1:E:522:ILE:HD11	1:E:556:ALA:HB1	1.94	0.50
1:B:245:ILE:HD13	1:B:283:ILE:HG13	1.94	0.50
1:E:245:ILE:HD13	1:E:283:ILE:HG13	1.94	0.49
1:A:245:ILE:HD13	1:A:283:ILE:HG13	1.94	0.49
1:A:445:CYS:O	1:A:494:THR:HA	2.12	0.49
1:B:456:GLN:HA	1:B:461:LYS:HD3	1.94	0.49
1:D:245:ILE:HD13	1:D:283:ILE:HG13	1.95	0.48
1:C:245:ILE:HD13	1:C:283:ILE:HG13	1.94	0.48
1:D:269:THR:CG2	1:D:272:LEU:HB2	2.43	0.48
1:E:219:HIS:CD2	1:E:395:GLU:HG3	2.49	0.48
1:E:388:LYS:HD2	1:E:389:TYR:CZ	2.48	0.48
1:A:452:GLN:HG2	1:A:468:HIS:HE2	1.78	0.48
1:C:442:ILE:HD12	1:C:491:LEU:HD23	1.95	0.48
1:D:467:LEU:HD11	1:D:476:ARG:HA	1.95	0.48
1:D:504:PRO:HA	1:D:527:ARG:HH21	1.79	0.48
1:D:269:THR:HG23	1:D:272:LEU:HB2	1.96	0.47
1:D:448:LYS:H	1:D:448:LYS:HE3	1.79	0.47
1:C:298:TYR:HB3	1:C:302:PHE:CE2	2.49	0.47
1:D:298:TYR:HB3	1:D:302:PHE:CE2	2.49	0.47
1:A:268:PRO:HD2	1:A:272:LEU:HD22	1.97	0.47
1:D:240:PHE:O	1:D:244:LEU:HB2	2.15	0.47
1:C:269:THR:HG22	1:C:272:LEU:HB2	1.97	0.47
1:A:412:GLU:HA	1:A:412:GLU:OE2	2.15	0.47
1:C:509:VAL:CG2	1:C:528:THR:HG21	2.44	0.47
1:E:465:GLN:HB2	1:E:488:PHE:CE2	2.50	0.46
1:B:298:TYR:HB3	1:B:302:PHE:CE2	2.51	0.46
1:A:240:PHE:O	1:A:244:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:GLN:HB2	1:A:488:PHE:CE2	2.51	0.46
1:B:504:PRO:HA	1:B:527:ARG:HH21	1.81	0.46
1:E:298:TYR:HB3	1:E:302:PHE:CE2	2.51	0.45
1:C:305:MET:HE1	1:C:322:HIS:ND1	2.32	0.45
1:E:448:LYS:HG2	1:E:468:HIS:HB2	1.98	0.44
1:A:298:TYR:HB3	1:A:302:PHE:CE2	2.52	0.44
1:B:305:MET:HE1	1:B:322:HIS:ND1	2.32	0.44
1:C:496:VAL:HA	1:C:499:ARG:HG3	1.98	0.44
1:D:504:PRO:HA	1:D:527:ARG:NH2	2.33	0.44
1:D:456:GLN:HA	1:D:461:LYS:HG3	2.00	0.44
1:A:305:MET:HE1	1:A:322:HIS:ND1	2.33	0.43
1:C:555:LYS:O	1:D:532:GLY:HA2	2.19	0.43
1:E:245:ILE:HD11	1:E:280:PHE:HD1	1.84	0.43
1:C:244:LEU:HD23	1:C:244:LEU:HA	1.85	0.43
1:D:220:VAL:CG1	1:D:244:LEU:HD13	2.49	0.43
1:E:215:LYS:HE3	1:E:399:LEU:HD21	1.99	0.43
1:B:504:PRO:HA	1:B:527:ARG:NH2	2.34	0.43
1:E:305:MET:HE1	1:E:322:HIS:ND1	2.34	0.43
1:A:363:LYS:HE3	1:A:388:LYS:HE3	2.00	0.43
1:A:334:LYS:HB2	1:A:335:HIS:CD2	2.54	0.42
1:A:302:PHE:HA	1:A:305:MET:HE3	2.02	0.42
1:B:446:GLU:HG2	1:B:450:GLU:OE1	2.19	0.42
1:C:265:VAL:HG11	1:C:276:VAL:HG11	2.02	0.42
1:C:302:PHE:HA	1:C:305:MET:HE3	2.02	0.42
1:B:245:ILE:HD11	1:B:280:PHE:HD1	1.84	0.42
1:D:468:HIS:H	1:D:471:ILE:HD12	1.85	0.42
1:E:280:PHE:O	1:E:284:THR:HG22	2.20	0.42
1:E:302:PHE:HA	1:E:305:MET:HE3	2.02	0.42
1:D:302:PHE:HA	1:D:305:MET:HE3	2.03	0.41
1:A:245:ILE:HD11	1:A:280:PHE:HD1	1.86	0.41
1:D:227:ILE:HD12	1:D:394:TYR:CE1	2.56	0.41
1:B:280:PHE:O	1:B:284:THR:HG22	2.21	0.41
1:D:476:ARG:O	1:D:480:LEU:HG	2.20	0.41
1:A:280:PHE:O	1:A:284:THR:HG22	2.20	0.41
1:A:267:ALA:HB1	1:A:272:LEU:HD23	2.02	0.41
1:A:302:PHE:HE1	1:A:327:LYS:HG3	1.85	0.41
1:D:269:THR:HG23	1:D:272:LEU:H	1.86	0.41
1:B:465:GLN:HB2	1:B:488:PHE:CE2	2.56	0.41
1:C:448:LYS:HE2	1:C:448:LYS:N	2.32	0.41
1:B:480:LEU:HB3	1:B:484:ARG:NH2	2.36	0.41
1:A:504:PRO:HA	1:A:527:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:PHE:O	1:C:284:THR:HG22	2.21	0.40
1:D:245:ILE:HD11	1:D:280:PHE:HD1	1.85	0.40
1:D:419:HIS:HB3	1:D:422:GLN:NE2	2.36	0.40
1:C:362:LYS:H	1:C:368:ASN:ND2	2.18	0.40
1:D:265:VAL:HG11	1:D:276:VAL:HG11	2.03	0.40
1:D:508:LEU:HD11	1:D:538:ILE:HD12	2.03	0.40
1:E:268:PRO:HG2	1:E:272:LEU:HD13	2.03	0.40
1:A:468:HIS:CE1	1:A:471:ILE:HG23	2.56	0.40
1:E:244:LEU:HD23	1:E:244:LEU:HA	1.84	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	362/377 (96%)	352 (97%)	8 (2%)	2 (1%)	21	44
1	B	362/377 (96%)	353 (98%)	7 (2%)	2 (1%)	21	44
1	C	362/377 (96%)	352 (97%)	8 (2%)	2 (1%)	21	44
1	D	362/377 (96%)	352 (97%)	10 (3%)	0	100	100
1	E	362/377 (96%)	354 (98%)	5 (1%)	3 (1%)	16	37
All	All	1810/1885 (96%)	1763 (97%)	38 (2%)	9 (0%)	24	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	363	LYS
1	A	255	ARG
1	E	189	SER
1	A	461	LYS
1	B	499	ARG

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Mol	Chain	Res	Type
1	C	367	ASP
1	E	255	ARG
1	B	326	GLY
1	C	326	GLY

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	314/323 (97%)	291 (93%)	23 (7%)	13	32
1	B	314/323 (97%)	292 (93%)	22 (7%)	14	34
1	C	314/323 (97%)	290 (92%)	24 (8%)	12	30
1	D	314/323 (97%)	286 (91%)	28 (9%)	9	23
1	E	314/323 (97%)	290 (92%)	24 (8%)	12	30
All	All	1570/1615 (97%)	1449 (92%)	121 (8%)	12	30

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
1	A	231	ARG
1	A	232	THR
1	A	244	LEU
1	A	245	ILE
1	A	253	GLN
1	A	270	ARG
1	A	272	LEU
1	A	296	THR
1	A	303	GLU
1	A	366	GLU
1	A	371	THR
1	A	380	HIS
1	A	412	GLU
1	A	422	GLN

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Mol	Chain	Res	Type
1	A	449	LYS
1	A	452	GLN
1	A	461	LYS
1	A	463	ASP
1	A	496	VAL
1	A	539	CYS
1	A	546	GLU
1	A	561	LYS
1	B	190	ASN
1	B	199	LYS
1	B	231	ARG
1	B	245	ILE
1	B	254	ASP
1	B	272	LEU
1	B	296	THR
1	B	362	LYS
1	B	364	ASP
1	B	371	THR
1	B	384	ASN
1	B	398	ASP
1	B	422	GLN
1	B	446	GLU
1	B	448	LYS
1	B	456	GLN
1	B	463	ASP
1	B	480	LEU
1	B	519	GLU
1	B	525	SER
1	B	539	CYS
1	B	546	GLU
1	C	190	ASN
1	C	196	GLU
1	C	199	LYS
1	C	232	THR
1	C	245	ILE
1	C	256	LYS
1	C	269	THR
1	C	270	ARG
1	C	272	LEU
1	C	296	THR
1	C	303	GLU
1	C	355	GLU

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Mol	Chain	Res	Type
1	C	371	THR
1	C	380	HIS
1	C	438	GLN
1	C	448	LYS
1	C	462	GLN
1	C	473	GLN
1	C	496	VAL
1	C	519	GLU
1	C	524	ARG
1	C	525	SER
1	C	528	THR
1	C	539	CYS
1	D	190	ASN
1	D	195	GLU
1	D	231	ARG
1	D	232	THR
1	D	244	LEU
1	D	245	ILE
1	D	252	LEU
1	D	254	ASP
1	D	257	ARG
1	D	270	ARG
1	D	272	LEU
1	D	296	THR
1	D	325	ASN
1	D	327	LYS
1	D	328	LEU
1	D	371	THR
1	D	380	HIS
1	D	398	ASP
1	D	414	LEU
1	D	438	GLN
1	D	446	GLU
1	D	448	LYS
1	D	453	GLU
1	D	478	ILE
1	D	519	GLU
1	D	525	SER
1	D	539	CYS
1	D	548	GLN
1	E	195	GLU
1	E	231	ARG

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Mol	Chain	Res	Type
1	E	245	ILE
1	E	269	THR
1	E	272	LEU
1	E	296	THR
1	E	306	ARG
1	E	315	THR
1	E	327	LYS
1	E	363	LYS
1	E	371	THR
1	E	380	HIS
1	E	388	LYS
1	E	422	GLN
1	E	446	GLU
1	E	463	ASP
1	E	473	GLN
1	E	480	LEU
1	E	516	LYS
1	E	519	GLU
1	E	525	SER
1	E	539	CYS
1	E	546	GLU
1	E	548	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	GLN
1	A	456	GLN
1	A	495	ASN
1	B	324	GLN
1	B	325	ASN
1	B	352	GLN
1	B	422	GLN
1	B	475	GLN
1	C	218	HIS
1	C	301	GLN
1	C	325	ASN
1	C	368	ASN
1	C	422	GLN
1	C	456	GLN
1	C	495	ASN
1	D	262	GLN

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Mol	Chain	Res	Type
1	D	352	GLN
1	D	437	HIS
1	D	452	GLN
1	D	456	GLN
1	E	219	HIS
1	E	274	ASN
1	E	422	GLN
1	E	473	GLN

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](#)

5 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	$\# Z > 2$
2	AMP	C	601	-	25,25,25	0.23	0	37,38,38	0.44	0
2	AMP	E	601	-	25,25,25	0.29	0	37,38,38	0.38	0
2	AMP	B	601	-	25,25,25	0.41	0	37,38,38	0.46	0
2	AMP	D	601	-	25,25,25	0.42	0	37,38,38	0.49	0
2	AMP	A	601	-	25,25,25	0.27	0	37,38,38	0.43	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
2	AMP	C	601	-	-	0/10/26/26	0/3/3/3
2	AMP	E	601	-	-	0/10/26/26	0/3/3/3
2	AMP	B	601	-	-	0/10/26/26	0/3/3/3
2	AMP	D	601	-	-	0/10/26/26	0/3/3/3
2	AMP	A	601	-	-	0/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

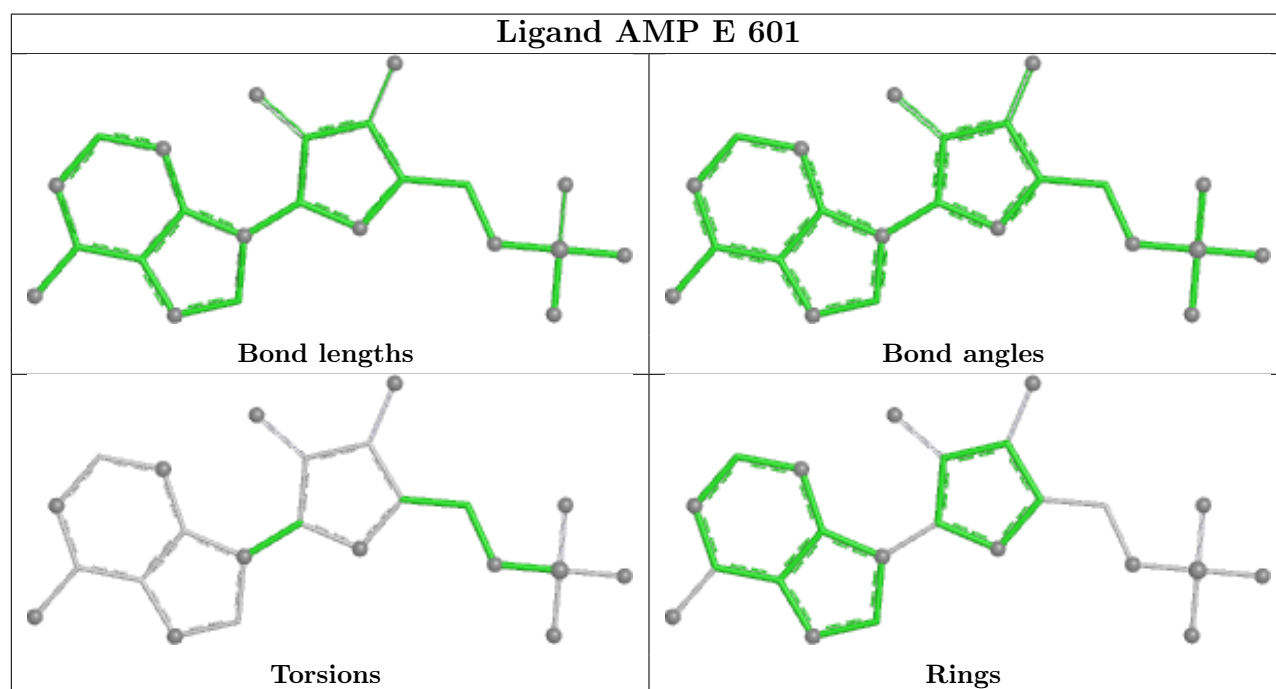
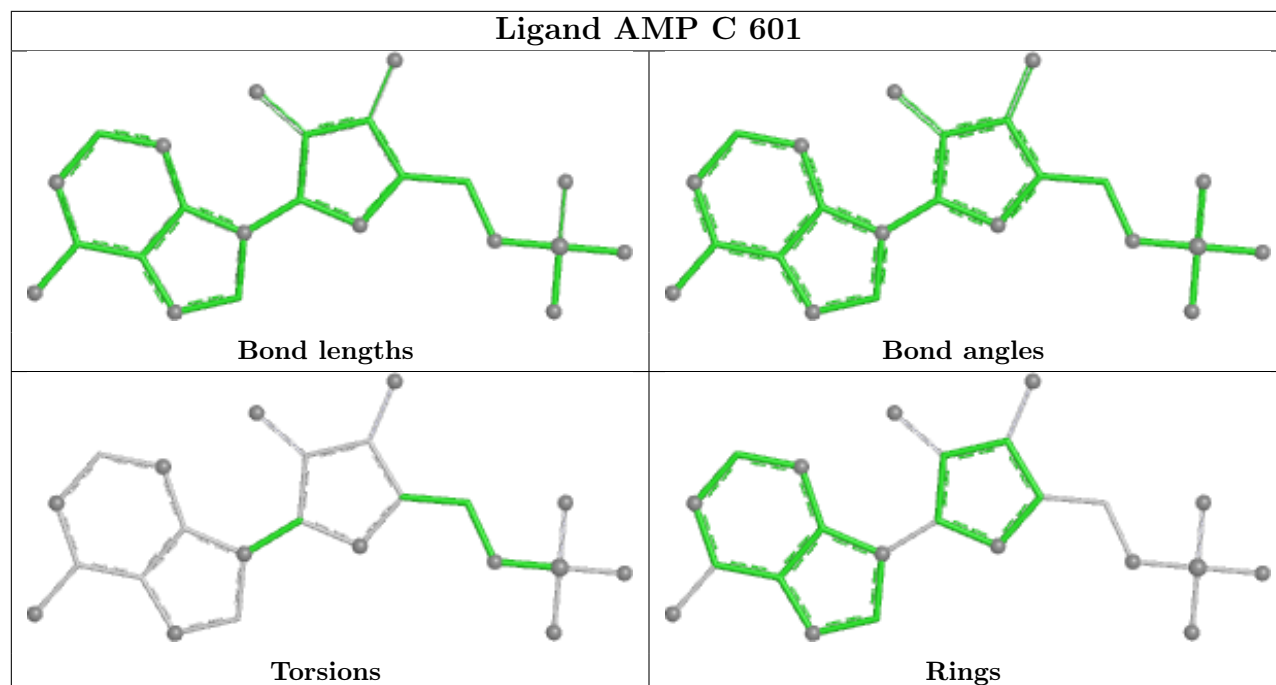
There are no chirality outliers.

There are no torsion outliers.

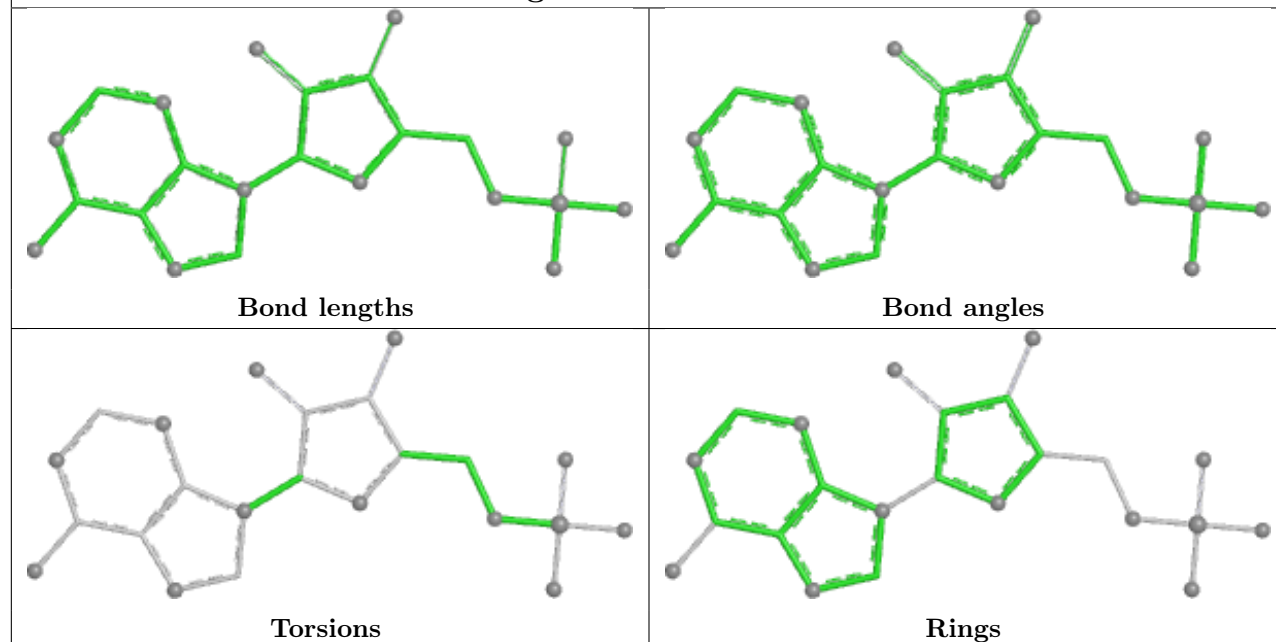
There are no ring outliers.

No monomer is involved in short contacts.

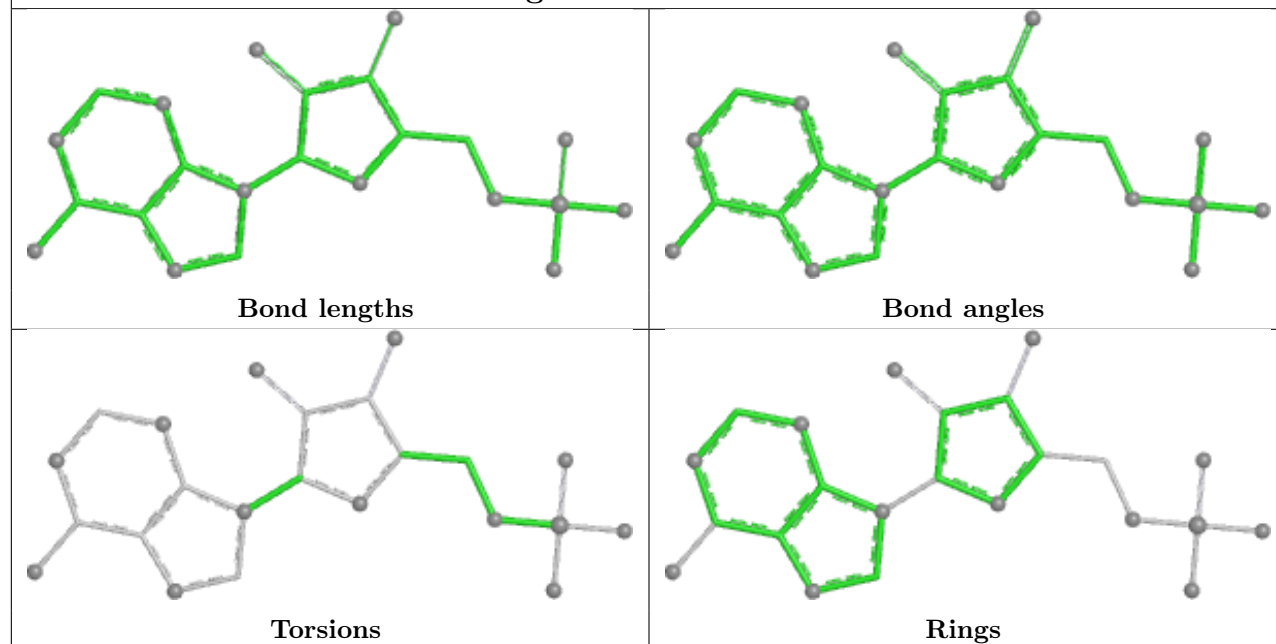
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

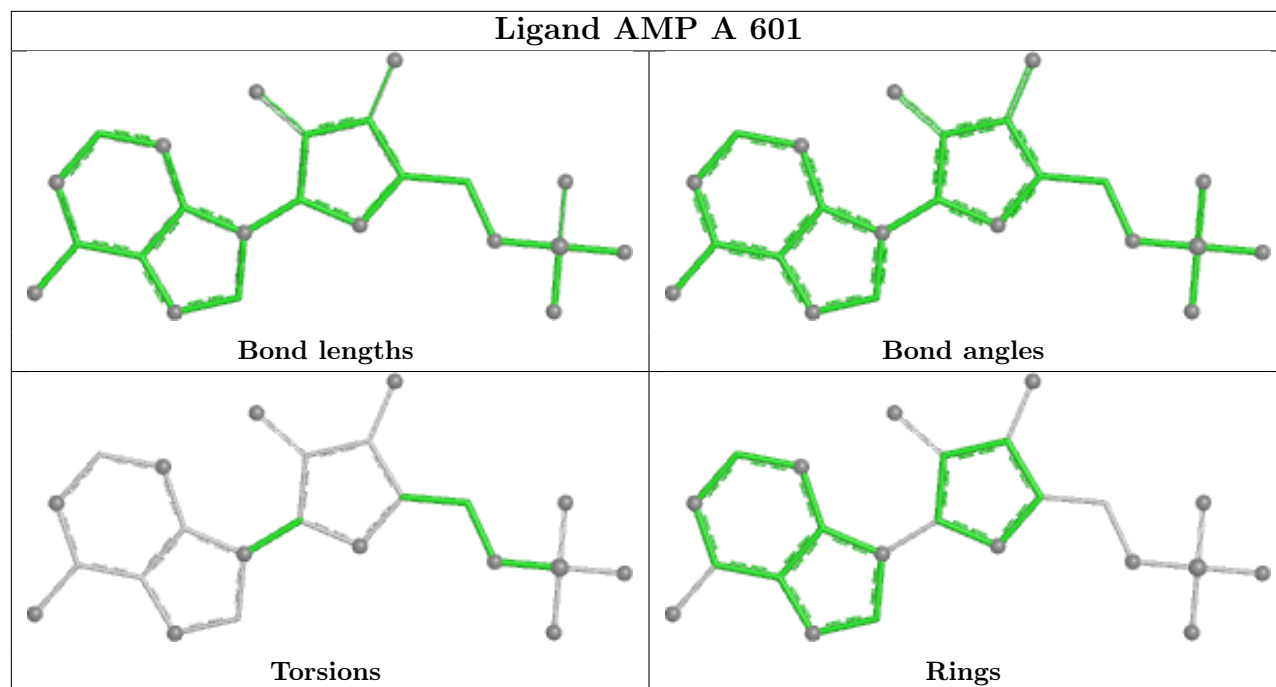


Ligand AMP B 601



Ligand AMP D 601





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	A	366/377 (97%)	0.60	28 (7%)	19	17	4, 23, 54, 73	0
1	B	366/377 (97%)	0.42	22 (6%)	27	24	3, 19, 52, 64	0
1	C	366/377 (97%)	0.44	20 (5%)	30	27	4, 24, 53, 71	0
1	D	366/377 (97%)	0.66	33 (9%)	15	13	3, 25, 56, 68	0
1	E	366/377 (97%)	0.48	28 (7%)	19	17	3, 21, 52, 67	0
All	All	1830/1885 (97%)	0.52	131 (7%)	21	18	3, 23, 54, 73	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	458	SER	4.0
1	A	367	ASP	3.6
1	A	364	ASP	3.6
1	A	399	LEU	3.6
1	E	437	HIS	3.5
1	B	461	LYS	3.5
1	E	462	GLN	3.4
1	C	324	GLN	3.4
1	B	447	THR	3.3
1	C	399	LEU	3.3
1	D	365	SER	3.3
1	E	461	LYS	3.2
1	B	460	ILE	3.2
1	A	499	ARG	3.2
1	D	256	LYS	3.2
1	C	501	LEU	3.1
1	B	462	GLN	3.1
1	B	437	HIS	3.1
1	D	450	GLU	3.1
1	A	461	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	364	ASP	3.1
1	D	399	LEU	3.1
1	E	524	ARG	3.1
1	D	476	ARG	3.0
1	B	455	SER	3.0
1	A	254	ASP	3.0
1	C	294	GLY	3.0
1	B	399	LEU	2.9
1	A	474	LYS	2.9
1	E	327	LYS	2.9
1	D	474	LYS	2.9
1	B	475	GLN	2.8
1	C	462	GLN	2.8
1	E	501	LEU	2.8
1	A	501	LEU	2.7
1	A	497	ALA	2.7
1	D	196	GLU	2.7
1	A	325	ASN	2.7
1	D	325	ASN	2.7
1	D	519	GLU	2.7
1	D	462	GLN	2.6
1	E	519	GLU	2.6
1	D	327	LYS	2.6
1	A	470	ASP	2.6
1	D	367	ASP	2.6
1	D	252	LEU	2.6
1	C	437	HIS	2.6
1	C	500	GLY	2.6
1	A	232	THR	2.6
1	D	254	ASP	2.5
1	C	461	LYS	2.5
1	A	190	ASN	2.5
1	E	470	ASP	2.5
1	B	473	GLN	2.5
1	E	189	SER	2.5
1	E	520	SER	2.5
1	A	463	ASP	2.5
1	A	450	GLU	2.5
1	A	460	ILE	2.5
1	D	460	ILE	2.5
1	B	367	ASP	2.5
1	A	468	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	459	ALA	2.5
1	E	459	ALA	2.5
1	E	476	ARG	2.4
1	A	519	GLU	2.4
1	B	446	GLU	2.4
1	D	446	GLU	2.4
1	C	469	GLY	2.4
1	D	473	GLN	2.4
1	B	519	GLU	2.4
1	D	501	LEU	2.4
1	C	254	ASP	2.4
1	D	481	LYS	2.4
1	D	437	HIS	2.3
1	B	364	ASP	2.3
1	A	257	ARG	2.3
1	D	459	ALA	2.3
1	E	256	LYS	2.3
1	E	472	PRO	2.3
1	E	399	LEU	2.3
1	D	232	THR	2.3
1	E	471	ILE	2.3
1	D	447	THR	2.3
1	B	517	ASP	2.3
1	D	194	SER	2.2
1	E	299	GLY	2.2
1	A	380	HIS	2.2
1	C	470	ASP	2.2
1	E	398	ASP	2.2
1	C	459	ALA	2.2
1	A	393	THR	2.2
1	D	452	GLN	2.2
1	B	189	SER	2.2
1	C	327	LYS	2.2
1	C	355	GLU	2.2
1	E	355	GLU	2.2
1	C	325	ASN	2.2
1	D	449	LYS	2.2
1	E	199	LYS	2.2
1	E	555	LYS	2.2
1	E	380	HIS	2.2
1	D	253	GLN	2.1
1	D	298	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	253	GLN	2.1
1	A	459	ALA	2.1
1	B	331	THR	2.1
1	A	462	GLN	2.1
1	B	436	GLY	2.1
1	A	496	VAL	2.1
1	C	517	ASP	2.1
1	D	281	SER	2.1
1	D	458	SER	2.1
1	E	365	SER	2.1
1	B	388	LYS	2.1
1	B	448	LYS	2.1
1	E	325	ASN	2.1
1	D	496	VAL	2.1
1	A	365	SER	2.1
1	A	476	ARG	2.1
1	C	497	ALA	2.1
1	A	471	ILE	2.1
1	E	518	VAL	2.1
1	E	477	GLU	2.0
1	C	474	LYS	2.0
1	D	456	GLN	2.0
1	C	460	ILE	2.0
1	A	516	LYS	2.0
1	B	456	GLN	2.0
1	D	469	GLY	2.0
1	B	476	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 oligosaccharides in this entry.

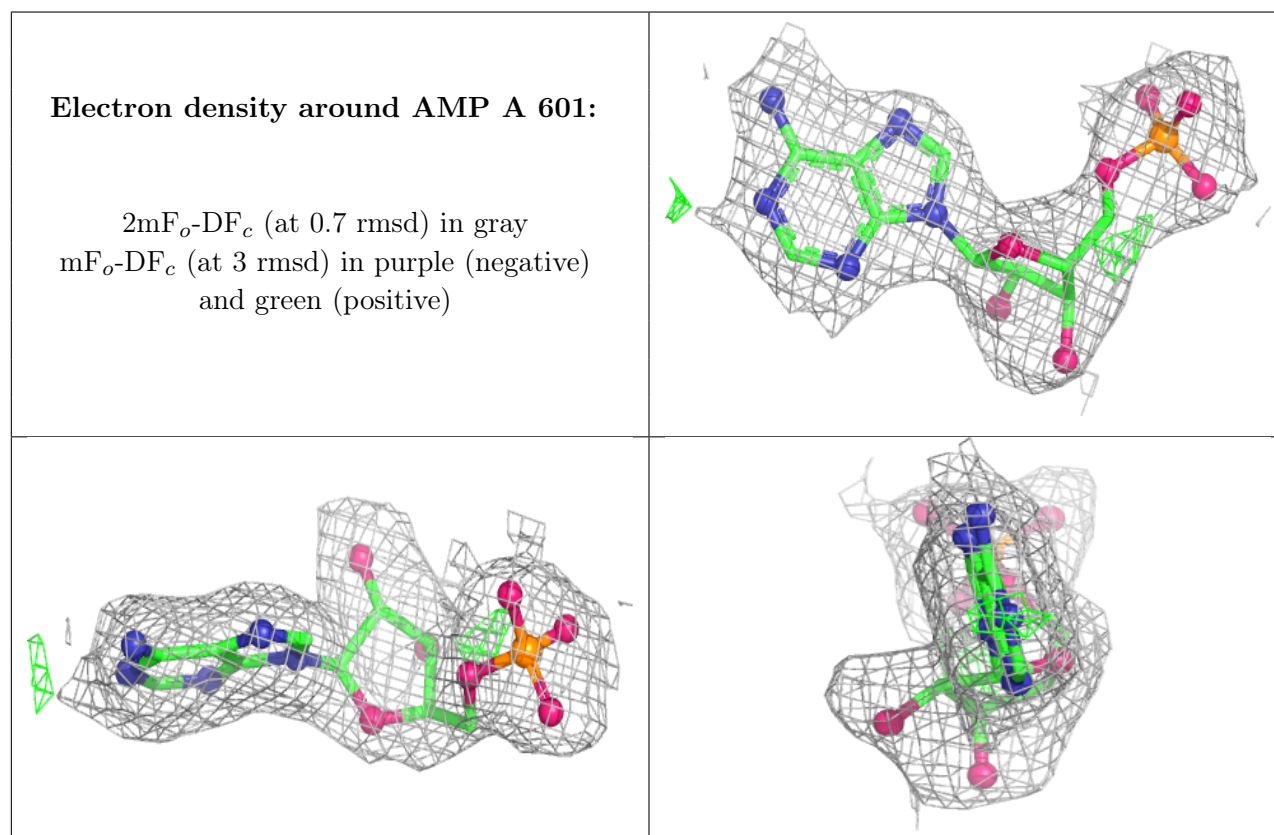
6.4 Ligands [i](#)

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.

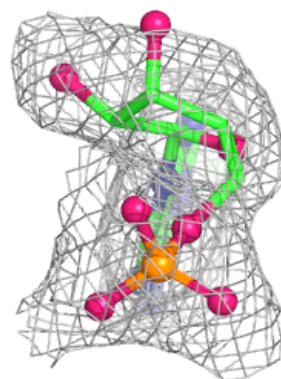
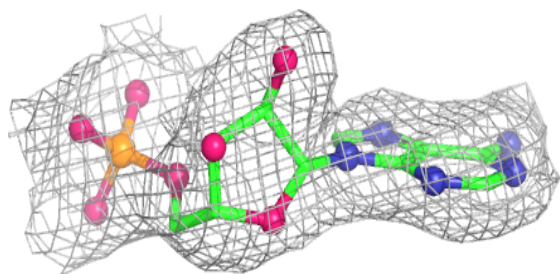
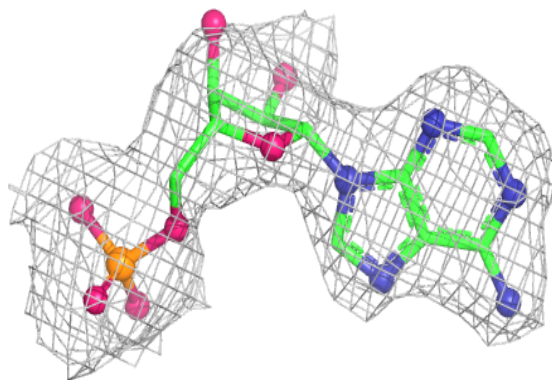
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AMP	A	601	23/23	0.92	0.10	4,23,29,30	0
2	AMP	C	601	23/23	0.92	0.10	22,29,33,37	0
2	AMP	B	601	23/23	0.93	0.09	4,21,30,30	0
2	AMP	D	601	23/23	0.93	0.09	7,23,28,31	0
2	AMP	E	601	23/23	0.94	0.08	6,19,27,28	0

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.

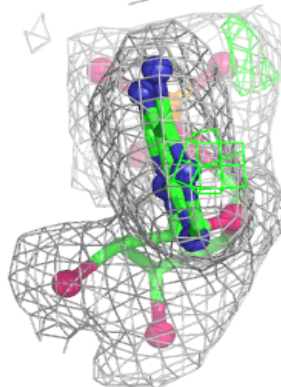
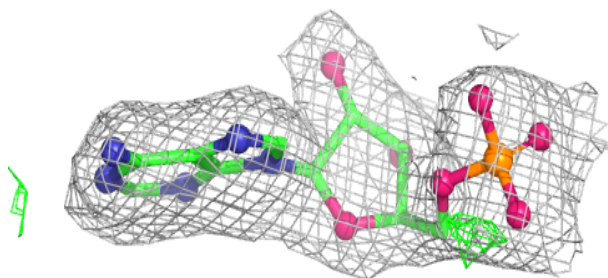
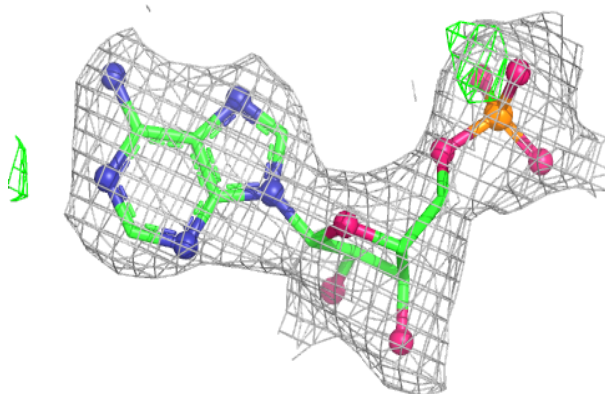


Electron density around AMP C 601:

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

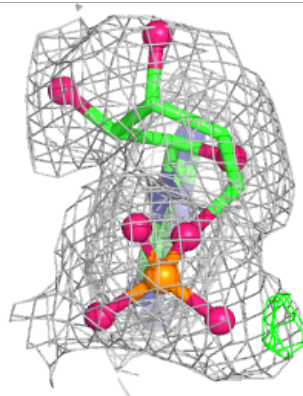
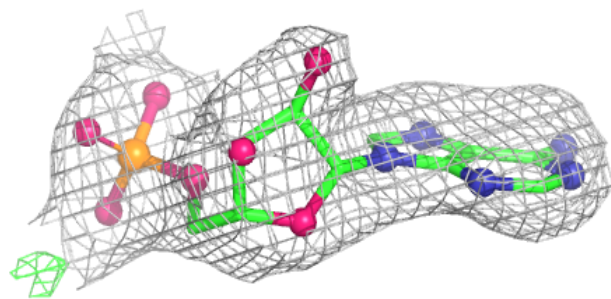
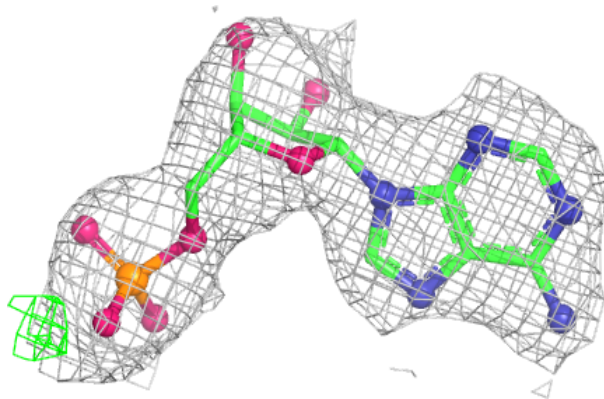
**Electron density around AMP B 601:**

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

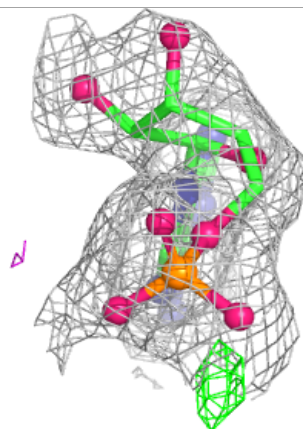
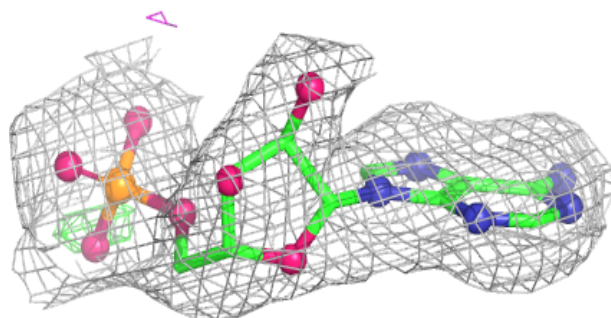
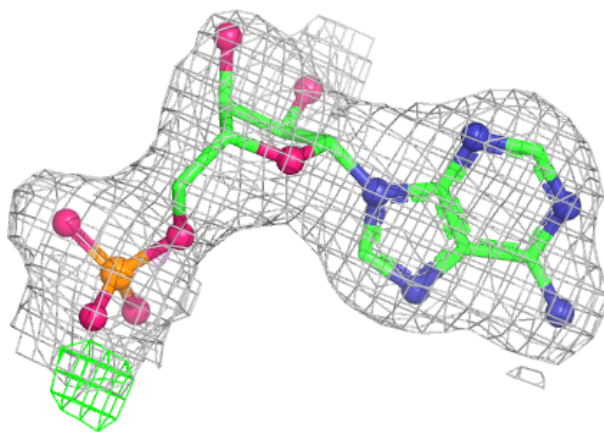


Electron density around AMP D 601:

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

**Electron density around AMP E 601:**

$2mF_o-DF_c$ (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.