Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 01:34 AM EDT

PDB ID	:	6L5M
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:

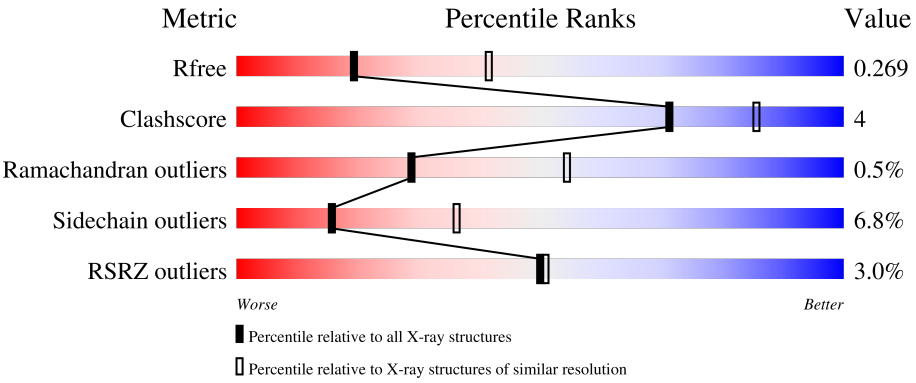
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	2% 84% 12%
1	B	377	3% 85% 11%
1	C	377	2% 84% 12%
1	D	377	5% 81% 15%
1	E	377	2% 84% 12%

2 Entry composition (i)

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.

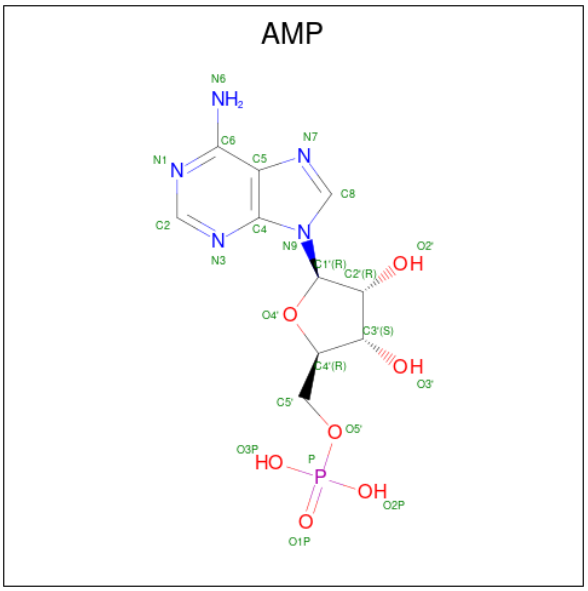
- Molecule 1 is a protein called Nucleolar RNA helicase 2.

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 (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (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.

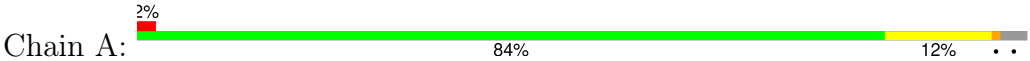
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total	O	0	0
			15	15		
3	B	13	Total	O	0	0
			13	13		
3	C	11	Total	O	0	0
			11	11		
3	D	10	Total	O	0	0
			10	10		
3	E	9	Total	O	0	0
			9	9		

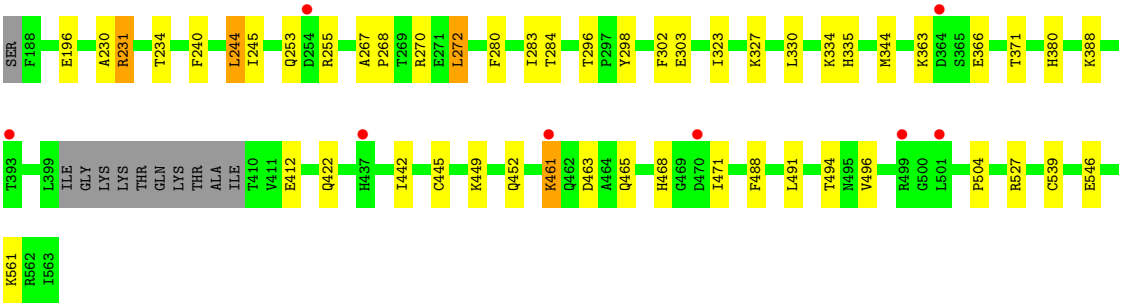
3 Residue-property plots (i)

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

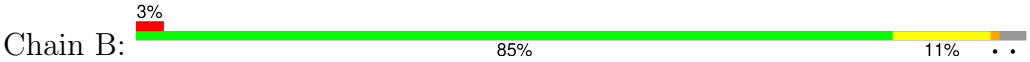
Chain A:

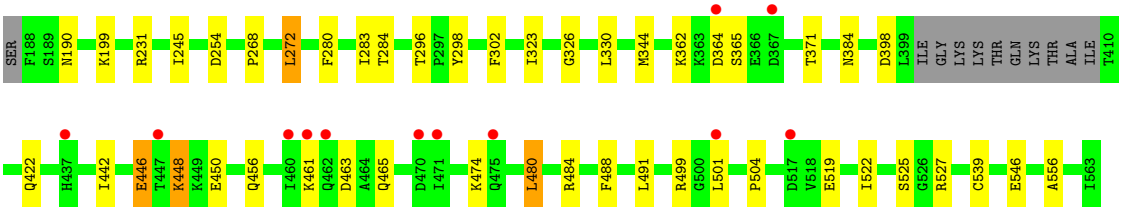




• Molecule 1: Nucleolar RNA helicase 2

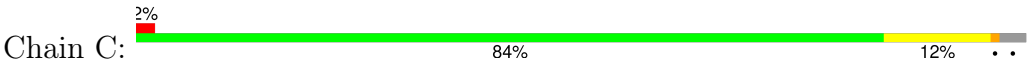
Chain B:

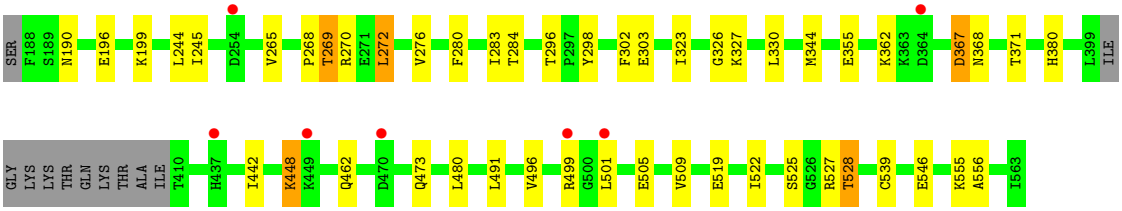




• Molecule 1: Nucleolar RNA helicase 2

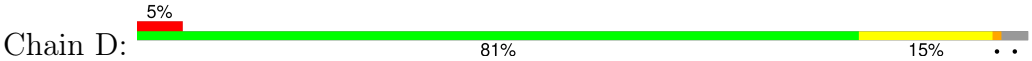
Chain C:

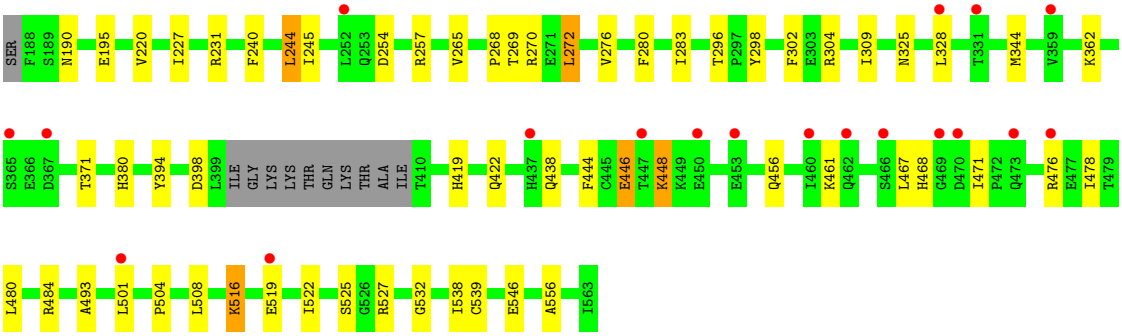




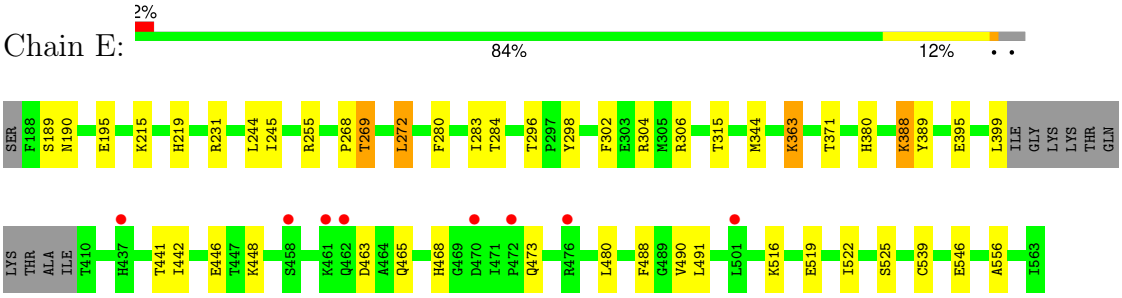
• Molecule 1: Nucleolar RNA helicase 2

Chain D:





• Molecule 1: Nucleolar RNA helicase 2



4 Data and refinement statistics (i)

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) 95.9 (36.51-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [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 (4.97%)	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 , 40.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.49	0/2949	0.68	0/3972
1	B	0.51	0/2949	0.69	0/3972
1	C	0.50	0/2949	0.69	0/3972
1	D	0.49	0/2949	0.69	0/3972
1	E	0.50	0/2949	0.70	0/3972
All	All	0.50	0/14745	0.69	0/19860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2894	0	2926	22	0
1	B	2894	0	2926	17	0
1	C	2894	0	2926	21	0
1	D	2894	0	2926	27	0
1	E	2894	0	2926	17	0
2	A	23	0	12	0	0
2	B	23	0	12	0	0
2	C	23	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	103	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 (103) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:C:496:VAL:HA	1:C:499:ARG:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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
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%)	25 50
1	B	362/377 (96%)	353 (98%)	7 (2%)	2 (1%)	25 50
1	C	362/377 (96%)	352 (97%)	8 (2%)	2 (1%)	25 50
1	D	362/377 (96%)	352 (97%)	10 (3%)	0	100 100
1	E	362/377 (96%)	354 (98%)	5 (1%)	3 (1%)	19 43
All	All	1810/1885 (96%)	1763 (97%)	38 (2%)	9 (0%)	29 54

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
1	C	367	ASP
1	E	255	ARG
1	B	326	GLY
1	C	326	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	314/323 (97%)	295 (94%)	19 (6%)	18 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	314/323 (97%)	292 (93%)	22 (7%)	15 35
1	C	314/323 (97%)	294 (94%)	20 (6%)	17 39
1	D	314/323 (97%)	290 (92%)	24 (8%)	13 30
1	E	314/323 (97%)	292 (93%)	22 (7%)	15 35
All	All	1570/1615 (97%)	1463 (93%)	107 (7%)	16 36

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
1	A	231	ARG
1	A	244	LEU
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	422	GLN
1	A	449	LYS
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	254	ASP
1	B	272	LEU
1	B	296	THR
1	B	362	LYS
1	B	364	ASP
1	B	365	SER
1	B	371	THR
1	B	384	ASN
1	B	398	ASP
1	B	422	GLN

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Mol	Chain	Res	Type
1	B	446	GLU
1	B	448	LYS
1	B	463	ASP
1	B	474	LYS
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	269	THR
1	C	270	ARG
1	C	272	LEU
1	C	296	THR
1	C	303	GLU
1	C	355	GLU
1	C	367	ASP
1	C	371	THR
1	C	380	HIS
1	C	448	LYS
1	C	462	GLN
1	C	473	GLN
1	C	519	GLU
1	C	525	SER
1	C	528	THR
1	C	539	CYS
1	C	546	GLU
1	D	190	ASN
1	D	195	GLU
1	D	231	ARG
1	D	244	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	328	LEU
1	D	362	LYS
1	D	371	THR

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Mol	Chain	Res	Type
1	D	380	HIS
1	D	398	ASP
1	D	438	GLN
1	D	446	GLU
1	D	448	LYS
1	D	478	ILE
1	D	516	LYS
1	D	519	GLU
1	D	525	SER
1	D	539	CYS
1	D	546	GLU
1	E	190	ASN
1	E	195	GLU
1	E	231	ARG
1	E	269	THR
1	E	272	LEU
1	E	296	THR
1	E	304	ARG
1	E	306	ARG
1	E	315	THR
1	E	363	LYS
1	E	371	THR
1	E	380	HIS
1	E	388	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	ASN
1	B	352	GLN
1	B	437	HIS
1	B	475	GLN
1	C	301	GLN

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Mol	Chain	Res	Type
1	C	368	ASN
1	C	495	ASN
1	D	325	ASN
1	D	352	GLN
1	D	422	GLN
1	D	452	GLN
1	D	456	GLN
1	E	274	ASN
1	E	422	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

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	D	601	-	21,25,25	0.74	0	23,38,38	0.82	1 (4%)
2	AMP	A	601	-	21,25,25	0.69	0	23,38,38	0.73	1 (4%)
2	AMP	B	601	-	21,25,25	0.76	0	23,38,38	0.78	1 (4%)
2	AMP	C	601	-	21,25,25	0.65	0	23,38,38	0.77	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	AMP	E	601	-	21,25,25	0.67	0	23,38,38	0.72	1 (4%)

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	D	601	-	-	0/6/26/26	0/3/3/3
2	AMP	A	601	-	-	0/6/26/26	0/3/3/3
2	AMP	B	601	-	-	0/6/26/26	0/3/3/3
2	AMP	C	601	-	-	0/6/26/26	0/3/3/3
2	AMP	E	601	-	-	0/6/26/26	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	AMP	C5-C6-N6	2.20	123.66	120.31
2	D	601	AMP	C5-C6-N6	2.16	123.59	120.31
2	B	601	AMP	C5-C6-N6	2.15	123.58	120.31
2	A	601	AMP	C5-C6-N6	2.08	123.48	120.31
2	E	601	AMP	C5-C6-N6	2.06	123.45	120.31

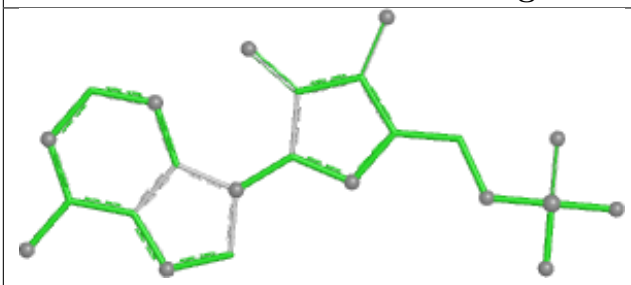
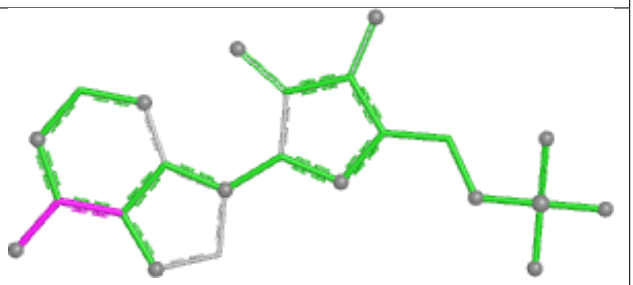
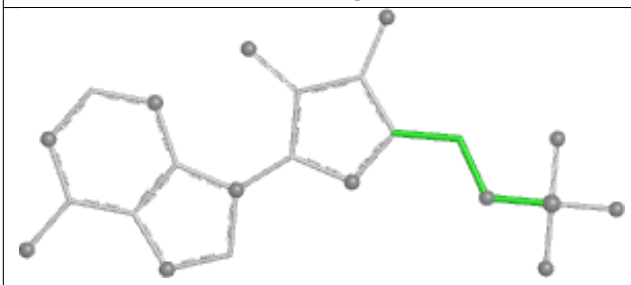
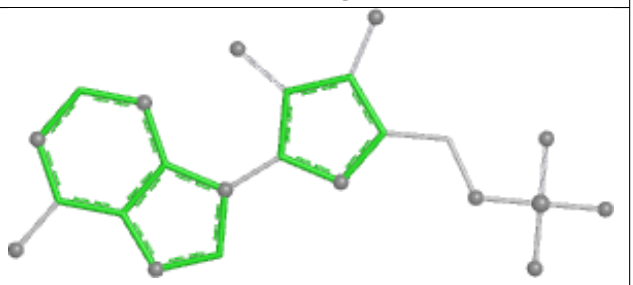
There are no chirality outliers.

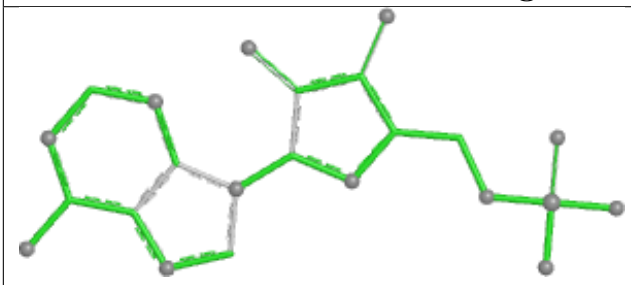
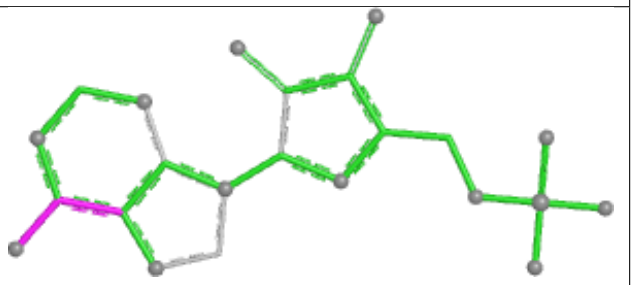
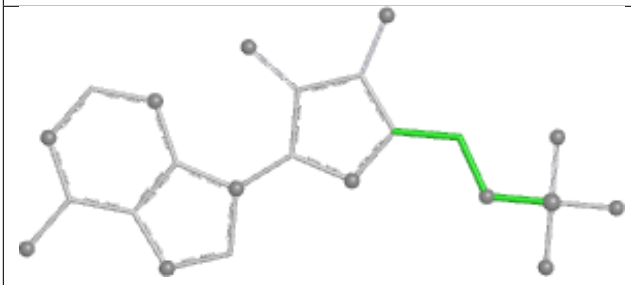
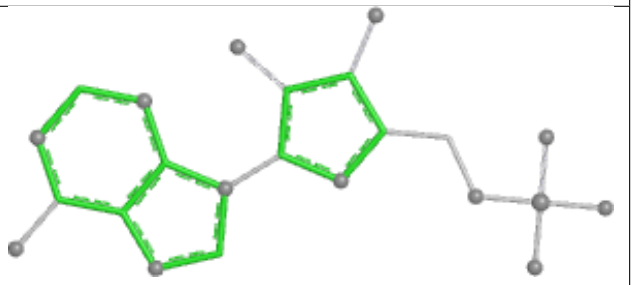
There are no torsion outliers.

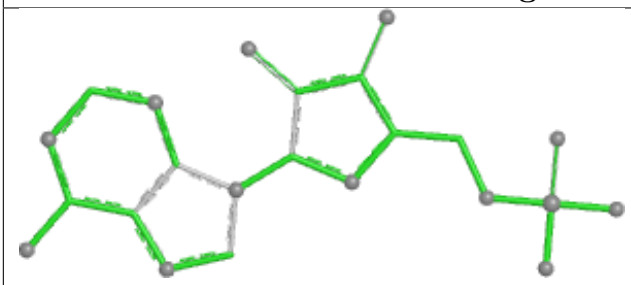
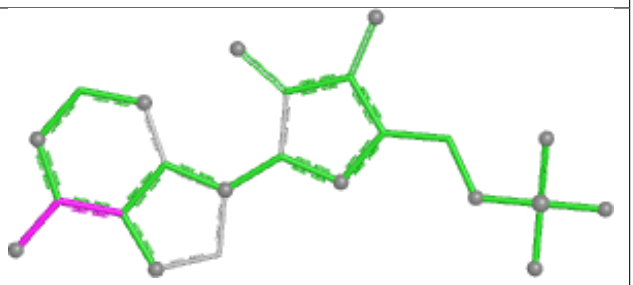
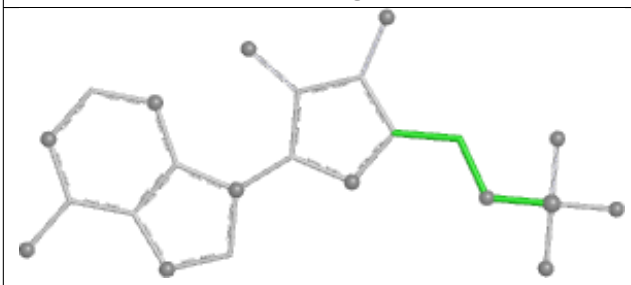
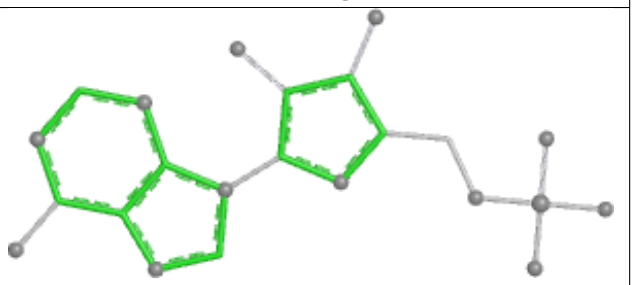
There are no ring outliers.

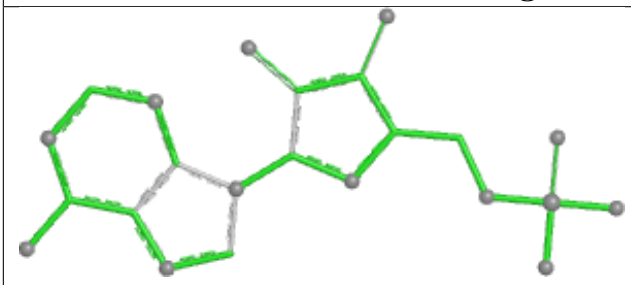
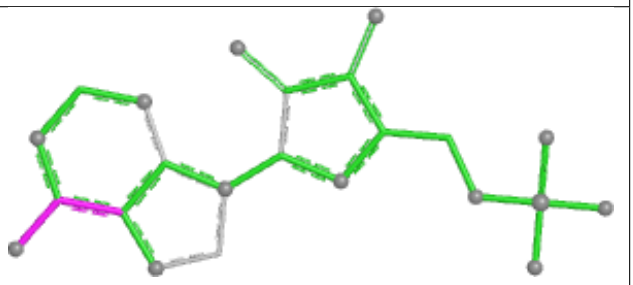
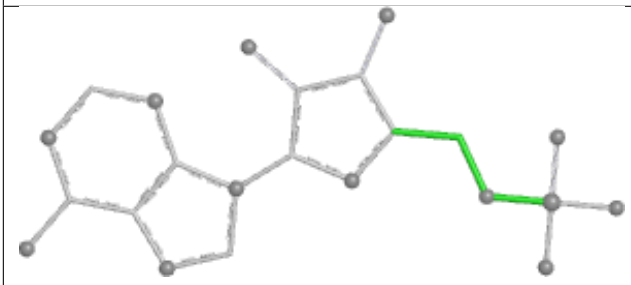
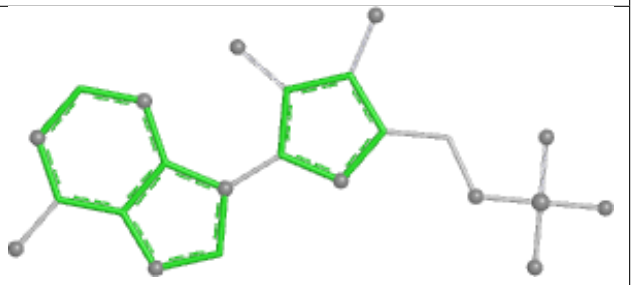
No monomer is involved in short contacts.

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 then 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.

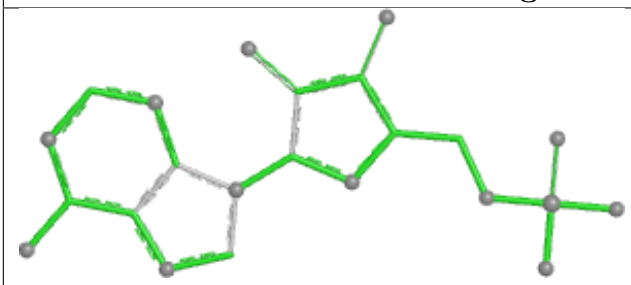
Ligand AMP D 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP A 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

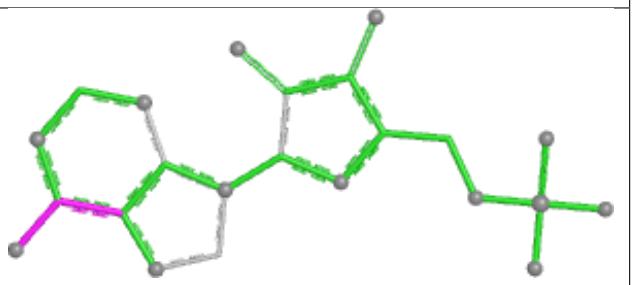
Ligand AMP B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand AMP C 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

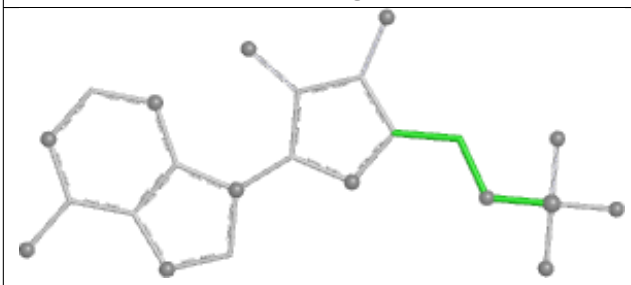
Ligand AMP E 601



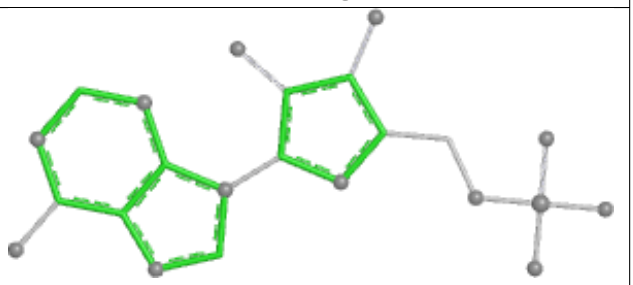
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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%)	0.14	8 (2%)	62 63	4, 23, 54, 73	0
1	B	366/377 (97%)	0.04	12 (3%)	46 46	3, 19, 52, 64	0
1	C	366/377 (97%)	0.04	7 (1%)	66 69	4, 24, 53, 71	0
1	D	366/377 (97%)	0.21	19 (5%)	27 25	3, 25, 56, 68	0
1	E	366/377 (97%)	0.04	8 (2%)	62 63	3, 21, 52, 67	0
All	All	1830/1885 (97%)	0.09	54 (2%)	50 51	3, 23, 54, 73	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	ASP	4.2
1	D	437	HIS	4.1
1	C	470	ASP	4.1
1	A	470	ASP	4.0
1	E	470	ASP	4.0
1	B	437	HIS	4.0
1	D	476	ARG	3.6
1	A	437	HIS	3.5
1	B	462	GLN	3.4
1	E	476	ARG	3.3
1	C	254	ASP	3.3
1	B	470	ASP	3.2
1	C	437	HIS	3.2
1	D	501	LEU	3.2
1	E	472	PRO	3.1
1	D	460	ILE	3.0
1	E	437	HIS	3.0
1	E	501	LEU	3.0
1	E	462	GLN	3.0
1	D	462	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	447	THR	2.7
1	B	364	ASP	2.6
1	A	461	LYS	2.6
1	C	501	LEU	2.6
1	D	367	ASP	2.6
1	B	501	LEU	2.5
1	C	364	ASP	2.5
1	E	461	LYS	2.5
1	B	447	THR	2.5
1	D	469	GLY	2.4
1	A	499	ARG	2.4
1	D	470	ASP	2.4
1	A	393	THR	2.4
1	A	364	ASP	2.4
1	B	367	ASP	2.4
1	D	473	GLN	2.3
1	D	466	SER	2.3
1	B	475	GLN	2.3
1	D	331	THR	2.2
1	D	519	GLU	2.2
1	B	460	ILE	2.2
1	C	499	ARG	2.2
1	D	252	LEU	2.2
1	D	328	LEU	2.1
1	D	450	GLU	2.1
1	D	359	VAL	2.1
1	D	453	GLU	2.1
1	B	461	LYS	2.1
1	E	458	SER	2.1
1	A	501	LEU	2.1
1	D	365	SER	2.1
1	C	449	LYS	2.1
1	B	517	ASP	2.0
1	B	471	ILE	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)

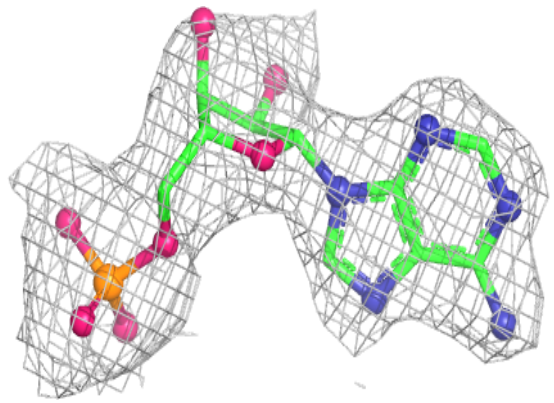
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

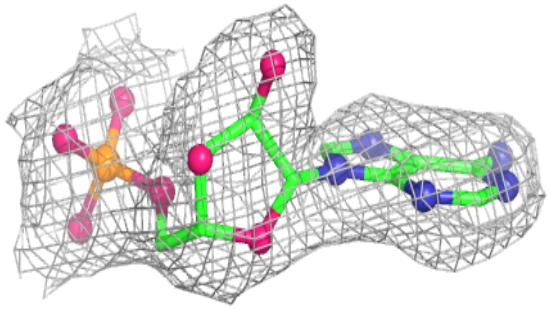
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AMP	C	601	23/23	0.94	0.15	22,29,33,37	0
2	AMP	A	601	23/23	0.95	0.16	4,23,29,30	0
2	AMP	B	601	23/23	0.96	0.13	4,21,30,30	0
2	AMP	D	601	23/23	0.96	0.14	7,23,28,31	0
2	AMP	E	601	23/23	0.96	0.14	6,19,27,28	0

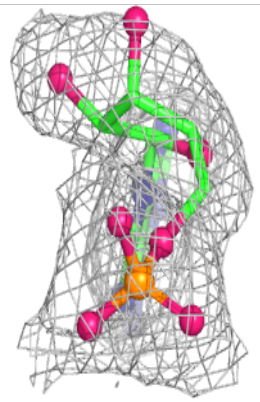
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

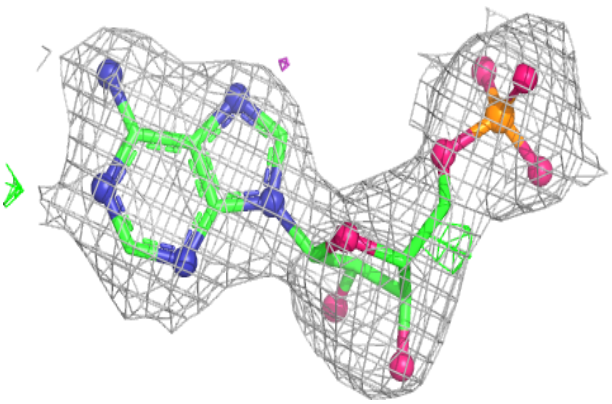


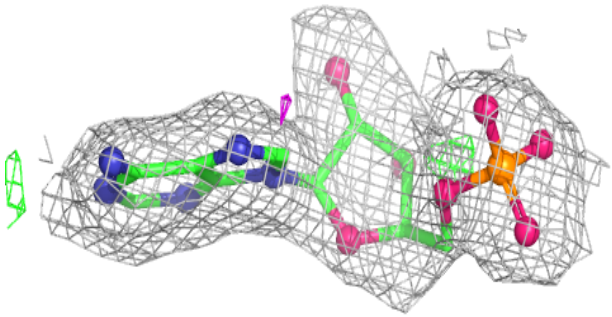


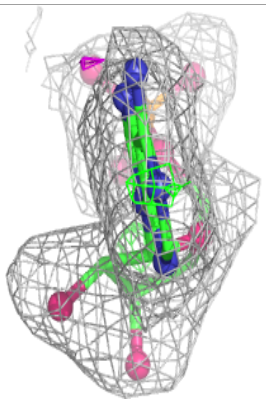


Electron density around AMP A 601:

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

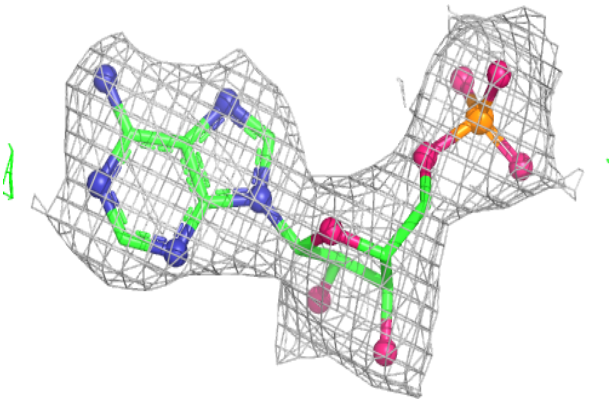


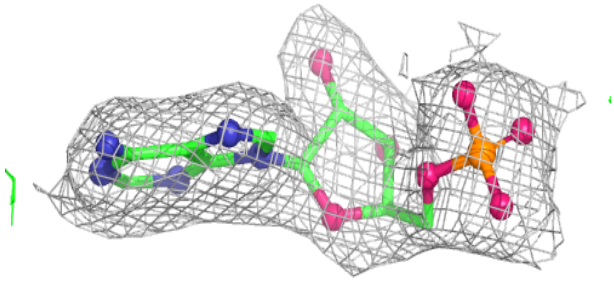


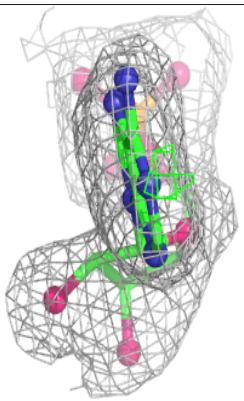


Electron density around AMP B 601:

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

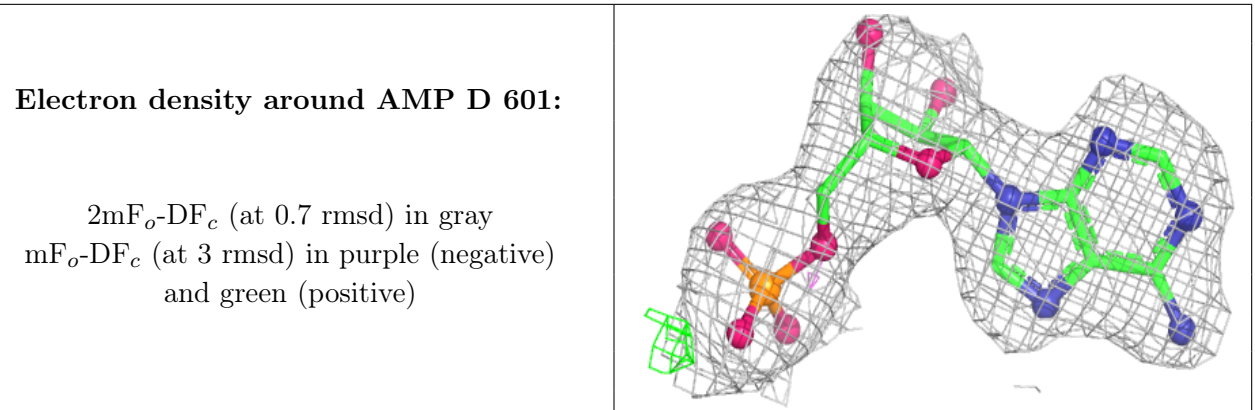


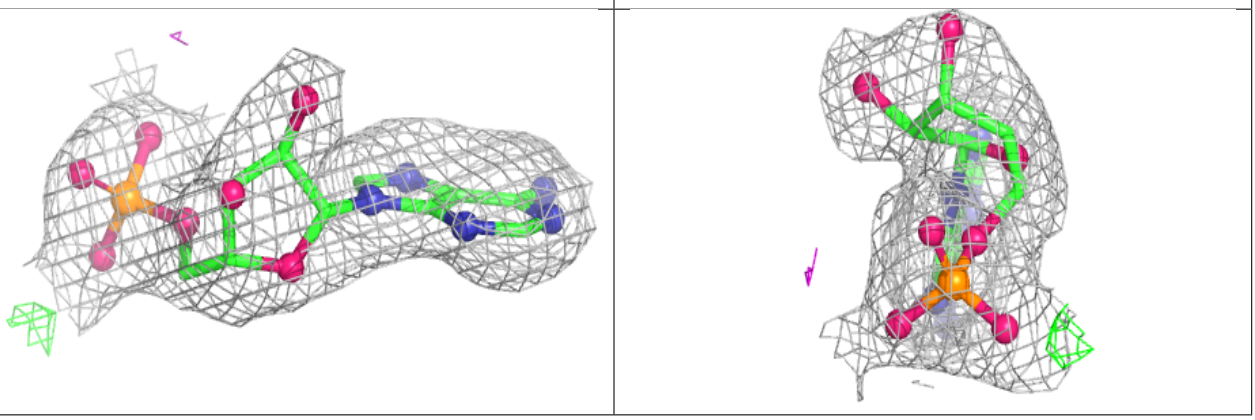




Electron density around AMP D 601:

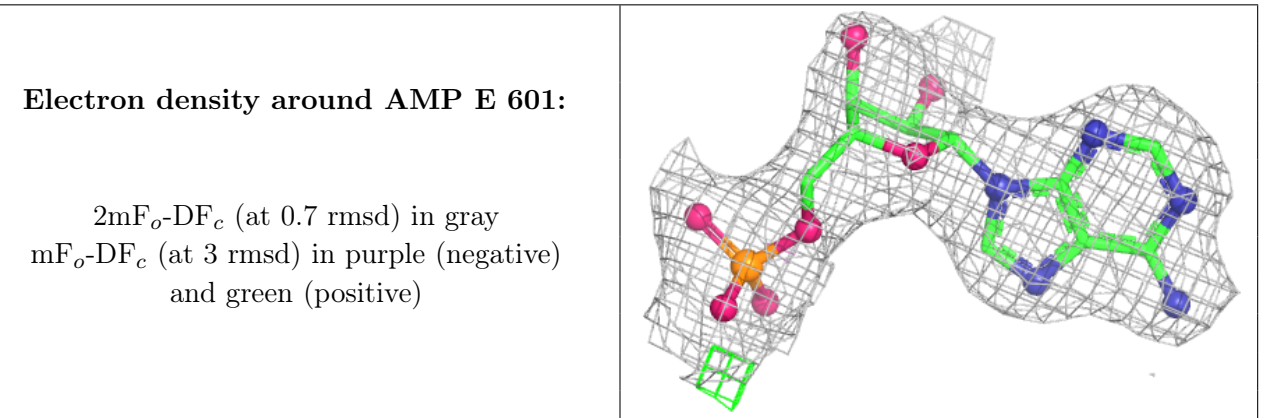
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

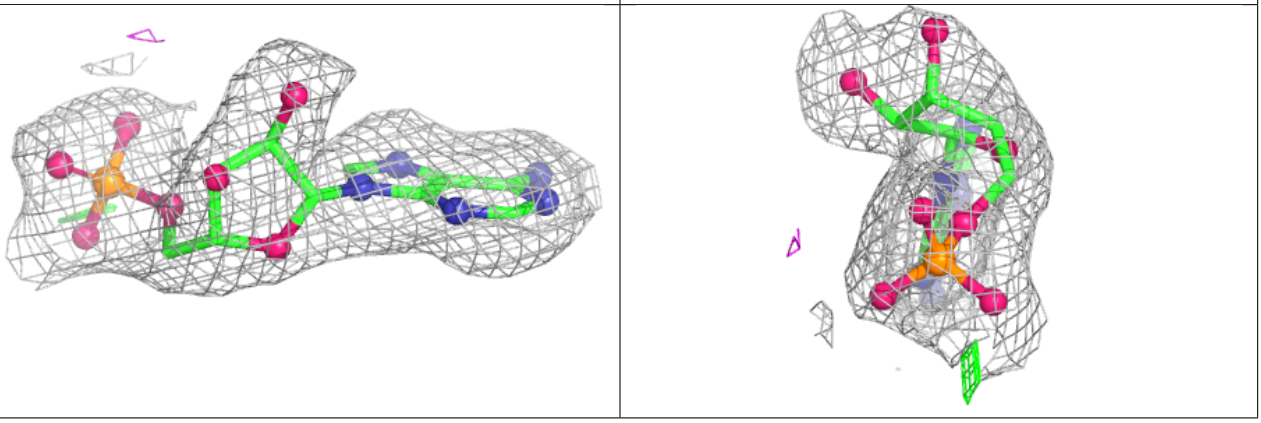




Electron density around AMP E 601:

$2mF_o$-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.