



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:36 AM UTC

PDB ID : 6E4W / pdb_00006e4w
Title : Structure of AMPK bound to activator
Authors : Calabrese, M.F.; Kurumbail, R.G.
Deposited on : 2018-07-18
Resolution : 3.35 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

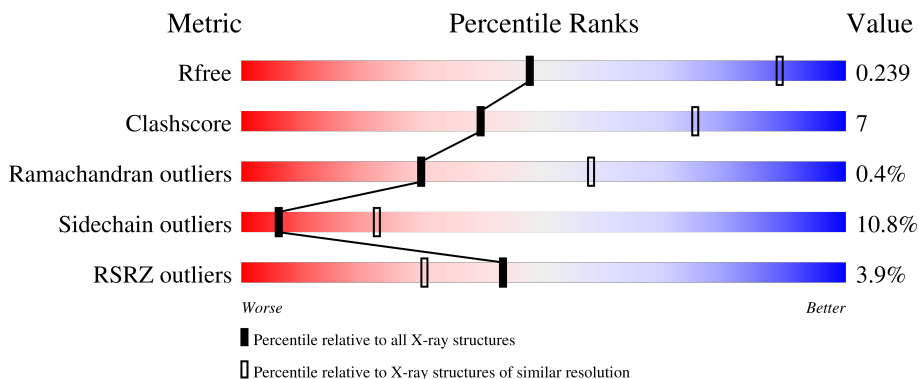
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	503	2% 55% 15% • 28%
2	B	204	3% 58% 19% • 22%
3	C	330	5% 63% 18% • 16%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6498 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 5'-AMP-activated protein kinase catalytic subunit alpha-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	P	S	0	0	0
			2933	1882	510	522	1	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P54645
A	517	ALA	-	linker	UNP P54645
A	518	SER	-	linker	UNP P54645
A	519	GLY	-	linker	UNP P54645
A	520	GLY	-	linker	UNP P54645
A	521	PRO	-	linker	UNP P54645
A	522	GLY	-	linker	UNP P54645
A	523	GLY	-	linker	UNP P54645
A	524	SER	-	linker	UNP P54645

- Molecule 2 is a protein called 5'-AMP-activated protein kinase subunit beta-1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	159	Total	C	N	O	P	S	0	0	0
			1251	812	210	225	1	3			

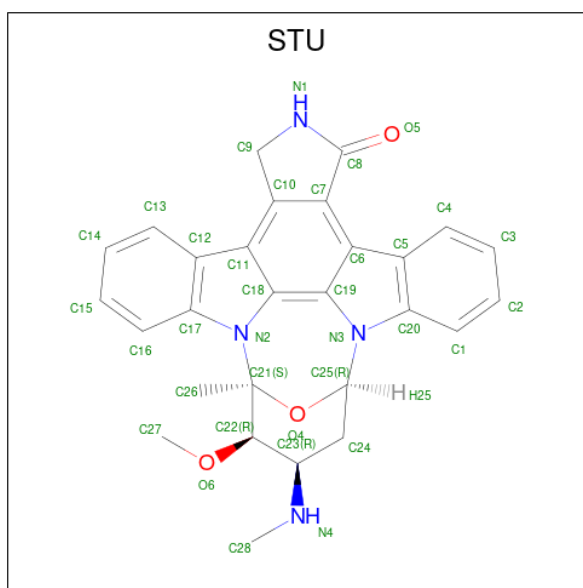
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	67	MET	-	initiating methionine	UNP P80386

- Molecule 3 is a protein called 5'-AMP-activated protein kinase subunit gamma-1.

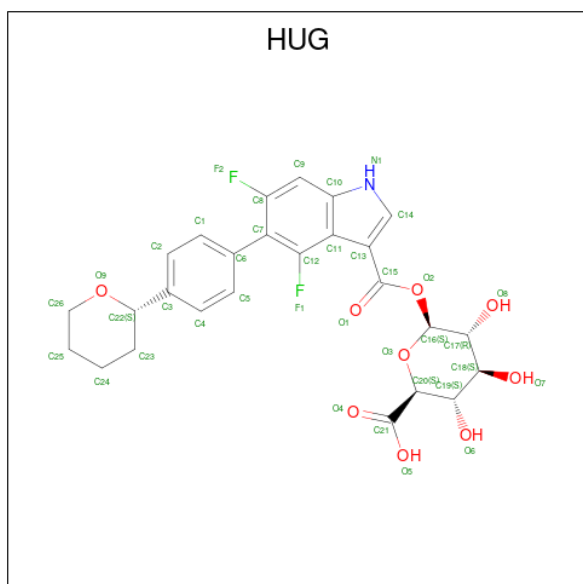
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	278	Total	C	N	O	S	0	0	0
			2160	1400	363	391	6			

- Molecule 4 is STAUROSPORINE (CCD ID: STU) (formula: $C_{28}H_{26}N_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 5 is 1-O-(4,6-difluoro-5-{4-[(2S)-oxan-2-yl]phenyl}-1H-indole-3-carbonyl)-beta-D-glucopyranuronic acid (CCD ID: HUG) (formula: $C_{26}H_{25}F_2NO_9$).

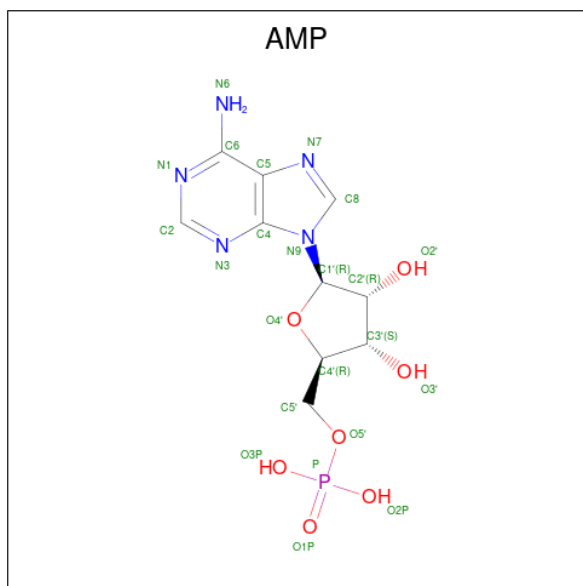


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			38	26	2	1	9		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

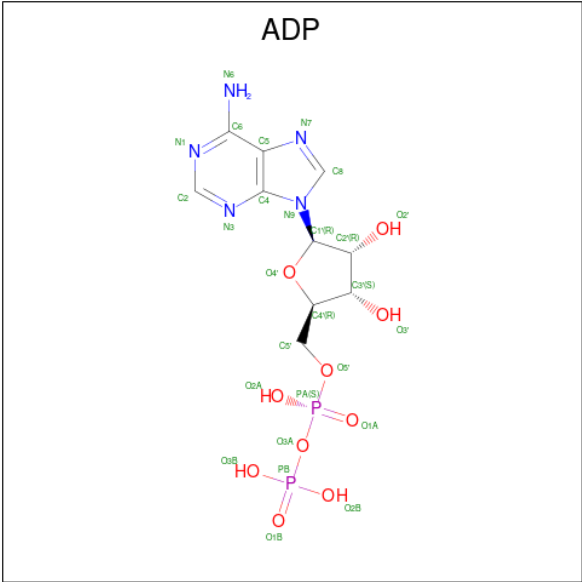
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total Cl 3 3	0	0

- Molecule 7 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



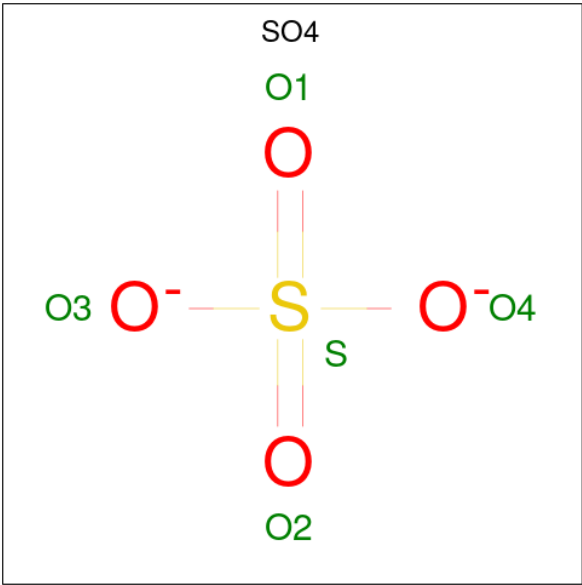
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C N O P 23 10 5 7 1	0	0
7	C	1	Total C N O P 23 10 5 7 1	0	0

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

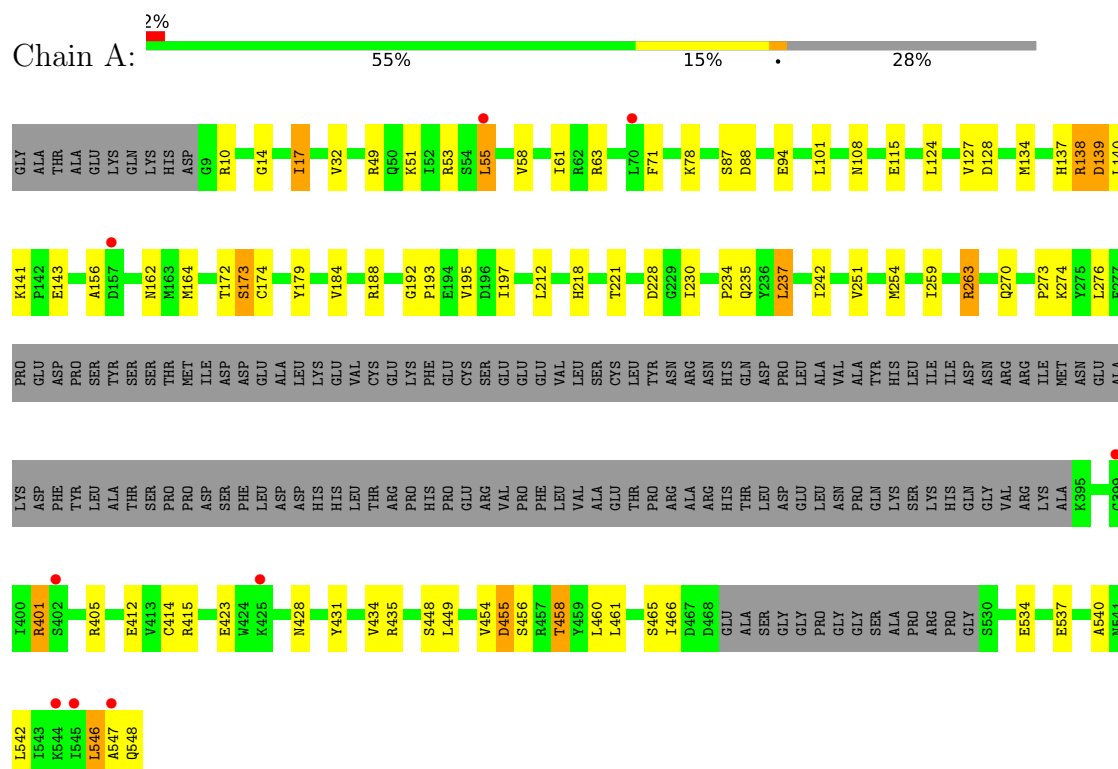


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	O	S	0	0
			5	4	1		

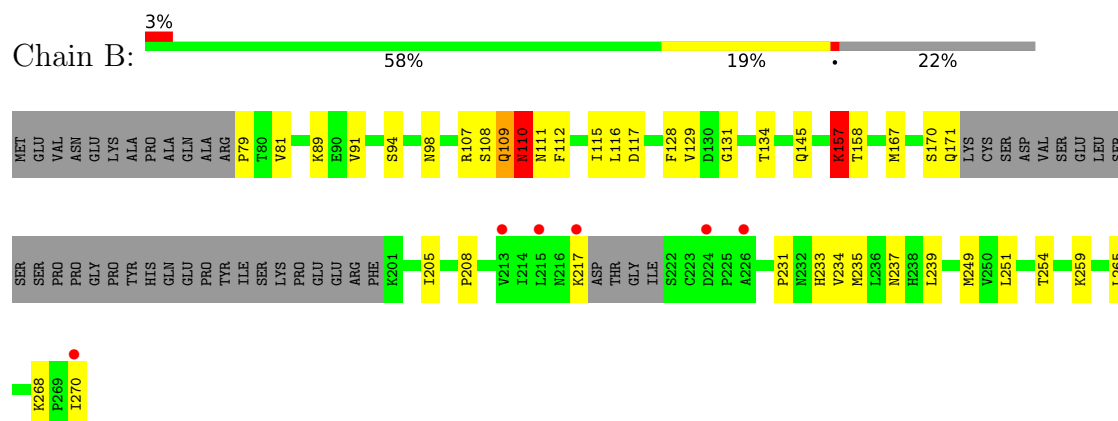
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

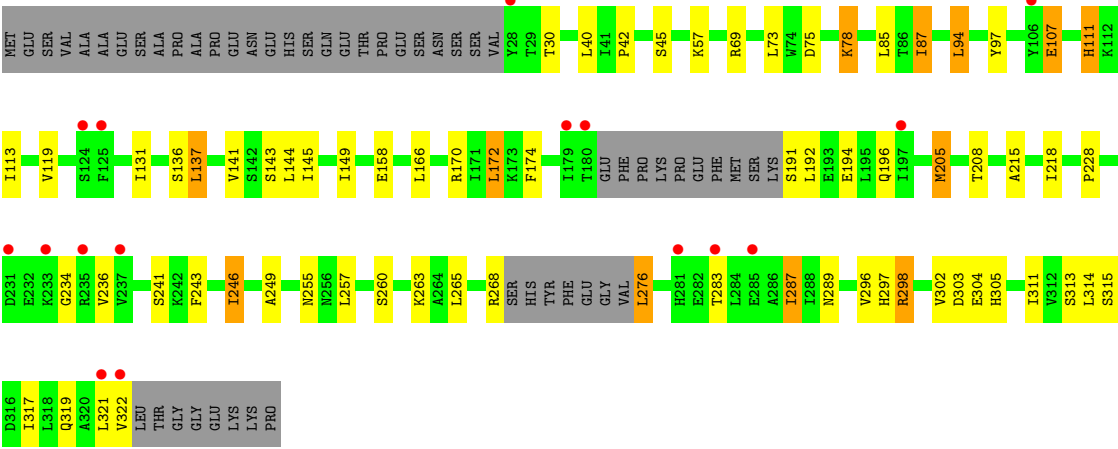
- Molecule 1: 5'-AMP-activated protein kinase catalytic subunit alpha-1



- Molecule 2: 5'-AMP-activated protein kinase subunit beta-1



- Molecule 3: 5'-AMP-activated protein kinase subunit gamma-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.97Å 123.97Å 402.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.58 – 3.35 40.58 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.58-3.35) 99.8 (40.58-3.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.209 , 0.244 0.205 , 0.239	Depositor DCC
R_{free} test set	1369 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.589	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 109.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6498	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HUG, AMP, SEP, ADP, STU, CL, TPO, SO4

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	0.90	0/2987	1.46	25/4029 (0.6%)
2	B	0.91	0/1274	1.34	11/1735 (0.6%)
3	C	0.85	0/2200	1.40	11/2998 (0.4%)
All	All	0.89	0/6461	1.42	47/8762 (0.5%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ALA	CA-C-N	-8.69	110.77	122.85
1	A	156	ALA	C-N-CA	-8.69	110.77	122.85
1	A	108	ASN	N-CA-C	-7.97	98.73	110.52
1	A	55	LEU	N-CA-C	-7.71	97.50	109.76
1	A	273	PRO	CA-C-N	7.58	130.29	120.44
1	A	273	PRO	C-N-CA	7.58	130.29	120.44
1	A	156	ALA	N-CA-C	6.52	121.86	113.18
1	A	139	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	546	LEU	CA-C-N	6.45	132.61	122.17
1	A	546	LEU	C-N-CA	6.45	132.61	122.17
1	A	14	GLY	N-CA-C	-6.28	99.31	110.86
1	A	456	SER	N-CA-C	-6.21	105.71	113.28
2	B	110	ASN	CA-CB-CG	6.08	118.68	112.60
1	A	138	ARG	N-CA-C	-6.00	102.79	110.53
1	A	455	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	17	ILE	CB-CA-C	5.96	118.17	110.96
1	A	547	ALA	N-CA-C	5.93	118.44	108.23
1	A	174	CYS	N-CA-C	5.90	120.13	111.34
2	B	157	LYS	CA-C-N	5.89	128.45	120.38
2	B	157	LYS	C-N-CA	5.89	128.45	120.38
1	A	101	LEU	N-CA-C	-5.89	104.99	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	PHE	CA-CB-CG	5.71	119.50	113.80
3	C	303	ASP	CA-CB-CG	5.69	118.29	112.60
3	C	315	SER	CA-C-N	5.68	127.89	120.28
3	C	315	SER	C-N-CA	5.68	127.89	120.28
2	B	208	PRO	CA-C-N	5.67	128.14	120.38
2	B	208	PRO	C-N-CA	5.67	128.14	120.38
2	B	233	HIS	CA-C-N	5.63	129.36	120.47
2	B	233	HIS	C-N-CA	5.63	129.36	120.47
2	B	110	ASN	CA-C-N	5.54	130.81	123.05
2	B	110	ASN	C-N-CA	5.54	130.81	123.05
2	B	98	ASN	CA-CB-CG	5.44	118.04	112.60
2	B	89	LYS	N-CA-C	-5.33	104.37	111.24
1	A	63	ARG	CA-C-N	5.26	127.59	120.38
1	A	63	ARG	C-N-CA	5.26	127.59	120.38
3	C	145	ILE	CA-C-N	5.25	127.62	120.54
3	C	145	ILE	C-N-CA	5.25	127.62	120.54
3	C	119	VAL	CA-C-N	5.24	128.68	120.82
3	C	119	VAL	C-N-CA	5.24	128.68	120.82
1	A	173	SER	CA-C-N	-5.18	115.38	121.90
1	A	173	SER	C-N-CA	-5.18	115.38	121.90
3	C	249	ALA	CA-C-N	5.18	127.99	120.79
3	C	249	ALA	C-N-CA	5.18	127.99	120.79
1	A	53	ARG	CA-C-N	5.10	127.07	120.44
1	A	53	ARG	C-N-CA	5.10	127.07	120.44
3	C	289	ASN	CA-C-N	5.07	127.03	120.44
3	C	289	ASN	C-N-CA	5.07	127.03	120.44

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	2933	0	2952	37	0
2	B	1251	0	1242	15	0
3	C	2160	0	2175	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	26	8	0
5	A	38	0	0	0	0
6	A	3	0	0	0	0
7	C	46	0	24	3	0
8	C	27	0	12	1	0
9	C	5	0	0	0	0
All	All	6498	0	6431	86	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 7.

All (86) 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)
4:A:601:STU:H283	4:A:601:STU:H272	1.09	1.05
1:A:263:ARG:HH11	1:A:263:ARG:HG3	1.14	1.05
4:A:601:STU:H283	4:A:601:STU:C27	1.91	1.00
4:A:601:STU:H272	4:A:601:STU:C28	1.93	0.98
1:A:218:HIS:CD2	1:A:221:THR:HG23	2.04	0.93
1:A:218:HIS:HD2	1:A:221:THR:HG23	1.35	0.91
3:C:97:TYR:CG	3:C:107:GLU:HG3	2.06	0.90
3:C:97:TYR:CD1	3:C:107:GLU:HG3	2.13	0.84
4:A:601:STU:H261	4:A:601:STU:H16	1.60	0.81
1:A:263:ARG:HG3	1:A:263:ARG:NH1	1.92	0.80
3:C:107:GLU:O	3:C:111:HIS:HB2	1.83	0.77
3:C:87:ILE:HG23	3:C:246:ILE:HG23	1.71	0.73
3:C:265:LEU:HD22	3:C:268:ARG:HH21	1.57	0.69
3:C:40:LEU:HD21	3:C:174:PHE:HB2	1.76	0.68
1:A:263:ARG:HH11	1:A:263:ARG:CG	1.98	0.68
2:B:91:VAL:HG22	2:B:129:VAL:HG13	1.83	0.60
3:C:107:GLU:CD	3:C:107:GLU:H	2.08	0.60
1:A:197:ILE:HD11	1:A:259:ILE:HG13	1.83	0.60
3:C:298:ARG:HB2	3:C:313:SER:HA	1.85	0.59
1:A:188:ARG:HB3	2:B:205:ILE:HD11	1.86	0.58
2:B:81:VAL:HG22	2:B:115:ILE:HG12	1.86	0.58
1:A:78:LYS:H	1:A:94:GLU:HG2	1.70	0.57
3:C:97:TYR:CG	3:C:107:GLU:CG	2.85	0.57
3:C:243:PHE:HB3	7:C:402:AMP:H5'1	1.86	0.57
3:C:241:SER:OG	7:C:402:AMP:H5'2	2.05	0.56
3:C:40:LEU:HD22	3:C:170:ARG:HG3	1.89	0.55
1:A:540:ALA:HB2	2:B:251:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:SER:H	3:C:263:LYS:HD2	1.71	0.55
1:A:401:ARG:O	1:A:548:GLN:HB3	2.07	0.54
2:B:79:PRO:HA	2:B:117:ASP:HA	1.89	0.54
1:A:228:ASP:HB3	1:A:230:ILE:HD12	1.90	0.54
3:C:42:PRO:HG2	3:C:45:SER:HB3	1.91	0.52
1:A:141:LYS:HG3	1:A:143:GLU:HB2	1.91	0.51
3:C:215:ALA:HA	3:C:218:ILE:HD12	1.93	0.51
3:C:75:ASP:HB3	3:C:78:LYS:HB2	1.92	0.50
1:A:127:VAL:HG22	1:A:140:LEU:HD21	1.94	0.50
2:B:91:VAL:HG13	2:B:129:VAL:HG22	1.94	0.50
3:C:205:MET:HB3	3:C:228:PRO:HD2	1.92	0.50
4:A:601:STU:H261	4:A:601:STU:C16	2.29	0.49
1:A:465:SER:HB3	2:B:237:ASN:HB3	1.95	0.49
3:C:69:ARG:HG2	3:C:87:ILE:HD11	1.95	0.49
1:A:423:GLU:HB2	1:A:435:ARG:HB3	1.95	0.48
1:A:137:HIS:HE1	1:A:139:ASP:O	1.96	0.48
3:C:40:LEU:HD12	3:C:137:LEU:HD11	1.95	0.48
3:C:73:LEU:HD21	3:C:85:LEU:HB2	1.94	0.48
1:A:448:SER:HB3	1:A:466:ILE:HD11	1.96	0.47
1:A:134:MET:HA	1:A:164:MET:HE3	1.95	0.47
1:A:143:GLU:O	4:A:601:STU:H281	2.14	0.47
3:C:107:GLU:CD	3:C:107:GLU:N	2.73	0.47
2:B:249:MET:HE3	2:B:270:ILE:HG21	1.97	0.47
1:A:234:PRO:HD2	1:A:237:LEU:HD22	1.96	0.46
3:C:144:LEU:HD23	3:C:149:ILE:HG23	1.98	0.46
3:C:149:ILE:HD11	8:C:403:ADP:C8	2.51	0.46
1:A:173:SER:HA	1:A:184:VAL:HG13	1.97	0.46
1:A:428:ASN:H	1:A:431:TYR:HB3	1.79	0.46
2:B:109:GLN:C	2:B:111:ASN:H	2.23	0.45
1:A:455:ASP:HB2	1:A:458:THR:HG22	1.98	0.45
3:C:172:LEU:HD13	3:C:314:LEU:HG	1.99	0.45
1:A:537:GLU:HG2	2:B:268:LYS:HE3	2.00	0.44
3:C:137:LEU:O	3:C:141:VAL:HG23	2.17	0.44
1:A:412:GLU:HG2	1:A:415:ARG:HH21	1.82	0.44
1:A:179:TYR:OH	1:A:212:LEU:HD21	2.18	0.44
1:A:449:LEU:HB3	1:A:461:LEU:HD11	1.99	0.43
4:A:601:STU:C16	4:A:601:STU:C26	2.95	0.43
1:A:193:PRO:O	1:A:197:ILE:HG12	2.17	0.43
2:B:145:GLN:H	2:B:145:GLN:CD	2.26	0.43
1:A:192:GLY:O	1:A:195:VAL:HG22	2.18	0.43
1:A:51:LYS:O	1:A:55:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HB3	1:A:242:ILE:HD11	2.02	0.42
2:B:107:ARG:HB2	2:B:112:PHE:CE2	2.54	0.42
3:C:73:LEU:HD22	3:C:113:ILE:HG21	2.01	0.41
2:B:128:PHE:CZ	2:B:131:GLY:HA2	2.55	0.41
3:C:192:LEU:HD13	3:C:287:ILE:HD13	2.02	0.41
3:C:297:HIS:HA	3:C:314:LEU:HD22	2.03	0.41
2:B:157:LYS:H	2:B:157:LYS:HG2	1.52	0.41
1:A:128:ASP:HB2	1:A:259:ILE:HG21	2.02	0.41
1:A:78:LYS:N	1:A:94:GLU:HG2	2.33	0.41
1:A:259:ILE:O	1:A:263:ARG:HB2	2.21	0.41
3:C:191:SER:HA	3:C:283:THR:HA	2.02	0.41
1:A:138:ARG:CZ	1:A:162:ASN:HB2	2.51	0.41
2:B:231:PRO:HG3	2:B:254:THR:HG21	2.03	0.41
3:C:276:LEU:HB2	7:C:402:AMP:N1	2.36	0.41
1:A:138:ARG:NH2	1:A:162:ASN:HB2	2.37	0.40
3:C:276:LEU:HD13	3:C:296:VAL:HG21	2.03	0.40
1:A:143:GLU:O	4:A:601:STU:C28	2.69	0.40
3:C:94:LEU:HG	3:C:257:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

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	A	355/503 (71%)	336 (95%)	19 (5%)	0	100	100
2	B	152/204 (74%)	139 (91%)	11 (7%)	2 (1%)	9	32
3	C	272/330 (82%)	256 (94%)	15 (6%)	1 (0%)	30	58
All	All	779/1037 (75%)	731 (94%)	45 (6%)	3 (0%)	30	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	234	GLY
2	B	110	ASN
2	B	170	SER

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	323/448 (72%)	295 (91%)	28 (9%)	9	32
2	B	137/184 (74%)	122 (89%)	15 (11%)	6	22
3	C	235/299 (79%)	203 (86%)	32 (14%)	3	15
All	All	695/931 (75%)	620 (89%)	75 (11%)	6	22

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	17	ILE
1	A	32	VAL
1	A	49	ARG
1	A	58	VAL
1	A	61	ILE
1	A	87	SER
1	A	88	ASP
1	A	115	GLU
1	A	124	LEU
1	A	235	GLN
1	A	237	LEU
1	A	251	VAL
1	A	254	MET
1	A	263	ARG
1	A	270	GLN
1	A	274	LYS
1	A	276	LEU
1	A	401	ARG
1	A	405	ARG

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Mol	Chain	Res	Type
1	A	414	CYS
1	A	434	VAL
1	A	454	VAL
1	A	458	THR
1	A	460	LEU
1	A	534	GLU
1	A	542	LEU
1	A	546	LEU
2	B	94	SER
2	B	109	GLN
2	B	110	ASN
2	B	116	LEU
2	B	134	THR
2	B	157	LYS
2	B	158	THR
2	B	167	MET
2	B	171	GLN
2	B	217	LYS
2	B	234	VAL
2	B	235	MET
2	B	239	LEU
2	B	259	LYS
2	B	265	LEU
3	C	30	THR
3	C	57	LYS
3	C	78	LYS
3	C	87	ILE
3	C	94	LEU
3	C	107	GLU
3	C	111	HIS
3	C	131	ILE
3	C	136	SER
3	C	137	LEU
3	C	143	SER
3	C	158	GLU
3	C	166	LEU
3	C	172	LEU
3	C	194	GLU
3	C	196	GLN
3	C	205	MET
3	C	208	THR
3	C	236	VAL

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Mol	Chain	Res	Type
3	C	246	ILE
3	C	255	ASN
3	C	276	LEU
3	C	287	ILE
3	C	298	ARG
3	C	302	VAL
3	C	304	GLU
3	C	305	HIS
3	C	311	ILE
3	C	317	ILE
3	C	319	GLN
3	C	321	LEU
3	C	322	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	A	428	ASN
1	A	541	ASN
2	B	98	ASN
2	B	154	GLN
2	B	233	HIS
3	C	92	ASN
3	C	111	HIS
3	C	168	HIS
3	C	221	GLN
3	C	247	ASN
3	C	255	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	SEP	B	108	2	8,9,10	1.27	1 (12%)	7,12,14	3.68	3 (42%)
1	TPO	A	172	1	8,10,11	1.31	1 (12%)	10,14,16	1.92	3 (30%)

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	SEP	B	108	2	-	6/6/8/10	-
1	TPO	A	172	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	TPO	P-OG1	-3.35	1.53	1.59
2	B	108	SEP	P-OG	-2.65	1.52	1.60

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	SEP	OG-CB-CA	7.67	115.61	108.14
2	B	108	SEP	O3P-P-OG	4.22	117.68	106.67
1	A	172	TPO	O3P-P-O2P	3.84	122.19	107.80
2	B	108	SEP	O2P-P-O1P	-3.60	96.82	110.83
1	A	172	TPO	O3P-P-O1P	-2.72	100.22	110.83
1	A	172	TPO	P-OG1-CB	-2.64	116.16	123.33

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	108	SEP	N-CA-CB-OG
2	B	108	SEP	C-CA-CB-OG
2	B	108	SEP	CB-OG-P-O2P
2	B	108	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
2	B	108	SEP	CB-OG-P-O1P
2	B	108	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
9	SO4	C	404	-	4,4,4	0.25	0	6,6,6	0.25	0
7	AMP	C	401	-	25,25,25	0.18	0	37,38,38	0.39	0
8	ADP	C	403	-	28,29,29	0.45	0	43,45,45	0.70	1 (2%)
5	HUG	A	602	-	42,42,42	0.85	1 (2%)	57,62,62	0.94	2 (3%)
4	STU	A	601	-	39,42,42	2.53	14 (35%)	50,68,68	2.74	17 (34%)
7	AMP	C	402	-	25,25,25	0.31	0	37,38,38	0.80	1 (2%)

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
7	AMP	C	401	-	-	3/10/26/26	0/3/3/3
8	ADP	C	403	-	-	1/16/32/32	0/3/3/3
5	HUG	A	602	-	-	4/20/48/48	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	STU	A	601	-	-	2/4/42/42	-
7	AMP	C	402	-	-	3/10/26/26	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	STU	C12-C17	5.21	1.49	1.41
4	A	601	STU	C9-C10	-5.10	1.46	1.50
4	A	601	STU	C5-C20	5.07	1.48	1.41
4	A	601	STU	C11-C10	4.87	1.49	1.40
4	A	601	STU	C6-C7	4.70	1.49	1.40
4	A	601	STU	C7-C10	4.34	1.47	1.39
4	A	601	STU	C19-C18	4.10	1.49	1.40
4	A	601	STU	C25-N3	3.67	1.48	1.45
4	A	601	STU	C11-C18	3.56	1.48	1.41
4	A	601	STU	C18-N2	-3.53	1.36	1.40
4	A	601	STU	C9-N1	3.36	1.49	1.45
4	A	601	STU	C6-C19	2.92	1.46	1.41
4	A	601	STU	O5-C8	2.42	1.29	1.23
4	A	601	STU	C17-N2	-2.40	1.37	1.40
5	A	602	HUG	C7-C6	-2.09	1.46	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C11-C10-C7	-7.13	116.56	121.25
4	A	601	STU	C18-N2-C17	5.60	114.14	107.37
4	A	601	STU	C28-N4-C23	5.44	120.88	114.39
4	A	601	STU	C12-C17-N2	-5.41	105.39	108.94
4	A	601	STU	C6-C7-C10	5.36	124.50	120.76
4	A	601	STU	C9-C10-C11	5.22	132.69	128.73
4	A	601	STU	C16-C17-N2	5.00	137.72	130.22
4	A	601	STU	C10-C7-C8	-4.51	104.32	108.09
4	A	601	STU	C1-C20-C5	-4.27	116.59	121.59
4	A	601	STU	C16-C17-C12	-4.02	116.89	121.59
4	A	601	STU	C7-C8-N1	3.98	110.18	106.38
7	C	402	AMP	O2P-P-O5'	3.56	115.95	106.67
4	A	601	STU	C4-C5-C20	3.40	123.17	119.24
4	A	601	STU	C13-C12-C17	3.07	122.79	119.24
4	A	601	STU	C1-C20-N3	2.88	134.65	129.73
4	A	601	STU	C9-N1-C8	-2.77	111.34	113.86
4	A	601	STU	O5-C8-C7	-2.44	124.92	128.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C9-C10-C7	2.36	110.75	109.88
5	A	602	HUG	O4-C21-C20	2.11	128.41	120.81
5	A	602	HUG	C13-C14-N1	-2.09	108.80	110.22
8	C	403	ADP	O2B-PB-O3A	2.05	111.51	104.64

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	STU	C22-C23-N4-C28
7	C	401	AMP	C5'-O5'-P-O2P
7	C	401	AMP	C5'-O5'-P-O3P
7	C	402	AMP	C5'-O5'-P-O2P
7	C	402	AMP	C5'-O5'-P-O3P
7	C	401	AMP	C5'-O5'-P-O1P
7	C	402	AMP	C5'-O5'-P-O1P
8	C	403	ADP	C5'-O5'-PA-O1A
5	A	602	HUG	C23-C22-C3-C4
4	A	601	STU	C24-C23-N4-C28
5	A	602	HUG	C23-C22-C3-C2
5	A	602	HUG	O9-C22-C3-C2
5	A	602	HUG	O9-C22-C3-C4

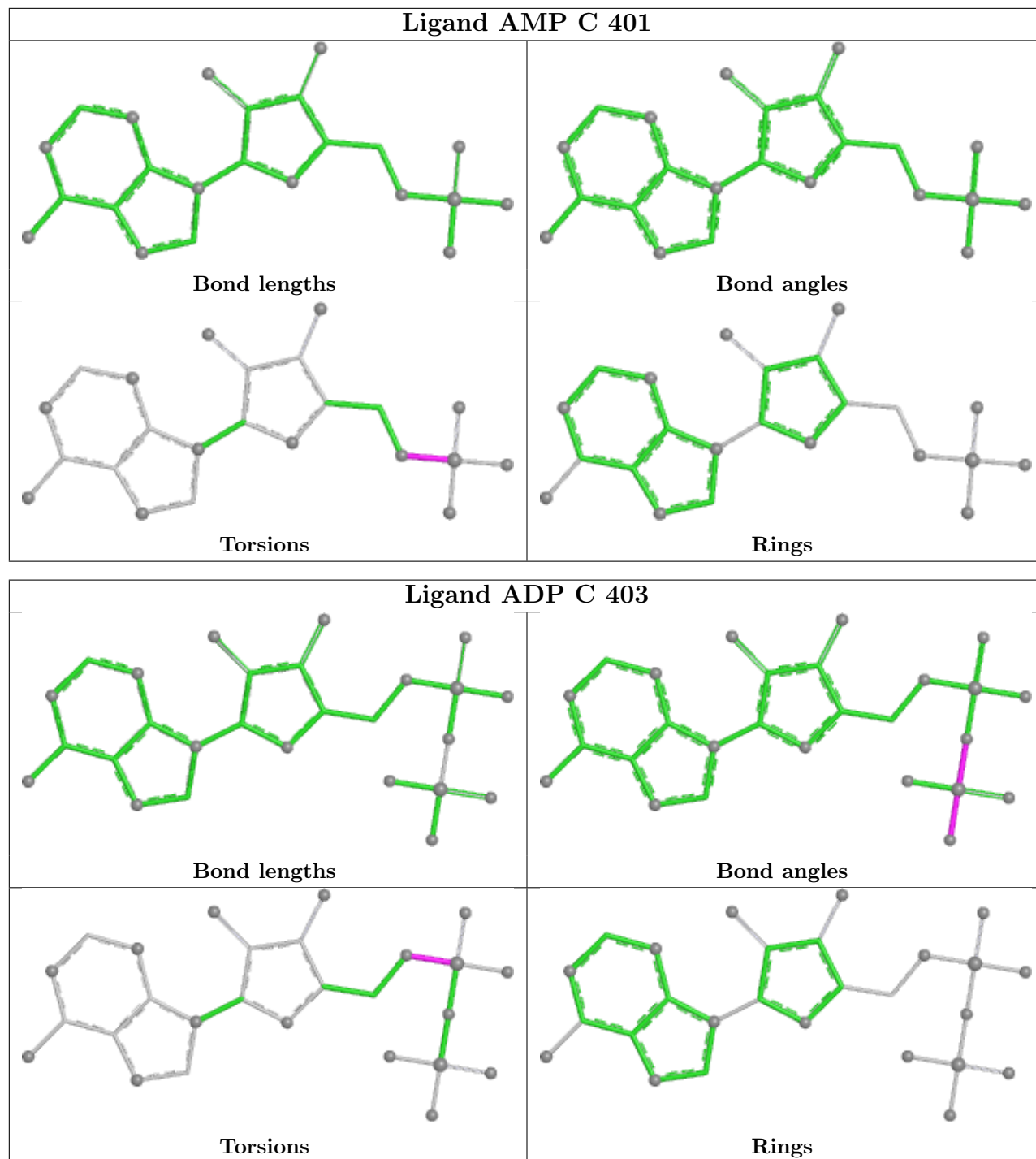
There are no ring outliers.

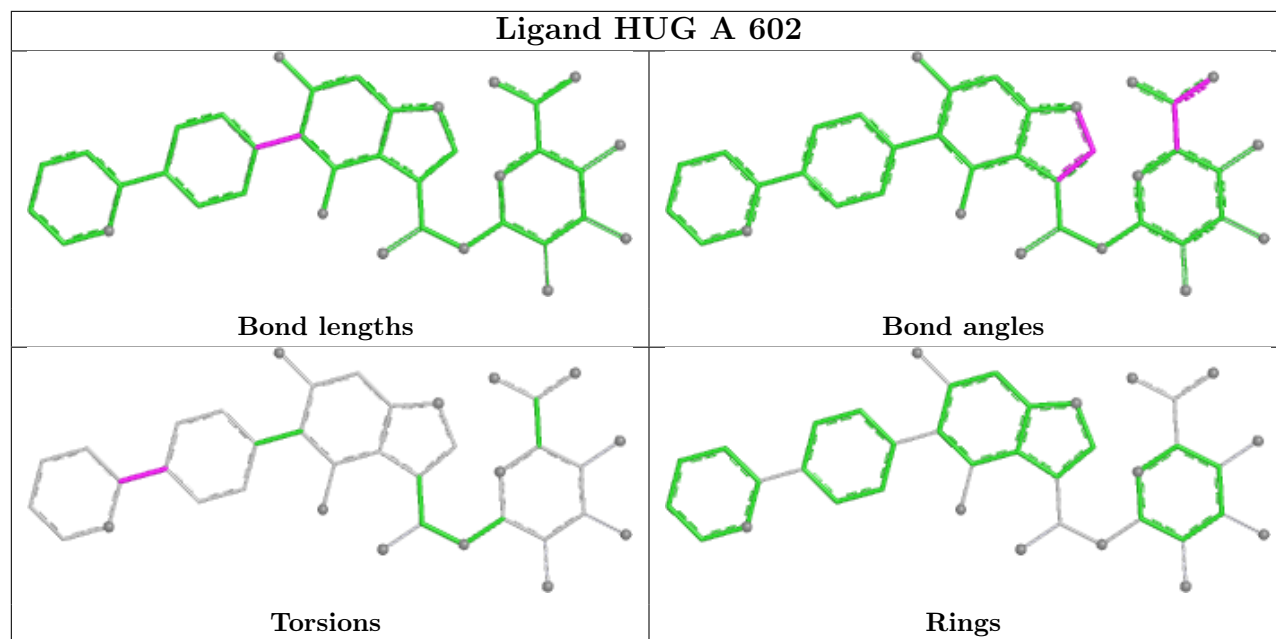
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	403	ADP	1	0
4	A	601	STU	8	0
7	C	402	AMP	3	0

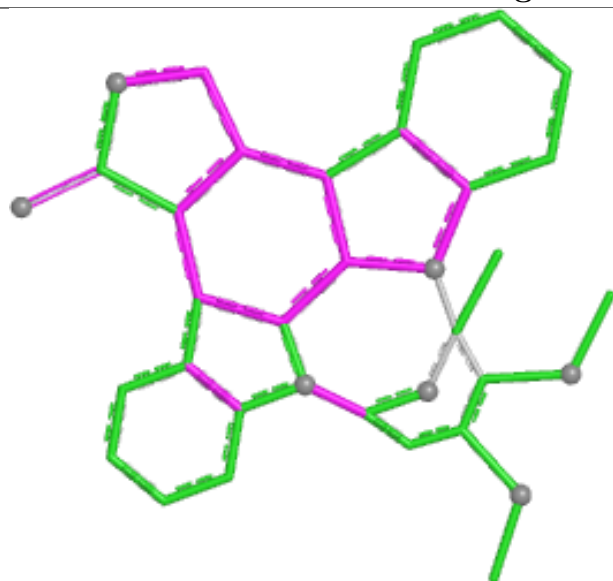
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

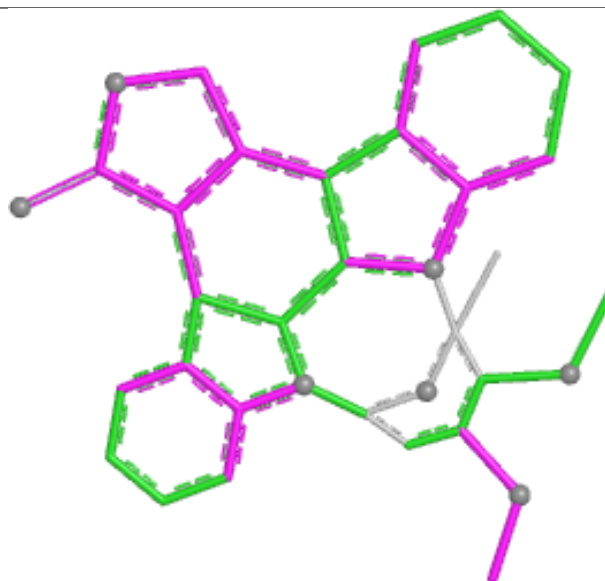




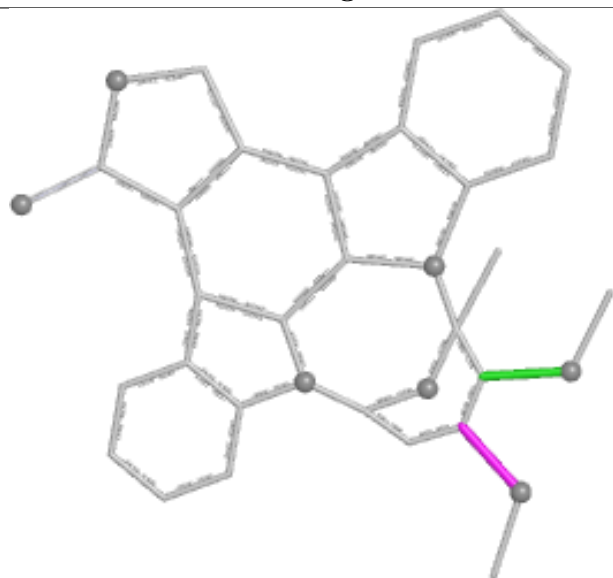
Ligand STU A 601



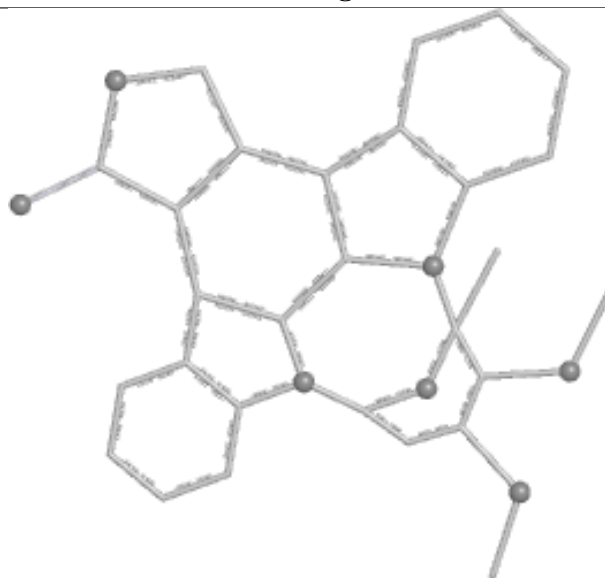
Bond lengths



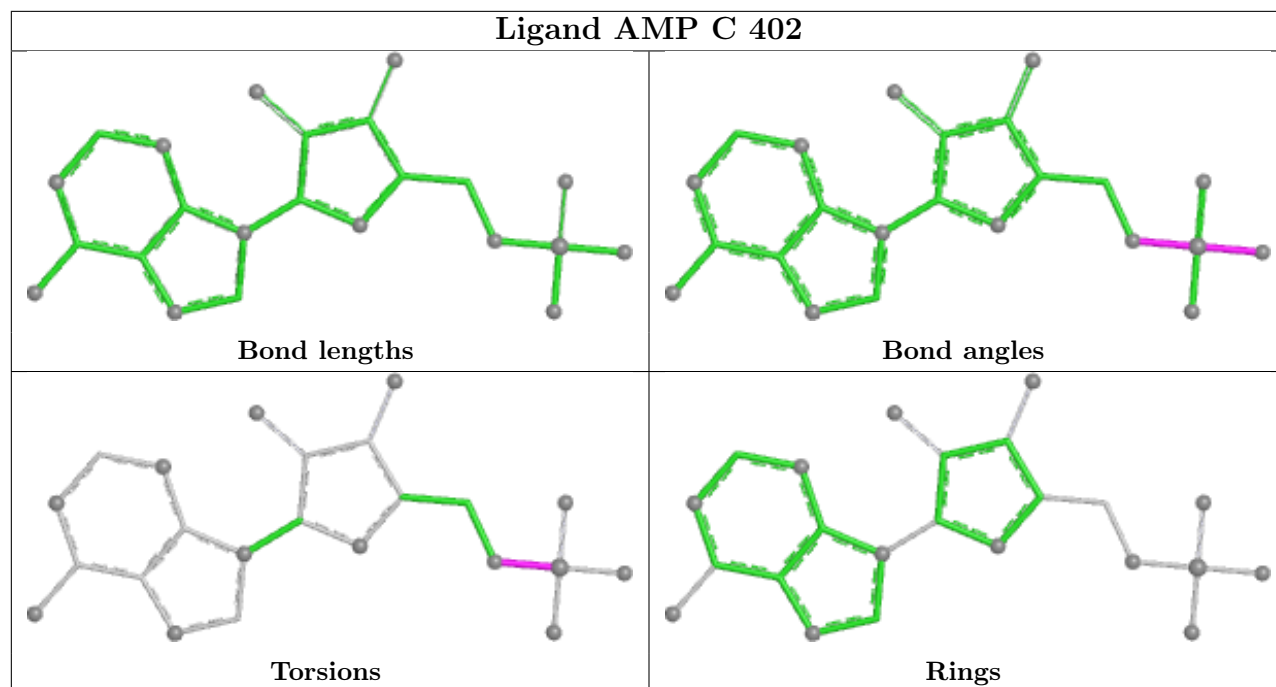
Bond angles



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, 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	361/503 (71%)	-0.06	9 (2%) 58 43	58, 86, 197, 215	0
2	B	158/204 (77%)	0.13	6 (3%) 44 31	71, 101, 147, 167	0
3	C	278/330 (84%)	0.22	16 (5%) 29 21	83, 129, 200, 210	0
All	All	797/1037 (76%)	0.08	31 (3%) 43 30	58, 105, 196, 215	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	ALA	3.7
3	C	285	GLU	3.6
3	C	179	ILE	3.4
3	C	106	TYR	3.3
2	B	226	ALA	3.3
3	C	231	ASP	3.2
1	A	70	LEU	3.1
3	C	322	VAL	3.0
3	C	321	LEU	3.0
1	A	399	GLY	2.8
3	C	28	TYR	2.6
3	C	124	SER	2.6
1	A	55	LEU	2.5
3	C	235	ARG	2.5
2	B	224	ASP	2.4
3	C	283	THR	2.4
1	A	402	SER	2.4
3	C	197	ILE	2.4
3	C	233	LYS	2.4
2	B	270	ILE	2.3
1	A	425	LYS	2.3
2	B	213	VAL	2.3
2	B	215	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	180	THR	2.2
1	A	545	ILE	2.1
2	B	217	LYS	2.1
3	C	281	HIS	2.1
3	C	125	PHE	2.1
1	A	157	ASP	2.0
1	A	544	LYS	2.0
3	C	237	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	SEP	B	108	10/11	0.92	0.09	100,104,110,112	0
1	TPO	A	172	11/12	0.96	0.07	85,89,93,95	0

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.

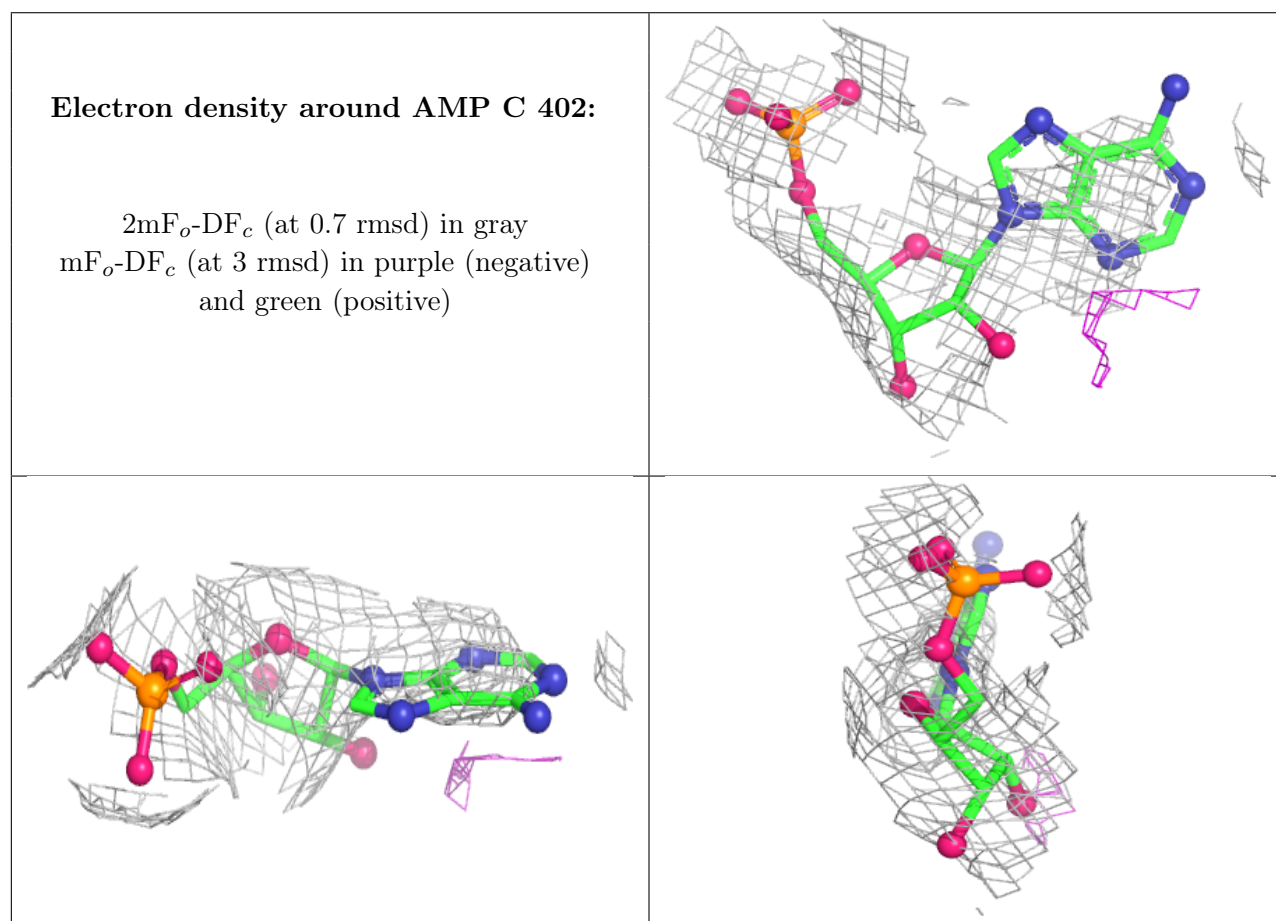
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	CL	A	605	1/1	0.82	0.12	133,133,133,133	0
7	AMP	C	402	23/23	0.89	0.12	171,183,191,193	0
9	SO4	C	404	5/5	0.90	0.10	150,150,152,152	0
8	ADP	C	403	27/27	0.91	0.11	184,194,203,205	0
7	AMP	C	401	23/23	0.94	0.10	147,152,156,161	0
5	HUG	A	602	38/38	0.94	0.10	76,99,144,146	0
4	STU	A	601	35/35	0.96	0.11	56,65,70,75	0
6	CL	A	604	1/1	0.97	0.08	92,92,92,92	0

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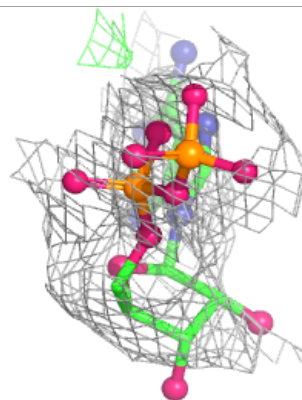
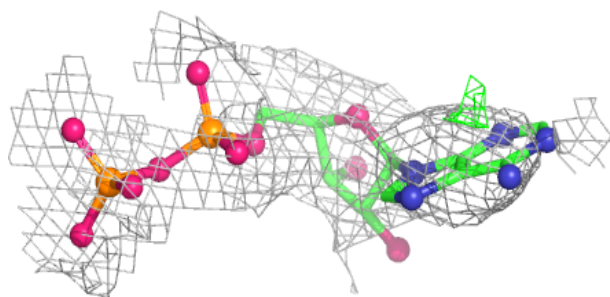
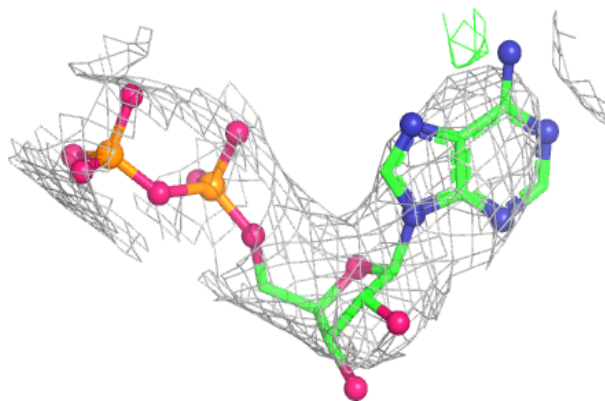
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CL	A	603	1/1	0.97	0.13	73,73,73,73	0

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.



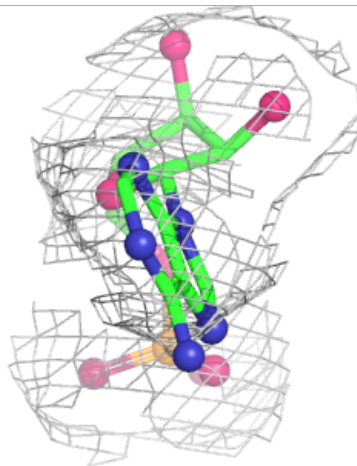
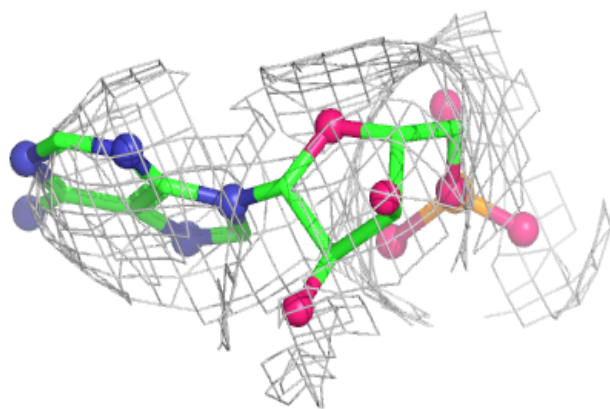
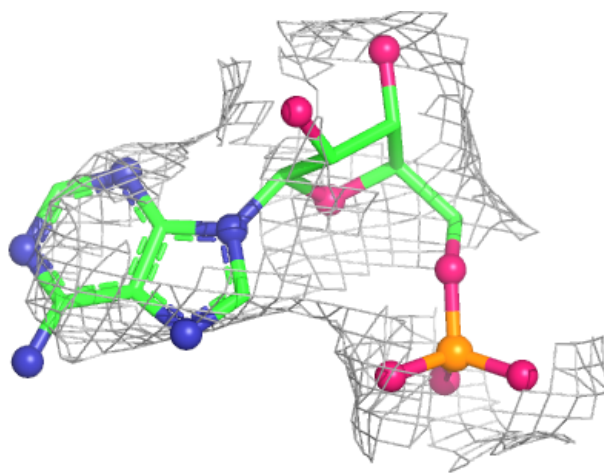
Electron density around ADP C 403:

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



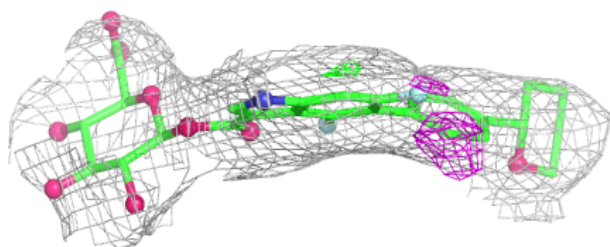
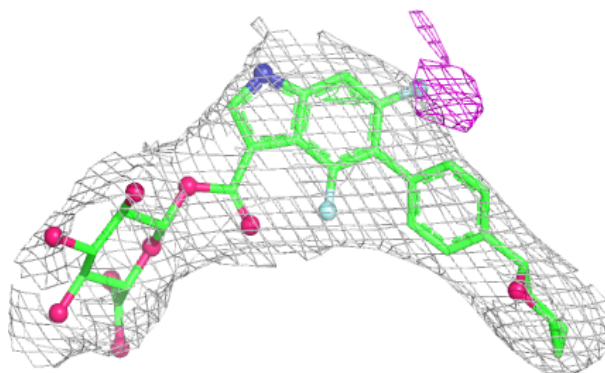
Electron density around AMP C 401:

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



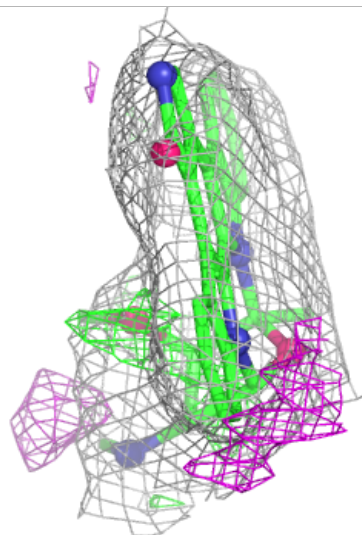
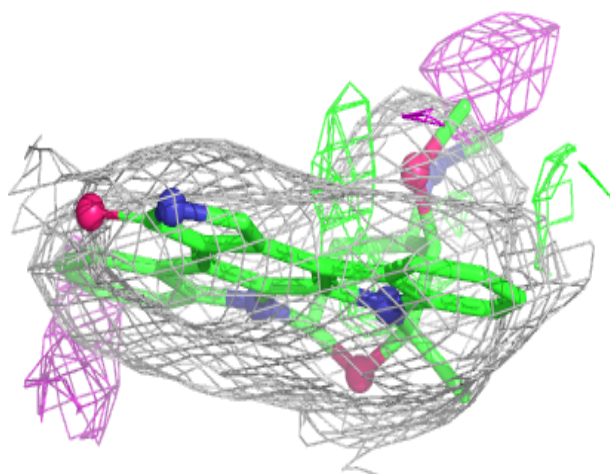
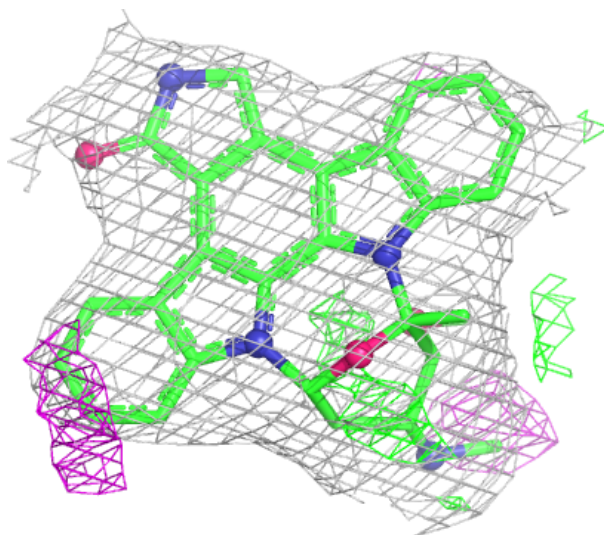
Electron density around HUG A 602:

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



Electron density around STU 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.