



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 PM UTC

PDB ID : 5ISO / pdb_00005iso
Title : STRUCTURE OF FULL LENGTH HUMAN AMPK (NON-PHOSPHORYLATED AT T-LOOP) IN COMPLEX WITH A SMALL MOLECULE ACTIVATOR, A BENZIMIDAZOLE DERIVATIVE (991)
Authors : Xiao, B.; Hubbard, J.A.; Gamblin, S.J.
Deposited on : 2016-03-15
Resolution : 2.63 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

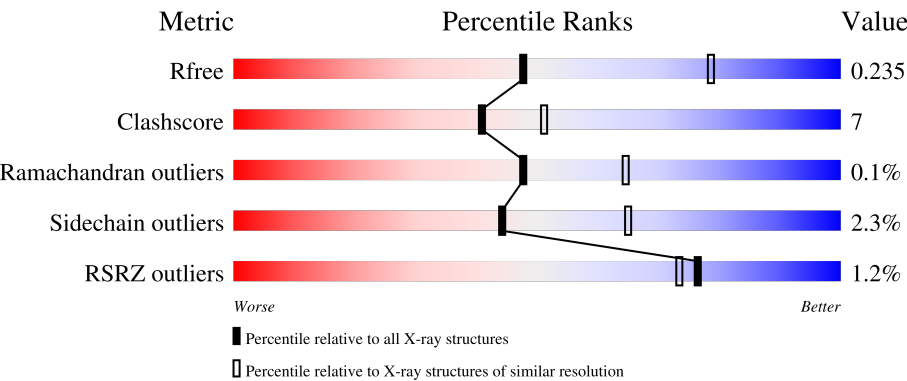
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	552	68%13%18%
1	C	552	2% 64%13%22%
2	B	286	51%12%36%
2	D	286	3% 45%14%40%

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Mol	Chain	Length	Quality of chain
3	E	331	 78%12%10%
3	F	331	 75%15%10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14898 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3614	2319	624	646	25			
1	C	429	Total	C	N	O	S	0	0	0
			3374	2169	579	603	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	P S	0	0	0
			1458	940	242	270	1 5			
2	D	173	Total	C	N	O	P S	0	0	0
			1343	874	224	240	1 4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP Q9Y478
B	-14	GLY	-	expression tag	UNP Q9Y478
B	-13	LEU	-	expression tag	UNP Q9Y478
B	-12	ASN	-	expression tag	UNP Q9Y478
B	-11	ASP	-	expression tag	UNP Q9Y478
B	-10	ILE	-	expression tag	UNP Q9Y478
B	-9	PHE	-	expression tag	UNP Q9Y478
B	-8	GLU	-	expression tag	UNP Q9Y478
B	-7	ALA	-	expression tag	UNP Q9Y478
B	-6	GLN	-	expression tag	UNP Q9Y478
B	-5	LYS	-	expression tag	UNP Q9Y478
B	-4	ILE	-	expression tag	UNP Q9Y478
B	-3	GLU	-	expression tag	UNP Q9Y478
B	-2	TRP	-	expression tag	UNP Q9Y478
B	-1	HIS	-	expression tag	UNP Q9Y478
B	0	GLU	-	expression tag	UNP Q9Y478

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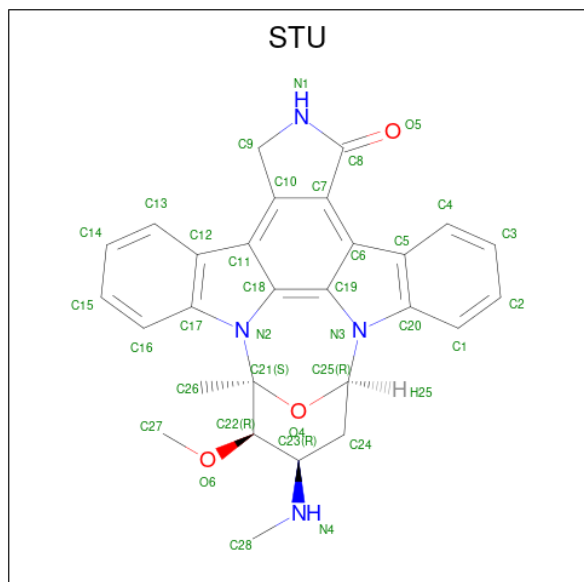
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	MET	-	initiating methionine	UNP Q9Y478
D	-14	GLY	-	expression tag	UNP Q9Y478
D	-13	LEU	-	expression tag	UNP Q9Y478
D	-12	ASN	-	expression tag	UNP Q9Y478
D	-11	ASP	-	expression tag	UNP Q9Y478
D	-10	ILE	-	expression tag	UNP Q9Y478
D	-9	PHE	-	expression tag	UNP Q9Y478
D	-8	GLU	-	expression tag	UNP Q9Y478
D	-7	ALA	-	expression tag	UNP Q9Y478
D	-6	GLN	-	expression tag	UNP Q9Y478
D	-5	LYS	-	expression tag	UNP Q9Y478
D	-4	ILE	-	expression tag	UNP Q9Y478
D	-3	GLU	-	expression tag	UNP Q9Y478
D	-2	TRP	-	expression tag	UNP Q9Y478
D	-1	HIS	-	expression tag	UNP Q9Y478
D	0	GLU	-	expression tag	UNP Q9Y478

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

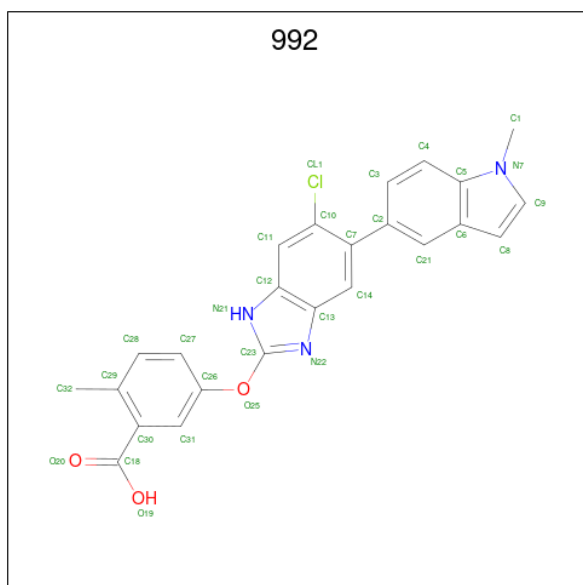
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	298	Total	C	N	O	S	0	0	0
			2384	1549	397	431	7			
3	F	299	Total	C	N	O	S	0	0	0
			2375	1547	393	428	7			

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



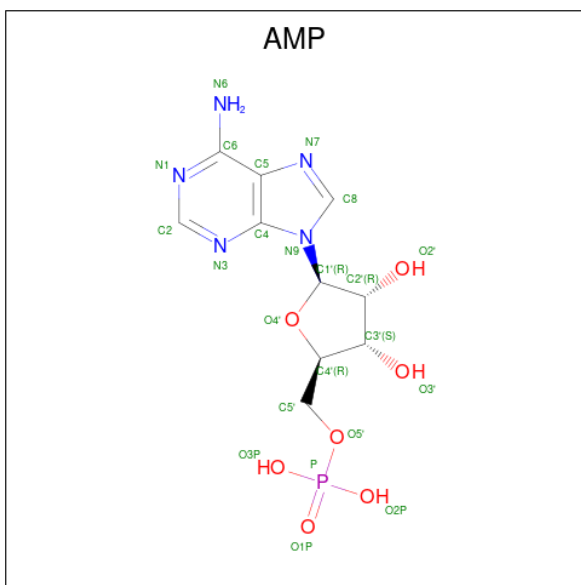
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	C	1	Total	C	N	O	0	0
			35	28	4	3		

- Molecule 5 is 5-[[6-chloranyl-5-(1-methylindol-5-yl)-1H-benzimidazol-2-yl]oxy]-2-methyl-benzoic acid (CCD ID: 992) (formula: C₂₄H₁₈ClN₃O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			31	24	1	3	3		
5	C	1	Total	C	Cl	N	O	0	0
			31	24	1	3	3		

- Molecule 6 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

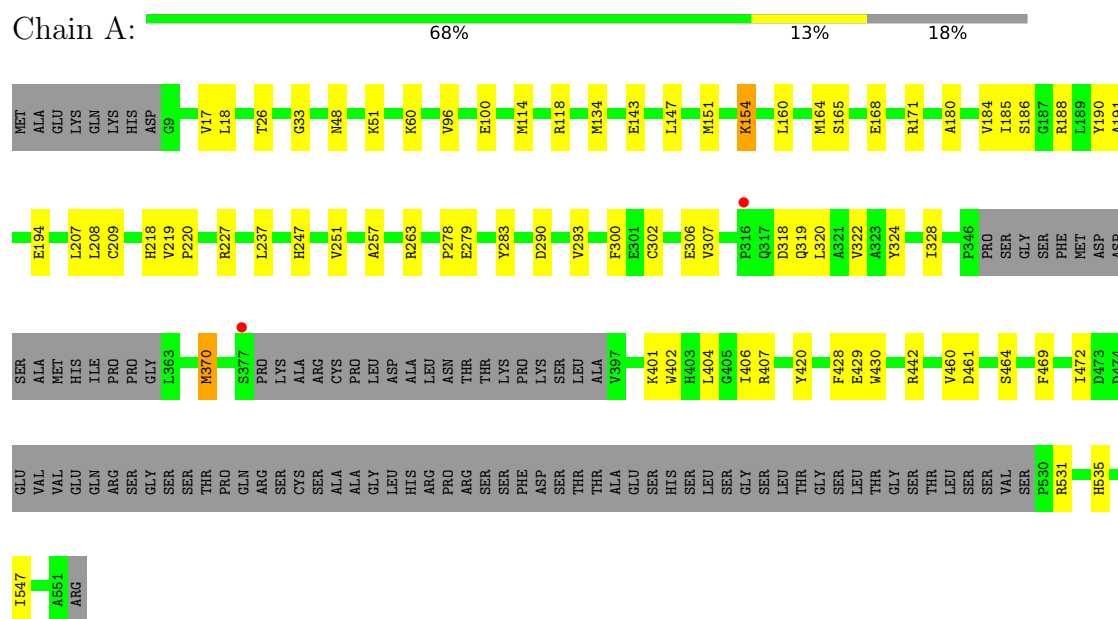
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	24	Total	O	0	0
			24	24		
7	B	7	Total	O	0	0
			7	7		
7	E	8	Total	O	0	0
			8	8		
7	C	29	Total	O	0	0
			29	29		
7	D	6	Total	O	0	0
			6	6		
7	F	6	Total	O	0	0
			6	6		

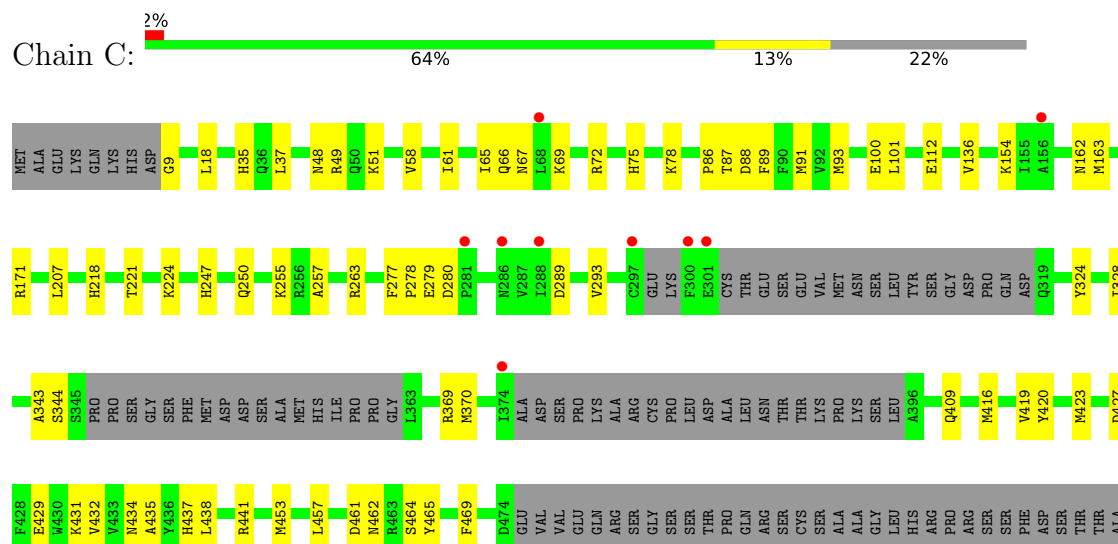
3 Residue-property plots

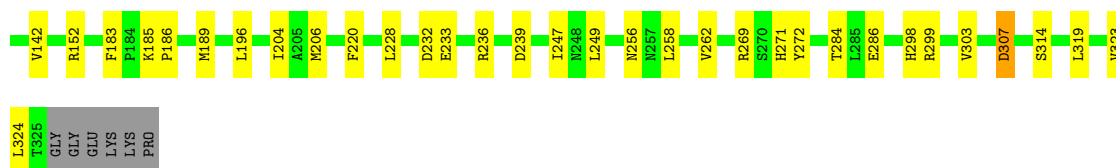
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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-2



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.42Å 129.39Å 139.28Å 90.00° 92.73° 90.00°	Depositor
Resolution (Å)	19.97 – 2.63 19.97 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.97-2.63) 94.1 (19.97-2.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.63Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.178 , 0.230 0.191 , 0.235	Depositor DCC
R_{free} test set	3884 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14898	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: AMP, 992, SEP, STU

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	0.26	0/3698	0.49	0/5000
1	C	0.25	0/3450	0.46	0/4668
2	B	0.26	0/1488	0.45	0/2027
2	D	0.23	0/1370	0.44	0/1869
3	E	0.26	0/2435	0.46	0/3309
3	F	0.26	0/2426	0.49	0/3299
All	All	0.26	0/14867	0.47	0/20172

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	3614	0	3588	48	0
1	C	3374	0	3306	53	0
2	B	1458	0	1437	22	0
2	D	1343	0	1301	30	0
3	E	2384	0	2430	30	0
3	F	2375	0	2421	32	0
4	A	35	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	35	0	26	2	0
5	A	31	0	17	2	0
5	C	31	0	17	3	0
6	E	69	0	36	0	0
6	F	69	0	36	1	0
7	A	24	0	0	0	0
7	B	7	0	0	0	0
7	C	29	0	0	1	0
7	D	6	0	0	0	0
7	E	8	0	0	1	0
7	F	6	0	0	1	0
All	All	14898	0	14641	192	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 (192) 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:370:MET:HE2	3:E:247:ILE:HG21	1.62	0.81
1:A:134:MET:HA	1:A:164:MET:HE2	1.68	0.75
1:C:431:LYS:NZ	2:D:185:GLY:O	2.25	0.70
1:C:369:ARG:HH22	2:D:219:THR:HB	1.56	0.69
1:A:26:THR:HG21	1:A:160:LEU:HG	1.74	0.69
1:C:171:ARG:HH22	2:D:204:PRO:HB3	1.59	0.68
1:C:434:ASN:HB3	1:C:437:HIS:HB3	1.76	0.68
1:C:67:ASN:ND2	1:C:163:MET:SD	2.69	0.66
1:A:430:TRP:HH2	2:B:191:PRO:HA	1.60	0.65
1:C:344:SER:OG	2:D:223:CYS:SG	2.54	0.64
1:A:186:SER:OG	1:A:227:ARG:NH1	2.30	0.64
3:F:127:LYS:HD2	3:F:128:PRO:HD2	1.79	0.64
1:C:457:LEU:HD21	1:C:465:TYR:HB3	1.80	0.63
1:C:48:ASN:ND2	1:C:88:ASP:OD1	2.30	0.62
2:D:140:PRO:HG2	2:D:152:ILE:HG13	1.81	0.62
3:E:239:ASP:OD1	3:E:269:ARG:NH2	2.33	0.62
1:A:118:ARG:NH2	1:A:151:MET:O	2.33	0.62
2:B:124:GLN:HG2	2:B:152:ILE:HG22	1.82	0.61
3:F:239:ASP:OD1	3:F:269:ARG:NH2	2.34	0.61
1:C:278:PRO:O	1:C:279:GLU:HG2	2.01	0.60
3:F:303:VAL:HG11	3:F:307:ASP:HA	1.84	0.59
4:A:601:STU:H261	4:A:601:STU:H16	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:99:TYR:O	7:E:501:HOH:O	2.17	0.58
1:C:18:LEU:HB2	5:C:602:992:H8	1.86	0.58
2:D:123:HIS:HB2	2:D:153:ILE:HD11	1.86	0.58
1:A:402:TRP:HB2	2:B:213:VAL:HG11	1.85	0.58
1:A:278:PRO:HA	1:A:283:TYR:CG	2.39	0.58
2:B:206:LEU:HD12	2:B:207:PRO:HD2	1.85	0.57
3:E:233:GLU:H	3:E:233:GLU:CD	2.13	0.57
1:A:531:ARG:HH12	1:A:535:HIS:HB2	1.70	0.57
1:C:35:HIS:HE1	1:C:37:LEU:HD12	1.69	0.57
1:A:185:ILE:HD11	1:A:227:ARG:HG3	1.86	0.57
1:C:434:ASN:OD1	1:C:435:ALA:N	2.38	0.56
2:B:249:MET:HE2	2:B:251:LEU:HD21	1.88	0.56
1:A:100:GLU:OE2	4:A:601:STU:N4	2.39	0.56
1:C:427:ASP:OD1	2:D:189:GLN:NE2	2.39	0.55
1:C:324:TYR:CE2	1:C:328:ILE:HD11	2.41	0.55
1:C:461:ASP:OD1	1:C:462:ASN:N	2.40	0.55
4:C:601:STU:H261	4:C:601:STU:H16	1.88	0.55
1:A:429:GLU:HB3	2:B:187:TYR:HB3	1.89	0.54
1:C:420:TYR:CG	2:D:191:PRO:HB3	2.43	0.54
3:F:323:VAL:HG23	3:F:324:LEU:HD12	1.88	0.54
3:F:70:ARG:NE	3:F:152:ARG:HH21	2.06	0.54
1:C:263:ARG:NH1	1:C:279:GLU:OE2	2.39	0.53
1:C:75:HIS:O	1:C:154:LYS:HA	2.08	0.53
1:A:247:HIS:CG	1:A:257:ALA:HB2	2.44	0.53
3:E:278:LYS:O	3:E:291:ARG:NH1	2.41	0.53
1:A:300:PHE:HD2	1:A:320:LEU:HD23	1.74	0.52
1:C:51:LYS:NZ	5:C:602:992:O20	2.42	0.52
1:A:319:GLN:HA	1:A:322:VAL:HG12	1.90	0.52
1:C:9:GLY:N	7:C:701:HOH:O	2.42	0.52
3:F:232:ASP:OD1	3:F:236:ARG:N	2.40	0.52
1:A:165:SER:HB2	1:A:168:GLU:HG3	1.91	0.51
1:A:208:LEU:HB3	1:A:237:LEU:HD21	1.92	0.51
3:F:142:VAL:HG11	3:F:323:VAL:HG21	1.92	0.51
3:F:204:ILE:HG22	3:F:206:MET:HG3	1.92	0.51
1:A:180:ALA:HB1	1:A:184:VAL:CG2	2.41	0.51
1:A:407:ARG:HH11	1:A:460:VAL:HG11	1.75	0.51
1:C:100:GLU:OE2	4:C:601:STU:N4	2.43	0.51
1:C:432:VAL:HG12	1:C:438:LEU:HD23	1.92	0.51
2:D:107:ARG:HG2	2:D:108:SEP:O	2.11	0.50
3:E:41:LEU:HD13	3:E:138:LEU:HD21	1.93	0.50
1:A:318:ASP:OD1	1:A:319:GLN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:MET:HG2	3:F:75:TRP:CE2	2.46	0.50
3:F:41:LEU:HD11	3:F:138:LEU:HD11	1.93	0.50
3:F:319:LEU:O	3:F:323:VAL:HG22	2.10	0.50
1:A:143:GLU:N	1:A:143:GLU:OE1	2.44	0.49
3:F:41:LEU:HD13	3:F:138:LEU:HD21	1.94	0.49
3:F:91:PHE:CZ	3:F:95:LEU:HD11	2.48	0.49
3:E:49:VAL:O	3:E:73:PRO:HD2	2.13	0.49
3:E:246:VAL:O	3:E:249:LEU:HB2	2.13	0.49
1:C:87:THR:HG22	1:C:88:ASP:OD1	2.12	0.49
2:D:125:TYR:O	2:D:150:ASN:HB2	2.12	0.49
3:E:33:MET:HE3	3:E:138:LEU:HB3	1.95	0.48
1:C:250:GLN:HG2	1:C:255:LYS:HB2	1.94	0.48
3:E:187:GLU:CD	3:E:187:GLU:H	2.21	0.48
1:C:420:TYR:HE1	1:C:438:LEU:HD21	1.78	0.48
1:A:307:VAL:HG22	1:A:320:LEU:HD22	1.94	0.48
2:B:108:SEP:OG	2:B:109:HIS:N	2.43	0.48
2:D:224:ASP:HB3	2:D:227:LEU:HG	1.94	0.48
2:D:165:ALA:O	2:D:169:ASP:HB2	2.13	0.48
1:C:91:MET:HE2	1:C:93:MET:HE3	1.96	0.48
3:F:220:PHE:CE1	3:F:228:LEU:HG	2.49	0.48
1:C:224:LYS:HD2	1:C:224:LYS:HA	1.66	0.48
1:C:48:ASN:HA	1:C:88:ASP:OD1	2.14	0.47
1:C:429:GLU:OE1	1:C:441:ARG:NH2	2.24	0.47
1:A:263:ARG:NH2	1:A:279:GLU:OE2	2.44	0.47
1:A:218:HIS:NE2	1:A:220:PRO:HG2	2.29	0.47
1:A:278:PRO:HA	1:A:283:TYR:CD2	2.50	0.47
2:B:105:LEU:HD22	2:B:114:ALA:HB2	1.96	0.47
3:F:99:TYR:CG	3:F:258:LEU:HD12	2.50	0.47
3:F:323:VAL:HG23	3:F:324:LEU:N	2.29	0.47
1:A:218:HIS:CE1	1:A:220:PRO:HG2	2.50	0.47
2:B:174:SER:O	2:B:178:GLU:HG2	2.15	0.47
1:C:218:HIS:HB3	1:C:221:THR:OG1	2.15	0.47
1:A:302:CYS:HB2	1:A:306:GLU:OE1	2.15	0.47
1:C:66:GLN:O	1:C:69:LYS:HG2	2.14	0.47
1:C:289:ASP:OD2	1:C:293:VAL:HG23	2.14	0.47
1:C:409:GLN:H	1:C:409:GLN:CD	2.23	0.46
3:F:57:VAL:HG22	3:F:112:HIS:O	2.15	0.46
3:F:303:VAL:CG1	3:F:307:ASP:HA	2.45	0.46
1:A:461:ASP:HB2	1:A:464:SER:OG	2.16	0.46
1:C:49:ARG:HG2	1:C:89:PHE:CE2	2.50	0.46
1:A:469:PHE:HB2	2:B:239:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:O	1:A:33:GLY:HA2	2.16	0.46
1:A:406:ILE:HD11	1:A:547:ILE:HG12	1.96	0.46
2:B:91:VAL:HG22	2:B:129:VAL:HG22	1.97	0.46
1:C:247:HIS:CG	1:C:257:ALA:HB2	2.51	0.46
2:D:102:LYS:HE2	2:D:133:TRP:CZ2	2.50	0.46
2:D:162:VAL:O	2:D:166:LEU:HD12	2.15	0.46
1:A:420:TYR:CD2	2:B:191:PRO:HB3	2.51	0.46
1:C:344:SER:HG	2:D:223:CYS:HG	1.60	0.46
3:E:29:TYR:O	3:E:33:MET:HG2	2.15	0.46
3:E:99:TYR:CG	3:E:258:LEU:HD12	2.50	0.46
1:C:112:GLU:H	1:C:112:GLU:CD	2.24	0.46
1:A:370:MET:HE3	3:E:244:PHE:CE1	2.50	0.46
3:E:99:TYR:HD1	3:E:106:ILE:HD11	1.80	0.45
2:D:249:MET:HB2	2:D:270:ILE:HD11	1.98	0.45
1:C:419:VAL:O	1:C:423:MET:HG3	2.16	0.45
1:A:401:LYS:HA	1:A:401:LYS:HD3	1.82	0.45
2:B:228:LEU:HD11	3:E:47:LYS:HB3	1.99	0.45
2:D:84:TRP:HZ3	2:D:87:GLY:O	2.00	0.45
2:D:128:PHE:HB2	2:D:133:TRP:CZ3	2.52	0.45
3:F:119:GLU:O	3:F:123:GLN:HG3	2.16	0.45
1:A:428:PHE:HE1	1:A:442:ARG:HD3	1.82	0.45
3:E:274:GLU:O	3:E:274:GLU:HG3	2.17	0.45
1:C:461:ASP:OD1	1:C:464:SER:HB2	2.17	0.45
3:F:319:LEU:HD23	3:F:319:LEU:HA	1.83	0.44
2:D:120:GLU:H	2:D:120:GLU:HG3	1.49	0.44
1:A:290:ASP:HA	1:A:293:VAL:HG12	2.00	0.44
3:E:206:MET:HE2	3:E:231:VAL:HG11	1.99	0.44
1:C:431:LYS:HD2	2:D:187:TYR:CZ	2.53	0.44
1:A:18:LEU:CB	5:A:602:992:H8	2.48	0.44
1:A:96:VAL:HG11	1:A:154:LYS:HD3	1.98	0.44
2:B:252:SER:HA	2:B:264:THR:O	2.17	0.44
3:F:299:ARG:HH12	6:F:402:AMP:P	2.41	0.44
3:E:41:LEU:HD23	3:E:167:LEU:HD11	1.98	0.44
3:F:298:HIS:HB3	3:F:299:ARG:CZ	2.48	0.44
3:F:271:HIS:NE2	3:F:272:TYR:HD2	2.16	0.44
2:B:188:HIS:ND1	2:B:190:GLU:HG3	2.33	0.43
1:C:61:ILE:O	1:C:65:ILE:HG12	2.18	0.43
3:E:234:LYS:HD3	3:E:236:ARG:NH2	2.33	0.43
1:C:101:LEU:HD11	1:C:207:LEU:HD21	2.01	0.43
1:C:420:TYR:CE1	1:C:438:LEU:HD21	2.54	0.43
3:F:185:LYS:NZ	3:F:286:GLU:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:VAL:HG12	2:D:240:TYR:CE2	2.54	0.43
1:A:114:MET:HE2	1:A:114:MET:HB3	1.90	0.43
3:E:41:LEU:HD11	3:E:138:LEU:HD11	2.00	0.43
1:C:343:ALA:HB1	2:D:219:THR:HG23	1.99	0.43
3:E:305:GLU:H	3:E:305:GLU:CD	2.25	0.43
1:C:72:ARG:HG3	1:C:78:LYS:HE3	2.01	0.43
1:A:171:ARG:HH22	2:B:204:PRO:HB3	1.84	0.42
3:E:157:ASP:OD1	3:E:159:GLU:HG2	2.19	0.42
3:F:127:LYS:HD2	3:F:128:PRO:CD	2.47	0.42
1:A:18:LEU:HB2	5:A:602:992:H8	2.00	0.42
2:B:125:TYR:HE1	2:B:153:ILE:HG23	1.85	0.42
3:E:185:LYS:HE3	3:E:185:LYS:HB2	1.81	0.42
2:B:244:ILE:H	2:B:244:ILE:HG12	1.61	0.42
1:A:48:ASN:HB3	1:A:51:LYS:HD2	2.02	0.42
1:C:86:PRO:HG2	2:D:155:VAL:HG12	2.01	0.42
3:F:28:VAL:HG21	3:F:183:PHE:HB3	2.02	0.42
2:B:245:LYS:HD2	2:B:245:LYS:HA	1.75	0.42
1:C:58:VAL:HG11	2:D:170:SER:HA	2.02	0.42
1:A:184:VAL:HG12	1:A:190:TYR:CE2	2.54	0.42
3:E:85:MET:HE3	3:E:85:MET:HB3	1.78	0.42
3:F:118:ARG:NH1	7:F:501:HOH:O	2.53	0.42
3:E:194:GLU:HB2	3:E:281:LEU:HB3	2.02	0.41
1:C:469:PHE:HE2	1:C:546:LEU:HD22	1.84	0.41
3:F:55:LEU:HD23	3:F:60:ALA:HB2	2.02	0.41
3:F:186:PRO:HD2	3:F:189:MET:HG3	2.02	0.41
1:C:277:PHE:O	1:C:280:ASP:HB2	2.19	0.41
2:D:120:GLU:HA	2:D:155:VAL:HG23	2.03	0.41
1:A:324:TYR:O	1:A:328:ILE:HG12	2.21	0.41
2:D:142:VAL:HB	2:D:152:ILE:HG21	2.02	0.41
1:A:404:LEU:HD22	2:B:210:LEU:HB3	2.01	0.41
1:A:188:ARG:NH1	2:B:205:ILE:HD13	2.35	0.41
2:D:171:GLN:N	2:D:171:GLN:OE1	2.54	0.41
3:F:233:GLU:H	3:F:233:GLU:CD	2.28	0.41
2:D:167:MET:HE3	2:D:167:MET:HA	2.02	0.41
3:E:173:LEU:HD22	3:E:315:LEU:HD22	2.03	0.41
3:E:284:THR:O	3:E:288:ILE:HG12	2.20	0.41
2:D:94:SER:O	2:D:126:LYS:N	2.54	0.41
3:F:247:ILE:HD12	3:F:247:ILE:HA	1.93	0.41
3:E:208:ARG:HH12	3:E:233:GLU:HA	1.85	0.41
1:C:18:LEU:CB	5:C:602:992:H8	2.50	0.41
1:C:370:MET:HE2	3:F:68:GLY:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:O	2:B:234:VAL:HG23	2.21	0.40
3:E:319:LEU:HA	3:E:319:LEU:HD23	1.77	0.40
1:C:416:MET:SD	1:C:457:LEU:HD12	2.61	0.40
2:D:232:ASN:O	2:D:235:MET:HG3	2.22	0.40
1:A:191:ALA:N	1:A:194:GLU:OE2	2.49	0.40
3:E:234:LYS:HE2	3:E:236:ARG:HE	1.86	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	445/552 (81%)	435 (98%)	10 (2%)	0	100	100
1	C	417/552 (76%)	407 (98%)	10 (2%)	0	100	100
2	B	176/286 (62%)	171 (97%)	5 (3%)	0	100	100
2	D	162/286 (57%)	160 (99%)	2 (1%)	0	100	100
3	E	296/331 (89%)	288 (97%)	8 (3%)	0	100	100
3	F	297/331 (90%)	293 (99%)	3 (1%)	1 (0%)	36	50
All	All	1793/2338 (77%)	1754 (98%)	38 (2%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	307	ASP

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	391/487 (80%)	382 (98%)	9 (2%)	44	65
1	C	358/487 (74%)	354 (99%)	4 (1%)	65	79
2	B	164/253 (65%)	155 (94%)	9 (6%)	19	32
2	D	144/253 (57%)	138 (96%)	6 (4%)	26	44
3	E	268/304 (88%)	265 (99%)	3 (1%)	65	79
3	F	266/304 (88%)	260 (98%)	6 (2%)	44	65
All	All	1591/2088 (76%)	1554 (98%)	37 (2%)	44	65

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	147	LEU
1	A	154	LYS
1	A	207	LEU
1	A	209	CYS
1	A	219	VAL
1	A	251	VAL
1	A	370	MET
1	A	472	ILE
2	B	90	GLU
2	B	113	VAL
2	B	120	GLU
2	B	134	THR
2	B	190	GLU
2	B	221	ILE
2	B	244	ILE
2	B	248	VAL
2	B	260	LYS
3	E	178	LEU
3	E	249	LEU
3	E	267	GLN
1	C	136	VAL
1	C	162	ASN
1	C	453	MET
1	C	537	MET
2	D	118	LEU

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Mol	Chain	Res	Type
2	D	120	GLU
2	D	134	THR
2	D	135	HIS
2	D	153	ILE
2	D	249	MET
3	F	196	LEU
3	F	249	LEU
3	F	256	ASN
3	F	262	VAL
3	F	284	THR
3	F	314	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	178	ASN
1	A	286	ASN
2	B	150	ASN
3	E	80	GLN
3	E	96	HIS
3	E	135	ASN
3	E	256	ASN
3	E	298	HIS
1	C	178	ASN
3	F	36	HIS
3	F	223	HIS
3	F	320	GLN

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	D	108	2	8,9,10	0.94	0	7,12,14	0.77	0
2	SEP	B	108	2	8,9,10	0.85	0	7,12,14	1.59	2 (28%)

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	D	108	2	-	1/6/8/10	-
2	SEP	B	108	2	-	1/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	SEP	OG-CB-CA	3.27	111.33	108.14
2	B	108	SEP	OG-P-O1P	2.35	112.79	106.44

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	108	SEP	N-CA-CB-OG
2	B	108	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	108	SEP	1	0
2	B	108	SEP	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	STU	C	601	-	39,42,42	0.86	2 (5%)	50,68,68	2.31	11 (22%)
6	AMP	E	401	-	25,25,25	1.41	4 (16%)	37,38,38	1.90	7 (18%)
5	992	A	602	-	33,35,35	1.30	3 (9%)	50,52,52	1.80	9 (18%)
4	STU	A	601	-	39,42,42	0.86	1 (2%)	50,68,68	2.22	12 (24%)
6	AMP	F	402	-	25,25,25	1.45	4 (16%)	37,38,38	1.89	7 (18%)
5	992	C	602	-	33,35,35	1.38	2 (6%)	50,52,52	1.78	14 (28%)
6	AMP	E	403	-	25,25,25	1.44	4 (16%)	37,38,38	1.93	7 (18%)
6	AMP	F	403	-	25,25,25	1.43	4 (16%)	37,38,38	1.98	9 (24%)
6	AMP	E	402	-	25,25,25	1.46	4 (16%)	37,38,38	1.77	7 (18%)
6	AMP	F	401	-	25,25,25	1.40	4 (16%)	37,38,38	2.00	8 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	STU	C	601	-	-	1/4/42/42	-
6	AMP	E	401	-	-	5/10/26/26	0/3/3/3
5	992	A	602	-	-	4/10/12/12	0/5/5/5
4	STU	A	601	-	-	1/4/42/42	-
6	AMP	F	402	-	-	3/10/26/26	0/3/3/3
5	992	C	602	-	-	4/10/12/12	0/5/5/5
6	AMP	E	403	-	-	5/10/26/26	0/3/3/3
6	AMP	F	403	-	-	0/10/26/26	0/3/3/3
6	AMP	E	402	-	-	3/10/26/26	0/3/3/3
6	AMP	F	401	-	-	3/10/26/26	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	602	992	C9-N7	-5.60	1.32	1.37
6	F	401	AMP	C5-C4	4.86	1.47	1.39
6	E	403	AMP	C5-C4	4.85	1.47	1.39
6	E	402	AMP	C5-C4	4.83	1.47	1.39
6	E	401	AMP	C5-C4	4.79	1.47	1.39
5	A	602	992	C9-N7	-4.76	1.33	1.37
6	F	402	AMP	C5-C4	4.72	1.47	1.39
6	F	403	AMP	C5-C4	4.67	1.47	1.39
6	F	402	AMP	C5-C6	2.84	1.48	1.41
6	F	403	AMP	C5-C6	2.81	1.48	1.41
6	E	402	AMP	C5-C6	2.76	1.48	1.41
6	E	403	AMP	C5-N7	-2.72	1.34	1.39
6	E	401	AMP	C5-C6	2.62	1.48	1.41
6	F	403	AMP	C5-N7	-2.62	1.34	1.39
6	F	401	AMP	C5-C6	2.60	1.48	1.41
6	E	403	AMP	C5-C6	2.57	1.48	1.41
6	E	402	AMP	C8-N7	2.51	1.36	1.31
6	E	402	AMP	C5-N7	-2.42	1.34	1.39
6	E	401	AMP	C8-N7	2.33	1.36	1.31
6	E	403	AMP	C8-N7	2.32	1.36	1.31
6	F	401	AMP	C5-N7	-2.31	1.34	1.39
6	F	402	AMP	C5-N7	-2.28	1.34	1.39
4	C	601	STU	C19-N3	-2.27	1.35	1.39
4	A	601	STU	O4-C25	-2.24	1.39	1.43
6	F	401	AMP	C8-N7	2.21	1.35	1.31
6	F	402	AMP	C8-N7	2.19	1.35	1.31
5	A	602	992	C12-C13	2.16	1.43	1.40
6	E	401	AMP	C5-N7	-2.15	1.35	1.39
4	C	601	STU	C26-C21	2.13	1.54	1.51
5	A	602	992	C11-C10	2.08	1.42	1.38
6	F	403	AMP	C8-N7	2.08	1.35	1.31
5	C	602	992	C12-C13	2.02	1.42	1.40

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C9-C10-C7	-8.19	106.88	109.88
4	C	601	STU	C9-C10-C7	-7.64	107.08	109.88
4	C	601	STU	C28-N4-C23	-6.70	106.38	114.39
6	E	403	AMP	C5-C4-N3	-6.34	117.98	126.72
6	F	401	AMP	C5-C4-N3	-6.27	118.08	126.72
6	F	403	AMP	C5-C4-N3	-6.24	118.12	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	402	AMP	C5-C4-N3	-6.21	118.16	126.72
6	E	402	AMP	C5-C4-N3	-5.90	118.60	126.72
6	E	401	AMP	C5-C4-N3	-5.71	118.86	126.72
5	C	602	992	C5-N7-C9	5.49	111.79	108.35
5	A	602	992	C5-N7-C9	5.35	111.70	108.35
6	F	401	AMP	N3-C4-N9	5.28	136.15	127.17
4	C	601	STU	C9-N1-C8	-5.21	109.11	113.86
4	C	601	STU	C9-C10-C11	5.16	132.65	128.73
6	F	403	AMP	N3-C4-N9	5.11	135.86	127.17
4	A	601	STU	C9-N1-C8	-5.07	109.24	113.86
6	E	401	AMP	N3-C4-N9	4.84	135.40	127.17
5	A	602	992	C1-N7-C5	-4.83	121.21	125.69
6	F	402	AMP	N3-C4-N9	4.81	135.35	127.17
6	E	403	AMP	N3-C4-N9	4.76	135.26	127.17
4	A	601	STU	C28-N4-C23	-4.67	108.81	114.39
5	A	602	992	C3-C2-C7	-4.54	113.40	120.91
6	E	402	AMP	N3-C4-N9	4.33	134.54	127.17
4	A	601	STU	C9-C10-C11	4.23	131.94	128.73
4	A	601	STU	C10-C9-N1	4.19	105.83	101.75
4	C	601	STU	C10-C9-N1	3.90	105.55	101.75
5	C	602	992	C3-C2-C7	-3.88	114.47	120.91
6	F	401	AMP	C2-N3-C4	3.80	121.11	111.83
5	A	602	992	C21-C2-C7	3.79	126.96	120.61
6	F	402	AMP	C2-N3-C4	3.79	121.08	111.83
6	E	402	AMP	C2-N3-C4	3.78	121.05	111.83
4	A	601	STU	C7-C8-N1	3.77	109.98	106.38
6	E	401	AMP	C2-N3-C4	3.76	121.01	111.83
6	F	403	AMP	C2-N3-C4	3.74	120.96	111.83
6	E	403	AMP	C4-C5-N7	-3.68	106.37	110.58
6	E	403	AMP	C2-N3-C4	3.64	120.71	111.83
4	C	601	STU	C7-C8-N1	3.63	109.84	106.38
4	C	601	STU	C27-O6-C22	-3.62	108.34	114.46
6	F	402	AMP	C4-C5-N7	-3.61	106.45	110.58
5	C	602	992	C21-C2-C7	3.56	126.58	120.61
6	E	401	AMP	N3-C2-N1	-3.53	123.23	128.58
6	F	403	AMP	C4-C5-N7	-3.39	106.71	110.58
5	C	602	992	C1-N7-C5	-3.36	122.58	125.69
6	E	402	AMP	C4-C5-N7	-3.34	106.77	110.58
4	A	601	STU	C6-C7-C10	-3.27	118.48	120.76
6	E	402	AMP	N3-C2-N1	-3.26	123.64	128.58
6	F	401	AMP	N3-C2-N1	-3.16	123.80	128.58
5	C	602	992	C4-C5-N7	3.03	134.04	129.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C16-C17-C12	-2.97	118.12	121.59
6	F	402	AMP	N3-C2-N1	-2.96	124.11	128.58
4	C	601	STU	C13-C12-C17	2.93	122.62	119.24
6	F	401	AMP	C4-C5-N7	-2.90	107.26	110.58
6	E	401	AMP	C4-C5-N7	-2.86	107.32	110.58
6	E	403	AMP	N3-C2-N1	-2.83	124.31	128.58
6	E	401	AMP	C4-N9-C8	2.82	108.70	105.74
6	F	403	AMP	N3-C2-N1	-2.82	124.31	128.58
5	C	602	992	C4-C3-C2	2.76	124.66	121.12
4	C	601	STU	O5-C8-C7	-2.72	124.52	128.47
6	E	403	AMP	C5-N7-C8	2.70	107.70	103.45
4	A	601	STU	C13-C12-C17	2.70	122.36	119.24
6	F	403	AMP	C5-N7-C8	2.62	107.57	103.45
6	F	403	AMP	C4-N9-C8	2.54	108.40	105.74
6	F	401	AMP	C4-N9-C8	2.51	108.37	105.74
5	A	602	992	C4-C5-N7	2.51	133.33	129.91
5	C	602	992	C6-C21-C2	-2.51	117.47	121.77
5	C	602	992	C26-O25-C23	-2.48	113.15	118.13
5	A	602	992	C6-C21-C2	-2.45	117.56	121.77
4	C	601	STU	C16-C17-C12	-2.43	118.75	121.59
6	F	403	AMP	O3P-P-O2P	2.41	116.85	107.80
6	F	402	AMP	C5-N7-C8	2.39	107.21	103.45
6	F	401	AMP	C5-N7-C8	2.29	107.06	103.45
6	F	402	AMP	C4-N9-C8	2.24	108.09	105.74
6	E	401	AMP	C5-N7-C8	2.20	106.91	103.45
5	C	602	992	C11-C12-C13	-2.20	118.91	122.17
5	A	602	992	C4-C3-C2	2.20	123.94	121.12
5	C	602	992	C12-C13-N22	-2.18	106.43	109.42
5	C	602	992	C21-C6-C5	2.18	121.76	119.56
5	C	602	992	C8-C9-N7	-2.15	108.36	110.39
5	A	602	992	C8-C9-N7	-2.13	108.37	110.39
6	E	403	AMP	O3P-P-O2P	2.13	115.79	107.80
6	F	403	AMP	O2P-P-O5'	-2.13	101.12	106.67
4	C	601	STU	C19-N3-C20	2.11	110.69	107.90
6	E	402	AMP	C6-C5-N7	2.06	136.06	132.09
4	A	601	STU	C6-C7-C8	2.06	133.44	130.53
5	A	602	992	C11-C12-C13	-2.05	119.13	122.17
6	E	402	AMP	C5-N7-C8	2.04	106.66	103.45
5	C	602	992	C14-C13-N22	2.03	133.69	129.31
6	F	401	AMP	C3'-C2'-C1'	2.03	105.30	101.46
5	C	602	992	C4-C5-C6	-2.01	119.30	121.78
4	A	601	STU	C3-C4-C5	-2.01	116.91	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	STU	C16-C17-N2	2.00	133.22	130.22

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	401	AMP	C5'-O5'-P-O1P
6	E	401	AMP	C5'-O5'-P-O2P
6	E	401	AMP	C5'-O5'-P-O3P
6	E	401	AMP	O4'-C4'-C5'-O5'
6	E	402	AMP	C5'-O5'-P-O2P
6	E	402	AMP	C5'-O5'-P-O3P
6	E	403	AMP	C5'-O5'-P-O1P
6	E	403	AMP	C5'-O5'-P-O2P
6	E	403	AMP	C5'-O5'-P-O3P
6	F	401	AMP	C5'-O5'-P-O1P
6	F	401	AMP	C5'-O5'-P-O2P
6	F	401	AMP	C5'-O5'-P-O3P
6	F	402	AMP	C5'-O5'-P-O1P
6	F	402	AMP	C5'-O5'-P-O2P
6	F	402	AMP	C5'-O5'-P-O3P
6	E	401	AMP	C3'-C4'-C5'-O5'
6	E	402	AMP	C5'-O5'-P-O1P
5	C	602	992	O20-C18-C30-C31
5	C	602	992	O19-C18-C30-C31
6	E	403	AMP	O4'-C4'-C5'-O5'
5	A	602	992	O20-C18-C30-C31
5	A	602	992	O19-C18-C30-C31
5	C	602	992	O20-C18-C30-C29
5	C	602	992	O19-C18-C30-C29
5	A	602	992	O20-C18-C30-C29
4	C	601	STU	C24-C23-N4-C28
5	A	602	992	O19-C18-C30-C29
4	A	601	STU	C24-C23-N4-C28
6	E	403	AMP	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	STU	2	0

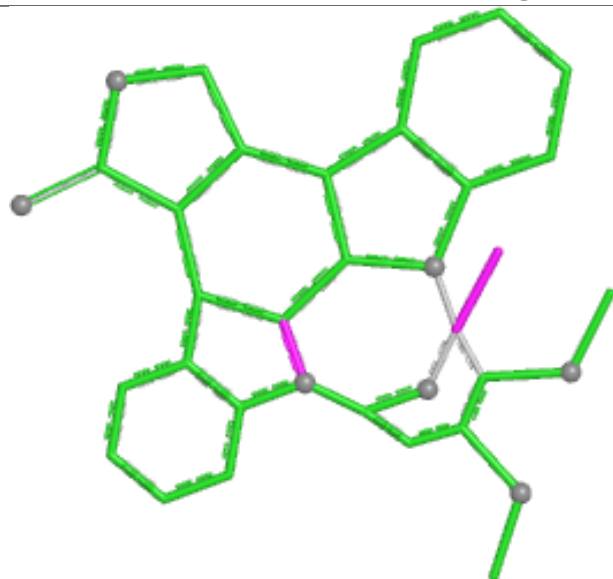
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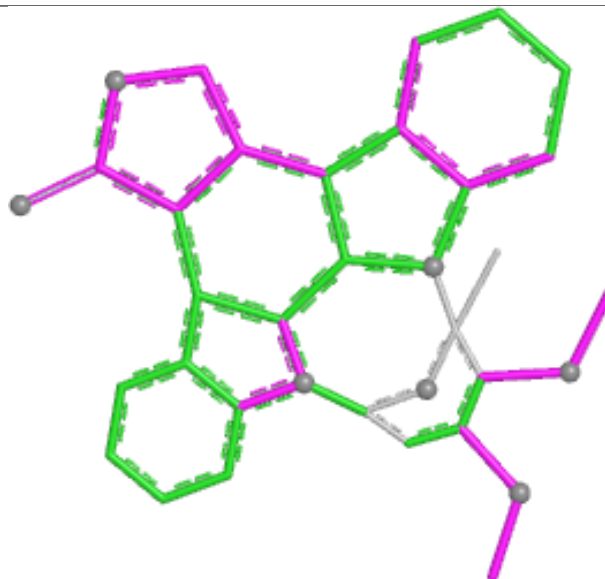
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	602	992	2	0
4	A	601	STU	2	0
6	F	402	AMP	1	0
5	C	602	992	3	0

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.

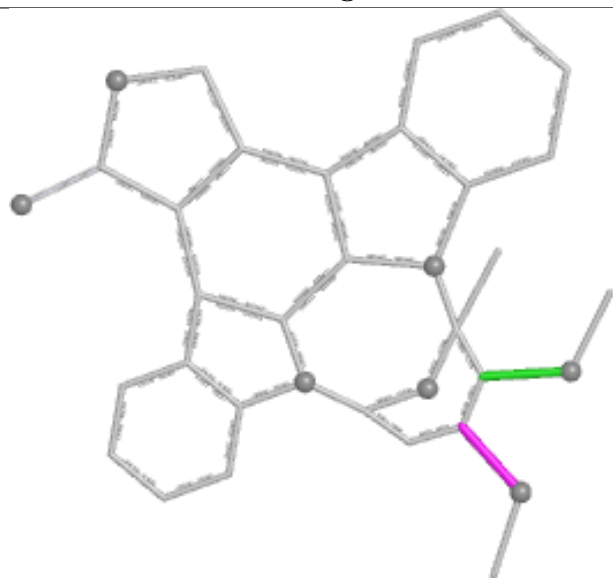
Ligand STU C 601



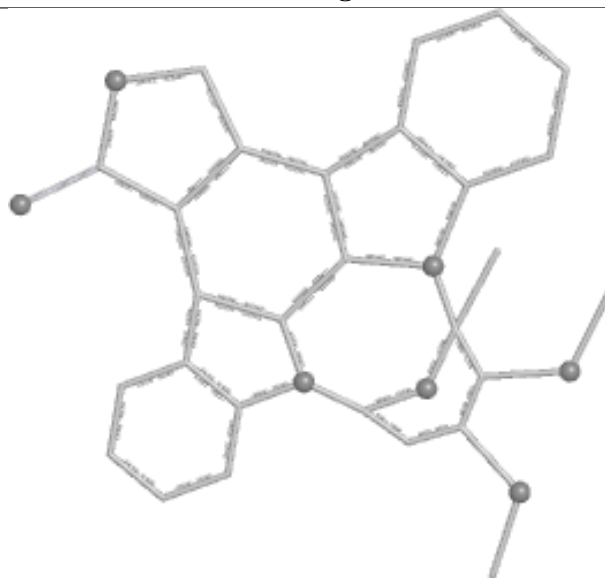
Bond lengths



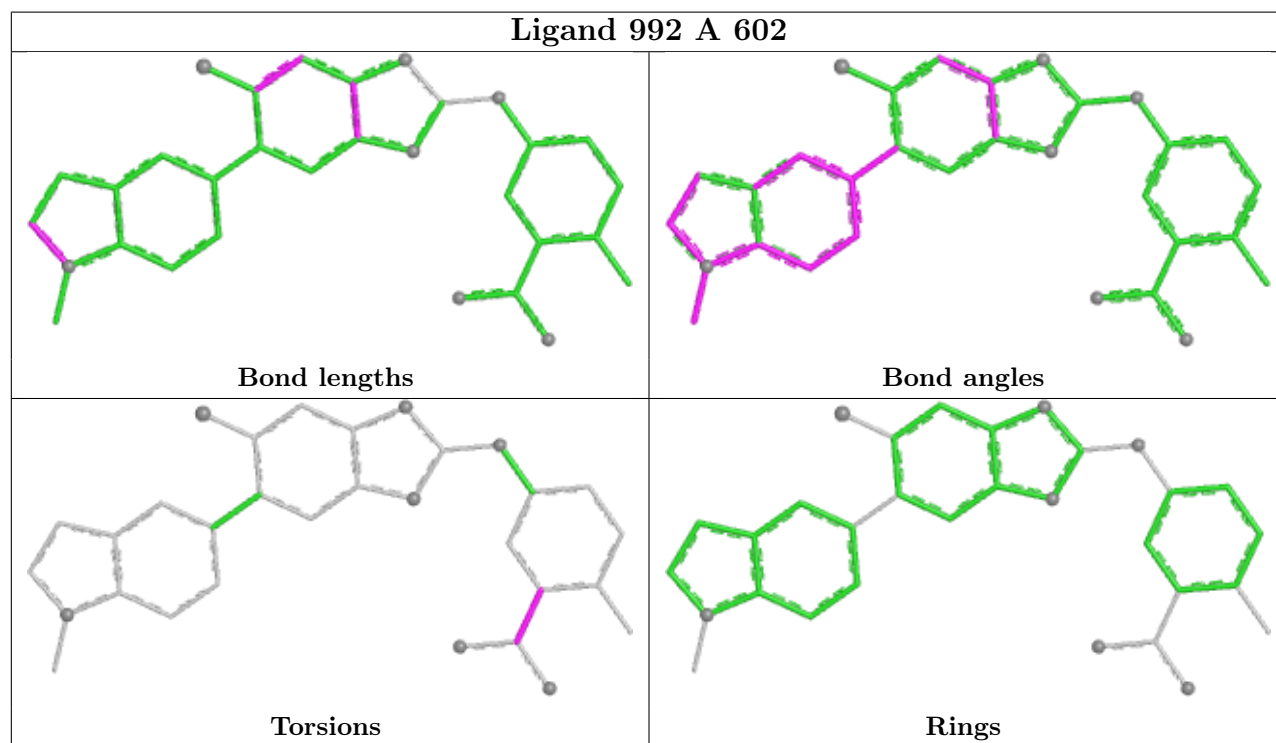
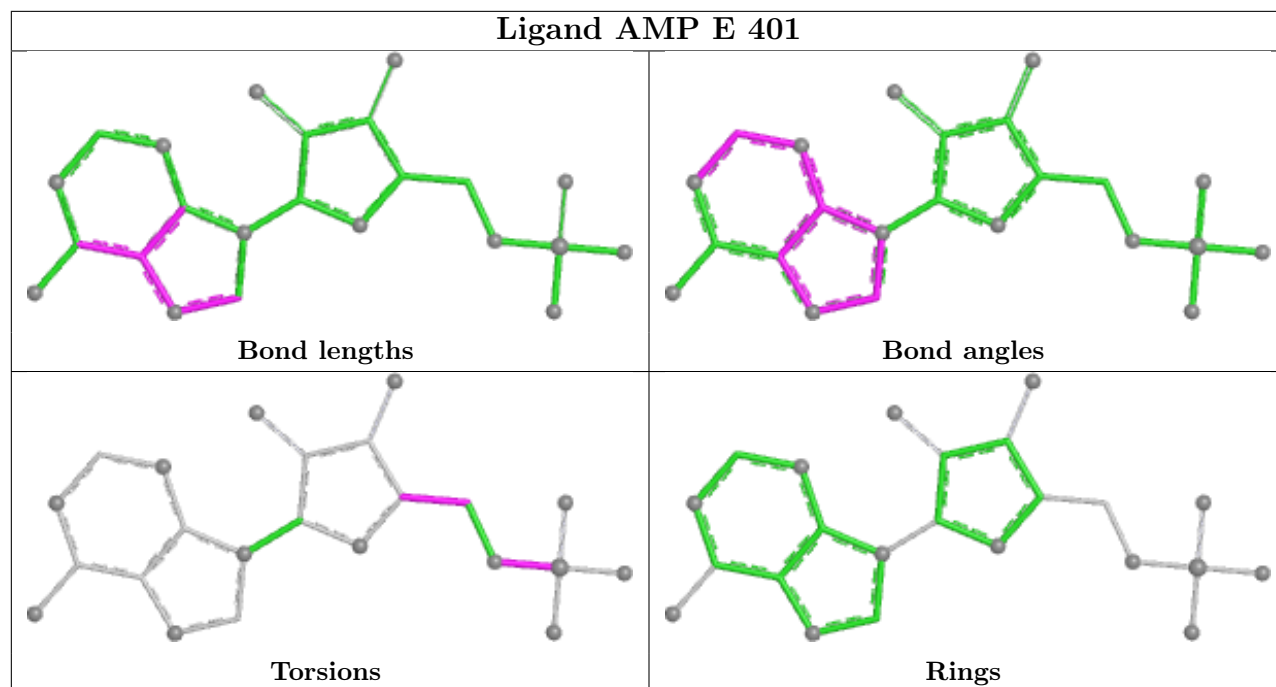
Bond angles



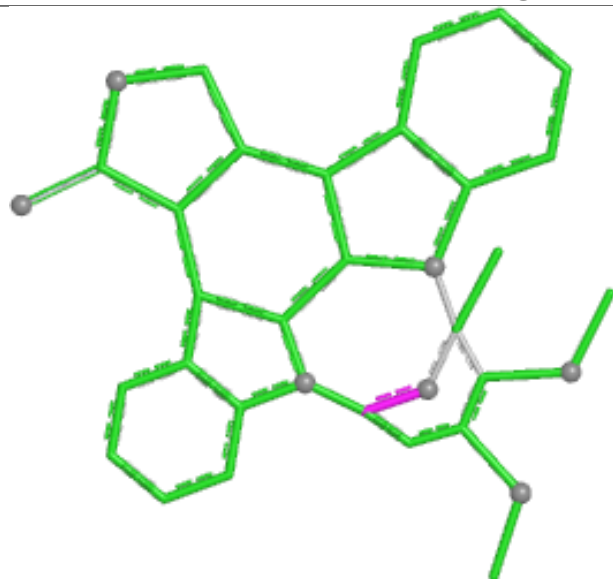
Torsions



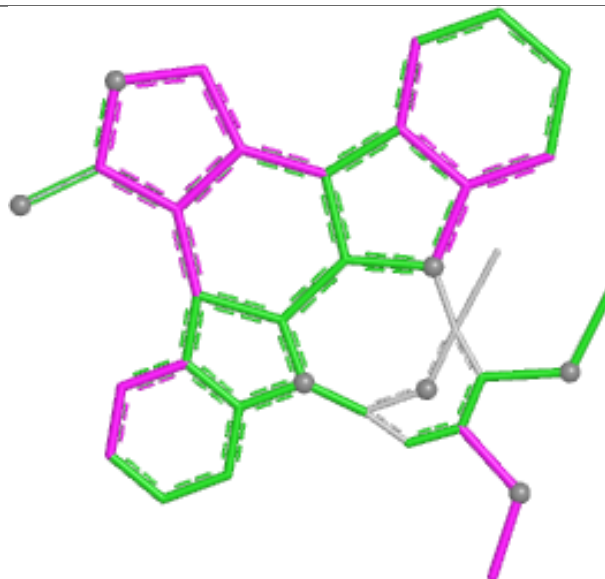
Rings



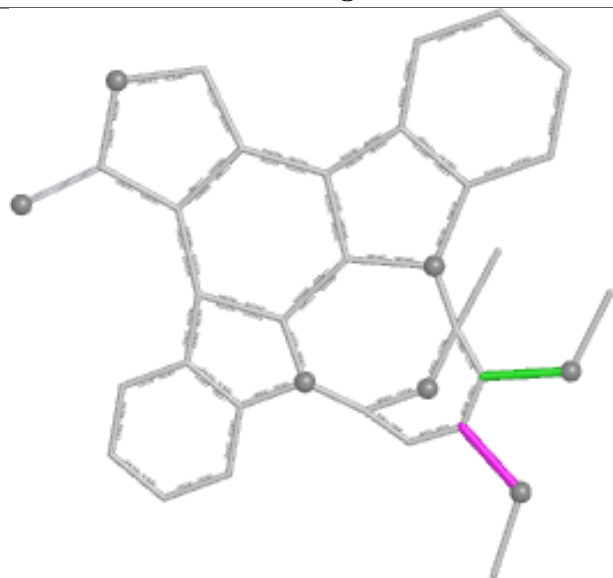
Ligand STU A 601



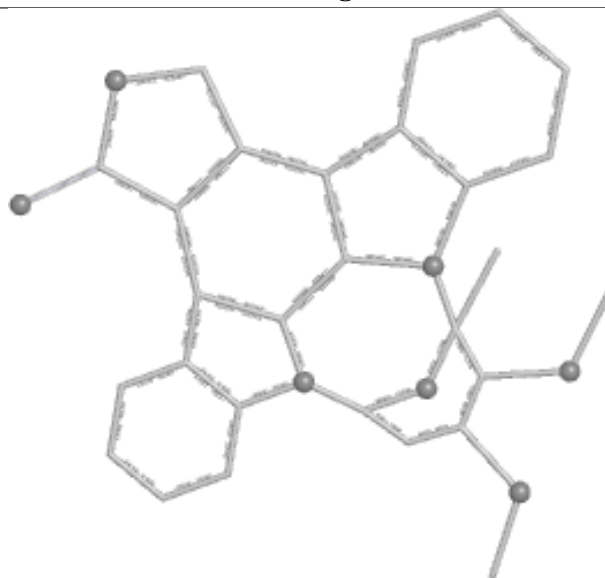
Bond lengths



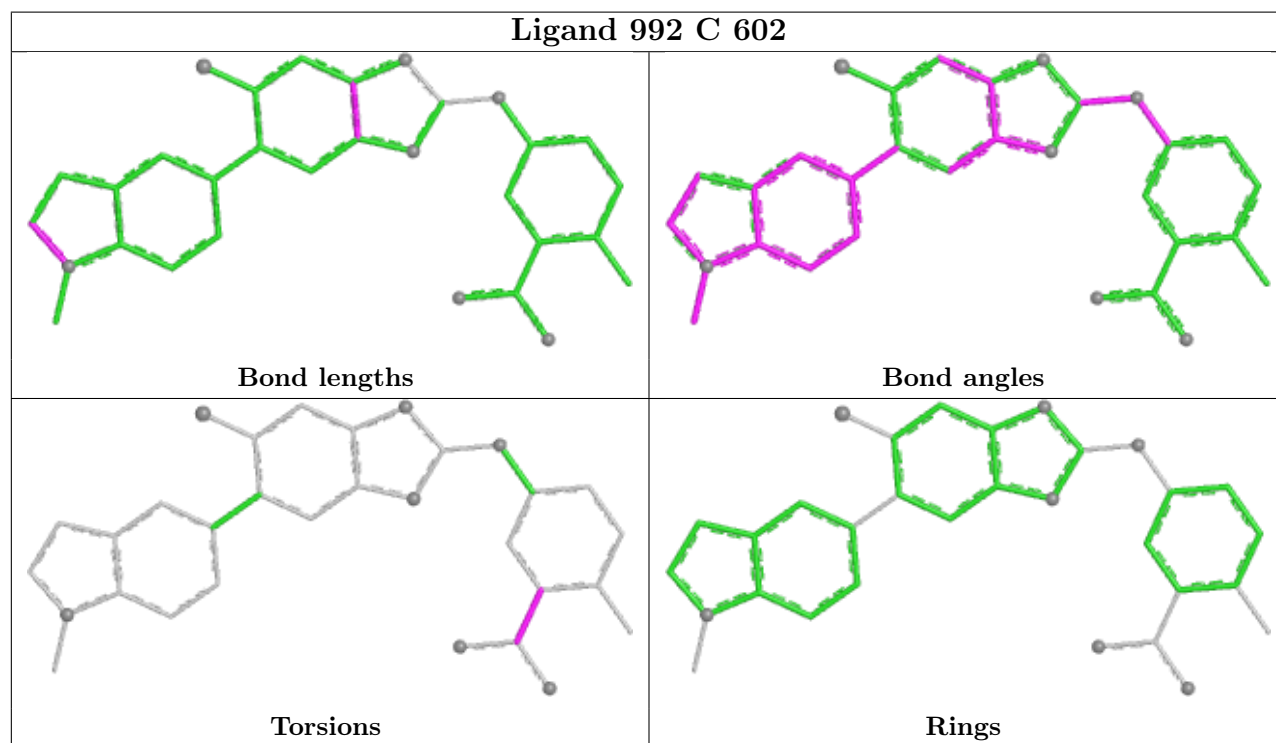
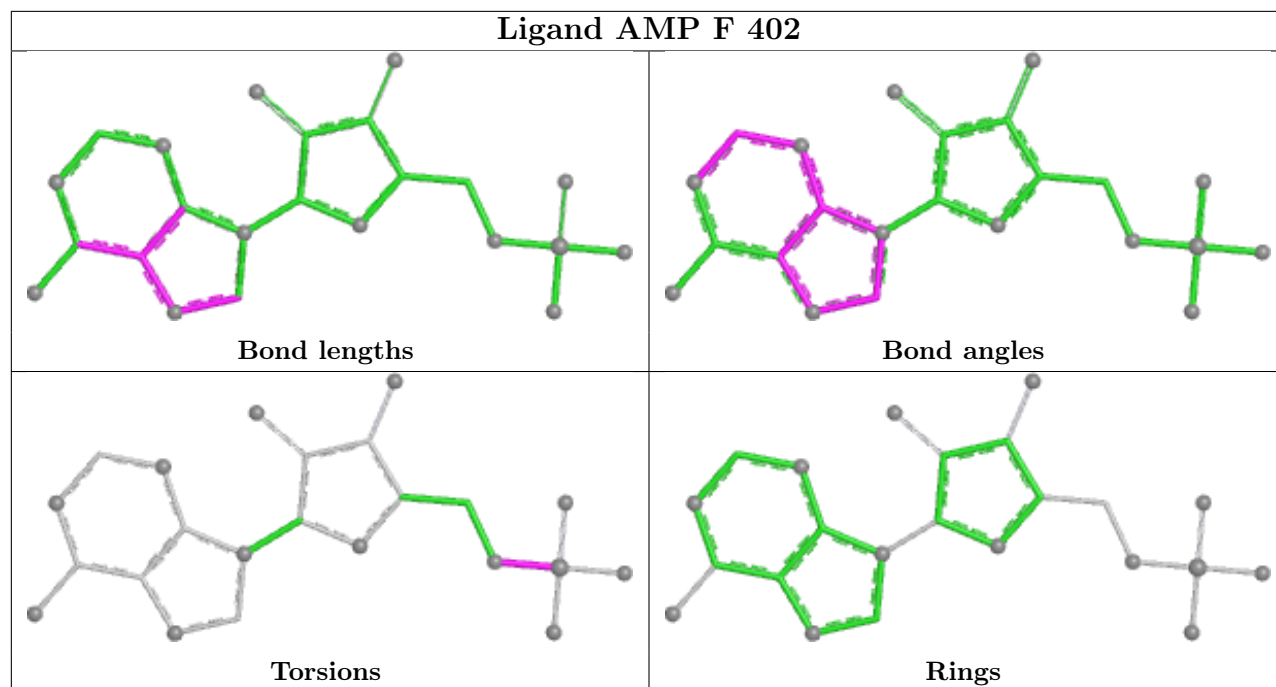
Bond angles

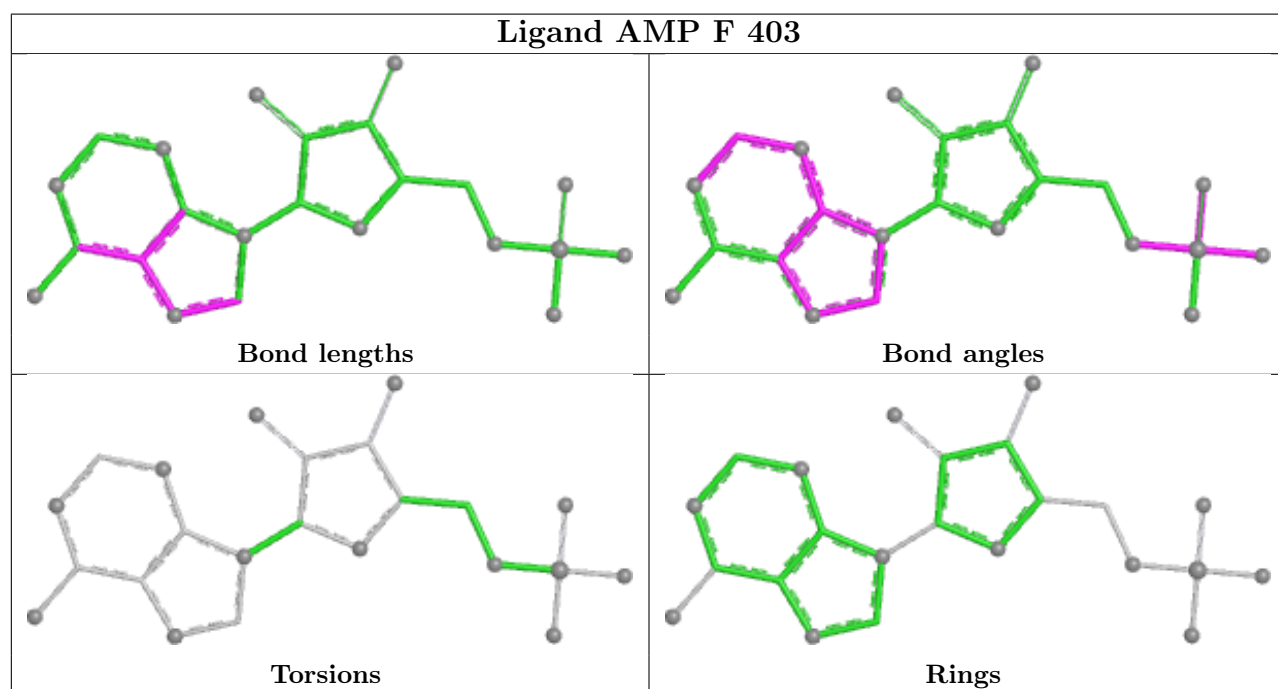
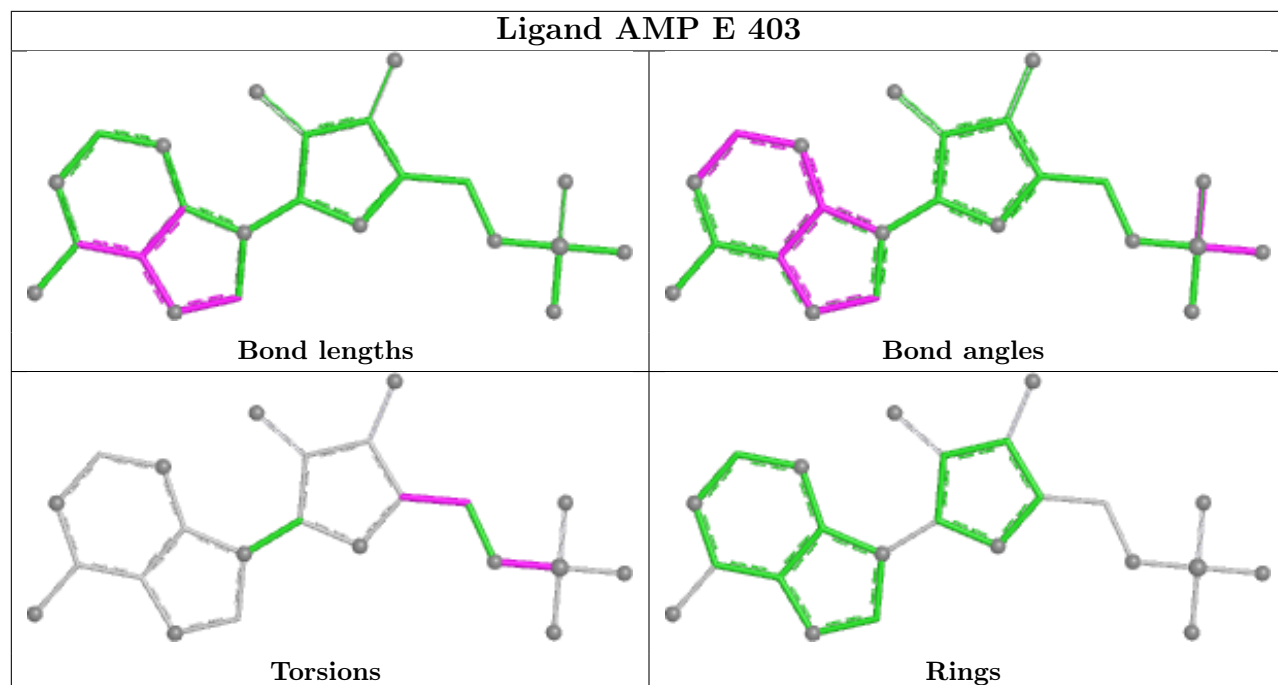


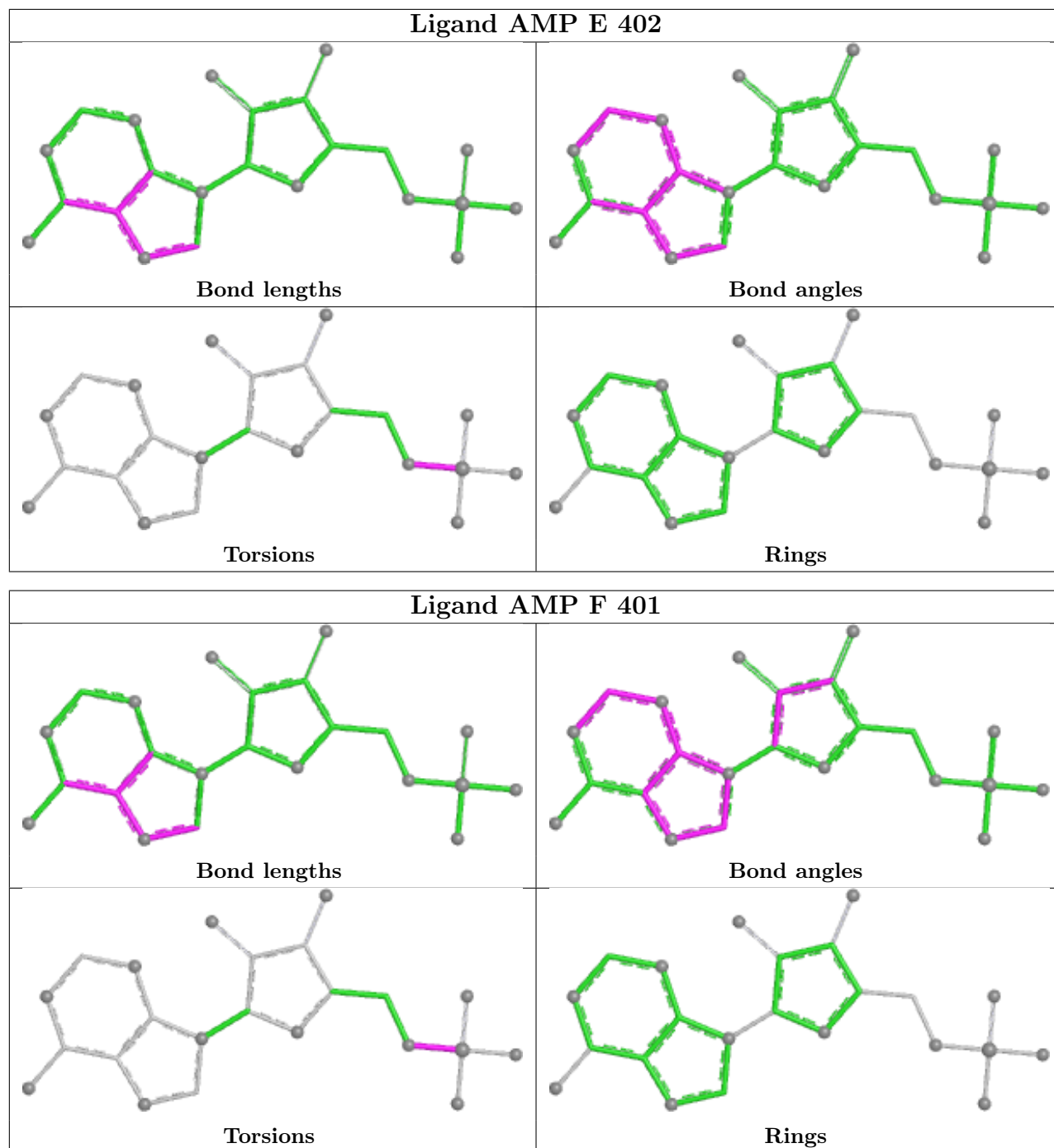
Torsions



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	453/552 (82%)	-0.37	2 (0%) 88 87	49, 79, 133, 171	0
1	C	429/552 (77%)	-0.25	10 (2%) 61 57	47, 80, 146, 172	0
2	B	182/286 (63%)	-0.40	0 100 100	48, 76, 116, 147	0
2	D	172/286 (60%)	0.15	10 (5%) 29 24	45, 97, 159, 179	0
3	E	298/331 (90%)	-0.58	0 100 100	48, 71, 116, 173	0
3	F	299/331 (90%)	-0.46	0 100 100	49, 72, 129, 180	0
All	All	1833/2338 (78%)	-0.34	22 (1%) 76 73	45, 77, 136, 180	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	136	ASP	3.7
2	D	148	THR	3.7
2	D	143	THR	3.3
1	C	281	PRO	3.1
2	D	193	VAL	3.1
2	D	246	ASP	3.0
1	C	550	LEU	3.0
2	D	172	LYS	2.6
1	C	301	GLU	2.5
1	A	316	PRO	2.5
2	D	150	ASN	2.5
1	C	68	LEU	2.5
1	C	374	ILE	2.4
2	D	137	PRO	2.4
1	C	156	ALA	2.4
1	C	286	ASN	2.2
1	A	377	SER	2.2
1	C	300	PHE	2.1
2	D	134	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	288	ILE	2.1
1	C	297	CYS	2.0
2	D	192	TYR	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	0.07	58,67,89,93	0
2	SEP	D	108	10/11	0.92	0.09	94,105,121,124	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.

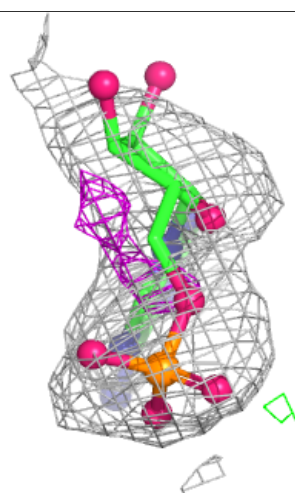
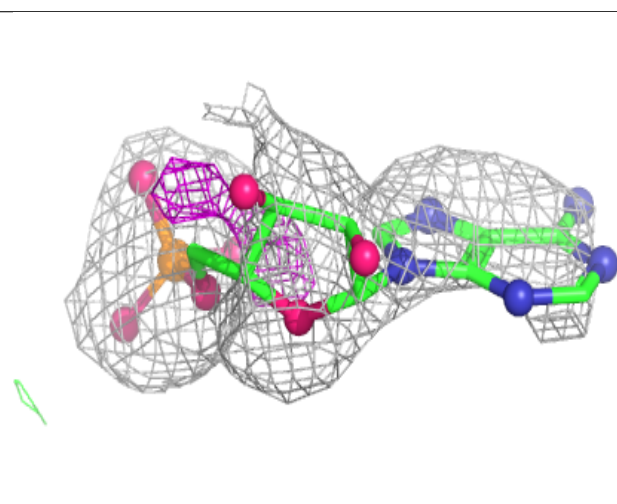
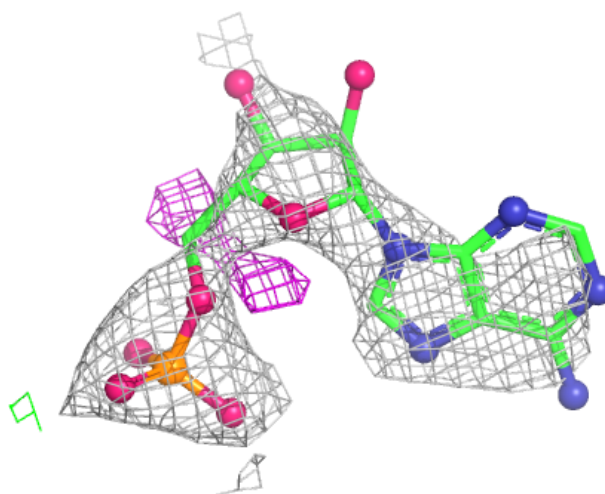
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	AMP	E	401	23/23	0.81	0.14	125,136,153,154	0
6	AMP	F	401	23/23	0.89	0.12	110,134,147,151	0
5	992	A	602	31/31	0.95	0.09	50,70,87,97	0
5	992	C	602	31/31	0.96	0.09	67,83,106,120	0
4	STU	A	601	35/35	0.98	0.05	42,51,61,61	0
6	AMP	E	402	23/23	0.98	0.05	57,61,66,69	0
6	AMP	E	403	23/23	0.98	0.05	56,66,73,80	0
4	STU	C	601	35/35	0.98	0.06	41,51,63,65	0
6	AMP	F	402	23/23	0.98	0.05	56,65,71,76	0
6	AMP	F	403	23/23	0.98	0.05	55,72,77,83	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.

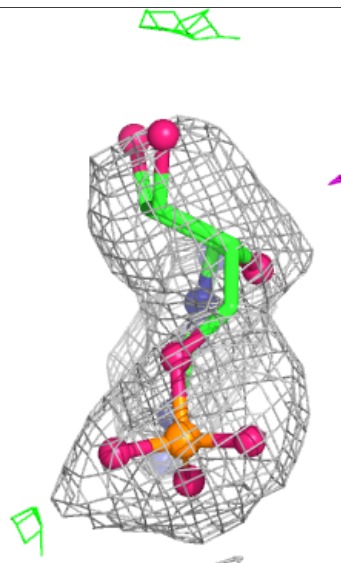
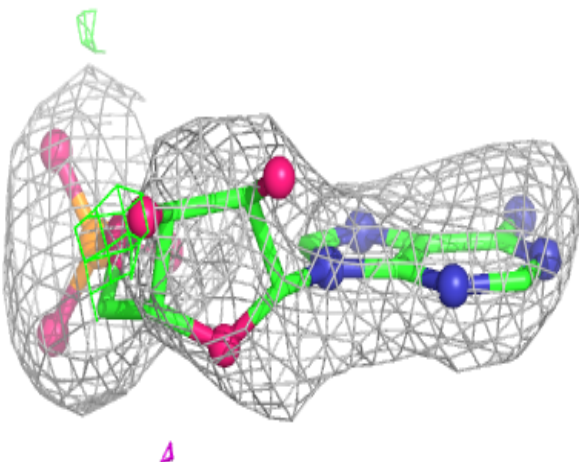
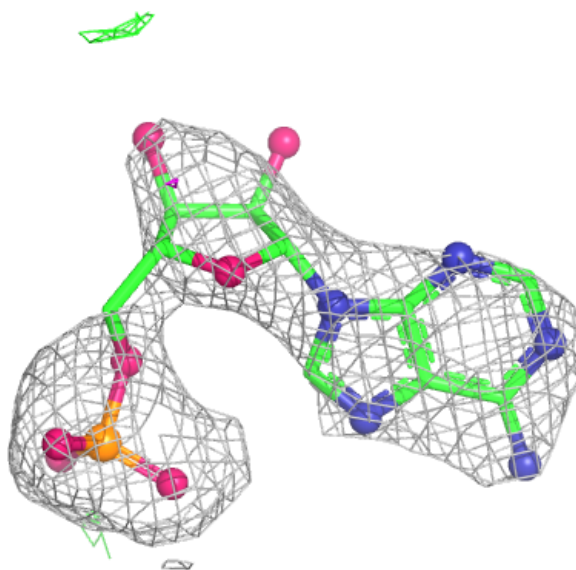
Electron density around AMP E 401:

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



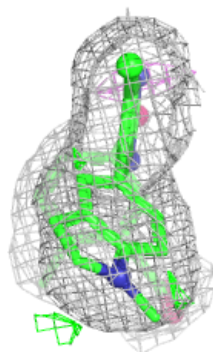
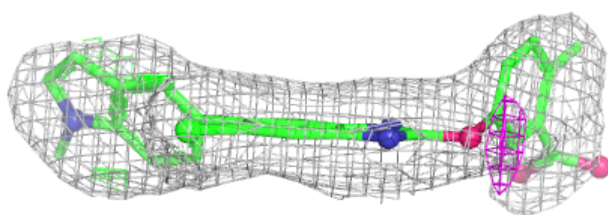
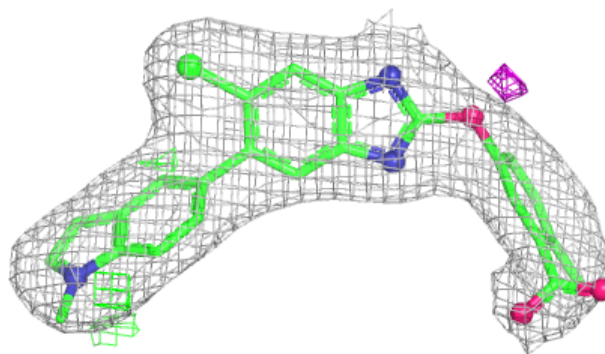
Electron density around AMP F 401:

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and green (positive)

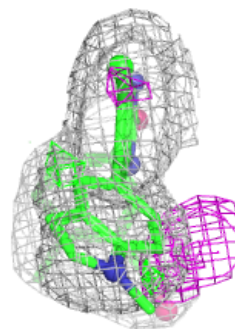
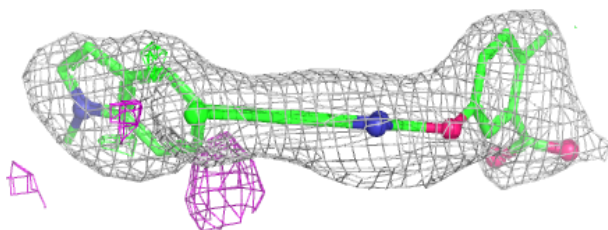
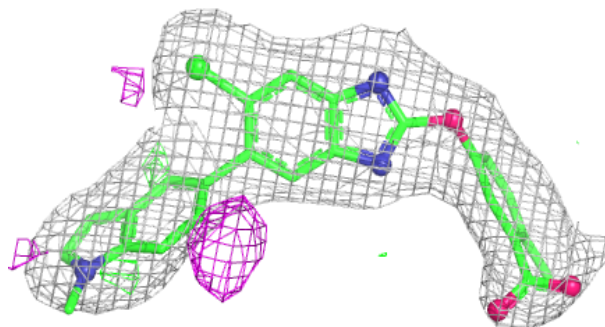


Electron density around 992 A 602:

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and green (positive)

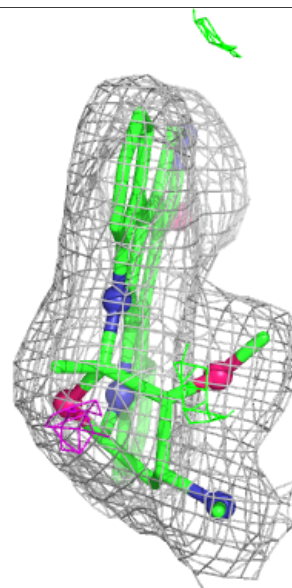
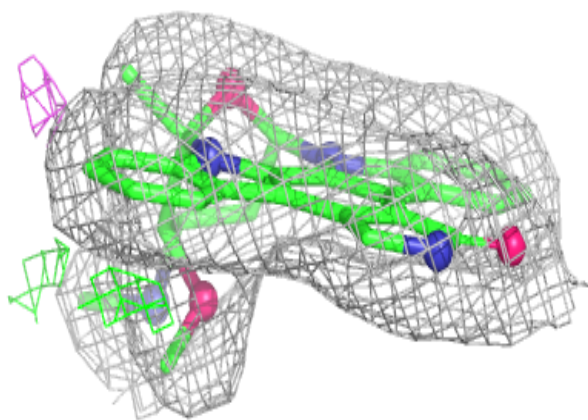
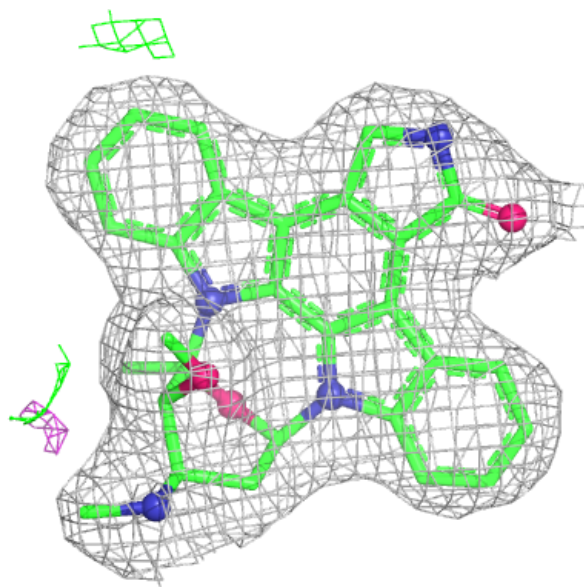
**Electron density around 992 C 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



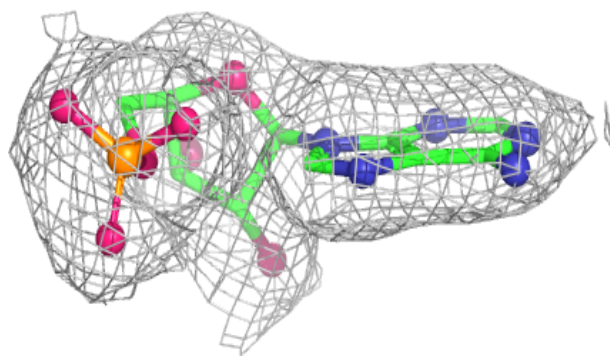
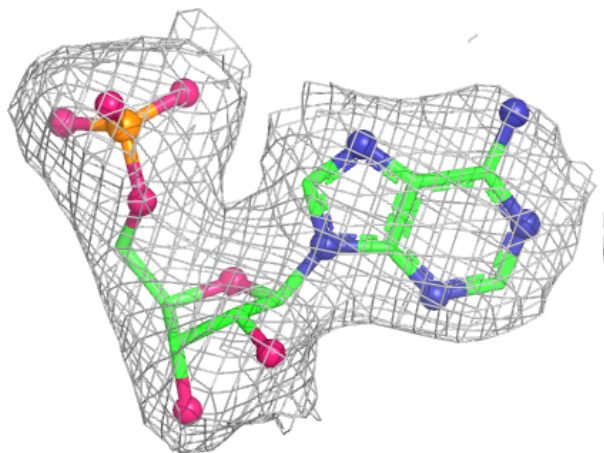
Electron density around STU A 601:

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and green (positive)



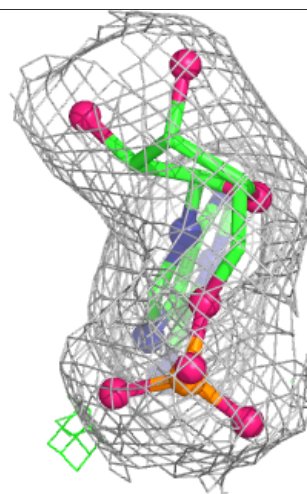
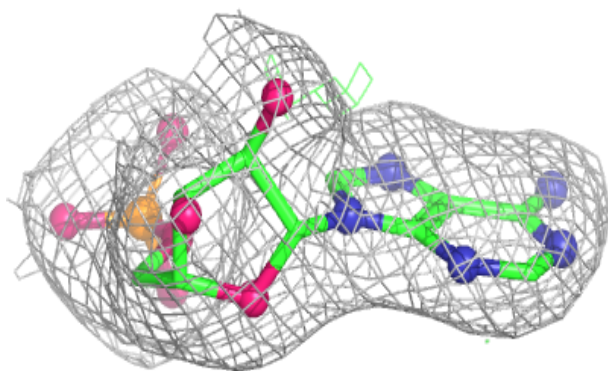
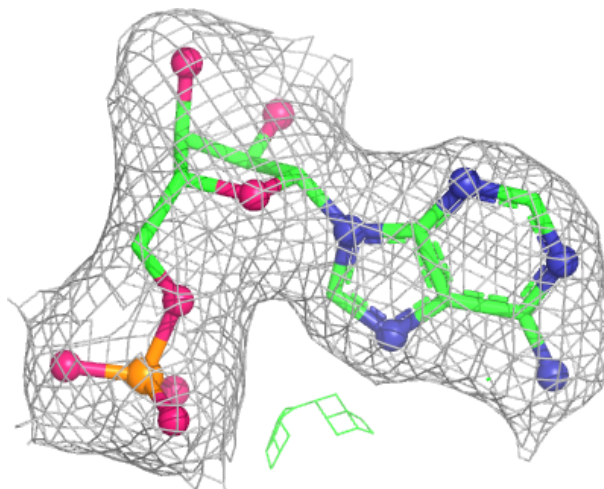
Electron density around AMP E 402:

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and green (positive)



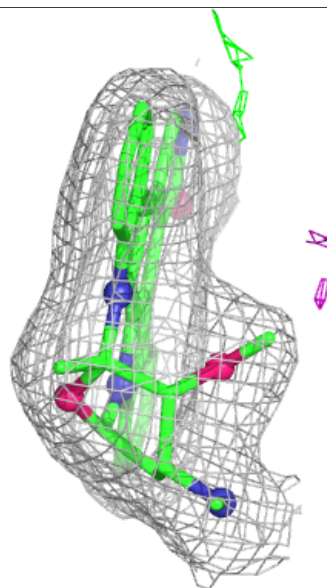
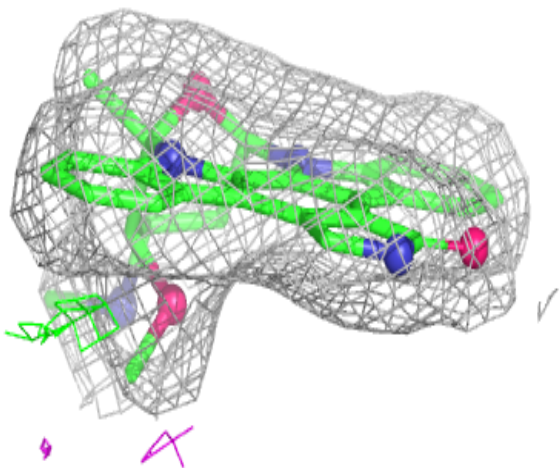
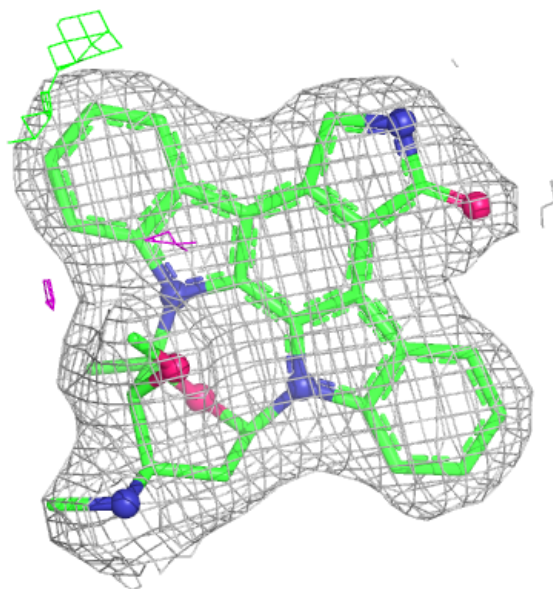
Electron density around AMP E 403:

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



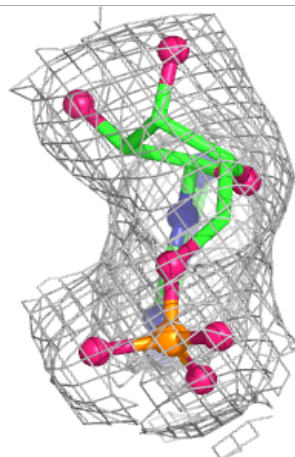
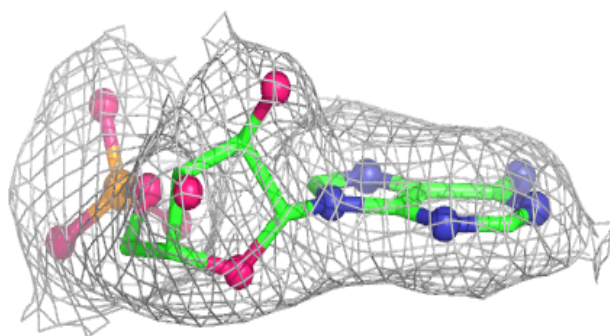
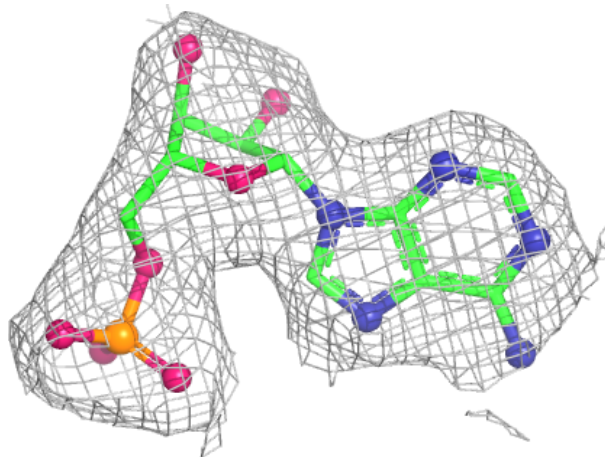
Electron density around STU C 601:

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



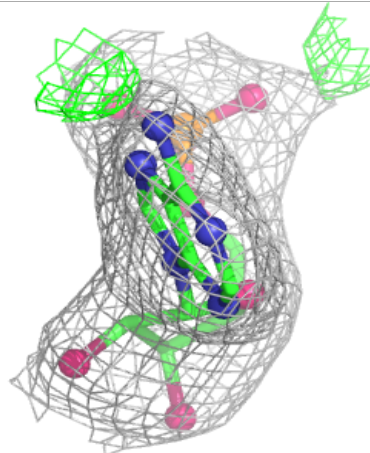
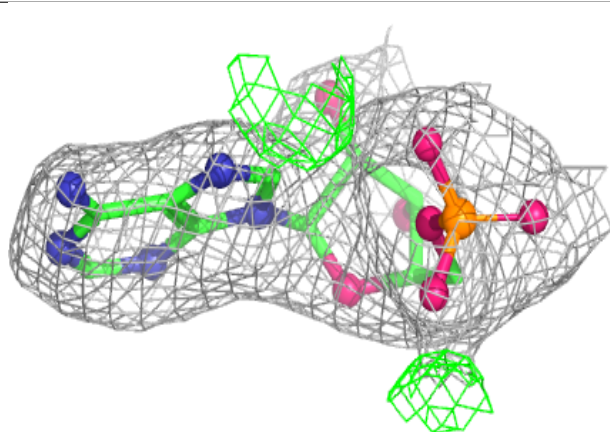
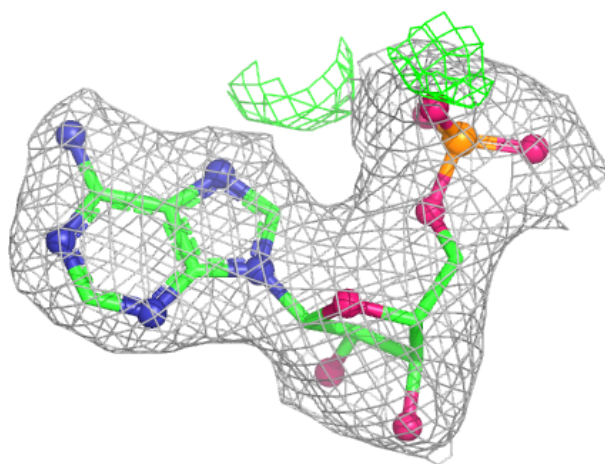
Electron density around AMP F 402:

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



Electron density around AMP F 403:

$2mF_o-DF_c$ (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.