



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 PM UTC

PDB ID : 4CFF / pdb_00004cff
Title : Structure of full length human AMPK in complex with a small molecule activator, a thienopyridone derivative (A-769662)
Authors : Xiao, B.; Sanders, M.J.; Carmena, D.; Bright, N.J.; Haire, L.F.; Underwood, E.; Patel, B.R.; Heath, R.B.; Walker, P.A.; Hallen, S.; Giordanetto, F.; Martin, S.R.; Carling, D.; Gamblin, S.J.
Deposited on : 2013-11-14
Resolution : 3.92 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](#) ①) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (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

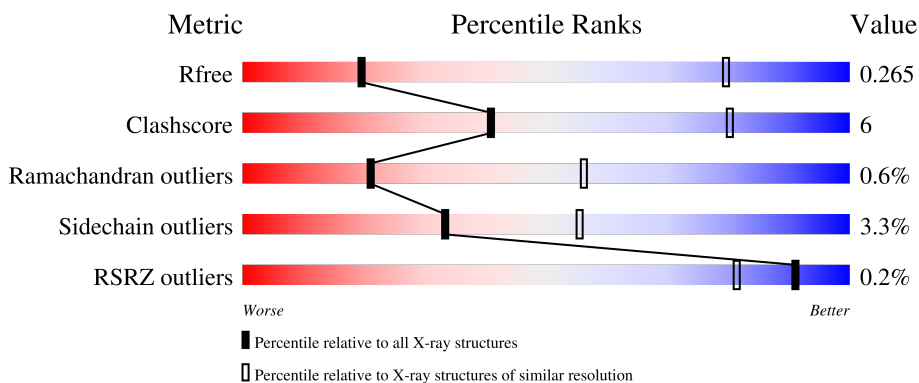
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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	571	
1	C	571	
2	B	286	
2	D	286	
3	E	331	

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Mol	Chain	Length	Quality of chain
3	F	331	 69% 18% 12%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 14484 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 SUB-UNIT ALPHA-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	425	3403	2187	592	601	1	22	0	0	0
1	C	423	3394	2182	590	599	1	22	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P54646
A	-17	SER	-	expression tag	UNP P54646
A	-16	HIS	-	expression tag	UNP P54646
A	-15	HIS	-	expression tag	UNP P54646
A	-14	HIS	-	expression tag	UNP P54646
A	-13	HIS	-	expression tag	UNP P54646
A	-12	HIS	-	expression tag	UNP P54646
A	-11	HIS	-	expression tag	UNP P54646
A	-10	SER	-	expression tag	UNP P54646
A	-9	SER	-	expression tag	UNP P54646
A	-8	GLY	-	expression tag	UNP P54646
A	-7	LEU	-	expression tag	UNP P54646
A	-6	GLU	-	expression tag	UNP P54646
A	-5	VAL	-	expression tag	UNP P54646
A	-4	LEU	-	expression tag	UNP P54646
A	-3	PHE	-	expression tag	UNP P54646
A	-2	GLN	-	expression tag	UNP P54646
A	-1	GLY	-	expression tag	UNP P54646
A	0	PRO	-	expression tag	UNP P54646
C	-18	MET	-	expression tag	UNP P54646
C	-17	SER	-	expression tag	UNP P54646
C	-16	HIS	-	expression tag	UNP P54646
C	-15	HIS	-	expression tag	UNP P54646
C	-14	HIS	-	expression tag	UNP P54646

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	expression tag	UNP P54646
C	-12	HIS	-	expression tag	UNP P54646
C	-11	HIS	-	expression tag	UNP P54646
C	-10	SER	-	expression tag	UNP P54646
C	-9	SER	-	expression tag	UNP P54646
C	-8	GLY	-	expression tag	UNP P54646
C	-7	LEU	-	expression tag	UNP P54646
C	-6	GLU	-	expression tag	UNP P54646
C	-5	VAL	-	expression tag	UNP P54646
C	-4	LEU	-	expression tag	UNP P54646
C	-3	PHE	-	expression tag	UNP P54646
C	-2	GLN	-	expression tag	UNP P54646
C	-1	GLY	-	expression tag	UNP P54646
C	0	PRO	-	expression tag	UNP P54646

- Molecule 2 is a protein called 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT BETA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	P	S			
2	B	171	1351	872	227	246	1	5	0	0	0
2	D	172	1356	875	228	247	1	5	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	expression tag	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

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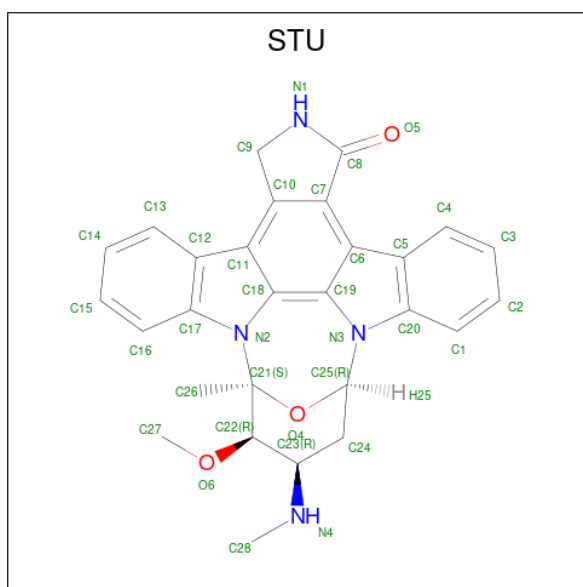
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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLU	-	expression tag	UNP Q9Y478
D	-15	MET	-	expression tag	UNP Q9Y478
D	-14	GLY	-	expression tag	UNP Q9Y478
D	-13	LEU	-	expression tag	UNP Q9Y478
D	-12	ASN	-	expression tag	UNP Q9Y478
D	-11	ASP	-	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.

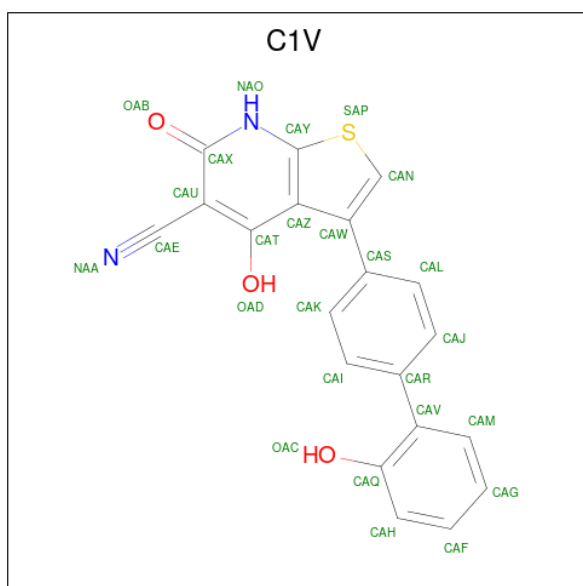
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	299	2412	1568	400	437	7	0	0	0
3	F	292	2354	1531	391	425	7	0	0	0

- Molecule 4 is STAUROSPORINE (CCD ID: STU) (formula: C₂₈H₂₆N₄O₃).



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

- Molecule 5 is 3-[4-(2-hydroxyphenyl)phenyl]-4-oxidanyl-6-oxidanylidene-7H-thieno[2,3-b]pyridine-5-carbonitrile (CCD ID: C1V) (formula: $C_{20}H_{12}N_2O_3S$).



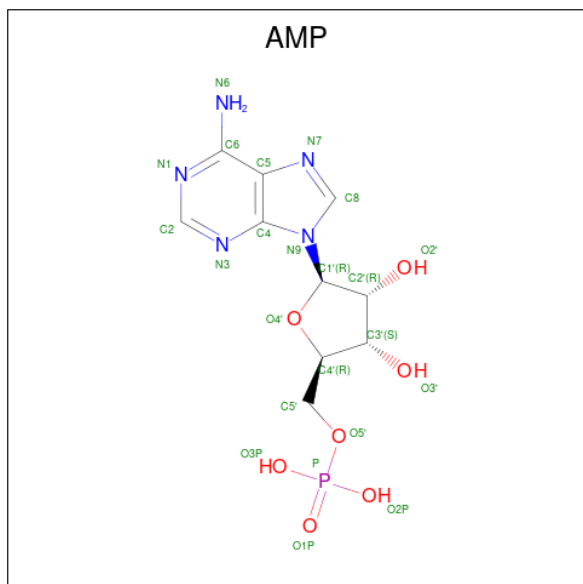
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	B	1	26	20	2	3	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	C	1	26	20	2	3	1	0	0

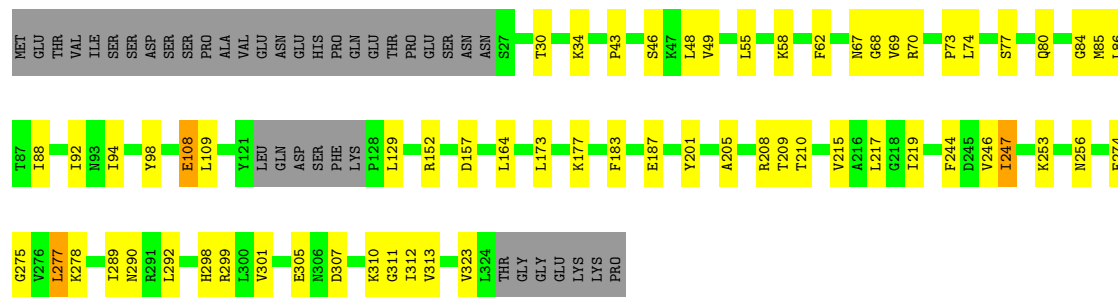
- Molecule 6 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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

- Molecule 3: 5'-AMP-ACTIVATED PROTEIN KINASE SUBUNIT GAMMA-1

Chain F:  69% 18% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.02Å 134.79Å 141.29Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	19.93 – 3.92 19.93 – 3.92	Depositor EDS
% Data completeness (in resolution range)	94.1 (19.93-3.92) 93.4 (19.93-3.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.94Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.208 , 0.264 0.210 , 0.265	Depositor DCC
R_{free} test set	1208 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	124.8	Xtrriage
Anisotropy	0.604	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14484	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: STU, SEP, AMP, TPO, C1V

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	0.29	0/3470	0.71	2/4687 (0.0%)
1	C	0.29	0/3461	0.71	2/4675 (0.0%)
2	B	0.31	0/1376	0.76	2/1872 (0.1%)
2	D	0.30	0/1381	0.79	4/1879 (0.2%)
3	E	0.32	0/2463	0.73	2/3344 (0.1%)
3	F	0.30	0/2403	0.71	2/3261 (0.1%)
All	All	0.30	0/14554	0.73	14/19718 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	191(D)	PRO	N-CA-CB	7.40	110.33	103.15
1	C	277	PHE	CA-C-N	6.72	126.23	119.24
1	C	277	PHE	C-N-CA	6.72	126.23	119.24
2	B	191(B)	PRO	N-CA-CB	6.58	110.16	103.25
2	D	196(D)	PRO	N-CA-CB	6.31	109.94	103.00
3	F	183	PHE	CA-C-N	5.57	125.57	119.89
3	F	183	PHE	C-N-CA	5.57	125.57	119.89
2	B	189(B)	GLN	N-CA-C	5.28	115.52	108.23
3	E	273	PHE	CB-CA-C	-5.18	110.19	117.23
1	A	277	PHE	CA-C-N	5.05	124.65	119.05
1	A	277	PHE	C-N-CA	5.05	124.65	119.05
2	D	193(D)	VAL	CA-C-N	5.04	130.77	121.70
2	D	193(D)	VAL	C-N-CA	5.04	130.77	121.70
3	E	124	ASP	CB-CA-C	5.03	115.96	109.28

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	3403	0	3394	49	0
1	C	3394	0	3386	45	0
2	B	1351	0	1329	23	0
2	D	1356	0	1329	23	0
3	E	2412	0	2483	35	0
3	F	2354	0	2426	31	0
4	A	35	0	26	3	0
4	C	35	0	26	3	0
5	B	26	0	12	1	0
5	C	26	0	12	0	0
6	E	46	0	24	1	0
6	F	46	0	24	2	0
All	All	14484	0	14471	188	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 6.

All (188) 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:C:370:MET:HG3	3:F:68:GLY:HA2	1.66	0.77
1:A:179:TYR:HA	1:A:202:VAL:HG11	1.73	0.71
1:C:430:TRP:HB3	1:C:440:VAL:HA	1.71	0.70
2:D:122:GLU:HG2	2:D:154:GLN:HG2	1.74	0.70
1:C:402:TRP:HB2	2:D:213:VAL:HG11	1.74	0.69
2:B:264:THR:HG22	3:E:48:LEU:HD23	1.75	0.68
3:F:98:TYR:CG	3:F:108:GLU:HG3	2.29	0.67
1:A:194:GLU:O	1:A:256:ARG:NH1	2.24	0.67
3:E:92:ILE:HG23	3:E:217:LEU:HD22	1.77	0.67
3:E:98:TYR:CG	3:E:108:GLU:HG3	2.31	0.65
1:A:100:GLU:OE2	4:A:1552:STU:N4	2.31	0.64
1:C:194:GLU:O	1:C:256:ARG:NH1	2.29	0.64
1:C:179:TYR:HA	1:C:202:VAL:HG11	1.79	0.64
3:F:94:ILE:HG21	3:F:109:LEU:HD13	1.81	0.63
3:F:88:ILE:HG23	3:F:247:ILE:HG23	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:74:LEU:HD21	3:E:86:LEU:HB2	1.80	0.62
1:A:423:MET:HB3	1:A:428:PHE:HB2	1.83	0.61
2:D:269:PRO:HG3	3:F:55:LEU:HA	1.81	0.61
1:C:158:PHE:O	1:C:160:LEU:N	2.33	0.61
1:C:63:ARG:NH2	1:C:162:ASN:OD1	2.34	0.61
4:C:1552:STU:H261	4:C:1552:STU:H16	1.83	0.61
3:E:244:PHE:HB3	6:E:1326:AMP:H5'1	1.84	0.60
1:A:142:PRO:HD3	1:A:203:ILE:HG12	1.82	0.60
3:F:277:LEU:HB2	6:F:1325:AMP:N1	2.17	0.59
1:C:423:MET:HB3	1:C:428:PHE:HB2	1.83	0.59
3:E:43:PRO:HG2	3:E:46:SER:HB3	1.85	0.58
1:C:454:SER:HB3	1:C:470:LYS:HB3	1.86	0.57
4:A:1552:STU:H261	4:A:1552:STU:H16	1.86	0.57
2:B:248:VAL:HA	2:B:269:PRO:HA	1.85	0.57
3:E:37:ARG:HD3	3:E:39:TYR:HB3	1.86	0.57
3:F:278:LYS:NZ	3:F:307:ASP:OD1	2.35	0.57
1:A:82:VAL:HG13	2:B:162:VAL:HG21	1.86	0.57
1:C:462:ASN:OD1	1:C:462:ASN:N	2.38	0.57
1:A:134:MET:HA	1:A:164:MET:HE2	1.86	0.56
1:A:165:SER:HB2	1:A:168:GLU:HB2	1.86	0.56
1:A:63:ARG:O	1:A:67:ASN:ND2	2.32	0.56
1:A:218:HIS:CD2	1:A:220:PRO:HD2	2.40	0.56
1:A:11:VAL:HG22	2:B:115:ILE:HD12	1.88	0.56
1:A:22:LEU:HD21	1:A:32:ILE:HB	1.88	0.56
2:B:206:LEU:HD12	2:B:207:PRO:HD2	1.87	0.55
1:A:428:PHE:HE1	1:A:442:ARG:HD3	1.71	0.55
1:C:428:PHE:HE1	1:C:442:ARG:HD3	1.71	0.55
3:E:304:ASP:O	3:E:306:ASN:N	2.39	0.55
3:F:209:THR:HG23	3:F:210:THR:HG23	1.89	0.54
1:C:85:THR:HG22	2:D:79:PRO:HG2	1.89	0.54
1:A:469:PHE:HE2	1:A:546:LEU:HD23	1.72	0.54
1:A:429:GLU:OE1	1:A:441:ARG:NH1	2.41	0.54
2:B:122:GLU:HG2	2:B:154:GLN:HG2	1.90	0.54
1:A:454:SER:HB3	1:A:470:LYS:HB3	1.90	0.53
1:A:412:PRO:HG3	1:A:465:TYR:CZ	2.44	0.53
2:D:267:TYR:HE1	3:F:67:ASN:HD21	1.57	0.52
3:E:56:GLN:NE2	3:E:110:GLU:O	2.42	0.52
3:E:88:ILE:HG23	3:E:247:ILE:HG23	1.90	0.52
3:F:92:ILE:HG23	3:F:217:LEU:HD22	1.90	0.52
1:A:469:PHE:HB2	2:B:239:LEU:HB3	1.92	0.52
3:F:84:GLY:HA2	3:F:129:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:HIS:CG	1:C:74:PRO:HD2	2.45	0.51
3:E:33:MET:O	3:E:139:PHE:N	2.43	0.51
2:D:126:LYS:HE3	2:D:133:TRP:CE3	2.45	0.51
1:C:132:ARG:CZ	1:C:278:PRO:HG2	2.41	0.51
3:E:70:ARG:HH21	3:E:244:PHE:HB2	1.75	0.51
1:A:369:ARG:NH2	2:B:220:GLY:O	2.45	0.50
3:F:298:HIS:HB3	3:F:299:ARG:NH2	2.26	0.50
2:D:224:ASP:HB3	2:D:227:LEU:HG	1.92	0.50
3:F:74:LEU:HD21	3:F:86:LEU:HB2	1.93	0.50
3:E:173:LEU:HD21	3:E:289:ILE:HG23	1.94	0.50
2:B:108:SEP:OG	2:B:109:HIS:N	2.38	0.50
1:C:218:HIS:CD2	1:C:220:PRO:HD2	2.46	0.49
2:B:256:ARG:NH1	2:B:258:LYS:O	2.36	0.49
1:A:443:LYS:NZ	1:A:448:GLY:O	2.45	0.49
2:D:81:VAL:HG22	2:D:115:ILE:HG12	1.94	0.49
3:F:77:SER:O	3:F:80:GLN:NE2	2.34	0.49
1:C:366:HIS:HB3	1:C:369:ARG:HG2	1.93	0.49
1:C:434:ASN:HB3	1:C:437:HIS:HB3	1.94	0.48
2:D:84:TRP:HB3	2:D:112:PHE:HB2	1.95	0.48
3:F:58:LYS:HE2	3:F:62:PHE:CE2	2.49	0.48
1:A:229:GLY:HA3	1:A:251:VAL:HG22	1.95	0.48
3:E:94:ILE:HG21	3:E:109:LEU:HD13	1.95	0.48
3:E:73:PRO:HD3	3:E:166:ILE:HD11	1.95	0.48
2:D:206:LEU:HD12	2:D:207:PRO:HD2	1.96	0.47
1:A:26:THR:HG21	1:A:160:LEU:HG	1.95	0.47
1:C:157:ASP:HB2	4:C:1552:STU:H273	1.96	0.47
3:E:145:LEU:HD13	3:E:169:HIS:CD2	2.50	0.47
1:A:247:HIS:CG	1:A:257:ALA:HB2	2.49	0.47
1:C:112:GLU:HG2	1:C:114:MET:H	1.80	0.47
1:C:272:LEU:HD12	1:C:273:PRO:HD2	1.97	0.47
3:E:101:SER:OG	3:E:102:ALA:N	2.48	0.47
2:D:221:ILE:H	2:D:221:ILE:HD13	1.79	0.47
1:A:278:PRO:HA	1:A:283:TYR:CG	2.49	0.47
1:C:66:GLN:HA	1:C:69:LYS:HE3	1.96	0.47
3:E:49:VAL:O	3:E:73:PRO:HD2	2.15	0.47
1:C:123:ILE:HD11	1:C:145:VAL:HG11	1.95	0.47
1:A:430:TRP:HB3	1:A:440:VAL:HG12	1.96	0.47
3:E:41:LEU:HD21	3:E:172:ILE:HA	1.97	0.47
1:A:35:HIS:HB3	1:A:39:GLY:H	1.79	0.47
1:A:402:TRP:HB2	2:B:213:VAL:HG11	1.97	0.47
1:C:21:THR:HG22	1:C:23:GLY:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:GLU:HB3	2:D:164:ASP:HB2	1.97	0.46
1:A:366:HIS:HB3	1:A:369:ARG:HG2	1.97	0.46
1:C:117:ARG:NH1	1:C:267:TRP:O	2.44	0.46
1:C:60:LYS:HA	1:C:63:ARG:HH11	1.81	0.46
1:C:85:THR:OG1	1:C:88:ASP:O	2.28	0.46
1:C:365:PRO:HA	2:D:221:ILE:O	2.16	0.45
2:B:84:TRP:HB3	2:B:112:PHE:HB2	1.97	0.45
3:E:212:PRO:HB2	3:E:215:VAL:HG23	1.99	0.45
3:F:49:VAL:O	3:F:73:PRO:HD2	2.16	0.45
1:A:63:ARG:HH21	1:A:163:MET:HG2	1.81	0.45
1:A:138:ARG:HH12	1:A:172:TPO:HB	1.82	0.45
2:D:118:LEU:HA	2:D:119:PRO:HD3	1.87	0.45
3:F:85:MET:HB3	3:F:85:MET:HE3	1.88	0.45
1:A:112:GLU:HG2	1:A:114:MET:H	1.81	0.45
3:F:177:LYS:NZ	3:F:290:ASN:OD1	2.49	0.45
3:E:108:GLU:H	3:E:108:GLU:HG2	1.50	0.45
3:F:62:PHE:CZ	3:F:253:LYS:HE3	2.52	0.45
3:F:274:GLU:HA	3:F:275:GLY:HA3	1.69	0.45
1:A:434:ASN:HB3	1:A:437:HIS:HB3	1.99	0.44
1:C:247:HIS:CG	1:C:257:ALA:HB2	2.52	0.44
2:D:193(D):VAL:HA	2:D:194(D):CYS:CB	2.47	0.44
3:E:298:HIS:HB3	3:E:299:ARG:NH2	2.33	0.44
3:F:70:ARG:HH21	3:F:244:PHE:HB2	1.82	0.44
1:A:182:PRO:HD3	1:A:198:TRP:CE2	2.52	0.44
1:C:134:MET:HE3	1:C:164:MET:HB2	1.99	0.44
3:E:37:ARG:NH1	3:E:40:ASP:OD2	2.51	0.44
1:A:30:VAL:HG21	4:A:1552:STU:C17	2.47	0.44
1:A:214:PHE:HE2	1:A:230:VAL:H	1.65	0.44
3:E:123:GLN:OE1	3:E:124:ASP:N	2.51	0.44
2:B:224:ASP:HB3	2:B:227:LEU:HG	2.00	0.44
1:C:168:GLU:OE2	1:C:470:LYS:NZ	2.47	0.44
2:B:239:LEU:HD11	2:B:251:LEU:HB3	2.00	0.43
3:F:157:ASP:HB2	3:F:164:LEU:HD11	2.00	0.43
1:C:53:ARG:NH2	2:D:169:ASP:OD1	2.52	0.43
2:B:84:TRP:CZ2	2:B:129:VAL:HG21	2.53	0.43
2:B:108:SEP:P	2:B:109:HIS:H	2.41	0.43
1:C:12:LYS:HG2	1:C:17:VAL:HG22	1.99	0.43
1:A:126:ALA:HB3	1:A:155:ILE:HD13	1.98	0.43
3:E:70:ARG:NH2	3:E:244:PHE:HB2	2.34	0.43
1:A:167:GLY:HA2	2:B:234:VAL:O	2.19	0.43
1:C:322:VAL:HG12	1:C:326:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:315:LEU:HD12	3:E:315:LEU:HA	1.83	0.43
1:A:31:LYS:NZ	2:B:108:SEP:O3P	2.47	0.43
1:C:192:GLY:N	1:C:194:GLU:OE2	2.45	0.43
3:E:239:ASP:OD1	3:E:240:ILE:N	2.46	0.43
3:F:173:LEU:HD21	3:F:289:ILE:HG23	2.01	0.43
1:A:370:MET:HA	1:A:371:PRO:HD3	1.94	0.43
1:A:536:THR:OG1	3:E:162:ASN:ND2	2.52	0.43
1:C:469:PHE:HB2	2:D:239:LEU:HB3	2.01	0.43
3:E:122:LEU:HD22	3:E:125:SER:OG	2.19	0.43
1:C:83:ILE:HB	1:C:90:PHE:HB2	2.01	0.42
1:C:123:ILE:HG23	1:C:155:ILE:HD11	2.01	0.42
1:C:62:LYS:HB2	2:D:166:LEU:HD13	2.01	0.42
3:F:215:VAL:O	3:F:219:ILE:HG13	2.19	0.42
3:F:205:ALA:N	6:F:1326:AMP:N1	2.60	0.42
1:A:79:LEU:HD13	1:A:93:MET:HE2	2.01	0.42
1:A:139:ASP:O	1:A:144:ASN:ND2	2.40	0.42
1:A:51:LYS:HD2	1:A:51:LYS:HA	1.81	0.42
3:F:201:TYR:CD1	3:F:311:GLY:HA3	2.54	0.42
1:A:73:HIS:CG	1:A:74:PRO:HD2	2.54	0.42
1:A:107:LYS:HG2	1:A:108:HIS:ND1	2.35	0.42
1:A:101:LEU:O	1:A:105:ILE:HG13	2.20	0.41
1:A:11:VAL:HG21	2:B:113:VAL:HG13	2.02	0.41
1:C:87:THR:OG1	2:D:81:VAL:HB	2.20	0.41
2:D:203:PRO:HA	2:D:204:PRO:HD3	1.88	0.41
3:F:30:THR:HG22	3:F:34:LYS:HE3	2.03	0.41
2:B:268:LYS:HA	2:B:269:PRO:HD2	1.95	0.41
3:F:301:VAL:HA	3:F:312:ILE:HD13	2.02	0.41
2:B:106:THR:HG22	5:B:1271:CIV:HAG	2.02	0.41
3:E:278:LYS:NZ	3:E:307:ASP:OD1	2.53	0.41
1:C:96:VAL:HG11	1:C:154:LYS:HG3	2.02	0.41
2:D:232:ASN:OD1	2:D:233:HIS:N	2.53	0.41
2:D:264:THR:HG22	3:F:48:LEU:HB3	2.03	0.41
3:E:85:MET:HE3	3:E:85:MET:HB3	1.92	0.41
1:C:48:ASN:O	1:C:52:ILE:HG12	2.21	0.41
3:F:43:PRO:HG2	3:F:46:SER:HB3	2.02	0.41
1:A:218:HIS:ND1	1:A:221:THR:OG1	2.46	0.41
2:B:161:GLU:HB3	2:B:164:ASP:HB2	2.03	0.41
3:E:209:THR:O	3:E:263:THR:OG1	2.28	0.40
3:F:92:ILE:HG12	3:F:246:VAL:HG11	2.03	0.40
1:C:193:PRO:O	1:C:197:ILE:HG12	2.20	0.40
4:C:1552:STU:H22	4:C:1552:STU:H283	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:98:TYR:CD2	3:E:108:GLU:HG3	2.56	0.40
3:E:209:THR:HG23	3:E:210:THR:HG23	2.03	0.40
1:A:8:ASP:HA	1:A:10:ARG:NH1	2.36	0.40
2:B:136:ASP:HA	2:B:137:PRO:HD3	1.93	0.40
1:C:31:LYS:HD2	1:C:46:ILE:HD11	2.04	0.40
1:C:406:ILE:HD12	1:C:406:ILE:HA	1.99	0.40
1:C:412:PRO:HG3	1:C:465:TYR:CZ	2.55	0.40
2:D:248:VAL:HA	2:D:269:PRO:HA	2.02	0.40
3:E:167:LEU:HD12	3:E:167:LEU:HA	1.93	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	414/571 (72%)	388 (94%)	26 (6%)	0	100	100
1	C	412/571 (72%)	390 (95%)	21 (5%)	1 (0%)	43	75
2	B	164/286 (57%)	157 (96%)	5 (3%)	2 (1%)	10	41
2	D	165/286 (58%)	153 (93%)	9 (6%)	3 (2%)	6	34
3	E	297/331 (90%)	278 (94%)	15 (5%)	4 (1%)	9	40
3	F	288/331 (87%)	275 (96%)	12 (4%)	1 (0%)	36	70
All	All	1740/2376 (73%)	1641 (94%)	88 (5%)	11 (1%)	21	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	191(B)	PRO
1	C	159	GLY
3	E	184	PRO

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Mol	Chain	Res	Type
3	F	277	LEU
2	D	193(D)	VAL
2	D	195(D)	LYS
3	E	186	PRO
3	E	305	GLU
2	B	190(B)	GLU
2	D	221	ILE
3	E	276	VAL

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	364/503 (72%)	356 (98%)	8 (2%)	45	64
1	C	364/503 (72%)	352 (97%)	12 (3%)	33	55
2	B	149/253 (59%)	145 (97%)	4 (3%)	39	60
2	D	149/253 (59%)	147 (99%)	2 (1%)	61	72
3	E	275/304 (90%)	261 (95%)	14 (5%)	21	46
3	F	268/304 (88%)	256 (96%)	12 (4%)	24	48
All	All	1569/2120 (74%)	1517 (97%)	52 (3%)	33	55

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	24	VAL
1	A	82	VAL
1	A	140	LEU
1	A	168	GLU
1	A	171	ARG
1	A	194	GLU
1	A	202	VAL
2	B	98	ASN
2	B	150	ASN

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Mol	Chain	Res	Type
2	B	221	ILE
2	B	234	VAL
1	C	10	ARG
1	C	24	VAL
1	C	82	VAL
1	C	136	VAL
1	C	140	LEU
1	C	168	GLU
1	C	171	ARG
1	C	194	GLU
1	C	202	VAL
1	C	326	LEU
1	C	432	VAL
1	C	462	ASN
2	D	98	ASN
2	D	221	ILE
3	E	37	ARG
3	E	98	TYR
3	E	108	GLU
3	E	123	GLN
3	E	124	ASP
3	E	126	PHE
3	E	208	ARG
3	E	247	ILE
3	E	256	ASN
3	E	273	PHE
3	E	276	VAL
3	E	292	LEU
3	E	313	VAL
3	E	315	LEU
3	F	69	VAL
3	F	108	GLU
3	F	152	ARG
3	F	187	GLU
3	F	208	ARG
3	F	247	ILE
3	F	256	ASN
3	F	292	LEU
3	F	305	GLU
3	F	310	LYS
3	F	313	VAL
3	F	323	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	535	HIS
2	B	98	ASN
2	B	109	HIS
2	B	135	HIS
1	C	178	ASN
1	C	250	GLN
1	C	335	ASN
1	C	336	GLN
2	D	111	ASN
2	D	124	GLN
2	D	154	GLN
2	D	233	HIS
3	E	36	HIS
3	E	112	HIS
3	E	162	ASN
3	F	56	GLN
3	F	67	ASN
3	F	267	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 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	$\# Z > 2$
1	TPO	A	172	1	8,10,11	0.86	0	10,14,16	1.12	1 (10%)
2	SEP	D	108	2	8,9,10	0.96	1 (12%)	7,12,14	0.85	0
1	TPO	C	172	1	8,10,11	0.85	0	10,14,16	1.14	1 (10%)

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	0.95	0	7,12,14	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	172	1	-	1/9/11/13	-
2	SEP	D	108	2	-	2/6/8/10	-
1	TPO	C	172	1	-	0/9/11/13	-
2	SEP	B	108	2	-	1/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	108	SEP	CA-N	-2.01	1.42	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	TPO	P-OG1-CB	-2.51	116.50	123.33
1	A	172	TPO	CG2-CB-CA	-2.08	109.21	113.26

There are no chirality outliers.

All (4) 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
2	D	108	SEP	CB-OG-P-O2P
1	A	172	TPO	CB-OG1-P-O2P

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	172	TPO	1	0
2	B	108	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
6	AMP	F	1325	-	25,25,25	1.41	4 (16%)	37,38,38	1.89	10 (27%)
4	STU	C	1552	-	39,42,42	0.73	2 (5%)	50,68,68	2.40	13 (26%)
6	AMP	E	1327	-	25,25,25	1.42	4 (16%)	37,38,38	1.89	8 (21%)
5	C1V	B	1271	-	28,29,29	2.56	9 (32%)	32,42,42	2.75	5 (15%)
6	AMP	F	1326	-	25,25,25	1.41	4 (16%)	37,38,38	1.91	9 (24%)
6	AMP	E	1326	-	25,25,25	1.44	4 (16%)	37,38,38	1.89	8 (21%)
4	STU	A	1552	-	39,42,42	0.74	2 (5%)	50,68,68	2.45	13 (26%)
5	C1V	C	1553	-	28,29,29	2.57	10 (35%)	32,42,42	2.80	5 (15%)

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
6	AMP	F	1325	-	-	1/10/26/26	0/3/3/3
4	STU	C	1552	-	-	1/4/42/42	-
6	AMP	E	1327	-	-	3/10/26/26	0/3/3/3
5	C1V	B	1271	-	-	0/8/10/10	0/4/4/4
6	AMP	F	1326	-	-	0/10/26/26	0/3/3/3
6	AMP	E	1326	-	-	3/10/26/26	0/3/3/3
4	STU	A	1552	-	-	1/4/42/42	-
5	C1V	C	1553	-	-	4/8/10/10	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1553	C1V	OAB-CAX	9.02	1.40	1.23
5	B	1271	C1V	OAB-CAX	8.89	1.40	1.23
6	E	1326	AMP	C5-C4	4.81	1.47	1.39
5	B	1271	C1V	CAS-CAW	4.73	1.55	1.48
6	E	1327	AMP	C5-C4	4.67	1.47	1.39
6	F	1325	AMP	C5-C4	4.66	1.47	1.39
6	F	1326	AMP	C5-C4	4.60	1.47	1.39
5	C	1553	C1V	CAS-CAW	4.52	1.55	1.48
5	C	1553	C1V	CAE-CAU	4.09	1.52	1.43
5	B	1271	C1V	CAE-CAU	3.92	1.51	1.43
5	B	1271	C1V	CAX-NAO	-3.51	1.32	1.38
5	C	1553	C1V	CAX-NAO	-3.27	1.32	1.38
5	C	1553	C1V	CAV-CAR	3.27	1.55	1.49
5	B	1271	C1V	CAU-CAX	-3.24	1.39	1.44
5	B	1271	C1V	CAV-CAR	3.09	1.55	1.49
5	C	1553	C1V	CAY-NAO	-2.87	1.34	1.38
5	B	1271	C1V	CAY-NAO	-2.85	1.34	1.38
5	C	1553	C1V	CAU-CAX	-2.82	1.40	1.44
5	C	1553	C1V	OAC-CAQ	2.82	1.42	1.36
6	E	1326	AMP	C5-C6	2.81	1.48	1.41
6	F	1326	AMP	C5-C6	2.78	1.48	1.41
5	B	1271	C1V	OAC-CAQ	2.78	1.41	1.36
6	F	1325	AMP	C5-C6	2.73	1.48	1.41
6	E	1327	AMP	C5-C6	2.68	1.48	1.41
5	C	1553	C1V	CAW-CAZ	2.63	1.50	1.44
5	B	1271	C1V	CAW-CAZ	2.56	1.50	1.44
6	E	1327	AMP	C8-N7	2.53	1.36	1.31
6	F	1326	AMP	C8-N7	2.39	1.36	1.31
4	A	1552	STU	O4-C25	-2.38	1.39	1.43
6	F	1325	AMP	C8-N7	2.36	1.36	1.31
6	E	1326	AMP	C8-N7	2.33	1.36	1.31
6	E	1327	AMP	C5-N7	-2.32	1.34	1.39
6	F	1326	AMP	C5-N7	-2.30	1.34	1.39
6	F	1325	AMP	C5-N7	-2.28	1.34	1.39
6	E	1326	AMP	C5-N7	-2.28	1.34	1.39
4	A	1552	STU	C19-N3	-2.24	1.35	1.39
4	C	1552	STU	O4-C25	-2.23	1.39	1.43
4	C	1552	STU	C19-N3	-2.16	1.35	1.39
5	C	1553	C1V	OAD-CAT	2.08	1.40	1.33

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1553	C1V	CAN-SAP-CAY	12.24	99.07	90.33
5	B	1271	C1V	CAN-SAP-CAY	11.88	98.81	90.33
4	A	1552	STU	C9-C10-C7	-8.74	106.67	109.88
4	C	1552	STU	C9-C10-C7	-8.67	106.70	109.88
5	C	1553	C1V	CAU-CAX-NAO	7.63	121.71	114.81
5	B	1271	C1V	CAU-CAX-NAO	7.16	121.29	114.81
4	C	1552	STU	C28-N4-C23	-6.21	106.97	114.39
6	F	1326	AMP	C5-C4-N3	-6.06	118.38	126.72
6	E	1327	AMP	C5-C4-N3	-6.00	118.46	126.72
4	A	1552	STU	C9-N1-C8	-5.99	108.40	113.86
6	E	1326	AMP	C5-C4-N3	-5.92	118.56	126.72
4	A	1552	STU	C28-N4-C23	-5.83	107.42	114.39
4	C	1552	STU	C9-N1-C8	-5.73	108.64	113.86
6	F	1325	AMP	C5-C4-N3	-5.72	118.84	126.72
4	A	1552	STU	C9-C10-C11	4.86	132.42	128.73
6	E	1326	AMP	N3-C4-N9	4.70	135.16	127.17
6	E	1327	AMP	N3-C4-N9	4.67	135.12	127.17
6	F	1326	AMP	N3-C4-N9	4.62	135.02	127.17
4	C	1552	STU	C9-C10-C11	4.58	132.21	128.73
4	A	1552	STU	C7-C8-N1	4.56	110.73	106.38
4	A	1552	STU	C10-C9-N1	4.55	106.18	101.75
6	F	1325	AMP	N3-C4-N9	4.55	134.91	127.17
4	C	1552	STU	C10-C9-N1	4.48	106.11	101.75
4	C	1552	STU	C7-C8-N1	4.30	110.48	106.38
4	A	1552	STU	C27-O6-C22	-4.02	107.67	114.46
4	C	1552	STU	C27-O6-C22	-3.79	108.05	114.46
6	F	1326	AMP	C4-C5-N7	-3.78	106.26	110.58
6	E	1326	AMP	C2-N3-C4	3.73	120.94	111.83
6	F	1326	AMP	C2-N3-C4	3.67	120.80	111.83
6	F	1325	AMP	C2-N3-C4	3.67	120.79	111.83
6	E	1327	AMP	C2-N3-C4	3.62	120.68	111.83
6	E	1327	AMP	C4-C5-N7	-3.60	106.47	110.58
5	C	1553	C1V	CAZ-CAY-SAP	-3.53	107.74	112.74
5	B	1271	C1V	CAZ-CAY-SAP	-3.53	107.75	112.74
6	E	1326	AMP	C4-C5-N7	-3.49	106.60	110.58
6	F	1325	AMP	C4-C5-N7	-3.48	106.60	110.58
6	F	1325	AMP	N3-C2-N1	-3.31	123.57	128.58
6	E	1326	AMP	N3-C2-N1	-3.24	123.67	128.58
4	A	1552	STU	C16-C17-C12	-3.20	117.85	121.59
4	A	1552	STU	C13-C12-C17	3.09	122.81	119.24
6	E	1327	AMP	N3-C2-N1	-2.97	124.09	128.58
4	C	1552	STU	C16-C17-C12	-2.89	118.20	121.59
6	F	1326	AMP	N3-C2-N1	-2.89	124.20	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1553	C1V	OAB-CAX-CAU	-2.80	118.90	124.27
6	F	1326	AMP	C5-N7-C8	2.79	107.83	103.45
5	B	1271	C1V	OAB-CAX-CAU	-2.78	118.94	124.27
6	F	1325	AMP	C4-N9-C8	2.78	108.66	105.74
4	C	1552	STU	C13-C12-C17	2.73	122.39	119.24
6	E	1327	AMP	C5-N7-C8	2.72	107.73	103.45
6	E	1327	AMP	C4-N9-C8	2.64	108.51	105.74
6	F	1326	AMP	C4-N9-C8	2.61	108.48	105.74
6	F	1325	AMP	C5-N7-C8	2.56	107.47	103.45
6	E	1326	AMP	C4-N9-C8	2.55	108.42	105.74
6	E	1326	AMP	C5-N7-C8	2.55	107.46	103.45
4	A	1552	STU	O5-C8-C7	-2.38	125.02	128.47
6	F	1326	AMP	N9-C8-N7	-2.19	110.83	113.94
4	A	1552	STU	C16-C17-N2	2.18	133.49	130.22
6	E	1327	AMP	N9-C8-N7	-2.16	110.87	113.94
5	C	1553	C1V	CAW-CAN-SAP	-2.16	107.90	114.23
6	F	1326	AMP	C6-C5-N7	2.11	136.15	132.09
4	C	1552	STU	O5-C8-C7	-2.10	125.43	128.47
4	C	1552	STU	C19-N3-C20	2.08	110.65	107.90
4	A	1552	STU	C19-N3-C20	2.08	110.65	107.90
5	B	1271	C1V	CAW-CAN-SAP	-2.08	108.15	114.23
6	F	1325	AMP	C6-C5-N7	2.06	136.06	132.09
6	F	1325	AMP	C2-N1-C6	2.06	122.12	118.73
6	F	1325	AMP	N9-C8-N7	-2.05	111.03	113.94
4	C	1552	STU	C6-C7-C10	-2.04	119.34	120.76
4	C	1552	STU	C3-C4-C5	-2.03	116.86	120.23
6	E	1326	AMP	C6-C5-N7	2.01	135.97	132.09
4	A	1552	STU	C3-C4-C5	-2.00	116.91	120.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1326	AMP	C5'-O5'-P-O2P
6	E	1326	AMP	C5'-O5'-P-O3P
6	E	1327	AMP	C5'-O5'-P-O2P
6	E	1327	AMP	C5'-O5'-P-O3P
5	C	1553	C1V	CAK-CAS-CAW-CAZ
5	C	1553	C1V	CAL-CAS-CAW-CAZ
6	F	1325	AMP	C5'-O5'-P-O1P
4	C	1552	STU	C24-C23-N4-C28
4	A	1552	STU	C24-C23-N4-C28

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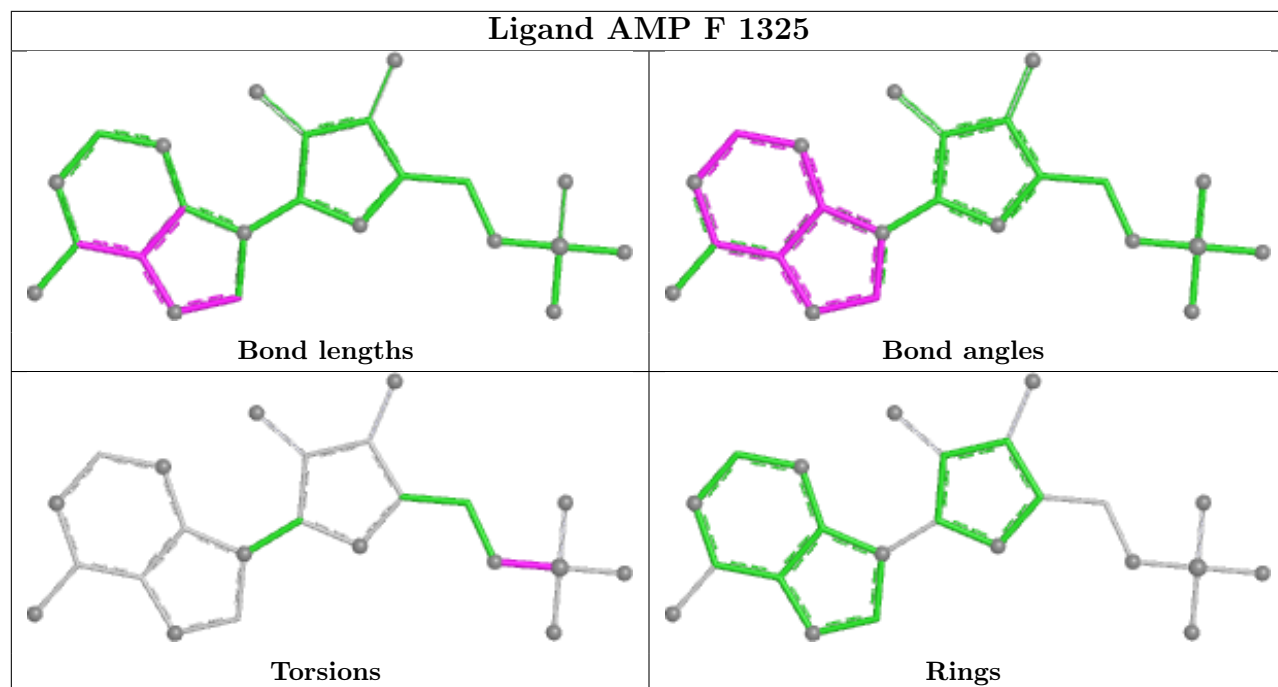
Mol	Chain	Res	Type	Atoms
5	C	1553	C1V	CAL-CAS-CAW-CAN
5	C	1553	C1V	CAK-CAS-CAW-CAN
6	E	1327	AMP	O4'-C4'-C5'-O5'
6	E	1326	AMP	C5'-O5'-P-O1P

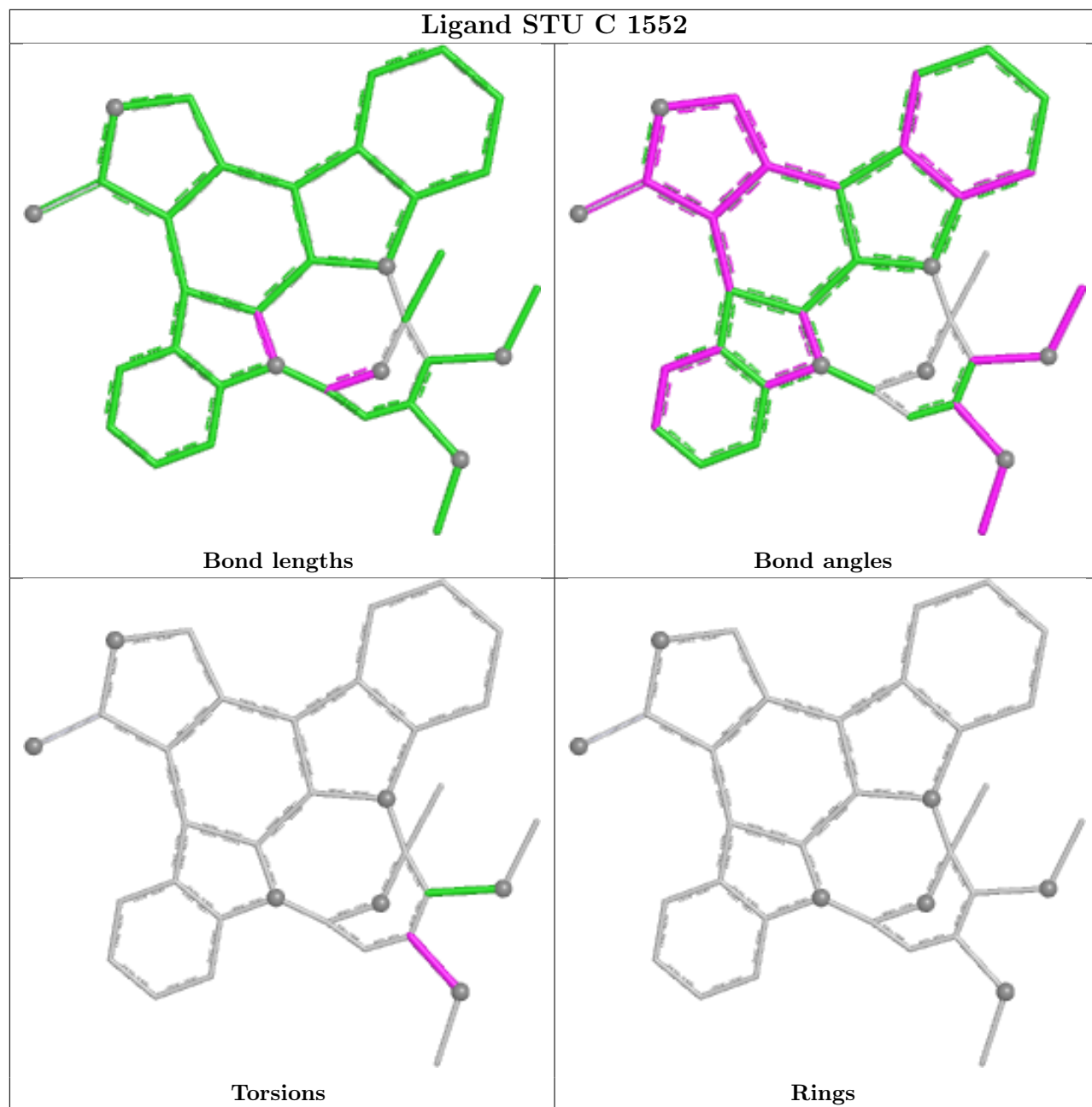
There are no ring outliers.

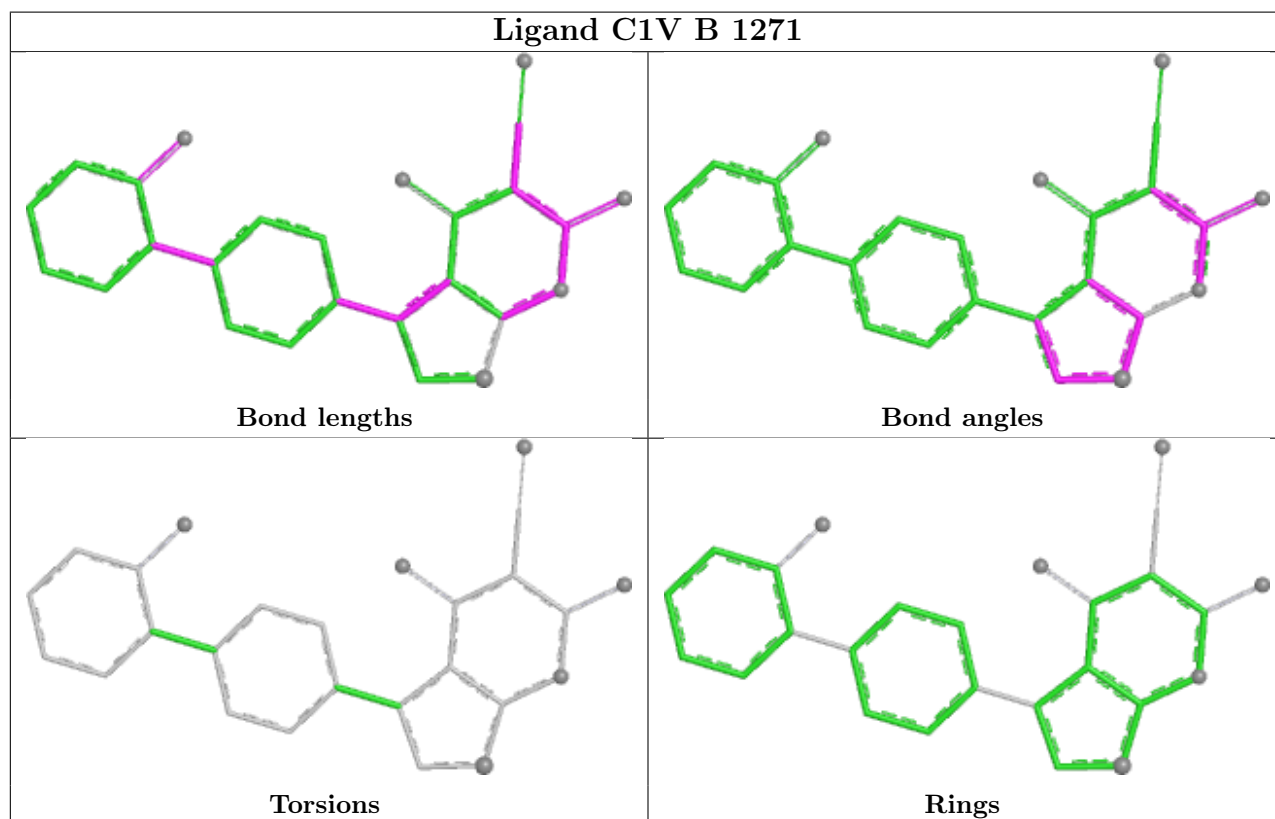
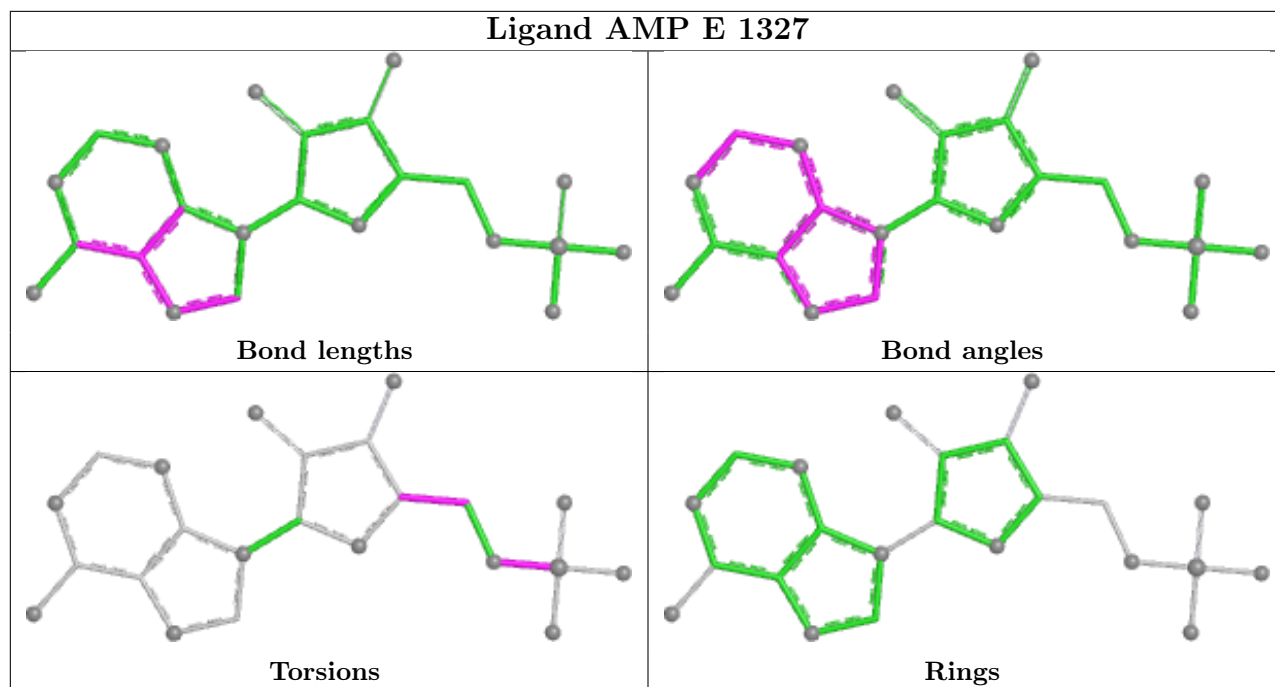
6 monomers are involved in 10 short contacts:

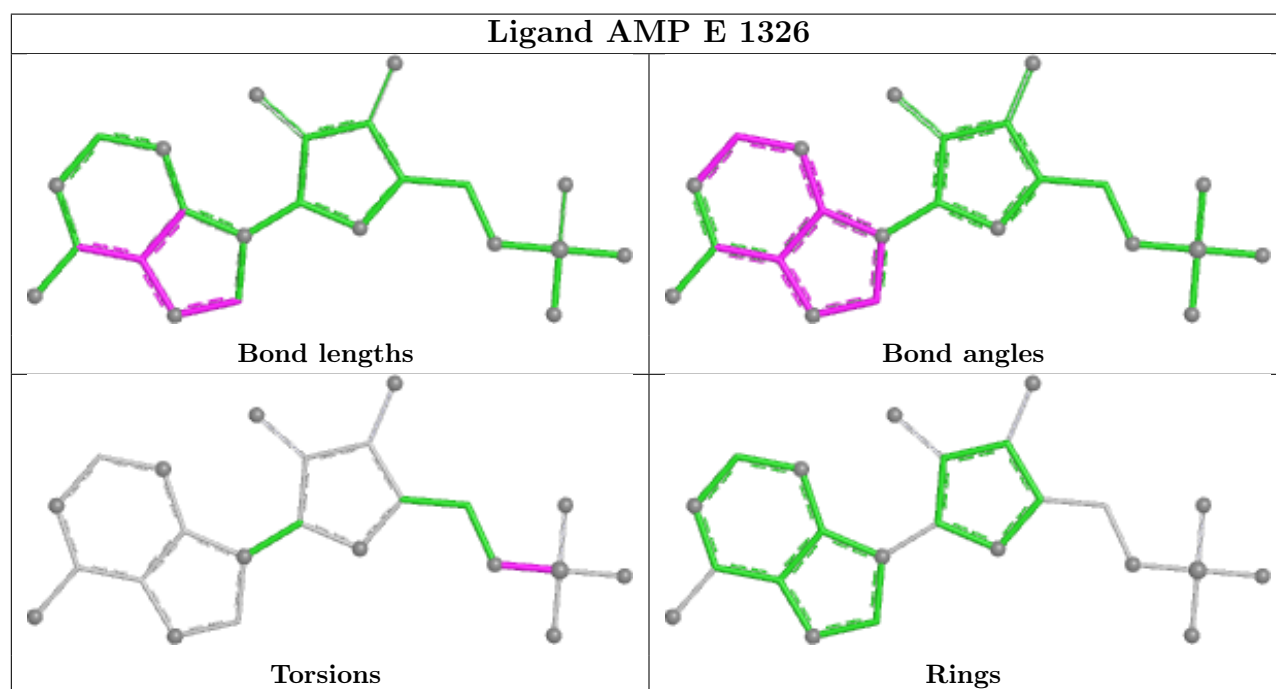
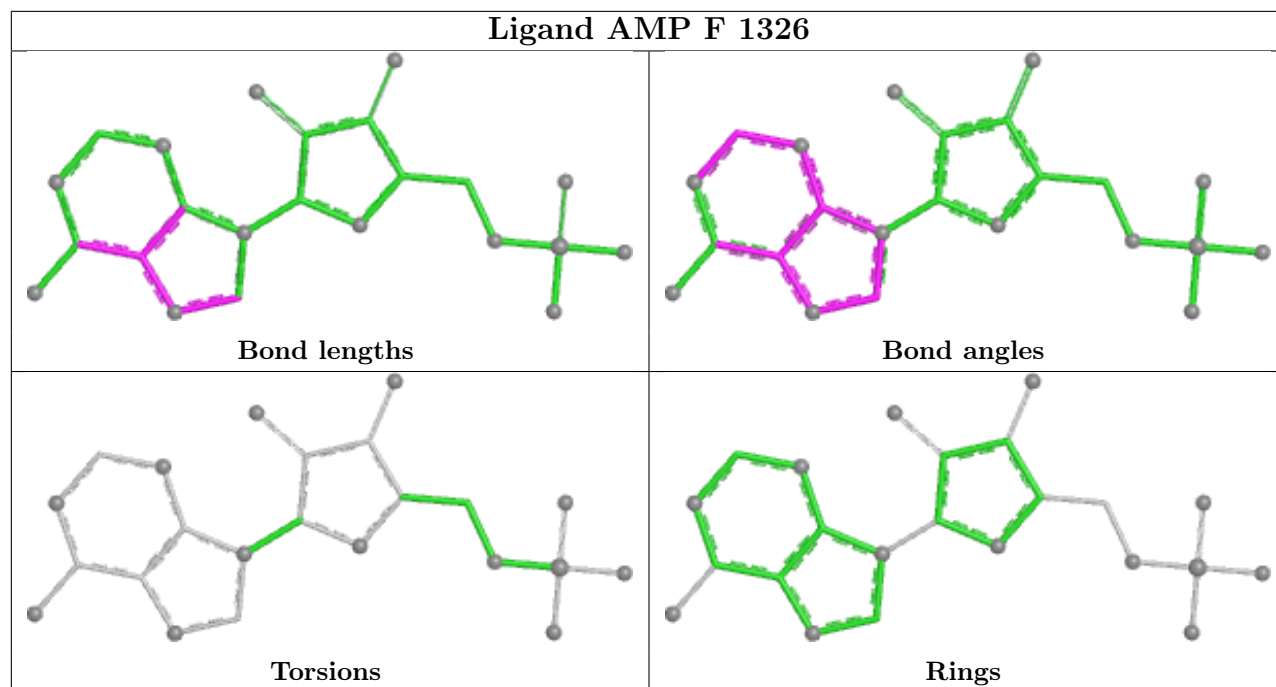
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1325	AMP	1	0
4	C	1552	STU	3	0
5	B	1271	C1V	1	0
6	F	1326	AMP	1	0
6	E	1326	AMP	1	0
4	A	1552	STU	3	0

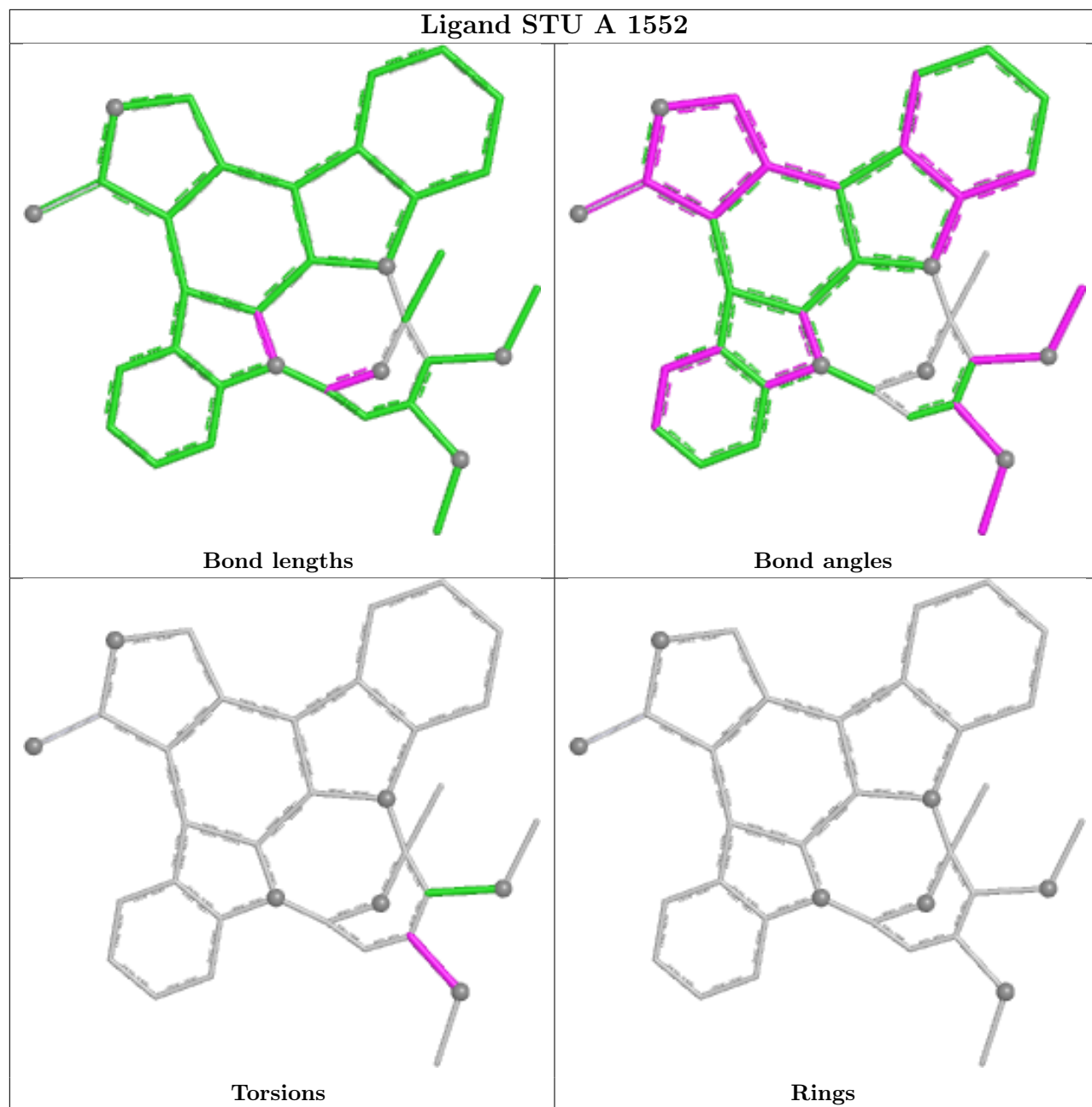
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

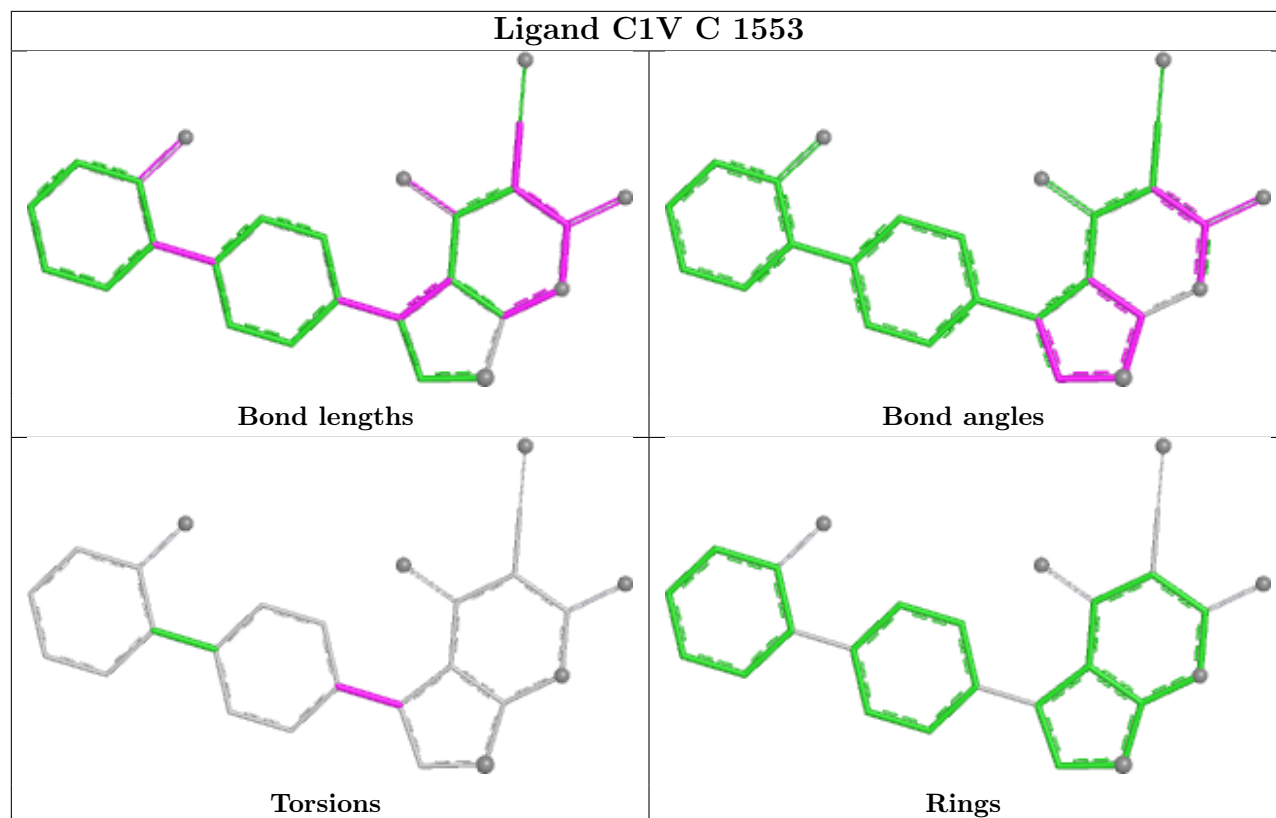












5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	424/571 (74%)	-0.47	1 (0%) 91 81	32, 79, 136, 159	0
1	C	422/571 (73%)	-0.51	0 100 100	50, 92, 140, 161	0
2	B	170/286 (59%)	-0.36	0 100 100	48, 100, 152, 182	0
2	D	171/286 (59%)	-0.40	0 100 100	58, 101, 145, 173	0
3	E	299/331 (90%)	-0.57	2 (0%) 84 67	29, 68, 140, 192	0
3	F	292/331 (88%)	-0.63	0 100 100	44, 73, 124, 147	0
All	All	1778/2376 (74%)	-0.50	3 (0%) 91 81	29, 83, 141, 192	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	184	PRO	2.4
1	A	52	ILE	2.2
3	E	124	ASP	2.2

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	D	108	10/11	0.88	0.07	83,98,109,111	0
2	SEP	B	108	10/11	0.89	0.06	93,103,114,115	0
1	TPO	C	172	11/12	0.93	0.06	66,92,95,95	0
1	TPO	A	172	11/12	0.96	0.05	54,71,75,76	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

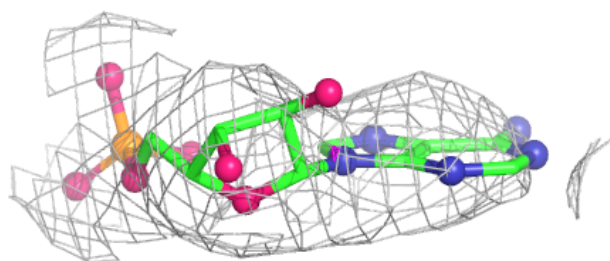
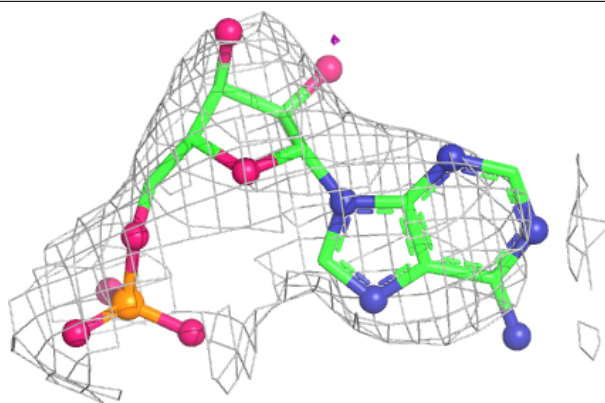
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	AMP	E	1326	23/23	0.87	0.07	80,83,99,101	0
5	C1V	B	1271	26/26	0.90	0.10	90,90,94,94	0
4	STU	A	1552	35/35	0.91	0.09	102,107,111,114	0
6	AMP	E	1327	23/23	0.94	0.06	71,75,79,81	0
4	STU	C	1552	35/35	0.96	0.07	119,122,127,127	0
5	C1V	C	1553	26/26	0.96	0.08	92,96,108,110	0
6	AMP	F	1325	23/23	0.96	0.05	52,59,69,74	0
6	AMP	F	1326	23/23	0.96	0.06	52,55,62,64	0

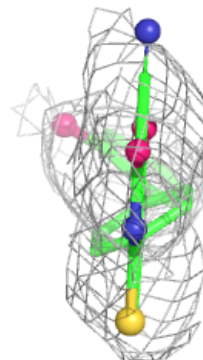
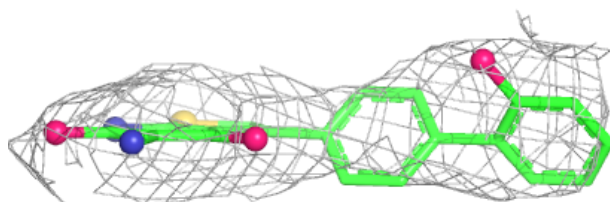
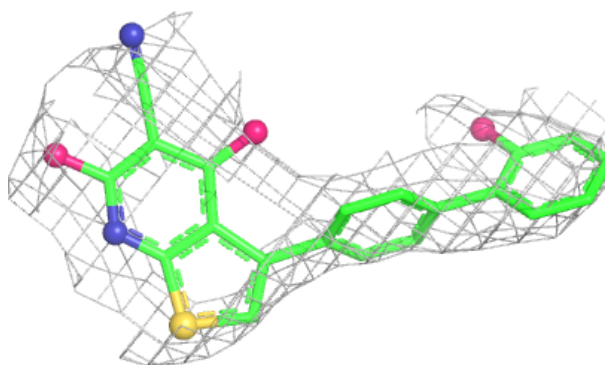
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP E 1326:

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

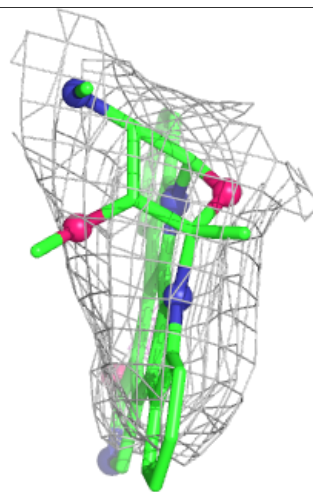
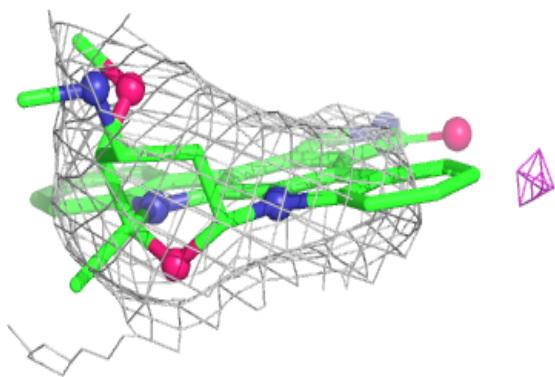
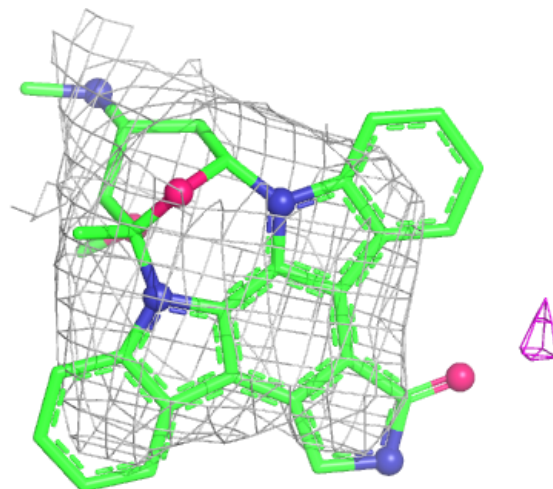
**Electron density around C1V B 1271:**

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



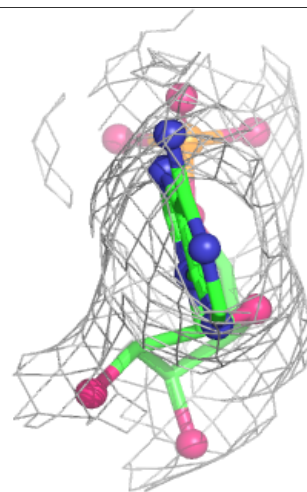
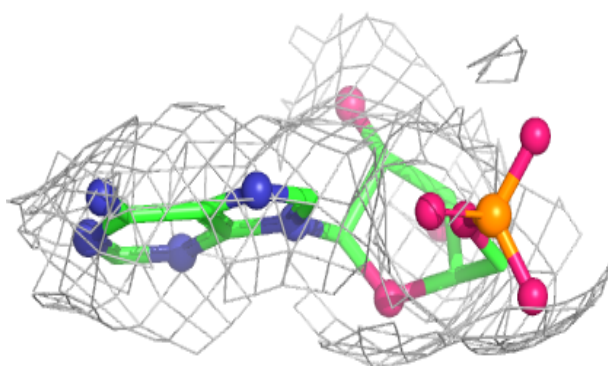
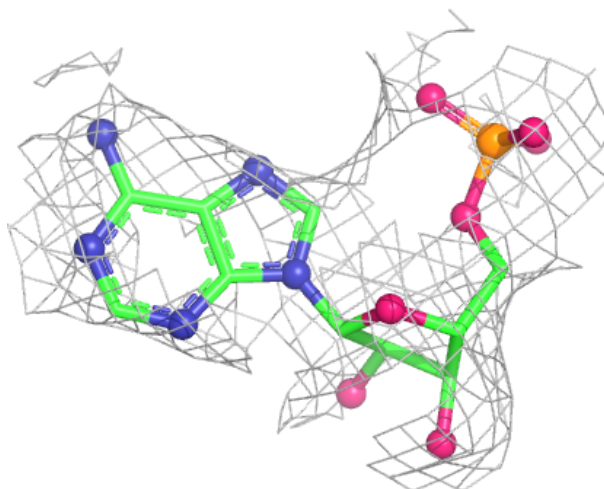
Electron density around STU A 1552:

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



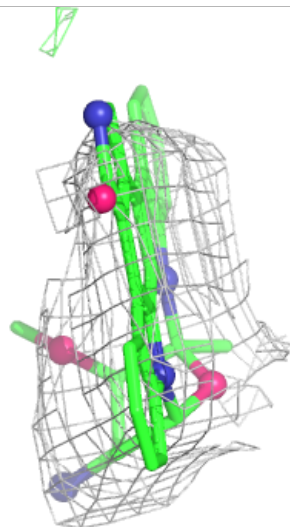
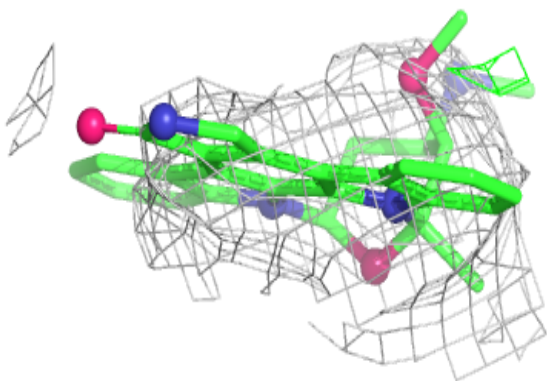
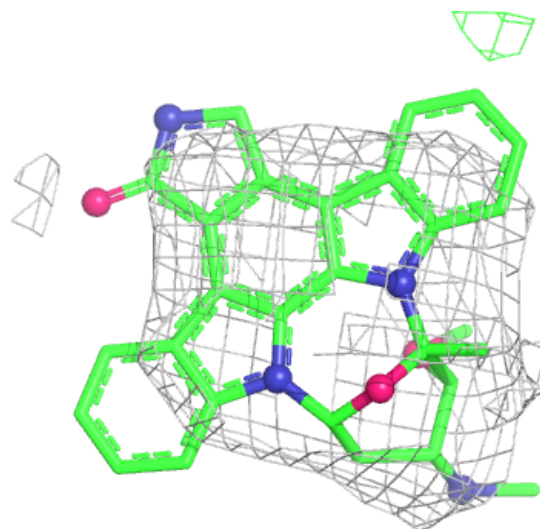
Electron density around AMP E 1327:

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



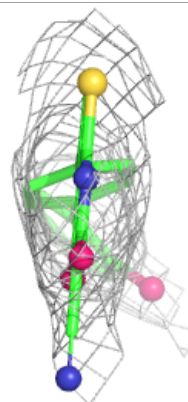
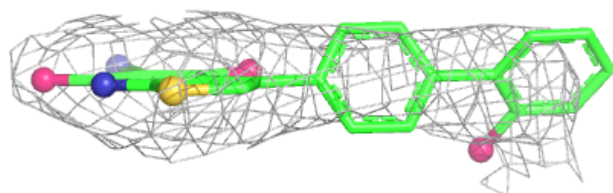
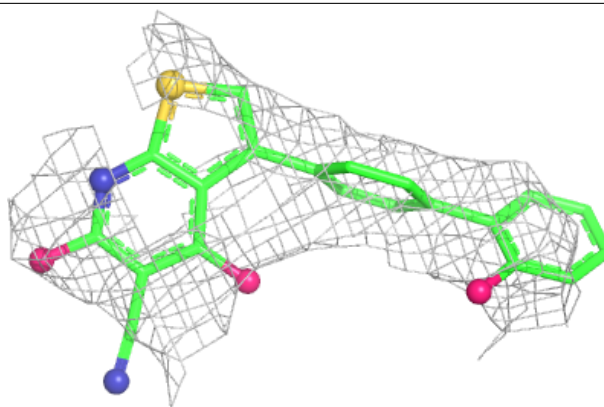
Electron density around STU C 1552:

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

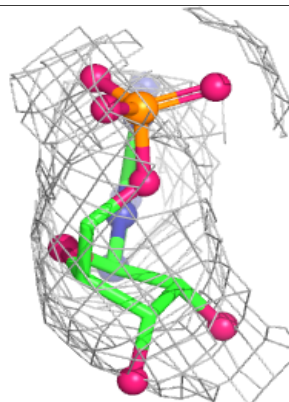
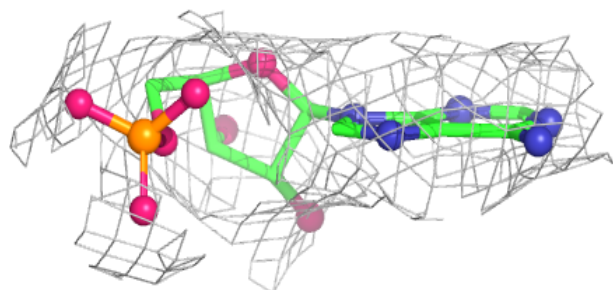
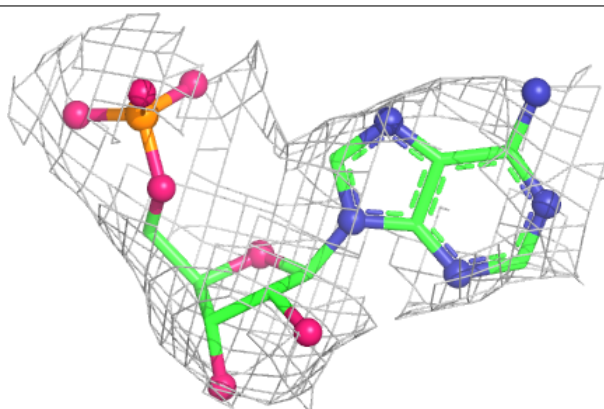


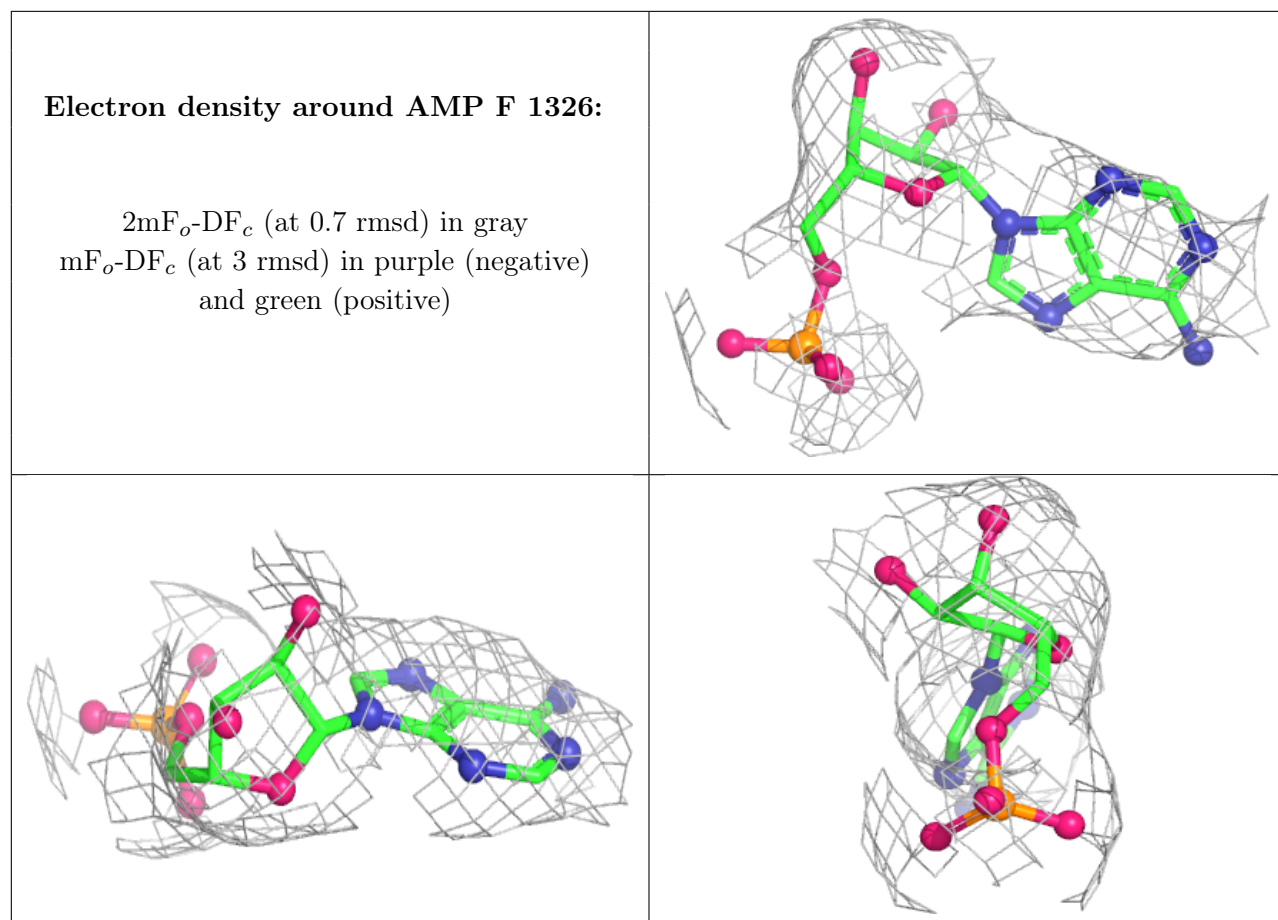
Electron density around C1V C 1553:

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

**Electron density around AMP F 1325:**

$2mF_o-DF_c$ (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.