



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:42 AM UTC

PDB ID : 6SY7 / pdb_00006sy7
Title : Structure of Trypanosome Brucei Phosphofructokinase in complex with AMP.
Authors : McNae, I.W.; Vasquez-Valdivieso, M.G.; Walkinshaw, M.D.
Deposited on : 2019-09-27
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

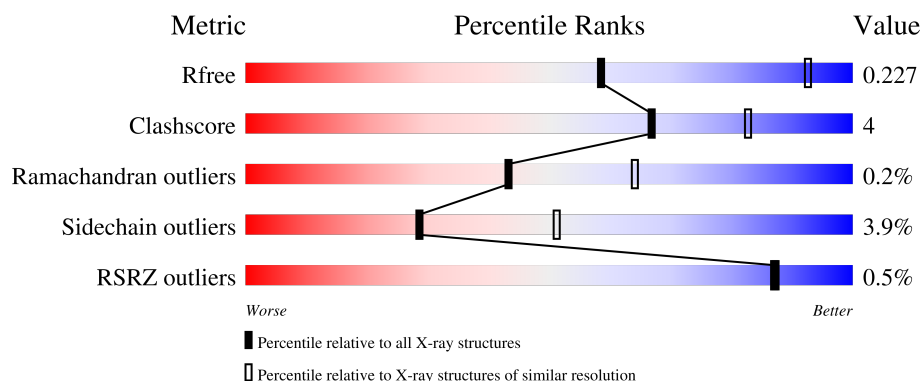
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	487	% 84% 8% 7%
1	B	487	84% 9% 7%
1	C	487	81% 11% 7%
1	D	487	% 81% 11% 7%
1	E	487	82% 9% 8%

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Mol	Chain	Length	Quality of chain
1	F	487	82% 9% • 8%
1	G	487	84% 8% • 7%
1	H	487	% 84% 9% • 7%

2 Entry composition

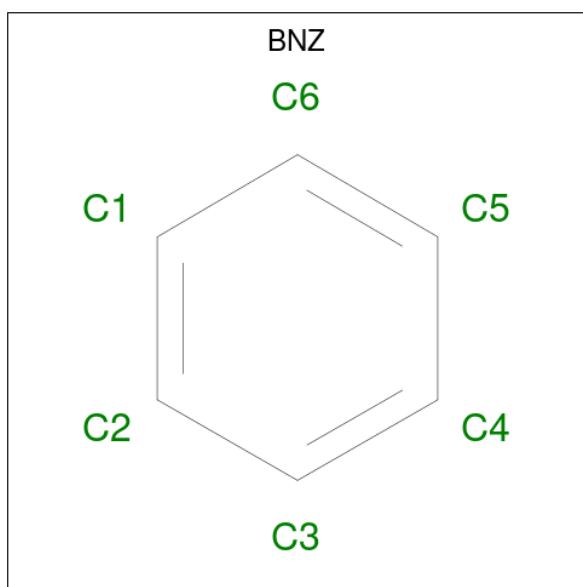
There are 5 unique types of molecules in this entry. The entry contains 28937 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent 6-phosphofructokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3522	2208	643	654	17			
1	B	454	Total	C	N	O	S	0	0	0
			3514	2203	642	653	16			
1	C	451	Total	C	N	O	S	0	0	0
			3492	2190	638	648	16			
1	D	452	Total	C	N	O	S	0	0	0
			3498	2191	640	651	16			
1	E	450	Total	C	N	O	S	0	0	0
			3485	2185	637	647	16			
1	F	450	Total	C	N	O	S	0	0	0
			3486	2185	637	648	16			
1	G	452	Total	C	N	O	S	0	0	0
			3502	2195	640	651	16			
1	H	454	Total	C	N	O	S	0	0	0
			3518	2206	642	653	17			

- Molecule 2 is BENZENE (CCD ID: BNZ) (formula: C₆H₆).



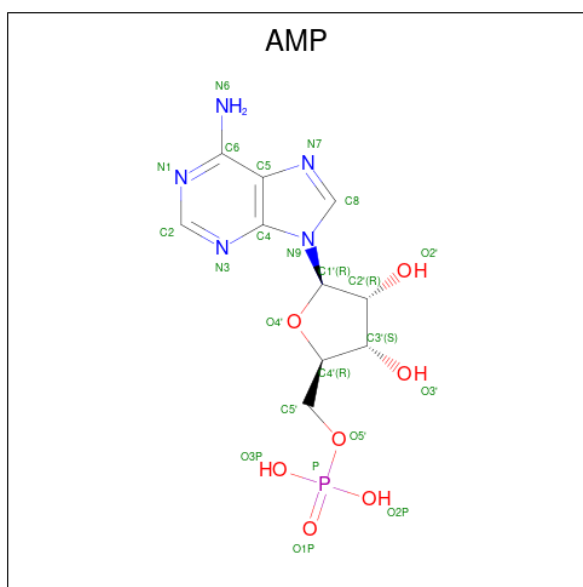
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 6 6	0	0
2	B	1	Total C 6 6	0	0
2	C	1	Total C 6 6	0	0
2	D	1	Total C 6 6	0	0
2	E	1	Total C 6 6	0	0
2	F	1	Total C 6 6	0	0
2	G	1	Total C 6 6	0	0
2	H	1	Total C 6 6	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	F	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	H	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	99	Total	O	0	0
			99	99		
5	B	96	Total	O	0	0
			96	96		
5	C	81	Total	O	0	0
			81	81		
5	D	74	Total	O	0	0
			74	74		

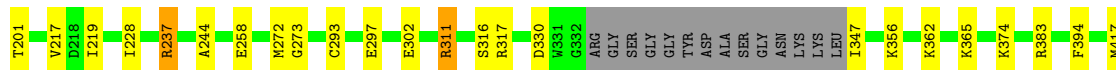
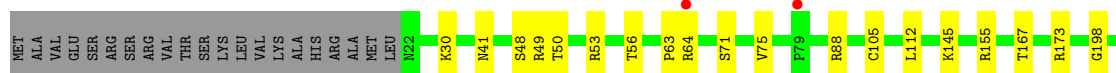
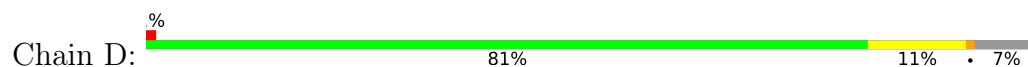
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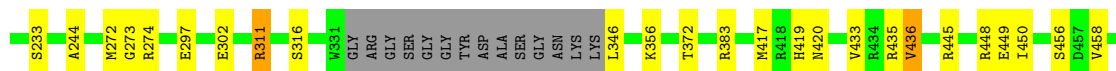
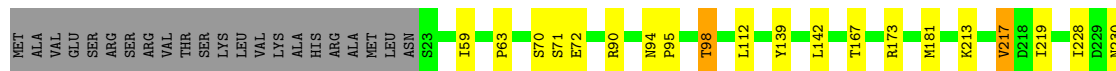
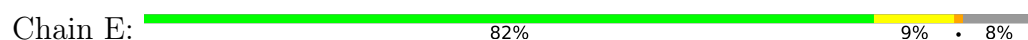
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	62	Total 62	O 62	0	0
5	F	70	Total 70	O 70	0	0
5	G	58	Total 58	O 58	0	0
5	H	100	Total 100	O 100	0	0



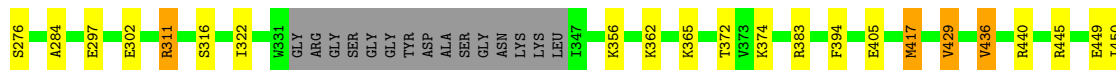
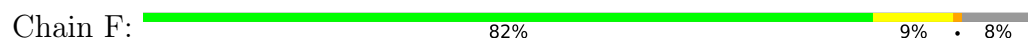
- Molecule 1: ATP-dependent 6-phosphofructokinase



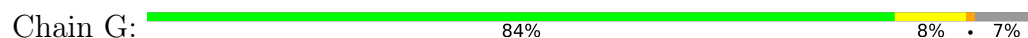
- Molecule 1: ATP-dependent 6-phosphofructokinase

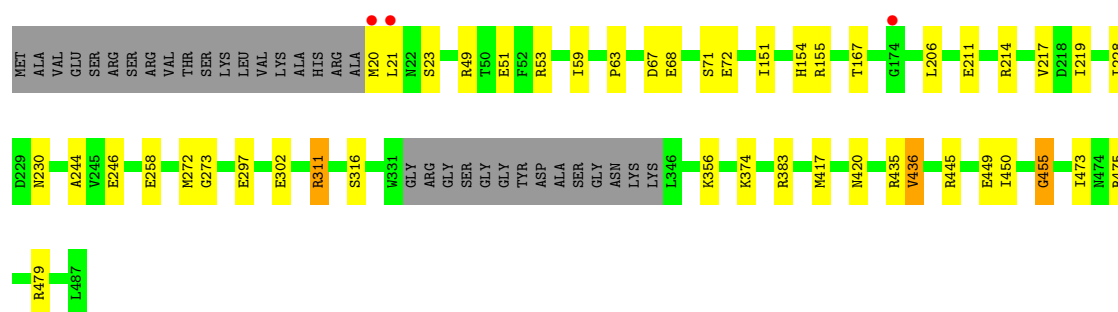


- Molecule 1: ATP-dependent 6-phosphofructokinase



- Molecule 1: ATP-dependent 6-phosphofructokinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.39Å 133.71Å 271.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.81 – 2.75 39.81 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.81-2.75) 98.8 (39.81-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	(Not available) , (Not available) 0.205 , 0.227	Depositor DCC
R_{free} test set	5586 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	51.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 21.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	28937	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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: BNZ, AMP, GOL

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	1.00	0/3582	1.40	0/4846
1	B	0.99	0/3574	1.40	3/4836 (0.1%)
1	C	0.99	0/3551	1.40	3/4803 (0.1%)
1	D	1.01	0/3558	1.41	6/4814 (0.1%)
1	E	0.99	1/3545 (0.0%)	1.39	0/4798
1	F	1.00	0/3546	1.40	3/4798 (0.1%)
1	G	1.01	0/3562	1.41	4/4820 (0.1%)
1	H	1.01	0/3578	1.40	1/4841 (0.0%)
All	All	1.00	1/28496 (0.0%)	1.40	20/38556 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	H	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	484	LEU	C-O	5.33	1.30	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	ARG	CB-CG-CD	7.79	129.22	111.30
1	D	486	LYS	CA-C-N	6.89	134.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	486	LYS	C-N-CA	6.89	134.10	121.70
1	F	33	ARG	NE-CZ-NH1	-6.71	114.79	121.50
1	C	476	ASN	CA-CB-CG	6.70	119.30	112.60
1	D	237	ARG	CG-CD-NE	6.32	125.89	112.00
1	H	155	ARG	CB-CG-CD	6.23	125.64	111.30
1	B	49	ARG	CB-CG-CD	6.10	125.33	111.30
1	G	155	ARG	CB-CA-C	5.78	120.38	110.79
1	F	246	GLU	CB-CG-CD	5.62	122.15	112.60
1	G	66	ARG	CG-CD-NE	5.55	124.22	112.00
1	F	33	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	C	155	ARG	CB-CA-C	5.43	119.80	110.79
1	G	131	ARG	CG-CD-NE	5.32	123.71	112.00
1	C	246	GLU	CB-CG-CD	5.21	121.45	112.60
1	D	477	ARG	CB-CG-CD	5.17	123.20	111.30
1	G	155	ARG	CG-CD-NE	-5.17	100.64	112.00
1	B	471	GLU	CB-CG-CD	5.12	121.31	112.60
1	B	198	GLY	CA-C-O	-5.09	117.19	122.28
1	D	330	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	455	GLY	Peptide
1	H	455	GLY	Peptide

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	3522	0	3573	29	0
1	B	3514	0	3564	26	0
1	C	3492	0	3541	39	0
1	D	3498	0	3542	37	0
1	E	3485	0	3533	34	0
1	F	3486	0	3533	24	0
1	G	3502	0	3550	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	3518	0	3570	28	0
2	A	6	0	6	0	0
2	B	6	0	6	0	0
2	C	6	0	6	0	0
2	D	6	0	6	0	0
2	E	6	0	6	0	0
2	F	6	0	6	0	0
2	G	6	0	6	0	0
2	H	6	0	6	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
3	D	6	0	8	1	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
4	A	23	0	12	1	0
4	B	23	0	12	2	0
4	C	23	0	12	2	0
4	D	23	0	12	1	0
4	F	46	0	24	2	0
4	G	23	0	12	2	0
4	H	23	0	12	1	0
5	A	99	0	0	1	0
5	B	96	0	0	1	0
5	C	81	0	0	3	0
5	D	74	0	0	2	0
5	E	62	0	0	5	0
5	F	70	0	0	0	0
5	G	58	0	0	3	0
5	H	100	0	0	3	0
All	All	28937	0	28614	213	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (213) 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:60:MET:HE1	1:B:60:MET:SD	1.57	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:TYR:CD1	1:E:181:MET:HE1	1.87	1.10
1:D:105:CYS:HB2	1:D:201:THR:HG21	1.46	0.95
1:B:473:ILE:HG23	1:C:473:ILE:HG23	1.50	0.94
1:A:60:MET:CE	1:B:60:MET:SD	2.53	0.93
1:C:139:TYR:CD1	1:C:181:MET:HE1	2.04	0.92
1:D:311:ARG:HG2	1:D:311:ARG:HH11	1.34	0.92
1:E:139:TYR:HD1	1:E:181:MET:HE1	1.43	0.83
1:H:23:SER:HA	5:H:1167:HOH:O	1.82	0.79
1:C:150:ALA:O	1:D:475:ARG:NH2	2.17	0.77
1:H:67:ASP:O	1:H:68:GLU:HB2	1.84	0.77
1:A:60:MET:HE2	1:B:63:PRO:HA	1.66	0.76
1:A:427:ILE:O	1:A:431:THR:HG22	1.85	0.76
1:D:347:ILE:HA	5:D:1173:HOH:O	1.86	0.76
1:G:450:ILE:HG22	4:G:503:AMP:C5	2.22	0.74
1:A:473:ILE:HG23	1:D:473:ILE:HG23	1.70	0.73
1:G:150:ALA:O	1:H:475:ARG:NH2	2.21	0.72
1:E:479:ARG:HD2	5:E:657:HOH:O	1.90	0.71
1:F:28:ASP:HB3	1:F:429:VAL:HG11	1.72	0.70
1:E:467:ARG:NH1	1:E:471:GLU:OE2	2.26	0.69
1:C:181:MET:CE	1:C:208:ILE:HD11	2.23	0.69
1:E:94:ASN:O	1:E:98:THR:CG2	2.41	0.68
1:E:473:ILE:HG23	1:G:473:ILE:HG23	1.76	0.68
1:B:450:ILE:HG22	4:B:1001:AMP:C5	2.29	0.67
1:F:473:ILE:HG23	1:H:473:ILE:HG23	1.77	0.66
1:A:60:MET:HE3	1:A:63:PRO:HA	1.78	0.66
1:F:311:ARG:HG2	1:F:311:ARG:HH21	1.59	0.66
1:E:142:LEU:HB2	1:E:181:MET:HE3	1.78	0.65
1:E:448:ARG:HH22	1:F:47:SER:HB3	1.62	0.65
1:G:131:ARG:NH1	1:G:152:GLU:OE2	2.30	0.65
1:C:152:GLU:OE2	1:D:475:ARG:NH1	2.30	0.64
1:A:477:ARG:HD3	1:D:477:ARG:NH2	2.13	0.64
1:D:311:ARG:HH11	1:D:311:ARG:CG	2.06	0.64
1:E:94:ASN:O	1:E:98:THR:HG23	1.98	0.64
1:C:181:MET:HE2	1:C:208:ILE:HD11	1.78	0.63
1:A:311:ARG:NH2	1:A:456:SER:O	2.34	0.61
1:G:348:ASP:HB3	1:G:351:VAL:HG22	1.80	0.61
1:H:311:ARG:NH1	1:H:455:GLY:H	1.97	0.61
1:F:28:ASP:HB3	1:F:429:VAL:CG1	2.30	0.61
4:C:503:AMP:O1P	1:D:155:ARG:HD3	2.01	0.61
1:B:289:GLN:HG2	5:B:1189:HOH:O	2.01	0.60
5:G:647:HOH:O	1:H:246:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:LEU:C	1:E:484:LEU:HD23	2.27	0.60
1:C:75:VAL:HG12	1:D:75:VAL:HG22	1.84	0.59
1:C:139:TYR:CE1	1:C:181:MET:HE1	2.36	0.59
1:D:105:CYS:HB2	1:D:201:THR:CG2	2.28	0.59
1:B:311:ARG:NH2	1:B:456:SER:O	2.36	0.59
1:C:181:MET:HE2	1:C:208:ILE:CD1	2.33	0.59
1:C:28:ASP:HB3	1:C:429:VAL:CG1	2.32	0.59
1:G:311:ARG:NH2	1:G:456:SER:O	2.36	0.59
1:D:237:ARG:NH2	1:D:394:PHE:HB2	2.19	0.58
1:C:139:TYR:CD1	1:C:181:MET:CE	2.84	0.58
1:C:46:TYR:C	1:D:448:ARG:HH21	2.13	0.57
1:H:311:ARG:HH21	1:H:311:ARG:CG	2.17	0.57
1:B:450:ILE:HG22	4:B:1001:AMP:C6	2.40	0.57
1:E:484:LEU:HD23	1:E:485:ALA:N	2.20	0.56
1:C:293:CYS:H	3:C:502:GOL:H31	1.71	0.56
1:G:63:PRO:HB3	1:H:63:PRO:HB3	1.86	0.56
1:F:394:PHE:CE1	1:F:417:MET:HE3	2.40	0.56
1:D:105:CYS:CB	1:D:201:THR:HG21	2.27	0.55
1:E:433:VAL:HG23	5:E:645:HOH:O	2.05	0.55
1:E:458:VAL:HG22	5:E:644:HOH:O	2.05	0.55
1:H:217:VAL:HG12	1:H:219:ILE:HG13	1.88	0.55
1:C:63:PRO:HB3	1:D:63:PRO:HB3	1.88	0.55
1:B:217:VAL:HG12	1:B:219:ILE:HG13	1.89	0.55
1:E:311:ARG:NH2	1:E:456:SER:O	2.40	0.54
1:G:450:ILE:HG22	4:G:503:AMP:C6	2.42	0.54
1:A:63:PRO:HB3	1:B:63:PRO:HB3	1.88	0.54
1:C:66:ARG:HB3	1:C:75:VAL:HG23	1.90	0.54
1:F:33:ARG:NH1	1:F:405:GLU:OE1	2.27	0.53
1:H:272:MET:HE1	1:H:383:ARG:HD3	1.90	0.53
1:B:311:ARG:HE	1:B:454:LEU:HA	1.74	0.53
1:G:419:HIS:HD2	5:G:618:HOH:O	1.91	0.53
1:C:217:VAL:HG12	1:C:219:ILE:HG13	1.90	0.52
1:G:372:THR:HG22	1:G:374:LYS:HE2	1.89	0.52
1:E:419:HIS:HE1	5:E:641:HOH:O	1.92	0.52
1:F:450:ILE:HG22	4:F:1001:AMP:C5	2.45	0.52
1:A:297:GLU:HG2	1:A:436:VAL:HG13	1.92	0.51
1:C:297:GLU:HG2	1:C:436:VAL:HG13	1.93	0.51
1:F:217:VAL:HG12	1:F:219:ILE:HG13	1.91	0.51
1:D:217:VAL:HG12	1:D:219:ILE:HG13	1.91	0.51
1:E:417:MET:HE3	1:E:420:ASN:H	1.75	0.51
1:C:28:ASP:HB3	1:C:429:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:THR:HG22	1:D:88:ARG:HH12	1.76	0.51
1:C:63:PRO:CB	1:D:63:PRO:HB3	2.41	0.51
1:D:48:SER:OG	1:D:50:THR:HG22	2.10	0.51
1:E:94:ASN:O	1:E:98:THR:HG22	2.10	0.51
1:C:63:PRO:HB3	1:D:63:PRO:CB	2.41	0.51
1:F:297:GLU:HG2	1:F:436:VAL:HG13	1.93	0.50
1:H:417:MET:HE3	1:H:420:ASN:H	1.75	0.50
1:E:297:GLU:HG2	1:E:436:VAL:HG13	1.93	0.50
1:H:211:GLU:OE1	1:H:214:ARG:NH1	2.44	0.50
1:G:56:THR:HG22	1:G:88:ARG:HH12	1.77	0.50
1:A:272:MET:HE1	1:A:383:ARG:HD3	1.94	0.50
1:B:211:GLU:OE1	1:B:214:ARG:NH1	2.44	0.50
1:H:297:GLU:HG2	1:H:436:VAL:HG13	1.93	0.50
1:A:56:THR:HG22	1:A:88:ARG:HH12	1.77	0.50
1:D:41:ASN:O	1:D:49:ARG:NH2	2.45	0.49
1:A:417:MET:HE3	1:A:420:ASN:H	1.77	0.49
1:H:154:HIS:HE1	5:H:1193:HOH:O	1.94	0.49
1:A:60:MET:HE2	1:B:63:PRO:CA	2.37	0.49
1:E:63:PRO:HB3	1:F:63:PRO:HB3	1.94	0.49
1:E:476:ASN:HA	1:E:479:ARG:HG2	1.95	0.49
1:G:272:MET:HE1	1:G:383:ARG:HD3	1.95	0.49
1:D:417:MET:HE3	1:D:420:ASN:H	1.76	0.48
1:B:297:GLU:HG2	1:B:436:VAL:HG13	1.94	0.48
1:G:417:MET:HE3	1:G:420:ASN:H	1.77	0.48
1:A:311:ARG:NE	1:A:454:LEU:HA	2.28	0.48
1:D:272:MET:HE1	1:D:383:ARG:HD3	1.95	0.48
1:F:272:MET:HE1	1:F:383:ARG:HD3	1.95	0.48
1:G:297:GLU:HG2	1:G:436:VAL:HG13	1.95	0.48
1:C:272:MET:HE1	1:C:383:ARG:HD3	1.95	0.47
1:D:297:GLU:HG2	1:D:436:VAL:HG13	1.96	0.47
1:F:276:SER:HA	1:F:297:GLU:OE1	2.14	0.47
1:C:304:GLU:HB3	5:C:652:HOH:O	2.13	0.47
1:C:450:ILE:HG22	4:C:503:AMP:C5	2.49	0.47
1:B:311:ARG:NE	1:B:454:LEU:HA	2.29	0.47
1:C:160:ASN:ND2	5:C:607:HOH:O	2.47	0.47
1:B:272:MET:HE1	1:B:383:ARG:HD3	1.95	0.47
1:H:53:ARG:NH1	5:H:1106:HOH:O	2.48	0.46
1:D:311:ARG:NH2	1:D:456:SER:O	2.47	0.46
1:E:272:MET:HE1	1:E:383:ARG:HD3	1.96	0.46
1:D:105:CYS:CB	1:D:201:THR:CG2	2.92	0.46
1:E:228:ILE:HD11	1:E:244:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PRO:HB3	1:B:63:PRO:CB	2.46	0.45
1:C:28:ASP:HB3	1:C:429:VAL:HG13	1.96	0.45
1:G:311:ARG:HE	1:G:458:VAL:HG13	1.81	0.45
1:B:317:ARG:HD3	1:B:317:ARG:HA	1.71	0.45
1:C:246:GLU:HG2	5:C:625:HOH:O	2.16	0.45
1:F:302:GLU:CD	1:F:356:LYS:HD3	2.41	0.45
1:F:311:ARG:HH21	1:F:311:ARG:CG	2.29	0.45
1:A:349:ILE:HG22	5:A:602:HOH:O	2.17	0.45
1:E:173:ARG:NH2	5:E:604:HOH:O	2.49	0.45
1:A:228:ILE:HD11	1:A:244:ALA:HB2	1.99	0.45
1:F:311:ARG:NH1	1:F:456:SER:O	2.48	0.45
1:A:450:ILE:HG22	4:A:503:AMP:C5	2.52	0.45
1:D:228:ILE:HD11	1:D:244:ALA:HB2	1.99	0.45
1:A:63:PRO:CB	1:B:63:PRO:HB3	2.46	0.45
1:A:311:ARG:HE	1:A:454:LEU:HA	1.82	0.45
1:D:317:ARG:HD3	1:D:317:ARG:HA	1.71	0.44
1:F:362:LYS:O	1:F:365:LYS:HG3	2.17	0.44
1:G:228:ILE:HD11	1:G:244:ALA:HB2	1.98	0.44
1:E:139:TYR:HD1	1:E:181:MET:CE	2.24	0.44
1:C:362:LYS:O	1:C:365:LYS:HG3	2.17	0.44
1:D:362:LYS:O	1:D:365:LYS:HG3	2.17	0.44
1:H:302:GLU:CD	1:H:356:LYS:HD3	2.43	0.44
1:H:311:ARG:HH12	1:H:455:GLY:H	1.61	0.44
1:A:302:GLU:CD	1:A:356:LYS:HD3	2.42	0.44
1:G:212:ALA:O	1:G:217:VAL:HG22	2.18	0.44
1:B:66:ARG:HG3	1:B:67:ASP:N	2.32	0.44
1:C:184:THR:O	1:C:188:LEU:HD13	2.18	0.44
1:C:228:ILE:HD11	1:C:244:ALA:HB2	2.00	0.44
1:D:198:GLY:O	1:D:201:THR:OG1	2.26	0.44
1:D:293:CYS:O	3:D:1003:GOL:H31	2.17	0.44
1:G:246:GLU:HG3	5:G:634:HOH:O	2.16	0.44
1:G:448:ARG:HH22	1:H:51:GLU:CD	2.25	0.44
1:E:450:ILE:HG22	4:F:1002:AMP:C5	2.53	0.43
1:G:348:ASP:HB3	1:G:351:VAL:CG2	2.46	0.43
1:B:302:GLU:CD	1:B:356:LYS:HD3	2.43	0.43
1:E:230:ASN:O	1:E:435:ARG:NH1	2.51	0.43
1:C:203:ARG:NH1	1:C:431:THR:O	2.51	0.43
1:D:302:GLU:CD	1:D:356:LYS:HD3	2.44	0.43
1:B:230:ASN:O	1:B:435:ARG:NH1	2.52	0.43
1:E:302:GLU:CD	1:E:356:LYS:HD3	2.43	0.43
1:A:152:GLU:OE1	1:B:475:ARG:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:ALA:HA	1:F:322:ILE:CD1	2.49	0.43
1:C:302:GLU:CD	1:C:356:LYS:HD3	2.44	0.42
1:C:445:ARG:O	1:C:449:GLU:HG2	2.19	0.42
1:D:445:ARG:O	1:D:449:GLU:HG2	2.19	0.42
1:D:258:GLU:HB3	1:D:374:LYS:HG3	2.02	0.42
1:A:229:ASP:OD2	1:A:273:GLY:HA2	2.20	0.42
1:A:258:GLU:HB3	1:A:374:LYS:HG3	2.01	0.42
1:B:445:ARG:O	1:B:449:GLU:HG2	2.20	0.42
1:C:181:MET:HE1	1:C:208:ILE:HD11	2.00	0.42
1:H:228:ILE:HD11	1:H:244:ALA:HB2	2.01	0.42
1:H:230:ASN:O	1:H:435:ARG:NH1	2.53	0.42
1:H:450:ILE:HG22	4:H:1001:AMP:C5	2.54	0.42
1:A:230:ASN:O	1:A:435:ARG:NH1	2.52	0.42
1:A:445:ARG:O	1:A:449:GLU:HG2	2.20	0.42
1:H:258:GLU:HB3	1:H:374:LYS:HG3	2.02	0.42
1:F:445:ARG:O	1:F:449:GLU:HG2	2.20	0.42
1:E:95:PRO:HA	1:E:98:THR:HG23	2.00	0.42
1:F:228:ILE:HD11	1:F:244:ALA:HB2	2.02	0.42
1:D:201:THR:HG22	5:D:1165:HOH:O	2.19	0.42
1:G:258:GLU:HB3	1:G:374:LYS:HG3	2.02	0.42
1:G:372:THR:HG22	1:G:374:LYS:CE	2.50	0.42
1:B:362:LYS:O	1:B:365:LYS:HG3	2.19	0.41
1:C:440:ARG:NH2	1:D:50:THR:HG23	2.36	0.41
1:E:95:PRO:CA	1:E:98:THR:HG23	2.50	0.41
1:D:450:ILE:HG22	4:D:1001:AMP:C5	2.56	0.41
1:E:274:ARG:HE	1:E:346:LEU:HD13	1.85	0.41
1:E:445:ARG:O	1:E:449:GLU:HG2	2.20	0.41
1:G:317:ARG:HD3	1:G:317:ARG:HA	1.71	0.41
1:E:217:VAL:HG13	1:E:219:ILE:HG13	2.02	0.41
1:F:258:GLU:HB3	1:F:374:LYS:HG3	2.03	0.41
1:H:151:ILE:HD13	1:H:151:ILE:HG21	1.85	0.41
1:B:228:ILE:HD11	1:B:244:ALA:HB2	2.02	0.41
1:F:394:PHE:CE1	1:F:417:MET:CE	3.04	0.41
1:A:217:VAL:HG13	1:A:219:ILE:HG13	2.02	0.41
1:E:63:PRO:HB3	1:F:63:PRO:CB	2.50	0.41
1:G:44:LYS:HD2	1:H:455:GLY:O	2.20	0.41
1:A:317:ARG:HD3	1:A:317:ARG:HA	1.71	0.41
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.97	0.41
1:C:487:LEU:HD23	1:C:487:LEU:HA	1.93	0.41
1:C:258:GLU:HB3	1:C:374:LYS:HG3	2.04	0.40
1:G:465:GLU:OE2	1:H:154:HIS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:LEU:HD12	1:H:206:LEU:HA	1.90	0.40
1:F:61:TYR:HE2	1:F:234:PHE:CD1	2.40	0.40
1:H:445:ARG:O	1:H:449:GLU:HG2	2.20	0.40
1:C:203:ARG:NH1	1:C:431:THR:HB	2.35	0.40
1:C:460:LEU:HD13	1:C:460:LEU:C	2.47	0.40
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.97	0.40
1:H:311:ARG:HH21	1:H:311:ARG:HG2	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	451/487 (93%)	441 (98%)	9 (2%)	1 (0%)	43 64
1	B	450/487 (92%)	440 (98%)	9 (2%)	1 (0%)	43 64
1	C	445/487 (91%)	435 (98%)	9 (2%)	1 (0%)	43 64
1	D	448/487 (92%)	438 (98%)	9 (2%)	1 (0%)	43 64
1	E	446/487 (92%)	436 (98%)	9 (2%)	1 (0%)	43 64
1	F	446/487 (92%)	436 (98%)	9 (2%)	1 (0%)	43 64
1	G	448/487 (92%)	437 (98%)	10 (2%)	1 (0%)	43 64
1	H	450/487 (92%)	437 (97%)	12 (3%)	1 (0%)	43 64
All	All	3584/3896 (92%)	3500 (98%)	76 (2%)	8 (0%)	43 64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	273	GLY
1	F	273	GLY
1	A	273	GLY

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Mol	Chain	Res	Type
1	B	273	GLY
1	D	273	GLY
1	G	273	GLY
1	H	273	GLY
1	C	273	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/405 (94%)	368 (97%)	13 (3%)	32	57
1	B	380/405 (94%)	365 (96%)	15 (4%)	28	51
1	C	377/405 (93%)	361 (96%)	16 (4%)	26	49
1	D	378/405 (93%)	363 (96%)	15 (4%)	28	50
1	E	377/405 (93%)	361 (96%)	16 (4%)	26	49
1	F	377/405 (93%)	358 (95%)	19 (5%)	22	42
1	G	379/405 (94%)	366 (97%)	13 (3%)	32	57
1	H	381/405 (94%)	370 (97%)	11 (3%)	37	61
All	All	3030/3240 (94%)	2912 (96%)	118 (4%)	28	51

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ILE
1	A	71	SER
1	A	72	GLU
1	A	112	LEU
1	A	167	THR
1	A	217	VAL
1	A	316	SER
1	A	372	THR
1	A	436	VAL
1	A	463	LYS

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Mol	Chain	Res	Type
1	A	471	GLU
1	A	477	ARG
1	A	479	ARG
1	B	30	LYS
1	B	49	ARG
1	B	53	ARG
1	B	59	ILE
1	B	66	ARG
1	B	71	SER
1	B	72	GLU
1	B	167	THR
1	B	316	SER
1	B	417	MET
1	B	434	ARG
1	B	436	VAL
1	B	442	GLN
1	B	467	ARG
1	B	479	ARG
1	C	24	VAL
1	C	50	THR
1	C	71	SER
1	C	155	ARG
1	C	167	THR
1	C	171	SER
1	C	311	ARG
1	C	316	SER
1	C	372	THR
1	C	417	MET
1	C	420	ASN
1	C	429	VAL
1	C	436	VAL
1	C	452	VAL
1	C	467	ARG
1	C	475	ARG
1	D	30	LYS
1	D	64	ARG
1	D	71	SER
1	D	112	LEU
1	D	145	LYS
1	D	167	THR
1	D	173	ARG
1	D	311	ARG

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Mol	Chain	Res	Type
1	D	316	SER
1	D	436	VAL
1	D	440	ARG
1	D	452	VAL
1	D	458	VAL
1	D	475	ARG
1	D	487	LEU
1	E	59	ILE
1	E	70	SER
1	E	71	SER
1	E	72	GLU
1	E	90	ARG
1	E	98	THR
1	E	167	THR
1	E	213	LYS
1	E	217	VAL
1	E	233	SER
1	E	311	ARG
1	E	316	SER
1	E	372	THR
1	E	436	VAL
1	E	467	ARG
1	E	479	ARG
1	F	33	ARG
1	F	59	ILE
1	F	71	SER
1	F	72	GLU
1	F	167	THR
1	F	211	GLU
1	F	246	GLU
1	F	311	ARG
1	F	316	SER
1	F	372	THR
1	F	417	MET
1	F	429	VAL
1	F	436	VAL
1	F	440	ARG
1	F	452	VAL
1	F	471	GLU
1	F	479	ARG
1	F	482	GLU
1	F	486	LYS

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Mol	Chain	Res	Type
1	G	59	ILE
1	G	66	ARG
1	G	71	SER
1	G	72	GLU
1	G	155	ARG
1	G	167	THR
1	G	179	LYS
1	G	274	ARG
1	G	316	SER
1	G	436	VAL
1	G	449	GLU
1	G	458	VAL
1	G	475	ARG
1	H	20	MET
1	H	21	LEU
1	H	49	ARG
1	H	59	ILE
1	H	71	SER
1	H	72	GLU
1	H	167	THR
1	H	311	ARG
1	H	316	SER
1	H	436	VAL
1	H	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	HIS
1	B	163	HIS
1	B	442	GLN
1	C	163	HIS
1	C	176	GLN
1	C	263	ASN
1	C	442	GLN
1	D	22	ASN
1	D	163	HIS
1	D	250	GLN
1	D	442	GLN
1	E	160	ASN
1	E	163	HIS
1	E	210	GLN

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Mol	Chain	Res	Type
1	E	250	GLN
1	E	442	GLN
1	F	163	HIS
1	F	442	GLN
1	G	250	GLN
1	G	315	HIS
1	H	154	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BNZ	H	1002	-	6,6,6	1.26	1 (16%)	6,6,6	1.03	0
2	BNZ	E	501	-	6,6,6	0.78	0	6,6,6	0.42	0
3	GOL	G	502	-	5,5,5	0.13	0	5,5,5	0.45	0
4	AMP	H	1001	-	25,25,25	0.39	0	37,38,38	0.53	0
2	BNZ	D	1002	-	6,6,6	0.66	0	6,6,6	0.52	0
3	GOL	A	502	-	5,5,5	0.15	0	5,5,5	0.54	0
2	BNZ	C	501	-	6,6,6	0.69	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	H	1003	-	5,5,5	0.21	0	5,5,5	0.34	0
4	AMP	C	503	-	25,25,25	0.41	0	37,38,38	0.57	0
3	GOL	E	502	-	5,5,5	0.10	0	5,5,5	0.32	0
4	AMP	F	1001	-	25,25,25	0.40	0	37,38,38	0.53	0
3	GOL	F	1004	-	5,5,5	0.11	0	5,5,5	0.28	0
2	BNZ	A	501	-	6,6,6	0.75	0	6,6,6	0.43	0
2	BNZ	F	1003	-	6,6,6	0.69	0	6,6,6	0.35	0
3	GOL	D	1003	-	5,5,5	0.23	0	5,5,5	0.38	0
4	AMP	A	503	-	25,25,25	0.30	0	37,38,38	0.74	0
3	GOL	C	502	-	5,5,5	0.18	0	5,5,5	0.22	0
2	BNZ	B	1002	-	6,6,6	0.95	0	6,6,6	0.54	0
2	BNZ	G	501	-	6,6,6	0.62	0	6,6,6	0.49	0
4	AMP	D	1001	-	25,25,25	0.37	0	37,38,38	0.78	1 (2%)
4	AMP	F	1002	-	25,25,25	0.35	0	37,38,38	0.59	0
3	GOL	B	1003	-	5,5,5	0.19	0	5,5,5	0.53	0
4	AMP	B	1001	-	25,25,25	0.48	0	37,38,38	0.72	0
4	AMP	G	503	-	25,25,25	0.48	0	37,38,38	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BNZ	H	1002	-	-	-	0/1/1/1
2	BNZ	E	501	-	-	-	0/1/1/1
3	GOL	G	502	-	-	2/4/4/4	-
4	AMP	H	1001	-	-	4/10/26/26	0/3/3/3
2	BNZ	D	1002	-	-	-	0/1/1/1
3	GOL	A	502	-	-	2/4/4/4	-
2	BNZ	C	501	-	-	-	0/1/1/1
3	GOL	H	1003	-	-	3/4/4/4	-
4	AMP	C	503	-	-	5/10/26/26	0/3/3/3
3	GOL	E	502	-	-	2/4/4/4	-
4	AMP	F	1001	-	-	4/10/26/26	0/3/3/3
3	GOL	F	1004	-	-	4/4/4/4	-
2	BNZ	A	501	-	-	-	0/1/1/1
3	GOL	D	1003	-	-	0/4/4/4	-
2	BNZ	F	1003	-	-	-	0/1/1/1
4	AMP	A	503	-	-	5/10/26/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	502	-	-	0/4/4/4	-
2	BNZ	B	1002	-	-	-	0/1/1/1
2	BNZ	G	501	-	-	-	0/1/1/1
4	AMP	D	1001	-	-	2/10/26/26	0/3/3/3
4	AMP	F	1002	-	-	2/10/26/26	0/3/3/3
3	GOL	B	1003	-	-	2/4/4/4	-
4	AMP	B	1001	-	-	0/10/26/26	0/3/3/3
4	AMP	G	503	-	-	2/10/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1002	BNZ	C2-C1	2.31	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1001	AMP	O3P-P-O5'	-2.50	100.15	106.67

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	E	502	GOL	O1-C1-C2-C3
3	G	502	GOL	C1-C2-C3-O3
3	H	1003	GOL	C1-C2-C3-O3
3	B	1003	GOL	C1-C2-C3-O3
3	F	1004	GOL	O1-C1-C2-C3
3	F	1004	GOL	C1-C2-C3-O3
3	B	1003	GOL	O2-C2-C3-O3
3	E	502	GOL	O1-C1-C2-O2
3	F	1004	GOL	O1-C1-C2-O2
3	G	502	GOL	O2-C2-C3-O3
3	H	1003	GOL	O2-C2-C3-O3
4	C	503	AMP	O4'-C4'-C5'-O5'
4	C	503	AMP	C3'-C4'-C5'-O5'
3	F	1004	GOL	O2-C2-C3-O3
4	A	503	AMP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	F	1001	AMP	C2'-C1'-N9-C8
4	C	503	AMP	C4'-C5'-O5'-P
4	A	503	AMP	C4'-C5'-O5'-P
4	F	1001	AMP	C4'-C5'-O5'-P
4	H	1001	AMP	O4'-C4'-C5'-O5'
4	H	1001	AMP	C4'-C5'-O5'-P
4	A	503	AMP	C3'-C4'-C5'-O5'
4	F	1002	AMP	O4'-C4'-C5'-O5'
4	G	503	AMP	C4'-C5'-O5'-P
3	H	1003	GOL	O1-C1-C2-O2
4	A	503	AMP	C2'-C1'-N9-C8
4	D	1001	AMP	C4'-C5'-O5'-P
4	F	1002	AMP	C4'-C5'-O5'-P
4	C	503	AMP	C5'-O5'-P-O1P
4	H	1001	AMP	C3'-C4'-C5'-O5'
4	F	1001	AMP	O4'-C1'-N9-C8
4	H	1001	AMP	C2'-C1'-N9-C8
4	F	1001	AMP	O4'-C4'-C5'-O5'
4	A	503	AMP	O4'-C1'-N9-C8
4	C	503	AMP	C2'-C1'-N9-C8
4	D	1001	AMP	C2'-C1'-N9-C8
4	G	503	AMP	C2'-C1'-N9-C8

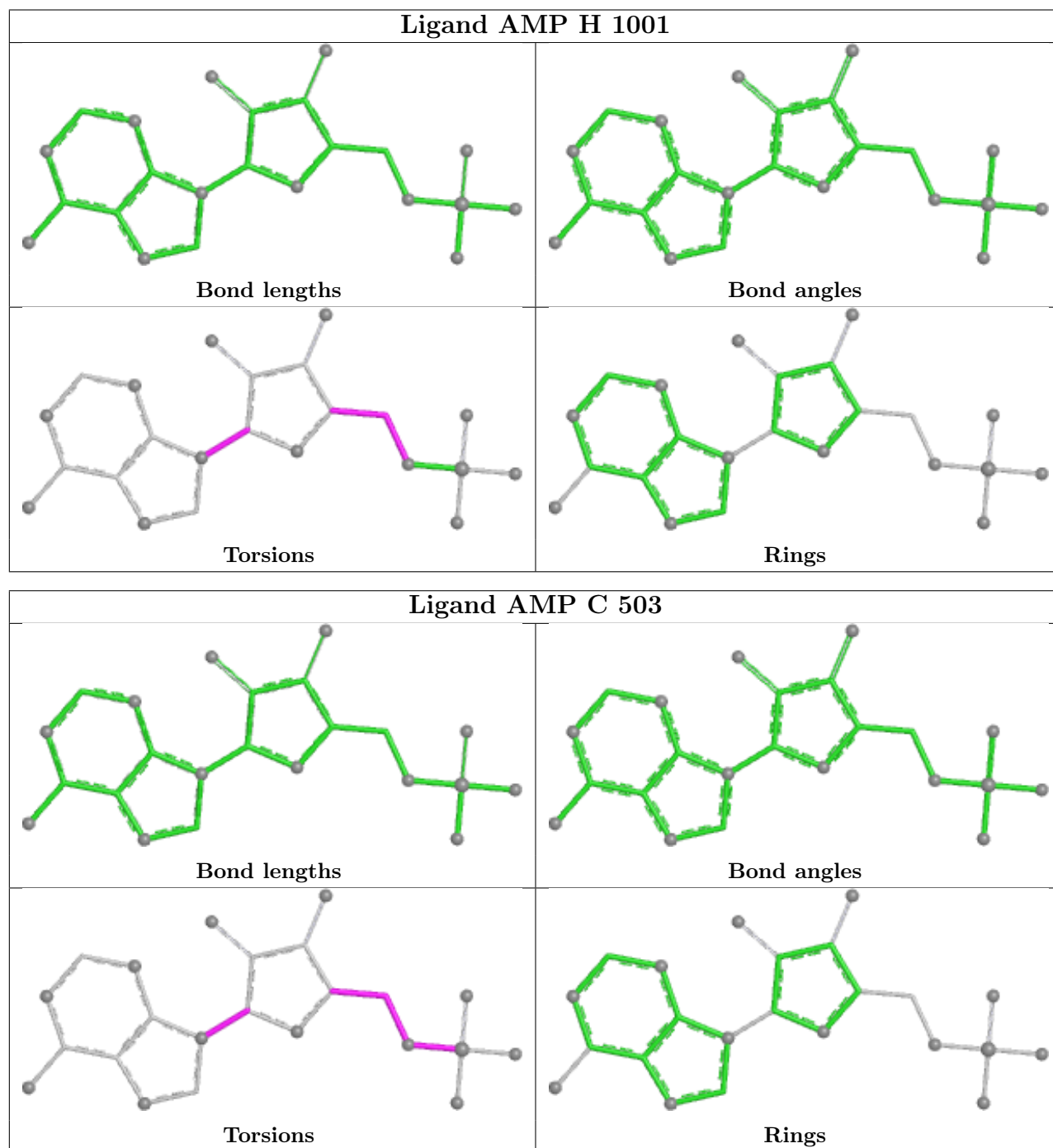
There are no ring outliers.

10 monomers are involved in 13 short contacts:

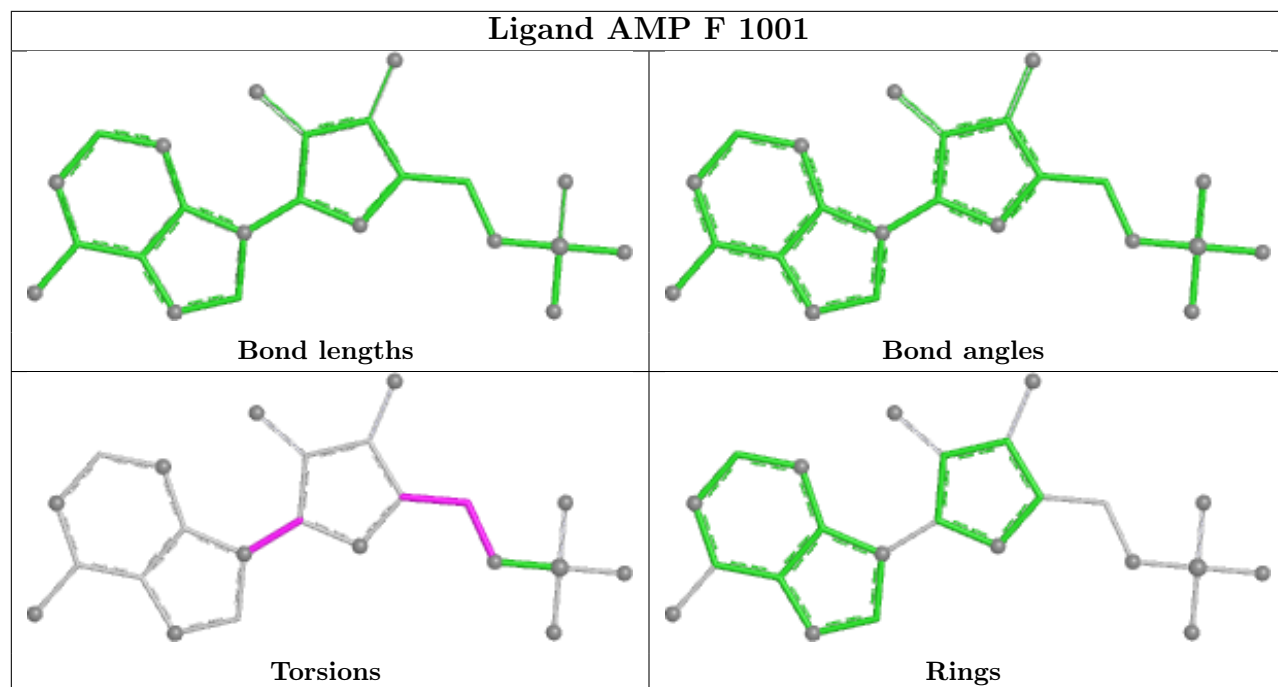
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1001	AMP	1	0
4	C	503	AMP	2	0
4	F	1001	AMP	1	0
3	D	1003	GOL	1	0
4	A	503	AMP	1	0
3	C	502	GOL	1	0
4	D	1001	AMP	1	0
4	F	1002	AMP	1	0
4	B	1001	AMP	2	0
4	G	503	AMP	2	0

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

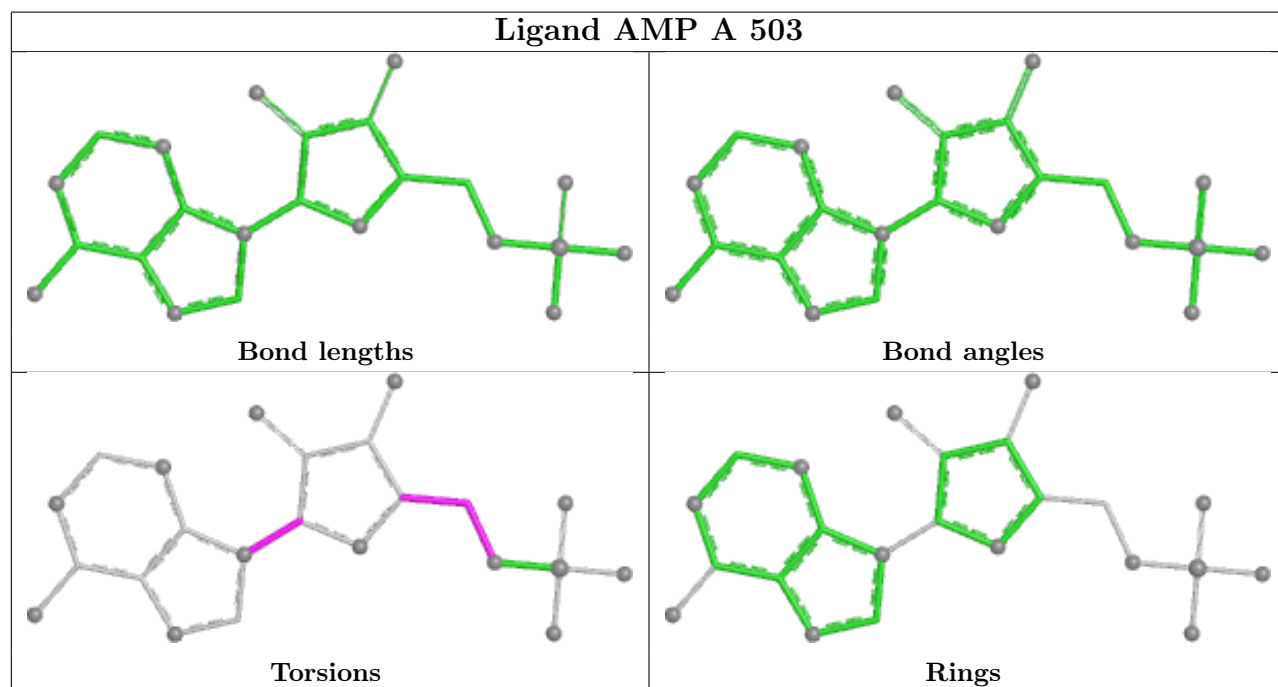
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



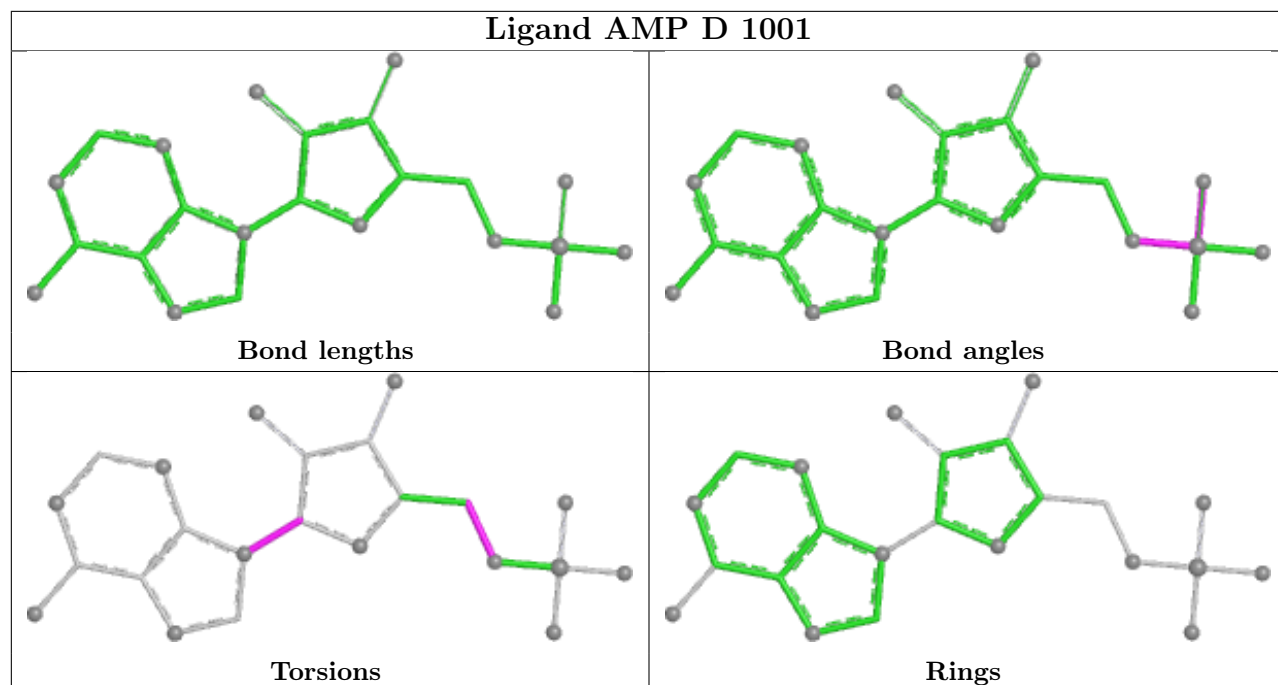
Ligand AMP F 1001



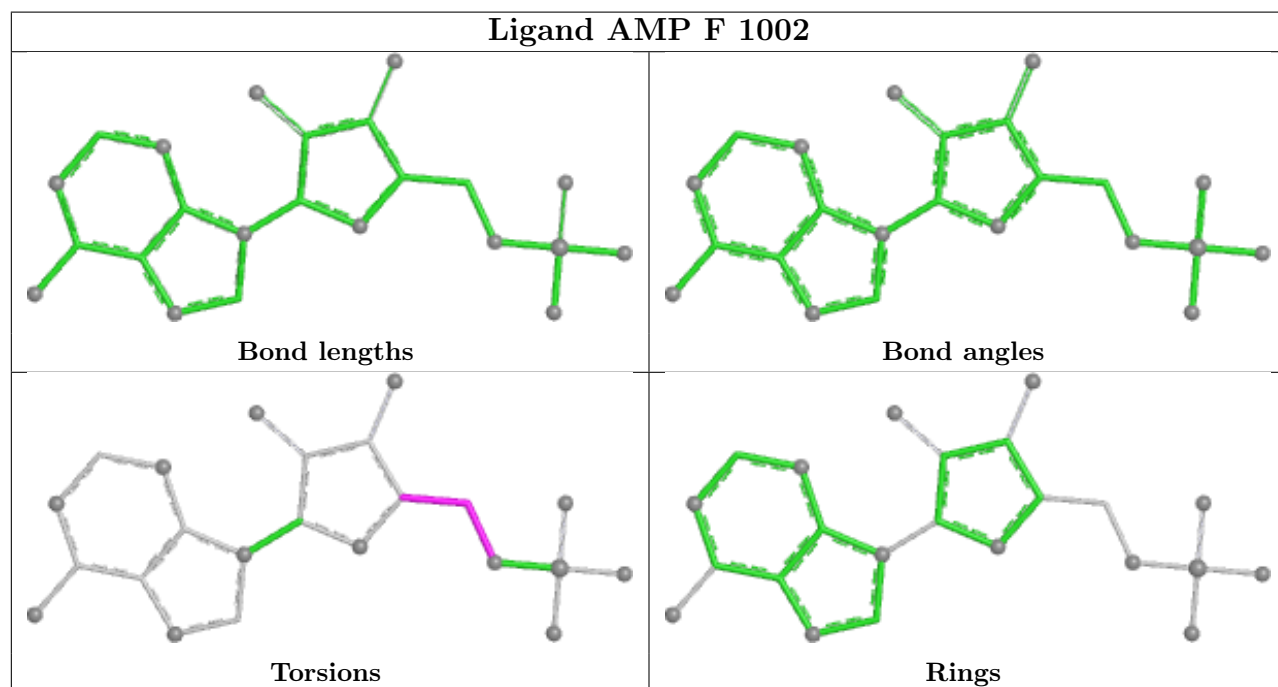
Ligand AMP A 503

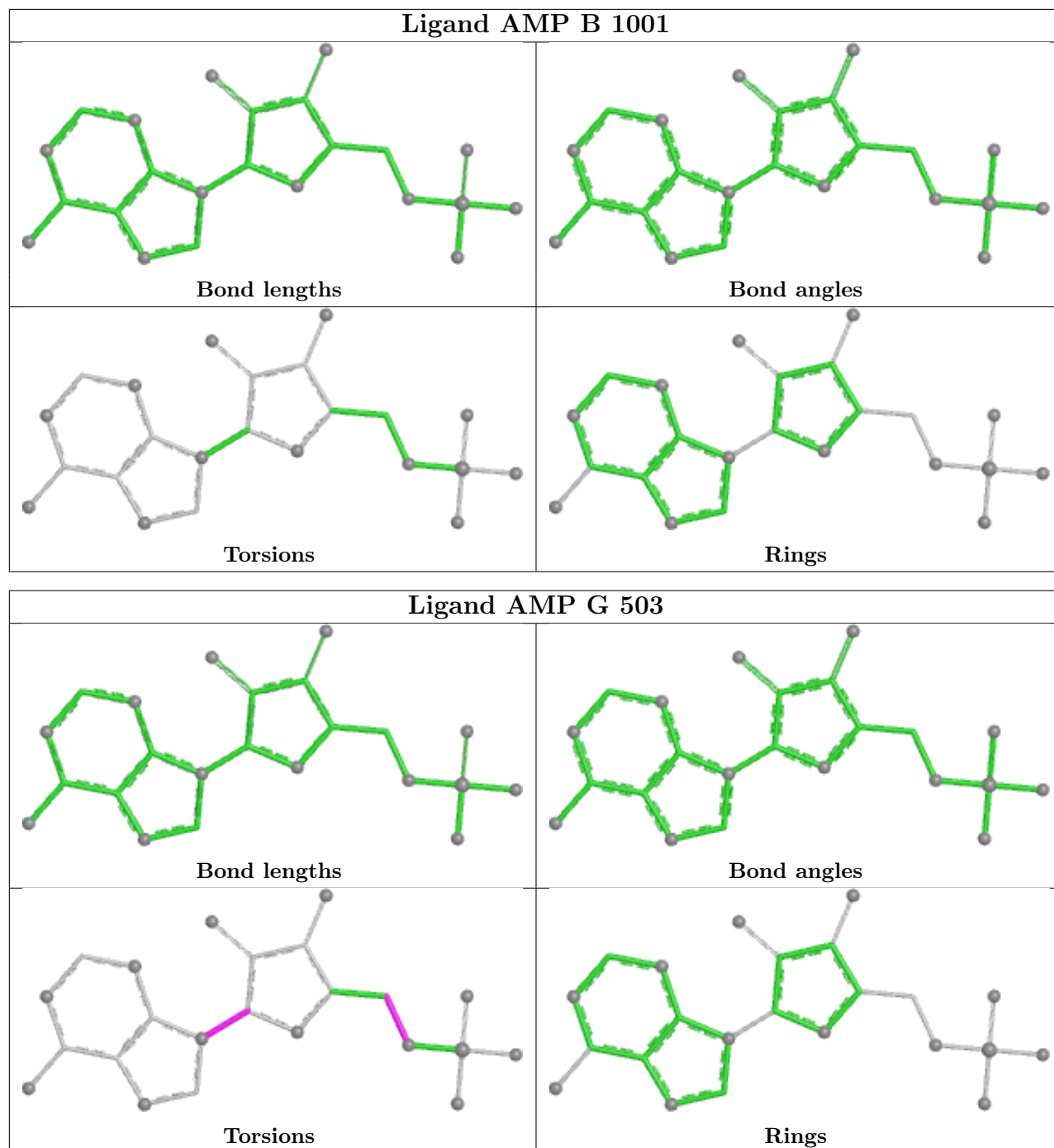


Ligand AMP D 1001



Ligand AMP F 1002





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	455/487 (93%)	-0.34	5 (1%) 78 77	15, 28, 55, 82	0
1	B	454/487 (93%)	-0.38	2 (0%) 88 89	14, 26, 50, 85	0
1	C	451/487 (92%)	-0.20	2 (0%) 88 89	19, 32, 58, 83	0
1	D	452/487 (92%)	-0.11	3 (0%) 84 84	20, 32, 58, 79	0
1	E	450/487 (92%)	-0.13	0 100 100	20, 35, 58, 73	0
1	F	450/487 (92%)	-0.04	0 100 100	21, 36, 62, 87	0
1	G	452/487 (92%)	-0.12	2 (0%) 88 89	22, 34, 58, 76	0
1	H	454/487 (93%)	-0.23	3 (0%) 84 84	17, 28, 55, 101	0
All	All	3618/3896 (92%)	-0.19	17 (0%) 87 87	14, 32, 57, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	20	MET	4.1
1	D	487	LEU	3.3
1	G	27	GLU	3.2
1	D	64	ARG	3.1
1	B	21	LEU	3.0
1	B	346	LEU	2.8
1	A	332	GLY	2.6
1	A	20	MET	2.4
1	C	69	PRO	2.4
1	H	21	LEU	2.4
1	A	346	LEU	2.3
1	C	346	LEU	2.3
1	H	174	GLY	2.2
1	G	485	ALA	2.1
1	A	475	ARG	2.1
1	A	487	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	79	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

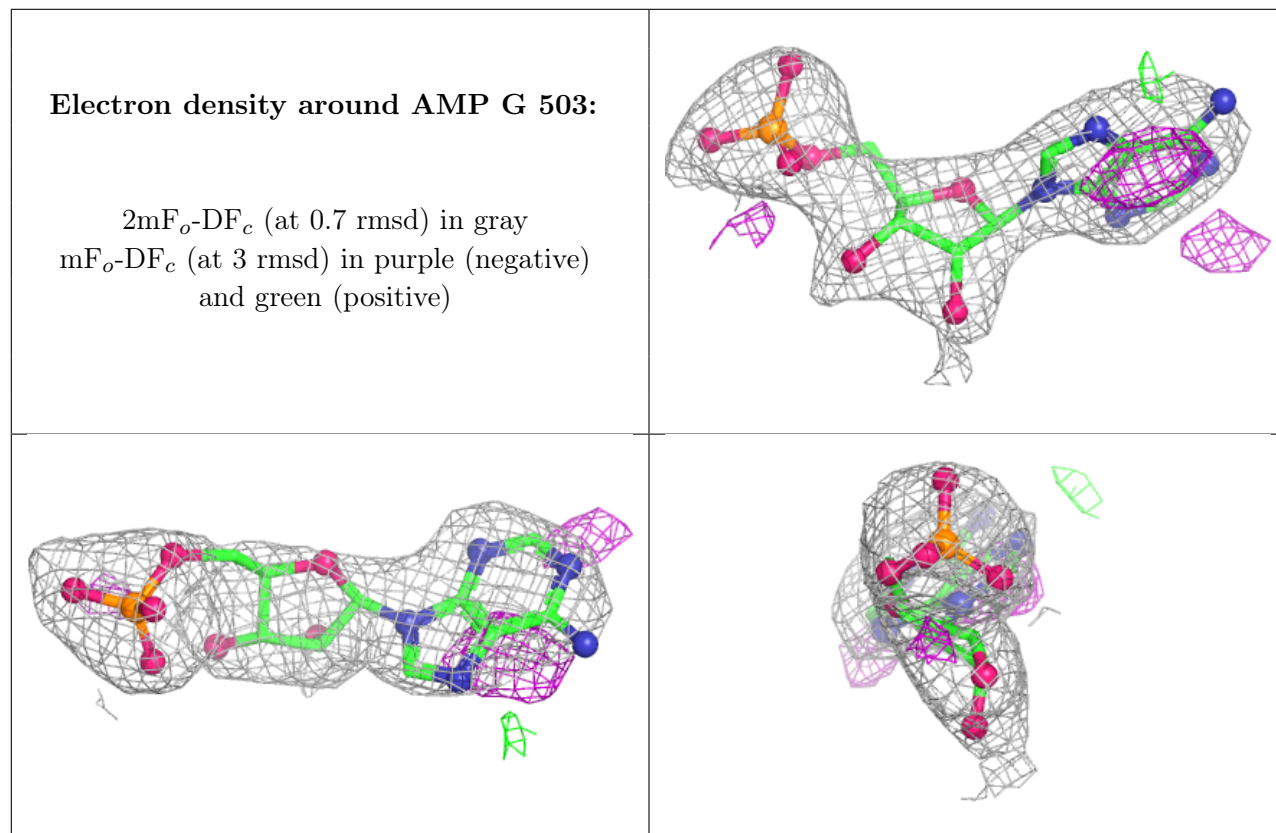
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BNZ	F	1003	6/6	0.54	0.24	57,58,59,59	0
2	BNZ	D	1002	6/6	0.58	0.21	46,51,51,52	0
2	BNZ	B	1002	6/6	0.68	0.19	31,32,32,33	0
2	BNZ	H	1002	6/6	0.68	0.20	29,29,30,31	0
2	BNZ	G	501	6/6	0.70	0.18	44,45,45,46	0
2	BNZ	C	501	6/6	0.72	0.17	42,43,44,44	0
3	GOL	H	1003	6/6	0.72	0.19	39,42,55,60	0
2	BNZ	E	501	6/6	0.76	0.18	44,45,46,46	0
2	BNZ	A	501	6/6	0.80	0.14	30,31,31,32	0
3	GOL	F	1004	6/6	0.88	0.09	22,24,25,27	0
3	GOL	D	1003	6/6	0.88	0.10	24,25,26,28	0
3	GOL	E	502	6/6	0.89	0.11	36,40,44,45	0
4	AMP	G	503	23/23	0.90	0.10	40,43,46,46	0
3	GOL	C	502	6/6	0.92	0.08	26,28,29,30	0
3	GOL	G	502	6/6	0.92	0.08	27,28,28,29	0
3	GOL	A	502	6/6	0.92	0.08	25,25,26,26	0
4	AMP	B	1001	23/23	0.92	0.09	35,37,41,42	0
3	GOL	B	1003	6/6	0.92	0.09	25,26,28,31	0
4	AMP	D	1001	23/23	0.93	0.07	42,46,51,52	0
4	AMP	C	503	23/23	0.94	0.07	41,44,46,47	0
4	AMP	F	1002	23/23	0.95	0.06	36,38,44,46	0
4	AMP	F	1001	23/23	0.95	0.07	33,39,42,42	0

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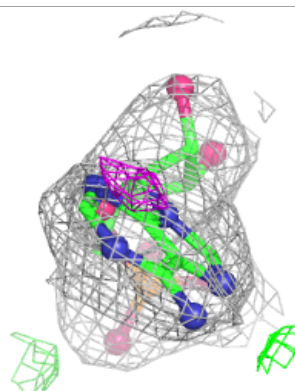
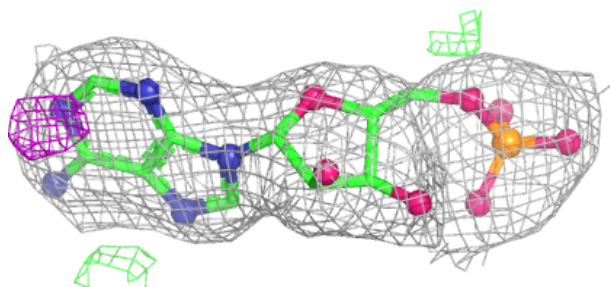
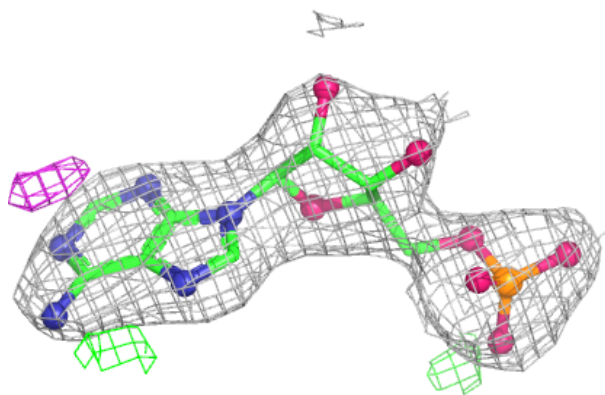
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AMP	H	1001	23/23	0.95	0.06	36,38,40,40	0
4	AMP	A	503	23/23	0.98	0.05	24,26,27,27	0

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.

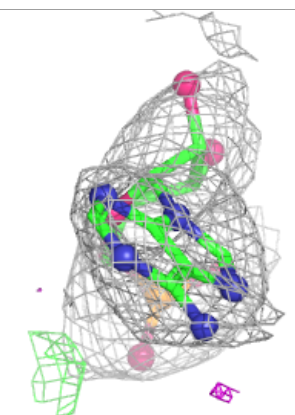
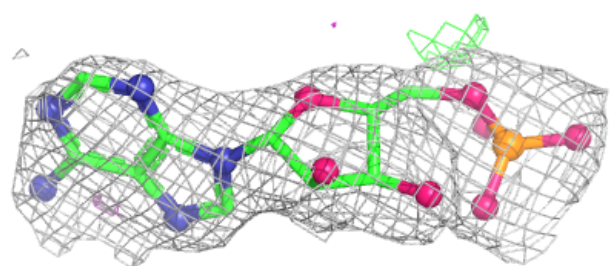
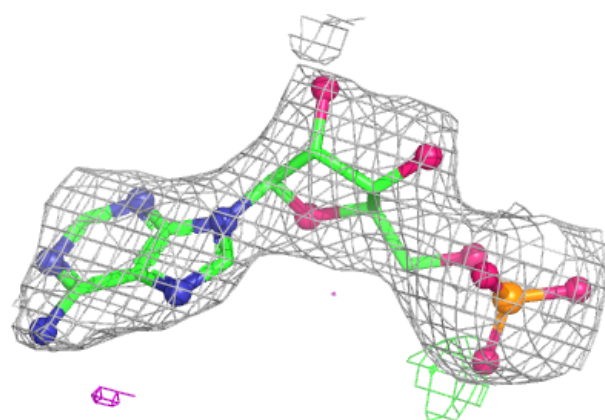


Electron density around AMP B 1001:

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

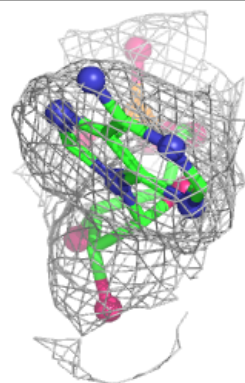
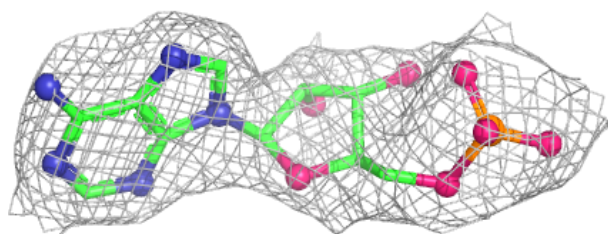
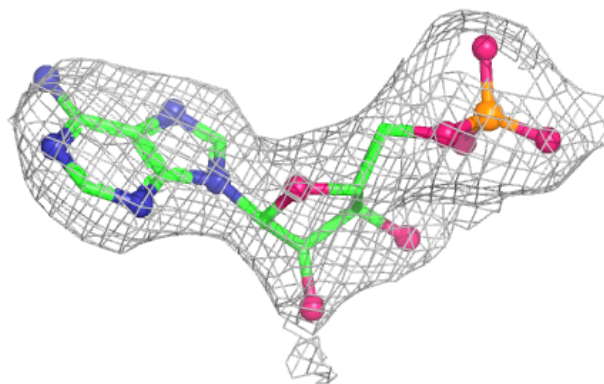
**Electron density around AMP D 1001:**

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

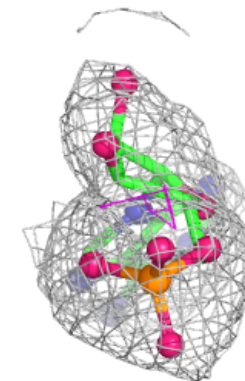
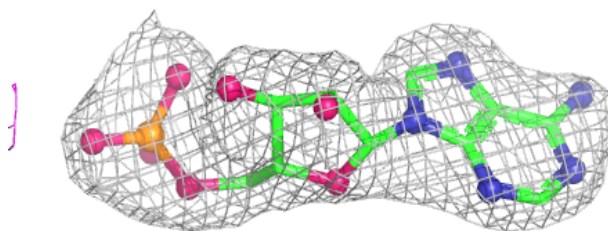
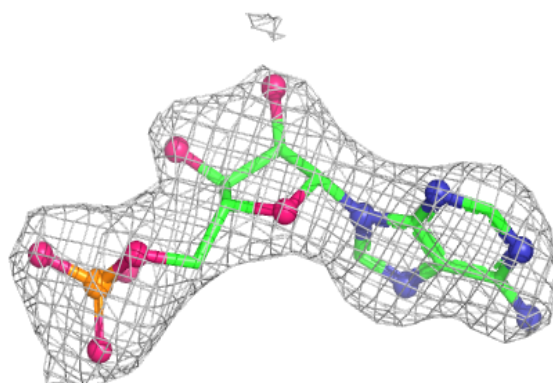


Electron density around AMP C 503:

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

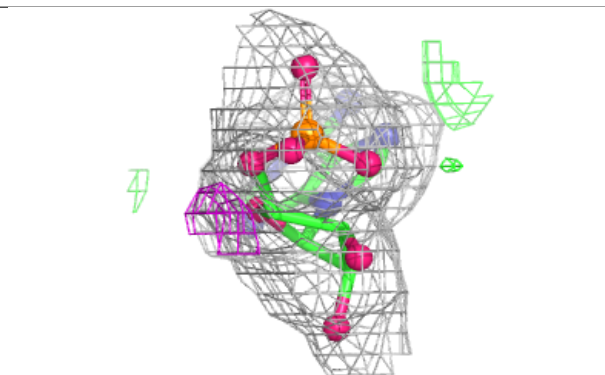
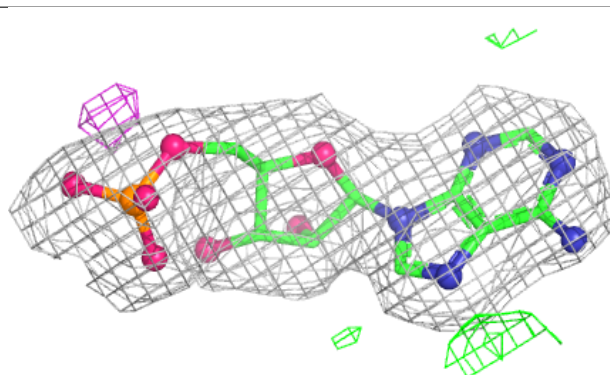
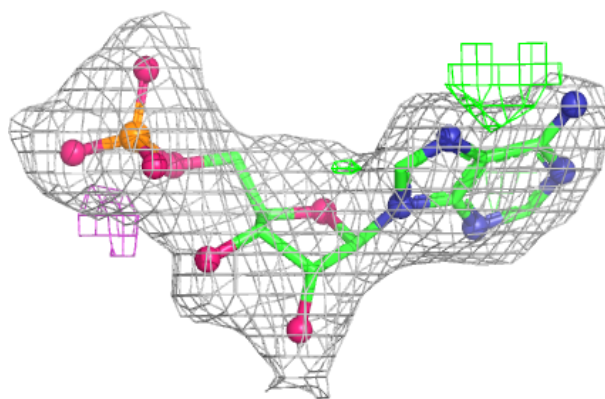
**Electron density around AMP F 1002:**

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

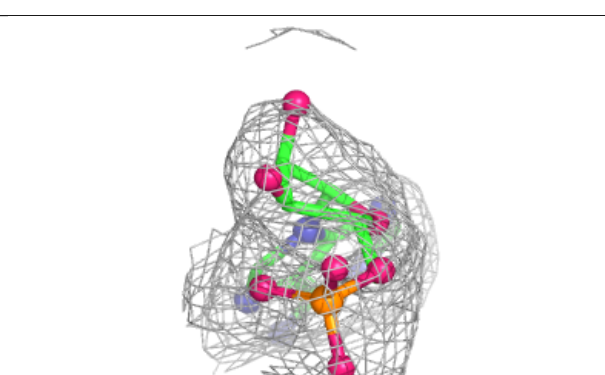
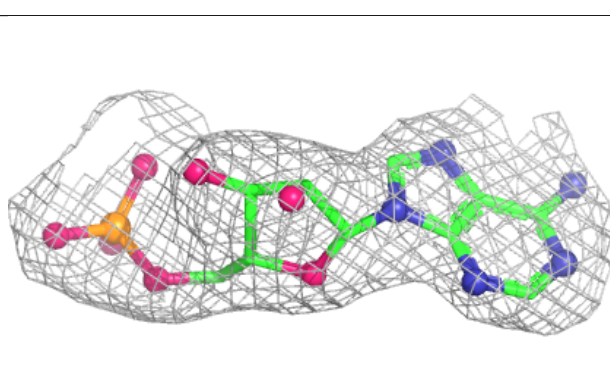
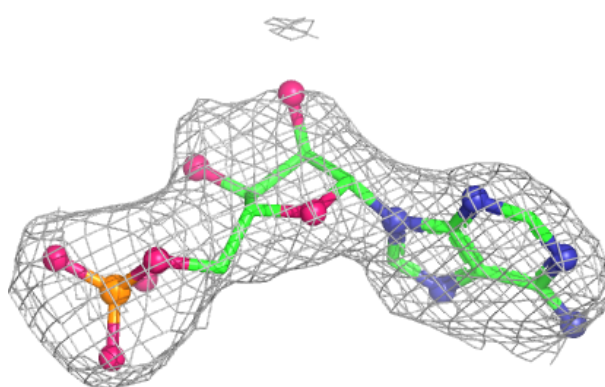


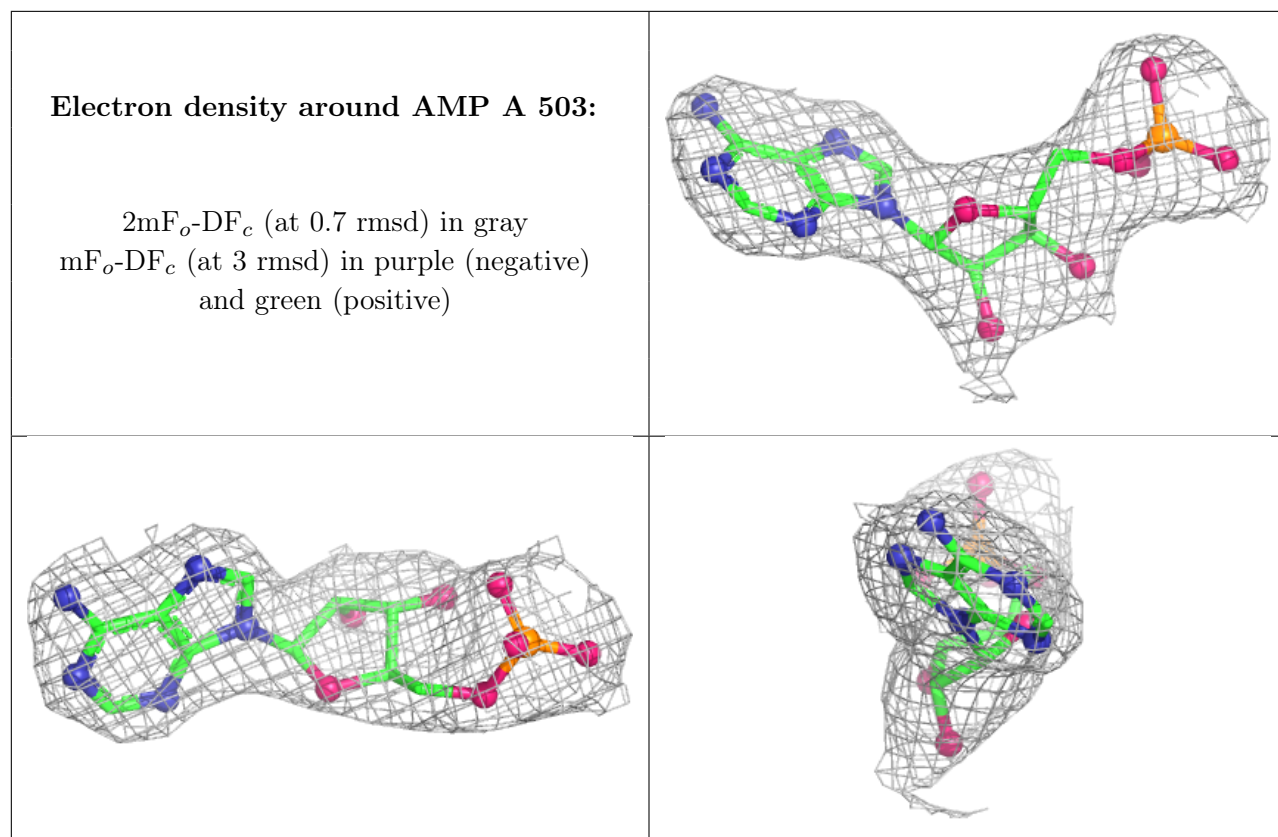
Electron density around AMP F 1001:

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

**Electron density around AMP H 1001:**

$2mF_o-DF_c$ (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.