



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:17 AM UTC

PDB ID : 3T94 / pdb_00003t94
Title : Crystal structure of 5'-deoxy-5'-methylthioadenosine phosphorylase (MTAP)
II complexed with 5'-deoxy-5'-methylthioadenosine and sulfate
Authors : Zhang, Y.; Ealick, S.E.
Deposited on : 2011-08-02
Resolution : 1.45 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:

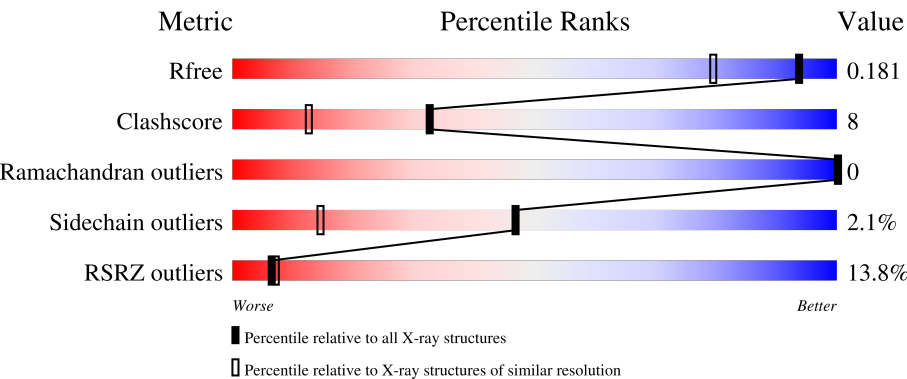
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	270	14% 87% 13%
1	B	270	14% 86% 14% .
1	C	270	14% 86% 14%
1	D	270	15% 84% 15% .
1	E	270	12% 84% 15% .

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Mol	Chain	Length	Quality of chain
1	F	270	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment on the left labeled '13%', a green segment in the middle labeled '88%', and a yellow segment on the right labeled '11%'.

2 Entry composition [i](#)

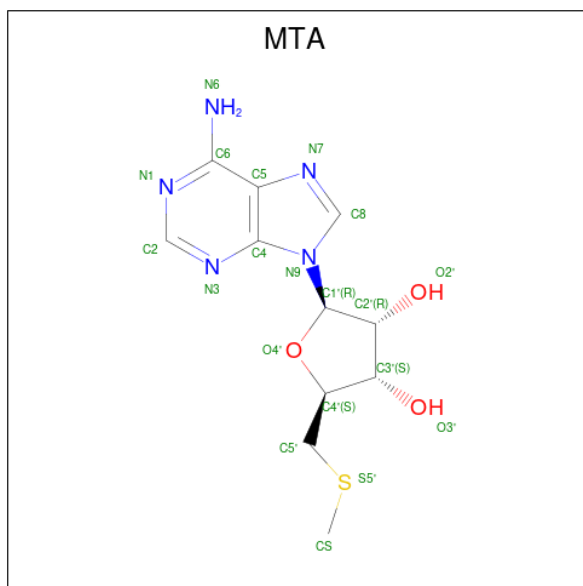
There are 4 unique types of molecules in this entry. The entry contains 14787 atoms, of which 0 are hydrogens and 0 are deuteriums.

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'-methylthioadenosine phosphorylase (MtaP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	13	0
			2145	1375	361	390	19			
1	B	270	Total	C	N	O	S	0	23	0
			2237	1433	374	410	20			
1	C	270	Total	C	N	O	S	0	23	0
			2246	1445	371	410	20			
1	D	270	Total	C	N	O	S	0	22	0
			2226	1427	376	404	19			
1	E	270	Total	C	N	O	S	0	31	0
			2286	1465	385	417	19			
1	F	270	Total	C	N	O	S	0	17	0
			2185	1403	364	399	19			

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	D	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	E	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
2	F	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	1
			10	8	2		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	1
			10	8	2		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

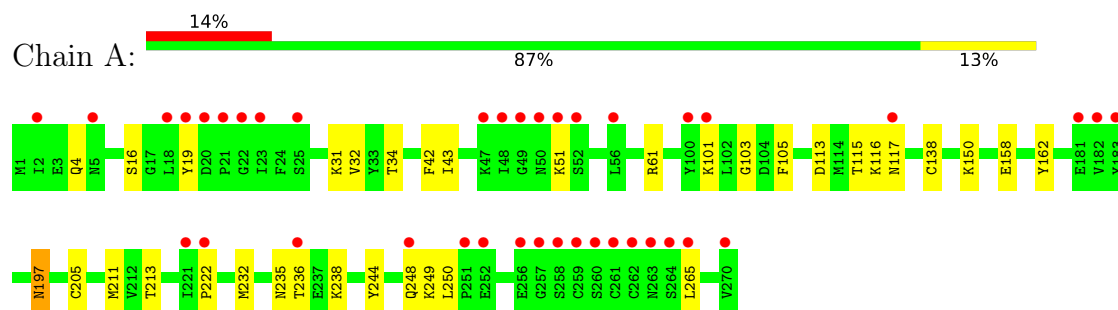
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	1
			196	196		
4	B	230	Total	O	0	0
			230	230		
4	C	208	Total	O	0	0
			208	208		
4	D	219	Total	O	0	0
			219	219		
4	E	221	Total	O	0	1
			222	222		
4	F	202	Total	O	0	0
			202	202		

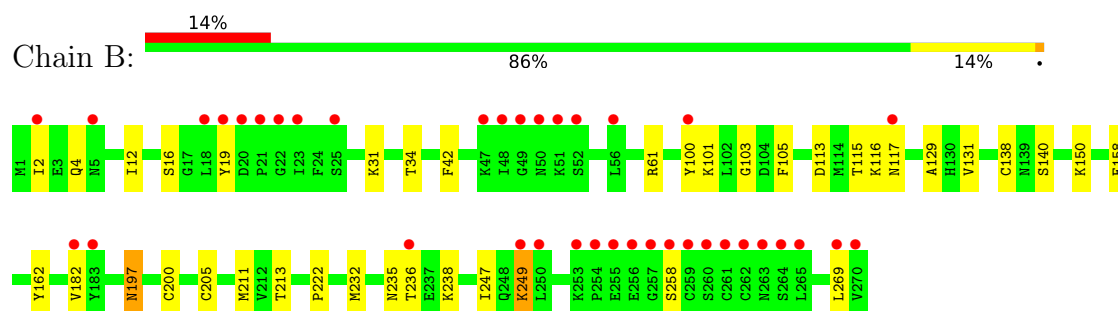
3 Residue-property plots [i](#)

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

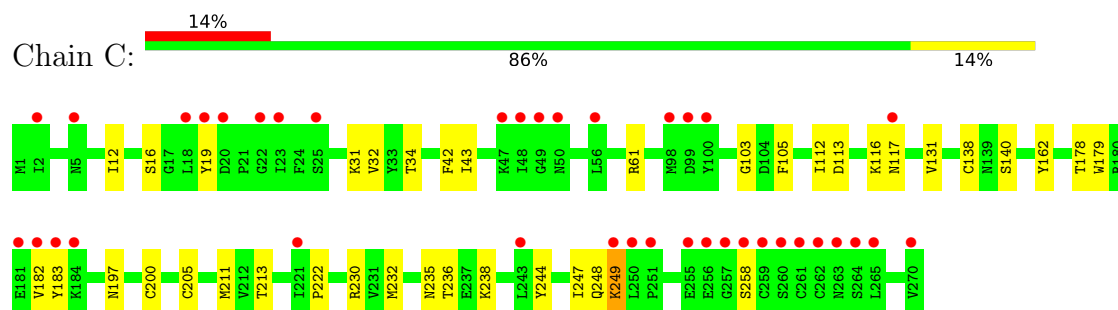
- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)



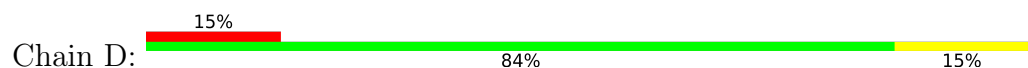
- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)

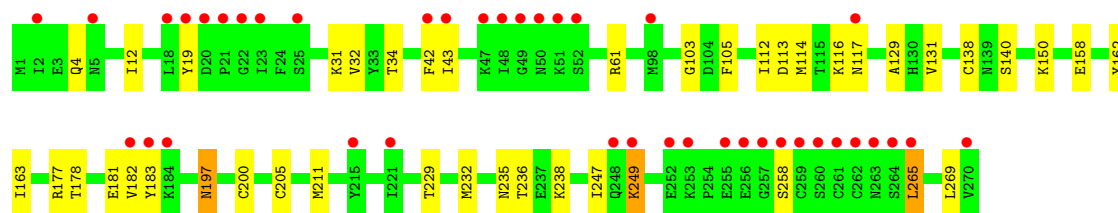


- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)

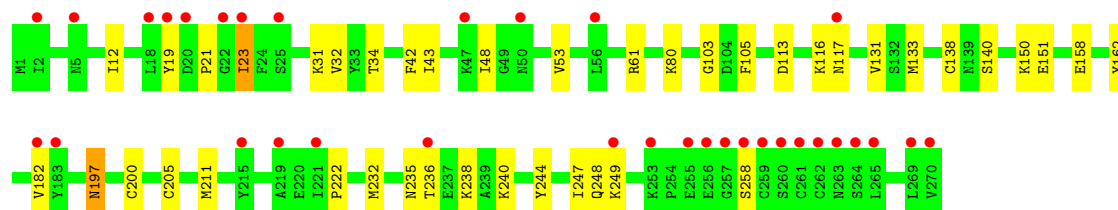
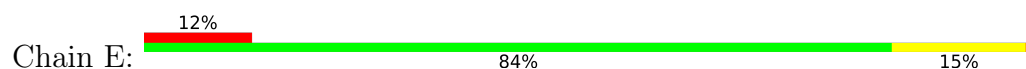


- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)

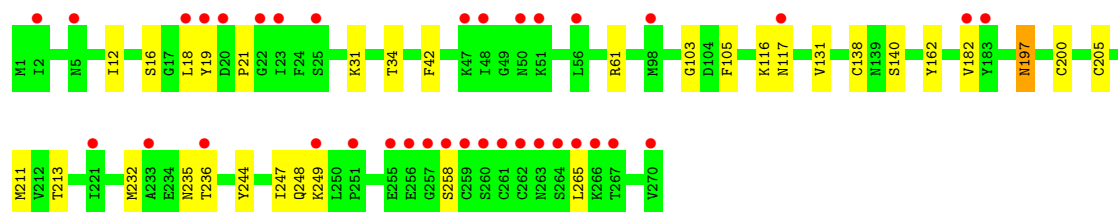
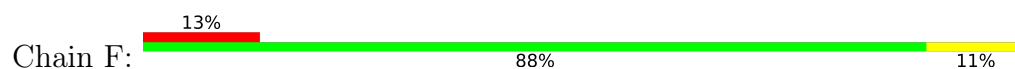




- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)



- Molecule 1: 5'-methylthioadenosine phosphorylase (MtaP)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	135.16Å 138.09Å 96.56Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	39.67 – 1.45 39.67 – 1.45	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.67-1.45) 97.0 (39.67-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.169 , 0.185 0.165 , 0.181	Depositor DCC
R_{free} test set	20910 reflections (6.93%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.000 for -1/2*h-1/2*k-l,1/2*h+1/2*k-l,1/2 *h-1/2*k 0.000 for -1/2*h-1/2*k+l,1/2*h+1/2*k+l,-1 /2*h+1/2*k 0.000 for -1/2*h+1/2*k+l,-1/2*h+1/2*k-l,- 1/2*h-1/2*k 0.000 for -1/2*h+1/2*k-l,-1/2*h+1/2*k+l,1 /2*h+1/2*k 0.041 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2 *h-1/2*k 0.034 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/ 2*h+1/2*k 0.000 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2 *h-1/2*k 0.000 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1 /2*h+1/2*k 0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14787	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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.

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.0813e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MTA, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.38	0/2191	0.69	1/2969 (0.0%)
1	B	0.38	0/2284	0.68	1/3095 (0.0%)
1	C	0.37	0/2294	0.69	0/3106
1	D	0.37	0/2273	0.68	1/3080 (0.0%)
1	E	0.38	0/2332	0.67	1/3158 (0.0%)
1	F	0.37	0/2231	0.67	1/3023 (0.0%)
All	All	0.37	0/13605	0.68	5/18431 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	ASN	CB-CA-C	-5.67	101.98	110.88
1	D	197	ASN	CB-CA-C	-5.42	102.37	110.88
1	F	197	ASN	CB-CA-C	-5.36	102.47	110.88
1	E	197	ASN	CB-CA-C	-5.22	102.68	110.88
1	B	197	ASN	CB-CA-C	-5.12	102.85	110.88

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	2145	0	2102	33	0
1	B	2237	0	2190	43	0
1	C	2246	0	2208	42	0
1	D	2226	0	2188	49	0
1	E	2286	0	2262	41	0
1	F	2185	0	2154	30	0
2	A	20	0	15	1	0
2	B	20	0	15	0	0
2	C	20	0	15	1	0
2	D	20	0	15	1	0
2	E	20	0	15	1	0
2	F	20	0	15	1	0
3	A	15	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	0	0
3	D	15	0	0	0	0
3	E	10	0	0	0	0
3	F	5	0	0	0	0
4	A	196	0	0	2	0
4	B	230	0	0	3	0
4	C	208	0	0	2	0
4	D	219	0	0	1	0
4	E	222	0	0	2	0
4	F	202	0	0	1	0
All	All	14787	0	13194	211	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 8.

All (211) 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:F:12[B]:ILE:HD11	1:F:247:ILE:HD11	1.48	0.92
1:B:12[A]:ILE:HD11	1:B:247:ILE:HD11	1.52	0.90
1:E:131[B]:VAL:HG11	1:E:200:CYS:SG	2.15	0.87
1:B:131[B]:VAL:HG11	1:B:200:CYS:SG	2.14	0.86
1:F:131[B]:VAL:HG11	1:F:200:CYS:SG	2.15	0.86
1:E:117[B]:ASN:HB3	1:F:117[B]:ASN:HA	1.59	0.83
1:C:131[B]:VAL:HG11	1:C:200:CYS:SG	2.19	0.83
1:B:117[B]:ASN:HB3	1:C:117[B]:ASN:HA	1.58	0.83
1:D:117[B]:ASN:HA	1:F:117[B]:ASN:HB3	1.60	0.82
1:D:131[B]:VAL:HG11	1:D:200:CYS:SG	2.19	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12[B]:ILE:HD11	1:C:247:ILE:HD11	1.63	0.80
1:D:12[B]:ILE:HD11	1:D:247:ILE:HD11	1.64	0.80
1:A:117[B]:ASN:HA	1:C:117[B]:ASN:HD22	1.51	0.76
1:E:12[B]:ILE:HD11	1:E:247:ILE:HD11	1.67	0.76
1:A:117[B]:ASN:HA	1:C:117[B]:ASN:HB3	1.69	0.74
1:A:117[B]:ASN:HB3	1:B:117[B]:ASN:HA	1.68	0.74
1:B:2:ILE:HD11	4:B:423:HOH:O	1.87	0.74
1:D:182[B]:VAL:HG13	1:F:182:VAL:HG11	1.68	0.73
1:D:117[B]:ASN:HB3	1:E:117[B]:ASN:HA	1.71	0.71
1:A:117[B]:ASN:HD22	1:B:117[B]:ASN:HA	1.54	0.71
1:B:117[B]:ASN:HD22	1:C:117[B]:ASN:HA	1.58	0.68
1:E:236[A]:THR:HG22	1:E:240:LYS:HE3	1.76	0.65
1:B:105:PHE:HE2	1:B:238:LYS:HE3	1.61	0.65
1:B:138:CYS:SG	1:B:205[B]:CYS:HB3	2.36	0.65
1:D:138:CYS:SG	1:D:205[B]:CYS:HB3	2.36	0.65
1:E:23:ILE:HD12	1:E:48[B]:ILE:HD13	1.80	0.64
1:E:222:PRO:HB2	4:F:397:HOH:O	1.99	0.63
1:D:4:GLN:NE2	4:D:1209:HOH:O	2.28	0.62
1:B:105:PHE:CE2	1:B:238:LYS:HE3	2.34	0.61
1:A:213:THR:HG21	1:A:232[B]:MET:HG2	1.80	0.61
1:A:211[A]:MET:HE1	1:A:232[A]:MET:HA	1.81	0.61
1:E:48[A]:ILE:HG22	1:E:248[A]:GLN:OE1	2.01	0.60
1:E:244:TYR:O	1:E:248[A]:GLN:HG2	2.01	0.60
1:A:138:CYS:SG	1:A:205[B]:CYS:HB3	2.42	0.60
1:D:117[B]:ASN:HD22	1:E:117[B]:ASN:HA	1.67	0.59
1:E:48[B]:ILE:HD12	1:E:53[B]:VAL:HG21	1.83	0.59
1:E:117[B]:ASN:HD22	1:F:117[B]:ASN:HA	1.67	0.59
1:D:182[B]:VAL:HG12	1:D:183[B]:TYR:CD2	2.37	0.59
1:F:211[A]:MET:HE1	1:F:232[A]:MET:HA	1.83	0.59
1:E:211[A]:MET:SD	1:E:235:ASN:CB	2.91	0.58
1:D:114:MET:SD	1:D:183[B]:TYR:HE1	2.27	0.58
1:E:138:CYS:SG	1:E:205[B]:CYS:HB3	2.44	0.58
1:A:244:TYR:CE2	1:A:248:GLN:NE2	2.72	0.58
1:C:32:VAL:HG21	1:C:43[B]:ILE:HD12	1.85	0.58
1:C:103:GLY:HA2	1:C:211[B]:MET:SD	2.44	0.58
1:D:211[A]:MET:HE1	1:D:232[A]:MET:HA	1.86	0.58
1:D:105:PHE:CE1	1:D:211[B]:MET:HE2	2.40	0.57
1:E:116[B]:LYS:O	1:E:117[B]:ASN:OD1	2.22	0.57
1:D:32:VAL:HG21	1:D:43[B]:ILE:HD12	1.87	0.57
1:A:103:GLY:HA2	1:A:211[B]:MET:SD	2.45	0.57
1:C:16:SER:O	1:C:232[B]:MET:HE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211[A]:MET:SD	1:B:235:ASN:CB	2.93	0.56
1:D:163:ILE:CD1	1:D:183[B]:TYR:HD1	2.18	0.56
1:C:112:ILE:HD13	1:C:183[B]:TYR:HB3	1.87	0.56
1:E:211[A]:MET:SD	1:E:235:ASN:HB2	2.46	0.56
4:A:1122:HOH:O	1:C:222:PRO:HB2	2.04	0.56
1:E:211[A]:MET:HE1	1:E:232[A]:MET:HA	1.87	0.56
1:A:4:GLN:NE2	4:A:402:HOH:O	2.35	0.56
1:C:213:THR:HG21	1:C:232[B]:MET:HG2	1.88	0.55
1:D:19:TYR:CE1	1:D:61:ARG:HA	2.41	0.55
1:E:105:PHE:CE2	1:E:238:LYS:HE3	2.41	0.55
1:D:163:ILE:HD12	1:D:183[B]:TYR:HD1	1.71	0.55
1:A:105:PHE:HE2	1:A:238:LYS:HE3	1.70	0.55
1:F:213:THR:HG21	1:F:232[B]:MET:HG2	1.89	0.55
1:B:232[A]:MET:O	1:B:236:THR:HG23	2.07	0.55
1:F:105:PHE:CE1	1:F:211[B]:MET:HE2	2.42	0.55
1:D:112:ILE:CD1	1:D:183[B]:TYR:HB3	2.38	0.54
1:B:222:PRO:HB2	4:C:386:HOH:O	2.08	0.54
1:F:16:SER:O	1:F:232[B]:MET:HE2	2.08	0.54
1:B:213:THR:HG21	1:B:232[B]:MET:HG2	1.89	0.54
1:D:178:THR:HG23	1:D:182[B]:VAL:HG21	1.90	0.54
1:E:105:PHE:HE2	1:E:238:LYS:HE3	1.71	0.54
1:C:105:PHE:CE1	1:C:211[B]:MET:HE2	2.43	0.54
1:B:117[B]:ASN:HB3	1:C:117[B]:ASN:CA	2.34	0.54
1:A:16:SER:O	1:A:232[B]:MET:HE2	2.07	0.53
1:B:2:ILE:C	1:B:2:ILE:HD12	2.33	0.53
1:C:138:CYS:SG	1:C:205[B]:CYS:HB3	2.47	0.53
1:A:105:PHE:CE2	1:A:238:LYS:HE3	2.43	0.53
1:B:211[A]:MET:SD	1:B:235:ASN:HB2	2.49	0.53
1:C:112:ILE:CD1	1:C:183[B]:TYR:HB3	2.39	0.53
1:F:103:GLY:HA2	1:F:211[B]:MET:SD	2.49	0.53
1:A:31:LYS:HG2	1:A:42[B]:PHE:CE1	2.44	0.52
1:B:4:GLN:NE2	4:B:423:HOH:O	2.42	0.52
1:F:18:LEU:HD11	1:F:21:PRO:HA	1.91	0.52
1:D:103:GLY:HA2	1:D:211[B]:MET:SD	2.49	0.52
1:F:116[B]:LYS:O	1:F:117[B]:ASN:OD1	2.27	0.52
1:B:103:GLY:HA2	1:B:211[B]:MET:SD	2.49	0.52
1:F:131[B]:VAL:CG1	1:F:200:CYS:SG	2.94	0.52
1:C:31:LYS:HG2	1:C:42[A]:PHE:CE2	2.44	0.52
1:D:140:SER:HB3	1:D:258:SER:CB	2.40	0.52
1:F:138:CYS:SG	1:F:205[B]:CYS:HB3	2.49	0.52
1:A:232[A]:MET:O	1:A:236:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211[A]:MET:HE1	1:B:232[A]:MET:HA	1.92	0.52
1:D:116[B]:LYS:O	1:D:117[B]:ASN:OD1	2.27	0.52
1:B:105:PHE:CE1	1:B:211[B]:MET:HE2	2.45	0.52
1:E:117[B]:ASN:CB	1:F:117[B]:ASN:HA	2.38	0.52
1:A:222:PRO:HB2	4:B:509:HOH:O	2.10	0.51
1:B:117[B]:ASN:CB	1:C:117[B]:ASN:HA	2.36	0.51
1:D:112:ILE:HD13	1:D:183[B]:TYR:HB3	1.92	0.51
1:E:32:VAL:HG21	1:E:43[B]:ILE:HD12	1.91	0.51
1:D:211[A]:MET:SD	1:D:235:ASN:CB	3.00	0.50
1:D:211[A]:MET:SD	1:D:235:ASN:HB2	2.50	0.50
1:E:131[B]:VAL:CG1	1:E:200:CYS:SG	2.96	0.50
1:F:31:LYS:HG2	1:F:42[A]:PHE:CE1	2.46	0.50
1:F:140:SER:HB3	1:F:258:SER:CB	2.42	0.50
1:D:117[B]:ASN:HA	1:F:117[B]:ASN:HD22	1.76	0.50
1:A:105:PHE:CE1	1:A:211[B]:MET:HE2	2.47	0.50
1:E:131[B]:VAL:HG12	1:E:133[B]:MET:HG3	1.93	0.49
1:D:178:THR:HG23	1:D:182[B]:VAL:CG2	2.43	0.49
1:B:140:SER:HB3	1:B:258:SER:CB	2.42	0.49
1:A:211[A]:MET:SD	1:A:235:ASN:HB2	2.53	0.48
1:C:178:THR:HG23	1:C:182[B]:VAL:HG21	1.93	0.48
1:B:31:LYS:HG2	1:B:42[A]:PHE:CE2	2.48	0.48
1:E:31:LYS:HG2	1:E:42[A]:PHE:CE2	2.47	0.48
1:E:150:LYS:HE3	1:E:158:GLU:OE2	2.13	0.48
1:C:19:TYR:CE1	1:C:61:ARG:HA	2.48	0.48
1:A:117[B]:ASN:HA	1:C:117[B]:ASN:ND2	2.26	0.48
1:C:244:TYR:CE2	1:C:248:GLN:NE2	2.82	0.48
1:D:112:ILE:HD13	1:D:183[A]:TYR:HD1	1.79	0.48
1:A:19:TYR:CE1	1:A:61:ARG:HA	2.48	0.48
1:A:116[B]:LYS:O	1:A:117[B]:ASN:OD1	2.31	0.47
1:A:117[B]:ASN:CA	1:C:117[B]:ASN:HB3	2.43	0.47
1:E:105:PHE:CE1	1:E:211[B]:MET:HE2	2.49	0.47
1:A:211[A]:MET:SD	1:A:235:ASN:CB	3.02	0.47
1:A:116[A]:LYS:HE3	1:B:113:ASP:OD2	2.13	0.47
1:C:131[B]:VAL:CG1	1:C:200:CYS:SG	3.00	0.47
1:E:19:TYR:CE1	1:E:61:ARG:HA	2.49	0.47
1:C:211[A]:MET:SD	1:C:235:ASN:CB	3.03	0.47
1:B:182:VAL:HG11	1:C:182[B]:VAL:HG13	1.96	0.47
1:D:182[A]:VAL:HG11	1:E:182:VAL:HG13	1.96	0.47
1:C:116[B]:LYS:O	1:C:117[B]:ASN:OD1	2.33	0.47
1:E:232[B]:MET:O	1:E:236[B]:THR:HG23	2.15	0.47
1:D:182[B]:VAL:HG12	1:D:183[B]:TYR:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116[A]:LYS:HE3	1:E:113:ASP:OD2	2.14	0.46
1:D:117[B]:ASN:HA	1:F:117[B]:ASN:CB	2.37	0.46
1:E:103:GLY:HA2	1:E:211[B]:MET:SD	2.55	0.46
1:D:31:LYS:HG2	1:D:42[B]:PHE:CE1	2.50	0.46
1:D:113:ASP:OD2	1:F:116[A]:LYS:HE3	2.14	0.46
1:E:12[B]:ILE:HD11	1:E:247:ILE:CD1	2.43	0.46
1:B:100[A]:TYR:O	1:B:101[A]:LYS:HD3	2.16	0.46
1:B:19:TYR:CE1	1:B:61:ARG:HA	2.50	0.46
1:F:19:TYR:CE1	1:F:61:ARG:HA	2.51	0.45
1:B:129:ALA:HB2	1:B:269:LEU:HD23	1.99	0.45
1:F:211[A]:MET:SD	1:F:235:ASN:CB	3.05	0.45
1:B:116[B]:LYS:O	1:B:117[B]:ASN:OD1	2.34	0.45
1:E:140:SER:HB3	1:E:258:SER:CB	2.46	0.45
1:E:236[A]:THR:CG2	1:E:240:LYS:HE3	2.44	0.45
1:D:114:MET:SD	1:D:183[B]:TYR:CE1	3.09	0.45
1:C:230:ARG:NH1	4:C:1204:HOH:O	2.38	0.45
1:F:211[A]:MET:SD	1:F:235:ASN:HB2	2.57	0.45
1:B:117[B]:ASN:ND2	1:C:117[B]:ASN:HA	2.30	0.44
1:A:51:LYS:NZ	1:A:250:LEU:O	2.46	0.44
1:D:105:PHE:CZ	1:D:211[B]:MET:HE2	2.52	0.44
1:E:23:ILE:HD12	1:E:48[B]:ILE:CD1	2.46	0.44
1:D:117[B]:ASN:CA	1:F:117[B]:ASN:HB3	2.38	0.44
1:A:116[B]:LYS:HD3	1:B:115:THR:O	2.17	0.44
1:F:244:TYR:CE2	1:F:248:GLN:NE2	2.86	0.44
1:A:101:LYS:HB3	1:A:101:LYS:NZ	2.32	0.43
1:A:150:LYS:HE3	1:A:158:GLU:OE2	2.17	0.43
1:D:131[B]:VAL:CG1	1:D:200:CYS:SG	2.99	0.43
2:A:901:MTA:H2'	2:A:901:MTA:N3	2.34	0.43
1:D:12[B]:ILE:HD11	1:D:247:ILE:CD1	2.42	0.43
1:D:105:PHE:HE2	1:D:238:LYS:HE2	1.84	0.43
1:B:105:PHE:CZ	1:B:211[B]:MET:HE2	2.54	0.43
1:A:113:ASP:OD2	1:C:116[A]:LYS:HE3	2.19	0.43
1:C:211[A]:MET:HE1	1:C:232[A]:MET:HA	2.01	0.43
1:E:21:PRO:HB2	1:E:23:ILE:CD1	2.48	0.43
1:B:131[B]:VAL:CG1	1:B:200:CYS:SG	2.97	0.43
1:C:12[B]:ILE:HD11	1:C:247:ILE:CD1	2.41	0.43
1:D:232[A]:MET:O	1:D:236:THR:HG23	2.19	0.43
1:C:178:THR:HG23	1:C:182[B]:VAL:CG2	2.49	0.43
1:C:179:TRP:O	1:C:183[A]:TYR:HB2	2.19	0.43
2:C:901:MTA:N3	2:C:901:MTA:H2'	2.34	0.43
1:D:265:LEU:HD23	1:D:265:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232[A]:MET:O	1:F:236:THR:HG23	2.19	0.43
1:C:105:PHE:CZ	1:C:211[B]:MET:HE2	2.54	0.42
1:D:229[B]:THR:HG21	4:E:1227:HOH:O	2.18	0.42
1:B:16:SER:O	1:B:232[B]:MET:HE2	2.19	0.42
1:C:105:PHE:CZ	1:C:211[B]:MET:CE	3.03	0.42
1:D:249:LYS:HB2	1:D:249:LYS:NZ	2.35	0.42
1:F:105:PHE:CZ	1:F:211[B]:MET:HE2	2.54	0.42
1:B:2:ILE:HD12	1:B:2:ILE:O	2.20	0.42
1:B:116[A]:LYS:HE3	1:C:113:ASP:CG	2.45	0.42
1:F:105:PHE:CZ	1:F:211[B]:MET:CE	3.03	0.42
1:A:117[B]:ASN:CB	1:B:117[B]:ASN:HA	2.45	0.42
1:C:232[A]:MET:O	1:C:236:THR:HG23	2.20	0.42
2:D:901:MTA:H2'	2:D:901:MTA:N3	2.35	0.42
1:C:249:LYS:NZ	1:C:249:LYS:HB2	2.35	0.41
1:D:150:LYS:HE3	1:D:158:GLU:OE1	2.19	0.41
1:E:211[A]:MET:SD	1:E:235:ASN:HB3	2.59	0.41
1:C:140:SER:HB3	1:C:258:SER:CB	2.50	0.41
1:A:115:THR:O	1:C:116[B]:LYS:HD3	2.19	0.41
1:B:150:LYS:HE3	1:B:158:GLU:OE2	2.20	0.41
1:D:105:PHE:CZ	1:D:211[B]:MET:CE	3.03	0.41
1:D:129:ALA:HB2	1:D:269:LEU:HD23	2.03	0.41
1:D:232[B]:MET:O	1:D:236:THR:HG23	2.19	0.41
1:E:211[A]:MET:HE2	1:E:211[A]:MET:HB3	1.99	0.41
1:B:249:LYS:HZ2	1:B:249:LYS:HB2	1.86	0.41
1:D:238:LYS:HE2	1:D:238:LYS:HB3	1.89	0.41
1:E:151:GLU:OE1	1:E:249:LYS:NZ	2.52	0.41
1:E:80:LYS:HD2	4:E:881:HOH:O	2.21	0.41
1:E:105:PHE:CZ	1:E:211[B]:MET:CE	3.04	0.41
1:A:105:PHE:CZ	1:A:211[B]:MET:HE2	2.56	0.41
1:F:265:LEU:HD23	1:F:265:LEU:HA	1.85	0.41
1:A:32:VAL:HG21	1:A:43:ILE:HD12	2.02	0.40
1:B:211[A]:MET:SD	1:B:235:ASN:HB3	2.60	0.40
1:B:249:LYS:HB2	1:B:249:LYS:NZ	2.36	0.40
1:B:116[A]:LYS:HE3	1:C:113:ASP:OD2	2.21	0.40
1:D:177:ARG:O	1:D:181[B]:GLU:HB2	2.21	0.40
2:E:901:MTA:N3	2:E:901:MTA:H2'	2.37	0.40
2:F:901:MTA:H2'	2:F:901:MTA:N3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	281/270 (104%)	278 (99%)	3 (1%)	0	100	100
1	B	291/270 (108%)	289 (99%)	2 (1%)	0	100	100
1	C	291/270 (108%)	289 (99%)	2 (1%)	0	100	100
1	D	290/270 (107%)	289 (100%)	1 (0%)	0	100	100
1	E	299/270 (111%)	298 (100%)	1 (0%)	0	100	100
1	F	285/270 (106%)	280 (98%)	5 (2%)	0	100	100
All	All	1737/1620 (107%)	1723 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	222/231 (96%)	217 (98%)	5 (2%)	44	13
1	B	234/231 (101%)	230 (98%)	4 (2%)	53	21
1	C	234/231 (101%)	229 (98%)	5 (2%)	47	14
1	D	232/231 (100%)	227 (98%)	5 (2%)	45	13
1	E	239/231 (104%)	235 (98%)	4 (2%)	53	21
1	F	229/231 (99%)	225 (98%)	4 (2%)	53	21
All	All	1390/1386 (100%)	1363 (98%)	27 (2%)	47	17

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	162	TYR
1	A	197	ASN
1	A	249	LYS
1	A	265	LEU
1	B	34	THR
1	B	162	TYR
1	B	197	ASN
1	B	249	LYS
1	C	34	THR
1	C	162	TYR
1	C	197	ASN
1	C	238	LYS
1	C	249	LYS
1	D	34	THR
1	D	162	TYR
1	D	197	ASN
1	D	249	LYS
1	D	265	LEU
1	E	23	ILE
1	E	34	THR
1	E	162	TYR
1	E	197	ASN
1	F	34	THR
1	F	162	TYR
1	F	197	ASN
1	F	249	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	235	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

19 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
3	SO4	F	902	-	4,4,4	0.27	0	6,6,6	0.45	0
3	SO4	B	272	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	A	902	-	4,4,4	0.21	0	6,6,6	0.45	0
3	SO4	B	271	-	4,4,4	0.24	0	6,6,6	0.23	0
3	SO4	C	902	-	4,4,4	0.24	0	6,6,6	0.48	0
3	SO4	E	902	-	4,4,4	0.21	0	6,6,6	0.48	0
2	MTA	D	901	-	22,22,22	1.33	2 (9%)	32,32,32	2.30	10 (31%)
2	MTA	A	901	-	22,22,22	1.39	3 (13%)	32,32,32	2.27	10 (31%)
2	MTA	E	901	-	22,22,22	1.40	2 (9%)	32,32,32	2.27	13 (40%)
3	SO4	B	902	-	4,4,4	0.25	0	6,6,6	0.54	0
3	SO4	E	271	-	4,4,4	0.26	0	6,6,6	0.19	0
2	MTA	F	901	-	22,22,22	1.45	3 (13%)	32,32,32	2.32	10 (31%)
2	MTA	C	901	-	22,22,22	1.43	3 (13%)	32,32,32	2.27	11 (34%)
3	SO4	D	271[B]	-	4,4,4	0.27	0	6,6,6	0.15	0
3	SO4	A	271[B]	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	D	902	-	4,4,4	0.27	0	6,6,6	0.53	0
3	SO4	D	271[A]	-	4,4,4	0.24	0	6,6,6	0.17	0
2	MTA	B	901	-	22,22,22	1.46	3 (13%)	32,32,32	2.29	12 (37%)
3	SO4	A	271[A]	-	4,4,4	0.28	0	6,6,6	0.12	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	MTA	B	901	-	-	2/7/23/23	0/3/3/3
2	MTA	F	901	-	-	2/7/23/23	0/3/3/3
2	MTA	C	901	-	-	2/7/23/23	0/3/3/3
2	MTA	D	901	-	-	2/7/23/23	0/3/3/3
2	MTA	A	901	-	-	2/7/23/23	0/3/3/3
2	MTA	E	901	-	-	2/7/23/23	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	MTA	C5-C4	4.65	1.47	1.39
2	F	901	MTA	C5-C4	4.64	1.47	1.39
2	A	901	MTA	C5-C4	4.57	1.47	1.39
2	C	901	MTA	C5-C4	4.54	1.47	1.39
2	E	901	MTA	C5-C4	4.49	1.47	1.39
2	D	901	MTA	C5-C4	4.18	1.46	1.39
2	B	901	MTA	C5-N7	-2.36	1.34	1.39
2	E	901	MTA	C5-N7	-2.32	1.34	1.39
2	C	901	MTA	C5-N7	-2.29	1.34	1.39
2	F	901	MTA	C5-C6	2.29	1.47	1.41
2	D	901	MTA	C5-C6	2.27	1.47	1.41
2	F	901	MTA	C5-N7	-2.19	1.35	1.39
2	C	901	MTA	C5-C6	2.14	1.47	1.41
2	A	901	MTA	C5-N7	-2.13	1.35	1.39
2	B	901	MTA	C5-C6	2.09	1.46	1.41
2	A	901	MTA	C5-C6	2.02	1.46	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	MTA	O4'-C1'-N9	-6.44	95.72	108.09
2	E	901	MTA	O4'-C1'-N9	-6.38	95.84	108.09
2	C	901	MTA	O4'-C1'-N9	-5.97	96.61	108.09
2	F	901	MTA	C5-C4-N3	-5.76	118.79	126.72
2	F	901	MTA	O4'-C1'-N9	-5.67	97.19	108.09
2	D	901	MTA	O4'-C1'-N9	-5.67	97.19	108.09
2	B	901	MTA	O4'-C1'-N9	-5.56	97.41	108.09
2	C	901	MTA	C5-C4-N3	-5.43	119.23	126.72
2	D	901	MTA	C5-C4-N3	-5.37	119.32	126.72
2	A	901	MTA	C5-C4-N3	-5.37	119.33	126.72
2	B	901	MTA	C5-C4-N3	-5.30	119.41	126.72
2	F	901	MTA	N3-C4-N9	4.87	135.45	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	MTA	N3-C4-N9	4.58	134.95	127.17
2	D	901	MTA	N3-C4-N9	4.56	134.93	127.17
2	A	901	MTA	N3-C4-N9	4.53	134.87	127.17
2	B	901	MTA	N3-C4-N9	4.49	134.80	127.17
2	E	901	MTA	C5-C4-N3	-4.46	120.58	126.72
2	E	901	MTA	N3-C4-N9	4.07	134.09	127.17
2	E	901	MTA	N3-C2-N1	-3.36	123.50	128.58
2	B	901	MTA	N3-C2-N1	-3.33	123.55	128.58
2	D	901	MTA	C2-N3-C4	3.25	119.77	111.83
2	F	901	MTA	C4-C5-N7	-3.18	106.94	110.58
2	B	901	MTA	C2-N3-C4	3.16	119.56	111.83
2	F	901	MTA	C2-N3-C4	3.11	119.43	111.83
2	D	901	MTA	N3-C2-N1	-3.04	123.98	128.58
2	C	901	MTA	C2-N3-C4	3.01	119.18	111.83
2	A	901	MTA	C2-N3-C4	2.95	119.03	111.83
2	D	901	MTA	C4-C5-N7	-2.94	107.22	110.58
2	E	901	MTA	C2-N1-C6	2.93	123.55	118.73
2	B	901	MTA	C3'-C2'-C1'	2.89	106.93	101.46
2	F	901	MTA	C1'-N9-C8	-2.87	120.72	127.09
2	C	901	MTA	C4-C5-N7	-2.83	107.34	110.58
2	D	901	MTA	C1'-N9-C8	-2.80	120.87	127.09
2	E	901	MTA	C2-N3-C4	2.80	118.67	111.83
2	E	901	MTA	C1'-N9-C8	-2.78	120.92	127.09
2	B	901	MTA	C4-C5-N7	-2.77	107.41	110.58
2	B	901	MTA	C1'-N9-C8	-2.75	120.99	127.09
2	C	901	MTA	N3-C2-N1	-2.73	124.45	128.58
2	A	901	MTA	C4-C5-N7	-2.64	107.56	110.58
2	C	901	MTA	C1'-N9-C8	-2.64	121.24	127.09
2	F	901	MTA	C4-N9-C8	2.63	108.50	105.74
2	A	901	MTA	N3-C2-N1	-2.62	124.61	128.58
2	A	901	MTA	C1'-N9-C8	-2.60	121.32	127.09
2	E	901	MTA	C4-N9-C8	2.60	108.47	105.74
2	D	901	MTA	C4-N9-C8	2.58	108.44	105.74
2	F	901	MTA	C5-N7-C8	2.52	107.41	103.45
2	F	901	MTA	N3-C2-N1	-2.47	124.84	128.58
2	E	901	MTA	O4'-C1'-C2'	-2.47	101.34	106.62
2	C	901	MTA	C2'-C3'-C4'	2.46	107.37	102.61
2	B	901	MTA	O4'-C1'-C2'	-2.45	101.37	106.62
2	D	901	MTA	C5-N7-C8	2.43	107.26	103.45
2	B	901	MTA	C2-N1-C6	2.42	122.70	118.73
2	F	901	MTA	C3'-C2'-C1'	2.41	106.02	101.46
2	A	901	MTA	C3'-C2'-C1'	2.40	106.00	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	MTA	C3'-C2'-C1'	2.38	105.96	101.46
2	A	901	MTA	O4'-C1'-C2'	-2.37	101.55	106.62
2	C	901	MTA	C4-N9-C8	2.35	108.20	105.74
2	E	901	MTA	C4-C5-N7	-2.33	107.92	110.58
2	D	901	MTA	C3'-C2'-C1'	2.33	105.86	101.46
2	B	901	MTA	C4-N9-C8	2.28	108.14	105.74
2	E	901	MTA	C2'-C1'-N9	2.18	118.73	113.30
2	C	901	MTA	C5-N7-C8	2.13	106.80	103.45
2	E	901	MTA	N6-C6-N1	2.13	123.12	118.38
2	B	901	MTA	C5-N7-C8	2.10	106.74	103.45
2	C	901	MTA	C2-N1-C6	2.08	122.15	118.73
2	A	901	MTA	C4-N9-C8	2.06	107.90	105.74

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	MTA	C2'-C1'-N9-C4
2	B	901	MTA	C2'-C1'-N9-C4
2	C	901	MTA	C2'-C1'-N9-C4
2	D	901	MTA	C2'-C1'-N9-C4
2	E	901	MTA	C2'-C1'-N9-C4
2	F	901	MTA	C2'-C1'-N9-C4
2	A	901	MTA	C2'-C1'-N9-C8
2	B	901	MTA	C2'-C1'-N9-C8
2	C	901	MTA	C2'-C1'-N9-C8
2	D	901	MTA	C2'-C1'-N9-C8
2	E	901	MTA	C2'-C1'-N9-C8
2	F	901	MTA	C2'-C1'-N9-C8

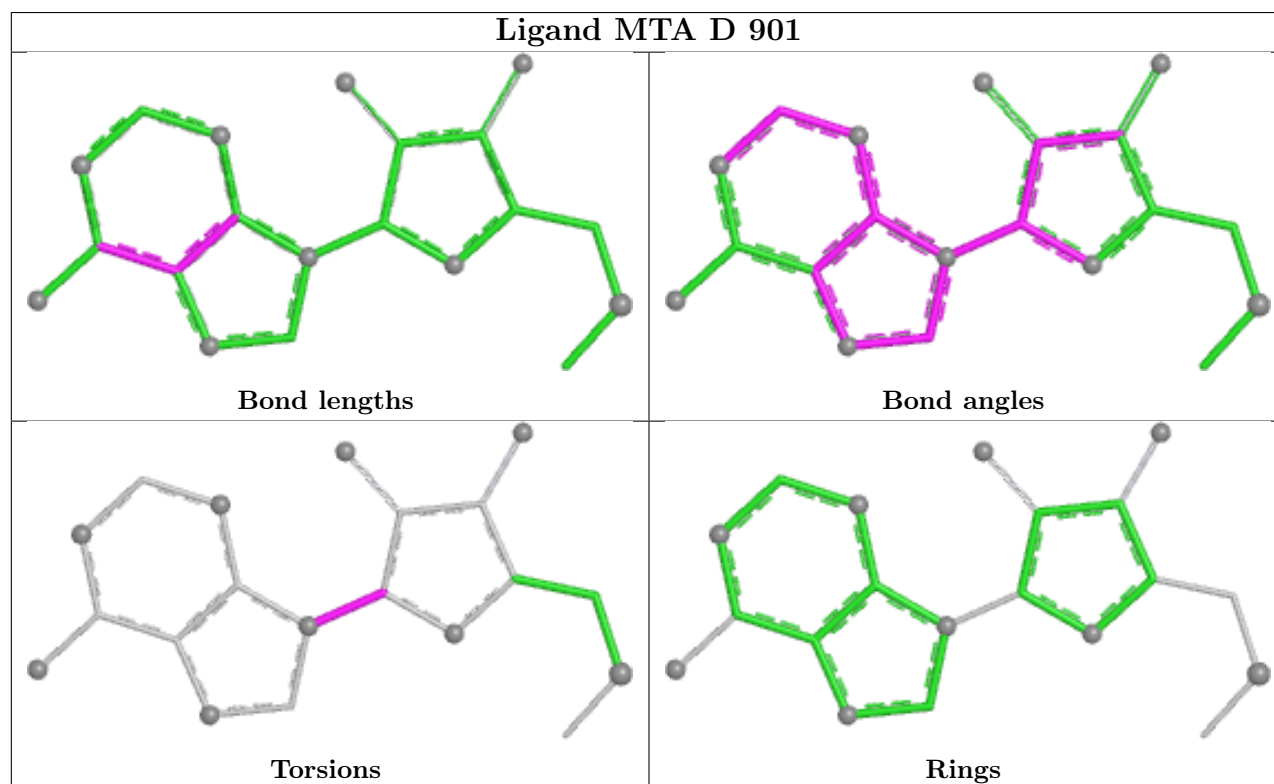
There are no ring outliers.

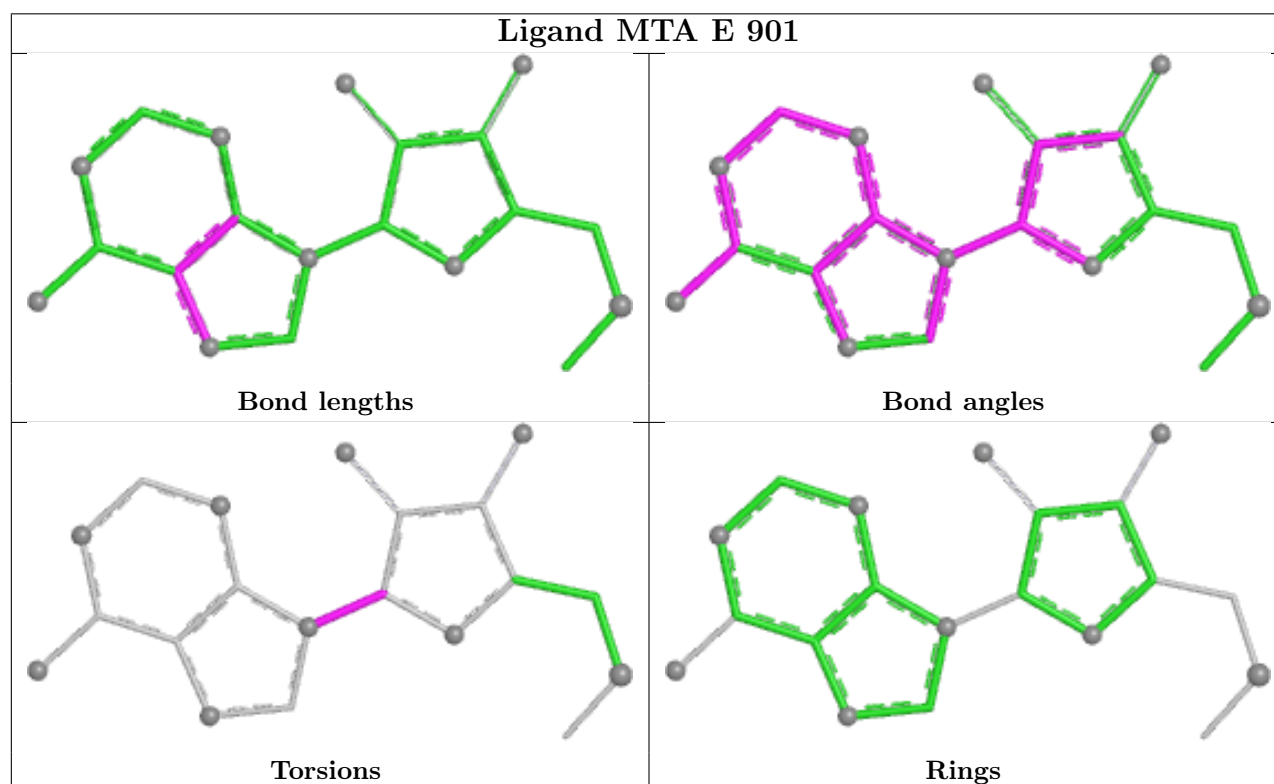
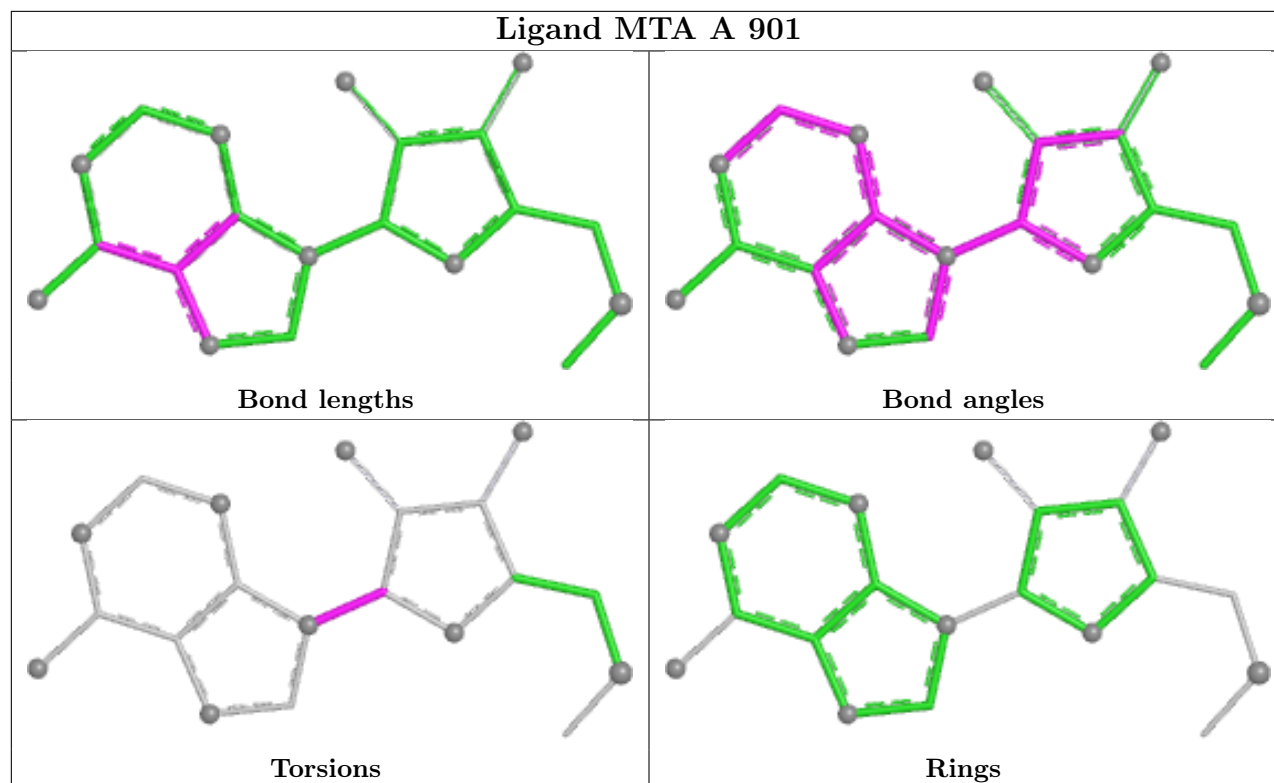
5 monomers are involved in 5 short contacts:

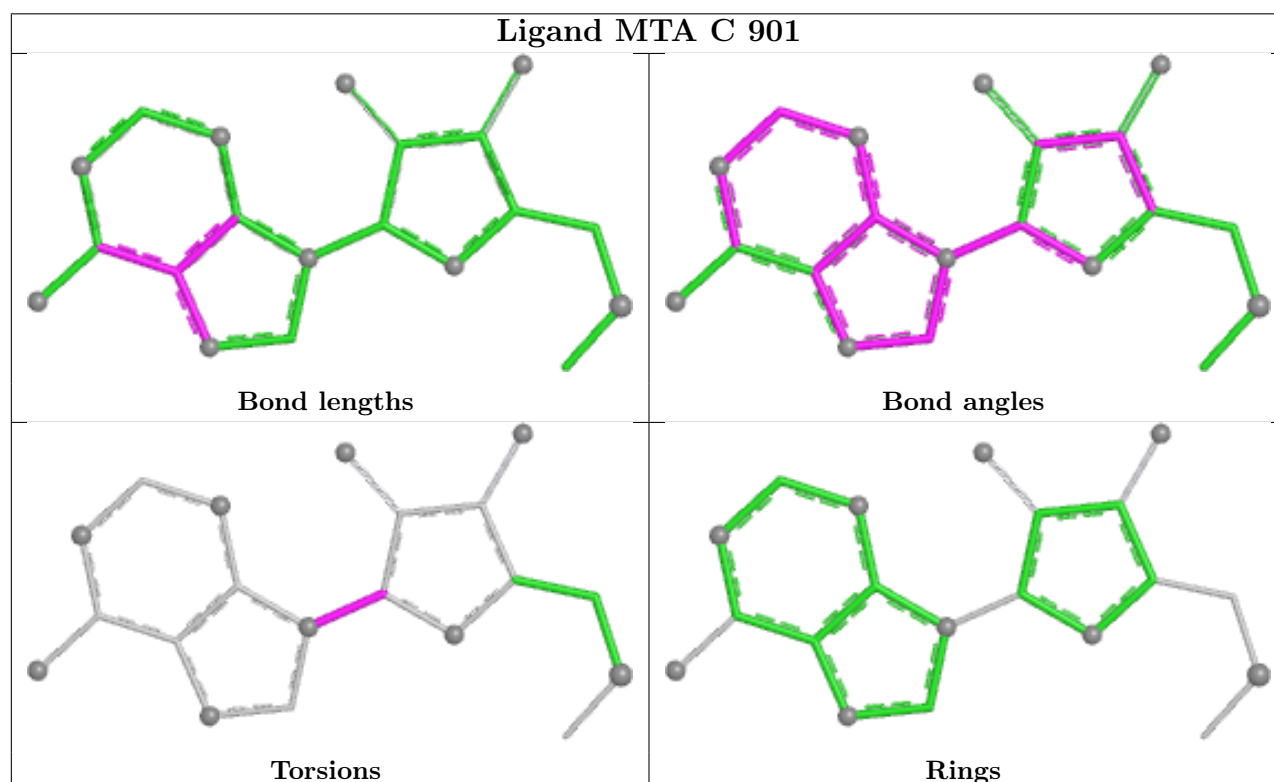
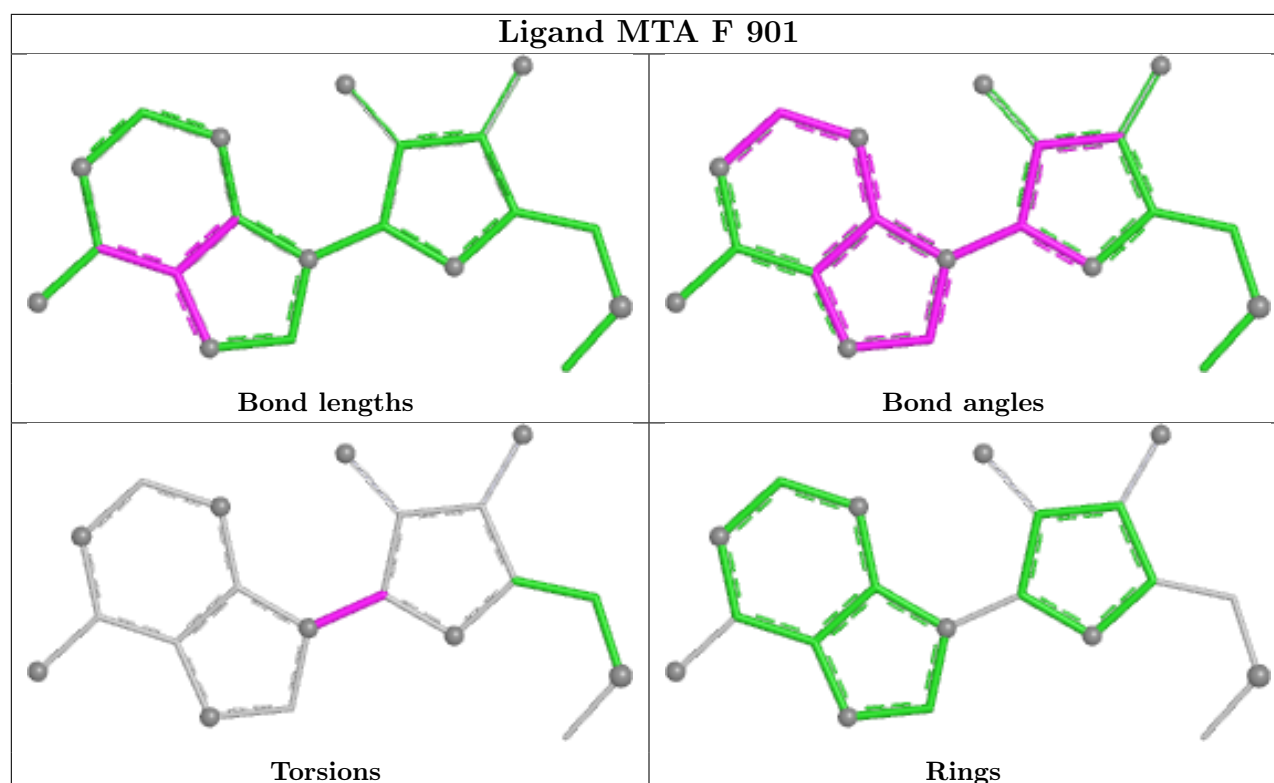
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	MTA	1	0
2	A	901	MTA	1	0
2	E	901	MTA	1	0
2	F	901	MTA	1	0
2	C	901	MTA	1	0

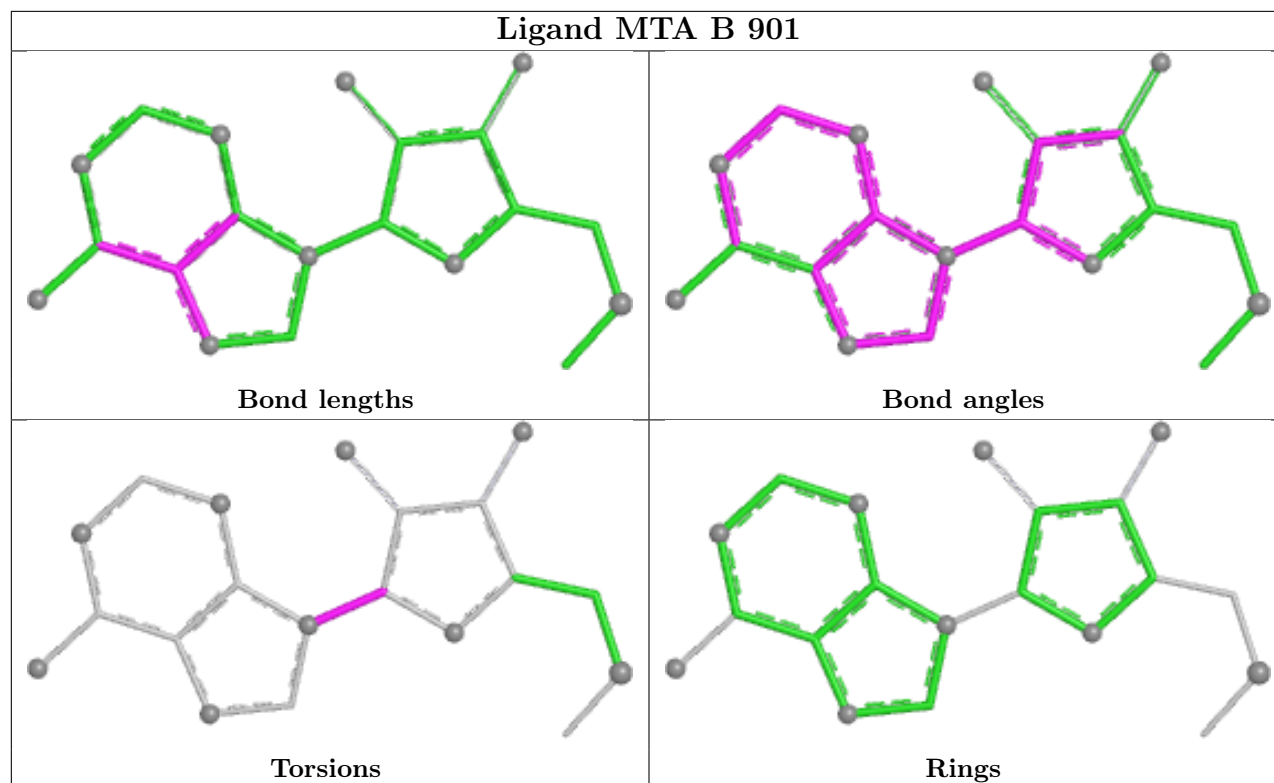
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

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	270/270 (100%)	0.83	39 (14%)	6 6	11, 25, 48, 88	13 (4%)
1	B	270/270 (100%)	0.80	38 (14%)	6 7	10, 23, 49, 90	23 (8%)
1	C	270/270 (100%)	0.83	38 (14%)	6 7	10, 24, 49, 91	23 (8%)
1	D	270/270 (100%)	0.86	40 (14%)	5 6	10, 25, 50, 88	22 (8%)
1	E	270/270 (100%)	0.75	33 (12%)	8 8	10, 22, 45, 90	31 (11%)
1	F	270/270 (100%)	0.87	36 (13%)	7 8	10, 26, 49, 98	17 (6%)
All	All	1620/1620 (100%)	0.82	224 (13%)	6 7	10, 24, 49, 98	129 (7%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	259	CYS	8.0
1	C	259	CYS	7.6
1	E	259	CYS	7.2
1	A	259	CYS	6.7
1	B	48	ILE	6.4
1	B	256	GLU	6.3
1	F	259	CYS	6.1
1	B	259	CYS	5.9
1	F	260	SER	5.8
1	E	263	ASN	5.8
1	D	48	ILE	5.7
1	D	262	CYS	5.7
1	F	256	GLU	5.6
1	E	262	CYS	5.5
1	A	263	ASN	5.5
1	A	48	ILE	5.3
1	C	263	ASN	5.1
1	E	260	SER	5.1
1	E	23	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	48	ILE	5.0
1	F	257	GLY	5.0
1	A	262	CYS	5.0
1	D	260	SER	5.0
1	C	264	SER	5.0
1	B	2	ILE	4.9
1	F	262	CYS	4.9
1	E	256	GLU	4.8
1	A	2	ILE	4.7
1	C	257	GLY	4.7
1	E	257	GLY	4.7
1	A	264	SER	4.7
1	D	261	CYS	4.6
1	F	261	CYS	4.6
1	D	256	GLU	4.6
1	A	256	GLU	4.5
1	C	262	CYS	4.5
1	F	255	GLU	4.5
1	B	257	GLY	4.5
1	B	258	SER	4.4
1	B	262	CYS	4.4
1	B	22	GLY	4.4
1	B	117[A]	ASN	4.3
1	E	50[A]	ASN	4.3
1	F	117[A]	ASN	4.3
1	E	255	GLU	4.3
1	F	183	TYR	4.3
1	E	117[A]	ASN	4.2
1	B	260	SER	4.2
1	D	2	ILE	4.2
1	E	261	CYS	4.2
1	C	255	GLU	4.2
1	C	256	GLU	4.1
1	A	260	SER	4.1
1	C	19	TYR	4.1
1	B	263	ASN	4.1
1	C	260	SER	4.1
1	D	264	SER	4.1
1	A	257	GLY	4.0
1	A	23	ILE	4.0
1	C	98[A]	MET	4.0
1	F	258	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	2	ILE	4.0
1	C	265	LEU	4.0
1	C	258	SER	3.9
1	F	19	TYR	3.9
1	D	257	GLY	3.9
1	F	48	ILE	3.9
1	F	263	ASN	3.8
1	B	23	ILE	3.8
1	B	255	GLU	3.8
1	E	236[A]	THR	3.8
1	A	258	SER	3.8
1	E	22	GLY	3.7
1	D	19	TYR	3.7
1	C	2	ILE	3.7
1	D	263	ASN	3.7
1	C	261	CYS	3.7
1	C	117[A]	ASN	3.6
1	B	261	CYS	3.6
1	C	182[A]	VAL	3.6
1	B	19	TYR	3.6
1	F	50	ASN	3.6
1	F	18	LEU	3.6
1	F	264	SER	3.6
1	F	265	LEU	3.6
1	D	258	SER	3.6
1	F	221	ILE	3.5
1	E	182	VAL	3.5
1	B	264	SER	3.5
1	E	270	VAL	3.5
1	F	270	VAL	3.5
1	B	270	VAL	3.5
1	A	18	LEU	3.4
1	E	258	SER	3.4
1	C	50	ASN	3.4
1	D	22	GLY	3.4
1	A	270	VAL	3.4
1	D	265	LEU	3.4
1	A	117[A]	ASN	3.4
1	A	19	TYR	3.3
1	A	22	GLY	3.3
1	B	265	LEU	3.3
1	F	2	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	23	ILE	3.2
1	D	50	ASN	3.2
1	B	50	ASN	3.2
1	D	183[A]	TYR	3.1
1	A	221	ILE	3.1
1	B	47	LYS	3.1
1	D	221	ILE	3.1
1	A	50	ASN	3.0
1	B	5[A]	ASN	3.0
1	D	117[A]	ASN	3.0
1	C	23	ILE	3.0
1	D	23	ILE	3.0
1	D	21	PRO	3.0
1	E	19	TYR	3.0
1	D	255	GLU	2.9
1	F	182	VAL	2.9
1	B	20	ASP	2.9
1	E	18	LEU	2.9
1	C	221	ILE	2.9
1	D	20	ASP	2.9
1	A	101	LYS	2.9
1	A	261	CYS	2.9
1	F	22	GLY	2.9
1	E	20	ASP	2.8
1	E	5[A]	ASN	2.8
1	E	47[A]	LYS	2.8
1	B	183	TYR	2.8
1	A	182	VAL	2.8
1	B	18	LEU	2.8
1	B	182	VAL	2.8
1	D	270	VAL	2.8
1	F	47	LYS	2.8
1	C	18	LEU	2.7
1	D	47	LYS	2.7
1	C	20	ASP	2.7
1	E	215	TYR	2.6
1	C	270	VAL	2.6
1	F	20	ASP	2.6
1	C	49	GLY	2.6
1	E	221	ILE	2.6
1	D	18	LEU	2.6
1	D	182[A]	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	22	GLY	2.6
1	A	183	TYR	2.5
1	C	183[A]	TYR	2.5
1	A	248	GLN	2.5
1	F	98	MET	2.5
1	A	49	GLY	2.5
1	F	25[A]	SER	2.5
1	A	20	ASP	2.5
1	C	100[A]	TYR	2.5
1	B	249	LYS	2.5
1	C	249	LYS	2.5
1	E	253	LYS	2.5
1	D	49	GLY	2.4
1	A	21	PRO	2.4
1	A	5	ASN	2.4
1	A	100	TYR	2.4
1	C	250	LEU	2.4
1	D	215	TYR	2.4
1	C	5	ASN	2.4
1	A	265	LEU	2.4
1	E	219	ALA	2.4
1	C	181[A]	GLU	2.4
1	F	251	PRO	2.4
1	B	56	LEU	2.4
1	E	265	LEU	2.4
1	B	49	GLY	2.4
1	E	249	LYS	2.3
1	A	25	SER	2.3
1	F	5	ASN	2.3
1	D	184[A]	LYS	2.3
1	D	253	LYS	2.3
1	F	249	LYS	2.3
1	A	52	SER	2.3
1	B	25	SER	2.3
1	D	52	SER	2.3
1	B	236	THR	2.3
1	A	56	LEU	2.3
1	B	250	LEU	2.3
1	D	43[A]	ILE	2.3
1	E	269	LEU	2.3
1	F	56	LEU	2.3
1	A	252	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	51	LYS	2.2
1	B	51	LYS	2.2
1	E	264	SER	2.2
1	C	251	PRO	2.2
1	A	47	LYS	2.2
1	A	236	THR	2.2
1	D	51	LYS	2.2
1	E	56	LEU	2.2
1	A	222	PRO	2.2
1	D	25	SER	2.2
1	C	56	LEU	2.1
1	B	100[A]	TYR	2.1
1	F	236	THR	2.1
1	A	181	GLU	2.1
1	C	184[A]	LYS	2.1
1	F	51	LYS	2.1
1	F	266	LYS	2.1
1	D	42[A]	PHE	2.1
1	A	251	PRO	2.1
1	B	254	PRO	2.1
1	E	25	SER	2.1
1	D	5[A]	ASN	2.1
1	D	98	MET	2.1
1	B	253	LYS	2.1
1	C	25	SER	2.1
1	D	252	GLU	2.1
1	F	267	THR	2.1
1	D	249	LYS	2.1
1	D	248	GLN	2.1
1	B	21	PRO	2.1
1	C	47	LYS	2.0
1	F	233	ALA	2.0
1	B	269	LEU	2.0
1	C	243	LEU	2.0
1	C	99[A]	ASP	2.0
1	B	52	SER	2.0
1	E	183	TYR	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

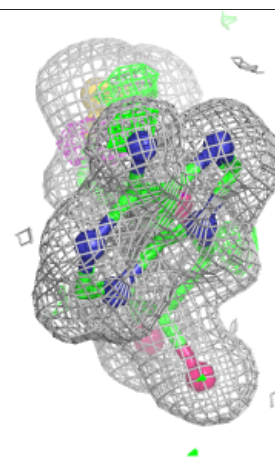
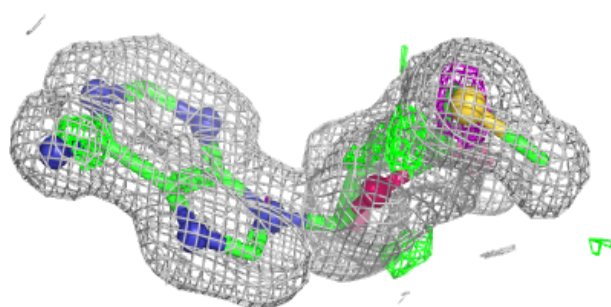
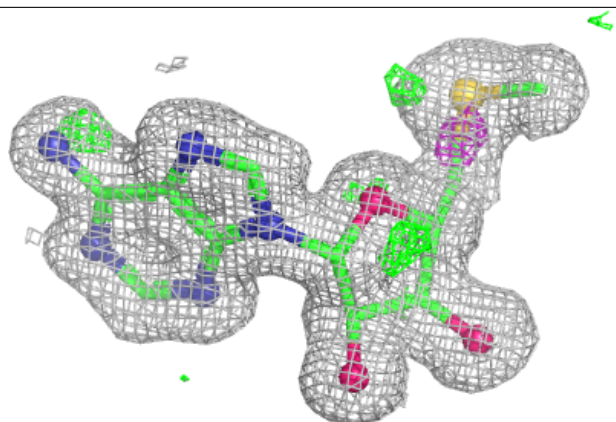
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	271[A]	5/5	0.88	0.13	25,26,29,32	5
3	SO4	A	271[B]	5/5	0.88	0.13	28,28,34,36	5
3	SO4	D	271[A]	5/5	0.89	0.12	28,31,34,35	5
3	SO4	D	271[B]	5/5	0.89	0.12	26,30,33,33	5
3	SO4	B	272	5/5	0.93	0.13	30,31,36,38	0
3	SO4	E	271	5/5	0.94	0.11	26,27,29,30	5
3	SO4	B	271	5/5	0.95	0.11	26,28,30,32	5
2	MTA	F	901	20/20	0.97	0.07	19,21,27,27	0
2	MTA	A	901	20/20	0.97	0.07	18,20,26,29	0
2	MTA	C	901	20/20	0.97	0.08	19,21,27,30	0
2	MTA	D	901	20/20	0.97	0.08	20,21,28,28	0
2	MTA	E	901	20/20	0.98	0.07	17,19,23,27	0
2	MTA	B	901	20/20	0.98	0.07	17,20,24,27	0
3	SO4	D	902	5/5	0.98	0.07	21,21,25,26	0
3	SO4	F	902	5/5	0.98	0.06	21,22,25,26	0
3	SO4	C	902	5/5	0.99	0.06	20,21,24,25	0
3	SO4	E	902	5/5	0.99	0.05	19,20,23,25	0
3	SO4	A	902	5/5	0.99	0.07	21,21,25,26	0
3	SO4	B	902	5/5	0.99	0.06	20,20,25,26	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.

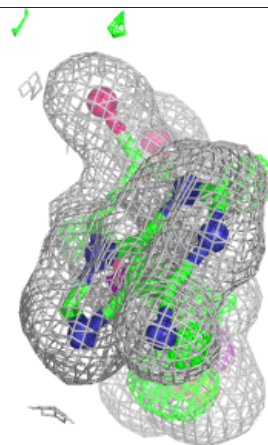
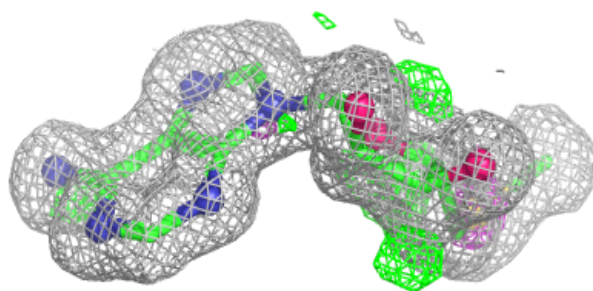
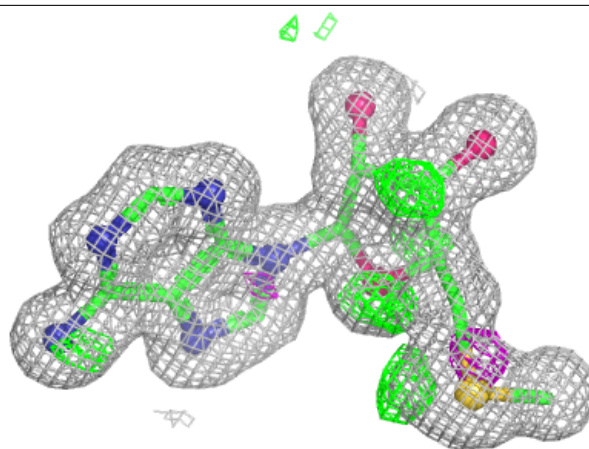
Electron density around MTA F 901:

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



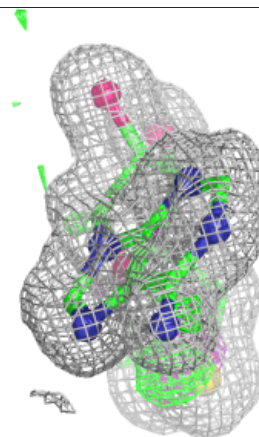
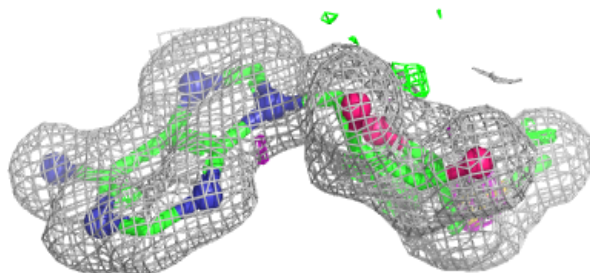
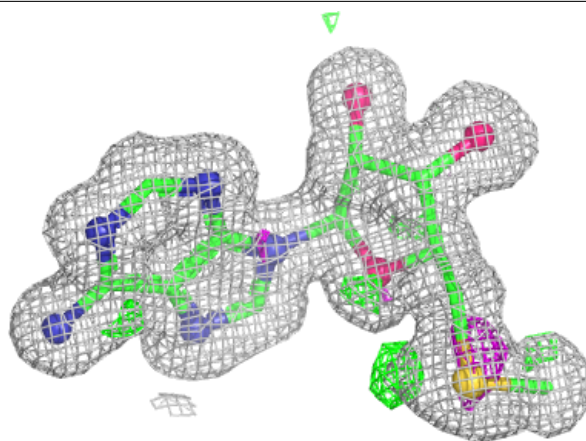
Electron density around MTA A 901:

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



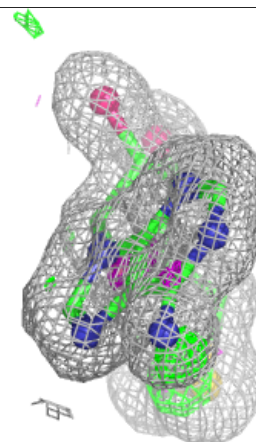
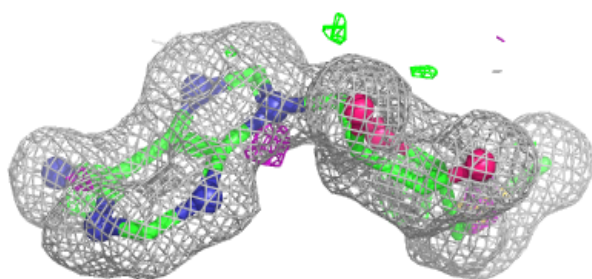
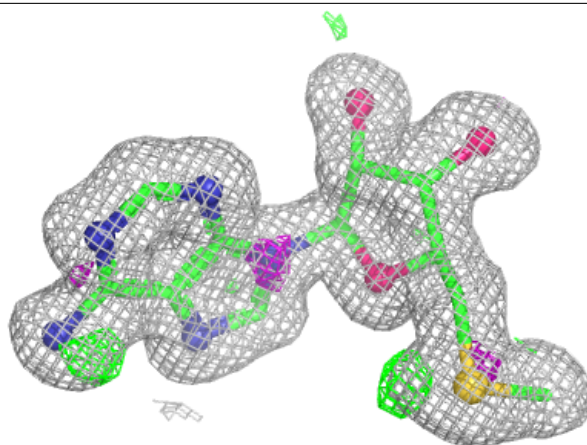
Electron density around MTA C 901:

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

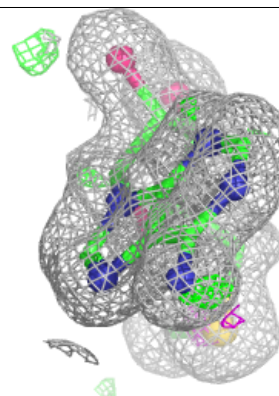
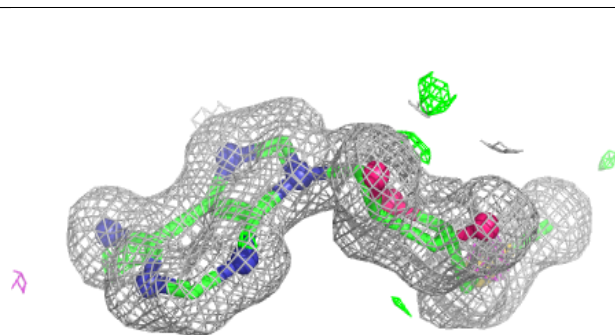
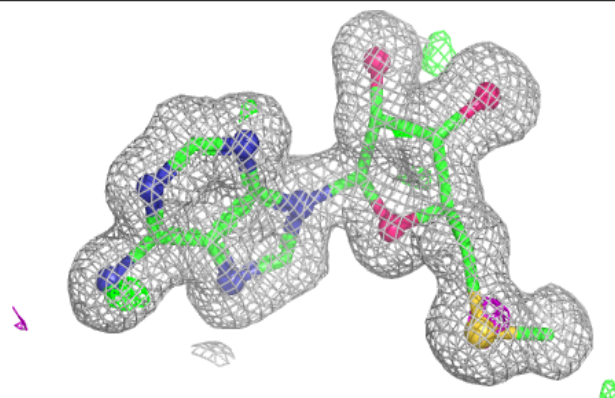


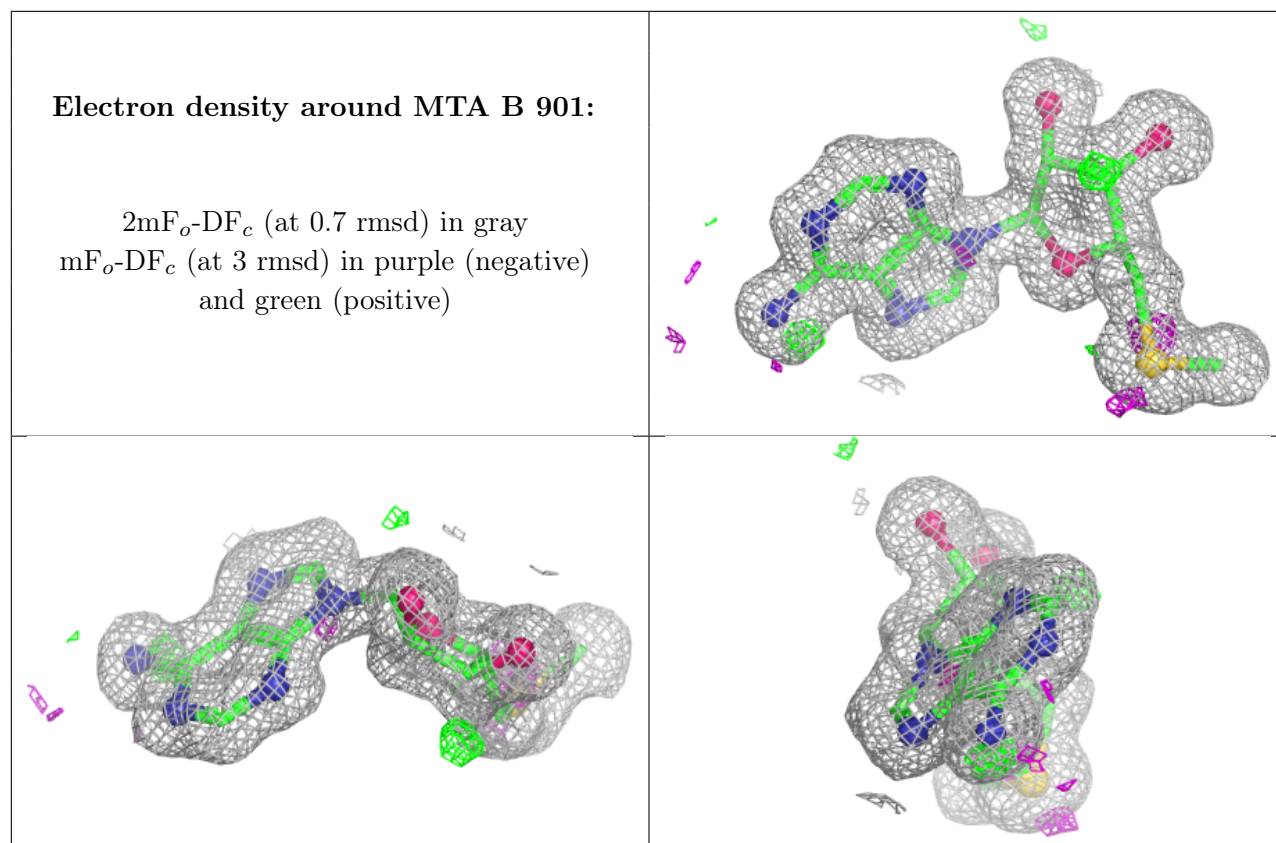
Electron density around MTA D 901:

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

**Electron density around MTA E 901:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.