Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2025 – 12:08 PM EST

PDB ID	:	9N3R
Title	:	Crystal structure of PRMT5:MEP50 in complex with MTA and TNG462
Authors	:	Whittington, D.A.
Deposited on	:	2025-01-31
Resolution	:	2.47 Å(reported)

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

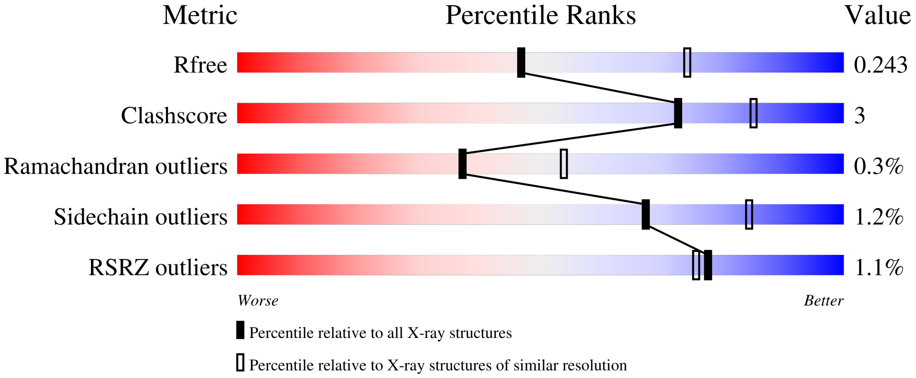
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

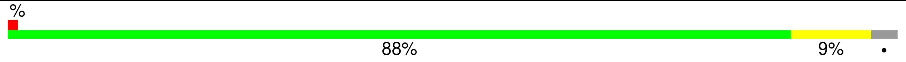
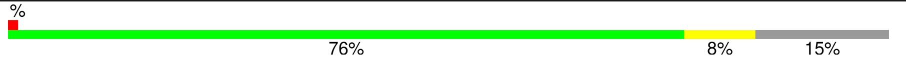
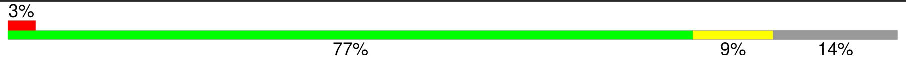
The reported resolution of this entry is 2.47 Å.

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}	164625	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

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 <=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	645	
1	C	645	
2	B	350	
2	D	350	

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 14937 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total 5072	C 3243	N 873	O 932	S 24	0	1	0
1	C	625	Total 5079	C 3248	N 873	O 933	S 25	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O14744
A	-6	ASP	-	expression tag	UNP O14744
A	-5	TYR	-	expression tag	UNP O14744
A	-4	LYS	-	expression tag	UNP O14744
A	-3	ASP	-	expression tag	UNP O14744
A	-2	ASP	-	expression tag	UNP O14744
A	-1	ASP	-	expression tag	UNP O14744
A	0	ASP	-	expression tag	UNP O14744
A	1	LYS	-	expression tag	UNP O14744
C	-7	MET	-	initiating methionine	UNP O14744
C	-6	ASP	-	expression tag	UNP O14744
C	-5	TYR	-	expression tag	UNP O14744
C	-4	LYS	-	expression tag	UNP O14744
C	-3	ASP	-	expression tag	UNP O14744
C	-2	ASP	-	expression tag	UNP O14744
C	-1	ASP	-	expression tag	UNP O14744
C	0	ASP	-	expression tag	UNP O14744
C	1	LYS	-	expression tag	UNP O14744

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	297	Total 2262	C 1421	N 387	O 443	S 11	0	1	0

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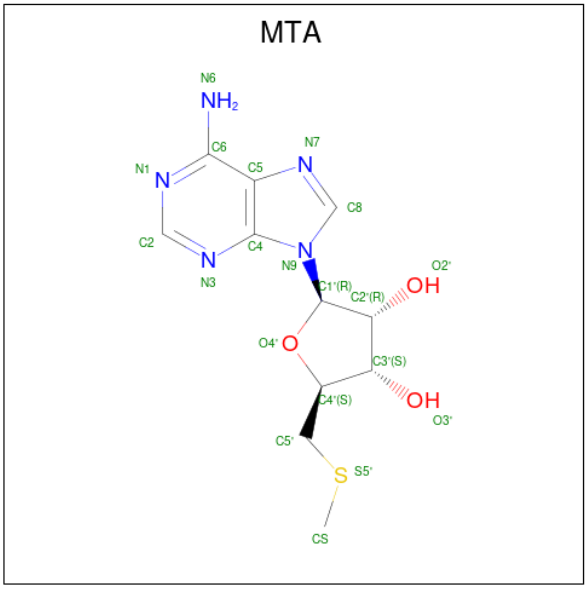
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	302	2294	1440	392	449	13	0	1	0

There are 18 discrepancies between the modelled and reference sequences:

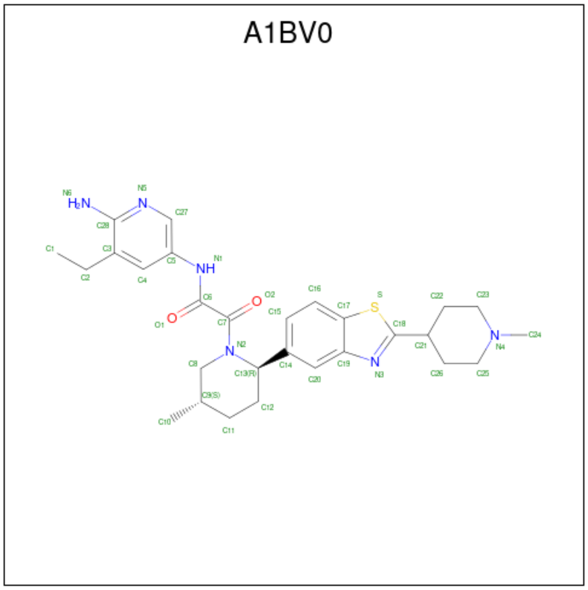
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag	UNP Q9BQA1
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1
D	-7	MET	-	initiating methionine	UNP Q9BQA1
D	-6	HIS	-	expression tag	UNP Q9BQA1
D	-5	HIS	-	expression tag	UNP Q9BQA1
D	-4	HIS	-	expression tag	UNP Q9BQA1
D	-3	HIS	-	expression tag	UNP Q9BQA1
D	-2	HIS	-	expression tag	UNP Q9BQA1
D	-1	HIS	-	expression tag	UNP Q9BQA1
D	0	HIS	-	expression tag	UNP Q9BQA1
D	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	20	11	5	3	1	0	0
			Total	C	N	O	S		
3	C	1	20	11	5	3	1	0	0

- Molecule 4 is N-(6-amino-5-ethylpyridin-3-yl)-2-{(2R,5S)-5-methyl-2-[2-(1-methylpiperidin-4-yl)-1,3-benzothiazol-5-yl]piperidin-1-yl}-2-oxoacetamide (three-letter code: A1BV0) (formula: $C_{28}H_{36}N_6O_2S$) (labeled as "Ligand of Interest" by depositor).

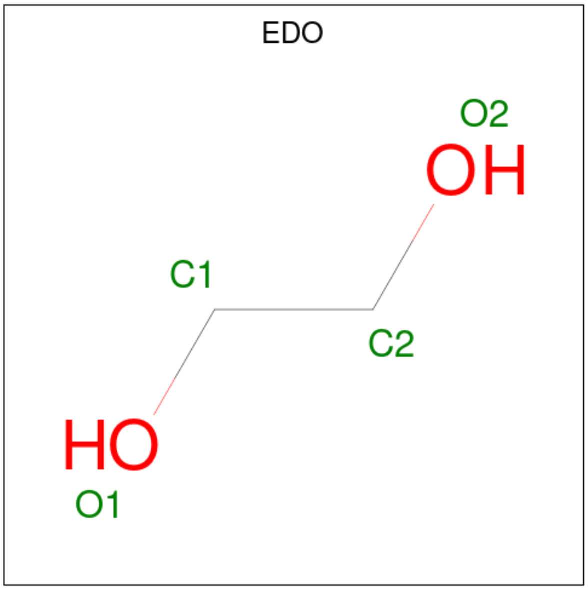


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	37	28	6	2	1	0	0
			Total	C	N	O	S		
4	C	1	37	28	6	2	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	2	2	2	0	0
			Total	Cl		
5	C	3	3	3	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

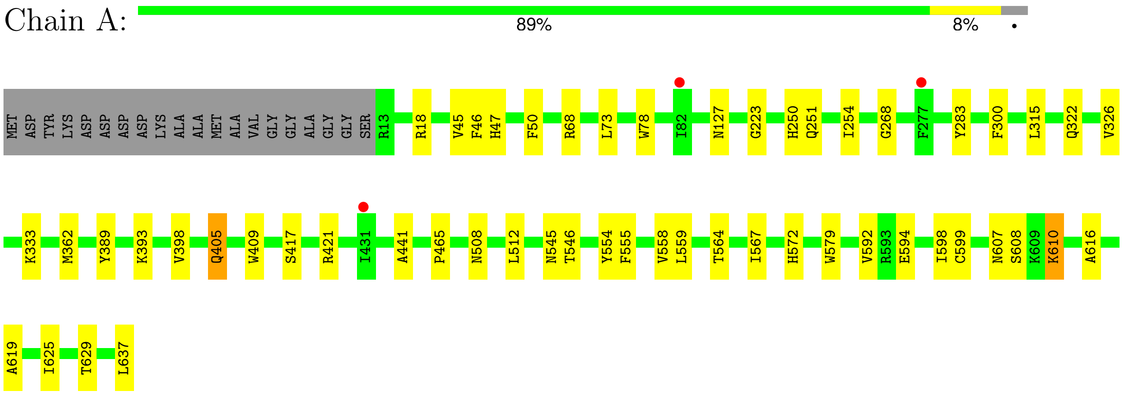
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	39	Total O 39 39	0	0
7	B	5	Total O 5 5	0	0
7	C	47	Total O 47 47	0	0
7	D	12	Total O 12 12	0	0

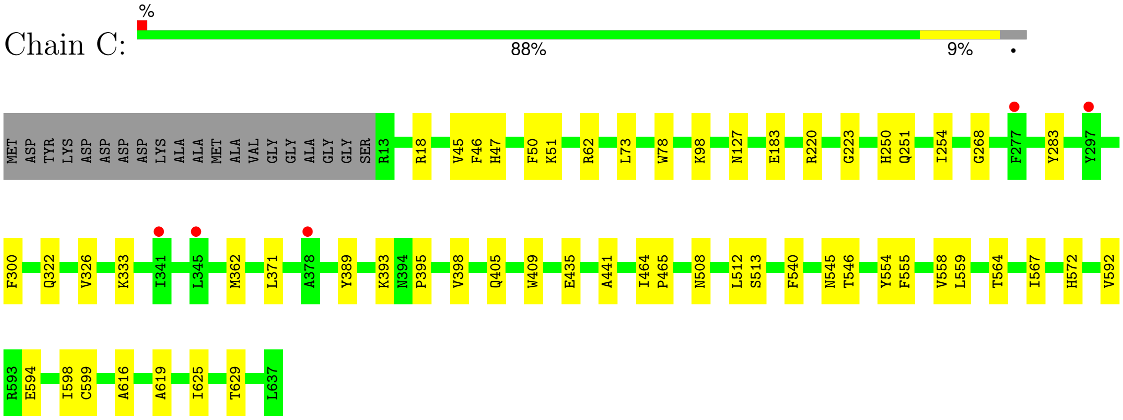
3 Residue-property plots ⓘ

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

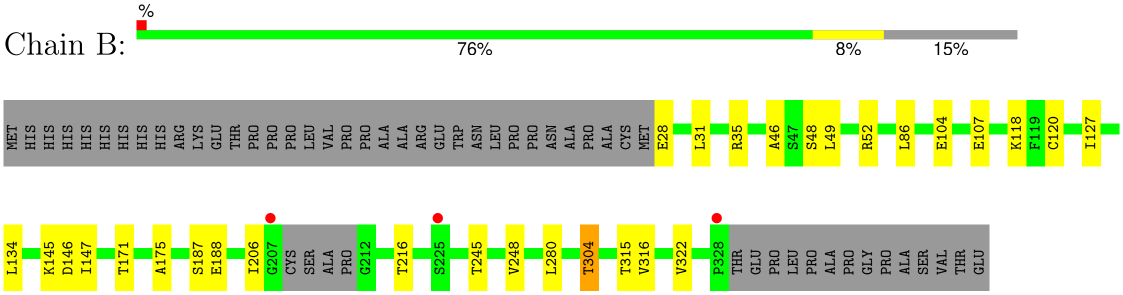
- Molecule 1: Protein arginine N-methyltransferase 5



- Molecule 1: Protein arginine N-methyltransferase 5

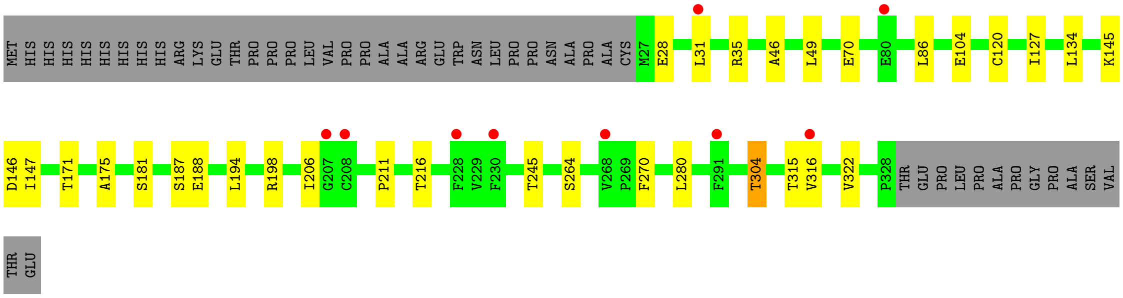


- Molecule 2: Methylosome protein 50



- Molecule 2: Methylosome protein 50

Chain D:



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.21Å 136.60Å 178.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 2.47 29.70 – 2.47	Depositor EDS
% Data completeness (in resolution range)	60.0 (29.70-2.47) 60.2 (29.70-2.47)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.49 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 5.8.0267	Depositor
R, R_{free}	0.210 , 0.243 0.210 , 0.243	Depositor DCC
R_{free} test set	4369 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	81.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14937	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.99 % 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 2.8640e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, A1BV0, MTA, CL

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	0.25	0/5214	0.47	0/7092
1	C	0.25	0/5222	0.48	0/7103
2	B	0.24	0/2314	0.50	0/3158
2	D	0.24	0/2348	0.49	0/3206
All	All	0.24	0/15098	0.48	0/20559

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5072	0	4964	28	0
1	C	5079	0	4966	30	0
2	B	2262	0	2183	16	0
2	D	2294	0	2215	19	0
3	A	20	0	15	0	0
3	C	20	0	15	0	0
4	A	37	0	0	0	0
4	C	37	0	0	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	3	0	0	0	0
6	C	4	0	6	0	0
6	D	4	0	6	0	0
7	A	39	0	0	0	0
7	B	5	0	0	0	0
7	C	47	0	0	0	0
7	D	12	0	0	0	0
All	All	14937	0	14370	89	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 3.

All (89) 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:220:ARG:HH22	1:C:545:ASN:HB2	1.59	0.68
1:C:545:ASN:OD1	1:C:594:GLU:N	2.31	0.62
1:C:220:ARG:NH2	1:C:545:ASN:HB2	2.16	0.61
2:D:280:LEU:HD22	2:D:315:THR:HG21	1.83	0.61
2:B:280:LEU:HD22	2:B:315:THR:HG21	1.84	0.60
2:D:35:ARG:NH1	2:D:86:LEU:O	2.35	0.59
2:B:35:ARG:NH1	2:B:86:LEU:O	2.36	0.59
1:C:51:LYS:O	1:C:62:ARG:NH2	2.35	0.59
1:C:465:PRO:HA	1:C:559:LEU:HA	1.85	0.59
2:B:127:ILE:HB	2:B:145:LYS:HD2	1.87	0.57
1:A:465:PRO:HA	1:A:559:LEU:HA	1.85	0.57
2:B:31:LEU:HD23	2:B:46:ALA:HB2	1.87	0.55
1:A:558:VAL:HA	1:A:564:THR:HG22	1.88	0.55
2:D:194:LEU:HB2	2:D:206:ILE:HD11	1.88	0.55
1:A:545:ASN:OD1	1:A:594:GLU:N	2.38	0.55
2:D:31:LEU:HD23	2:D:46:ALA:HB2	1.89	0.54
2:D:28:GLU:N	2:D:28:GLU:OE1	2.40	0.54
1:C:18:ARG:NH2	1:C:268:GLY:O	2.39	0.54
2:D:35:ARG:HA	2:D:304:THR:HG21	1.89	0.54
2:B:35:ARG:HA	2:B:304:THR:HG21	1.89	0.54
2:D:127:ILE:HB	2:D:145:LYS:HD2	1.90	0.54
1:C:558:VAL:HA	1:C:564:THR:HG22	1.90	0.53
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.91	0.53
1:C:512:LEU:HD22	1:C:546:THR:HG21	1.90	0.53
1:C:183:GLU:OE1	1:C:220:ARG:NH2	2.34	0.52
1:A:607:ASN:HD21	1:A:610:LYS:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HD22	1:A:546:THR:HG21	1.92	0.51
2:B:316:VAL:HG12	2:B:322:VAL:HG22	1.93	0.50
2:D:70:GLU:N	2:D:70:GLU:OE1	2.45	0.50
1:A:18:ARG:NH2	1:A:268:GLY:O	2.44	0.50
1:C:362:MET:HG2	1:C:389:TYR:HB2	1.94	0.49
1:A:405:GLN:HA	1:A:409:TRP:HB2	1.94	0.49
1:C:616:ALA:HB2	1:C:625:ILE:HA	1.94	0.48
2:D:134:LEU:HD23	2:D:175:ALA:HB1	1.96	0.48
1:A:68:ARG:NH1	2:B:52:ARG:O	2.46	0.48
1:A:616:ALA:HB2	1:A:625:ILE:HA	1.96	0.48
2:D:181:SER:OG	2:D:198:ARG:NH1	2.47	0.48
2:B:134:LEU:HD23	2:B:175:ALA:HB1	1.96	0.47
1:C:322:GLN:O	1:C:326:VAL:HG13	2.14	0.47
1:A:465:PRO:HB3	1:A:559:LEU:HD23	1.96	0.47
1:A:223:GLY:HA2	1:A:508:ASN:O	2.15	0.47
1:C:405:GLN:HA	1:C:409:TRP:HB2	1.97	0.47
1:A:250:HIS:O	1:A:254:ILE:HG12	2.15	0.47
1:C:371:LEU:HD11	1:C:435:GLU:HB2	1.97	0.47
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.50	0.47
2:B:28:GLU:OE1	2:B:28:GLU:N	2.47	0.46
1:A:599:CYS:HB3	1:A:619:ALA:HB3	1.98	0.46
1:C:223:GLY:HA2	1:C:508:ASN:O	2.15	0.46
1:A:322:GLN:O	1:A:326:VAL:HG13	2.16	0.46
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.97	0.46
1:C:73:LEU:HB2	1:C:78:TRP:CE2	2.51	0.46
1:C:441:ALA:HB2	1:C:555:PHE:HB2	1.97	0.46
1:C:250:HIS:O	1:C:254:ILE:HG12	2.16	0.45
1:C:599:CYS:HB3	1:C:619:ALA:HB3	1.99	0.45
2:B:171:THR:HG21	2:B:216:THR:HA	1.98	0.45
2:B:107:GLU:HB2	2:B:118:LYS:HG2	1.99	0.45
2:D:171:THR:HG21	2:D:216:THR:HA	1.99	0.45
1:C:465:PRO:HB3	1:C:559:LEU:HD23	1.98	0.44
2:D:316:VAL:HG12	2:D:322:VAL:HG22	1.98	0.44
1:A:50:PHE:HB2	2:B:49:LEU:HB3	1.99	0.44
1:A:421:ARG:NH2	1:A:637:LEU:OXT	2.46	0.44
2:B:104:GLU:HG3	2:B:120:CYS:HB2	1.99	0.44
1:C:554:TYR:HB3	1:C:567:ILE:HG13	2.00	0.44
1:A:47:HIS:HB3	1:A:50:PHE:HB2	2.00	0.43
2:B:28:GLU:HG2	2:B:48:SER:HB3	1.99	0.43
1:A:398:VAL:HG11	1:A:417:SER:HB2	2.01	0.42
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ILE:HG21	1:A:579:TRP:HB2	2.01	0.42
1:C:464:ILE:HG23	1:C:559:LEU:HB3	2.01	0.42
1:A:315:LEU:HD11	1:A:421:ARG:NH1	2.35	0.42
1:C:45:VAL:HG23	1:C:46:PHE:HD1	1.84	0.42
1:C:513:SER:CB	1:C:540:PHE:HB3	2.50	0.42
2:D:104:GLU:HG3	2:D:120:CYS:HB2	2.00	0.42
1:A:592:VAL:HG21	1:A:598:ILE:HD11	2.02	0.41
1:A:251:GLN:NE2	1:A:283:TYR:OH	2.53	0.41
1:C:395:PRO:HA	1:C:398:VAL:HB	2.03	0.41
1:C:592:VAL:HG21	1:C:598:ILE:HD11	2.03	0.41
1:A:607:ASN:ND2	1:A:610:LYS:HE2	2.36	0.41
1:C:98:LYS:H	1:C:98:LYS:HG3	1.72	0.41
2:B:187:SER:OG	2:B:188:GLU:N	2.54	0.41
2:D:187:SER:OG	2:D:188:GLU:N	2.52	0.41
1:C:251:GLN:NE2	1:C:283:TYR:OH	2.54	0.40
2:D:264:SER:OG	2:D:270:PHE:N	2.46	0.40
1:A:554:TYR:HB3	1:A:567:ILE:HG13	2.03	0.40
1:C:47:HIS:CE1	2:D:49:LEU:HD22	2.56	0.40
1:C:50:PHE:HB2	2:D:49:LEU:HB3	2.02	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	624/645 (97%)	600 (96%)	24 (4%)	0	100	100
1	C	625/645 (97%)	601 (96%)	24 (4%)	0	100	100
2	B	294/350 (84%)	279 (95%)	12 (4%)	3 (1%)	13	23
2	D	301/350 (86%)	284 (94%)	13 (4%)	4 (1%)	10	17
All	All	1844/1990 (93%)	1764 (96%)	73 (4%)	7 (0%)	37	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147[A]	ILE
2	B	147[B]	ILE
2	D	147[A]	ILE
2	D	147[B]	ILE
2	D	211	PRO
2	D	245	THR
2	B	245	THR

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	559/570 (98%)	550 (98%)	9 (2%)	58	79
1	C	560/570 (98%)	553 (99%)	7 (1%)	65	83
2	B	254/298 (85%)	251 (99%)	3 (1%)	67	84
2	D	258/298 (87%)	257 (100%)	1 (0%)	89	95
All	All	1631/1736 (94%)	1611 (99%)	20 (1%)	67	84

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	300	PHE
1	A	333	LYS
1	A	393	LYS
1	A	405	GLN
1	A	572	HIS
1	A	608	SER
1	A	610	LYS
1	A	629	THR
2	B	206	ILE
2	B	248	VAL
2	B	304	THR
1	C	127	ASN

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Mol	Chain	Res	Type
1	C	300	PHE
1	C	333	LYS
1	C	393	LYS
1	C	572[A]	HIS
1	C	572[B]	HIS
1	C	629	THR
2	D	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	251	GLN
1	A	322	GLN
2	B	294	GLN
1	C	79	ASN
1	C	251	GLN
1	C	359	GLN
2	D	294	GLN

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 ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	C	706	-	3,3,3	0.44	0	2,2,2	0.33	0
3	MTA	C	701	-	18,22,22	0.97	2 (11%)	18,32,32	0.86	0
3	MTA	A	701	-	18,22,22	0.96	2 (11%)	18,32,32	0.85	0
4	A1BV0	C	702	-	38,41,41	0.89	3 (7%)	45,59,59	1.56	9 (20%)
6	EDO	D	401	-	3,3,3	0.44	0	2,2,2	0.33	0
4	A1BV0	A	702	-	38,41,41	0.89	3 (7%)	45,59,59	1.55	7 (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	EDO	C	706	-	-	0/1/1/1	-
3	MTA	C	701	-	-	0/3/23/23	0/3/3/3
3	MTA	A	701	-	-	0/3/23/23	0/3/3/3
4	A1BV0	C	702	-	-	3/18/45/45	0/5/5/5
6	EDO	D	401	-	-	1/1/1/1	-
4	A1BV0	A	702	-	-	3/18/45/45	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	A1BV0	C7-C6	-3.40	1.49	1.53
4	C	702	A1BV0	C7-C6	-3.37	1.49	1.53
3	C	701	MTA	C8-N7	-2.36	1.30	1.34
3	A	701	MTA	C8-N7	-2.35	1.30	1.34
4	C	702	A1BV0	C3-C28	-2.19	1.39	1.42
4	A	702	A1BV0	C3-C28	-2.17	1.39	1.42
4	A	702	A1BV0	C28-N6	2.14	1.39	1.34
4	C	702	A1BV0	C28-N6	2.14	1.39	1.34
3	C	701	MTA	C1'-N9	-2.08	1.44	1.49
3	A	701	MTA	C1'-N9	-2.04	1.44	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	702	A1BV0	C7-C6-N1	3.56	118.54	112.28
4	C	702	A1BV0	C7-C6-N1	3.49	118.41	112.28
4	A	702	A1BV0	C27-N5-C28	3.45	121.97	118.64
4	C	702	A1BV0	C27-N5-C28	3.42	121.94	118.64
4	A	702	A1BV0	O2-C7-C6	3.42	120.05	116.72
4	A	702	A1BV0	C5-C27-N5	-3.29	121.34	124.07
4	C	702	A1BV0	C5-C27-N5	-3.26	121.37	124.07
4	C	702	A1BV0	O2-C7-C6	3.11	119.75	116.72
4	C	702	A1BV0	C4-C3-C28	3.08	119.18	116.42
4	A	702	A1BV0	C4-C3-C28	3.03	119.14	116.42
4	C	702	A1BV0	C19-C17-S	-2.94	107.96	111.85
4	A	702	A1BV0	C19-C17-S	-2.85	108.07	111.85
4	C	702	A1BV0	C25-C26-C21	-2.41	108.18	111.00
4	A	702	A1BV0	C20-C19-C17	-2.30	118.51	121.04
4	C	702	A1BV0	C23-C22-C21	-2.22	108.40	111.00
4	C	702	A1BV0	C20-C19-C17	-2.17	118.66	121.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

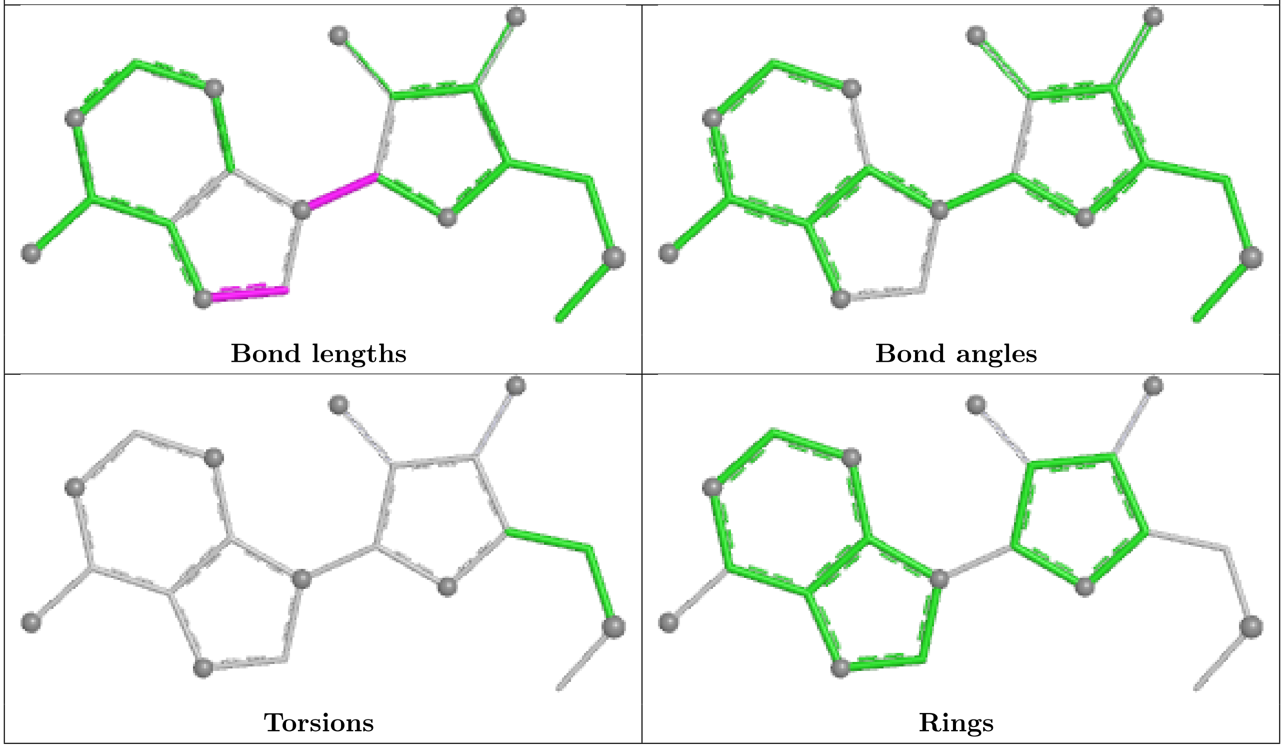
Mol	Chain	Res	Type	Atoms
4	A	702	A1BV0	N1-C6-C7-O2
4	C	702	A1BV0	N1-C6-C7-O2
6	D	401	EDO	O1-C1-C2-O2
4	C	702	A1BV0	C12-C13-C14-C15
4	C	702	A1BV0	C12-C13-C14-C20
4	A	702	A1BV0	C12-C13-C14-C20
4	A	702	A1BV0	C12-C13-C14-C15

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 MTA C 701



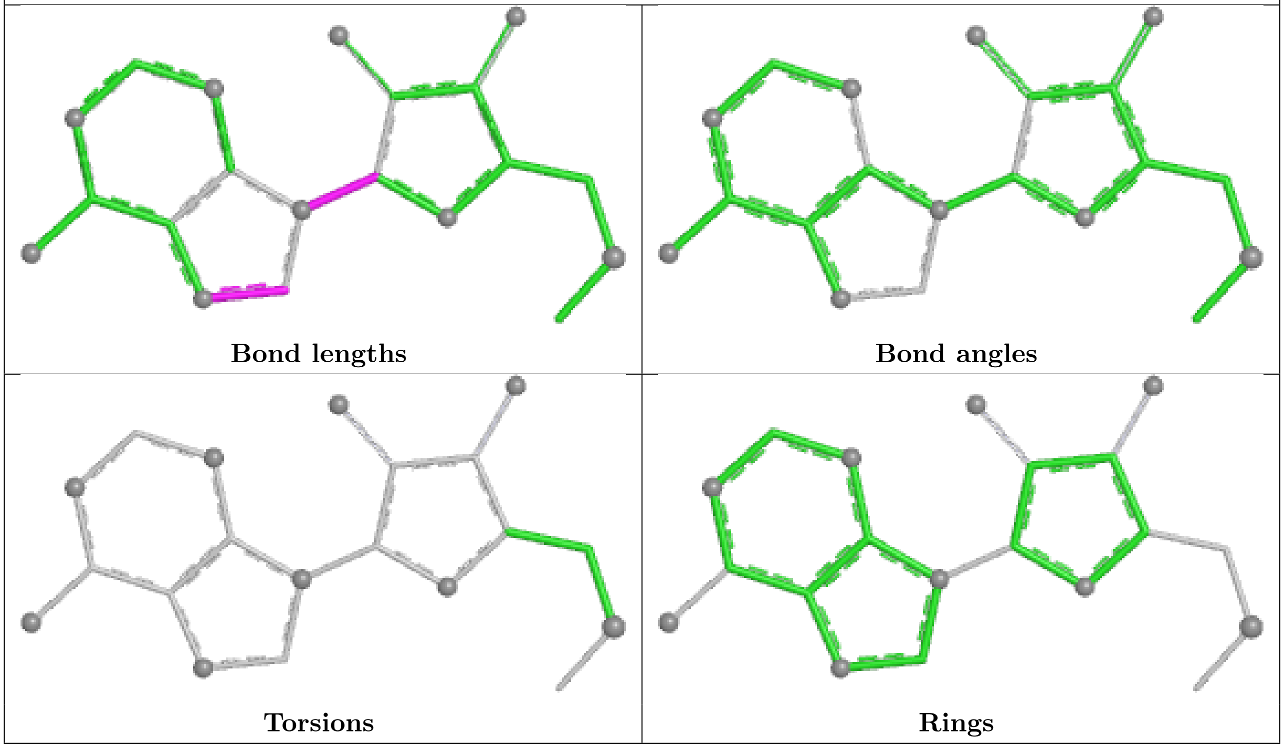
Bond lengths

Bond angles

Torsions

Rings

Ligand MTA A 701



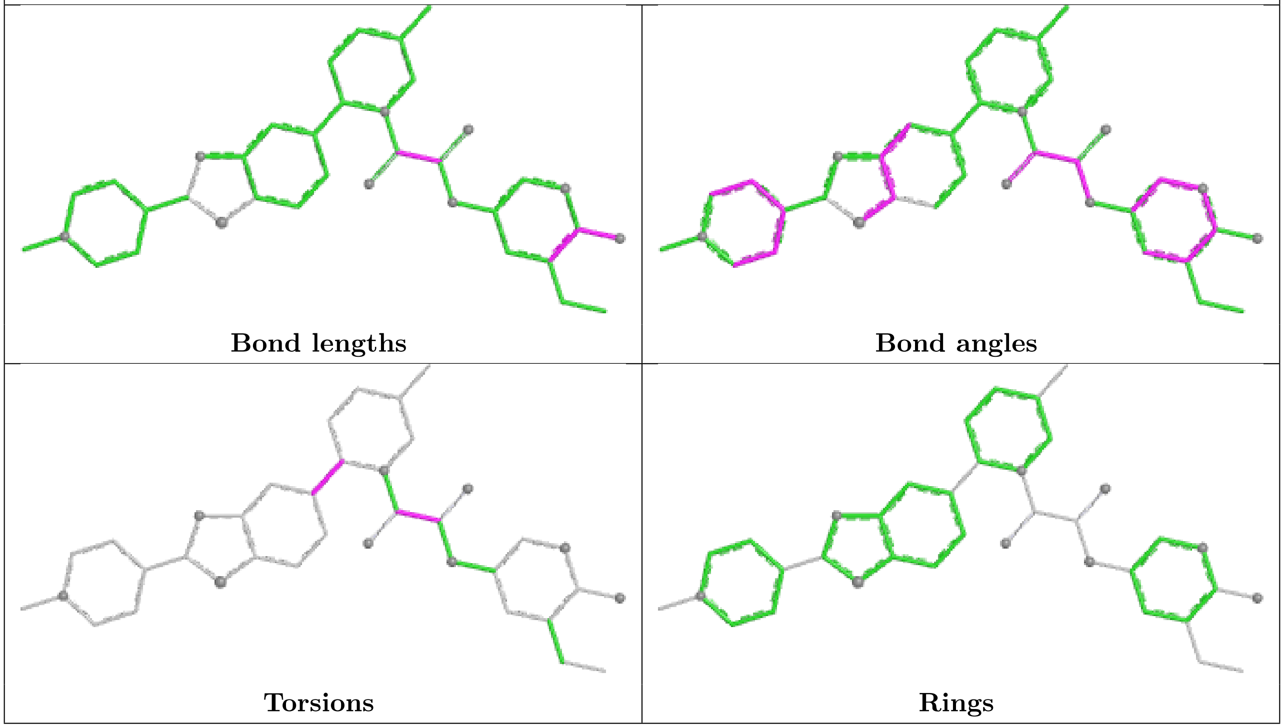
Bond lengths

Bond angles

Torsions

Rings

Ligand A1BV0 C 702



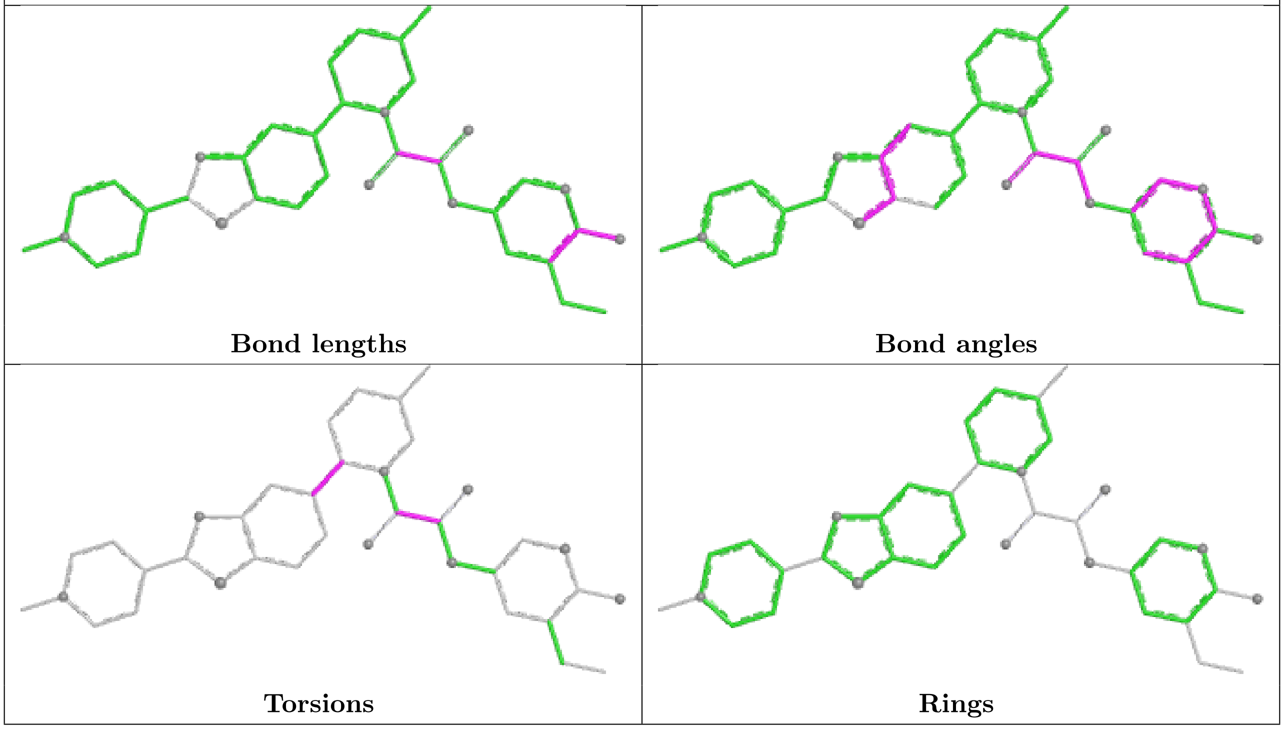
Bond lengths

Bond angles

Torsions

Rings

Ligand A1BV0 A 702



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	625/645 (96%)	-0.07	3 (0%)	87	85	33, 75, 122, 169	1 (0%)
1	C	625/645 (96%)	-0.12	5 (0%)	82	80	33, 70, 122, 178	2 (0%)
2	B	297/350 (84%)	0.23	3 (1%)	79	77	42, 96, 130, 174	1 (0%)
2	D	302/350 (86%)	0.23	9 (2%)	52	50	38, 96, 146, 188	1 (0%)
All	All	1849/1990 (92%)	0.01	20 (1%)	77	75	33, 83, 128, 188	5 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	277	PHE	4.5
1	A	277	PHE	3.5
2	D	268	VAL	3.0
1	A	82	ILE	3.0
2	D	291	PHE	2.8
2	B	225	SER	2.7
2	B	207	GLY	2.7
1	C	341	ILE	2.6
2	D	80	GLU	2.6
1	C	297	TYR	2.4
1	C	345	LEU	2.4
2	D	207	GLY	2.4
1	C	378	ALA	2.4
2	D	316	VAL	2.3
2	D	228	PHE	2.3
2	D	230	PHE	2.3
2	D	208	CYS	2.2
1	A	431	ILE	2.1
2	D	31	LEU	2.1
2	B	328	PRO	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 monosaccharides in this entry.

6.4 Ligands ⓘ

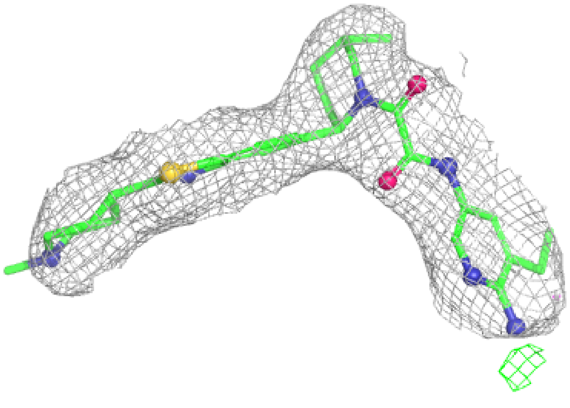
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

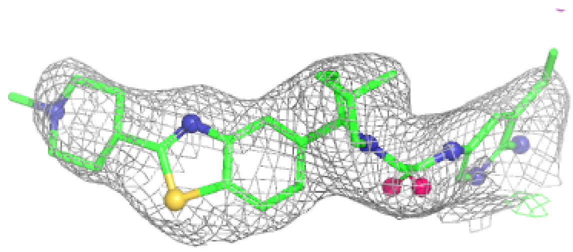
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	D	401	4/4	0.68	0.22	88,90,98,107	0
6	EDO	C	706	4/4	0.79	0.15	66,76,79,81	0
5	CL	C	703	1/1	0.87	0.12	71,71,71,71	0
5	CL	C	705	1/1	0.91	0.10	70,70,70,70	0
5	CL	C	704	1/1	0.92	0.06	71,71,71,71	0
4	A1BV0	C	702	37/37	0.94	0.09	56,66,87,102	0
5	CL	A	704	1/1	0.95	0.06	71,71,71,71	0
3	MTA	C	701	20/20	0.95	0.09	54,65,71,72	0
3	MTA	A	701	20/20	0.95	0.07	54,65,73,73	0
4	A1BV0	A	702	37/37	0.96	0.08	60,68,81,101	0
5	CL	A	703	1/1	0.98	0.03	63,63,63,63	0

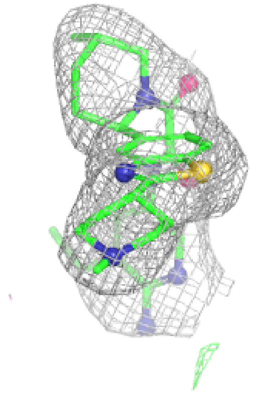
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1BV0 C 702:

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

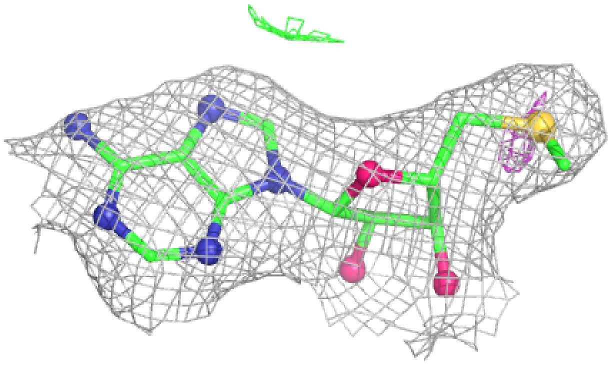


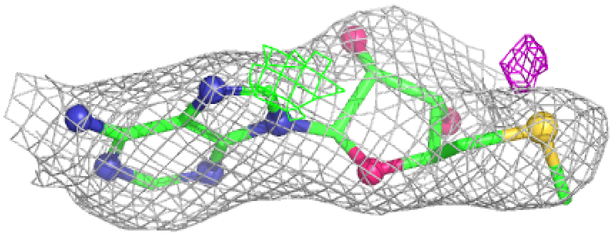


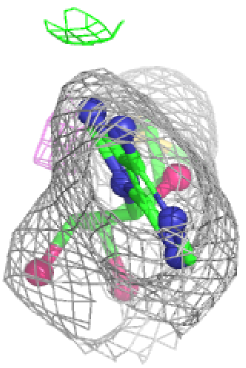


Electron density around MTA C 701:

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







Electron density around MTA A 701:

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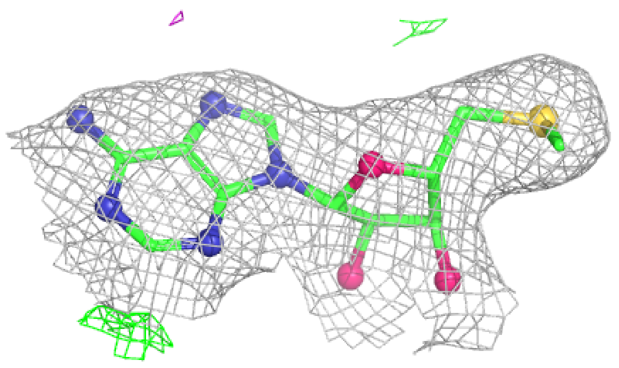
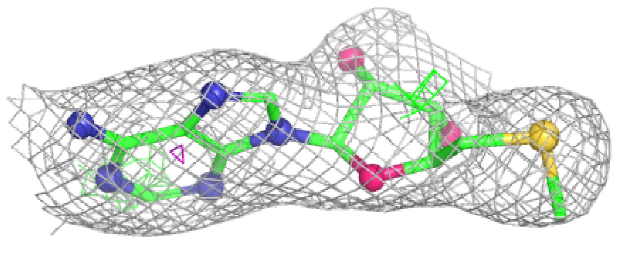
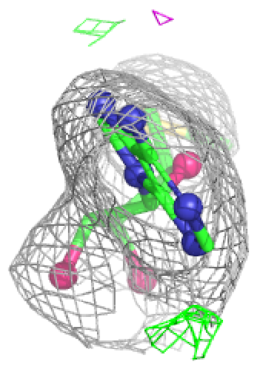
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

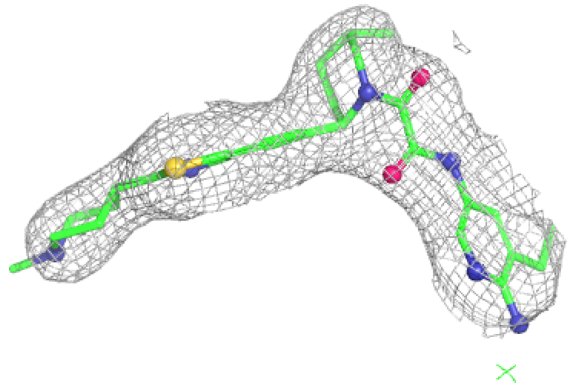


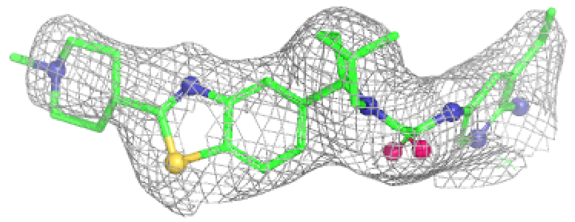


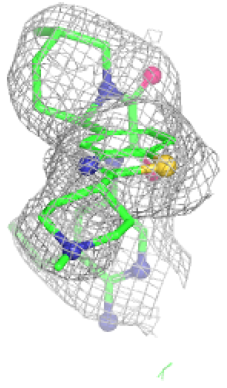


Electron density around A1BV0 A 702:

$2mF_o$-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.