



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2022 – 10:05 AM EST

PDB ID : 7S1S  
Title : PRMT5/MEP50 crystal structure with MTA and MRTX-1719 bound  
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Deposited on : 2021-09-02  
Resolution : 2.62 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

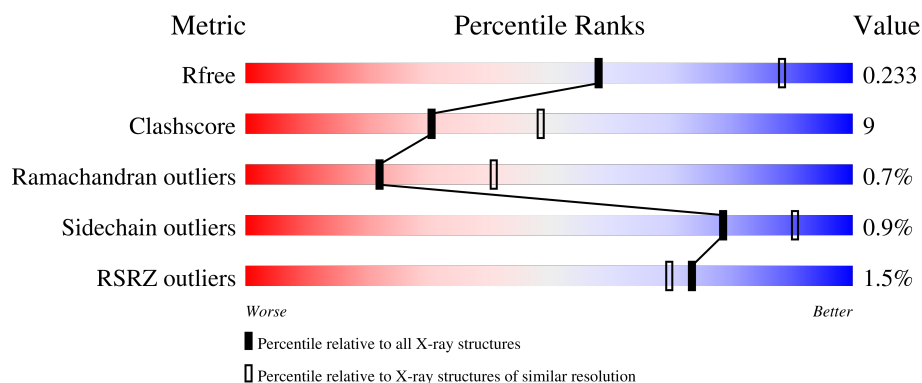
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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  $\geq 3$ , 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	645	<div> <div>0%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
2	B	350	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>18%</div> <div>.</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7478 atoms, of which 19 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	C	N	O	S	40	0	0
			5048	3231	865	928	24			

There are 9 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

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	302	Total	C	N	O	S	34	1	0
			2294	1442	392	447	13			

There are 9 discrepancies between the modelled and reference sequences:

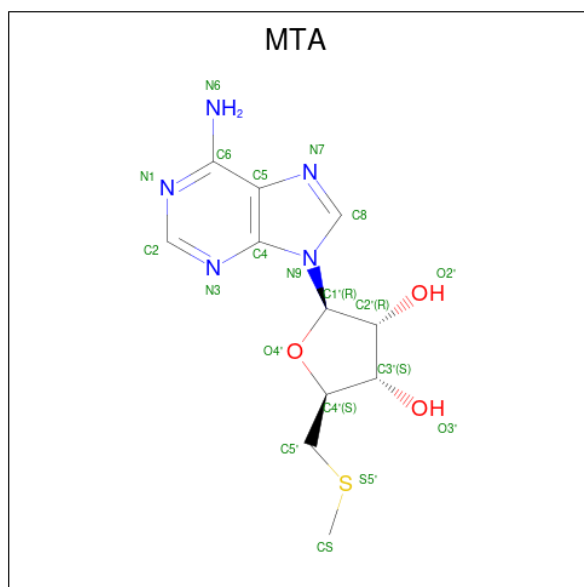
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag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

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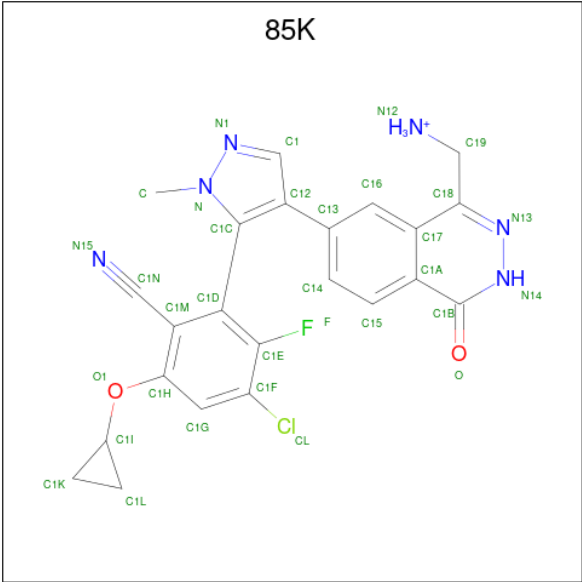
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- 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
3	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 4 is (7-{(5M)-5-[3-chloro-6-cyano-5-(cyclopropyloxy)-2-fluorophenyl]-1-methyl-1H-pyrazol-4-yl}-4-oxo-3,4-dihydrophthalazin-1-yl)methanaminium (three-letter code: 85K) (formula:  $C_{23}H_{19}ClFN_6O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	H	N	O	0	0
			52	23	1	1	19	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total	O	0	0
			59	59		
5	B	5	Total	O	0	0
			5	5		



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.14Å 138.09Å 178.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.64 – 2.62 46.64 – 2.62	Depositor EDS
% Data completeness (in resolution range)	88.0 (46.64-2.62) 88.0 (46.64-2.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.209 , 0.233 0.209 , 0.233	Depositor DCC
$R_{free}$ test set	1772 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.890	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7478	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MTA, 85K

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	0.24	0/5190	0.42	0/7062
2	B	0.24	0/2348	0.45	0/3207
All	All	0.24	0/7538	0.43	0/10269

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	5048	0	4933	80	0
2	B	2294	0	2210	54	0
3	A	20	0	14	0	0
4	A	33	19	0	0	0
5	A	59	0	0	1	0
5	B	5	0	0	1	0
All	All	7459	19	7157	132	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 9.

All (132) 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)
2:B:194:LEU:HB2	2:B:206:ILE:HD11	1.41	0.98
1:A:296:ALA:O	1:A:300:PHE:N	2.15	0.79
1:A:278:CYS:O	1:A:282:GLN:HG3	1.89	0.71
1:A:294:PRO:HD2	1:A:298:GLU:OE1	1.89	0.71
1:A:100:ARG:O	1:A:104:GLU:HG3	1.93	0.69
2:B:184:LEU:HB3	2:B:218:LEU:HD13	1.79	0.64
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.33	0.63
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.80	0.63
1:A:300:PHE:CE2	1:A:577:PHE:HB3	2.33	0.62
2:B:24:PRO:HG2	2:B:59:TRP:CZ2	2.36	0.61
2:B:126:ASP:OD1	2:B:127:ILE:N	2.29	0.61
1:A:364:LEU:HB3	1:A:420:MET:CE	2.31	0.60
2:B:274:LEU:H	2:B:274:LEU:HD13	1.68	0.58
1:A:140:ASN:HB3	5:A:818:HOH:O	2.03	0.58
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.85	0.58
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.40	0.57
2:B:30:GLN:HG2	2:B:49:LEU:HD12	1.85	0.57
1:A:232:PRO:O	1:A:235:ILE:HG12	2.03	0.57
2:B:27:MET:CE	2:B:68:PRO:HB2	2.35	0.56
1:A:617:VAL:O	1:A:622:CYS:HA	2.06	0.56
2:B:27:MET:HG3	2:B:59:TRP:NE1	2.20	0.56
2:B:28:GLU:OE1	2:B:28:GLU:N	2.36	0.56
1:A:362:MET:SD	1:A:429:ALA:HB2	2.45	0.55
1:A:430:ASP:OD1	1:A:458:LYS:HD2	2.05	0.55
2:B:274:LEU:HD13	2:B:274:LEU:N	2.20	0.55
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.71	0.55
2:B:280:LEU:HD22	2:B:315:THR:HG21	1.89	0.55
1:A:609:LYS:O	1:A:637:LEU:HB2	2.06	0.54
1:A:93:ASP:OD2	1:A:131:ASN:HA	2.08	0.53
1:A:437:LEU:HD21	1:A:468:TYR:CE1	2.44	0.53
1:A:369:GLY:N	1:A:370:PRO:CD	2.72	0.52
1:A:304:TYR:O	1:A:505:ARG:HB3	2.10	0.52
1:A:512:LEU:HD22	1:A:546:THR:HG21	1.91	0.52
1:A:454:GLN:OE1	1:A:525:ASN:N	2.39	0.52
1:A:493:ASP:HB3	1:A:496:ALA:HB2	1.92	0.52
2:B:130:THR:HG23	2:B:173:VAL:HG22	1.92	0.52
2:B:33:ALA:HB1	2:B:86:LEU:HD11	1.92	0.51
2:B:289:GLU:OE2	2:B:292:ARG:HB2	2.10	0.51
1:A:294:PRO:HD2	1:A:298:GLU:CD	2.31	0.51
2:B:134:LEU:HD12	2:B:139:GLN:HB2	1.91	0.51
2:B:221:HIS:HE1	2:B:223:GLN:HB2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LEU:N	2:B:20:PRO:HD3	2.26	0.50
1:A:16:SER:HB2	1:A:281:LEU:HD11	1.93	0.50
2:B:37:ARG:O	2:B:307:PRO:HG3	2.12	0.50
1:A:49:ARG:NH2	2:B:99:ASP:OD2	2.38	0.50
1:A:376:LEU:HD21	1:A:388:LEU:HD12	1.94	0.49
2:B:134:LEU:HD23	2:B:175:ALA:CB	2.43	0.49
1:A:82:ILE:O	1:A:120:PRO:HD2	2.13	0.49
1:A:435:GLU:O	1:A:435:GLU:HG2	2.13	0.49
2:B:134:LEU:HD23	2:B:175:ALA:HB1	1.95	0.49
1:A:285:GLU:O	1:A:289:GLN:HG2	2.13	0.48
2:B:260:GLY:N	2:B:274:LEU:HD22	2.28	0.48
2:B:27:MET:HE3	2:B:31:LEU:HD21	1.95	0.48
2:B:41:ALA:HB1	2:B:60:LEU:HD11	1.94	0.48
1:A:629:THR:HG22	1:A:629:THR:O	2.13	0.48
2:B:27:MET:HE2	2:B:68:PRO:HB2	1.94	0.48
1:A:364:LEU:HB3	1:A:420:MET:HE2	1.96	0.47
1:A:512:LEU:HD13	1:A:546:THR:HG21	1.96	0.47
1:A:369:GLY:H	1:A:370:PRO:HD2	1.78	0.47
2:B:259:THR:HB	2:B:274:LEU:HD23	1.96	0.47
1:A:222:LEU:HB3	1:A:510:HIS:HB2	1.97	0.47
1:A:614:GLU:HG2	1:A:627:ASN:O	2.14	0.47
1:A:73:LEU:HB2	1:A:78:TRP:NE1	2.29	0.47
1:A:578:SER:O	1:A:579:TRP:HB2	2.15	0.47
2:B:27:MET:HE1	2:B:68:PRO:HB2	1.97	0.47
1:A:405:GLN:HA	1:A:409:TRP:HB2	1.96	0.47
1:A:442:ASP:OD2	1:A:604:ARG:NE	2.44	0.46
1:A:605:CYS:HB2	1:A:612:TRP:CE2	2.50	0.46
1:A:16:SER:CB	1:A:281:LEU:HD11	2.46	0.46
1:A:208:ILE:HD12	1:A:253:LEU:HD21	1.97	0.46
1:A:557:THR:CG2	1:A:565:LEU:HB2	2.45	0.46
2:B:289:GLU:OE2	2:B:292:ARG:HD3	2.16	0.46
2:B:283:LEU:HA	2:B:288:SER:O	2.16	0.46
1:A:44:PRO:HB2	1:A:46:PHE:O	2.16	0.46
2:B:44:LEU:HB2	2:B:59:TRP:HB2	1.97	0.46
2:B:24:PRO:HG2	2:B:59:TRP:CH2	2.51	0.45
2:B:70:GLU:OE2	2:B:70:GLU:N	2.49	0.45
1:A:525:ASN:ND2	1:A:530:ILE:HG12	2.31	0.45
1:A:603:TRP:HE3	1:A:614:GLU:O	1.99	0.45
1:A:610:LYS:HB3	1:A:634:THR:HB	1.99	0.45
2:B:186:CYS:HB2	2:B:215:PRO:HG2	1.97	0.45
2:B:259:THR:HB	2:B:274:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:PRO:HG2	2:B:114:LEU:HD21	1.99	0.44
1:A:70:ASP:N	1:A:70:ASP:OD1	2.49	0.44
1:A:121:ALA:HA	1:A:150:MET:O	2.17	0.44
1:A:15:SER:HA	1:A:39:ASP:OD2	2.17	0.44
2:B:32:GLU:HB2	5:B:401:HOH:O	2.16	0.44
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.98	0.44
1:A:26:ILE:CD1	1:A:68:ARG:HD3	2.48	0.44
2:B:101:GLY:HA2	2:B:126:ASP:O	2.17	0.44
1:A:149:SER:HB3	1:A:201:ARG:HH21	1.83	0.43
1:A:294:PRO:HG2	1:A:298:GLU:OE2	2.17	0.43
1:A:557:THR:HG22	1:A:565:LEU:HB2	1.99	0.43
2:B:282:VAL:HB	2:B:291:PHE:HB3	2.00	0.43
1:A:453:ALA:HB1	1:A:456:PHE:CZ	2.53	0.43
2:B:147:ILE:O	2:B:147:ILE:HG22	2.17	0.43
1:A:554:TYR:HB3	1:A:567:ILE:HG13	2.01	0.43
2:B:194:LEU:CB	2:B:206:ILE:HD11	2.29	0.43
1:A:296:ALA:HB1	1:A:577:PHE:CE1	2.53	0.43
2:B:166:HIS:ND1	2:B:187:SER:HB3	2.34	0.43
1:A:217:VAL:O	1:A:220:ARG:HB2	2.18	0.43
1:A:440:PHE:O	1:A:441:ALA:HB3	2.18	0.43
1:A:537:THR:O	1:A:538:LEU:HD23	2.19	0.42
2:B:221:HIS:CE1	2:B:223:GLN:HB2	2.52	0.42
1:A:18:ARG:NE	1:A:20:LEU:HD21	2.34	0.42
1:A:495:GLU:HB3	1:A:587:LYS:HE2	2.00	0.42
1:A:519:PHE:CE1	1:A:534:ARG:HB3	2.54	0.42
2:B:130:THR:CG2	2:B:173:VAL:HG22	2.49	0.42
1:A:437:LEU:HD21	1:A:468:TYR:CD1	2.54	0.42
1:A:472:LEU:O	1:A:515:PRO:HA	2.20	0.42
2:B:146:ASP:O	2:B:147:ILE:HB	2.20	0.42
2:B:175:ALA:HA	2:B:183:PHE:CB	2.50	0.42
1:A:51:LYS:HD3	2:B:276:GLU:OE2	2.19	0.41
1:A:601:ARG:O	1:A:615:TRP:HA	2.20	0.41
1:A:445:LEU:HD21	1:A:611:VAL:HB	2.02	0.41
2:B:156:GLN:O	2:B:158:VAL:HG13	2.20	0.41
2:B:194:LEU:HB2	2:B:206:ILE:CD1	2.31	0.41
1:A:420:MET:SD	1:A:449:CYS:HB3	2.60	0.41
2:B:182:VAL:HA	2:B:195:TRP:O	2.19	0.41
1:A:144:THR:HG22	1:A:144:THR:O	2.19	0.41
2:B:127:ILE:HB	2:B:145:LYS:HD2	2.03	0.41
2:B:33:ALA:CB	2:B:86:LEU:HG	2.50	0.41
2:B:184:LEU:HG	2:B:220:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TYR:OH	1:A:505:ARG:NH1	2.53	0.41
1:A:18:ARG:O	1:A:41:LEU:HD12	2.22	0.40
1:A:67:THR:OG1	1:A:68:ARG:N	2.53	0.40
1:A:78:TRP:CZ3	1:A:117:LEU:HD13	2.56	0.40
2:B:37:ARG:HG3	2:B:39:ASP:OD1	2.21	0.40
1:A:434:SER:HB2	1:A:436:LEU:HG	2.03	0.40
1:A:57:GLU:HG2	1:A:61:ASN:OD1	2.21	0.40
1:A:315:LEU:HD11	1:A:421:ARG:NH2	2.36	0.40
1:A:556:GLU:OE1	1:A:568:ARG:HD3	2.20	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	623/645 (97%)	591 (95%)	27 (4%)	5 (1%)	19	36
2	B	297/350 (85%)	284 (96%)	12 (4%)	1 (0%)	41	62
All	All	920/995 (92%)	875 (95%)	39 (4%)	6 (1%)	22	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	PRO
2	B	147	ILE
1	A	293	PRO
1	A	441	ALA
1	A	300	PHE
1	A	294	PRO

### 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	555/570 (97%)	549 (99%)	6 (1%)	73	88
2	B	257/298 (86%)	256 (100%)	1 (0%)	91	97
All	All	812/868 (94%)	805 (99%)	7 (1%)	78	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ARG
1	A	237	LEU
1	A	284	LEU
1	A	299	LEU
1	A	393	LYS
1	A	594	GLU
2	B	274	LEU

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

Mol	Chain	Res	Type
2	B	320	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 monosaccharides in this entry.

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	85K	A	702	-	32,37,37	1.18	3 (9%)	36,55,55	2.14	7 (19%)
3	MTA	A	701	-	19,22,22	4.13	7 (36%)	19,32,32	1.82	3 (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
4	85K	A	702	-	-	1/14/18/18	0/5/5/5
3	MTA	A	701	-	-	0/3/23/23	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	MTA	C2'-C1'	-16.18	1.29	1.53
3	A	701	MTA	O3'-C3'	-4.22	1.33	1.43
4	A	702	85K	C12-C1C	-3.20	1.36	1.41
3	A	701	MTA	O2'-C2'	2.81	1.49	1.43
3	A	701	MTA	C5-N7	-2.70	1.29	1.39
3	A	701	MTA	C8-N7	-2.57	1.30	1.34
4	A	702	85K	C18-C17	2.53	1.46	1.43
4	A	702	85K	C19-C18	2.37	1.54	1.51
3	A	701	MTA	C6-N6	2.28	1.42	1.34
3	A	701	MTA	O4'-C1'	2.09	1.44	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	85K	C-N-C1C	-6.68	119.22	129.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	85K	C1B-N14-N13	5.26	124.15	119.32
3	A	701	MTA	N3-C2-N1	-4.85	121.10	128.68
4	A	702	85K	C1E-C1F-CL	4.66	121.29	119.50
3	A	701	MTA	CS-S5'-C5'	4.54	109.65	101.30
4	A	702	85K	C12-C1C-N	-4.04	105.84	108.75
4	A	702	85K	O1-C1H-C1M	3.96	118.43	115.09
4	A	702	85K	C1D-C1C-N	-3.01	118.81	123.31
4	A	702	85K	C1C-C1D-C1E	-2.48	118.27	122.36
3	A	701	MTA	C3'-C2'-C1'	2.26	104.38	100.98

There are no chirality outliers.

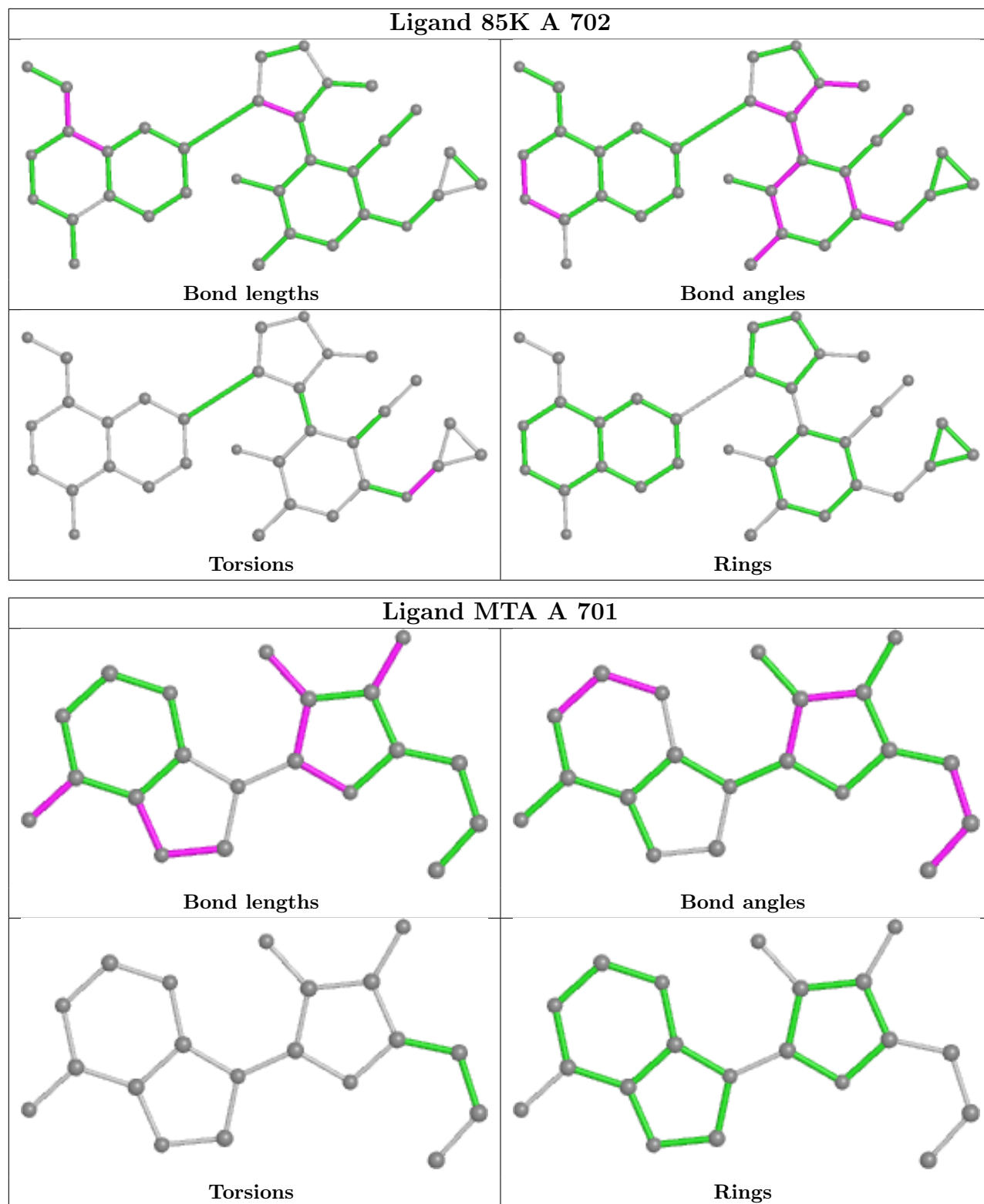
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	85K	C1K-C1I-O1-C1H

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 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 ⓘ

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	625/645 (96%)	-0.22	6 (0%) 82 80	34, 52, 100, 137	22 (3%)
2	B	302/350 (86%)	0.03	8 (2%) 56 50	48, 74, 108, 153	16 (5%)
All	All	927/995 (93%)	-0.14	14 (1%) 73 70	34, 61, 104, 153	38 (4%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	329	THR	5.1
1	A	299	LEU	3.4
1	A	272	HIS	3.1
2	B	114	LEU	2.9
1	A	295	ASN	2.9
2	B	21	PRO	2.7
1	A	240	LYS	2.4
2	B	41	ALA	2.4
2	B	24	PRO	2.3
1	A	239	ASN	2.2
2	B	266	HIS	2.1
1	A	243	PHE	2.0
2	B	19	LEU	2.0
2	B	60	LEU	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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

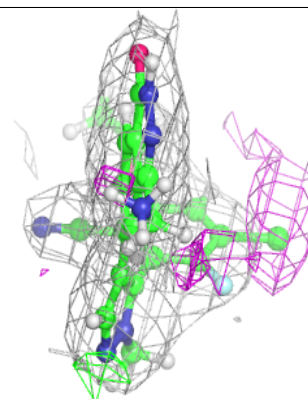
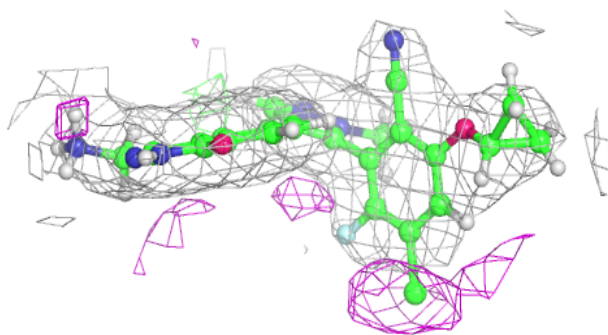
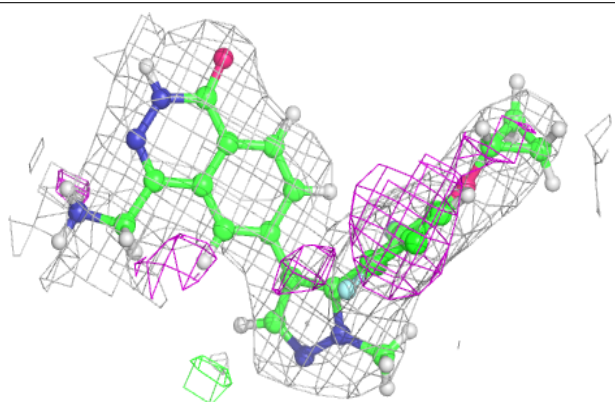
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

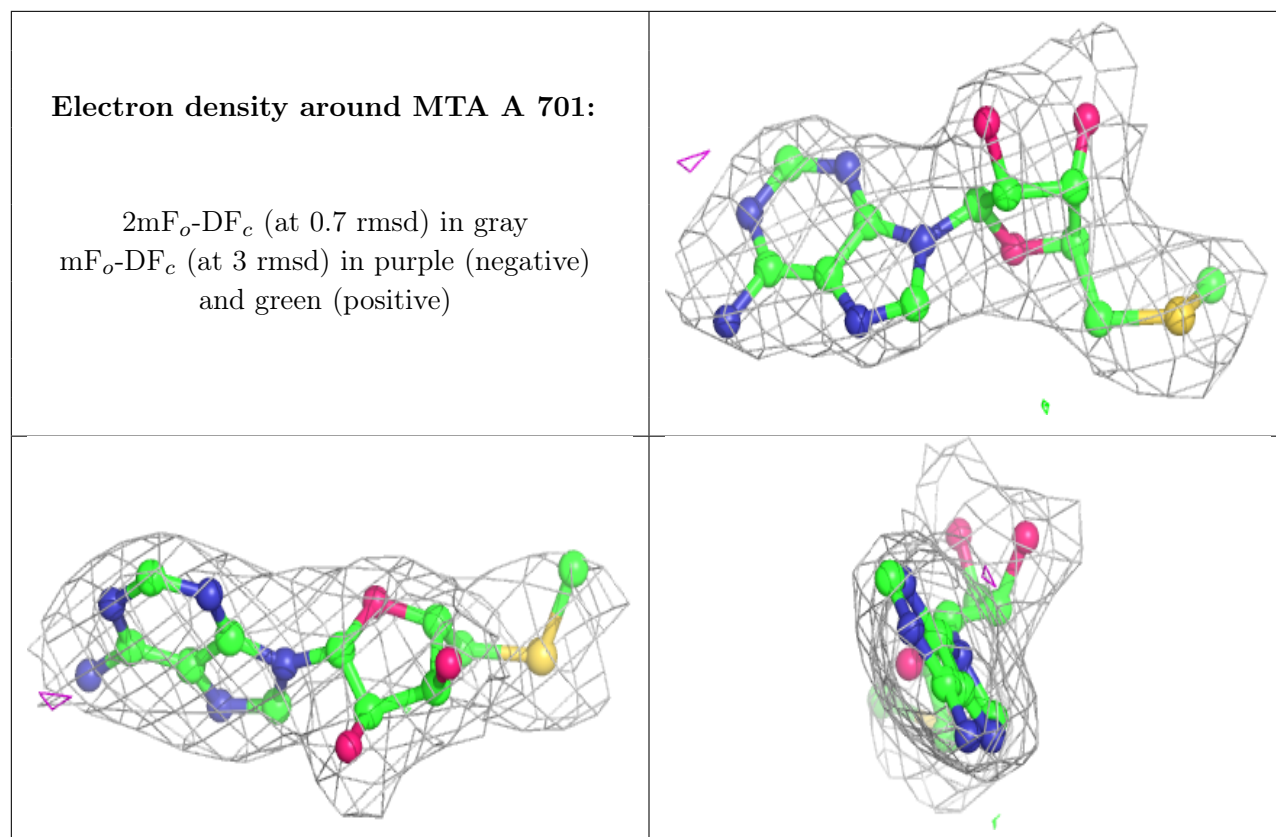
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	85K	A	702	33/33	0.93	0.17	39,52,66,100	0
3	MTA	A	701	20/20	0.98	0.14	40,41,45,46	0

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 85K A 702:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.