



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2022 – 05:21 pm BST

PDB ID : 7ZVL  
Title : HUMAN PRMT5:MEP50 Crystal Structure With MTA and Fragment Bound  
Authors : Ahmad, M.U.; Koelmel, W.; Arkhipova, V.; Lawson, J.D.; Smith, C.R.; Gunn, R.J.  
Deposited on : 2022-05-16  
Resolution : 2.39 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.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

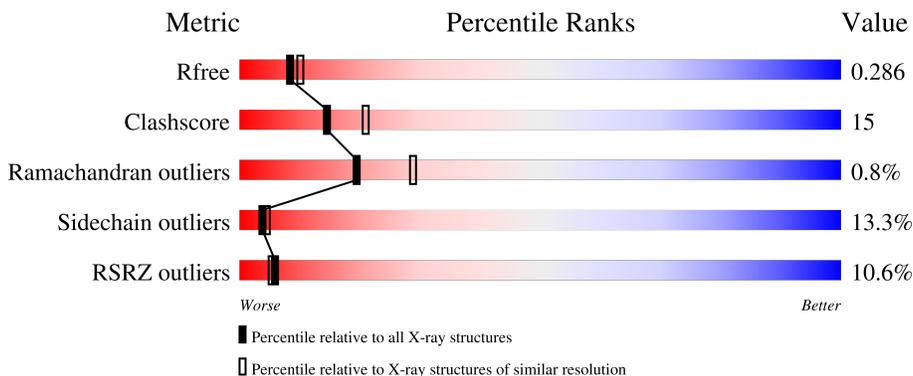
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	
2	B	350	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNL	A	702	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7594 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
			Total	C	N	O	S			
1	A	625	5068	3242	870	931	25	0	1	0

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
			Total	C	N	O	S			
2	B	310	2345	1471	401	458	15	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

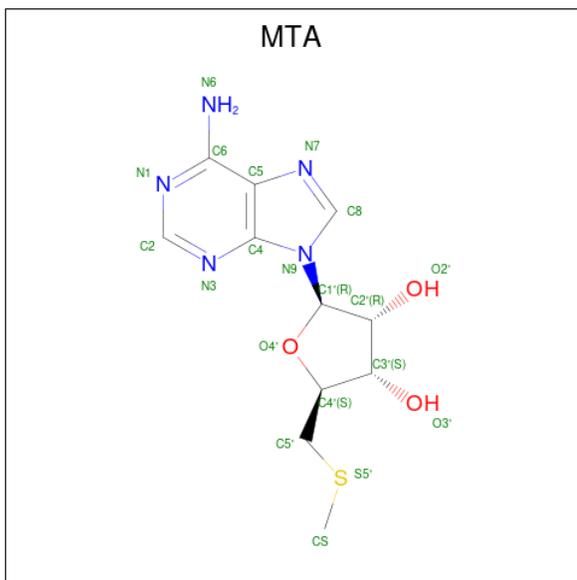
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag	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<sub>11</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C N		
4	A	1	13	10 3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

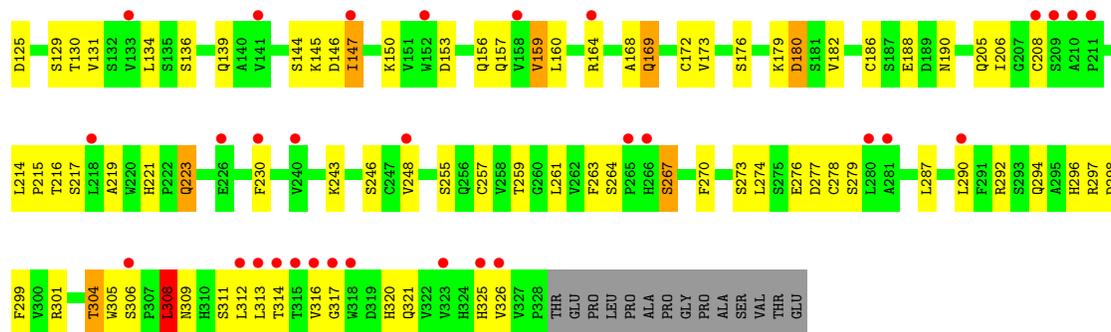
- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	111	Total O 111 111	0	0
7	B	24	Total O 24 24	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.58Å 138.39Å 178.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.37 – 2.39 109.37 – 2.39	Depositor EDS
% Data completeness (in resolution range)	43.8 (109.37-2.39) 43.8 (109.37-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.216 , 0.286 0.221 , 0.286	Depositor DCC
$R_{free}$ test set	1124 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 i

### 5.1 Standard geometry i

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

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	0.70	0/5210	0.89	2/7088 (0.0%)
2	B	0.73	0/2402	0.83	0/3283
All	All	0.71	0/7612	0.87	2/10371 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	PHE	CB-CA-C	7.06	124.51	110.40
1	A	604	ARG	NE-CZ-NH2	-5.43	117.58	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

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	5068	0	4960	146	0
2	B	2345	0	2260	83	0
3	A	20	0	15	1	0
4	A	13	0	0	5	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	111	0	0	4	0
7	B	24	0	0	3	0
All	All	7594	0	7251	225	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 15.

All (225) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:SER:HB2	1:A:216:HIS:HD2	1.48	0.79
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.19	0.78
1:A:219:ASP:O	1:A:222:LEU:HG	1.86	0.75
1:A:328:GLU:HG2	1:A:370:PRO:HG3	1.68	0.75
1:A:556:GLU:HG2	1:A:566:SER:HB2	1.68	0.74
2:B:66:ALA:HB1	2:B:72:PHE:HB2	1.70	0.74
2:B:58:LEU:HB2	2:B:77:VAL:HG12	1.68	0.73
1:A:214:SER:HB2	1:A:216:HIS:CD2	2.24	0.73
1:A:512:LEU:HG	1:A:546:THR:HG21	1.71	0.73
1:A:92:PRO:HG2	1:A:134:LEU:HD12	1.71	0.72
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.54	0.72
1:A:51:LYS:O	1:A:62:ARG:NH1	2.23	0.72
2:B:35:ARG:HA	2:B:304:THR:HG21	1.71	0.72
2:B:259:THR:HG21	2:B:301:ARG:NH2	2.05	0.71
1:A:629:THR:O	1:A:629:THR:HG23	1.93	0.68
1:A:327:PHE:C	1:A:327:PHE:HD2	1.95	0.68
2:B:36:TYR:H	2:B:304:THR:HG21	1.59	0.68
1:A:607:ASN:HB3	1:A:609:LYS:H	1.59	0.68
1:A:319:LEU:HD22	1:A:323:THR:HG21	1.76	0.67
2:B:105:LEU:HB3	2:B:119:PHE:HD2	1.59	0.67
2:B:313:LEU:HB3	2:B:325:HIS:HB2	1.78	0.66
2:B:312:LEU:HA	2:B:325:HIS:O	1.96	0.65
2:B:42:LEU:HD21	2:B:314:THR:HG21	1.79	0.65
1:A:360:VAL:HG13	1:A:430:ASP:H	1.61	0.64
2:B:147:ILE:HG23	2:B:168:ALA:O	1.98	0.64
2:B:130:THR:HG23	2:B:173:VAL:HG22	1.79	0.64
1:A:346:LEU:HD21	1:A:382:ALA:HB1	1.80	0.64
1:A:485:ARG:HG3	1:A:498:PHE:HZ	1.62	0.63
1:A:33:VAL:HG23	1:A:38:PHE:HB2	1.80	0.63
1:A:276:GLU:HG2	1:A:278:CYS:SG	2.39	0.62
2:B:276:GLU:O	7:B:501:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HD22	1:A:576:MET:SD	2.40	0.62
1:A:386:ILE:O	1:A:412:GLN:NE2	2.33	0.61
1:A:324:TYR:CB	1:A:368:ARG:HD2	2.30	0.61
1:A:327:PHE:C	1:A:327:PHE:CD2	2.74	0.61
1:A:185:THR:HG23	1:A:221:TRP:HZ2	1.66	0.61
1:A:553:GLY:HA3	1:A:582:ILE:HG22	1.83	0.61
1:A:629:THR:O	1:A:629:THR:CG2	2.47	0.60
1:A:157:LEU:HD22	1:A:213:PRO:HG3	1.83	0.60
2:B:186:CYS:HB2	2:B:215:PRO:HB2	1.85	0.59
1:A:434:SER:HB2	1:A:436:LEU:HG	1.84	0.59
1:A:134:LEU:HD23	1:A:192:PHE:CE1	2.37	0.59
1:A:193:ARG:NH1	1:A:224:GLU:OE2	2.36	0.59
2:B:147:ILE:HG12	2:B:168:ALA:C	2.23	0.58
1:A:13:ARG:HG2	1:A:289:GLN:HE21	1.68	0.58
2:B:172[A]:CYS:HB3	2:B:186:CYS:SG	2.43	0.57
1:A:444:GLU:O	1:A:445:LEU:HB2	2.04	0.57
1:A:52:ARG:NH2	1:A:109:GLN:OE1	2.29	0.57
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.86	0.57
1:A:300:PHE:CD2	1:A:577:PHE:HB2	2.40	0.57
1:A:358:VAL:HB	1:A:385:ARG:HB2	1.87	0.57
2:B:37:ARG:HB3	2:B:39:ASP:OD1	2.04	0.56
1:A:627:ASN:N	1:A:628:PRO:CD	2.69	0.56
1:A:53:GLU:HA	1:A:102:ASN:HD21	1.71	0.55
1:A:377:ARG:O	1:A:380:LYS:HG3	2.05	0.55
2:B:109:ASP:HB2	2:B:114:LEU:H	1.69	0.55
2:B:306:SER:HB3	2:B:312:LEU:HB3	1.88	0.55
1:A:340:ALA:HA	1:A:563:ILE:HD13	1.88	0.55
2:B:19:LEU:HD22	2:B:25:ALA:HA	1.89	0.55
2:B:264:SER:HB3	2:B:270:PHE:HB2	1.89	0.55
1:A:51:LYS:HG3	1:A:89:TRP:CE3	2.42	0.54
1:A:554:TYR:HB3	1:A:567:ILE:HG13	1.89	0.54
1:A:488:ARG:HD2	1:A:494:PRO:HA	1.89	0.54
1:A:96:VAL:HB	1:A:99:ILE:HD12	1.89	0.54
1:A:82:ILE:O	1:A:120:PRO:HD2	2.08	0.54
1:A:405:GLN:NE2	1:A:413:VAL:O	2.41	0.54
2:B:35:ARG:HA	2:B:304:THR:CG2	2.37	0.54
1:A:65:PRO:O	2:B:50:SER:OG	2.19	0.54
1:A:324:TYR:HB2	1:A:368:ARG:HD2	1.89	0.54
1:A:90:ILE:HG23	1:A:103:SER:HB3	1.89	0.53
1:A:106:ALA:O	1:A:110:GLU:HG3	2.07	0.53
1:A:487:CYS:O	1:A:492:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLY:N	1:A:370:PRO:HD2	2.24	0.53
2:B:188:GLU:HA	2:B:214:LEU:HD13	1.90	0.53
1:A:358:VAL:HA	1:A:385:ARG:O	2.08	0.53
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.91	0.53
1:A:170:ASN:ND2	2:B:205:GLN:O	2.42	0.53
2:B:87:THR:CG2	2:B:95:LEU:HB3	2.39	0.52
2:B:173:VAL:HG23	2:B:173:VAL:O	2.10	0.52
2:B:58:LEU:CD2	2:B:86:LEU:HD21	2.40	0.52
1:A:544:VAL:HG23	1:A:545:ASN:O	2.10	0.52
1:A:222:LEU:HD12	1:A:510:HIS:CD2	2.45	0.51
2:B:42:LEU:HB3	2:B:61:PHE:HB2	1.91	0.51
1:A:444:GLU:OE1	4:A:702:UNL:N1	2.44	0.51
1:A:396:ASN:O	1:A:399:VAL:HB	2.10	0.51
2:B:221:HIS:CE1	2:B:223:GLN:HB2	2.46	0.51
2:B:109:ASP:HB3	2:B:112:GLU:N	2.25	0.51
2:B:221:HIS:HE1	2:B:223:GLN:HB2	1.76	0.51
1:A:621:VAL:HG21	7:A:901:HOH:O	2.11	0.50
2:B:304:THR:O	2:B:313:LEU:HD12	2.09	0.50
1:A:392:GLU:OE2	1:A:393:LYS:N	2.44	0.50
2:B:96:VAL:HB	2:B:104:GLU:HG2	1.94	0.50
1:A:444:GLU:OE2	4:A:702:UNL:N2	2.45	0.49
1:A:276:GLU:CG	1:A:278:CYS:SG	3.00	0.49
1:A:342:TYR:CD1	1:A:381:GLN:HB3	2.47	0.49
1:A:18:ARG:NH1	1:A:19:ASP:O	2.46	0.49
2:B:150:LYS:HB3	2:B:159:VAL:CG1	2.43	0.49
1:A:362:MET:HG2	1:A:389:TYR:HB2	1.94	0.49
1:A:525:ASN:OD1	1:A:530:ILE:HG23	2.12	0.49
2:B:217:SER:O	2:B:230:PHE:HA	2.13	0.49
1:A:45:VAL:HG23	1:A:46:PHE:CD1	2.42	0.49
1:A:371:LEU:HD22	1:A:435:GLU:HG2	1.95	0.49
1:A:525:ASN:HD21	1:A:527:ASP:HB2	1.76	0.49
1:A:328:GLU:OE2	1:A:368:ARG:HB2	2.14	0.48
1:A:358:VAL:HB	1:A:385:ARG:CB	2.43	0.48
2:B:306:SER:CB	2:B:312:LEU:HB3	2.44	0.48
1:A:294:PRO:HB2	1:A:299:LEU:HD13	1.95	0.48
2:B:313:LEU:O	2:B:325:HIS:N	2.47	0.48
1:A:208:ILE:HD12	1:A:231:LEU:CD2	2.44	0.48
2:B:30:GLN:HB2	2:B:47:SER:O	2.13	0.48
1:A:430:ASP:OD1	1:A:458:LYS:NZ	2.40	0.47
2:B:172[B]:CYS:SG	2:B:216:THR:O	2.71	0.47
1:A:455:HIS:CE1	1:A:456:PHE:HD2	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:PRO:HD2	2:B:59:TRP:CH2	2.49	0.47
2:B:106:TRP:HA	2:B:117:SER:HA	1.97	0.47
2:B:306:SER:HB3	2:B:309:ASN:O	2.15	0.47
1:A:346:LEU:CD2	1:A:382:ALA:HB1	2.44	0.47
1:A:348:ARG:NH1	1:A:460:ASP:O	2.39	0.47
1:A:418:SER:OG	1:A:423:TRP:HB2	2.15	0.46
1:A:525:ASN:ND2	1:A:527:ASP:HB2	2.30	0.46
2:B:145:LYS:HA	2:B:169:GLN:HB3	1.97	0.46
1:A:62:ARG:NH2	2:B:298:ASP:OD1	2.48	0.46
1:A:53:GLU:OE2	1:A:56:GLN:N	2.43	0.46
1:A:297:TYR:HB2	7:A:865:HOH:O	2.15	0.46
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.49	0.46
2:B:153:ASP:O	2:B:157:GLN:N	2.48	0.46
1:A:333:LYS:HZ2	4:A:702:UNL:C9	2.29	0.46
2:B:306:SER:HB2	2:B:312:LEU:HD22	1.98	0.46
2:B:134:LEU:HD12	2:B:139:GLN:HB2	1.98	0.45
1:A:238:THR:HG22	1:A:242:GLY:HA2	1.98	0.45
1:A:290:ASN:N	1:A:290:ASN:HD22	2.15	0.45
1:A:469:THR:HA	1:A:519:PHE:O	2.16	0.45
1:A:485:ARG:HG3	1:A:498:PHE:CZ	2.45	0.45
1:A:560:TYR:O	1:A:563:ILE:HD12	2.16	0.45
1:A:205:ALA:HA	1:A:228:ALA:HB3	1.99	0.45
1:A:314:PRO:HB3	1:A:319:LEU:HD11	1.98	0.45
1:A:232:PRO:HA	1:A:267:THR:O	2.16	0.45
1:A:610:LYS:HE3	1:A:634:THR:HG21	1.99	0.45
2:B:255:SER:OG	2:B:277:ASP:HB2	2.16	0.45
1:A:405:GLN:HG3	1:A:406:PHE:N	2.32	0.45
1:A:101:ARG:O	1:A:104:GLU:HB2	2.17	0.44
2:B:20:PRO:HG2	2:B:74:SER:C	2.37	0.44
2:B:31:LEU:HA	2:B:46:ALA:CB	2.47	0.44
2:B:104:GLU:HA	2:B:119:PHE:O	2.17	0.44
2:B:124:HIS:CD2	2:B:144:SER:HB2	2.52	0.44
1:A:134:LEU:HD23	1:A:192:PHE:HE1	1.81	0.44
1:A:220:ARG:CZ	1:A:545:ASN:O	2.66	0.44
2:B:176:SER:HB3	2:B:182:VAL:HG12	1.98	0.44
1:A:327:PHE:HD2	1:A:328:GLU:N	2.15	0.44
1:A:457:LEU:HG	1:A:461:GLY:HA3	1.99	0.44
1:A:531:ASP:OD1	1:A:533:ASN:HB2	2.17	0.44
2:B:105:LEU:HB3	2:B:119:PHE:CD2	2.46	0.44
2:B:305:TRP:CD2	2:B:313:LEU:HD13	2.53	0.44
2:B:153:ASP:CG	2:B:156:GLN:HB2	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:SER:HA	1:A:264:PHE:O	2.18	0.44
1:A:185:THR:O	1:A:188:TRP:HB2	2.18	0.43
1:A:567:ILE:HG21	1:A:579:TRP:HB2	2.00	0.43
2:B:105:LEU:O	2:B:118:LYS:N	2.50	0.43
1:A:239:ASN:OD1	1:A:243:PHE:N	2.40	0.43
1:A:246:LEU:HB2	1:A:283:TYR:HE2	1.83	0.43
1:A:113:PHE:CE2	1:A:117:LEU:HD11	2.54	0.43
1:A:274:GLU:C	1:A:275:LYS:HG2	2.37	0.43
1:A:53:GLU:HA	1:A:102:ASN:ND2	2.34	0.43
2:B:219:ALA:HB2	2:B:261:LEU:O	2.19	0.43
1:A:419:ASP:OD1	1:A:421:ARG:HD3	2.19	0.43
2:B:83:VAL:HG23	2:B:83:VAL:O	2.18	0.43
2:B:146:ASP:O	2:B:147:ILE:HB	2.19	0.43
1:A:409:TRP:HB3	1:A:413:VAL:CG2	2.49	0.43
2:B:31:LEU:HD21	2:B:320:HIS:CE1	2.53	0.43
2:B:134:LEU:HD13	2:B:180:ASP:O	2.17	0.43
1:A:360:VAL:HG13	1:A:430:ASP:N	2.32	0.43
1:A:60:LYS:HE2	1:A:60:LYS:HB2	1.80	0.43
1:A:281:LEU:HA	1:A:284:LEU:HD12	2.00	0.43
2:B:278:CYS:SG	2:B:298:ASP:O	2.76	0.43
2:B:299:PHE:O	2:B:317:GLY:HA2	2.19	0.43
2:B:109:ASP:HB3	2:B:112:GLU:H	1.84	0.42
1:A:47:HIS:ND1	2:B:49:LEU:HD22	2.33	0.42
1:A:215:ASN:HD22	1:A:215:ASN:C	2.23	0.42
1:A:238:THR:HG23	1:A:272:HIS:CD2	2.53	0.42
1:A:405:GLN:HA	1:A:409:TRP:HB2	2.00	0.42
1:A:349:VAL:HG12	1:A:357:ASN:HB3	2.01	0.42
1:A:190:HIS:ND1	1:A:193:ARG:NH2	2.66	0.42
1:A:435:GLU:O	4:A:702:UNL:C10	2.67	0.42
2:B:27:MET:HG2	2:B:59:TRP:NE1	2.34	0.42
1:A:468:TYR:CE1	1:A:521:PHE:HB2	2.53	0.42
1:A:74:SER:OG	1:A:76:ARG:HB3	2.19	0.42
2:B:20:PRO:CB	2:B:21:PRO:HD2	2.50	0.42
2:B:188:GLU:C	2:B:190:ASN:H	2.23	0.42
2:B:34:ALA:HB2	2:B:316:VAL:HG13	2.02	0.42
1:A:353:GLU:HA	1:A:356:THR:HG22	2.02	0.42
2:B:87:THR:HG22	2:B:95:LEU:HB3	2.02	0.42
1:A:90:ILE:HD11	1:A:110:GLU:OE1	2.20	0.41
2:B:104:GLU:HB3	2:B:120:CYS:SG	2.60	0.41
1:A:26:ILE:HG22	7:B:509:HOH:O	2.19	0.41
1:A:497:GLN:H	1:A:497:GLN:CD	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:LEU:HD21	2:B:94:ILE:HG23	2.02	0.41
2:B:308:LEU:HD13	2:B:308:LEU:N	2.35	0.41
2:B:136:SER:N	2:B:180:ASP:OD1	2.41	0.41
1:A:60:LYS:HG3	1:A:61:ASN:N	2.35	0.41
1:A:369:GLY:N	1:A:370:PRO:CD	2.83	0.41
1:A:317:ASP:O	1:A:393:LYS:NZ	2.50	0.41
1:A:302:LYS:O	1:A:305:GLU:OE1	2.39	0.41
1:A:391:VAL:HG22	1:A:416:VAL:HB	2.02	0.41
1:A:553:GLY:CA	1:A:582:ILE:HG22	2.47	0.41
2:B:105:LEU:N	2:B:119:PHE:O	2.42	0.41
1:A:29:THR:O	1:A:33:VAL:HG13	2.20	0.41
1:A:333:LYS:NZ	4:A:702:UNL:C9	2.84	0.41
1:A:443:ASN:HB2	7:A:844:HOH:O	2.21	0.41
2:B:263:PHE:N	7:B:502:HOH:O	2.34	0.41
1:A:542:VAL:HG21	1:A:598:ILE:CD1	2.51	0.41
2:B:109:ASP:HB3	2:B:112:GLU:CA	2.50	0.41
1:A:346:LEU:HD21	1:A:382:ALA:CB	2.50	0.41
2:B:29:ARG:HD2	2:B:320:HIS:HB2	2.03	0.41
1:A:631:ARG:HG3	1:A:632:SER:N	2.36	0.41
2:B:34:ALA:HB2	2:B:316:VAL:CG1	2.52	0.41
2:B:92:ARG:HD3	2:B:92:ARG:HA	1.56	0.41
1:A:69:SER:OG	1:A:71:LEU:HG	2.22	0.40
1:A:216:HIS:O	1:A:219:ASP:HB2	2.20	0.40
1:A:391:VAL:HA	1:A:416:VAL:O	2.21	0.40
1:A:327:PHE:CZ	3:A:701:MTA:CS	3.04	0.40
1:A:419:ASP:HB3	1:A:422:GLU:HG2	2.03	0.40
1:A:62:ARG:HA	1:A:63:PRO:HD3	1.91	0.40
1:A:343:LYS:HD2	1:A:563:ILE:HD11	2.04	0.40
1:A:371:LEU:HB2	7:A:819:HOH:O	2.20	0.40
2:B:296:HIS:HE1	2:B:321:GLN:O	2.05	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	624/645 (97%)	585 (94%)	37 (6%)	2 (0%)	41	55
2	B	309/350 (88%)	281 (91%)	23 (7%)	5 (2%)	9	13
All	All	933/995 (94%)	866 (93%)	60 (6%)	7 (1%)	19	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
2	B	267	SER
1	A	261	GLU
1	A	210	ALA
2	B	25	ALA
2	B	208	CYS
2	B	308	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/570 (98%)	498 (89%)	61 (11%)	6	8
2	B	264/298 (89%)	216 (82%)	48 (18%)	1	2
All	All	823/868 (95%)	714 (87%)	109 (13%)	4	4

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	35	LYS
1	A	52	ARG
1	A	60	LYS
1	A	62	ARG
1	A	74	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	91	ARG
1	A	95	LYS
1	A	136	ARG
1	A	146	HIS
1	A	148	SER
1	A	163	LEU
1	A	169	GLU
1	A	170	ASN
1	A	174	THR
1	A	184	LYS
1	A	185	THR
1	A	193	ARG
1	A	199	SER
1	A	214	SER
1	A	215	ASN
1	A	220	ARG
1	A	240	LYS
1	A	245	VAL
1	A	247	SER
1	A	256	ARG
1	A	259	LYS
1	A	274	GLU
1	A	275	LYS
1	A	281	LEU
1	A	285	GLU
1	A	291	ARG
1	A	299	LEU
1	A	302	LYS
1	A	310	SER
1	A	327	PHE
1	A	335	SER
1	A	349	VAL
1	A	355	ASP
1	A	358	VAL
1	A	360	VAL
1	A	361	LEU
1	A	371	LEU
1	A	375	SER
1	A	387	LYS
1	A	393	LYS
1	A	405	GLN
1	A	458	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	463	SER
1	A	491	ASP
1	A	492	ARG
1	A	497	GLN
1	A	504	VAL
1	A	505	ARG
1	A	512	LEU
1	A	526	ARG
1	A	529	MET
1	A	543	GLU
1	A	559	LEU
1	A	608	SER
1	A	629	THR
2	B	19	LEU
2	B	22	ASN
2	B	36	TYR
2	B	42	LEU
2	B	50	SER
2	B	52	ARG
2	B	60	LEU
2	B	72	PHE
2	B	73	CYS
2	B	86	LEU
2	B	91	GLU
2	B	92	ARG
2	B	107	GLU
2	B	111	ASN
2	B	113	THR
2	B	114	LEU
2	B	116	VAL
2	B	118	LYS
2	B	119	PHE
2	B	121	LYS
2	B	125	ASP
2	B	129	SER
2	B	131	VAL
2	B	159	VAL
2	B	160	LEU
2	B	164	ARG
2	B	169	GLN
2	B	179	LYS
2	B	180	ASP

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Mol	Chain	Res	Type
2	B	206	ILE
2	B	223	GLN
2	B	243	LYS
2	B	246	SER
2	B	248	VAL
2	B	257	CYS
2	B	267	SER
2	B	273	SER
2	B	274	LEU
2	B	279	SER
2	B	287	LEU
2	B	290	LEU
2	B	292	ARG
2	B	294	GLN
2	B	297	ARG
2	B	304	THR
2	B	308	LEU
2	B	311	SER
2	B	326	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	216	HIS
1	A	251	GLN
1	A	282	GLN
1	A	289	GLN
1	A	290	ASN
1	A	359	GLN
1	A	455	HIS
1	A	510	HIS
1	A	525	ASN
1	A	545	ASN
2	B	224	GLN
2	B	310	HIS
2	B	321	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is unknown and 1 is monoatomic - leaving 3 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
3	MTA	A	701	-	19,22,22	1.27	2 (10%)	19,32,32	1.85	4 (21%)
5	GOL	B	401	-	5,5,5	0.12	0	5,5,5	0.38	0
5	GOL	A	703	-	5,5,5	0.07	0	5,5,5	0.17	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
3	MTA	A	701	-	-	0/3/23/23	0/3/3/3
5	GOL	B	401	-	-	2/4/4/4	-
5	GOL	A	703	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	MTA	C2-N3	2.83	1.36	1.32
3	A	701	MTA	C5-N7	-2.66	1.30	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	MTA	CS-S5'-C5'	-4.94	92.21	101.30
3	A	701	MTA	C4-C5-N7	-3.48	105.77	109.40
3	A	701	MTA	N3-C2-N1	-3.32	123.49	128.68
3	A	701	MTA	O4'-C1'-C2'	-2.54	103.22	106.93

There are no chirality outliers.

All (4) torsion outliers are listed below:

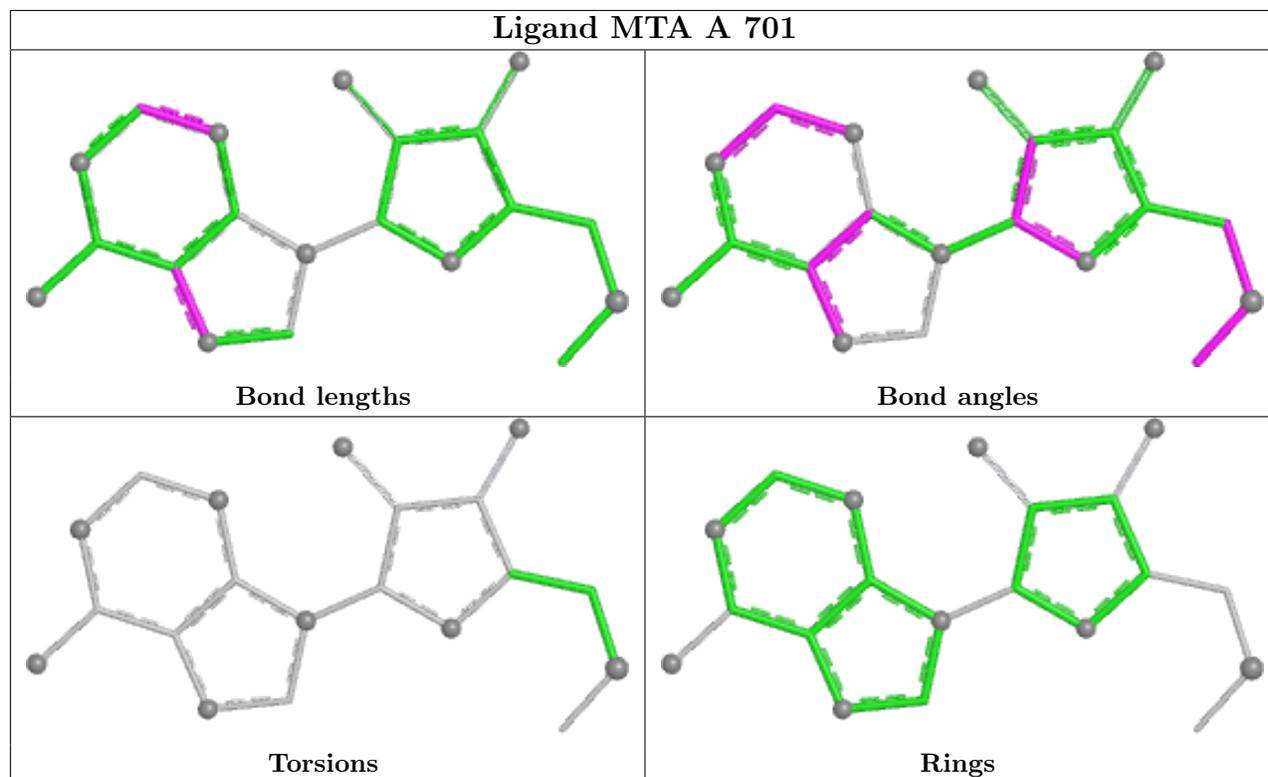
Mol	Chain	Res	Type	Atoms
5	A	703	GOL	C1-C2-C3-O3
5	A	703	GOL	O2-C2-C3-O3
5	B	401	GOL	O1-C1-C2-C3
5	B	401	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	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, 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%)	0.40	25 (4%) 38 37	21, 50, 97, 134	0
2	B	310/350 (88%)	1.54	74 (23%) 0 0	48, 87, 156, 224	0
All	All	935/995 (93%)	0.78	99 (10%) 6 5	21, 63, 119, 224	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	23	ALA	14.2
2	B	24	PRO	13.4
2	B	22	ASN	13.3
2	B	26	CYS	12.4
2	B	20	PRO	11.7
2	B	21	PRO	11.6
2	B	25	ALA	9.2
2	B	312	LEU	9.2
1	A	376	LEU	7.0
2	B	74	SER	6.9
2	B	59	TRP	6.8
2	B	73	CYS	6.4
2	B	69	ASN	5.9
2	B	66	ALA	5.6
2	B	64	PRO	5.6
2	B	209	SER	5.3
2	B	106	TRP	5.0
2	B	41	ALA	5.0
2	B	61	PHE	5.0
2	B	27	MET	4.7
2	B	72	PHE	4.7
2	B	67	ALA	4.7
2	B	280	LEU	4.6
2	B	313	LEU	4.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	107	GLU	4.4
1	A	431	ILE	4.2
1	A	409	TRP	4.1
2	B	19	LEU	4.1
2	B	152	TRP	4.1
1	A	341	ILE	3.8
2	B	50	SER	3.7
1	A	243	PHE	3.5
1	A	327	PHE	3.5
2	B	103	VAL	3.5
2	B	315	THR	3.4
2	B	208	CYS	3.4
2	B	87	THR	3.4
2	B	290	LEU	3.4
2	B	317	GLY	3.3
2	B	266	HIS	3.3
2	B	33	ALA	3.3
2	B	31	LEU	3.3
2	B	230	PHE	3.2
2	B	34	ALA	3.2
2	B	36	TYR	3.2
2	B	119	PHE	3.1
2	B	326	VAL	3.1
2	B	210	ALA	3.0
1	A	389	TYR	3.0
2	B	114	LEU	3.0
2	B	306	SER	3.0
2	B	44	LEU	2.9
1	A	387	LYS	2.9
2	B	318	TRP	2.9
2	B	63	ASP	2.9
1	A	406	PHE	2.9
1	A	358	VAL	2.9
2	B	43	LEU	2.8
2	B	314	THR	2.8
2	B	211	PRO	2.8
2	B	40	GLY	2.8
2	B	141	VAL	2.8
2	B	218	LEU	2.8
1	A	374	ALA	2.7
1	A	255	PHE	2.7
2	B	133	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	462	VAL	2.7
2	B	86	LEU	2.7
2	B	60	LEU	2.6
2	B	281	ALA	2.5
2	B	35	ARG	2.4
2	B	265	PRO	2.4
2	B	113	THR	2.4
1	A	361	LEU	2.4
1	A	146	HIS	2.3
2	B	164	ARG	2.3
2	B	75	ALA	2.3
2	B	56	GLY	2.3
2	B	325	HIS	2.3
2	B	323	VAL	2.3
2	B	90	GLY	2.2
1	A	529	MET	2.2
2	B	70	GLU	2.2
2	B	240	VAL	2.2
1	A	577	PHE	2.2
1	A	339	GLN	2.2
2	B	248	VAL	2.2
1	A	342	TYR	2.1
2	B	158	VAL	2.1
2	B	49	LEU	2.1
1	A	383	ASP	2.1
1	A	23	VAL	2.1
2	B	316	VAL	2.1
1	A	432	ILE	2.1
1	A	271	HIS	2.1
2	B	226	GLU	2.1
1	A	433	VAL	2.1
2	B	147	ILE	2.0
1	A	98	LYS	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](#)

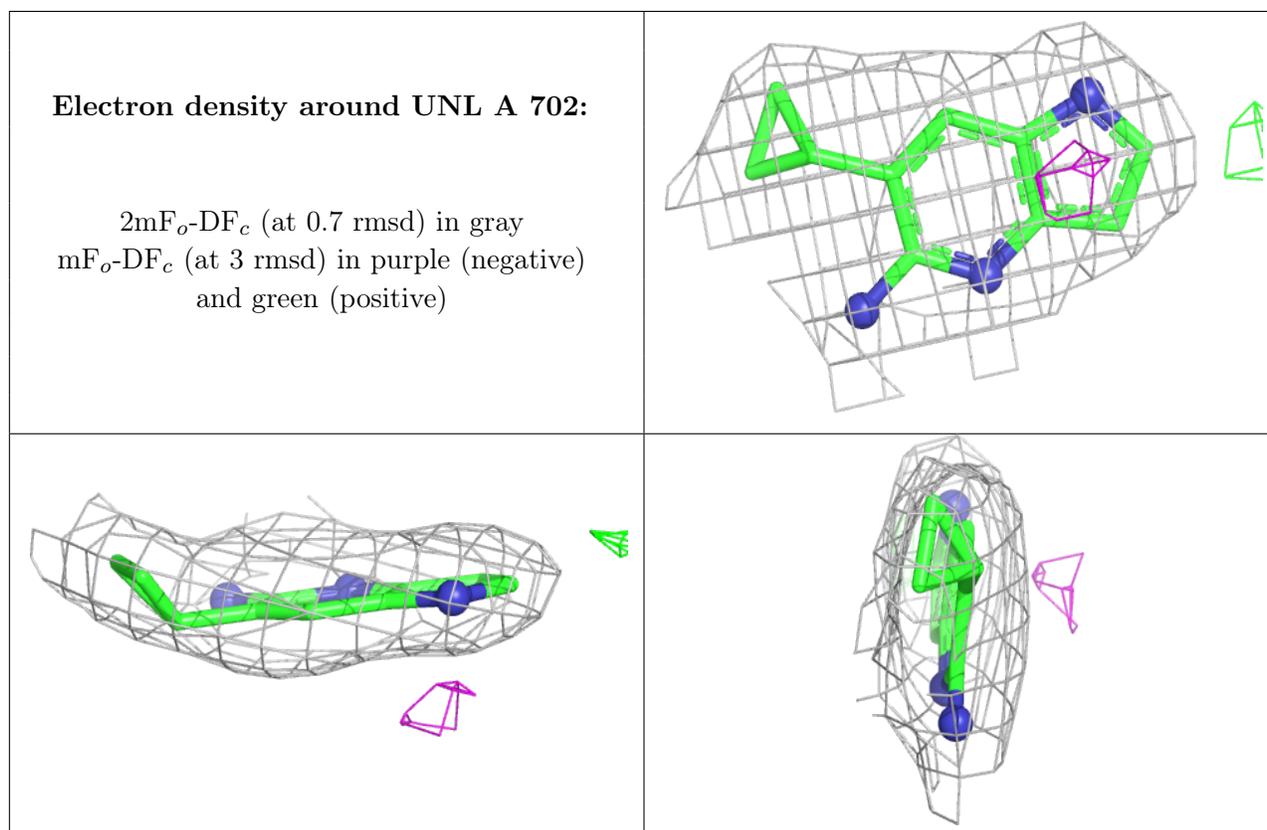
There are no monosaccharides in this entry.

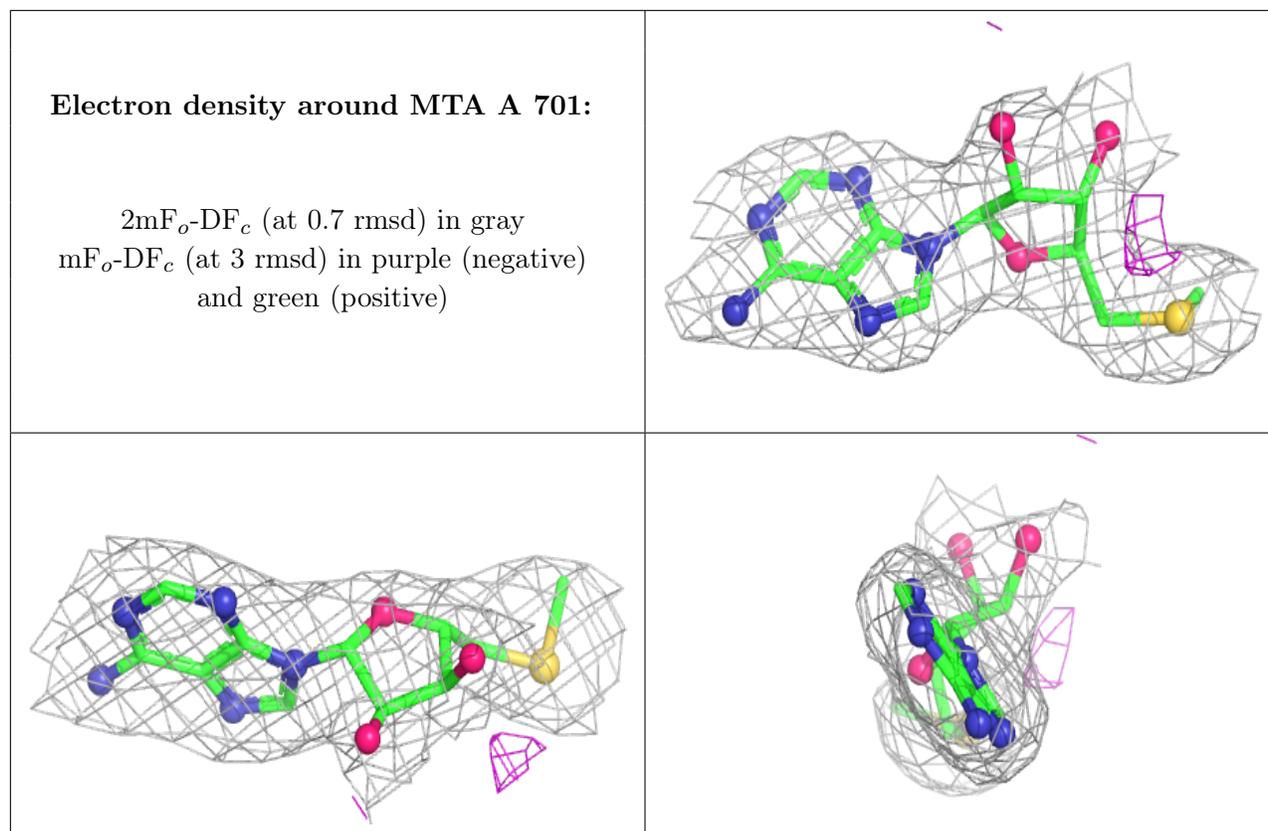
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	GOL	A	703	6/6	0.89	0.23	63,65,70,76	0
5	GOL	B	401	6/6	0.92	0.16	66,70,72,74	0
4	UNL	A	702	13/-	0.94	0.16	45,49,51,51	0
3	MTA	A	701	20/20	0.96	0.15	34,35,37,37	0
6	CL	A	704	1/1	0.97	0.06	38,38,38,38	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.