



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:46 AM UTC

PDB ID : 7ZVU / pdb_00007zvu
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 : 2022-05-17
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

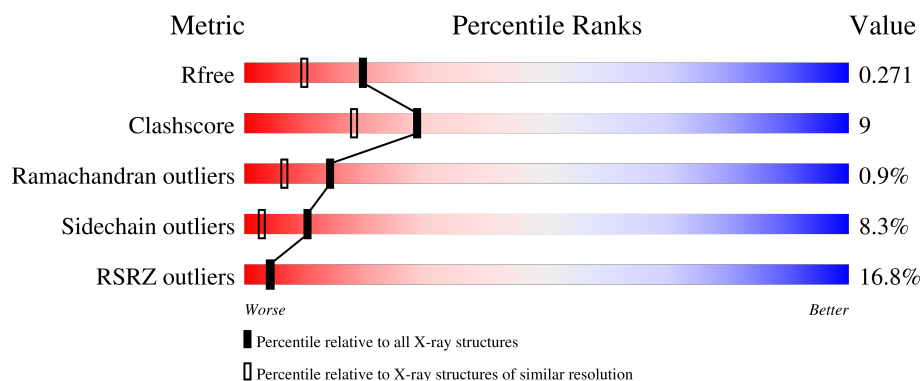
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	645	
2	B	350	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7793 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	5083	3252	872	934	25	0	3	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:

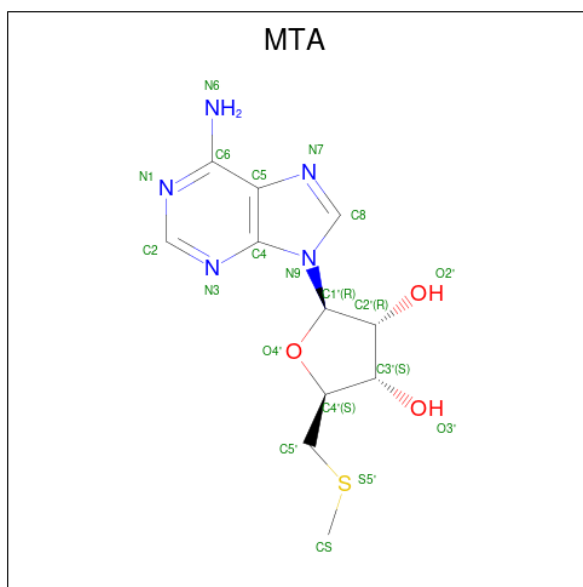
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag	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 (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$) (labeled as "Ligand of Interest" by depositor).



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

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			20	14	6		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

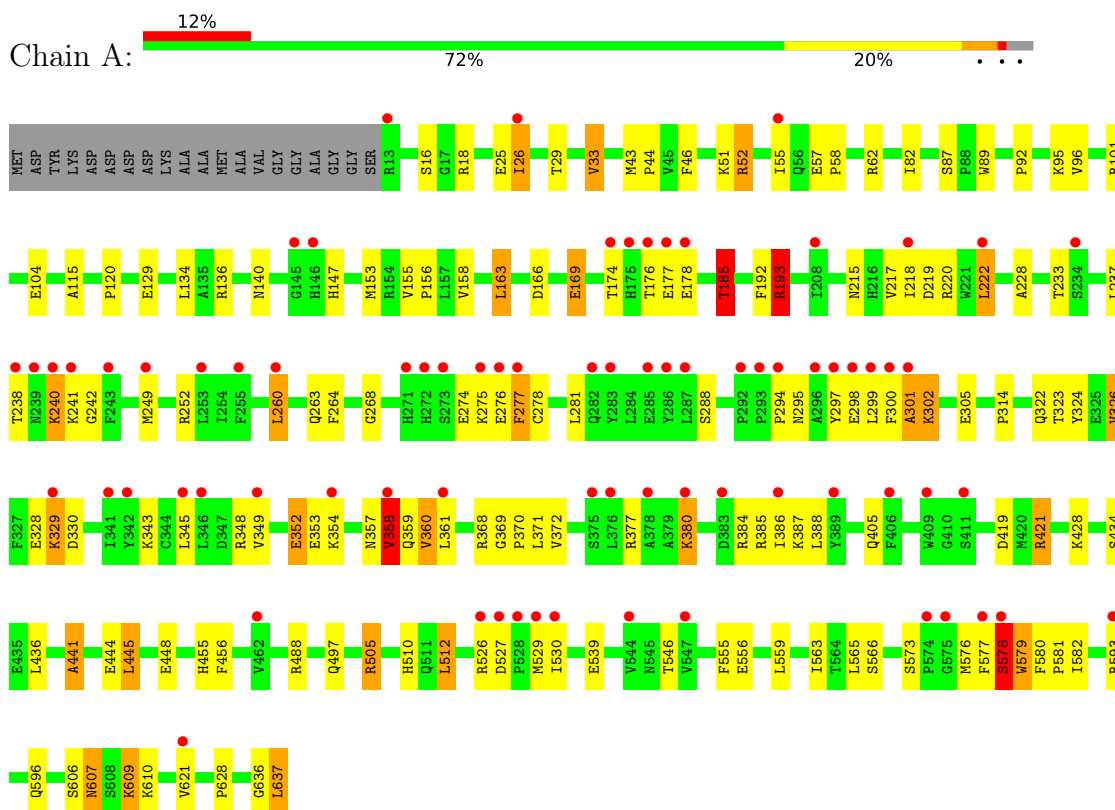
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	256	Total	O	0	0
			256	256		
6	B	57	Total	O	0	0
			57	57		

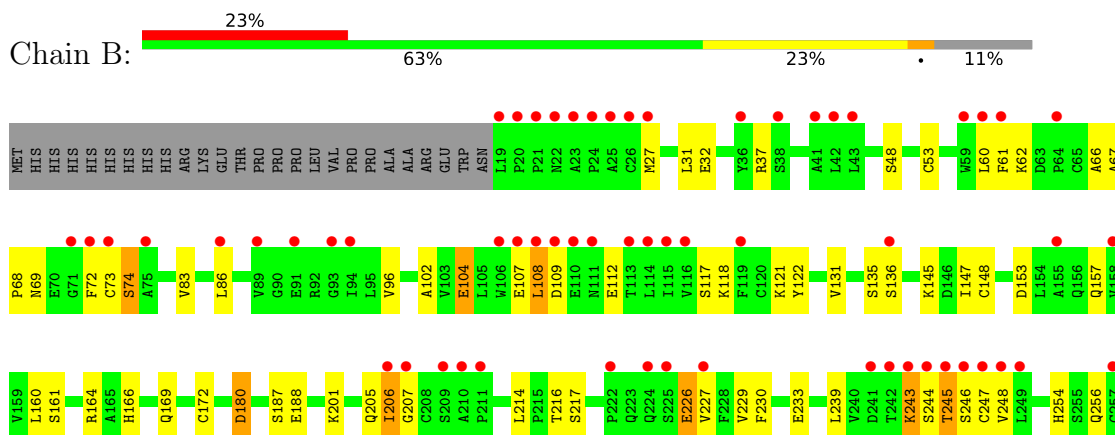
3 Residue-property plots

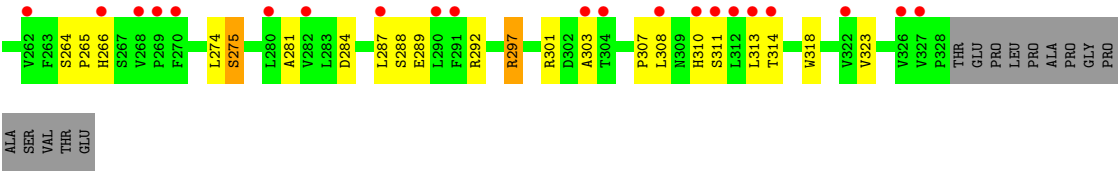
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 2: Methylosome protein 50





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	105.15Å 139.16Å 178.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.75 – 1.95 109.75 – 1.95	Depositor EDS
% Data completeness (in resolution range)	62.2 (109.75-1.95) 62.6 (109.75-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.237 , 0.266 0.242 , 0.271	Depositor DCC
R_{free} test set	3096 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7793	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MTA, 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	1.19	8/5228 (0.2%)	1.46	32/7111 (0.5%)
2	B	1.28	3/2402 (0.1%)	1.35	2/3283 (0.1%)
All	All	1.22	11/7630 (0.1%)	1.42	34/10394 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	ASP	C-O	5.94	1.30	1.23
1	A	488	ARG	C-O	-5.91	1.16	1.23
1	A	314	PRO	C-O	-5.46	1.16	1.24
1	A	581	PRO	C-O	-5.43	1.16	1.23
2	B	131	VAL	C-O	5.28	1.29	1.23
2	B	205	GLN	C-O	-5.19	1.17	1.24
1	A	358	VAL	N-CA	5.15	1.52	1.46
1	A	222	LEU	C-O	5.05	1.29	1.24
1	A	129	GLU	C-O	-5.03	1.18	1.24
2	B	275	SER	C-O	5.01	1.30	1.23
1	A	115	ALA	C-O	-5.01	1.18	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ASP	CA-CB-CG	9.48	122.08	112.60
1	A	607	ASN	CB-CA-C	-9.33	92.38	111.22
1	A	576	MET	CA-C-N	9.19	132.59	120.28
1	A	576	MET	C-N-CA	9.19	132.59	120.28
1	A	268	GLY	CA-C-O	-7.04	116.96	122.52
1	A	636	GLY	CA-C-O	-6.81	115.38	121.64
1	A	215	ASN	CB-CA-C	-6.65	99.75	110.79
1	A	539	GLU	CB-CG-CD	6.62	123.85	112.60
1	A	578	SER	CA-C-N	-6.00	110.08	121.54
1	A	578	SER	C-N-CA	-6.00	110.08	121.54
1	A	578	SER	N-CA-C	-5.81	98.42	110.80
1	A	215	ASN	N-CA-CB	5.76	118.59	110.12
2	B	226	GLU	CB-CG-CD	-5.76	102.81	112.60
1	A	140	ASN	CA-CB-CG	-5.67	106.92	112.60
1	A	233	THR	CA-C-N	5.50	127.92	120.38
1	A	233	THR	C-N-CA	5.50	127.92	120.38
1	A	606	SER	CA-C-N	5.47	133.61	123.32
1	A	606	SER	C-N-CA	5.47	133.61	123.32
1	A	26	ILE	CA-C-N	5.47	127.87	120.65
1	A	26	ILE	C-N-CA	5.47	127.87	120.65
1	A	217	VAL	CA-C-O	-5.45	115.39	121.17
1	A	530	ILE	CA-C-O	-5.45	114.70	120.48
1	A	52	ARG	CB-CG-CD	5.42	123.77	111.30
1	A	87	SER	CB-CA-C	5.39	118.04	109.52
1	A	456	PHE	CA-CB-CG	5.36	119.16	113.80
1	A	628	PRO	CA-C-N	5.31	129.89	122.08
1	A	628	PRO	C-N-CA	5.31	129.89	122.08
1	A	193	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	609	LYS	CA-CB-CG	-5.23	103.63	114.10
1	A	278	CYS	N-CA-C	-5.17	106.23	112.54
1	A	637	LEU	CA-C-O	-5.10	112.14	120.80
1	A	185	THR	CB-CA-C	5.09	119.51	110.85
1	A	62	ARG	NE-CZ-NH1	-5.07	116.43	121.50
2	B	227	VAL	CA-CB-CG2	5.02	118.94	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169[A]	GLU	Sidechain

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	5083	0	4978	82	0
2	B	2345	0	2260	50	0
3	A	20	0	15	0	0
4	A	20	0	0	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	256	0	0	9	0
6	B	57	0	0	6	0
All	All	7793	0	7269	130	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 (130) 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:578:SER:O	1:A:579:TRP:HB2	1.26	1.08
1:A:578:SER:O	1:A:579:TRP:CB	2.02	1.03
1:A:185:THR:HG22	6:A:922:HOH:O	1.72	0.89
2:B:201:LYS:O	6:B:501:HOH:O	1.97	0.81
1:A:156:PRO:O	1:A:185:THR:HG21	1.81	0.80
2:B:27:MET:HE3	2:B:31:LEU:HD21	1.64	0.80
1:A:324:TYR:CB	1:A:368:ARG:HD2	2.16	0.76
2:B:60:LEU:HD22	2:B:108:LEU:HD21	1.69	0.75
1:A:348:ARG:HE	1:A:359:GLN:HE22	1.36	0.72
1:A:297:TYR:CD2	1:A:577:PHE:HA	2.25	0.72
2:B:32:GLU:OE1	6:B:502:HOH:O	2.07	0.71
1:A:302:LYS:O	1:A:305:GLU:OE1	2.12	0.68
1:A:419:ASP:OD1	1:A:421:ARG:HD3	1.94	0.68
1:A:358:VAL:HA	1:A:385:ARG:O	1.96	0.66
2:B:157:GLN:OE1	6:B:503:HOH:O	2.12	0.66
1:A:26:ILE:HD12	1:A:43:MET:HE1	1.79	0.65
1:A:238:THR:HG22	1:A:242:GLY:HA2	1.78	0.64
1:A:324:TYR:HB2	1:A:368:ARG:HD2	1.80	0.64
1:A:348:ARG:HE	1:A:359:GLN:NE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HB2	1:A:298:GLU:HB2	1.81	0.61
1:A:156:PRO:O	1:A:185:THR:CG2	2.50	0.60
1:A:343:LYS:HE3	1:A:563:ILE:HD11	1.83	0.60
2:B:109:ASP:HB3	2:B:112:GLU:H	1.67	0.60
2:B:169:GLN:NE2	6:B:507:HOH:O	2.29	0.59
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.38	0.58
1:A:377:ARG:O	1:A:380:LYS:HG3	2.02	0.58
2:B:172[B]:CYS:SG	2:B:216:THR:O	2.62	0.57
1:A:158:VAL:HG11	1:A:163:LEU:HD13	1.85	0.57
1:A:324:TYR:HB3	1:A:368:ARG:HD2	1.86	0.57
2:B:109:ASP:HB3	2:B:112:GLU:N	2.21	0.56
1:A:444:GLU:OE2	4:A:702:UNL:N3	2.39	0.56
1:A:322:GLN:O	1:A:326:VAL:HG13	2.05	0.55
2:B:135:SER:OG	2:B:180:ASP:OD2	2.25	0.55
2:B:60:LEU:CD2	2:B:108:LEU:HD21	2.35	0.54
1:A:18:ARG:NH2	1:A:277:PHE:CZ	2.75	0.54
2:B:32:GLU:HG2	2:B:83:VAL:O	2.08	0.54
1:A:565:LEU:HA	1:A:573:SER:OG	2.07	0.54
1:A:607:ASN:HB3	1:A:609:LYS:H	1.71	0.54
1:A:29:THR:O	1:A:33:VAL:HG13	2.07	0.54
1:A:222:LEU:HD12	1:A:510:HIS:CG	2.44	0.53
1:A:295:ASN:OD1	1:A:297:TYR:HB3	2.08	0.53
1:A:434:SER:HB2	1:A:436:LEU:HG	1.91	0.53
1:A:444:GLU:O	1:A:445:LEU:HB2	2.07	0.53
1:A:55:ILE:HD13	6:A:919:HOH:O	2.08	0.52
1:A:301:ALA:HB1	1:A:505:ARG:HG3	1.91	0.52
1:A:360:VAL:HG11	1:A:428:LYS:O	2.10	0.52
1:A:448:GLU:O	6:A:803:HOH:O	2.19	0.52
1:A:300:PHE:HE1	1:A:329:LYS:HE2	1.76	0.51
1:A:577:PHE:CD1	1:A:578:SER:N	2.79	0.51
1:A:147:HIS:HB3	6:A:928:HOH:O	2.11	0.50
1:A:44:PRO:HB2	1:A:46:PHE:O	2.11	0.50
1:A:607:ASN:HB2	1:A:610:LYS:H	1.75	0.50
1:A:240:LYS:H	1:A:240:LYS:CE	2.25	0.50
1:A:386:ILE:HG13	1:A:386:ILE:O	2.12	0.49
1:A:349:VAL:HG23	1:A:384:ARG:HE	1.77	0.49
2:B:109:ASP:O	2:B:112:GLU:HG2	2.12	0.49
1:A:228:ALA:HA	1:A:263:GLN:O	2.12	0.49
1:A:596:GLN:OE1	6:A:804:HOH:O	2.20	0.49
1:A:297:TYR:CE2	1:A:577:PHE:HA	2.47	0.49
1:A:607:ASN:CB	1:A:609:LYS:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ALA:HA	2:B:121:LYS:O	2.13	0.48
2:B:148:CYS:SG	2:B:164:ARG:HG2	2.53	0.48
1:A:527:ASP:HB3	1:A:529:MET:O	2.14	0.48
2:B:96:VAL:HB	2:B:104:GLU:HG3	1.95	0.48
2:B:62:LYS:H	2:B:74:SER:HG	1.60	0.48
1:A:294:PRO:HB2	1:A:298:GLU:CB	2.43	0.48
2:B:281:ALA:HB2	2:B:292:ARG:NH1	2.29	0.48
1:A:219:ASP:O	1:A:222:LEU:HG	2.14	0.48
1:A:512:LEU:HG	1:A:546:THR:HG21	1.95	0.48
2:B:27:MET:HE1	2:B:68:PRO:CB	2.43	0.48
1:A:82:ILE:O	1:A:120:PRO:HD2	2.15	0.47
2:B:303:ALA:HB1	2:B:313:LEU:HD11	1.95	0.47
1:A:101:ARG:NH1	6:A:821:HOH:O	2.48	0.46
1:A:240:LYS:H	1:A:240:LYS:HE2	1.80	0.46
2:B:48:SER:OG	2:B:53:CYS:O	2.30	0.46
2:B:229:VAL:HG12	2:B:239:LEU:HA	1.98	0.46
2:B:244:SER:C	2:B:246:SER:N	2.73	0.46
2:B:217:SER:O	2:B:230:PHE:HA	2.15	0.46
1:A:455:HIS:HD2	6:A:1008:HOH:O	1.99	0.46
1:A:153:MET:HE2	1:A:192:PHE:CE2	2.51	0.46
2:B:264:SER:HB2	2:B:266:HIS:HD2	1.81	0.46
1:A:249:MET:SD	1:A:252:ARG:HD3	2.56	0.45
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.98	0.45
1:A:276:GLU:HG3	1:A:277:PHE:N	2.32	0.45
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.79	0.45
2:B:66:ALA:HB1	2:B:72:PHE:HB2	1.98	0.45
2:B:244:SER:HB3	2:B:246:SER:HB3	1.98	0.45
1:A:328:GLU:OE2	1:A:368:ARG:HD3	2.16	0.45
1:A:51:LYS:HG2	1:A:89:TRP:CD2	2.52	0.45
1:A:556:GLU:HG2	1:A:566:SER:HB2	1.99	0.45
2:B:145:LYS:HA	2:B:169:GLN:HB3	1.99	0.45
1:A:153:MET:HE2	1:A:192:PHE:CZ	2.52	0.44
1:A:372:VAL:HG13	1:A:388:LEU:HD13	1.98	0.44
2:B:254:HIS:CG	2:B:275:SER:HB2	2.51	0.44
2:B:265:PRO:HB2	2:B:310:HIS:CE1	2.53	0.44
1:A:345:LEU:O	1:A:349:VAL:HG22	2.18	0.44
1:A:371:LEU:HB2	6:A:872:HOH:O	2.18	0.44
2:B:32:GLU:OE2	2:B:301:ARG:HD3	2.18	0.44
1:A:16:SER:HA	1:A:264:PHE:O	2.18	0.44
1:A:369:GLY:N	1:A:370:PRO:CD	2.81	0.43
1:A:323:THR:O	1:A:326:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:HG12	1:A:357:ASN:CG	2.43	0.43
2:B:166:HIS:ND1	2:B:187:SER:HB3	2.34	0.43
2:B:243:LYS:HA	2:B:243:LYS:NZ	2.33	0.43
1:A:421:ARG:HH12	1:A:637:LEU:C	2.27	0.43
2:B:153:ASP:HB2	2:B:160:LEU:HD21	2.01	0.43
2:B:307:PRO:O	2:B:310:HIS:CD2	2.72	0.42
1:A:26:ILE:HG22	6:B:512:HOH:O	2.18	0.42
1:A:352:GLU:HG2	1:A:353:GLU:N	2.34	0.42
2:B:61:PHE:CG	2:B:67:ALA:HB2	2.54	0.42
2:B:264:SER:HB2	2:B:266:HIS:CD2	2.54	0.42
1:A:349:VAL:HG23	1:A:384:ARG:NE	2.35	0.42
2:B:69:ASN:OD1	2:B:69:ASN:C	2.62	0.41
2:B:289:GLU:OE2	2:B:292:ARG:HB2	2.20	0.41
1:A:240:LYS:H	1:A:240:LYS:HZ3	1.68	0.41
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.35	0.41
2:B:314:THR:HA	2:B:323:VAL:O	2.20	0.41
1:A:92:PRO:HG2	1:A:134:LEU:HD12	2.02	0.41
2:B:188:GLU:HG2	2:B:214:LEU:HD13	2.01	0.41
1:A:58:PRO:HG3	2:B:297:ARG:HA	2.02	0.41
2:B:244:SER:C	2:B:246:SER:H	2.29	0.41
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.84	0.41
2:B:86:LEU:HD11	2:B:96:VAL:HG22	2.03	0.41
2:B:206:ILE:HG13	2:B:207:GLY:N	2.35	0.41
1:A:193:ARG:HH11	1:A:193:ARG:HD3	1.62	0.41
1:A:505:ARG:HG2	1:A:580:PHE:CD1	2.56	0.40
2:B:256:GLN:NE2	6:B:511:HOH:O	2.54	0.40
2:B:284:ASP:OD2	2:B:288:SER:HB2	2.21	0.40
1:A:96:VAL:HG21	2:B:233:GLU:HG3	2.03	0.40
1:A:104:GLU:HB3	6:A:1033:HOH:O	2.22	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	626/645 (97%)	590 (94%)	31 (5%)	5 (1%)	16	8
2	B	309/350 (88%)	299 (97%)	7 (2%)	3 (1%)	12	5
All	All	935/995 (94%)	889 (95%)	38 (4%)	8 (1%)	14	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	TRP
2	B	147	ILE
1	A	578	SER
2	B	248	VAL
1	A	358	VAL
1	A	441	ALA
1	A	301	ALA
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	561/570 (98%)	513 (91%)	48 (9%)	10	2
2	B	264/298 (89%)	243 (92%)	21 (8%)	11	3
All	All	825/868 (95%)	756 (92%)	69 (8%)	10	3

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	33	VAL
1	A	52	ARG
1	A	57	GLU
1	A	95	LYS
1	A	136	ARG
1	A	155	VAL
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	169[A]	GLU
1	A	169[B]	GLU
1	A	174	THR
1	A	176	THR
1	A	177	GLU
1	A	178	GLU
1	A	185	THR
1	A	193	ARG
1	A	218	ILE
1	A	220	ARG
1	A	237	LEU
1	A	240	LYS
1	A	241	LYS
1	A	260	LEU
1	A	274	GLU
1	A	275	LYS
1	A	277	PHE
1	A	281	LEU
1	A	288	SER
1	A	299	LEU
1	A	302	LYS
1	A	326	VAL
1	A	329	LYS
1	A	352	GLU
1	A	354	LYS
1	A	360	VAL
1	A	361	LEU
1	A	380	LYS
1	A	387	LYS
1	A	405	GLN
1	A	421	ARG
1	A	445	LEU
1	A	497	GLN
1	A	505	ARG
1	A	512	LEU
1	A	526	ARG
1	A	559	LEU
1	A	582	ILE
1	A	593	ARG
1	A	621	VAL
2	B	37	ARG
2	B	73	CYS

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Mol	Chain	Res	Type
2	B	74	SER
2	B	104	GLU
2	B	107	GLU
2	B	108	LEU
2	B	117	SER
2	B	118	LYS
2	B	136	SER
2	B	161	SER
2	B	180	ASP
2	B	206	ILE
2	B	226	GLU
2	B	243	LYS
2	B	245	THR
2	B	247	CYS
2	B	274	LEU
2	B	287	LEU
2	B	297	ARG
2	B	308	LEU
2	B	311	SER

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	56	GLN
1	A	128	GLN
1	A	140	ASN
1	A	175	HIS
1	A	289	GLN
1	A	290	ASN
1	A	336	GLN
1	A	359	GLN
1	A	405	GLN
2	B	157	GLN
2	B	224	GLN
2	B	254	HIS
2	B	294	GLN
2	B	310	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is unknown - 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	$\# Z > 2$
5	GOL	A	703	-	5,5,5	0.13	0	5,5,5	0.20	0
5	GOL	B	401	-	5,5,5	0.12	0	5,5,5	0.28	0
3	MTA	A	701	-	22,22,22	1.53	5 (22%)	32,32,32	2.22	11 (34%)

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
5	GOL	A	703	-	-	2/4/4/4	-
5	GOL	B	401	-	-	3/4/4/4	-
3	MTA	A	701	-	-	0/7/23/23	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	MTA	C4-N9	-3.19	1.31	1.37
3	A	701	MTA	C5-C4	2.79	1.44	1.39
3	A	701	MTA	C5-N7	-2.49	1.34	1.39
3	A	701	MTA	C8-N9	-2.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	MTA	C8-N7	2.31	1.36	1.31

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	MTA	C4-N9-C8	5.10	111.09	105.74
3	A	701	MTA	C5-C4-N3	-5.07	119.74	126.72
3	A	701	MTA	N3-C4-N9	4.20	134.31	127.17
3	A	701	MTA	N9-C8-N7	-4.01	108.25	113.94
3	A	701	MTA	C4-C5-N7	-3.48	106.60	110.58
3	A	701	MTA	C2-N3-C4	3.41	120.15	111.83
3	A	701	MTA	N3-C2-N1	-3.38	123.47	128.58
3	A	701	MTA	C5-N7-C8	2.97	108.12	103.45
3	A	701	MTA	C6-C5-N7	2.21	136.36	132.09
3	A	701	MTA	O4'-C1'-N9	-2.17	103.92	108.09
3	A	701	MTA	C4-N9-C1'	-2.06	121.82	126.63

There are no chirality outliers.

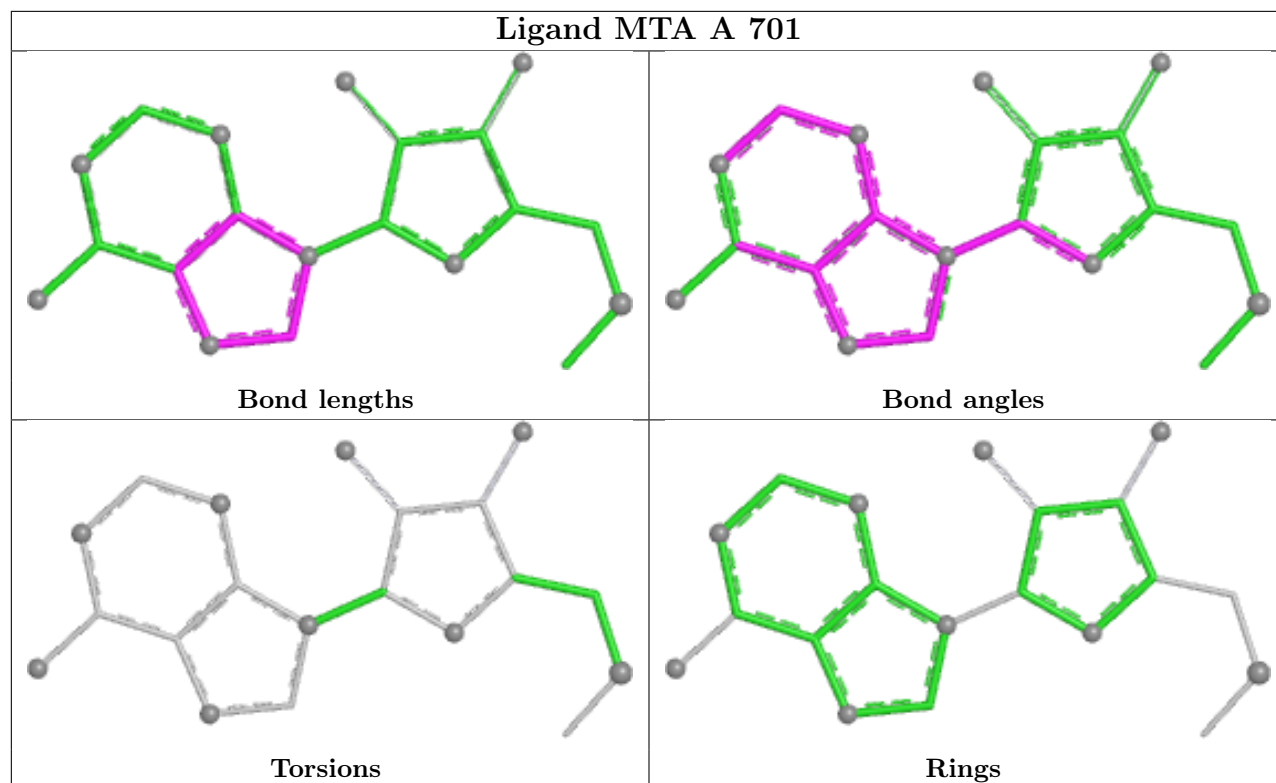
All (5) torsion outliers are listed below:

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

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 [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	625/645 (96%)	0.86	76 (12%)	8 10	11, 26, 60, 112	3 (0%)
2	B	310/350 (88%)	1.47	81 (26%)	1 1	13, 34, 69, 100	1 (0%)
All	All	935/995 (93%)	1.06	157 (16%)	4 4	11, 29, 67, 112	4 (0%)

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	LEU	9.4
2	B	21	PRO	9.2
1	A	577	PHE	7.1
1	A	277	PHE	6.6
1	A	293	PRO	6.4
2	B	20	PRO	6.2
1	A	578	SER	5.7
1	A	297	TYR	5.6
1	A	300	PHE	5.5
1	A	292	PRO	5.4
1	A	294	PRO	5.2
2	B	248	VAL	5.2
2	B	312	LEU	5.1
2	B	210	ALA	4.9
1	A	301	ALA	4.8
2	B	268	VAL	4.8
2	B	23	ALA	4.7
1	A	243	PHE	4.6
1	A	296	ALA	4.5
1	A	361	LEU	4.4
1	A	530	ILE	4.4
2	B	211	PRO	4.3
1	A	299	LEU	4.2
2	B	106	TRP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	349	VAL	4.1
2	B	114	LEU	4.1
1	A	176	THR	4.1
1	A	526	ARG	3.9
1	A	222	LEU	3.9
1	A	529	MET	3.9
2	B	22	ASN	3.8
2	B	290	LEU	3.8
1	A	575	GLY	3.8
1	A	255	PHE	3.8
2	B	207	GLY	3.7
1	A	574	PRO	3.6
1	A	342	TYR	3.6
1	A	13	ARG	3.6
2	B	60	LEU	3.6
2	B	249	LEU	3.6
2	B	26	CYS	3.4
2	B	108	LEU	3.4
2	B	313	LEU	3.4
2	B	72	PHE	3.4
2	B	27	MET	3.4
2	B	247	CYS	3.4
1	A	272	HIS	3.4
1	A	286	TYR	3.4
1	A	175	HIS	3.3
2	B	71	GLY	3.3
1	A	146	HIS	3.3
2	B	245	THR	3.3
1	A	345	LEU	3.2
2	B	242	THR	3.2
2	B	206	ILE	3.2
1	A	249	MET	3.2
2	B	246	SER	3.2
2	B	61	PHE	3.2
2	B	24	PRO	3.1
1	A	409	TRP	3.1
2	B	109	ASP	3.1
2	B	244	SER	3.1
1	A	380	LYS	3.1
2	B	113	THR	3.0
2	B	73	CYS	3.0
1	A	271	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	260	LEU	2.9
2	B	59	TRP	2.9
1	A	55	ILE	2.9
2	B	110	GLU	2.9
1	A	376	LEU	2.9
2	B	303	ALA	2.8
1	A	240	LYS	2.8
2	B	225	SER	2.8
1	A	145	GLY	2.8
2	B	42	LEU	2.8
2	B	116	VAL	2.8
2	B	262	VAL	2.8
2	B	41	ALA	2.7
2	B	25	ALA	2.7
1	A	358	VAL	2.7
2	B	327	VAL	2.7
1	A	26	ILE	2.7
1	A	177	GLU	2.7
1	A	178	GLU	2.7
2	B	115	ILE	2.7
2	B	311	SER	2.6
1	A	341	ILE	2.6
2	B	282	VAL	2.6
1	A	528	PRO	2.6
2	B	308	LEU	2.6
2	B	326	VAL	2.6
2	B	209	SER	2.6
2	B	314	THR	2.6
1	A	287	LEU	2.5
2	B	136	SER	2.5
2	B	75	ALA	2.5
2	B	86	LEU	2.5
1	A	174	THR	2.5
2	B	241	ASP	2.5
2	B	257	CYS	2.4
1	A	234	SER	2.4
1	A	386	ILE	2.4
2	B	222	PRO	2.4
2	B	111	ASN	2.4
1	A	329	LYS	2.4
1	A	238	THR	2.4
2	B	89	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	107	GLU	2.4
2	B	64	PRO	2.4
2	B	227	VAL	2.4
1	A	241	LYS	2.4
1	A	346	LEU	2.3
2	B	36	TYR	2.3
2	B	291	PHE	2.3
1	A	276	GLU	2.3
1	A	275	LYS	2.3
1	A	621	VAL	2.3
2	B	243	LYS	2.3
2	B	270	PHE	2.3
2	B	155	ALA	2.3
1	A	273	SER	2.3
2	B	38	SER	2.3
1	A	527	ASP	2.3
2	B	158	VAL	2.3
2	B	287	LEU	2.3
1	A	389	TYR	2.2
1	A	375	SER	2.2
1	A	383	ASP	2.2
2	B	310	HIS	2.2
2	B	43	LEU	2.2
1	A	406	PHE	2.2
1	A	282	GLN	2.2
1	A	544	VAL	2.2
2	B	266	HIS	2.1
1	A	239	ASN	2.1
1	A	208	ILE	2.1
1	A	411	SER	2.1
2	B	280	LEU	2.1
1	A	354	LYS	2.1
1	A	378	ALA	2.1
2	B	94	ILE	2.1
2	B	304	THR	2.1
1	A	547	VAL	2.1
1	A	298	GLU	2.1
1	A	218	ILE	2.1
1	A	593	ARG	2.1
2	B	224	GLN	2.1
2	B	269	PRO	2.1
1	A	253	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	285	GLU	2.0
2	B	119	PHE	2.0
1	A	462	VAL	2.0
2	B	91	GLU	2.0
2	B	93	GLY	2.0
1	A	283	TYR	2.0
2	B	322	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

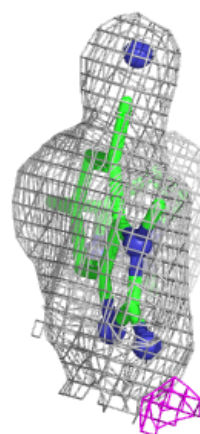
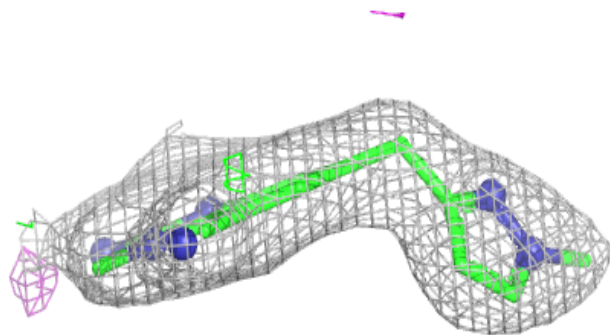
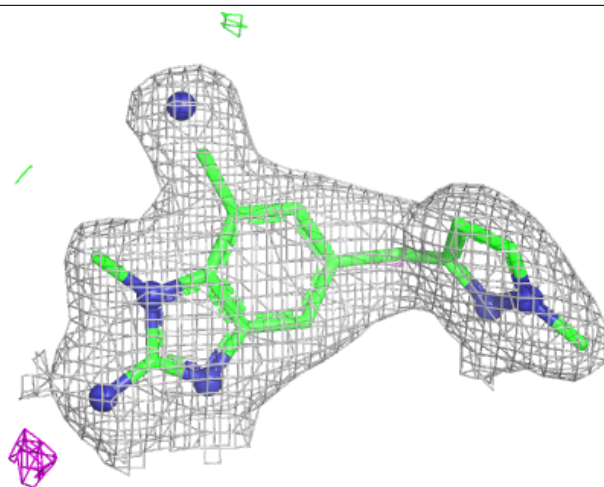
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

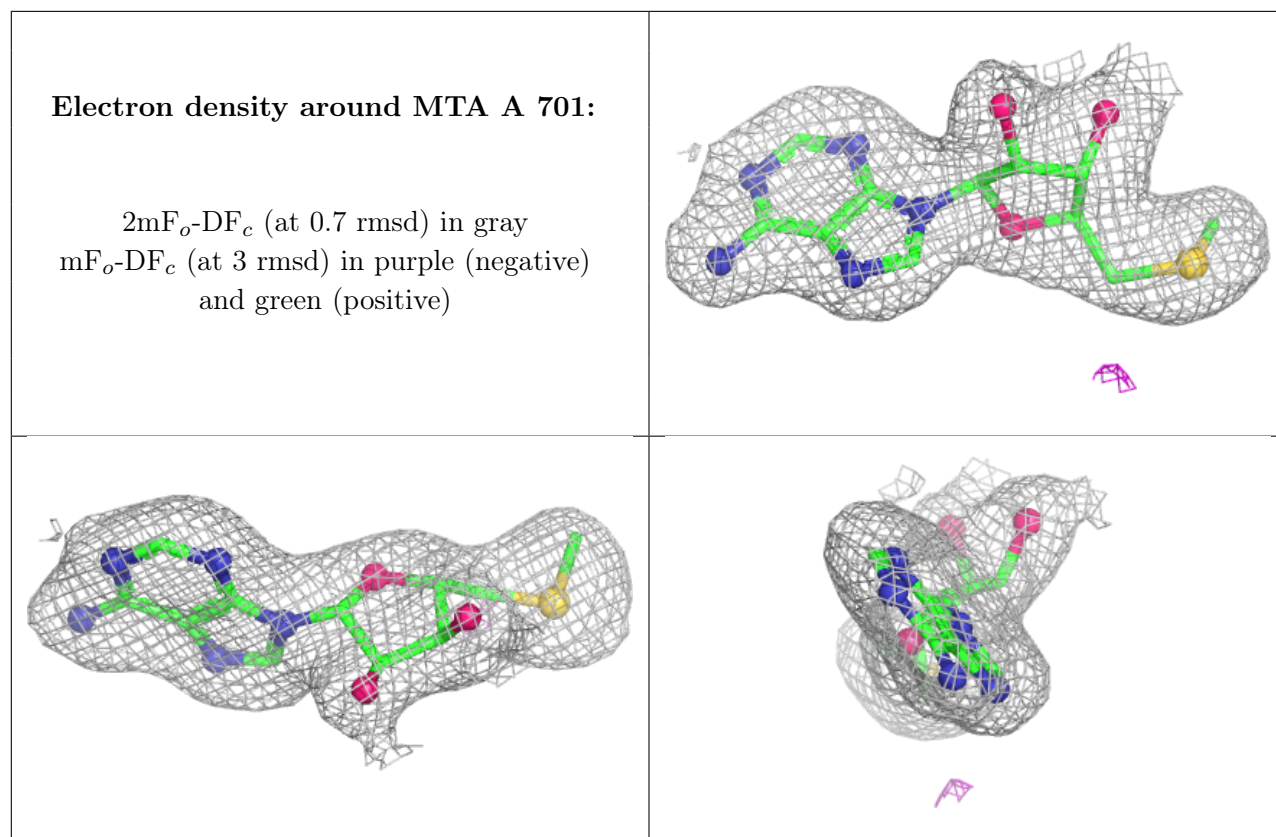
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	703	6/6	0.82	0.23	46,50,58,67	0
5	GOL	B	401	6/6	0.88	0.18	65,69,72,73	0
4	UNL	A	702	20/-	0.96	0.07	16,22,29,32	0
3	MTA	A	701	20/20	0.98	0.05	16,18,20,21	0

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 UNL 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 [i](#)

There are no such residues in this entry.