



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:26 AM UTC

PDB ID : 7ZUP / pdb_00007zup
Title : Human PRMT5:MEP50 structure with Fragment (Example 18) and MTA Bound
Authors : Ahmad, M.U.; Koelmel, W.; Arkhipova, V.; Lawson, J.D.; Smith, C.R.; Gunn, R.J.
Deposited on : 2022-05-12
Resolution : 2.01 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

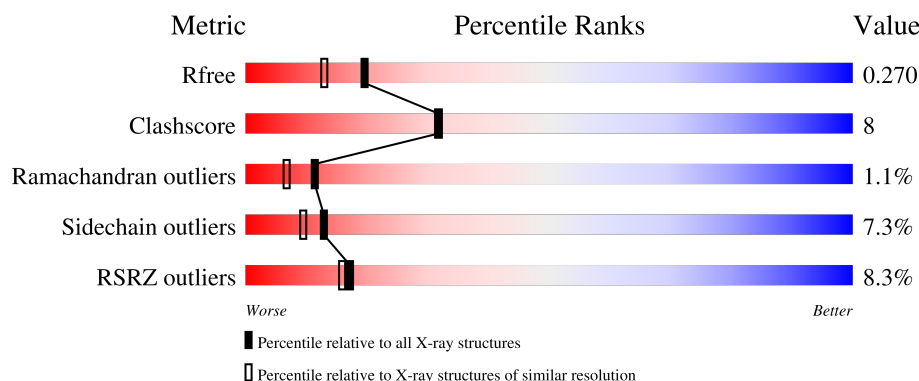
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	6% 75% 18% • •
2	B	350	11% 66% 21% • 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7691 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	C	N	O	S	0	3	0
			5085	3251	873	936	25			

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

There are 9 discrepancies between the modelled and reference sequences:

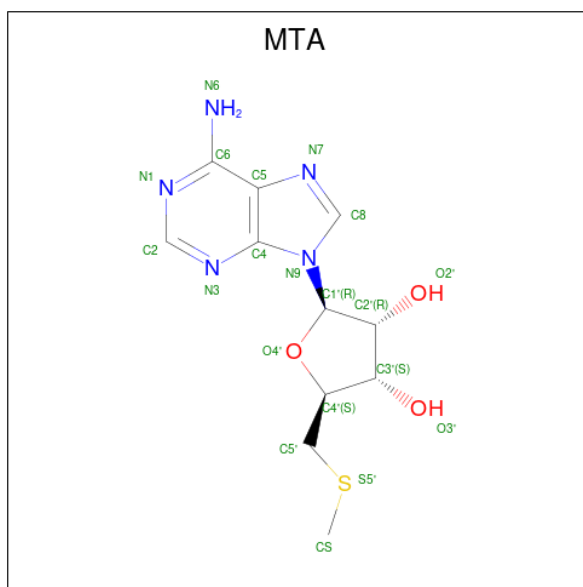
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag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

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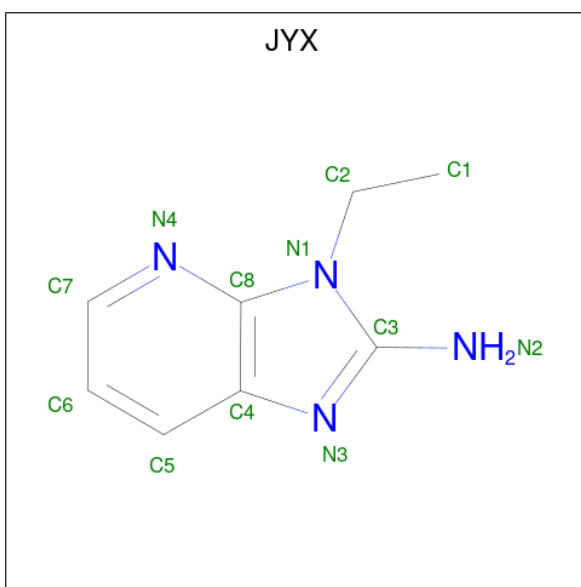
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

- 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 3-ethylimidazo[4,5-b]pyridin-2-amine (CCD ID: JYX) (formula: $C_8H_{10}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			12	8	4		

- 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		

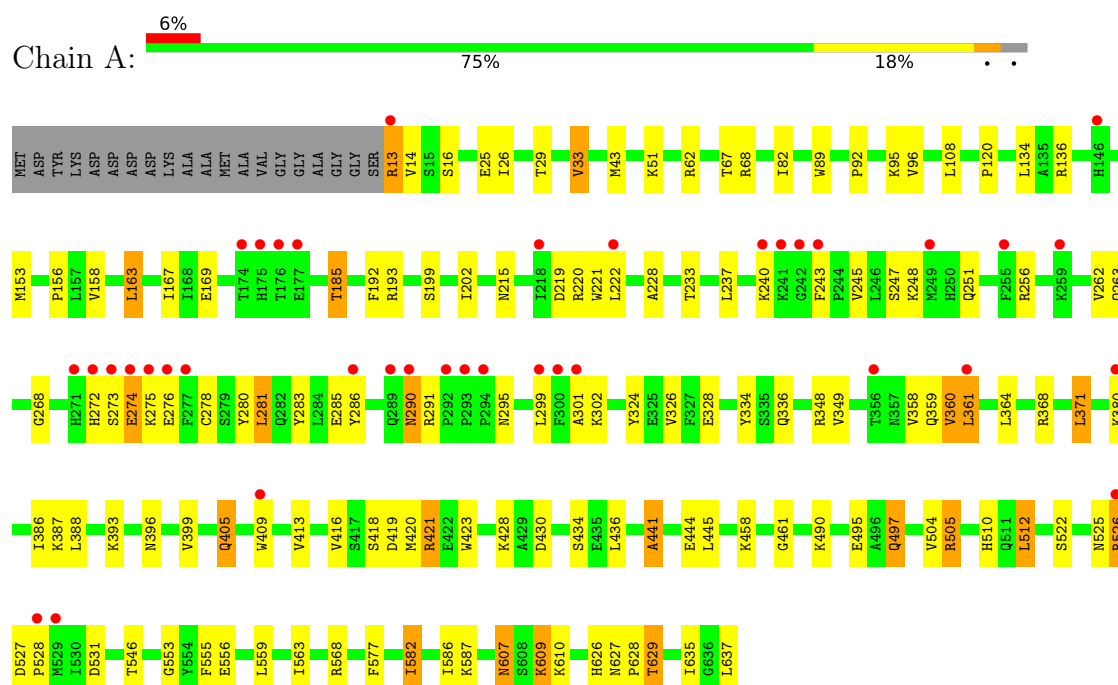
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	182	Total 182	O 182	0	0
6	B	35	Total 35	O 35	0	0

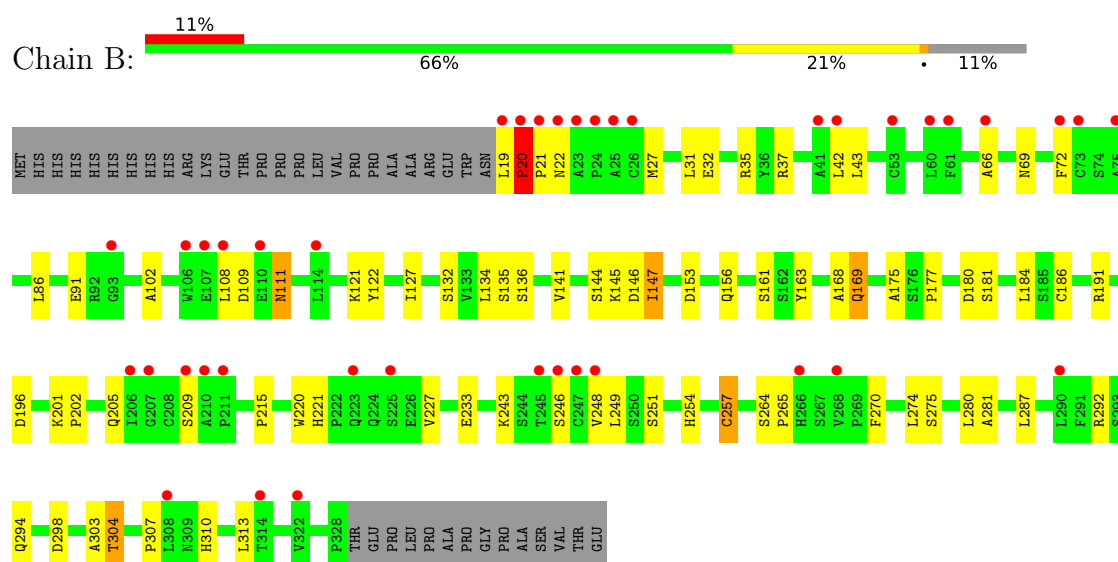
3 Residue-property plots [i](#)

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

- Molecule 1: 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	104.28Å 138.65Å 178.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.59 – 2.01 109.59 – 2.01	Depositor EDS
% Data completeness (in resolution range)	46.2 (109.59-2.01) 46.2 (109.59-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.02Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.219 , 0.271 0.223 , 0.270	Depositor DCC
R_{free} test set	1957 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7691	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 3.23% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.97	0/5227	1.39	6/7111 (0.1%)
2	B	1.10	0/2402	1.35	2/3283 (0.1%)
All	All	1.02	0/7629	1.38	8/10394 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	497	GLN	CB-CA-C	-6.69	99.30	110.68
1	A	607	ASN	CB-CA-C	-6.47	98.65	112.63
2	B	20	PRO	N-CA-C	5.79	117.77	110.70
2	B	109	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	268	GLY	CA-C-O	-5.56	117.45	122.57
1	A	262	VAL	CA-C-O	-5.42	117.40	121.68
1	A	272	HIS	CA-C-N	5.39	127.76	120.65
1	A	272	HIS	C-N-CA	5.39	127.76	120.65

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	5085	0	4970	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2345	0	2260	38	0
3	A	20	0	15	0	0
4	A	12	0	0	1	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	182	0	0	3	0
6	B	35	0	0	3	0
All	All	7691	0	7261	119	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (119) 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:35:ARG:HA	2:B:304:THR:HG21	1.66	0.77
2:B:135:SER:HB3	2:B:177:PRO:O	1.88	0.73
1:A:219:ASP:O	1:A:222:LEU:HG	1.89	0.73
1:A:421:ARG:HH12	1:A:637:LEU:C	1.97	0.73
1:A:324:TYR:CB	1:A:368:ARG:HD2	2.20	0.71
1:A:276:GLU:HB3	1:A:278:CYS:SG	2.32	0.70
2:B:153:ASP:OD2	2:B:156:GLN:HB2	1.92	0.69
1:A:607:ASN:HB2	1:A:609:LYS:H	1.61	0.64
1:A:405:GLN:NE2	1:A:413:VAL:O	2.29	0.64
2:B:27:MET:HE3	2:B:31:LEU:HD21	1.79	0.63
1:A:16:SER:OG	1:A:281:LEU:HD21	1.98	0.63
1:A:96:VAL:HG21	2:B:233:GLU:HG3	1.81	0.62
1:A:348:ARG:HE	1:A:359:GLN:HE22	1.50	0.60
1:A:430:ASP:OD1	1:A:458:LYS:NZ	2.32	0.60
1:A:336:GLN:NE2	1:A:563:ILE:HG23	2.17	0.59
1:A:273:SER:C	1:A:275:LYS:H	2.11	0.59
1:A:228:ALA:HA	1:A:263:GLN:O	2.03	0.59
1:A:248:LYS:HA	1:A:251:GLN:HE21	1.67	0.59
2:B:221:HIS:HB2	2:B:227:VAL:HG23	1.85	0.59
1:A:222:LEU:HD12	1:A:510:HIS:CD2	2.38	0.58
1:A:416:VAL:HG21	1:A:423:TRP:CZ2	2.38	0.58
1:A:243:PHE:CD1	1:A:275:LYS:HE2	2.39	0.58
1:A:324:TYR:HB2	1:A:368:ARG:HD2	1.85	0.57
1:A:62:ARG:HD3	2:B:298:ASP:OD2	2.05	0.57
1:A:29:THR:O	1:A:33:VAL:HG13	2.05	0.57
2:B:303:ALA:HB1	2:B:313:LEU:HD11	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LYS:HA	2:B:169:GLN:HB3	1.89	0.55
2:B:233:GLU:HA	2:B:257:CYS:HB2	1.88	0.55
1:A:51:LYS:O	1:A:62:ARG:NH1	2.33	0.54
2:B:66:ALA:HB1	2:B:72:PHE:HB3	1.89	0.54
1:A:92:PRO:HG2	1:A:134:LEU:HD12	1.89	0.54
2:B:281:ALA:HB2	2:B:292:ARG:NH1	2.23	0.54
1:A:324:TYR:HB3	1:A:368:ARG:HD2	1.90	0.54
1:A:26:ILE:HD12	1:A:43:MET:HE1	1.90	0.53
1:A:328:GLU:OE2	1:A:368:ARG:HD3	2.08	0.53
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.90	0.53
1:A:444:GLU:O	1:A:445:LEU:HB2	2.08	0.53
1:A:67:THR:OG1	1:A:68:ARG:N	2.42	0.53
1:A:334:TYR:HE1	1:A:371:LEU:HD13	1.72	0.53
2:B:37:ARG:O	2:B:307:PRO:HG3	2.09	0.53
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.43	0.52
2:B:265:PRO:HB2	2:B:310:HIS:CE1	2.45	0.52
2:B:201:LYS:O	6:B:501:HOH:O	2.19	0.52
2:B:102:ALA:HA	2:B:121:LYS:O	2.10	0.52
2:B:181:SER:O	2:B:196:ASP:HA	2.10	0.52
2:B:191:ARG:HG2	2:B:205:GLN:NE2	2.24	0.52
1:A:283:TYR:O	1:A:286:TYR:HB3	2.10	0.51
1:A:434:SER:HB2	1:A:436:LEU:HG	1.93	0.51
1:A:245:VAL:HG12	1:A:283:TYR:CE1	2.45	0.51
1:A:361:LEU:O	1:A:388:LEU:HA	2.11	0.51
1:A:419:ASP:OD1	1:A:421:ARG:HD3	2.12	0.50
2:B:32:GLU:OE1	6:B:502:HOH:O	2.19	0.50
2:B:144:SER:HB3	2:B:146:ASP:OD1	2.12	0.50
1:A:386:ILE:HG13	1:A:386:ILE:O	2.11	0.50
2:B:35:ARG:HA	2:B:304:THR:CG2	2.41	0.49
1:A:290:ASN:HD22	1:A:290:ASN:N	2.11	0.49
1:A:512:LEU:HG	1:A:546:THR:HG21	1.93	0.49
1:A:556:GLU:OE2	1:A:568:ARG:HD3	2.12	0.49
2:B:69:ASN:OD1	2:B:69:ASN:C	2.56	0.49
1:A:607:ASN:HD22	1:A:610:LYS:HG2	1.78	0.48
1:A:153:MET:HE2	1:A:192:PHE:CE2	2.48	0.48
1:A:458:LYS:O	1:A:461:GLY:N	2.43	0.48
2:B:35:ARG:NH1	2:B:86:LEU:O	2.46	0.48
1:A:334:TYR:CE1	1:A:371:LEU:HD13	2.48	0.47
1:A:531:ASP:C	1:A:531:ASP:OD1	2.55	0.47
1:A:158:VAL:HG11	1:A:163:LEU:HD13	1.96	0.47
1:A:627:ASN:N	1:A:628:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASN:O	1:A:399:VAL:HB	2.15	0.47
1:A:421:ARG:NH1	1:A:637:LEU:C	2.70	0.46
1:A:222:LEU:HD12	1:A:510:HIS:CG	2.51	0.46
1:A:185:THR:HG23	1:A:221:TRP:HZ2	1.80	0.46
1:A:364:LEU:HB3	1:A:420:MET:CE	2.44	0.46
1:A:82:ILE:O	1:A:120:PRO:HD2	2.15	0.46
1:A:199:SER:HB3	1:A:202:ILE:HD12	1.98	0.46
1:A:301:ALA:HB1	1:A:505:ARG:HG3	1.98	0.45
1:A:243:PHE:CD1	1:A:275:LYS:CE	3.00	0.45
1:A:215[B]:ASN:C	1:A:215[B]:ASN:ND2	2.75	0.45
1:A:525:ASN:C	1:A:525:ASN:HD22	2.23	0.45
1:A:444:GLU:OE2	4:A:702:JYX:N3	2.50	0.45
1:A:26:ILE:HG22	6:B:517:HOH:O	2.17	0.44
1:A:302:LYS:HA	1:A:302:LYS:HD2	1.77	0.44
2:B:280:LEU:O	2:B:292:ARG:HA	2.17	0.44
1:A:215[B]:ASN:C	1:A:215[B]:ASN:HD22	2.25	0.44
1:A:247:SER:O	1:A:251:GLN:HG3	2.18	0.44
2:B:161:SER:HB3	2:B:163:TYR:CZ	2.52	0.44
2:B:86:LEU:HD12	2:B:86:LEU:HA	1.75	0.44
1:A:215[B]:ASN:ND2	1:A:215[B]:ASN:O	2.51	0.44
1:A:607:ASN:ND2	1:A:610:LYS:HG2	2.33	0.43
1:A:586:ILE:HA	1:A:626:HIS:NE2	2.33	0.43
1:A:609:LYS:O	1:A:637:LEU:HB2	2.18	0.43
1:A:553:GLY:HA3	1:A:582:ILE:HG22	2.00	0.43
1:A:371:LEU:HB2	6:A:811:HOH:O	2.19	0.43
1:A:156:PRO:O	1:A:185:THR:HG21	2.18	0.43
1:A:405:GLN:HA	1:A:409:TRP:HB2	2.00	0.43
1:A:628:PRO:O	1:A:629:THR:HB	2.17	0.43
2:B:20:PRO:HB3	2:B:21:PRO:HD2	2.01	0.43
1:A:51:LYS:HG2	1:A:89:TRP:CD2	2.53	0.43
1:A:393:LYS:HD3	6:A:898:HOH:O	2.19	0.43
2:B:264:SER:OG	2:B:270:PHE:N	2.46	0.43
1:A:526:ARG:HA	6:A:966:HOH:O	2.19	0.43
1:A:233:THR:HG22	1:A:280:TYR:CZ	2.54	0.42
1:A:348:ARG:HE	1:A:359:GLN:NE2	2.15	0.42
1:A:295:ASN:OD1	1:A:295:ASN:C	2.62	0.42
1:A:360:VAL:HG11	1:A:428:LYS:O	2.20	0.42
2:B:254:HIS:CG	2:B:275:SER:HB2	2.55	0.41
2:B:184:LEU:HG	2:B:220:TRP:CZ2	2.55	0.41
1:A:167:ILE:HB	2:B:202:PRO:HD2	2.01	0.41
1:A:409:TRP:HB3	1:A:413:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:LEU:HD13	1:A:635:ILE:HG21	2.02	0.41
1:A:629:THR:O	1:A:629:THR:CG2	2.69	0.41
2:B:111:ASN:OD1	2:B:111:ASN:N	2.46	0.41
1:A:13:ARG:HB2	1:A:14:VAL:H	1.70	0.41
2:B:42:LEU:HD12	2:B:43:LEU:N	2.36	0.40
2:B:134:LEU:HD23	2:B:175:ALA:HB1	2.03	0.40
1:A:495:GLU:OE1	1:A:587:LYS:NZ	2.54	0.40
2:B:22:ASN:O	2:B:22:ASN:CG	2.64	0.40
2:B:147:ILE:HG23	2:B:168:ALA:O	2.22	0.40
2:B:186:CYS:HB2	2:B:215:PRO:HG2	2.04	0.40
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.84	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	626/645 (97%)	579 (92%)	43 (7%)	4 (1%)	21	17
2	B	309/350 (88%)	292 (94%)	11 (4%)	6 (2%)	6	3
All	All	935/995 (94%)	871 (93%)	54 (6%)	10 (1%)	11	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	A	274	GLU
2	B	20	PRO
2	B	243	LYS
2	B	248	VAL
1	A	441	ALA
1	A	527	ASP

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Mol	Chain	Res	Type
2	B	127	ILE
2	B	209	SER
1	A	528	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	561/570 (98%)	517 (92%)	44 (8%)	11	8
2	B	264/298 (89%)	247 (94%)	17 (6%)	16	12
All	All	825/868 (95%)	764 (93%)	61 (7%)	13	9

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	25	GLU
1	A	33	VAL
1	A	95	LYS
1	A	108	LEU
1	A	136	ARG
1	A	163	LEU
1	A	169[A]	GLU
1	A	169[B]	GLU
1	A	185	THR
1	A	193	ARG
1	A	220	ARG
1	A	237	LEU
1	A	240	LYS
1	A	256	ARG
1	A	274	GLU
1	A	281	LEU
1	A	285	GLU
1	A	290	ASN
1	A	291	ARG

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Mol	Chain	Res	Type
1	A	299	LEU
1	A	326	VAL
1	A	349	VAL
1	A	358	VAL
1	A	360	VAL
1	A	361	LEU
1	A	371	LEU
1	A	380	LYS
1	A	387	LYS
1	A	405	GLN
1	A	418	SER
1	A	421	ARG
1	A	490	LYS
1	A	497	GLN
1	A	504	VAL
1	A	505	ARG
1	A	512	LEU
1	A	522	SER
1	A	526	ARG
1	A	559	LEU
1	A	577	PHE
1	A	582	ILE
1	A	609	LYS
1	A	629	THR
2	B	19	LEU
2	B	91	GLU
2	B	108	LEU
2	B	111	ASN
2	B	132	SER
2	B	136	SER
2	B	141	VAL
2	B	169	GLN
2	B	180	ASP
2	B	246	SER
2	B	249	LEU
2	B	251	SER
2	B	257	CYS
2	B	274	LEU
2	B	287	LEU
2	B	294	GLN
2	B	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	147	HIS
1	A	251	GLN
1	A	263	GLN
1	A	271	HIS
1	A	289	GLN
1	A	290	ASN
1	A	336	GLN
1	A	359	GLN
1	A	533	ASN
1	A	607	ASN
2	B	224	GLN

5.3.3 RNA [i](#)

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](#)

4 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	$\# Z > 2$
5	GOL	A	703	-	5,5,5	0.09	0	5,5,5	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	JYX	A	702	-	13,13,13	0.50	0	13,18,18	0.81	0
5	GOL	B	401	-	5,5,5	0.08	0	5,5,5	0.19	0
3	MTA	A	701	-	22,22,22	1.49	3 (13%)	32,32,32	1.86	9 (28%)

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	-	-	4/4/4/4	-
4	JYX	A	702	-	-	0/2/2/2	0/2/2/2
5	GOL	B	401	-	-	2/4/4/4	-
3	MTA	A	701	-	-	0/7/23/23	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	MTA	C5-C4	3.81	1.45	1.39
3	A	701	MTA	C5-N7	-3.63	1.32	1.39
3	A	701	MTA	C4-N9	-2.58	1.32	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	MTA	C5-C4-N3	-5.22	119.52	126.72
3	A	701	MTA	N3-C4-N9	4.28	134.44	127.17
3	A	701	MTA	N3-C2-N1	-3.56	123.20	128.58
3	A	701	MTA	C2-N3-C4	3.24	119.75	111.83
3	A	701	MTA	C4-C5-N7	-2.79	107.40	110.58
3	A	701	MTA	C4-N9-C8	2.55	108.42	105.74
3	A	701	MTA	C5-N7-C8	2.40	107.22	103.45
3	A	701	MTA	C2-N1-C6	2.19	122.32	118.73
3	A	701	MTA	N9-C8-N7	-2.11	110.94	113.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	703	GOL	C1-C2-C3-O3

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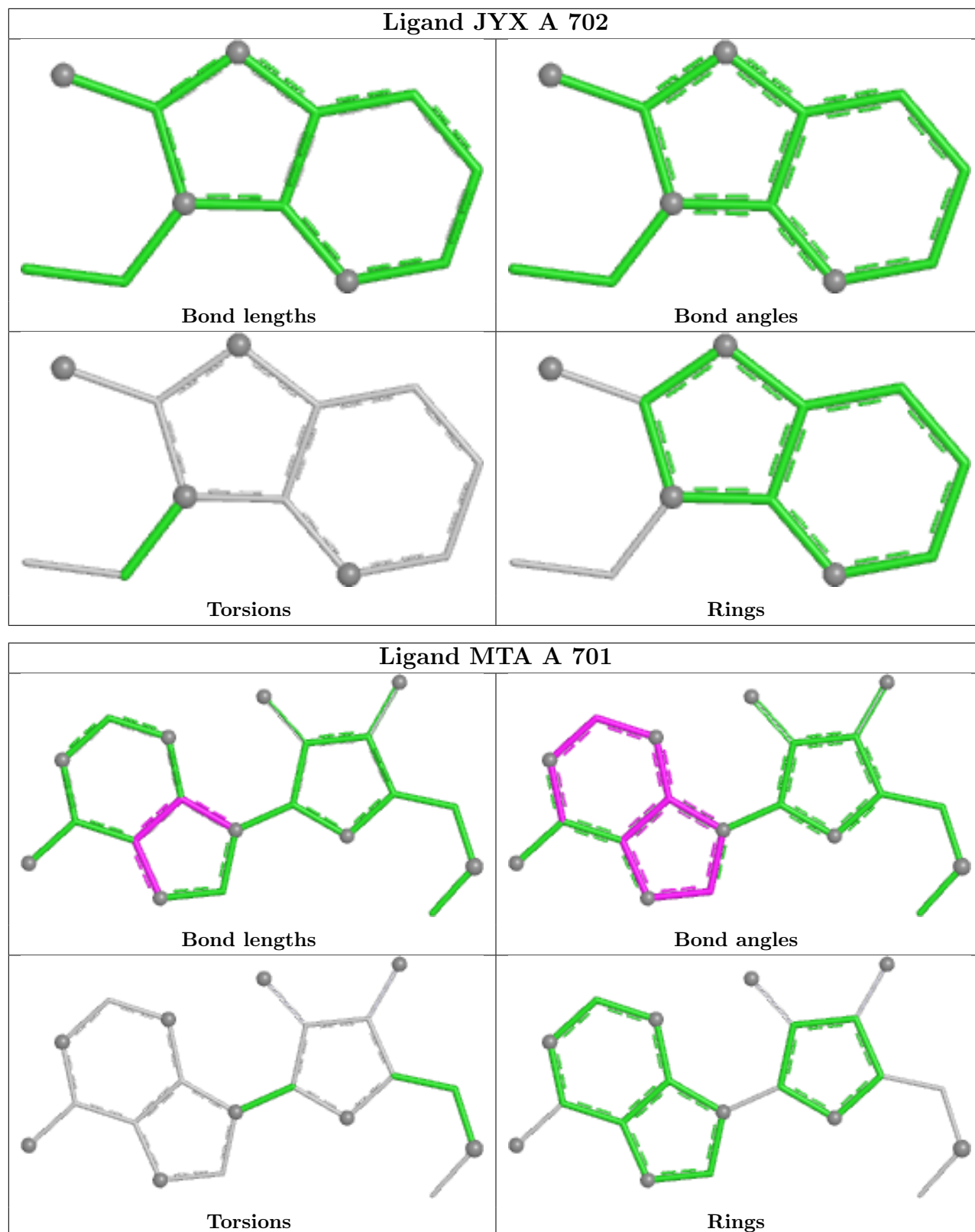
Mol	Chain	Res	Type	Atoms
5	B	401	GOL	C1-C2-C3-O3
5	B	401	GOL	O2-C2-C3-O3
5	A	703	GOL	O1-C1-C2-C3
5	A	703	GOL	O2-C2-C3-O3
5	A	703	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	702	JYX	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 ⓘ

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%)	0.37	38 (6%) 27 26	10, 26, 59, 90	3 (0%)
2	B	310/350 (88%)	1.04	40 (12%) 7 6	12, 38, 63, 102	1 (0%)
All	All	935/995 (93%)	0.59	78 (8%) 17 16	10, 30, 60, 102	4 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	LEU	9.1
2	B	21	PRO	7.6
1	A	277	PHE	5.5
1	A	243	PHE	5.3
2	B	210	ALA	5.2
2	B	268	VAL	4.8
2	B	20	PRO	4.8
2	B	24	PRO	4.7
1	A	292	PRO	4.7
1	A	293	PRO	4.5
2	B	25	ALA	4.1
1	A	222	LEU	3.9
1	A	299	LEU	3.9
1	A	526	ARG	3.8
2	B	211	PRO	3.7
2	B	207	GLY	3.6
2	B	246	SER	3.6
2	B	107	GLU	3.5
1	A	176	THR	3.5
2	B	72	PHE	3.5
2	B	23	ALA	3.4
1	A	380	LYS	3.3
2	B	206	ILE	3.3
1	A	529	MET	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	248	VAL	3.2
1	A	361	LEU	3.2
2	B	108	LEU	3.2
1	A	294	PRO	3.1
1	A	300	PHE	3.1
2	B	22	ASN	3.1
2	B	41	ALA	3.0
2	B	114	LEU	3.0
2	B	93	GLY	3.0
1	A	146	HIS	3.0
2	B	225	SER	2.9
1	A	255	PHE	2.9
1	A	290	ASN	2.9
1	A	275	LYS	2.9
1	A	272	HIS	2.9
2	B	26	CYS	2.8
2	B	290	LEU	2.8
1	A	249	MET	2.8
1	A	274	GLU	2.6
2	B	75	ALA	2.6
2	B	61	PHE	2.6
2	B	209	SER	2.6
1	A	177	GLU	2.6
2	B	247	CYS	2.6
1	A	528	PRO	2.6
2	B	73	CYS	2.6
1	A	271	HIS	2.5
2	B	106	TRP	2.5
2	B	53	CYS	2.4
2	B	314	THR	2.4
1	A	13	ARG	2.4
2	B	245	THR	2.4
2	B	266	HIS	2.3
2	B	110	GLU	2.3
1	A	409	TRP	2.3
1	A	286	TYR	2.3
1	A	242	GLY	2.3
1	A	301	ALA	2.3
2	B	66	ALA	2.3
2	B	322	VAL	2.2
1	A	241	LYS	2.2
2	B	42	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	60	LEU	2.2
1	A	289	GLN	2.2
1	A	273	SER	2.1
1	A	259	LYS	2.1
1	A	174	THR	2.1
1	A	218	ILE	2.1
1	A	276	GLU	2.1
2	B	223	GLN	2.1
1	A	175	HIS	2.0
2	B	308	LEU	2.0
1	A	240	LYS	2.0
1	A	356	THR	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](#)

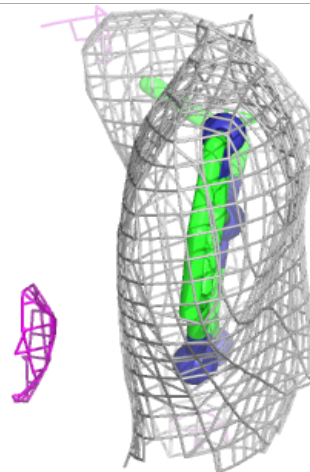
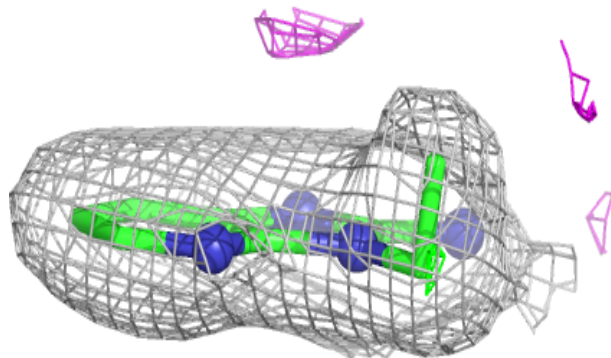
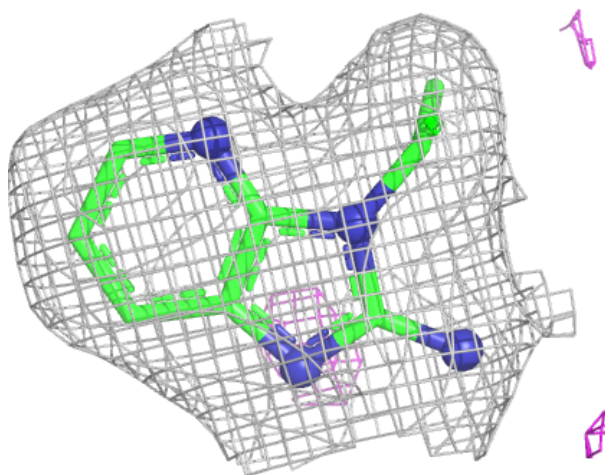
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

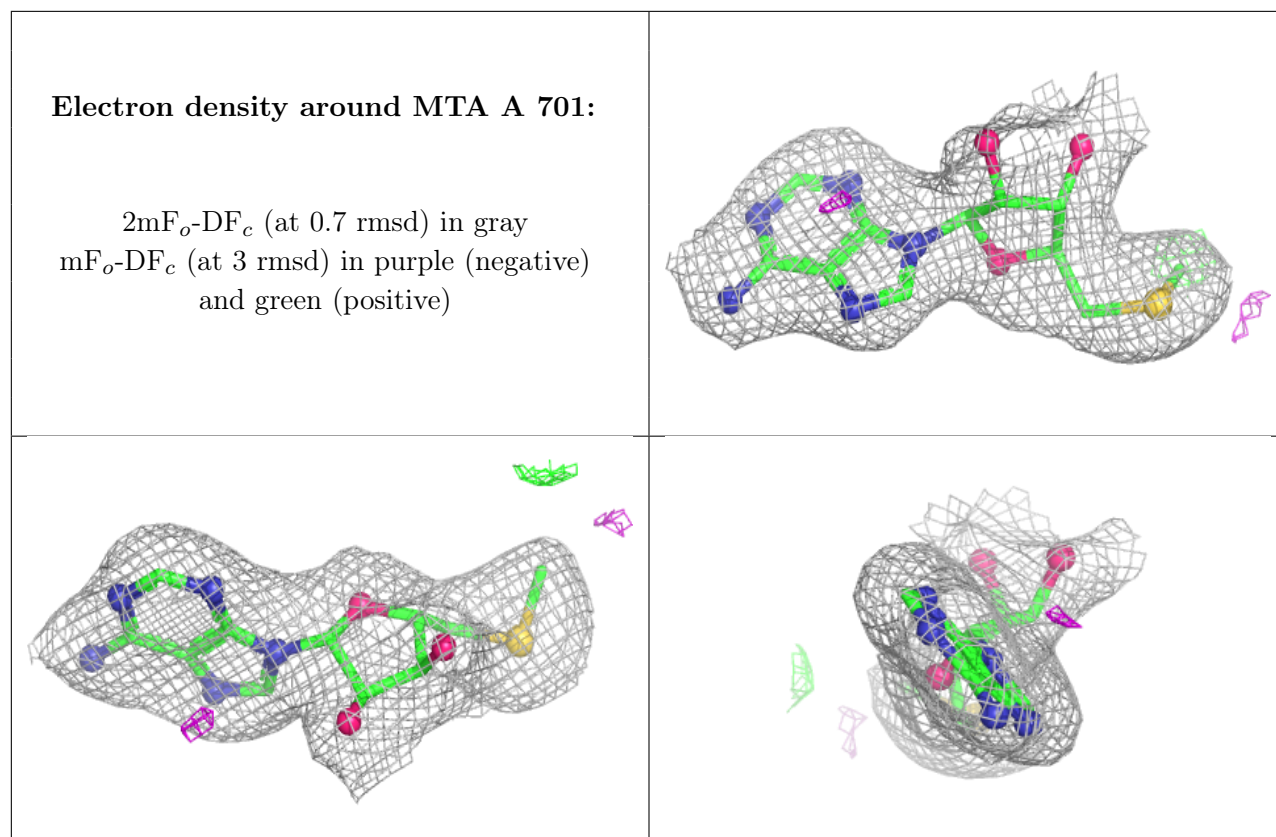
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	703	6/6	0.88	0.17	45,46,48,50	0
5	GOL	B	401	6/6	0.88	0.19	65,67,68,69	0
4	JYX	A	702	12/12	0.96	0.06	17,18,18,18	0
3	MTA	A	701	20/20	0.97	0.05	18,20,21,21	0

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 JYX 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.