



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:23 AM UTC

PDB ID : 7ZUQ / pdb_00007zuq
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 : 2022-05-13
Resolution : 2.48 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

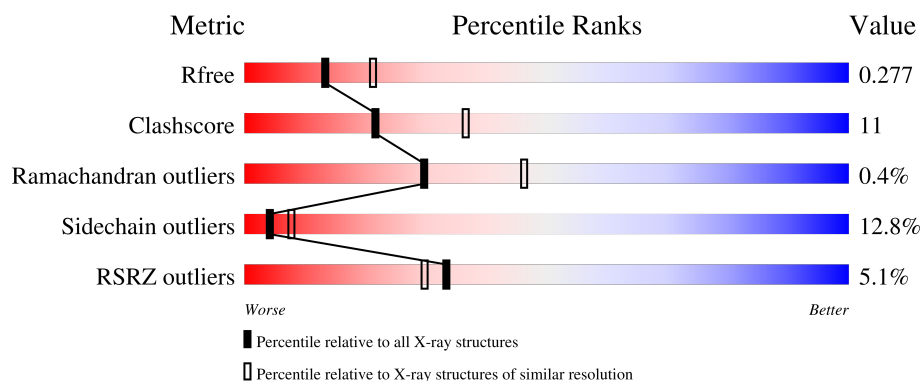
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 67% 26% . .
2	B	350	7% 59% 26% . 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7639 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	4	0
			5092	3255	874	938	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	2	0
			2354	1476	402	461	15			

There are 9 discrepancies between the modelled and reference sequences:

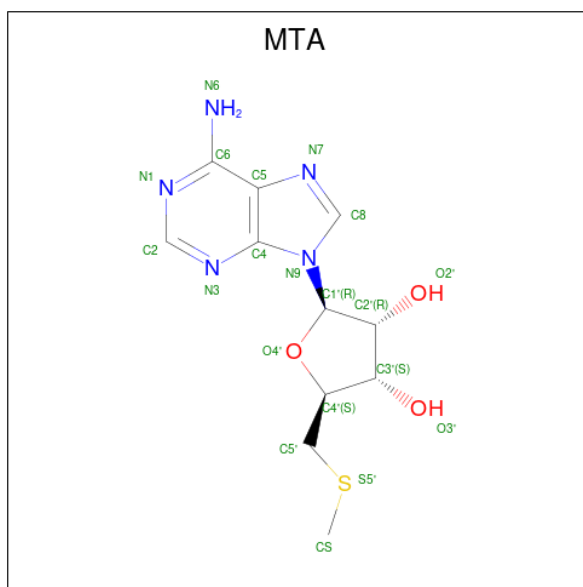
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag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

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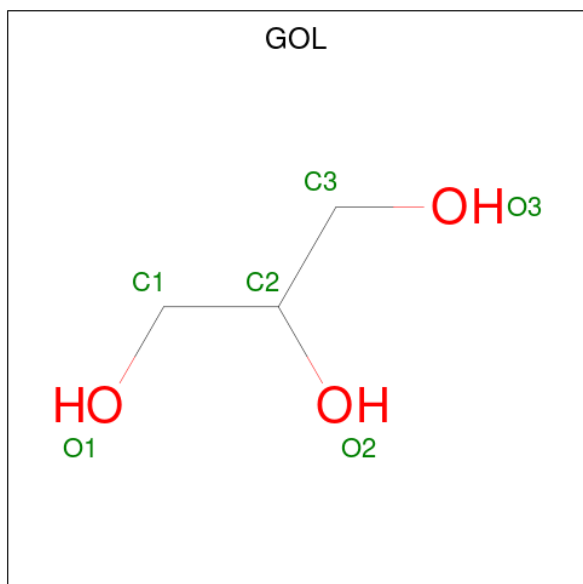
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1

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



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

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Br	C	N	O	0	0
			21	1	13	6	1		

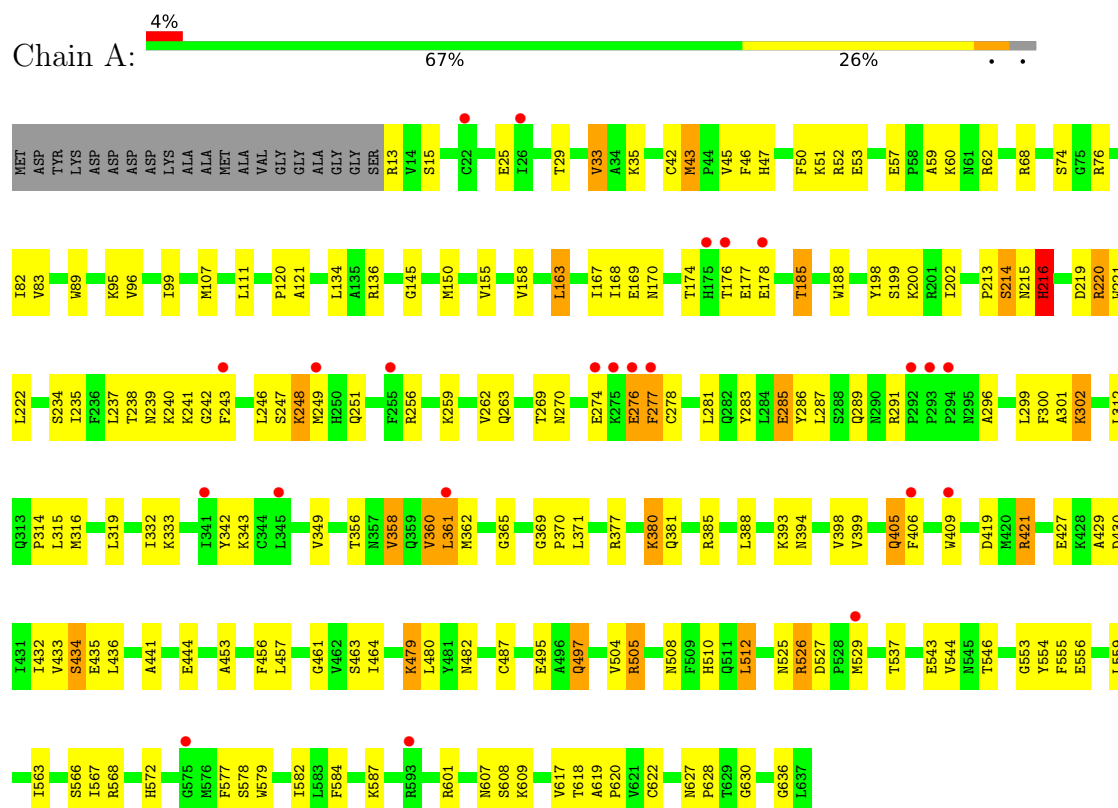
- Molecule 6 is water.

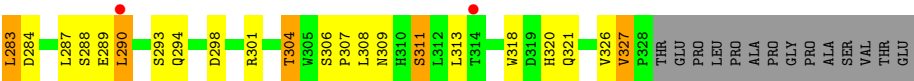
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	118	Total	O	0	0
			118	118		
6	B	22	Total	O	0	0
			22	22		

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





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.86Å 138.23Å 178.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.26 – 2.48 109.26 – 2.48	Depositor EDS
% Data completeness (in resolution range)	51.5 (109.26-2.48) 51.5 (109.26-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.227 , 0.279 0.229 , 0.277	Depositor DCC
R_{free} test set	1173 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7639	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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: MTA, UNL, 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	0.95	0/5234	1.33	3/7121 (0.0%)
2	B	1.06	0/2411	1.29	0/3295
All	All	0.99	0/7645	1.32	3/10416 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	HIS	N-CA-CB	-5.24	101.64	110.49
1	A	584	PHE	CB-CA-C	5.15	115.08	110.44
1	A	145	GLY	CA-C-O	-5.13	117.62	122.39

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	5092	0	4976	106	0
2	B	2354	0	2265	56	0
3	A	20	0	15	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
5	A	21	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	118	0	0	4	0
6	B	22	0	0	1	0
All	All	7639	0	7272	159	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 11.

All (159) 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:553:GLY:HA3	1:A:582:ILE:HG22	1.66	0.76
2:B:145:LYS:HA	2:B:169:GLN:HB2	1.70	0.74
2:B:109:ASP:HB2	2:B:114:LEU:HG	1.68	0.73
1:A:270:ASN:HB2	1:A:277:PHE:CE1	2.24	0.72
1:A:333:LYS:NZ	5:A:703:UNL:BR1	2.78	0.71
2:B:35:ARG:HA	2:B:304:THR:HG21	1.72	0.69
1:A:285:GLU:HG3	1:A:289:GLN:HE22	1.58	0.69
1:A:219:ASP:O	1:A:222:LEU:HG	1.92	0.69
1:A:198:TYR:O	1:A:482:ASN:ND2	2.27	0.68
2:B:29:ARG:HD2	2:B:320:HIS:HB2	1.75	0.68
1:A:453:ALA:HB1	1:A:456:PHE:CZ	2.29	0.67
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.30	0.66
1:A:248:LYS:HA	1:A:251:GLN:HE21	1.61	0.66
1:A:556:GLU:HG2	1:A:566:SER:HB2	1.79	0.65
1:A:537:THR:HG23	1:A:601:ARG:HD3	1.79	0.64
2:B:186:CYS:HB2	2:B:215:PRO:HB2	1.80	0.63
1:A:512:LEU:HG	1:A:546:THR:HG21	1.80	0.63
1:A:360:VAL:HG13	1:A:430:ASP:H	1.63	0.61
1:A:199:SER:HB3	1:A:202:ILE:HD12	1.83	0.60
1:A:222:LEU:HD12	1:A:510:HIS:CD2	2.37	0.60
1:A:301:ALA:HB1	1:A:505:ARG:HG3	1.85	0.59
2:B:217:SER:O	2:B:230:PHE:HA	2.03	0.58
1:A:377:ARG:O	1:A:380:LYS:HG3	2.03	0.58
2:B:87:THR:HG21	2:B:133:VAL:HG22	1.86	0.57
1:A:315:LEU:HD23	1:A:636:GLY:O	2.05	0.57
1:A:82:ILE:O	1:A:120:PRO:HD2	2.05	0.56
1:A:435:GLU:O	5:A:703:UNL:N1	2.38	0.56
1:A:526:ARG:HA	6:A:852:HOH:O	2.04	0.56
1:A:185:THR:HG23	1:A:221:TRP:HZ2	1.71	0.55
2:B:221:HIS:HB2	2:B:227:VAL:HG22	1.89	0.55
1:A:314:PRO:HB3	1:A:319:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:TYR:O	1:A:286:TYR:HB3	2.06	0.55
1:A:419:ASP:OD1	1:A:421:ARG:HD3	2.08	0.54
1:A:300:PHE:CD2	1:A:577:PHE:HB2	2.44	0.53
1:A:45:VAL:HG23	1:A:46:PHE:HD1	1.73	0.53
1:A:251:GLN:HG2	1:A:287:LEU:HD21	1.91	0.53
1:A:405:GLN:HA	1:A:409:TRP:HB2	1.90	0.53
1:A:215[A]:ASN:O	1:A:219:ASP:N	2.42	0.52
1:A:567:ILE:HA	1:A:572:HIS:CD2	2.45	0.52
2:B:27:MET:CE	2:B:68:PRO:HB2	2.39	0.52
1:A:312:LEU:HG	5:A:703:UNL:C8	2.40	0.52
1:A:235:ILE:HG13	1:A:246:LEU:HD21	1.92	0.52
2:B:134:LEU:HD12	2:B:139:GLN:CB	2.38	0.52
1:A:627:ASN:N	1:A:628:PRO:HD3	2.25	0.52
1:A:553:GLY:CA	1:A:582:ILE:HG22	2.39	0.51
2:B:230:PHE:CE1	2:B:238:SER:HB2	2.46	0.51
1:A:567:ILE:HG21	1:A:579:TRP:HB2	1.92	0.51
1:A:495:GLU:HB3	1:A:587:LYS:HE2	1.91	0.51
2:B:36:TYR:H	2:B:304:THR:HG21	1.75	0.51
2:B:134:LEU:HD12	2:B:139:GLN:HB2	1.92	0.51
1:A:441:ALA:HB2	1:A:555:PHE:HB2	1.93	0.51
2:B:28:GLU:HB3	2:B:47:SER:O	2.11	0.50
2:B:107:GLU:HB2	2:B:118:LYS:HG2	1.93	0.50
1:A:62:ARG:HD3	2:B:298:ASP:OD2	2.12	0.50
1:A:316:MET:HE3	1:A:636:GLY:HA3	1.94	0.50
1:A:619:ALA:HA	1:A:620:PRO:C	2.37	0.50
1:A:434:SER:HB2	1:A:436:LEU:HG	1.94	0.50
1:A:215[B]:ASN:O	1:A:219:ASP:N	2.45	0.50
1:A:107:MET:SD	1:A:134:LEU:HD12	2.52	0.49
2:B:27:MET:HE1	2:B:68:PRO:HB2	1.95	0.49
2:B:48:SER:N	2:B:55:ALA:O	2.43	0.49
2:B:32:GLU:HB2	6:B:502:HOH:O	2.13	0.49
1:A:222:LEU:HD12	1:A:510:HIS:CG	2.48	0.49
2:B:284:ASP:OD2	2:B:288:SER:HB2	2.13	0.49
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.95	0.48
1:A:53:GLU:O	1:A:60:LYS:HA	2.13	0.48
1:A:358:VAL:HA	1:A:385:ARG:O	2.13	0.48
1:A:222:LEU:O	1:A:508:ASN:OD1	2.32	0.48
1:A:158:VAL:HG11	1:A:163:LEU:HD13	1.96	0.48
1:A:241:LYS:HB2	1:A:243:PHE:CD2	2.48	0.48
1:A:607:ASN:HB3	1:A:609:LYS:H	1.79	0.48
1:A:51:LYS:HG3	1:A:89:TRP:CE3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:SER:HB3	2:B:189:ASP:OD1	2.13	0.48
1:A:29:THR:O	1:A:33:VAL:HG13	2.14	0.48
1:A:42:CYS:HA	1:A:83:VAL:O	2.13	0.48
1:A:479:LYS:HG3	1:A:480:LEU:N	2.29	0.47
2:B:118:LYS:HA	2:B:118:LYS:HD2	1.72	0.47
1:A:59:ALA:HB2	2:B:278:CYS:SG	2.55	0.47
1:A:51:LYS:O	1:A:62:ARG:NH1	2.48	0.47
1:A:525:ASN:C	1:A:525:ASN:HD22	2.20	0.47
2:B:301:ARG:HD2	2:B:318:TRP:CE2	2.49	0.47
1:A:52:ARG:HA	1:A:62:ARG:HH11	1.80	0.47
1:A:343:LYS:HE3	1:A:563:ILE:HD11	1.97	0.46
1:A:214:SER:HB2	1:A:216:HIS:HB3	1.97	0.46
1:A:246:LEU:HB2	1:A:283:TYR:HE2	1.80	0.46
1:A:487:CYS:C	1:A:497:GLN:HG2	2.40	0.46
1:A:618:THR:HB	6:A:849:HOH:O	2.15	0.46
2:B:235:GLY:HA2	2:B:258:VAL:HG23	1.97	0.46
1:A:276:GLU:HB3	1:A:278:CYS:SG	2.55	0.46
1:A:342:TYR:HD1	1:A:381:GLN:HB3	1.80	0.46
1:A:300:PHE:CE2	1:A:577:PHE:HB2	2.51	0.46
1:A:556:GLU:HG2	1:A:566:SER:CB	2.46	0.46
1:A:302:LYS:HD2	1:A:302:LYS:HA	1.62	0.45
1:A:237:LEU:HD12	1:A:237:LEU:H	1.81	0.45
1:A:617:VAL:O	1:A:622:CYS:HA	2.16	0.45
1:A:43:MET:HE3	1:A:43:MET:HB2	1.85	0.45
1:A:457:LEU:HG	1:A:461:GLY:HA3	1.98	0.45
2:B:58:LEU:HB2	2:B:77:VAL:HG12	1.98	0.45
1:A:52:ARG:HA	1:A:62:ARG:NH1	2.32	0.45
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.84	0.45
1:A:369:GLY:N	1:A:370:PRO:CD	2.80	0.45
1:A:554:TYR:HA	1:A:567:ILE:HD11	1.98	0.45
1:A:185:THR:O	1:A:188:TRP:HB2	2.17	0.44
1:A:342:TYR:CD1	1:A:381:GLN:HB3	2.52	0.44
2:B:290:LEU:H	2:B:290:LEU:HG	1.66	0.44
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.83	0.44
1:A:405:GLN:HG3	1:A:406:PHE:N	2.32	0.44
1:A:525:ASN:HD21	1:A:527:ASP:HB2	1.81	0.44
1:A:296:ALA:O	1:A:300:PHE:N	2.38	0.44
2:B:101:GLY:O	2:B:124:HIS:HB2	2.17	0.44
1:A:568:ARG:O	1:A:572:HIS:N	2.51	0.44
2:B:37:ARG:HD2	2:B:91[A]:GLU:HG3	2.00	0.44
1:A:525:ASN:C	1:A:525:ASN:ND2	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:MET:HE3	1:A:429:ALA:HB2	2.00	0.43
1:A:220:ARG:HD2	1:A:220:ARG:HA	1.75	0.43
1:A:433:VAL:HA	1:A:464:ILE:O	2.18	0.43
1:A:238:THR:CG2	1:A:242:GLY:HA2	2.48	0.43
1:A:222:LEU:N	6:A:801:HOH:O	2.51	0.43
2:B:304:THR:O	2:B:313:LEU:HD12	2.18	0.43
1:A:15:SER:HB3	1:A:263:GLN:HG2	2.01	0.43
2:B:124:HIS:CE1	2:B:150:LYS:HD2	2.54	0.43
2:B:244:SER:O	2:B:245:THR:HG22	2.19	0.43
2:B:172[B]:CYS:HB3	2:B:186:CYS:SG	2.59	0.43
1:A:167:ILE:HB	2:B:202:PRO:HD2	2.01	0.42
1:A:168:ILE:HG22	1:A:170:ASN:OD1	2.19	0.42
2:B:37:ARG:O	2:B:307:PRO:HG3	2.19	0.42
2:B:83:VAL:HG23	2:B:83:VAL:O	2.18	0.42
2:B:172[A]:CYS:HB3	2:B:186:CYS:SG	2.59	0.42
2:B:219:ALA:HB3	2:B:229:VAL:HG23	2.01	0.42
2:B:105:LEU:HB2	2:B:119:PHE:CE2	2.54	0.42
1:A:301:ALA:CB	1:A:505:ARG:HG3	2.48	0.42
2:B:134:LEU:HD12	2:B:139:GLN:HB3	2.01	0.42
2:B:301:ARG:HD2	2:B:318:TRP:NE1	2.34	0.42
2:B:259:THR:HG21	2:B:301:ARG:NH2	2.33	0.42
1:A:361:LEU:O	1:A:388:LEU:HA	2.20	0.42
1:A:214:SER:HB2	1:A:216:HIS:CD2	2.54	0.42
1:A:627:ASN:ND2	1:A:630:GLY:HA2	2.35	0.42
1:A:121:ALA:HA	1:A:150:MET:O	2.20	0.42
1:A:432:ILE:HG13	1:A:463:SER:HA	2.01	0.42
2:B:111:ASN:HB2	2:B:113:THR:HG23	2.01	0.42
2:B:37:ARG:HD2	2:B:91[B]:GLU:HG3	2.01	0.41
2:B:153:ASP:O	2:B:157:GLN:N	2.53	0.41
2:B:306:SER:HB3	2:B:309:ASN:O	2.19	0.41
2:B:153:ASP:OD2	2:B:156:GLN:HB2	2.19	0.41
1:A:96:VAL:HB	1:A:99:ILE:HD12	2.03	0.41
1:A:365:GLY:HA3	3:A:701:MTA:O4'	2.21	0.41
2:B:243:LYS:H	2:B:243:LYS:HG2	1.57	0.41
1:A:362:MET:SD	1:A:456:PHE:CE1	3.14	0.41
2:B:283:LEU:HA	2:B:288:SER:O	2.20	0.41
2:B:79:THR:OG1	2:B:81:ALA:O	2.34	0.41
1:A:394:ASN:O	1:A:398:VAL:HG23	2.21	0.40
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.94	0.40
1:A:434:SER:HB2	6:A:866:HOH:O	2.20	0.40
2:B:311:SER:O	2:B:327:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:ILE:HG23	2:B:168:ALA:O	2.21	0.40
2:B:188:GLU:HA	2:B:214:LEU:HD13	2.03	0.40
2:B:264:SER:N	2:B:270:PHE:O	2.52	0.40
1:A:444:GLU:OE2	5:A:703:UNL:N2	2.54	0.40
2:B:105:LEU:O	2:B:118:LYS:N	2.54	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	627/645 (97%)	601 (96%)	24 (4%)	2 (0%)	36	53
2	B	310/350 (89%)	293 (94%)	15 (5%)	2 (1%)	21	35
All	All	937/995 (94%)	894 (95%)	39 (4%)	4 (0%)	30	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
1	A	216	HIS
1	A	213	PRO
2	B	222	PRO

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	562/570 (99%)	494 (88%)	68 (12%)	5	9
2	B	265/298 (89%)	226 (85%)	39 (15%)	3	5
All	All	827/868 (95%)	720 (87%)	107 (13%)	4	7

All (107) 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	35	LYS
1	A	43	MET
1	A	57	GLU
1	A	68	ARG
1	A	74	SER
1	A	76	ARG
1	A	95	LYS
1	A	136	ARG
1	A	155	VAL
1	A	163	LEU
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	200	LYS
1	A	214	SER
1	A	216	HIS
1	A	220	ARG
1	A	234	SER
1	A	239	ASN
1	A	240	LYS
1	A	247	SER
1	A	248	LYS
1	A	249	MET
1	A	256	ARG
1	A	259	LYS
1	A	262	VAL
1	A	269	THR
1	A	274	GLU

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Mol	Chain	Res	Type
1	A	276	GLU
1	A	277	PHE
1	A	281	LEU
1	A	285	GLU
1	A	291	ARG
1	A	299	LEU
1	A	302	LYS
1	A	332	ILE
1	A	349	VAL
1	A	356	THR
1	A	358	VAL
1	A	360	VAL
1	A	361	LEU
1	A	371	LEU
1	A	380	LYS
1	A	393	LYS
1	A	399	VAL
1	A	405	GLN
1	A	421	ARG
1	A	427	GLU
1	A	434	SER
1	A	479	LYS
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	544	VAL
1	A	559	LEU
1	A	578	SER
1	A	608	SER
2	B	19	LEU
2	B	22	ASN
2	B	39	ASP
2	B	42	LEU
2	B	48	SER
2	B	80	GLU
2	B	91[A]	GLU
2	B	91[B]	GLU
2	B	104	GLU

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Mol	Chain	Res	Type
2	B	111	ASN
2	B	114	LEU
2	B	116	VAL
2	B	118	LYS
2	B	129	SER
2	B	131	VAL
2	B	132	SER
2	B	133	VAL
2	B	156	GLN
2	B	180	ASP
2	B	226	GLU
2	B	227	VAL
2	B	243	LYS
2	B	246	SER
2	B	248	VAL
2	B	249	LEU
2	B	274	LEU
2	B	279	SER
2	B	283	LEU
2	B	287	LEU
2	B	289	GLU
2	B	290	LEU
2	B	293	SER
2	B	294	GLN
2	B	304	THR
2	B	308	LEU
2	B	311	SER
2	B	321	GLN
2	B	326	VAL
2	B	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	140	ASN
1	A	216	HIS
1	A	250	HIS
1	A	289	GLN
1	A	290	ASN
1	A	336	GLN
1	A	359	GLN

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Mol	Chain	Res	Type
1	A	405	GLN
1	A	497	GLN
1	A	510	HIS
1	A	525	ASN
1	A	549	HIS
2	B	78	GLN
2	B	139	GLN
2	B	169	GLN
2	B	178	HIS
2	B	224	GLN
2	B	256	GLN
2	B	310	HIS

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](#)

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	$\# Z > 2$
4	GOL	A	702	-	5,5,5	0.15	0	5,5,5	0.32	0
4	GOL	B	401	-	5,5,5	0.13	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MTA	A	701	-	22,22,22	1.64	5 (22%)	32,32,32	1.88	8 (25%)

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	GOL	A	702	-	-	2/4/4/4	-
4	GOL	B	401	-	-	2/4/4/4	-
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	C5-C4	4.32	1.46	1.39
3	A	701	MTA	C5-N7	-3.32	1.33	1.39
3	A	701	MTA	C4-N9	-2.86	1.31	1.37
3	A	701	MTA	C8-N9	-2.39	1.33	1.37
3	A	701	MTA	C5-C6	2.31	1.47	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	MTA	C5-C4-N3	-5.21	119.54	126.72
3	A	701	MTA	N3-C4-N9	4.43	134.71	127.17
3	A	701	MTA	N3-C2-N1	-3.16	123.79	128.58
3	A	701	MTA	C2-N3-C4	3.14	119.49	111.83
3	A	701	MTA	C4-C5-N7	-3.11	107.02	110.58
3	A	701	MTA	C4-N9-C8	3.03	108.92	105.74
3	A	701	MTA	C5-N7-C8	2.27	107.02	103.45
3	A	701	MTA	C2-N1-C6	2.01	122.03	118.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

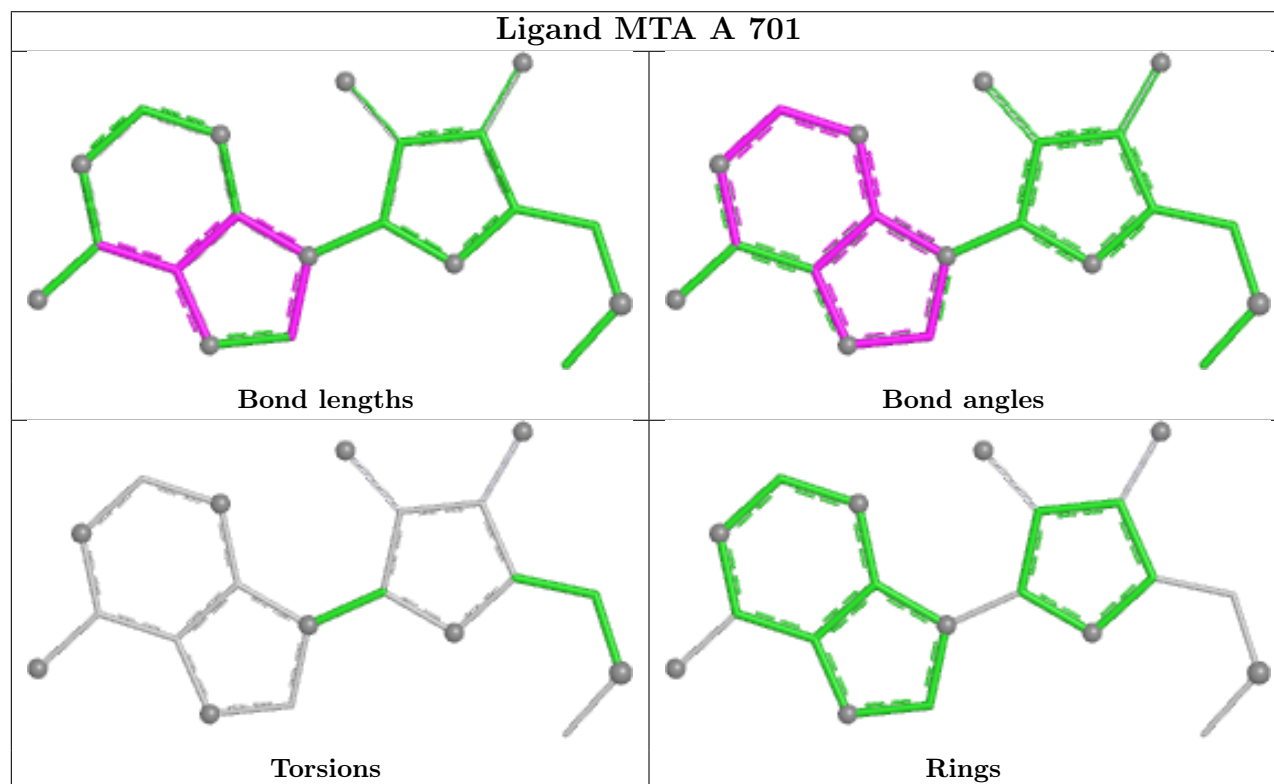
Mol	Chain	Res	Type	Atoms
4	A	702	GOL	C1-C2-C3-O3
4	B	401	GOL	O2-C2-C3-O3
4	B	401	GOL	C1-C2-C3-O3
4	A	702	GOL	O2-C2-C3-O3

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 ⓘ

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%)	0.33	23 (3%) 45 41	12, 32, 65, 106	4 (0%)
2	B	310/350 (88%)	0.74	25 (8%) 18 15	17, 43, 69, 99	2 (0%)
All	All	935/995 (93%)	0.47	48 (5%) 33 30	12, 36, 67, 106	6 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	LEU	6.2
2	B	21	PRO	5.6
2	B	22	ASN	4.0
2	B	210	ALA	3.9
1	A	409	TRP	3.5
1	A	274	GLU	3.4
2	B	114	LEU	3.4
2	B	23	ALA	3.3
2	B	25	ALA	3.3
2	B	245	THR	3.3
1	A	345	LEU	3.2
1	A	275	LYS	3.2
2	B	20	PRO	3.1
1	A	293	PRO	3.1
1	A	277	PHE	3.0
2	B	86	LEU	3.0
2	B	209	SER	2.8
1	A	361	LEU	2.8
1	A	406	PHE	2.8
1	A	292	PRO	2.7
2	B	246	SER	2.7
1	A	529	MET	2.5
1	A	341	ILE	2.5
2	B	41	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	314	THR	2.5
1	A	255	PHE	2.5
2	B	211	PRO	2.5
2	B	268	VAL	2.5
1	A	276	GLU	2.5
1	A	176	THR	2.4
1	A	249	MET	2.3
1	A	26	ILE	2.3
2	B	72	PHE	2.3
2	B	226	GLU	2.3
1	A	575	GLY	2.2
2	B	206	ILE	2.2
2	B	218	LEU	2.2
2	B	24	PRO	2.2
1	A	22	CYS	2.2
1	A	243	PHE	2.2
1	A	294	PRO	2.2
2	B	290	LEU	2.2
1	A	175	HIS	2.1
2	B	26	CYS	2.1
2	B	249	LEU	2.1
1	A	593	ARG	2.0
1	A	178	GLU	2.0
2	B	273	SER	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](#)

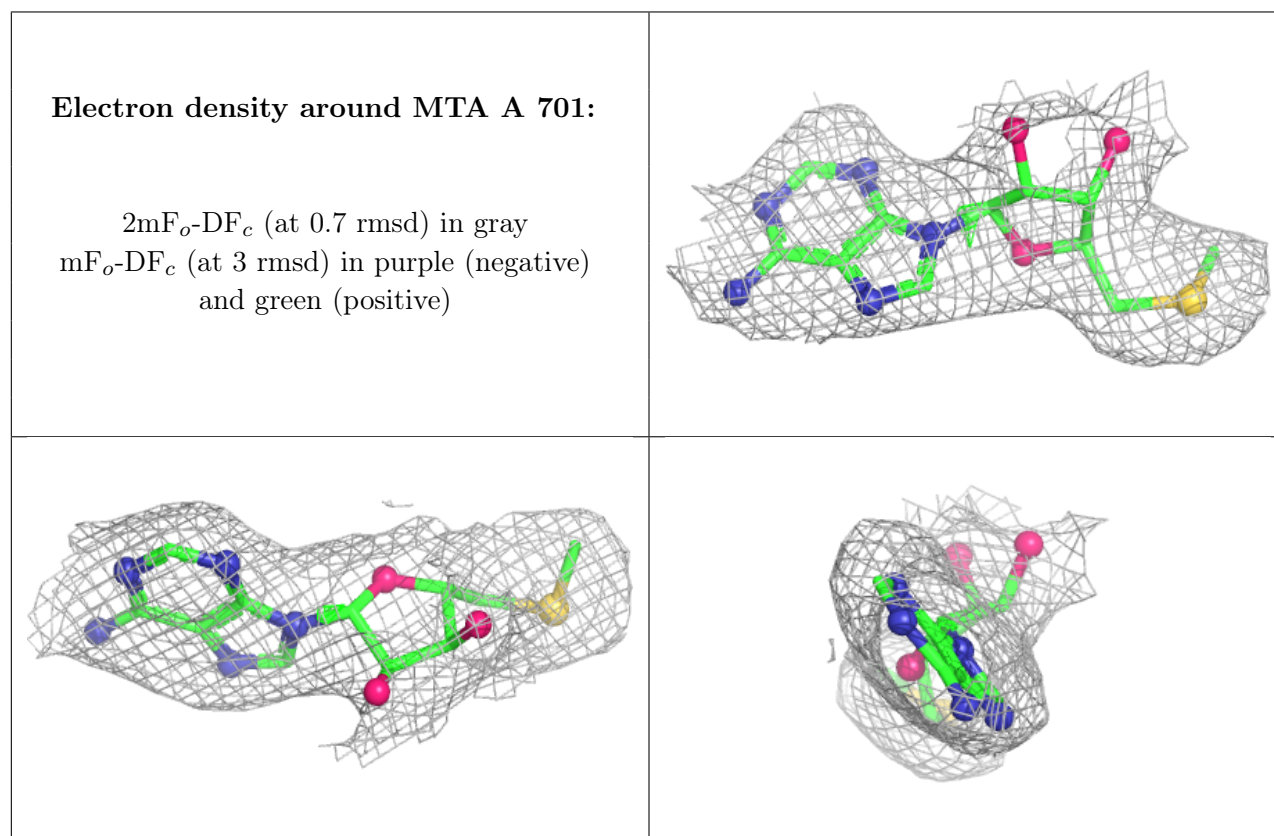
There are no oligosaccharides in this entry.

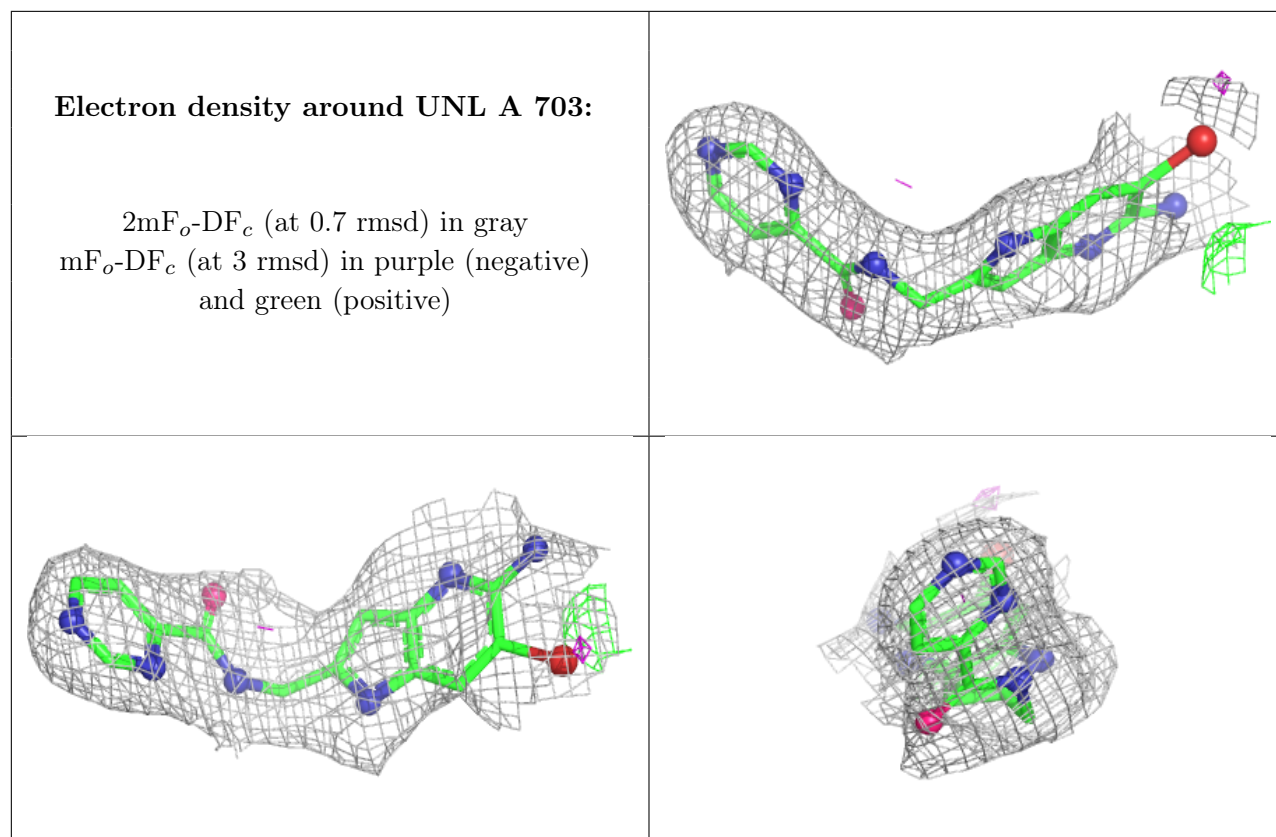
6.4 Ligands [i](#)

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
4	GOL	A	702	6/6	0.82	0.13	31,34,35,36	0
4	GOL	B	401	6/6	0.89	0.10	42,43,44,46	0
3	MTA	A	701	20/20	0.96	0.07	20,21,23,23	0
5	UNL	A	703	21/-	0.97	0.06	25,27,29,33	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.