



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:45 AM EDT

PDB ID : 7ZVL / pdb_00007zvl
Title : HUMAN PRMT5:MEP50 Crystal Structure With MTA and Fragment Bound
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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

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	:	NOT EXECUTED
Xtriage (Phenix)	:	2.0
EDS	:	NOT EXECUTED
Buster-report	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

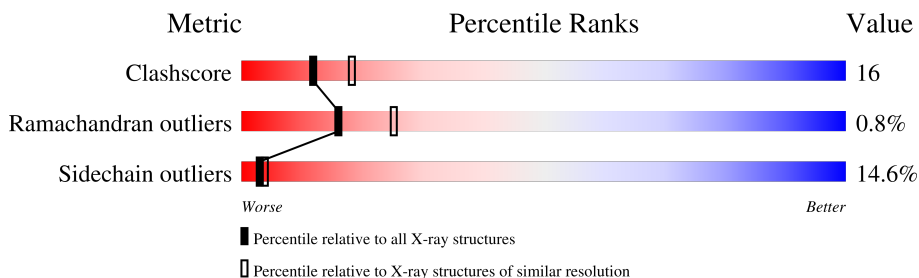
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 ≥ 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 $\leq 5\%$.

Note EDS was not executed.

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

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
1	A	625	Total	C	N	O	S	0	1	0
			5068	3242	870	931	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:

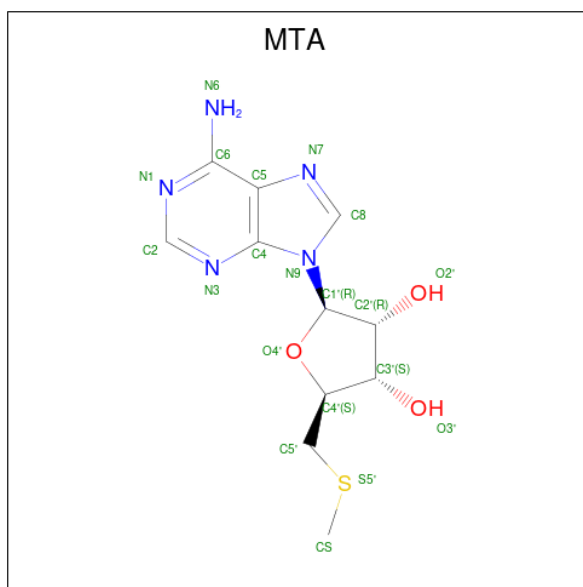
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag	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 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
			13	10	3		

- 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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 7 is water.

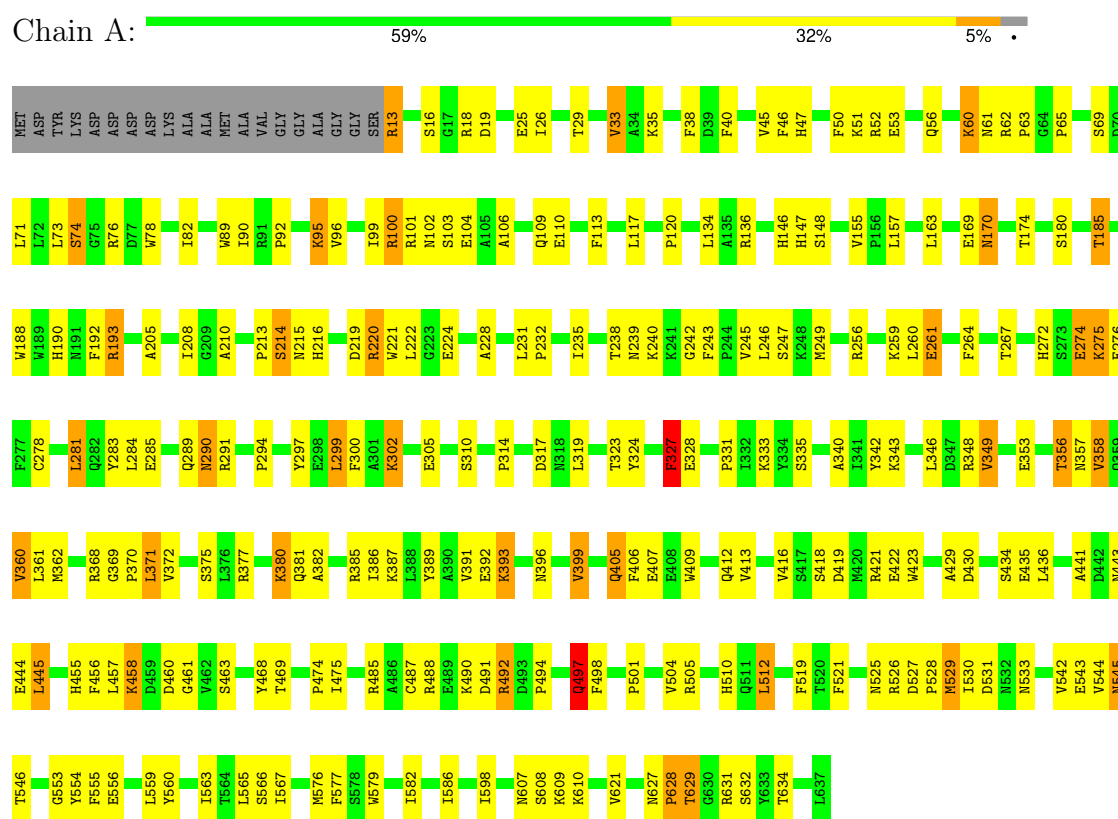
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	111	Total	O	0	0
			111	111		
7	B	24	Total	O	0	0
			24	24		

3 Residue-property plots

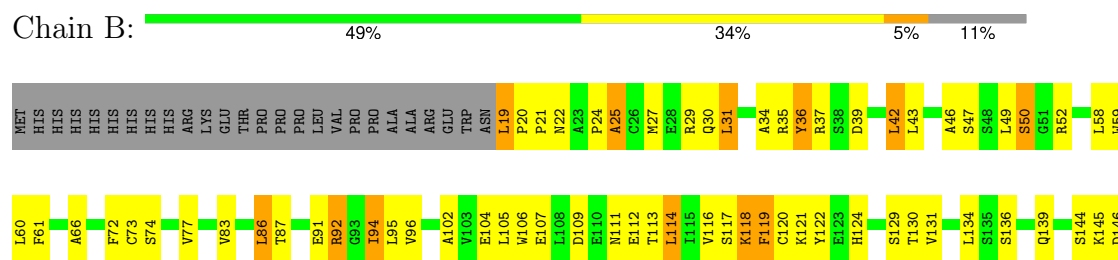
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Protein arginine N-methyltransferase 5



• Molecule 2: Methylosome protein 50





4 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.58Å 138.39Å 178.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.37 – 2.39	Depositor
% Data completeness (in resolution range)	43.8 (109.37-2.39)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.216 , 0.286	Depositor
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.193	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7594	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: CL, UNL, 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	1.04	2/5210 (0.0%)	1.44	14/7088 (0.2%)
2	B	1.12	0/2402	1.33	0/3283
All	All	1.07	2/7612 (0.0%)	1.41	14/10371 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	501	PRO	C-O	-5.37	1.17	1.23
1	A	474	PRO	C-O	-5.36	1.17	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	PHE	CB-CA-C	6.79	124.51	110.31
1	A	331	PRO	CA-C-N	5.97	128.30	120.60
1	A	331	PRO	C-N-CA	5.97	128.30	120.60
1	A	95	LYS	N-CA-C	-5.78	105.72	112.89
1	A	545	ASN	CB-CA-C	5.75	119.24	109.53
1	A	40	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	407	GLU	CA-C-O	-5.52	115.21	120.90
1	A	628	PRO	CB-CA-C	-5.48	104.73	111.64
1	A	586	ILE	CA-C-N	5.42	127.85	120.54
1	A	586	ILE	C-N-CA	5.42	127.85	120.54
1	A	180	SER	CA-C-N	5.36	125.93	119.98
1	A	180	SER	C-N-CA	5.36	125.93	119.98
1	A	100	ARG	N-CA-C	-5.25	105.47	111.14
1	A	497	GLN	CB-CA-C	-5.25	102.41	110.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5068	0	4960	151	0
2	B	2345	0	2260	84	0
3	A	20	0	15	3	0
4	A	13	0	0	4	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
6	A	1	0	0	0	0
7	A	111	0	0	4	0
7	B	24	0	0	3	0
All	All	7594	0	7251	232	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 16.

All (232) 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:327:PHE:CZ	3:A:701:MTA:HCS1	2.13	0.83
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
1:A:327:PHE:C	1:A:327:PHE:HD2	1.95	0.73
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:528:PRO:HG2	1:A:529:MET:HE2	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:327:PHE:C	1:A:327:PHE:CD2	2.74	0.66
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:327:PHE:HZ	3:A:701:MTA:HCS1	1.56	0.64
1:A:485:ARG:HG3	1:A:498:PHE:HZ	1.62	0.63
2:B:147:ILE:HG12	2:B:168:ALA:C	2.23	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:497:GLN:H	1:A:497:GLN:CD	2.19	0.50
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:27:MET:HE2	2:B:320:HIS:NE2	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:NH1	1:A:19:ASP:O	2.46	0.49
2:B:20:PRO:HG2	2:B:74:SER:C	2.37	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
2:B:153:ASP:CG	2:B:156:GLN:HB2	2.38	0.48
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
1:A:274:GLU:C	1:A:275:LYS:HG2	2.37	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
2:B:24:PRO:HD2	2:B:59:TRP:CH2	2.49	0.47
1:A:215:ASN:C	1:A:215:ASN:HD22	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:188:GLU:C	2:B:190:ASN:H	2.23	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:101:ARG:O	1:A:104:GLU:HB2	2.17	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:239:ASN:CG	1:A:243:PHE:HB2	2.42	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
1:A:362:MET:HE3	1:A:429:ALA:HB2	1.98	0.44
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:53:GLU:HA	1:A:102:ASN:ND2	2.34	0.43
1:A:260:LEU:O	1:A:261:GLU:C	2.60	0.43
1:A:405:GLN:HG3	1:A:406:PHE:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:A:701:MTA:H4'	3:A:701:MTA:HCS2	1.84	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: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
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: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:317:ASP:O	1:A:393:LYS:NZ	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:576:MET:HE2	1:A:576:MET:HB3	1.98	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%)	36	50
2	B	309/350 (88%)	281 (91%)	23 (7%)	5 (2%)	7	11
All	All	933/995 (94%)	866 (93%)	60 (6%)	7 (1%)	16	25

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 ⓘ

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%)	490 (88%)	69 (12%)	4	6
2	B	264/298 (89%)	213 (81%)	51 (19%)	1	2
All	All	823/868 (95%)	703 (85%)	120 (15%)	3	4

All (120) 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	60	LYS
1	A	74	SER
1	A	95	LYS
1	A	100	ARG
1	A	136	ARG
1	A	146	HIS
1	A	147	HIS
1	A	148	SER
1	A	155	VAL
1	A	163	LEU
1	A	169	GLU
1	A	170	ASN
1	A	174	THR
1	A	185	THR
1	A	193	ARG
1	A	214	SER
1	A	220	ARG
1	A	235	ILE
1	A	240	LYS
1	A	245	VAL
1	A	247	SER
1	A	249	MET
1	A	256	ARG

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Mol	Chain	Res	Type
1	A	259	LYS
1	A	274	GLU
1	A	275	LYS
1	A	281	LEU
1	A	285	GLU
1	A	290	ASN
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	356	THR
1	A	358	VAL
1	A	360	VAL
1	A	361	LEU
1	A	371	LEU
1	A	372	VAL
1	A	375	SER
1	A	380	LYS
1	A	387	LYS
1	A	393	LYS
1	A	399	VAL
1	A	405	GLN
1	A	445	LEU
1	A	458	LYS
1	A	463	SER
1	A	475	ILE
1	A	490	LYS
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

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Mol	Chain	Res	Type
2	B	19	LEU
2	B	22	ASN
2	B	31	LEU
2	B	36	TYR
2	B	42	LEU
2	B	50	SER
2	B	52	ARG
2	B	60	LEU
2	B	73	CYS
2	B	86	LEU
2	B	91	GLU
2	B	92	ARG
2	B	94	ILE
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	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
2	B	206	ILE
2	B	223	GLN
2	B	224	GLN
2	B	243	LYS
2	B	246	SER
2	B	248	VAL
2	B	249	LEU
2	B	257	CYS
2	B	267	SER
2	B	268	VAL
2	B	274	LEU
2	B	279	SER
2	B	287	LEU

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Mol	Chain	Res	Type
2	B	290	LEU
2	B	292	ARG
2	B	294	GLN
2	B	297	ARG
2	B	300	VAL
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 (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	216	HIS
1	A	250	HIS
1	A	251	GLN
1	A	263	GLN
1	A	282	GLN
1	A	289	GLN
1	A	290	ASN
1	A	336	GLN
1	A	359	GLN
1	A	396	ASN
1	A	405	GLN
1	A	508	ASN
1	A	510	HIS
1	A	511	GLN
1	A	525	ASN
1	A	545	ASN
2	B	190	ASN
2	B	205	GLN
2	B	223	GLN
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](#)

Mogul was not executed - this section is therefore empty.

5.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

5.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

5.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

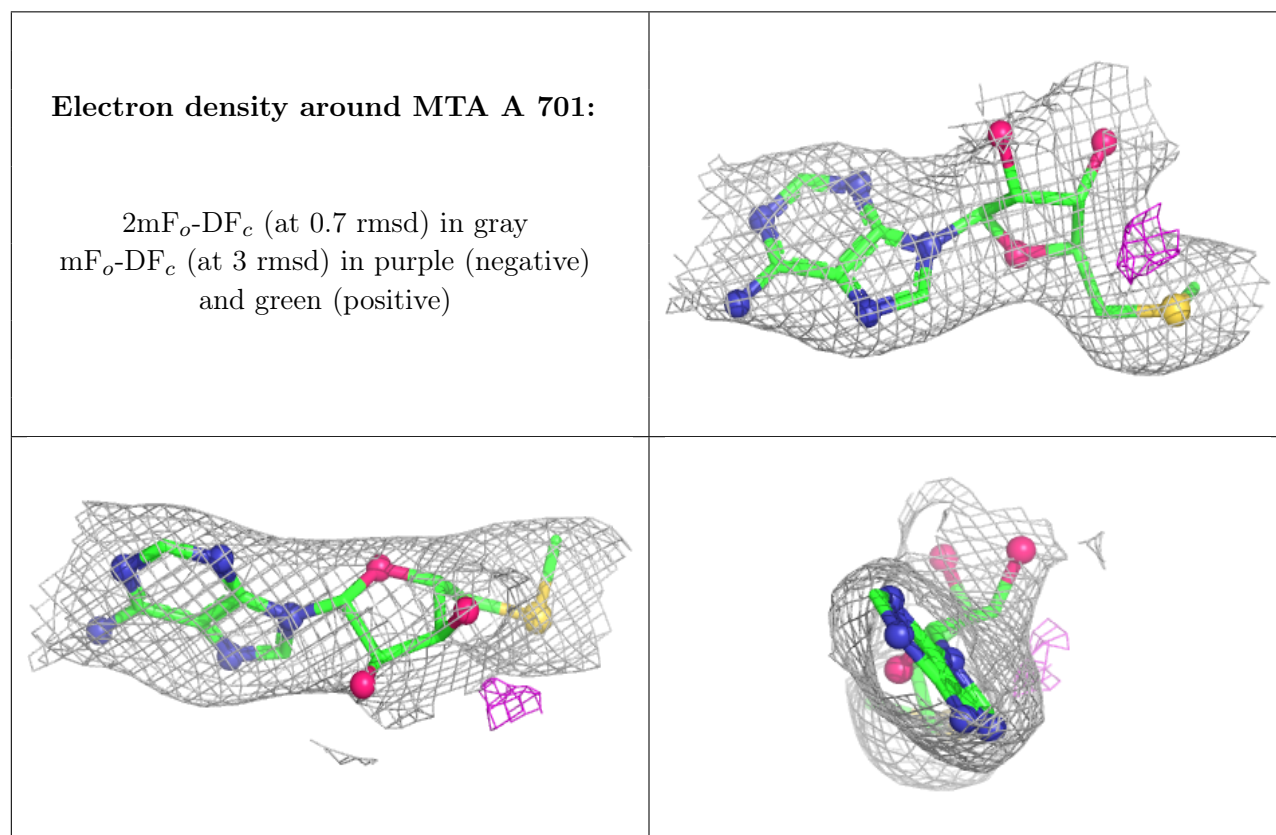
6.3 Carbohydrates [i](#)

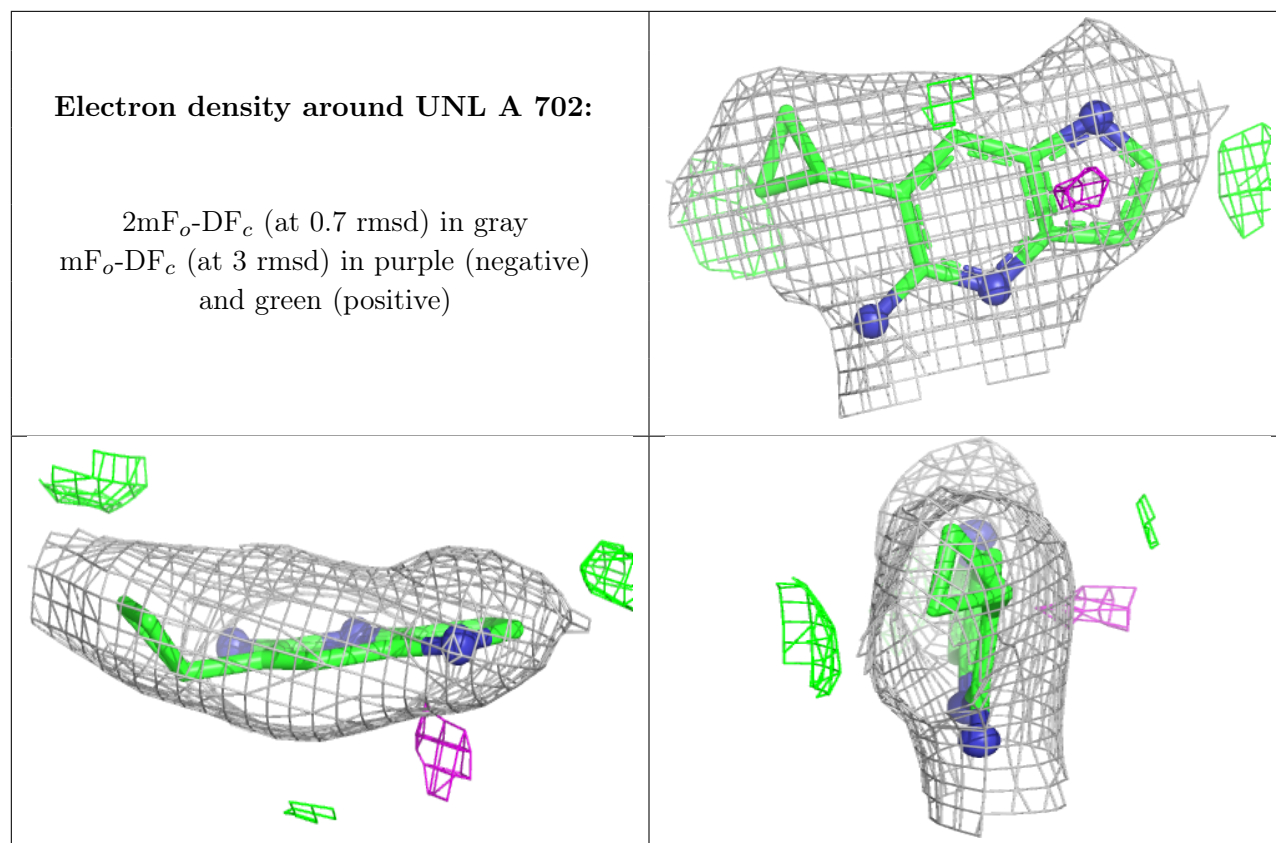
EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

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](#)

EDS was not executed - this section is therefore empty.