



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:56 AM UTC

PDB ID : 9OUC / pdb_00009ouc
Title : Influenza A Virus Nucleoprotein(8-498)NP complex with 5-(4-(morpholinomethyl)phenyl)-2-oxo-6-(trifluoromethyl)-1,2-dihydropyridine-3-carboxamide (Compound 3)
Authors : Mamo, M.
Deposited on : 2025-05-28
Resolution : 2.73 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

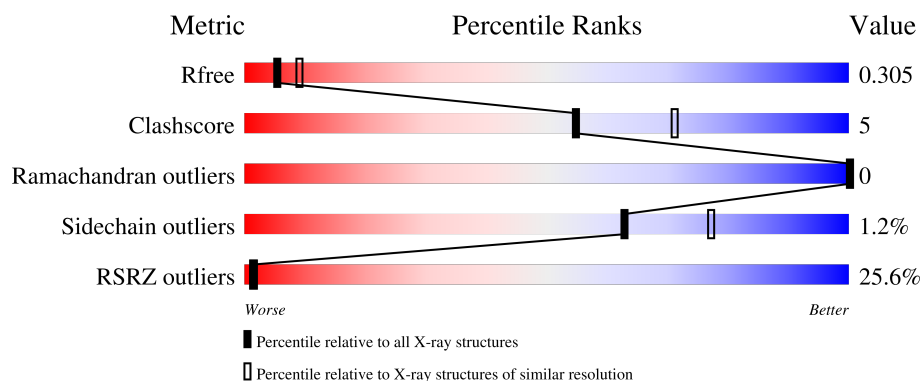
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	498	30% 73% 12% • 14%
1	B	498	14% 75% 10% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6845 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.

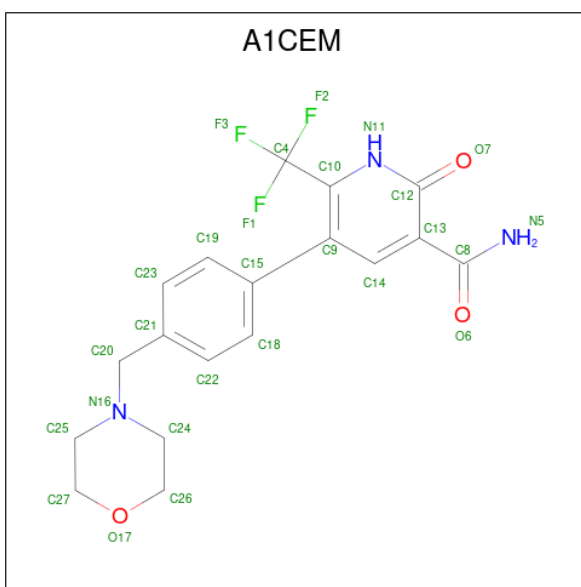
- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3260	2031	598	607	24			
1	B	427	Total	C	N	O	S	0	0	0
			3304	2062	597	618	27			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP P03466
A	499	HIS	-	expression tag	UNP P03466
A	500	HIS	-	expression tag	UNP P03466
A	501	HIS	-	expression tag	UNP P03466
A	502	HIS	-	expression tag	UNP P03466
A	503	HIS	-	expression tag	UNP P03466
A	504	HIS	-	expression tag	UNP P03466
B	7	MET	-	initiating methionine	UNP P03466
B	499	HIS	-	expression tag	UNP P03466
B	500	HIS	-	expression tag	UNP P03466
B	501	HIS	-	expression tag	UNP P03466
B	502	HIS	-	expression tag	UNP P03466
B	503	HIS	-	expression tag	UNP P03466
B	504	HIS	-	expression tag	UNP P03466

- Molecule 2 is 5-{4-[(morpholin-4-yl)methyl]phenyl}-2-oxo-6-(trifluoromethyl)-1,2-dihydropyridine-3-carboxamide (CCD ID: A1CEM) (formula: C₁₈H₁₈F₃N₃O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			27	18	3	3	3		
2	B	1	Total	C	F	N	O	0	0
			27	18	3	3	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

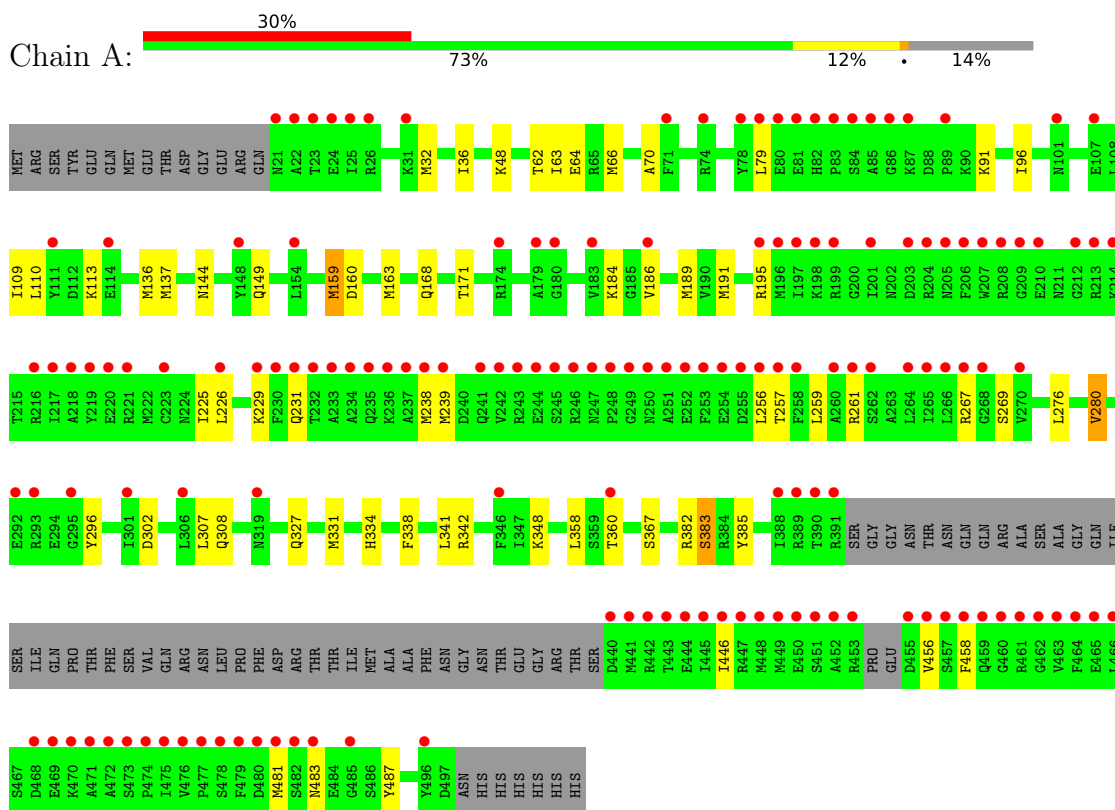
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	132	Total	O	0	0
			132	132		

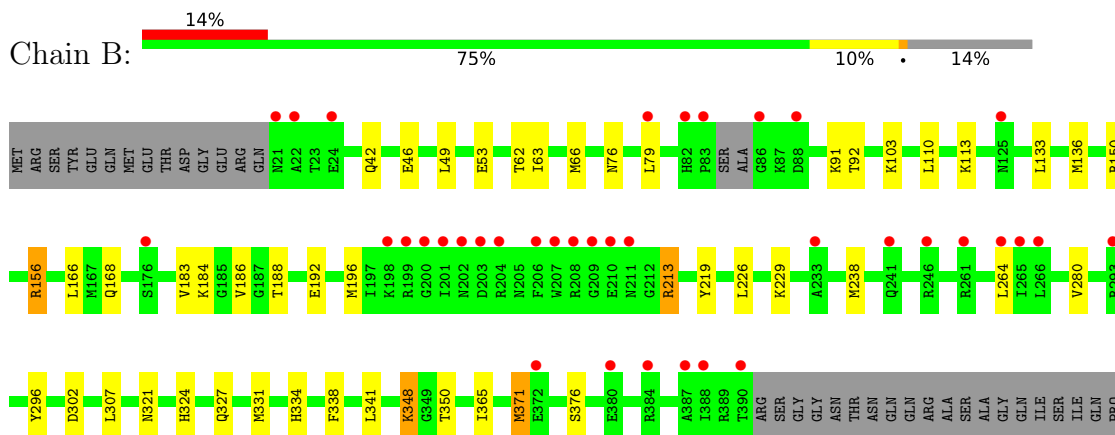
3 Residue-property plots

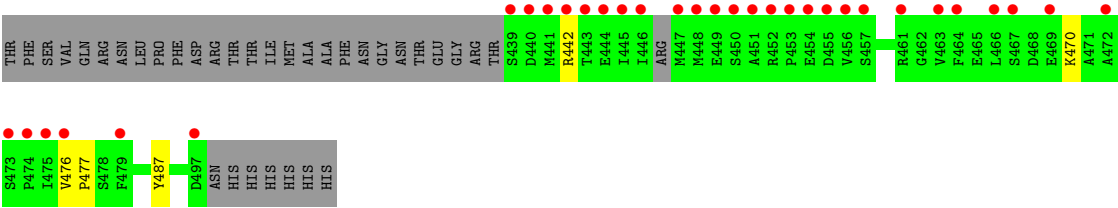
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Nucleoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	72.97Å 96.86Å 285.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	142.63 – 2.73 142.63 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.7 (142.63-2.73) 96.6 (142.63-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.266 , 0.307 0.257 , 0.305	Depositor DCC
R_{free} test set	1300 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6845	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: MG, A1CEM

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	0.68	0/3316	1.10	8/4472 (0.2%)
1	B	0.65	1/3362 (0.0%)	1.06	4/4527 (0.1%)
All	All	0.67	1/6678 (0.0%)	1.08	12/8999 (0.1%)

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	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	MET	SD-CE	-6.59	1.63	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ARG	CA-C-N	6.79	129.26	120.44
1	B	150	ARG	C-N-CA	6.79	129.26	120.44
1	A	458	PHE	CA-CB-CG	6.36	120.16	113.80
1	A	458	PHE	N-CA-C	-5.86	99.35	108.90
1	A	79	LEU	N-CA-CB	-5.45	103.28	111.56
1	A	280	VAL	N-CA-C	-5.37	107.55	111.90
1	B	280	VAL	N-CA-C	-5.33	107.58	111.90
1	A	195	ARG	CA-C-N	5.26	127.59	120.44
1	A	195	ARG	C-N-CA	5.26	127.59	120.44
1	A	267	ARG	N-CA-C	5.22	117.03	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ARG	CB-CA-C	5.22	119.45	110.79
1	A	149	GLN	N-CA-CB	-5.05	102.68	110.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	156	ARG	Sidechain
1	B	213	ARG	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	3260	0	3139	36	2
1	B	3304	0	3231	26	1
2	A	27	0	0	0	0
2	B	27	0	0	0	0
3	B	1	0	0	0	0
4	A	94	0	0	1	0
4	B	132	0	0	0	0
All	All	6845	0	6370	62	3

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 5.

All (62) 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:B:238:MET:HE1	1:B:442:ARG:HG2	1.45	0.97
1:B:238:MET:CE	1:B:442:ARG:HG2	1.96	0.96
1:A:36:ILE:HG23	1:A:136:MET:HE3	1.72	0.70
1:A:238:MET:HB3	1:A:259:LEU:HD11	1.75	0.69
1:B:238:MET:HE2	1:B:442:ARG:HG2	1.79	0.64
1:A:327:GLN:HG2	1:A:331:MET:HE2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:GLN:HG2	1:B:331:MET:HE2	1.81	0.63
1:A:342:ARG:HD3	1:A:483:ASN:O	1.99	0.62
1:A:348:LYS:HA	1:A:383:SER:HB2	1.80	0.61
1:B:365:ILE:HG21	1:B:371:MET:HE1	1.85	0.58
1:A:456:VAL:HG23	1:A:481:MET:HG3	1.88	0.56
1:B:348:LYS:HD2	1:B:350:THR:OG1	2.06	0.55
1:B:166:LEU:HD11	1:B:264:LEU:HD12	1.92	0.51
1:A:159:MET:HE1	1:A:191:MET:HA	1.93	0.51
1:A:331:MET:HE1	1:A:487:TYR:CE1	2.46	0.51
1:B:331:MET:HE1	1:B:487:TYR:CE1	2.46	0.50
1:A:64:GLU:HG2	1:A:136:MET:HE2	1.93	0.49
1:A:342:ARG:NH1	1:A:481:MET:O	2.45	0.49
1:A:189:MET:HE3	1:A:225:ILE:HG22	1.94	0.49
1:B:196:MET:HE3	1:B:219:TYR:HD1	1.77	0.48
1:A:70:ALA:HA	1:A:113:LYS:HD3	1.96	0.48
1:A:168:GLN:HG3	1:A:338:PHE:CD1	2.49	0.48
1:B:307:LEU:CD1	1:B:334:HIS:HE1	2.27	0.48
1:A:239:MET:HE1	1:A:256:LEU:HD23	1.95	0.48
1:A:307:LEU:CD1	1:A:334:HIS:HE1	2.27	0.48
1:B:62:THR:HG22	1:B:66:MET:HE2	1.96	0.47
1:A:62:THR:HG22	1:A:66:MET:HE2	1.96	0.47
1:A:91:LYS:HB3	1:A:110:LEU:HD22	1.96	0.47
1:B:133:LEU:HA	1:B:136:MET:HE3	1.97	0.47
1:A:184:LYS:HB2	1:A:189:MET:HE2	1.96	0.47
1:B:42:GLN:NE2	1:B:46:GLU:OE2	2.49	0.46
1:B:184:LYS:O	1:B:229:LYS:HE3	2.15	0.46
1:A:184:LYS:O	1:A:229:LYS:HE3	2.15	0.46
1:B:168:GLN:HG3	1:B:338:PHE:CD1	2.51	0.46
1:B:91:LYS:HB3	1:B:110:LEU:HD22	1.97	0.46
1:B:63:ILE:HA	1:B:66:MET:HE3	1.98	0.46
1:A:296:TYR:CE1	1:A:302:ASP:HB3	2.52	0.45
1:A:257:THR:O	1:A:261:ARG:HG3	2.16	0.44
1:B:296:TYR:CE1	1:B:302:ASP:HB3	2.52	0.44
1:B:186:VAL:HG13	1:B:226:LEU:HD11	1.98	0.44
1:B:476:VAL:HA	1:B:477:PRO:HD3	1.92	0.44
1:A:144:ASN:HB3	1:A:171:THR:HG21	1.99	0.44
1:A:231:GLN:NE2	1:A:269:SER:HB2	2.32	0.44
1:A:48:LYS:NZ	4:A:710:HOH:O	2.51	0.44
1:A:308:GLN:HA	1:A:382:ARG:HG2	2.00	0.44
1:A:63:ILE:HA	1:A:66:MET:HE3	2.00	0.43
1:B:76:ASN:HA	1:B:79:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:MET:HE2	1:A:137:MET:HB3	1.89	0.43
1:A:358:LEU:HB3	1:A:360:THR:HG22	2.01	0.43
1:B:188:THR:O	1:B:192:GLU:HG3	2.19	0.42
1:A:96:ILE:HG12	1:A:109:ILE:HG12	2.02	0.42
1:A:186:VAL:HG13	1:A:226:LEU:HD11	2.01	0.42
1:B:92:THR:HB	1:B:113:LYS:HE2	2.03	0.41
1:A:238:MET:HE1	1:A:446:ILE:HD13	2.03	0.41
1:B:49:LEU:HD22	1:B:53:GLU:HB3	2.03	0.41
1:A:383:SER:OG	1:A:385:TYR:O	2.39	0.41
1:A:307:LEU:HD12	1:A:334:HIS:HE1	1.85	0.41
1:A:276:LEU:HD13	1:A:280:VAL:HG11	2.03	0.41
1:B:321:ASN:ND2	1:B:324:HIS:CE1	2.90	0.40
1:A:341:LEU:HD11	1:A:487:TYR:HA	2.02	0.40
1:B:341:LEU:HD11	1:B:487:TYR:HA	2.03	0.40
1:A:160:ASP:HB3	1:A:163:MET:HG2	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ASN:OD1	1:A:483:ASN:ND2[4_555]	1.69	0.51
1:B:213:ARG:NH1	1:B:376:SER:O[5_445]	1.83	0.37
1:A:483:ASN:CG	1:A:483:ASN:ND2[4_555]	2.08	0.12

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	422/498 (85%)	416 (99%)	6 (1%)	0	100	100
1	B	421/498 (84%)	415 (99%)	6 (1%)	0	100	100
All	All	843/996 (85%)	831 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	326/420 (78%)	322 (99%)	4 (1%)	63	77
1	B	343/420 (82%)	339 (99%)	4 (1%)	63	77
All	All	669/840 (80%)	661 (99%)	8 (1%)	63	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	159	MET
1	A	367	SER
1	A	383	SER
1	B	103	LYS
1	B	183	VAL
1	B	348	LYS
1	B	470	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	125	ASN
1	A	149	GLN
1	A	231	GLN
1	B	76	ASN
1	B	370	ASN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
2	A1CEM	B	601	-	29,29,29	0.40	0	39,42,42	0.57	1 (2%)
2	A1CEM	A	601	-	29,29,29	0.32	0	39,42,42	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1CEM	B	601	-	-	5/18/26/26	0/3/3/3
2	A1CEM	A	601	-	-	5/18/26/26	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	A1CEM	C15-C9-C10	2.29	125.69	122.86

There are no chirality outliers.

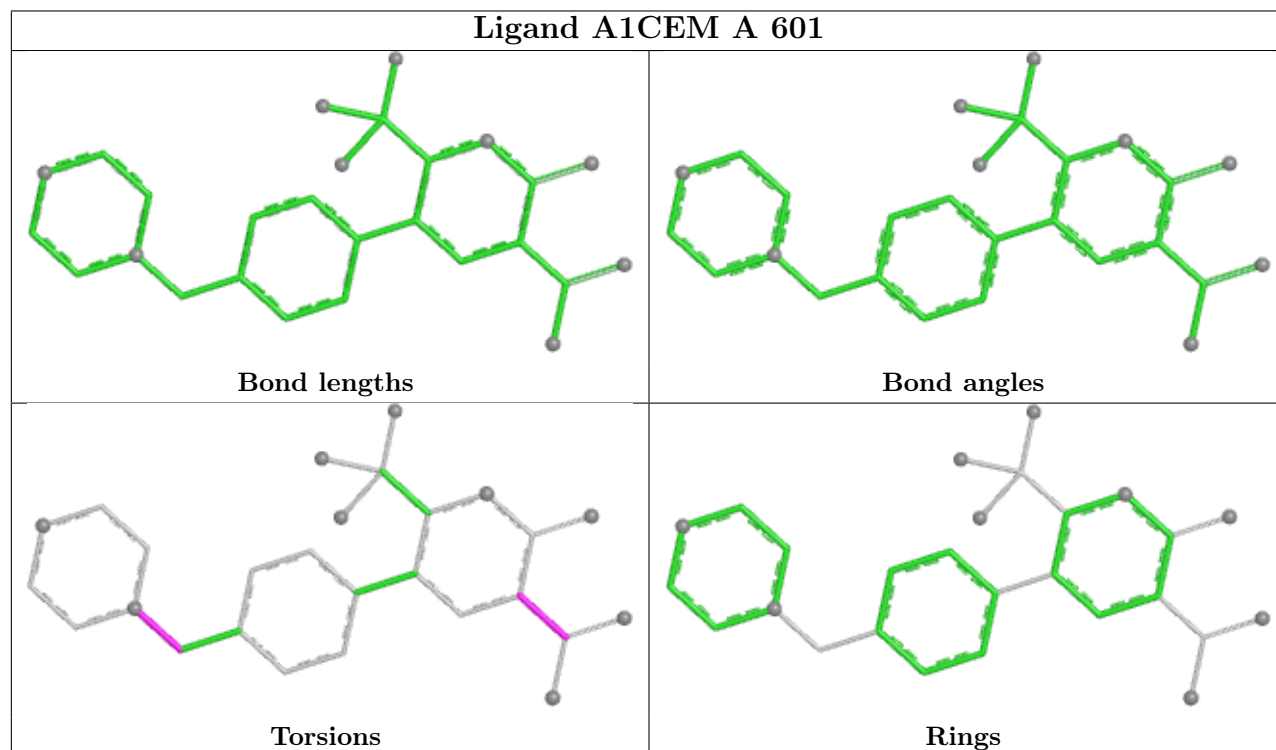
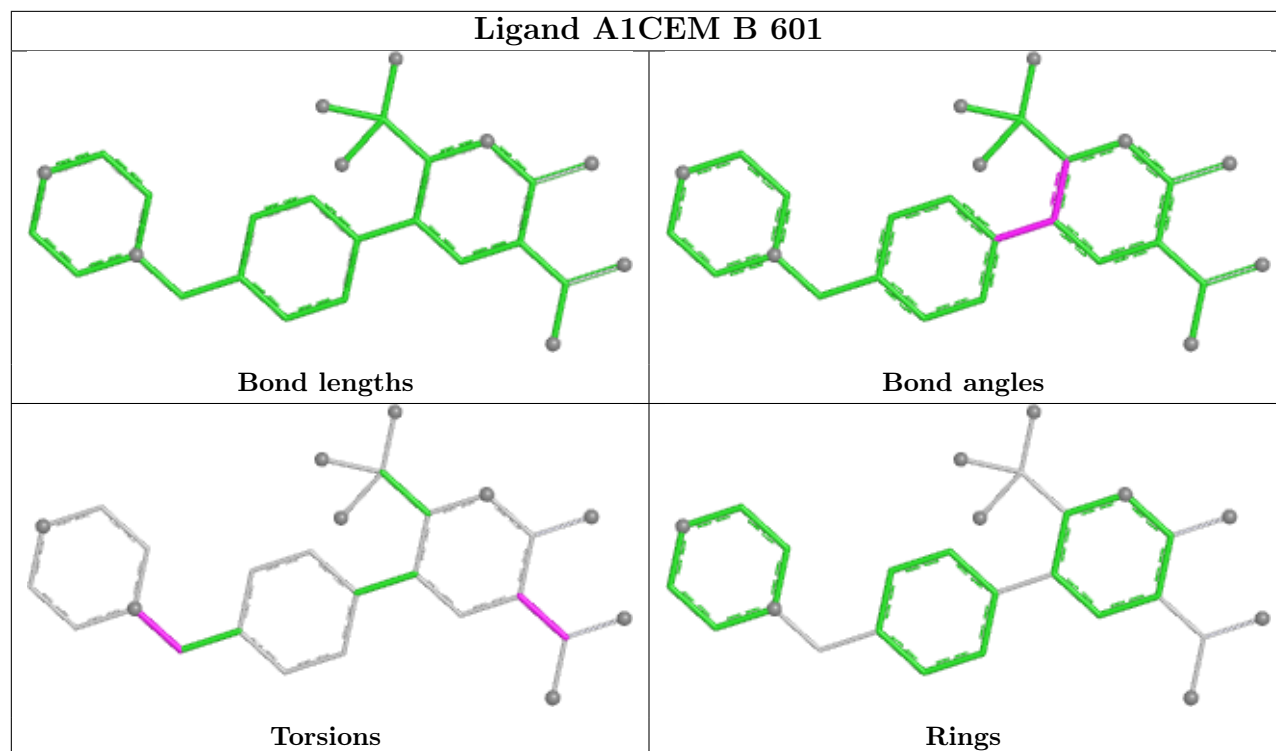
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1CEM	C12-C13-C8-N5
2	A	601	A1CEM	C14-C13-C8-N5
2	A	601	A1CEM	C14-C13-C8-O6
2	B	601	A1CEM	C12-C13-C8-N5
2	B	601	A1CEM	C12-C13-C8-O6
2	B	601	A1CEM	C14-C13-C8-N5
2	B	601	A1CEM	C14-C13-C8-O6
2	B	601	A1CEM	C21-C20-N16-C24
2	A	601	A1CEM	C12-C13-C8-O6
2	A	601	A1CEM	C21-C20-N16-C25

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 ⓘ

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	428/498 (85%)	1.68	150 (35%)  	18, 54, 116, 156	0
1	B	427/498 (85%)	1.13	69 (16%)  	24, 45, 86, 105	0
All	All	855/996 (85%)	1.40	219 (25%)  	18, 49, 106, 156	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	VAL	6.3
1	A	206	PHE	5.2
1	B	456	VAL	5.2
1	A	443	THR	5.1
1	B	455	ASP	5.0
1	A	458	PHE	5.0
1	A	223	CYS	4.9
1	A	453	ARG	4.9
1	A	452	ALA	4.8
1	A	456	VAL	4.8
1	A	462	GLY	4.7
1	A	442	ARG	4.7
1	B	380	GLU	4.7
1	B	439	SER	4.7
1	A	446	ILE	4.6
1	A	204	ARG	4.6
1	A	234	ALA	4.6
1	A	233	ALA	4.5
1	A	449	MET	4.5
1	A	85	ALA	4.5
1	A	464	PHE	4.5
1	A	255	ASP	4.5
1	A	251	ALA	4.4
1	A	209	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	440	ASP	4.2
1	A	22	ALA	4.2
1	A	472	ALA	4.2
1	A	481	MET	4.1
1	A	479	PHE	4.1
1	A	207	TRP	4.1
1	B	454	GLU	4.0
1	A	246	ARG	4.0
1	B	202	ASN	3.9
1	A	444	GLU	3.9
1	A	445	ILE	3.9
1	A	447	ARG	3.9
1	A	252	GLU	3.9
1	A	241	GLN	3.8
1	B	201	ILE	3.8
1	B	453	PRO	3.8
1	A	450	GLU	3.7
1	A	390	THR	3.7
1	A	203	ASP	3.7
1	A	480	ASP	3.7
1	A	217	ILE	3.7
1	A	249	GLY	3.7
1	B	387	ALA	3.7
1	A	451	SER	3.7
1	A	242	VAL	3.6
1	A	440	ASP	3.6
1	B	446	ILE	3.5
1	A	459	GLN	3.5
1	B	390	THR	3.5
1	A	196	MET	3.5
1	A	244	GLU	3.5
1	A	213	ARG	3.5
1	A	475	ILE	3.4
1	A	441	MET	3.4
1	A	478	SER	3.4
1	A	295	GLY	3.4
1	A	477	PRO	3.4
1	A	231	GLN	3.4
1	A	388	ILE	3.4
1	A	457	SER	3.4
1	A	86	GLY	3.4
1	A	179	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	451	ALA	3.4
1	A	253	PHE	3.4
1	A	256	LEU	3.4
1	A	248	PRO	3.3
1	B	83	PRO	3.3
1	B	82	HIS	3.3
1	A	448	MET	3.3
1	A	201	ILE	3.3
1	A	212	GLY	3.3
1	A	87	LYS	3.3
1	A	195	ARG	3.2
1	B	21	ASN	3.2
1	A	461	ARG	3.2
1	A	239	MET	3.2
1	A	473	SER	3.2
1	A	476	VAL	3.1
1	A	208	ARG	3.1
1	A	243	ARG	3.1
1	A	292	GLU	3.1
1	A	266	LEU	3.1
1	B	266	LEU	3.1
1	B	444	GLU	3.1
1	A	235	GLN	3.1
1	A	268	GLY	3.1
1	A	236	LYS	3.1
1	A	101	ASN	3.0
1	A	471	ALA	3.0
1	A	84	SER	3.0
1	B	461	ARG	3.0
1	A	455	ASP	3.0
1	B	467	SER	3.0
1	A	205	ASN	3.0
1	B	22	ALA	3.0
1	B	208	ARG	2.9
1	A	474	PRO	2.9
1	B	441	MET	2.9
1	B	372	GLU	2.9
1	A	78	TYR	2.9
1	A	485	GLY	2.9
1	A	265	ILE	2.9
1	A	219	TYR	2.9
1	A	460	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	245	SER	2.8
1	B	265	ILE	2.8
1	B	79	LEU	2.8
1	B	466	LEU	2.8
1	B	464	PHE	2.8
1	B	474	PRO	2.8
1	A	293	ARG	2.8
1	A	229	LYS	2.7
1	A	247	ASN	2.7
1	B	449	GLU	2.7
1	A	221	ARG	2.7
1	B	443	THR	2.7
1	A	31	LYS	2.7
1	A	250	ASN	2.7
1	A	469	GLU	2.7
1	A	230	PHE	2.7
1	A	257	THR	2.7
1	A	111	TYR	2.7
1	A	267	ARG	2.7
1	B	86	GLY	2.7
1	B	204	ARG	2.7
1	A	114	GLU	2.7
1	B	447	MET	2.6
1	A	79	LEU	2.6
1	A	482	SER	2.6
1	A	468	ASP	2.6
1	A	226	LEU	2.6
1	A	80	GLU	2.6
1	A	21	ASN	2.6
1	A	260	ALA	2.6
1	B	463	VAL	2.6
1	A	232	THR	2.6
1	B	199	ARG	2.6
1	A	82	HIS	2.6
1	B	206	PHE	2.6
1	B	445	ILE	2.5
1	A	261	ARG	2.5
1	A	220	GLU	2.5
1	B	209	GLY	2.5
1	A	346	PHE	2.5
1	B	233	ALA	2.5
1	A	23	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	391	ARG	2.5
1	B	246	ARG	2.5
1	B	448	MET	2.5
1	A	360	THR	2.4
1	A	465	GLU	2.4
1	A	198	LYS	2.4
1	A	270	VAL	2.4
1	A	237	ALA	2.4
1	A	466	LEU	2.4
1	A	210	GLU	2.4
1	B	261	ARG	2.4
1	A	319	ASN	2.4
1	A	74	ARG	2.4
1	A	216	ARG	2.3
1	B	176	SER	2.3
1	B	207	TRP	2.3
1	B	200	GLY	2.3
1	A	183	VAL	2.3
1	A	258	PHE	2.3
1	A	496	TYR	2.3
1	A	214	LYS	2.3
1	B	210	GLU	2.3
1	A	199	ARG	2.3
1	B	88	ASP	2.3
1	B	450	SER	2.3
1	A	174	ARG	2.2
1	B	203	ASP	2.2
1	A	470	LYS	2.2
1	B	198	LYS	2.2
1	B	388	ILE	2.2
1	B	479	PHE	2.2
1	B	472	ALA	2.2
1	A	24	GLU	2.2
1	B	293	ARG	2.2
1	A	264	LEU	2.2
1	B	475	ILE	2.2
1	B	264	LEU	2.2
1	A	83	PRO	2.1
1	A	154	LEU	2.1
1	A	197	ILE	2.1
1	B	457	SER	2.1
1	B	469	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	26	ARG	2.1
1	A	483	ASN	2.1
1	B	241	GLN	2.1
1	A	25	ILE	2.1
1	A	301	ILE	2.1
1	A	254	GLU	2.1
1	B	497	ASP	2.1
1	A	262	SER	2.1
1	A	81	GLU	2.1
1	B	24	GLU	2.1
1	B	384	ARG	2.1
1	A	238	MET	2.1
1	B	211	ASN	2.1
1	A	148	TYR	2.1
1	B	452	ARG	2.0
1	A	218	ALA	2.0
1	B	473	SER	2.0
1	A	306	LEU	2.0
1	A	186	VAL	2.0
1	A	71	PHE	2.0
1	B	442	ARG	2.0
1	A	107	GLU	2.0
1	A	89	PRO	2.0
1	A	180	GLY	2.0
1	B	125	ASN	2.0
1	A	389	ARG	2.0
1	B	476	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,

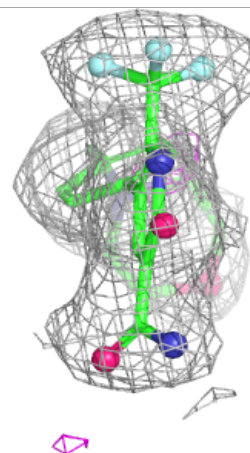
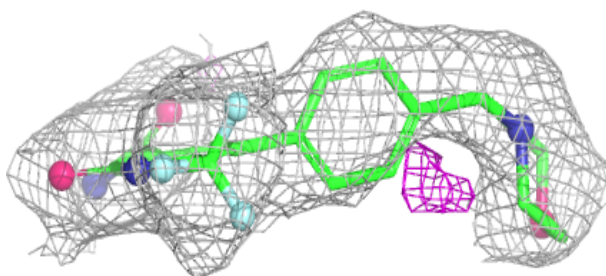
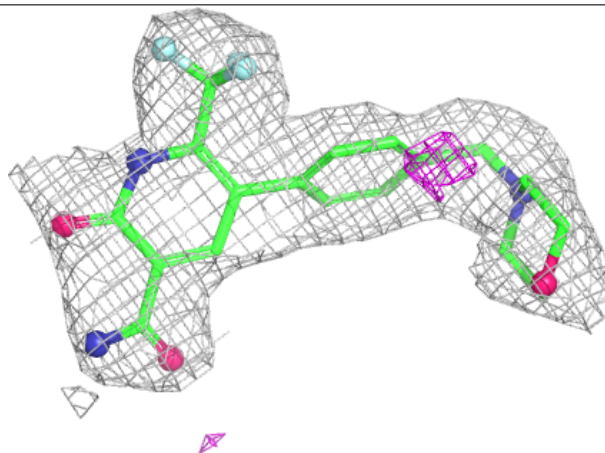
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1CEM	A	601	27/27	0.82	0.16	56,57,59,59	0
2	A1CEM	B	601	27/27	0.85	0.14	38,40,48,48	0
3	MG	B	602	1/1	0.87	0.17	33,33,33,33	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.

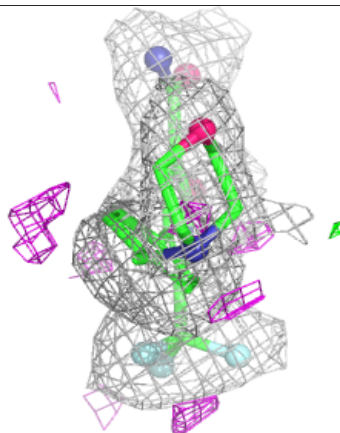
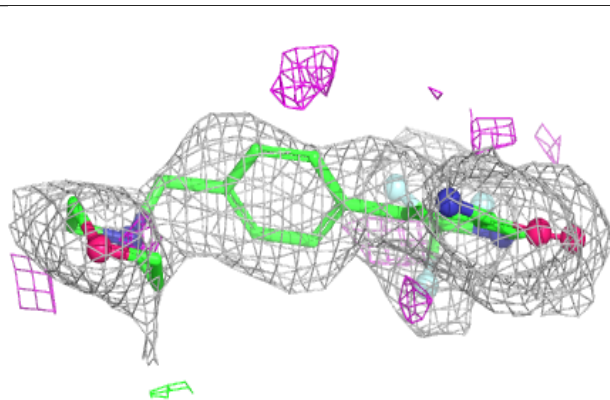
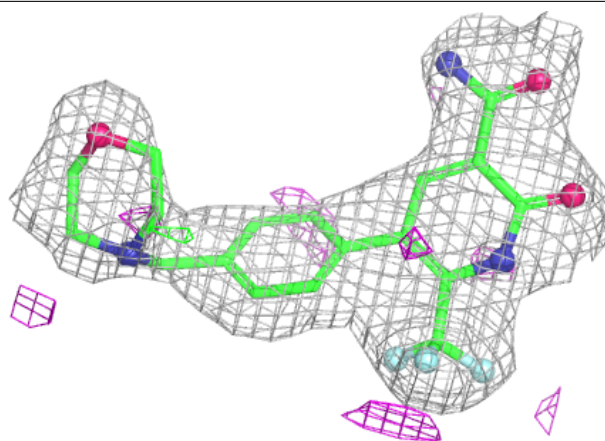
Electron density around A1CEM A 601:

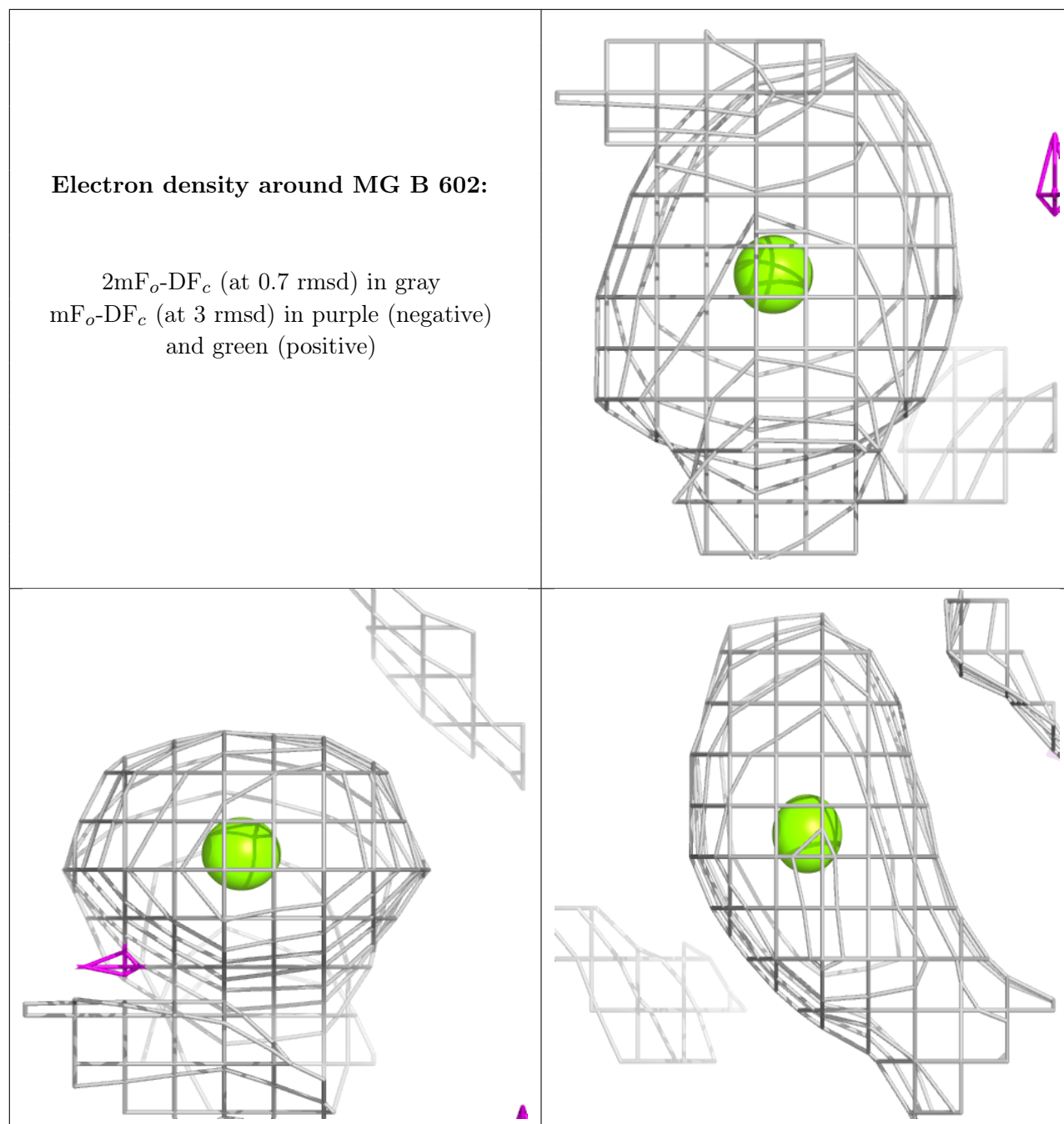
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1CEM B 601:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.