



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2021 – 04:08 PM EST

PDB ID : 7L6R  
Title : Crystal Structure of SARS-CoV-2 Nsp16/10 Heterodimer in Complex with (m7GpppA2m)pUpUpApApA (Cap-1), S-Adenosyl-L-homocysteine (SAH) and Manganese (Mn).  
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Deposited on : 2020-12-23  
Resolution : 1.98 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

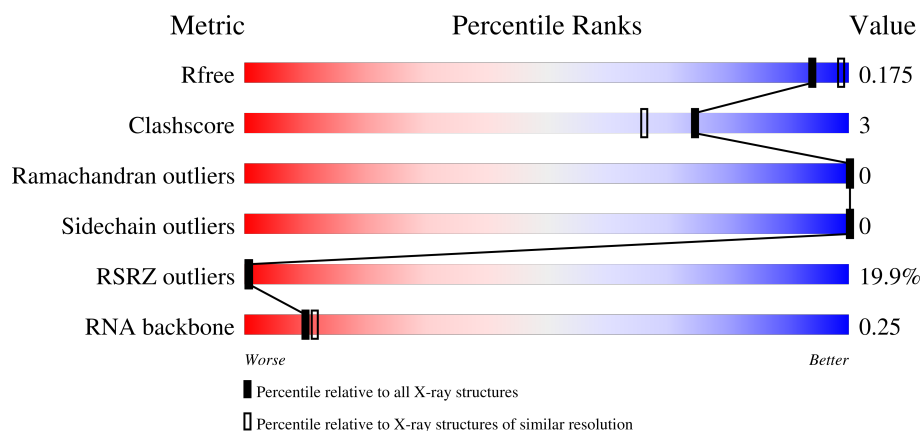
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)
RNA backbone	3102	1105 (2.50-1.46)

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  $\geq 3$ , 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	300	<div> <div>15%</div> <div>95%</div> <div>5%</div> </div>
2	B	141	<div> <div>26%</div> <div>75%</div> <div>23%</div> </div>
3	C	7	<div> <div>29%</div> <div>29%</div> <div>29%</div> <div>14%</div> </div>

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
8	GLC	A	7107	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 3873 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 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	16	0
			2482	1576	419	470	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6797	SER	-	expression tag	UNP P0DTD1
A	6798	ASN	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	109	Total	C	N	O	S	0	2	0
			820	510	137	157	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4252	SER	-	expression tag	UNP P0DTD1
B	4253	ASN	-	expression tag	UNP P0DTD1

- Molecule 3 is a RNA chain called RNA (5'-D\*(M7G))-R(P\*(A2M)P\*UP\*UP\*AP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	P	0	0	0
			118	50	19	42	7			

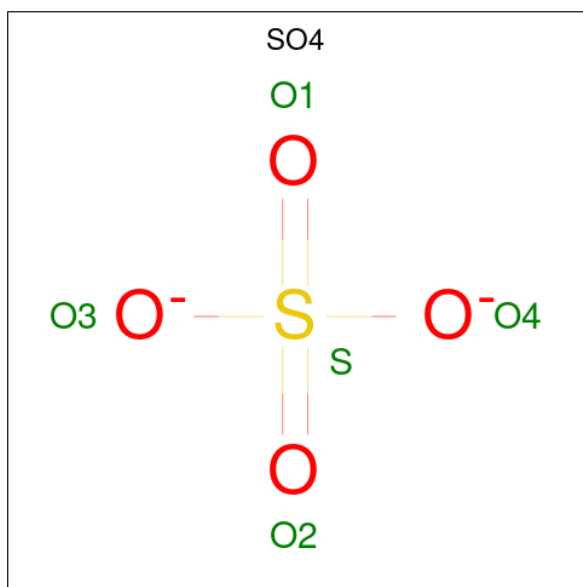
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

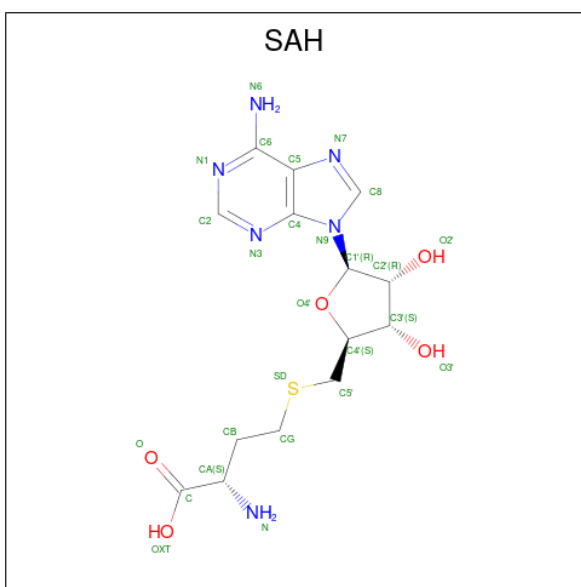
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	1
			3	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



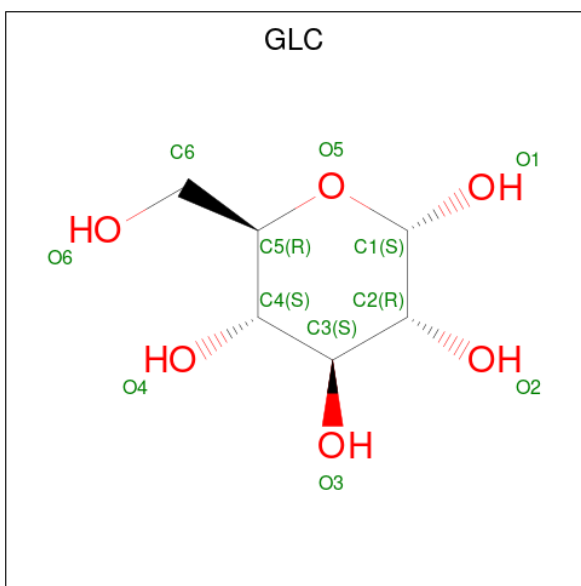
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 8 is alpha-D-glucopyranose (three-letter code: GLC) (formula:  $\text{C}_6\text{H}_{12}\text{O}_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	6	6		
8	A	1	Total	C	O	0	0
			12	6	6		
8	A	1	Total	C	O	0	0
			12	6	6		

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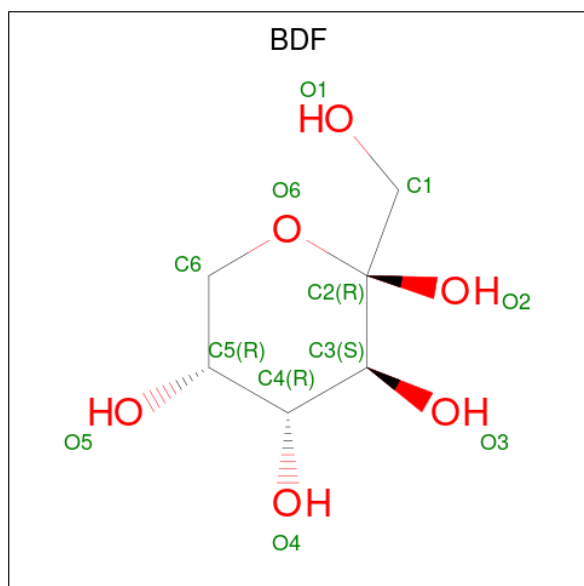
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Zn	0	0
			1	1		

- Molecule 10 is beta-D-fructopyranose (three-letter code: BDF) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			12	6	6		

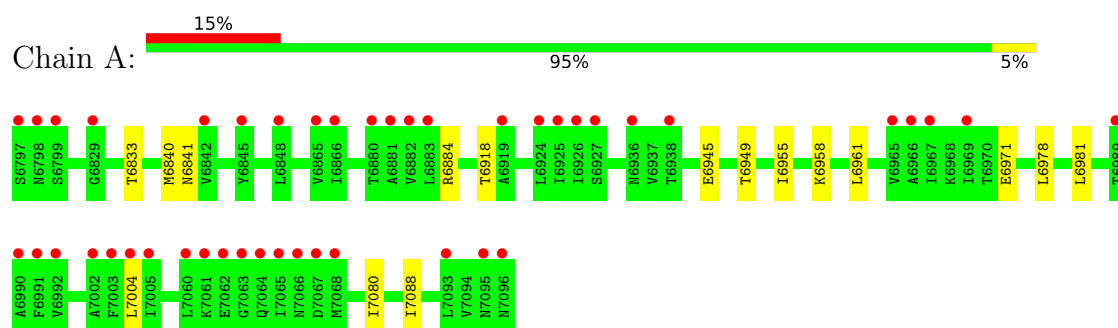
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	269	Total	O	0	17
			281	281		
11	B	50	Total	O	0	3
			53	53		
11	C	22	Total	O	0	2
			23	23		

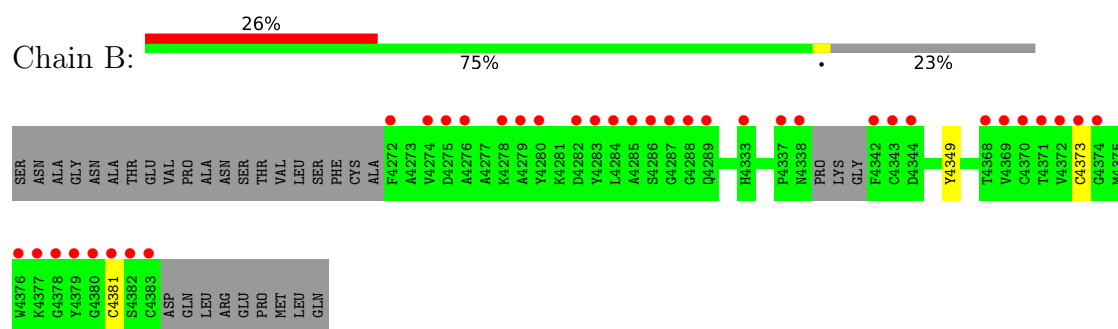
### 3 Residue-property plots

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.

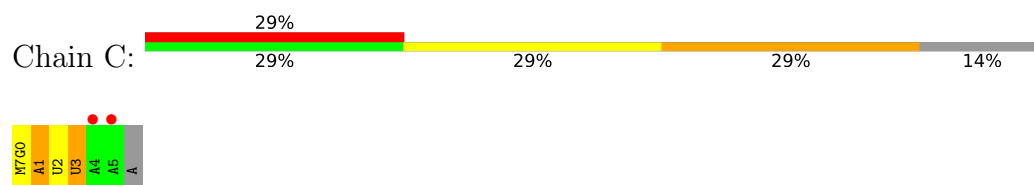
#### • Molecule 1: 2'-O-methyltransferase



#### • Molecule 2: Non-structural protein 10



#### • Molecule 3: RNA (5'-D\*(M7G))-R(P\*(A2M)P\*UP\*UP\*AP\*A)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.76 Å 168.76 Å 52.27 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.95 – 1.98 29.95 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.95-1.98) 99.9 (29.95-1.98)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.98 Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.150 , 0.166 0.158 , 0.175	Depositor DCC
$R_{free}$ test set	3093 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3873	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BDF, ZN, M7G, SO4, A2M, CL, GLC, SAH, MN

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	0.64	0/2534	0.72	0/3436
2	B	0.71	0/837	0.69	0/1133
3	C	0.26	0/73	0.71	0/114
All	All	0.65	0/3444	0.72	0/4683

There are no bond length outliers.

There are no bond angle outliers.

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	2482	0	2447	15	0
2	B	820	0	780	6	0
3	C	118	0	60	6	0
4	A	1	0	0	0	0
5	A	3	0	0	0	0
6	A	5	0	0	1	0
7	A	26	0	19	2	0
8	A	48	0	48	4	0
9	B	1	0	0	0	0
10	B	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	A	281	0	0	0	0
11	B	53	0	0	0	0
11	C	23	0	0	0	0
All	All	3873	0	3366	22	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 3.

All (22) 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:6833:THR:H	8:A:7107:GLC:H1	1.69	0.58
1:A:6840:MET:CE	3:C:3:U:C2	2.90	0.54
1:A:6918:THR:HG22	1:A:7088:ILE:HG22	1.89	0.54
1:A:6971:GLU:OE1	3:C:0:M7G:H82	2.07	0.54
1:A:6840:MET:HE2	3:C:3:U:N1	2.26	0.50
1:A:6833:THR:H	8:A:7107:GLC:C1	2.26	0.48
1:A:6978:LEU:HG	1:A:7004[B]:LEU:HD23	1.96	0.47
1:A:6945[B]:GLU:OE1	1:A:6949:THR:OG1	2.33	0.45
1:A:6840:MET:HE3	3:C:3:U:H1'	1.98	0.44
2:B:4373:CYS:CB	2:B:4381:CYS:SG	3.05	0.44
1:A:6841:ASN:ND2	3:C:2:U:H4'	2.32	0.44
1:A:6884[A]:ARG:HB3	2:B:4349:TYR:OH	2.18	0.44
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	2.00	0.43
2:B:4373:CYS:CB	2:B:4381:CYS:HG	2.32	0.43
2:B:4373:CYS:HG	2:B:4381:CYS:HG	1.68	0.42
1:A:6958:LYS:NZ	6:A:7104:SO4:O4	2.53	0.42
7:A:7105:SAH:H3'	8:A:7106:GLC:H1	2.02	0.42
2:B:4373:CYS:SG	2:B:4381:CYS:SG	3.18	0.41
1:A:6955:ILE:CG2	1:A:6981[B]:LEU:HD21	2.51	0.41
7:A:7105:SAH:SD	3:C:1:A2M:CM'	3.09	0.41
1:A:6833:THR:HB	8:A:7107:GLC:H1	2.03	0.41
2:B:4373:CYS:HB3	2:B:4381:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/300 (105%)	309 (98%)	5 (2%)	0	100	100
2	B	107/141 (76%)	103 (96%)	4 (4%)	0	100	100
All	All	421/441 (96%)	412 (98%)	9 (2%)	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	275/260 (106%)	275 (100%)	0	100	100
2	B	91/115 (79%)	91 (100%)	0	100	100
All	All	366/375 (98%)	366 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	3/7 (42%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	3	U

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
3	A2M	C	1	3	18,25,26	1.08	1 (5%)	18,36,39	1.38	3 (16%)

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
3	A2M	C	1	3	-	0/5/27/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	A2M	C5-C4	2.35	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	A2M	N3-C2-N1	-3.96	122.49	128.68
3	C	1	A2M	C4-C5-N7	-2.55	106.74	109.40
3	C	1	A2M	C2-N1-C6	2.15	122.44	118.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	A2M	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\# Z  > 2$
8	GLC	A	7107	-	12,12,12	0.56	0	17,17,17	1.08	2 (11%)
8	GLC	A	7106	-	12,12,12	0.44	0	17,17,17	1.11	1 (5%)
6	SO4	A	7104	-	4,4,4	0.38	0	6,6,6	0.06	0
8	GLC	A	7108	-	12,12,12	0.53	0	17,17,17	0.69	0
7	SAH	A	7105	-	21,28,28	0.62	0	20,40,40	0.87	1 (5%)
8	GLC	A	7109	-	12,12,12	0.47	0	17,17,17	0.54	0
10	BDF	B	4402	-	12,12,12	0.31	0	18,18,18	0.56	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
8	GLC	A	7107	-	-	0/2/22/22	0/1/1/1
8	GLC	A	7106	-	-	0/2/22/22	0/1/1/1
8	GLC	A	7108	-	-	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SAH	A	7105	-	-	0/7/31/31	0/3/3/3
8	GLC	A	7109	-	-	2/2/22/22	0/1/1/1
10	BDF	B	4402	-	-	0/3/23/23	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	7107	GLC	O5-C1-C2	2.84	115.36	110.28
7	A	7105	SAH	C5-C6-N6	2.18	123.66	120.35
8	A	7106	GLC	O5-C5-C6	2.12	111.72	106.44
8	A	7107	GLC	C1-O5-C5	2.07	117.57	113.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	7109	GLC	O5-C5-C6-O6
8	A	7108	GLC	C4-C5-C6-O6
8	A	7109	GLC	C4-C5-C6-O6
8	A	7108	GLC	O5-C5-C6-O6

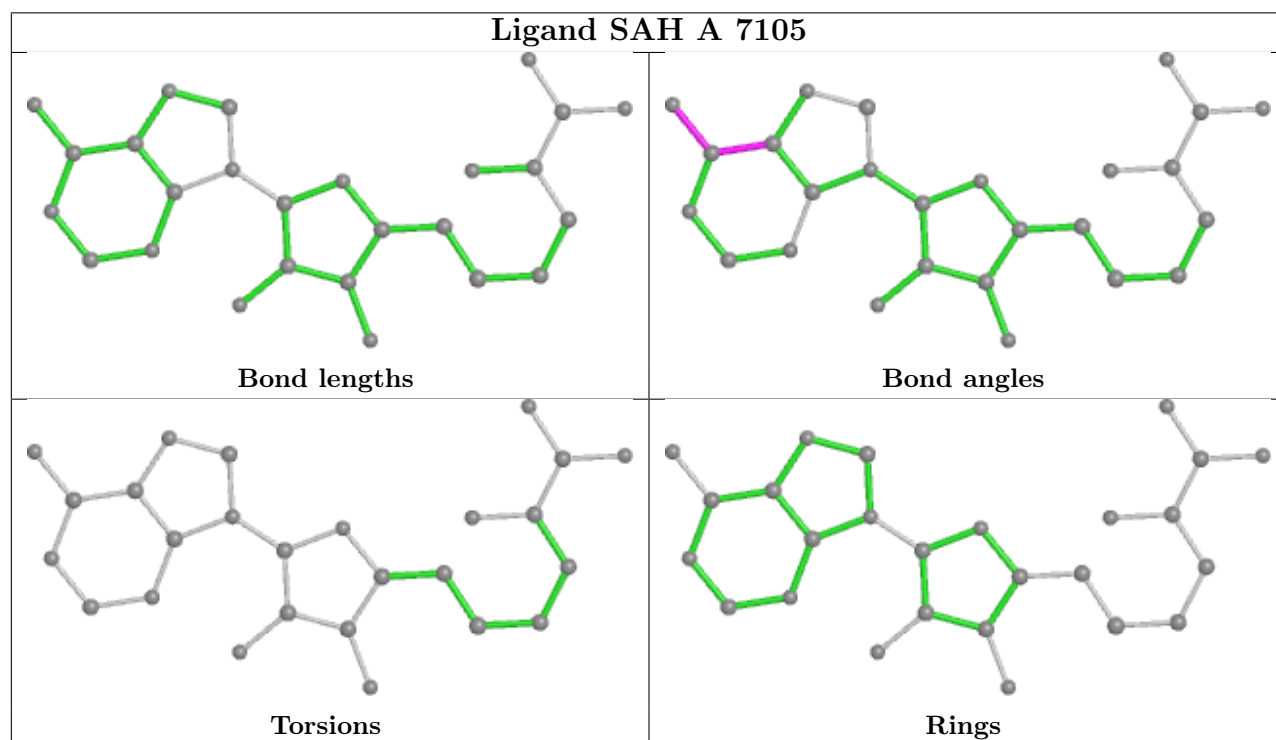
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	7107	GLC	3	0
8	A	7106	GLC	1	0
6	A	7104	SO4	1	0
7	A	7105	SAH	2	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 [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	300/300 (100%)	0.64	44 (14%) 2 2	23, 35, 67, 114	0
2	B	109/141 (77%)	1.61	36 (33%) 0 0	30, 58, 116, 146	0
3	C	4/7 (57%)	2.14	2 (50%) 0 0	49, 57, 117, 127	0
All	All	413/448 (92%)	0.91	82 (19%) 1 1	23, 39, 99, 146	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4383	CYS	12.7
2	B	4342	PHE	8.8
2	B	4372	VAL	8.3
2	B	4371	THR	8.3
1	A	6797	SER	7.8
2	B	4382	SER	7.8
2	B	4381	CYS	7.5
2	B	4373	CYS	6.7
2	B	4370	CYS	6.0
2	B	4285	ALA	5.7
1	A	7062	GLU	5.6
2	B	4377	LYS	5.5
2	B	4289	GLN	5.5
2	B	4287	GLY	5.2
1	A	7063	GLY	5.1
2	B	4338	ASN	5.1
2	B	4337	PRO	5.0
1	A	7004[A]	LEU	4.9
1	A	6967	ILE	4.8
1	A	6798	ASN	4.7
2	B	4286[A]	SER	4.6
2	B	4380	GLY	4.6
3	C	4	A	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	7068	MET	4.5
1	A	7003	PHE	4.4
2	B	4379	TYR	4.4
2	B	4283	TYR	4.3
1	A	6926	ILE	4.3
2	B	4378	GLY	4.2
2	B	4369	VAL	4.2
2	B	4288	GLY	4.2
1	A	7061	LYS	4.2
2	B	4284	LEU	4.2
2	B	4272	PHE	4.2
1	A	7096	ASN	4.1
1	A	6925	ILE	4.1
1	A	7002	ALA	3.9
3	C	5	A	3.7
1	A	6938	THR	3.6
2	B	4374	GLY	3.6
1	A	7005	ILE	3.6
1	A	6966	ALA	3.5
2	B	4282	ASP	3.4
1	A	6919[A]	ALA	3.3
1	A	6924	LEU	3.3
2	B	4274	VAL	3.3
1	A	6969	ILE	3.2
2	B	4278	LYS	3.2
1	A	6965	VAL	3.2
1	A	7064	GLN	3.1
1	A	6829	GLY	3.1
1	A	6848	LEU	3.0
1	A	7066	ASN	2.9
1	A	7067	ASP	2.8
2	B	4275	ASP	2.8
2	B	4280	TYR	2.8
1	A	7060	LEU	2.8
1	A	6990	ALA	2.7
1	A	6991	PHE	2.7
1	A	6866	ILE	2.6
2	B	4276	ALA	2.6
2	B	4376	TRP	2.6
1	A	6883	LEU	2.6
1	A	6936	ASN	2.6
2	B	4333	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	6845	TYR	2.6
1	A	6882	VAL	2.5
2	B	4279	ALA	2.4
1	A	6842	VAL	2.4
1	A	7093	LEU	2.4
1	A	6799	SER	2.4
1	A	6927	SER	2.3
1	A	6992	VAL	2.3
1	A	7065	ILE	2.3
2	B	4343	CYS	2.3
2	B	4368	THR	2.3
1	A	6881	ALA	2.2
1	A	7095	ASN	2.1
1	A	6989	THR	2.1
1	A	6865	VAL	2.1
1	A	6880	THR	2.1
2	B	4344	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	A2M	C	1	23/24	0.95	0.10	34,39,50,50	0

## 6.3 Carbohydrates [i](#)

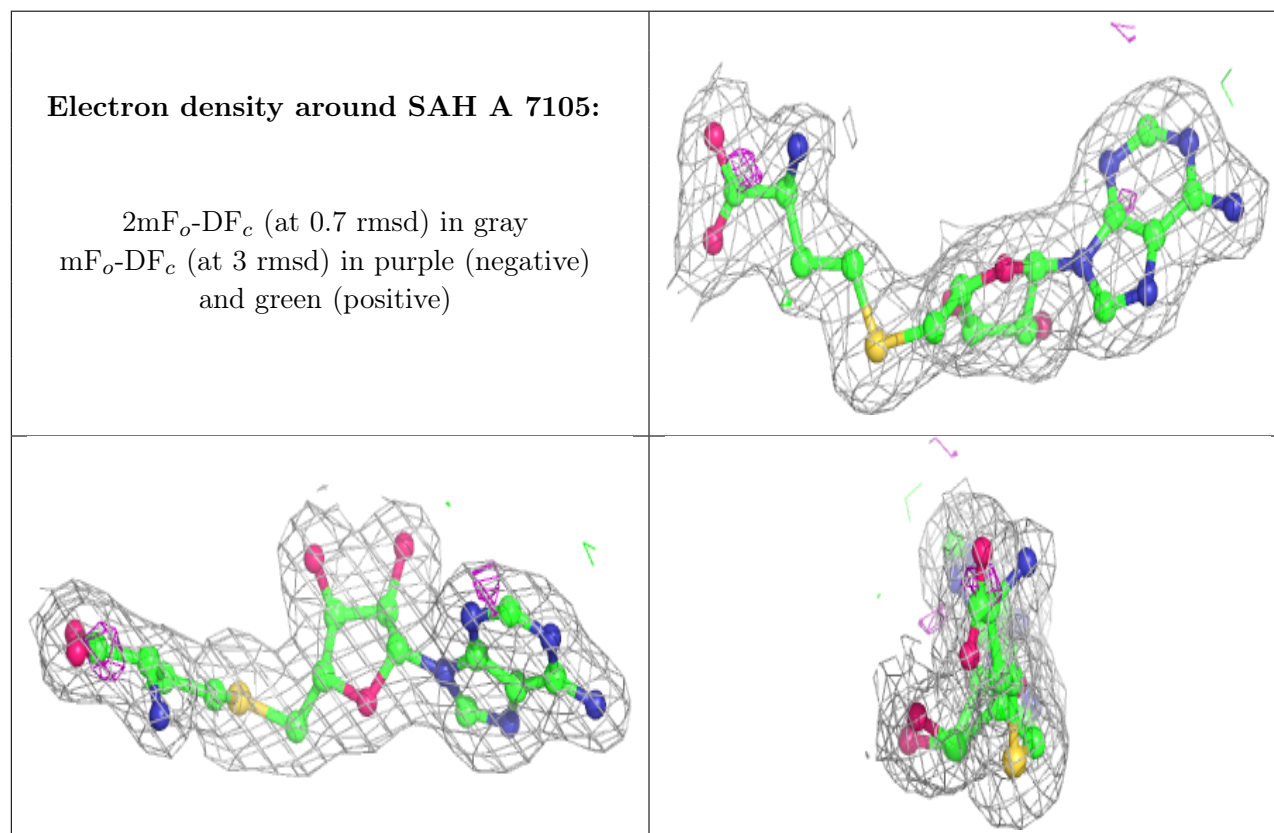
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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.

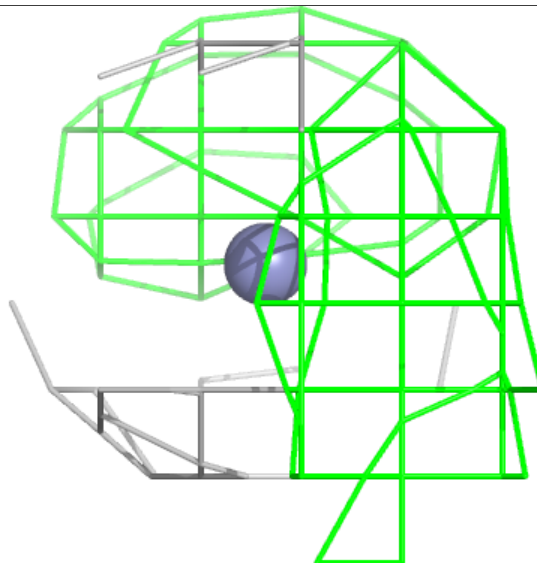
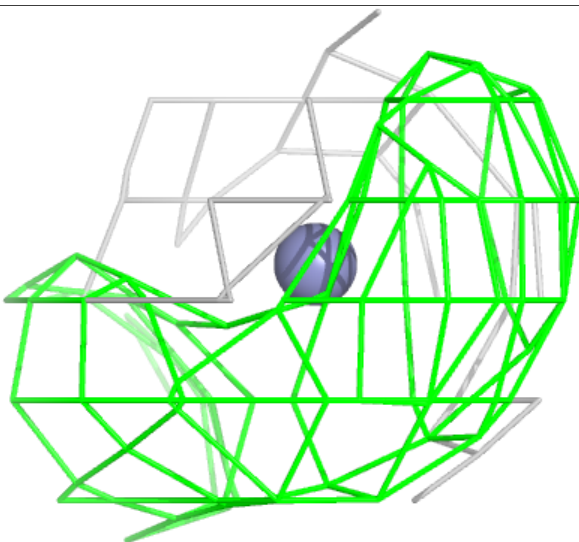
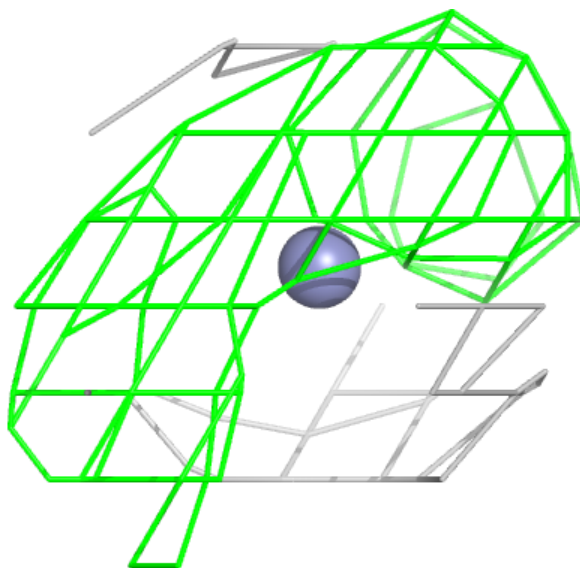
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	GLC	A	7107	12/12	0.76	0.42	46,68,73,79	0
8	GLC	A	7109	12/12	0.76	0.37	101,105,112,113	0
8	GLC	A	7108	12/12	0.80	0.22	53,78,86,89	0
8	GLC	A	7106	12/12	0.81	0.44	41,56,63,67	12
6	SO4	A	7104	5/5	0.91	0.21	52,61,66,67	5
10	BDF	B	4402	12/12	0.91	0.20	51,60,65,67	0
5	CL	A	7102	1/1	0.92	0.23	65,65,65,65	1
5	CL	A	7103[A]	1/1	0.94	0.08	54,54,54,54	1
5	CL	A	7103[B]	1/1	0.94	0.08	57,57,57,57	1
7	SAH	A	7105	26/26	0.96	0.08	31,32,34,36	0
9	ZN	B	4401	1/1	0.96	0.09	39,39,39,39	1
4	MN	A	7101	1/1	0.96	0.09	41,41,41,41	1

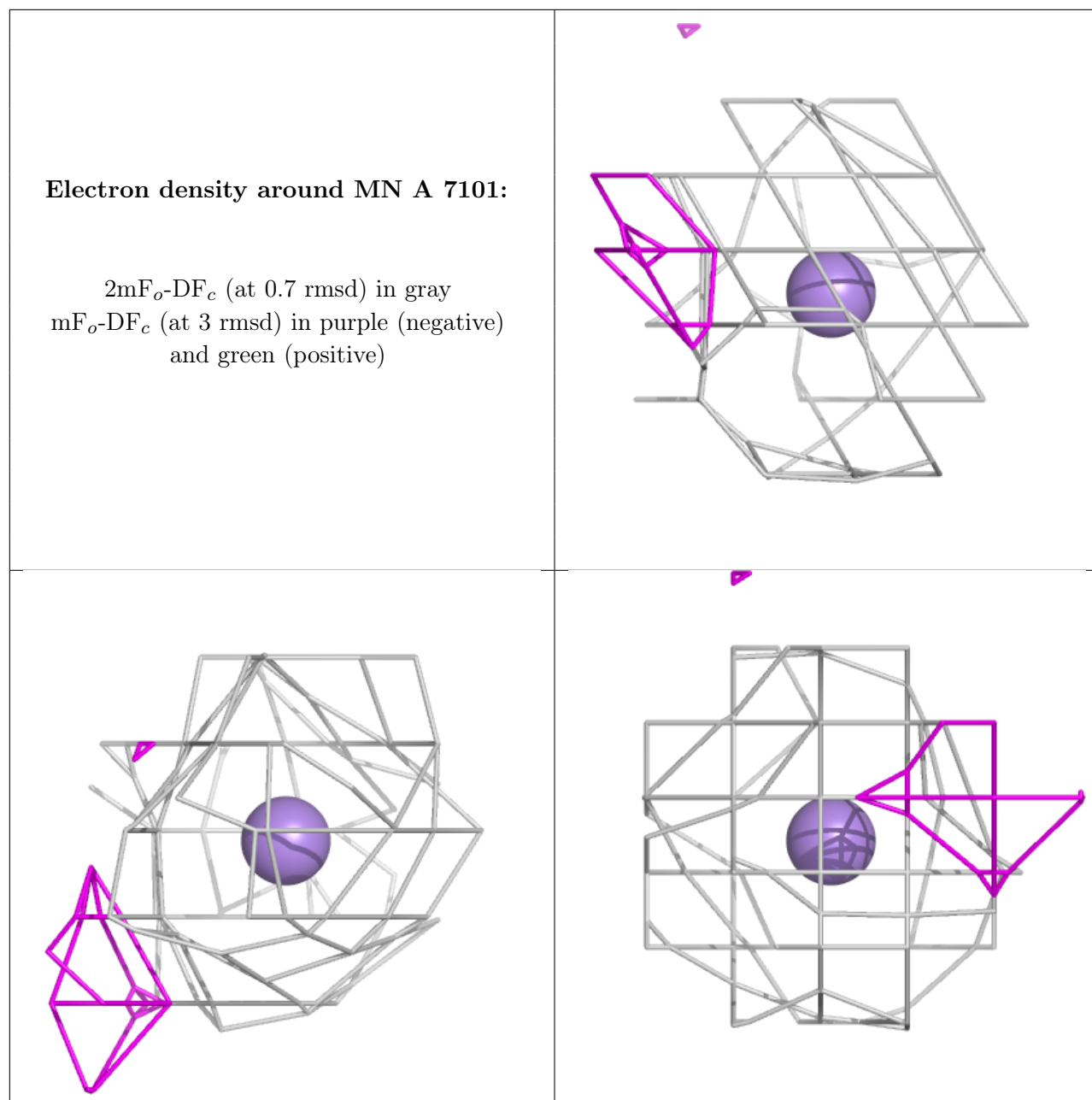
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around ZN B 4401:**

$2mF_o-DF_c$  (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.