



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2021 – 02:19 PM EST

PDB ID : 6WKQ
Title : 1.98 Angstrom Resolution Crystal Structure of NSP16-NSP10 Heterodimer from SARS-CoV-2 in Complex with Sinefungin
Authors : Minasov, G.; Shuvalova, L.; Rosas-Lemus, M.; Kiryukhina, O.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2020-04-16
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.16
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) : 2.16

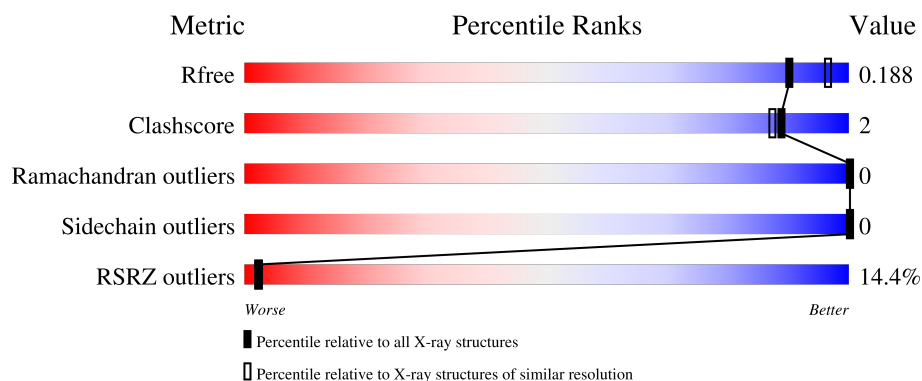
1 Overall quality at a glance

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)

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	301	<div> <div>13%</div> <div>94%</div> <div>5%</div> </div>
1	C	301	<div> <div>9%</div> <div>94%</div> <div>• •</div> </div>
2	B	142	<div> <div>18%</div> <div>82%</div> <div>• 14%</div> </div>
2	D	142	<div> <div>19%</div> <div>79%</div> <div>• 18%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7361 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	297	Total	C	N	O	S	0	13	0
			2430	1550	405	458	17			
1	C	294	Total	C	N	O	S	0	8	0
			2365	1510	396	442	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6796	SER	-	expression tag	UNP P0DTD1
A	6797	ASN	-	expression tag	UNP P0DTD1
A	6798	ALA	-	expression tag	UNP P0DTD1
C	6796	SER	-	expression tag	UNP P0DTD1
C	6797	ASN	-	expression tag	UNP P0DTD1
C	6798	ALA	-	expression tag	UNP P0DTD1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	1	0
			917	570	155	175	17			
2	D	116	Total	C	N	O	S	0	1	0
			864	539	145	165	15			

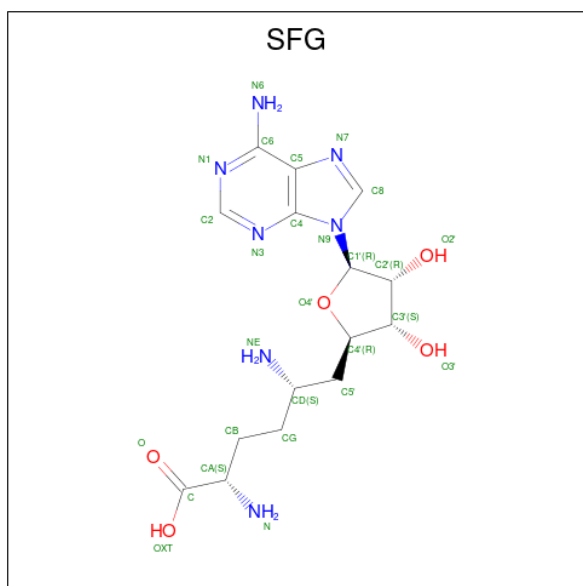
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4251	SER	-	expression tag	UNP P0DTD1
B	4252	ASN	-	expression tag	UNP P0DTD1
B	4253	ALA	-	expression tag	UNP P0DTD1
D	4251	SER	-	expression tag	UNP P0DTD1
D	4252	ASN	-	expression tag	UNP P0DTD1
D	4253	ALA	-	expression tag	UNP P0DTD1

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		

- Molecule 4 is SINEFUNGIN (three-letter code: SFG) (formula: C₁₅H₂₃N₇O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	15	7	5		
4	C	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Zn	0	0
			2	2		
6	D	2	Total	Zn	0	0
			2	2		

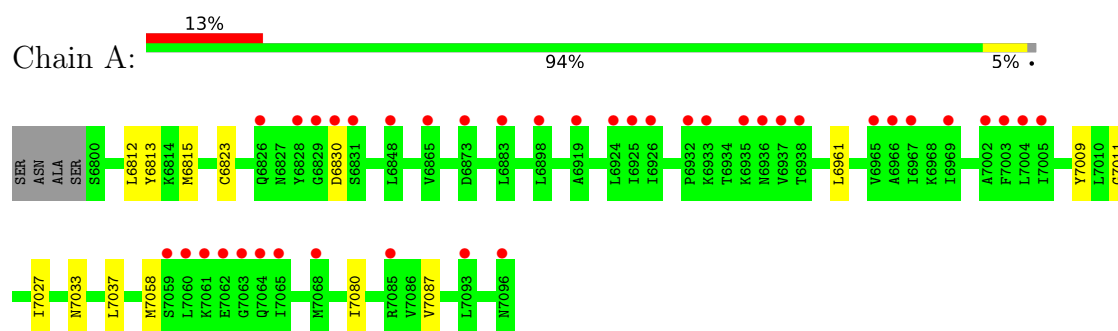
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	237	Total	O	0	24
			257	257		
7	B	81	Total	O	0	6
			87	87		
7	C	249	Total	O	0	16
			263	263		
7	D	69	Total	O	0	2
			71	71		

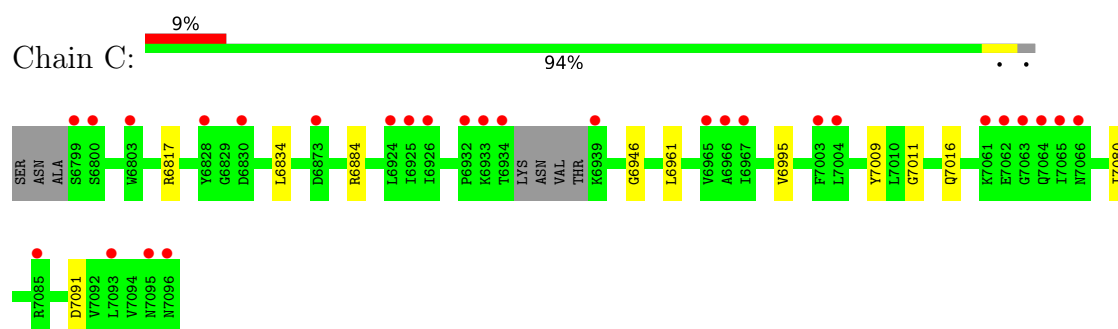
3 Residue-property plots [i](#)

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

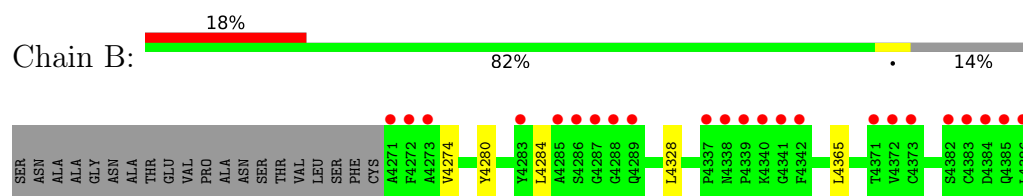
• Molecule 1: 2'-O-methyltransferase



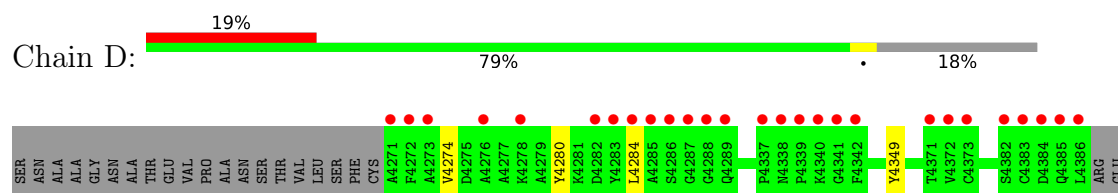
• Molecule 1: 2'-O-methyltransferase



• Molecule 2: Non-structural protein 10



• Molecule 2: Non-structural protein 10



PRO
MET
LEU
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	166.25Å 166.25Å 98.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 1.98 29.92 – 1.98	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.92-1.98) 100.0 (29.92-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.162 , 0.180 0.169 , 0.188	Depositor DCC
R_{free} test set	5357 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7361	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: NA, ZN, FMT, SFG

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	0/2482	0.74	0/3368
1	C	0.64	0/2415	0.73	0/3274
2	B	0.66	0/937	0.74	0/1268
2	D	0.66	0/883	0.74	0/1198
All	All	0.64	0/6717	0.74	0/9108

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	2430	0	2406	14	0
1	C	2365	0	2348	8	0
2	B	917	0	878	3	0
2	D	864	0	826	3	0
3	A	2	0	0	0	0
3	C	2	0	0	0	0
4	A	27	0	22	0	0
4	C	27	0	22	0	0
5	A	18	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	27	0	9	1	0
6	B	2	0	0	0	0
6	D	2	0	0	0	0
7	A	257	0	0	1	0
7	B	87	0	0	0	0
7	C	263	0	0	1	0
7	D	71	0	0	0	0
All	All	7361	0	6517	25	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 2.

All (25) 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:C:7016[B]:GLN:OE1	7:C:7299[B]:HOH:O	2.14	0.66
1:A:6812[A]:LEU:HD23	1:A:6815:MET:HE3	1.85	0.59
1:C:6884:ARG:HB3	2:D:4349:TYR:OH	2.06	0.55
1:C:6834:LEU:HD21	1:C:6995[B]:VAL:CG2	2.36	0.54
1:A:6812[B]:LEU:HA	1:A:6815:MET:HE2	1.92	0.52
1:C:6961:LEU:HB2	1:C:7080:ILE:HB	1.92	0.50
2:B:4280:TYR:CE2	2:B:4284:LEU:HD11	2.49	0.48
1:C:6946:GLY:N	5:C:7105:FMT:O2	2.42	0.47
1:A:6812[A]:LEU:HA	1:A:6815:MET:HE2	1.96	0.47
2:D:4280:TYR:CE2	2:D:4284:LEU:HD11	2.51	0.46
1:A:6823:CYS:HB2	1:A:7027[A]:ILE:HD12	1.97	0.46
1:A:7009:TYR:CZ	1:A:7011:GLY:HA2	2.50	0.46
1:A:6830:ASP:CB	1:A:7037:LEU:HD12	2.45	0.46
1:A:6830:ASP:HB3	1:A:7037:LEU:HD12	1.98	0.45
2:B:4328:LEU:HD22	2:B:4365:LEU:HD11	1.99	0.45
1:C:7009:TYR:CZ	1:C:7011:GLY:HA2	2.52	0.44
1:A:6812[A]:LEU:HD23	1:A:6815:MET:CE	2.47	0.44
2:B:4274:VAL:CG1	2:D:4274:VAL:HG11	2.48	0.44
1:A:7033:ASN:HB3	7:A:7387:HOH:O	2.19	0.43
1:A:6812[B]:LEU:HA	1:A:6815:MET:CE	2.50	0.42
1:A:7087:VAL:HG13	1:C:7091:ASP:HB3	2.00	0.41
1:A:6813:TYR:OH	1:A:7033:ASN:OD1	2.35	0.41
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	2.02	0.41
1:C:6817:ARG:O	1:C:6817:ARG:HG2	2.21	0.40
1:A:7058:MET:O	1:A:7080:ILE:HA	2.21	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	308/301 (102%)	299 (97%)	9 (3%)	0	100	100
1	C	298/301 (99%)	289 (97%)	9 (3%)	0	100	100
2	B	121/142 (85%)	116 (96%)	5 (4%)	0	100	100
2	D	115/142 (81%)	112 (97%)	3 (3%)	0	100	100
All	All	842/886 (95%)	816 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	269/260 (104%)	269 (100%)	0	100	100
1	C	261/260 (100%)	261 (100%)	0	100	100
2	B	101/115 (88%)	101 (100%)	0	100	100
2	D	95/115 (83%)	95 (100%)	0	100	100
All	All	726/750 (97%)	726 (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 ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 8 are monoatomic - leaving 17 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	$\# Z > 2$
5	FMT	C	7109	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SFG	C	7103	-	22,29,29	0.94	1 (4%)	18,42,42	1.47	3 (16%)
5	FMT	C	7105	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	7104	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	7104	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	7109	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	7107	-	0,2,2	0.00	-	0,1,1	0.00	-
4	SFG	A	7103	-	22,29,29	0.92	1 (4%)	18,42,42	1.45	3 (16%)
5	FMT	C	7110	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	7108	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	7107	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	7108	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	7106	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	7112	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	7106	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	7111	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	7105	-	0,2,2	0.00	-	0,1,1	0.00	-

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	SFG	C	7103	-	-	0/9/33/33	0/3/3/3
4	SFG	A	7103	-	-	0/9/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	7103	SFG	C5-C4	2.37	1.47	1.40
4	A	7103	SFG	C5-C4	2.06	1.46	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7103	SFG	N3-C2-N1	-3.81	122.73	128.68
4	C	7103	SFG	N3-C2-N1	-3.81	122.73	128.68
4	C	7103	SFG	C4-C5-N7	-2.67	106.62	109.40
4	A	7103	SFG	C4-C5-N7	-2.42	106.88	109.40
4	C	7103	SFG	O4'-C1'-C2'	-2.29	103.58	106.93
4	A	7103	SFG	O4'-C1'-C2'	-2.13	103.81	106.93

There are no chirality outliers.

There are no torsion outliers.

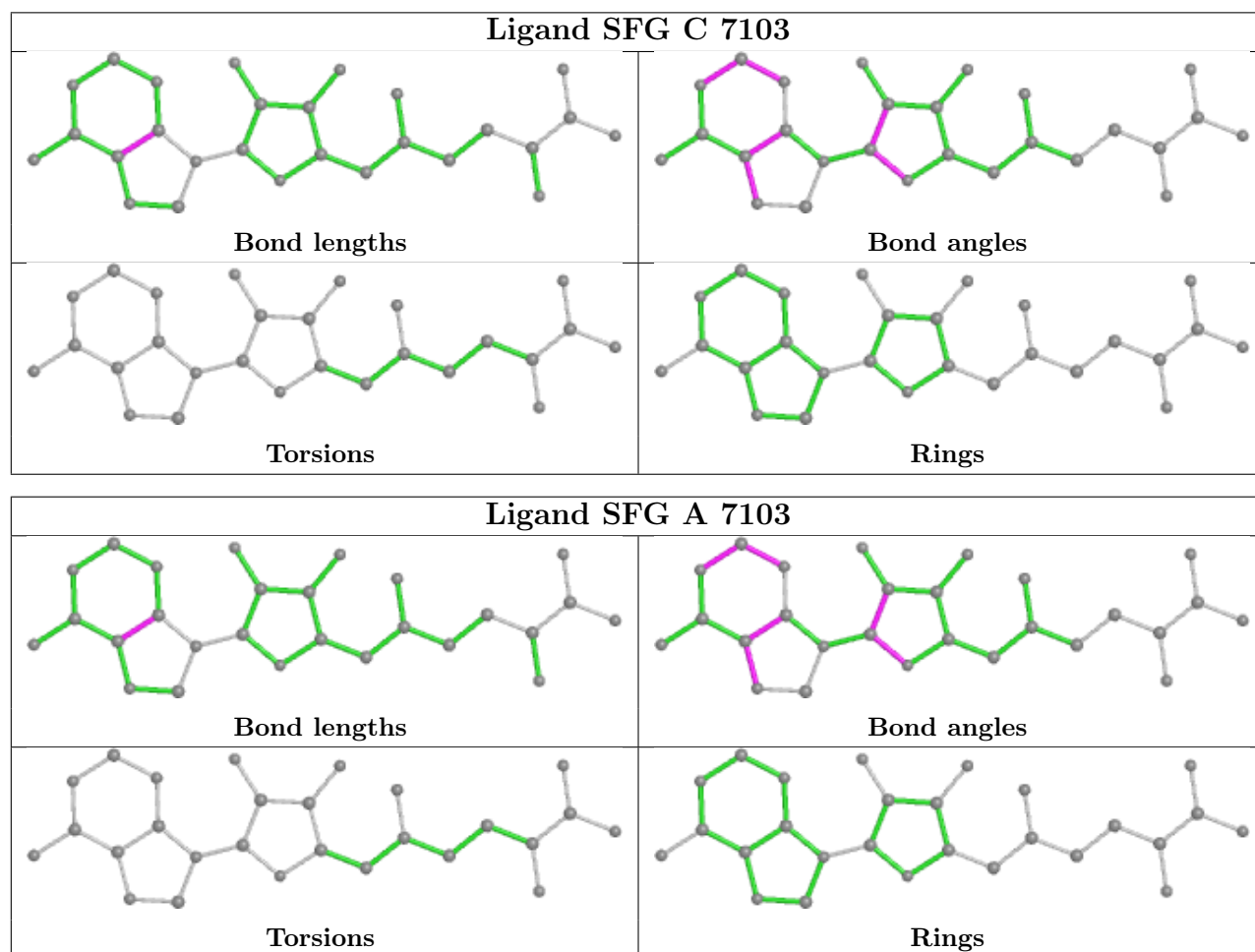
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	7105	FMT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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, 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	297/301 (98%)	0.59	39 (13%) 3 3	22, 34, 72, 113	0
1	C	294/301 (97%)	0.36	28 (9%) 8 9	23, 32, 64, 101	0
2	B	122/142 (85%)	0.98	25 (20%) 1 0	28, 47, 79, 112	0
2	D	116/142 (81%)	0.95	27 (23%) 0 0	26, 45, 82, 127	0
All	All	829/886 (93%)	0.61	119 (14%) 2 2	22, 35, 76, 127	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	4386	LEU	13.4
2	B	4386	LEU	8.4
1	A	6937	VAL	8.4
2	B	4339	PRO	7.5
2	D	4339	PRO	7.4
1	A	7061	LYS	7.0
1	A	6936	ASN	6.8
2	B	4340	LYS	6.6
1	C	6799	SER	6.2
2	B	4342	PHE	5.9
1	C	7062	GLU	5.6
2	B	4387	ARG	5.6
2	D	4383	CYS	5.5
2	D	4271	ALA	5.5
1	C	7096	ASN	5.3
1	A	6829	GLY	5.3
1	C	6934	THR	5.1
2	D	4286	SER	5.0
2	D	4285	ALA	4.9
2	B	4287	GLY	4.8
1	A	6828	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	4371	THR	4.8
1	C	6932	PRO	4.7
1	C	6933	LYS	4.6
1	C	6803	TRP	4.6
2	D	4340	LYS	4.6
1	A	6831	SER	4.6
2	B	4285	ALA	4.5
1	C	6800	SER	4.5
1	A	7085	ARG	4.3
2	D	4382	SER	4.3
1	A	6967	ILE	4.2
2	B	4384	ASP	4.2
2	D	4289	GLN	4.2
2	B	4271	ALA	4.1
1	A	6926	ILE	4.1
2	D	4385	GLN	4.1
2	D	4341	GLY	4.1
1	A	6830	ASP	4.0
2	B	4288	GLY	4.0
1	A	6938	THR	3.9
2	D	4273	ALA	3.9
1	C	6828	TYR	3.8
2	B	4385	GLN	3.8
1	A	7062	GLU	3.8
2	B	4372	VAL	3.6
2	B	4286	SER	3.6
1	A	6966	ALA	3.6
2	D	4372	VAL	3.6
1	A	7065	ILE	3.5
2	B	4283	TYR	3.5
2	D	4384	ASP	3.4
2	B	4382	SER	3.4
2	D	4287	GLY	3.4
1	A	7005	ILE	3.4
2	D	4342	PHE	3.4
2	D	4272	PHE	3.3
1	A	7064	GLN	3.3
1	C	7064	GLN	3.3
1	A	6925	ILE	3.2
1	A	6933	LYS	3.2
2	B	4373	CYS	3.2
1	A	6826	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	7061	LYS	3.1
2	D	4283	TYR	3.1
2	D	4278	LYS	3.1
2	D	4288	GLY	3.1
1	A	6932	PRO	3.1
2	B	4371	THR	3.1
2	B	4341	GLY	3.0
1	A	6965	VAL	3.0
1	A	7093	LEU	3.0
2	B	4338	ASN	2.9
1	A	7096	ASN	2.9
1	C	7004	LEU	2.9
1	C	7065	ILE	2.9
1	A	7004	LEU	2.8
1	C	6967	ILE	2.8
1	C	6926	ILE	2.8
2	B	4388	GLU	2.8
1	A	7003	PHE	2.8
1	C	6965	VAL	2.8
1	A	6924	LEU	2.8
1	C	7066	ASN	2.8
1	C	6830	ASP	2.7
2	B	4289	GLN	2.7
1	C	7063	GLY	2.7
2	D	4284	LEU	2.7
1	C	6925	ILE	2.6
2	D	4282	ASP	2.6
1	C	7095	ASN	2.6
2	B	4273	ALA	2.6
1	C	6939	LYS	2.5
1	A	6883	LEU	2.5
1	A	7063	GLY	2.5
2	B	4272	PHE	2.5
2	D	4338	ASN	2.5
1	A	7068	MET	2.4
1	A	6898[A]	LEU	2.4
1	C	7093	LEU	2.4
2	B	4337	PRO	2.4
1	C	7085	ARG	2.4
1	C	6873	ASP	2.3
1	C	7003	PHE	2.3
1	A	6969	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	6873	ASP	2.3
1	A	6935	LYS	2.3
1	A	6848	LEU	2.3
2	D	4373	CYS	2.2
1	A	6919	ALA	2.2
1	A	7002	ALA	2.2
1	C	6966	ALA	2.2
2	D	4337	PRO	2.2
2	D	4276	ALA	2.1
1	A	7059	SER	2.1
2	B	4383	CYS	2.1
1	C	6924	LEU	2.1
1	A	6865	VAL	2.0
1	A	7060	LEU	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 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, 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(\AA^2)	Q<0.9
3	NA	A	7102	1/1	0.83	0.17	53,53,53,53	1
5	FMT	C	7110	3/3	0.83	0.16	54,54,60,62	0
5	FMT	C	7105	3/3	0.88	0.22	41,41,44,46	0
3	NA	C	7102	1/1	0.89	0.10	55,55,55,55	1
5	FMT	C	7111	3/3	0.92	0.12	51,51,57,58	0
6	ZN	D	4402	1/1	0.93	0.07	54,54,54,54	0
3	NA	A	7101	1/1	0.93	0.10	48,48,48,48	0
5	FMT	C	7107	3/3	0.95	0.11	50,50,52,53	0
3	NA	C	7101	1/1	0.95	0.14	43,43,43,43	0

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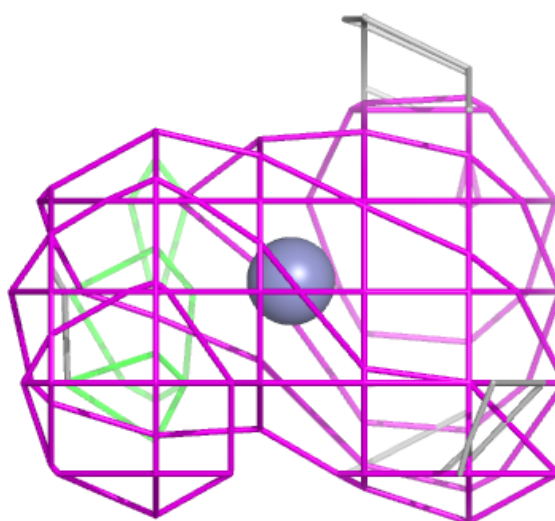
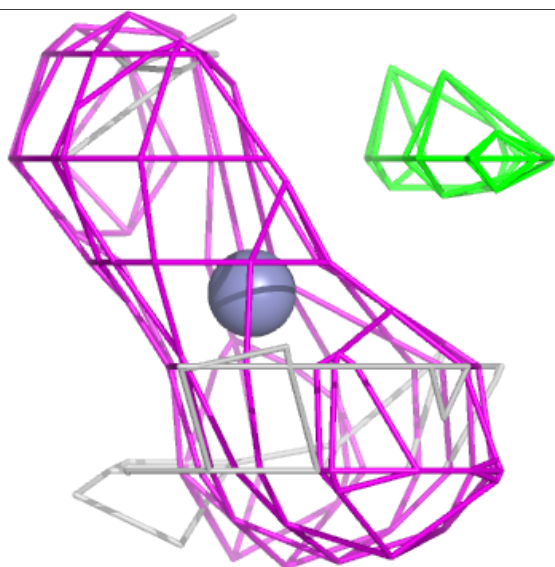
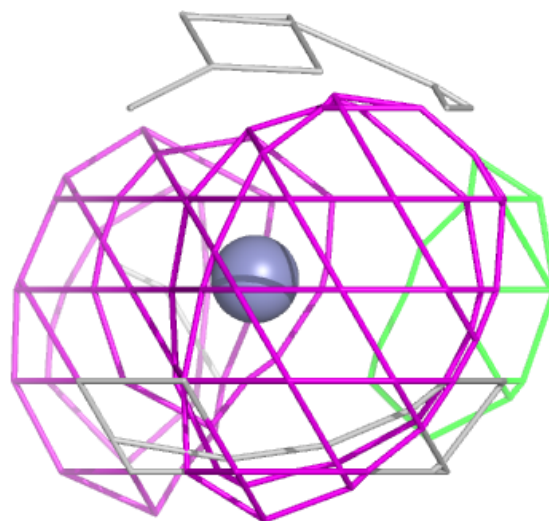
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FMT	C	7112	3/3	0.95	0.15	57,57,63,64	0
5	FMT	A	7104	3/3	0.95	0.10	48,48,52,54	0
5	FMT	A	7108	3/3	0.95	0.26	52,52,53,53	0
6	ZN	B	4402	1/1	0.96	0.11	49,49,49,49	0
5	FMT	C	7108	3/3	0.97	0.13	56,56,56,57	0
6	ZN	B	4401	1/1	0.97	0.06	39,39,39,39	0
4	SFG	A	7103	27/27	0.97	0.07	26,28,32,34	0
4	SFG	C	7103	27/27	0.97	0.07	24,27,29,30	0
5	FMT	A	7107	3/3	0.97	0.10	48,48,53,54	0
5	FMT	C	7104	3/3	0.97	0.08	33,33,33,34	0
5	FMT	A	7106	3/3	0.97	0.11	53,53,55,56	0
6	ZN	D	4401	1/1	0.98	0.06	36,36,36,36	0
5	FMT	A	7109	3/3	0.98	0.13	53,53,54,56	0
5	FMT	C	7109	3/3	0.98	0.19	38,38,41,50	0
5	FMT	A	7105	3/3	0.98	0.07	30,30,31,32	0
5	FMT	C	7106	3/3	0.99	0.08	38,38,39,39	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.

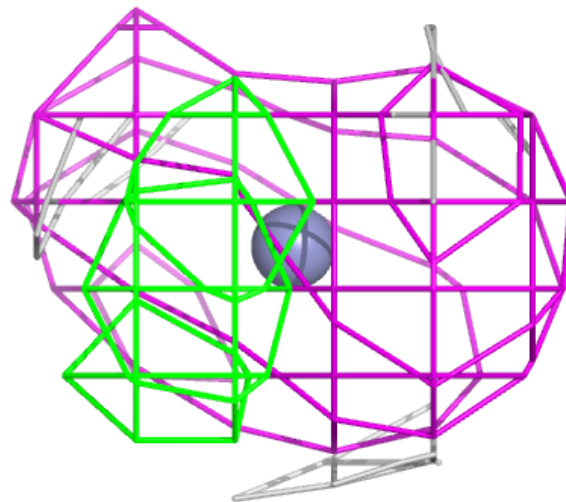
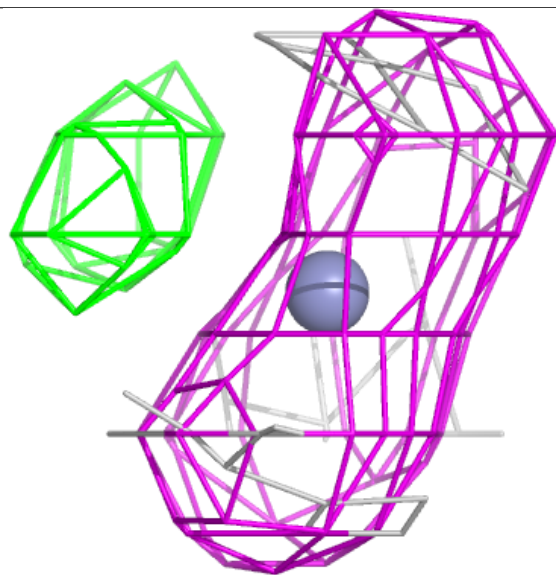
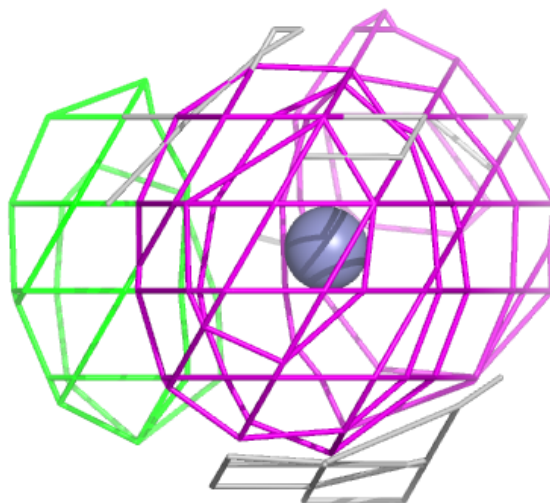
Electron density around ZN D 4402:

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



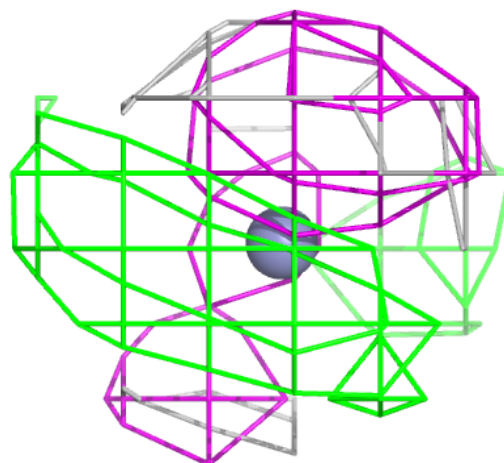
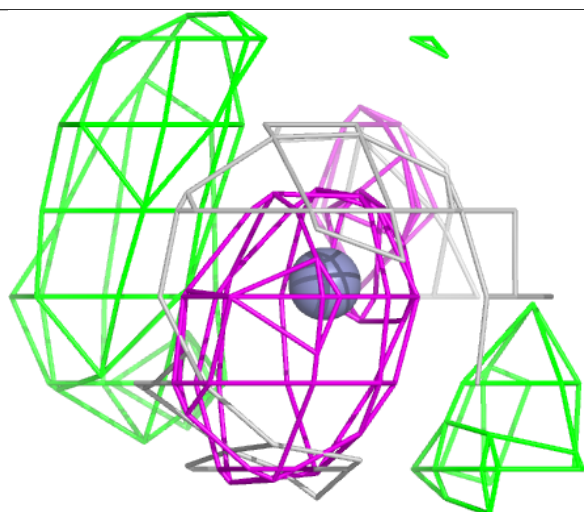
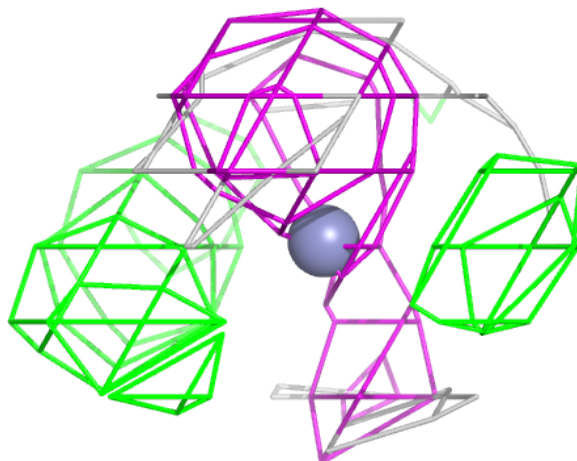
Electron density around ZN B 4402:

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



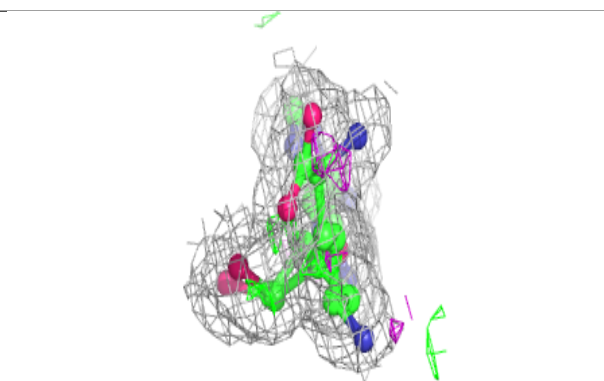
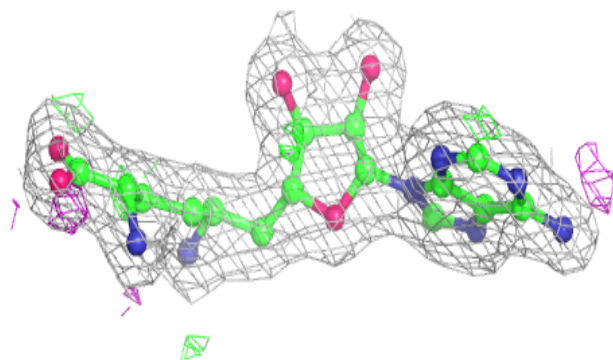
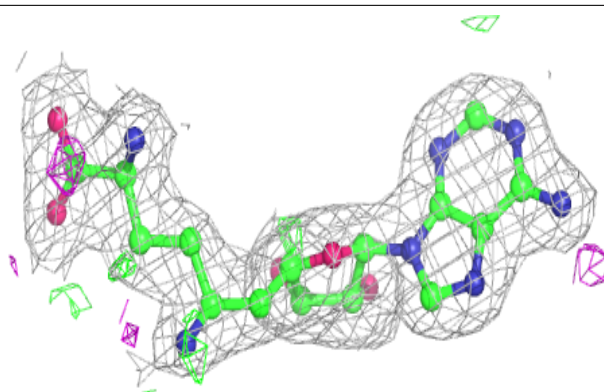
Electron density around ZN B 4401:

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

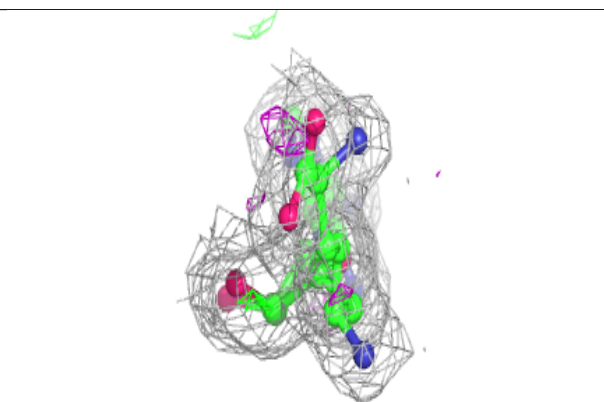
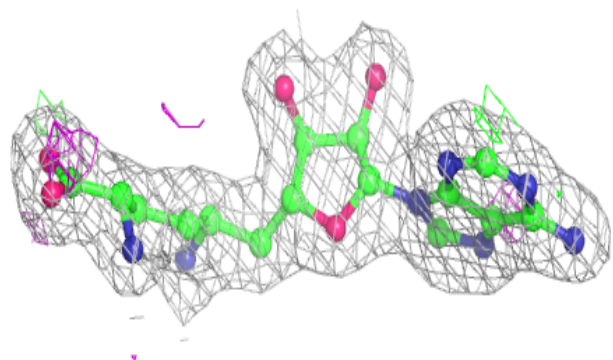
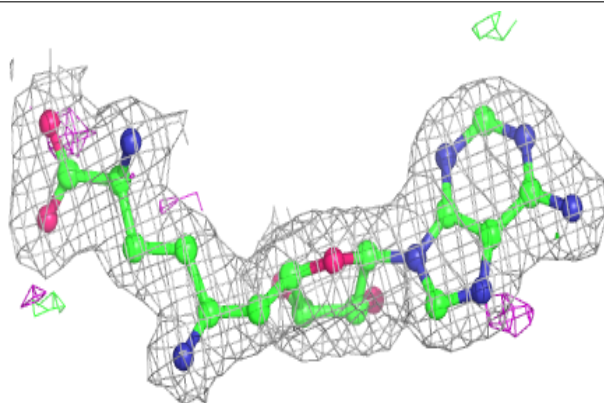


Electron density around SFG A 7103:

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

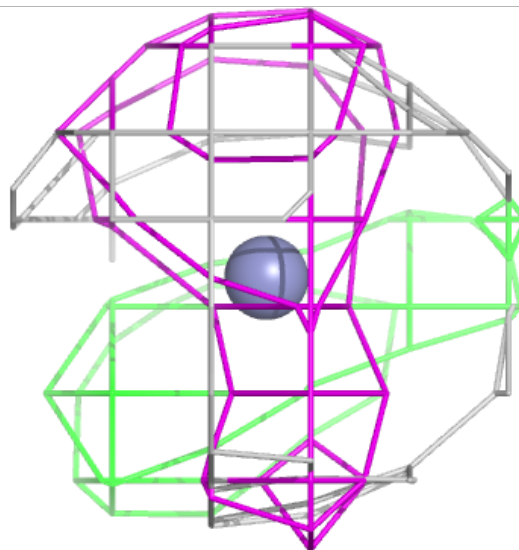
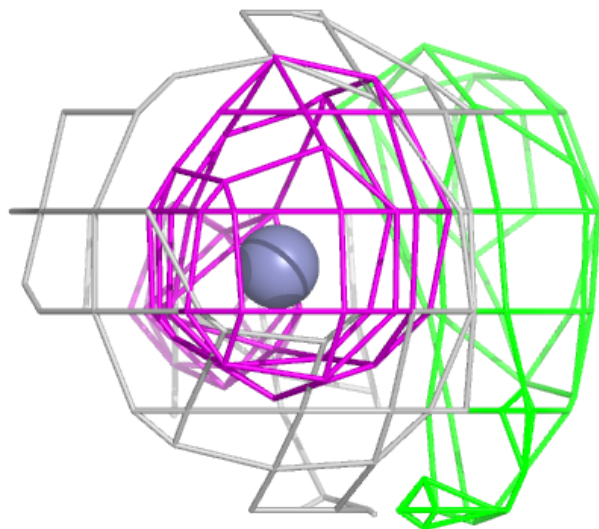
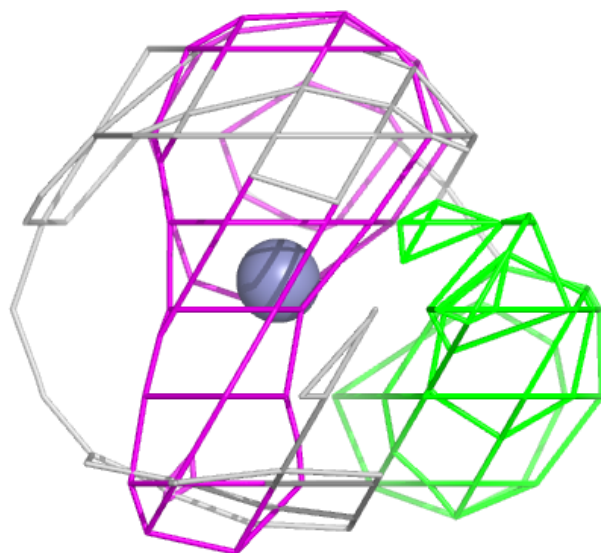
**Electron density around SFG C 7103:**

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



Electron density around ZN D 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 [i](#)

There are no such residues in this entry.