



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 03:35 PM EDT

PDB ID : 8F4S
Title : Crystal Structure of the SARS-CoV-2 2'-O-Methyltransferase with Compound 5a bound to the Cryptic Pocket of nsp16
Authors : Minasov, G.; Shuvalova, L.; Brunzelle, J.S.; Rosas-Lemus, M.; Kiryukhina, O.; Satchell, K.J.F.; Center for Structural Biology of Infectious Diseases (CSBID)
Deposited on : 2022-11-11
Resolution : 2.15 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

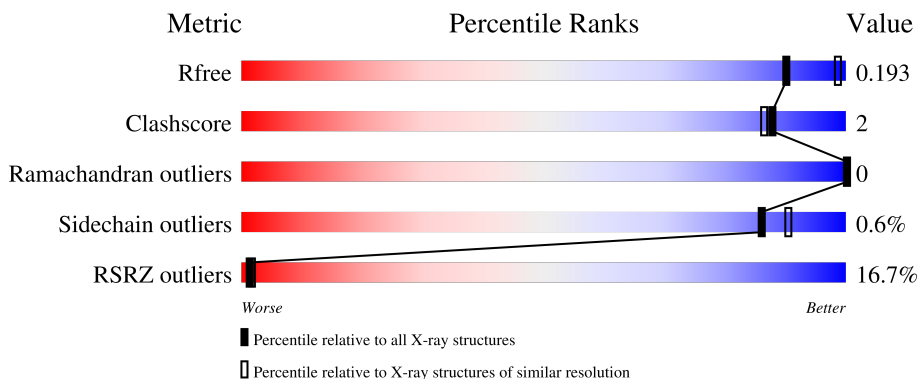
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	
2	B	142	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 3471 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
			Total	C	N	O	S			
1	A	298	2401	1531	404	447	19	0	7	0

There are 3 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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	109	817	506	138	157	16	0	2	0

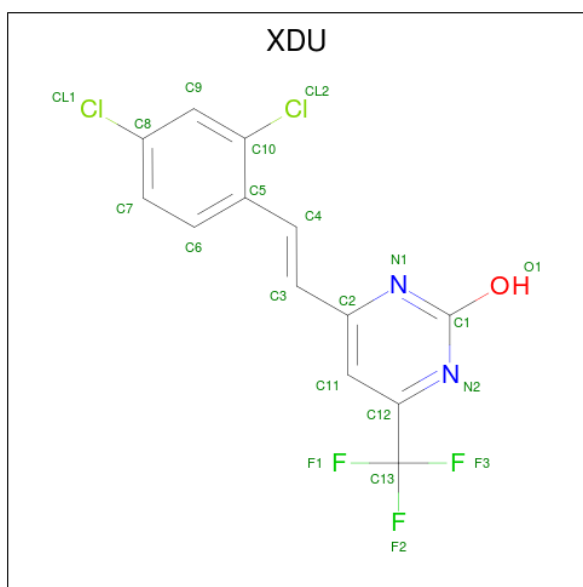
There are 3 discrepancies between the modelled and reference sequences:

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

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

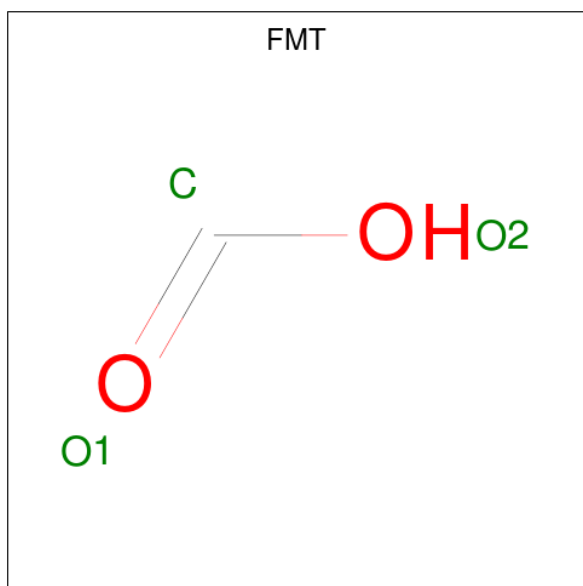
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is 4-[(E)-2-(2,4-dichlorophenyl)ethenyl]-6-(trifluoromethyl)pyrimidin-2-ol (three-letter code: XDU) (formula: C₁₃H₇Cl₂F₃N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
4	A	1	21	13	2	3	2	1	0	0

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



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

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

- 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 2 2	0	0

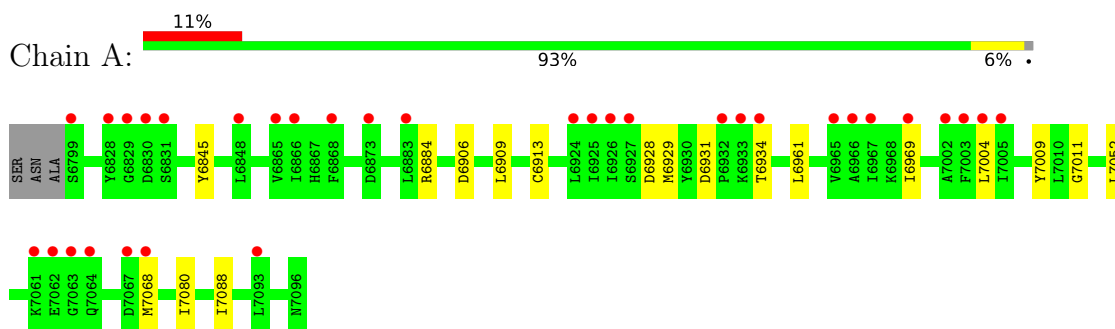
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	179	Total O 184 184	0	6
7	B	28	Total O 30 30	0	2

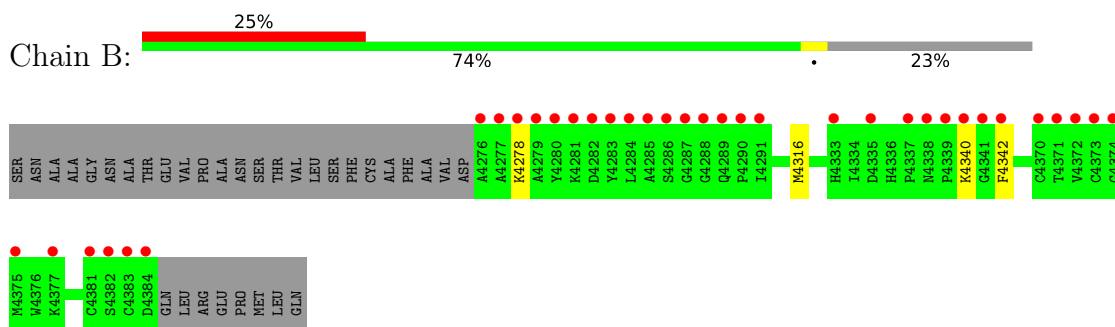
3 Residue-property plots [i](#)

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 2: Non-structural protein 10



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	170.85Å 170.85Å 51.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.59 – 2.15 29.59 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.59-2.15) 99.9 (29.59-2.15)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.16Å)	Xtrriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.166 , 0.191 0.171 , 0.193	Depositor DCC
R_{free} test set	2416 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtrriage
Anisotropy	0.145	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3471	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: ZN, XDU, NA, FMT

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	0.28	0/2453	0.62	0/3324
2	B	0.27	0/835	0.56	0/1131
All	All	0.27	0/3288	0.60	0/4455

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

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	2401	0	2386	10	0
2	B	817	0	777	2	0
3	A	1	0	0	0	0
4	A	21	0	0	3	0
5	A	15	0	5	0	0
6	B	2	0	0	0	0
7	A	184	0	0	0	0
7	B	30	0	0	0	0
All	All	3471	0	3168	13	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 (13) 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:6909:LEU:HD11	1:A:7088:ILE:HG21	1.65	0.77
1:A:6913:CYS:SG	4:A:7102:XDU:C4	2.95	0.55
4:A:7102:XDU:CL2	4:A:7102:XDU:C3	2.96	0.51
1:A:6931:ASP:O	1:A:6934:THR:HG22	2.14	0.48
1:A:6845:TYR:OH	1:A:6928:ASP:HB2	2.12	0.48
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	1.96	0.46
1:A:6969:ILE:HD13	1:A:7004:LEU:HG	1.98	0.44
1:A:6929:MET:HG2	4:A:7102:XDU:CL1	2.55	0.44
1:A:7052:LEU:HD12	1:A:7052:LEU:N	2.34	0.42
2:B:4340:LYS:HE3	2:B:4342:PHE:HB3	2.02	0.42
2:B:4278:LYS:N	2:B:4278:LYS:HD2	2.35	0.41
1:A:6884:ARG:HH22	1:A:6906:ASP:CG	2.24	0.41
1:A:7009:TYR:CZ	1:A:7011:GLY:HA2	2.56	0.41

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	303/301 (101%)	291 (96%)	12 (4%)	0	100	100
2	B	109/142 (77%)	105 (96%)	4 (4%)	0	100	100
All	All	412/443 (93%)	396 (96%)	16 (4%)	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	265/260 (102%)	264 (100%)	1 (0%)	91	93
2	B	91/115 (79%)	89 (98%)	2 (2%)	52	55
All	All	356/375 (95%)	353 (99%)	3 (1%)	86	86

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7068	MET
2	B	4316[A]	MET
2	B	4316[B]	MET

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	A	7106	-	2,2,2	0.34	0	1,1,1	0.23	0
4	XDU	A	7102	-	19,22,22	1.15	2 (10%)	26,32,32	3.07	14 (53%)
5	FMT	A	7103	-	2,2,2	0.31	0	1,1,1	0.24	0
5	FMT	A	7104	-	2,2,2	0.22	0	1,1,1	0.25	0
5	FMT	A	7107	-	2,2,2	0.37	0	1,1,1	0.22	0
5	FMT	A	7105	-	2,2,2	0.23	0	1,1,1	0.29	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
4	XDU	A	7102	-	-	2/11/11/11	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7102	XDU	C10-CL2	3.00	1.80	1.73
4	A	7102	XDU	C8-CL1	2.38	1.79	1.74

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7102	XDU	C13-C12-N2	7.78	123.39	114.56
4	A	7102	XDU	C5-C10-CL2	6.01	125.39	120.17
4	A	7102	XDU	C11-C2-C3	-4.35	110.60	121.48
4	A	7102	XDU	C10-C5-C4	4.13	125.01	121.86
4	A	7102	XDU	C3-C2-N1	4.04	128.21	117.75
4	A	7102	XDU	C5-C4-C3	-3.96	114.49	126.46
4	A	7102	XDU	C9-C10-C5	-3.74	119.67	122.46
4	A	7102	XDU	C6-C5-C10	3.56	119.94	116.69
4	A	7102	XDU	C6-C5-C4	-3.35	114.51	121.12
4	A	7102	XDU	C11-C12-C13	-2.58	116.84	120.10
4	A	7102	XDU	F3-C13-C12	-2.32	108.50	112.47
4	A	7102	XDU	F1-C13-C12	-2.28	108.57	112.47
4	A	7102	XDU	C9-C10-CL2	-2.22	114.91	118.49
4	A	7102	XDU	C11-C12-N2	-2.19	119.77	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

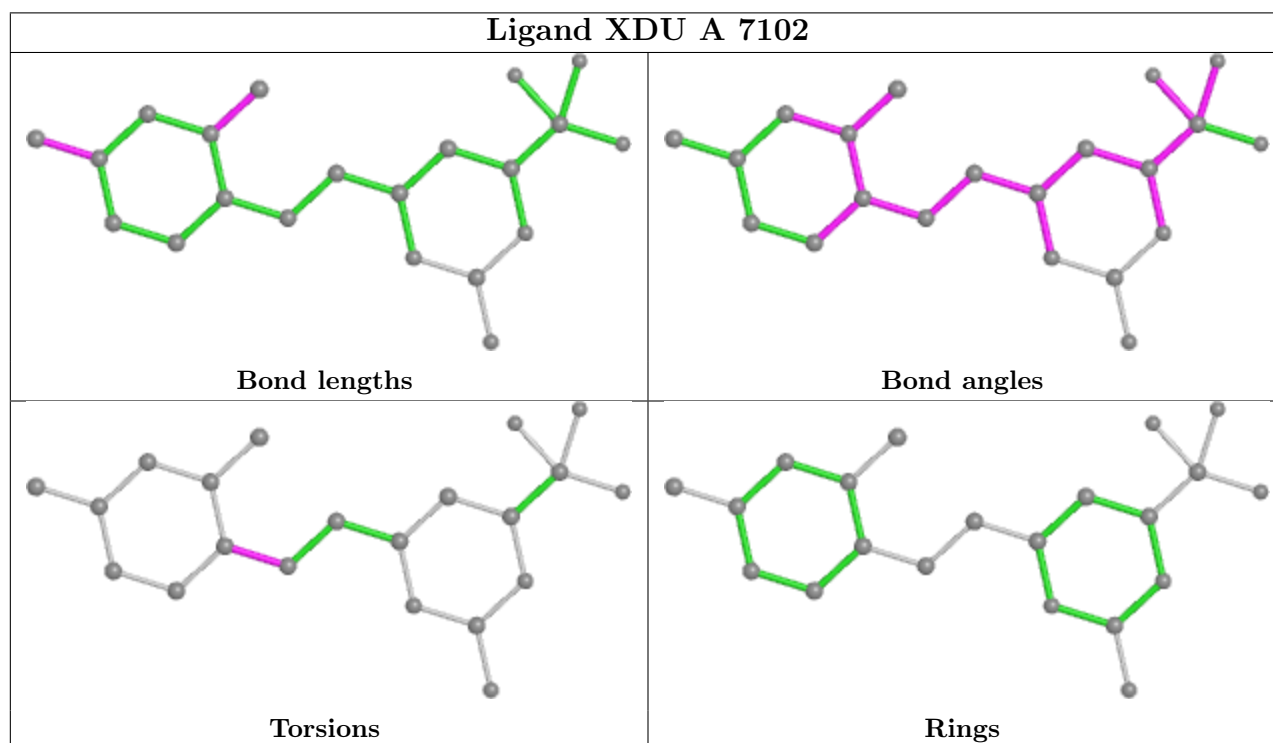
Mol	Chain	Res	Type	Atoms
4	A	7102	XDU	C3-C4-C5-C10
4	A	7102	XDU	C3-C4-C5-C6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	7102	XDU	3	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	298/301 (99%)	0.43	33 (11%) 5 7	34, 50, 98, 159	0
2	B	109/142 (76%)	1.70	35 (32%) 0 0	42, 81, 170, 195	0
All	All	407/443 (91%)	0.77	68 (16%) 1 2	34, 55, 144, 195	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4286[A]	SER	12.9
2	B	4287	GLY	10.5
2	B	4289	GLN	9.2
2	B	4383	CYS	8.6
2	B	4339	PRO	8.5
2	B	4284	LEU	8.0
2	B	4276	ALA	7.9
1	A	6799	SER	7.5
2	B	4280	TYR	7.0
2	B	4288	GLY	6.3
2	B	4372	VAL	6.0
2	B	4342	PHE	5.7
2	B	4285	ALA	5.7
2	B	4340	LYS	5.5
2	B	4373	CYS	5.2
2	B	4338	ASN	4.8
2	B	4382	SER	4.8
2	B	4283	TYR	4.6
1	A	6925	ILE	4.5
2	B	4384	ASP	4.4
1	A	7062	GLU	4.3
1	A	6829	GLY	4.2
2	B	4341	GLY	4.2
2	B	4337	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	6926	ILE	4.1
2	B	4335	ASP	4.1
2	B	4282	ASP	4.1
1	A	7061	LYS	3.9
1	A	7093	LEU	3.8
1	A	7063	GLY	3.7
1	A	7004	LEU	3.7
1	A	6965	VAL	3.7
1	A	6924	LEU	3.6
1	A	6967	ILE	3.6
1	A	6828	TYR	3.6
2	B	4290	PRO	3.6
2	B	4281	LYS	3.5
2	B	4370	CYS	3.5
1	A	6966	ALA	3.5
2	B	4371	THR	3.5
1	A	6866	ILE	3.4
2	B	4381	CYS	3.1
1	A	6933	LYS	3.1
2	B	4279	ALA	3.0
1	A	6830	ASP	3.0
1	A	6883	LEU	3.0
1	A	6873	ASP	2.9
1	A	6865	VAL	2.8
1	A	7002	ALA	2.7
1	A	6934	THR	2.7
2	B	4375	MET	2.7
2	B	4278	LYS	2.6
1	A	7064	GLN	2.6
1	A	7003	PHE	2.6
2	B	4374	GLY	2.6
1	A	6927	SER	2.5
1	A	7005	ILE	2.5
1	A	7068	MET	2.5
1	A	6969	ILE	2.5
2	B	4277	ALA	2.4
2	B	4333	HIS	2.4
2	B	4291	ILE	2.3
1	A	6932	PRO	2.3
1	A	6831	SER	2.2
1	A	6868	PHE	2.2
2	B	4377	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	6848	LEU	2.0
1	A	7067	ASP	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](#)

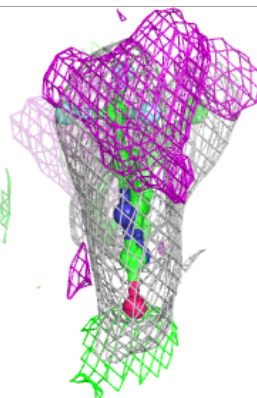
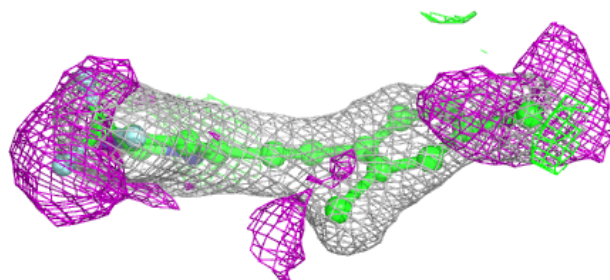
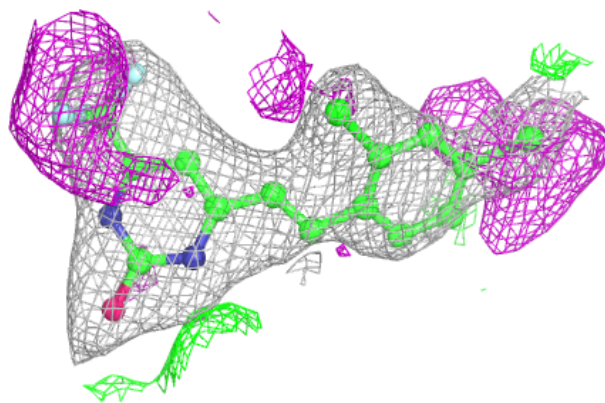
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	FMT	A	7106	3/3	0.83	0.24	78,78,98,101	0
5	FMT	A	7107	3/3	0.83	0.32	71,71,84,91	0
5	FMT	A	7103	3/3	0.88	0.15	84,84,102,110	0
3	NA	A	7101	1/1	0.90	0.15	58,58,58,58	0
4	XDU	A	7102	21/21	0.93	0.13	60,80,91,104	0
6	ZN	B	4402	1/1	0.95	0.16	115,115,115,115	0
6	ZN	B	4401	1/1	0.96	0.04	73,73,73,73	0
5	FMT	A	7104	3/3	0.98	0.11	60,60,64,64	0
5	FMT	A	7105	3/3	0.98	0.21	58,58,58,60	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.

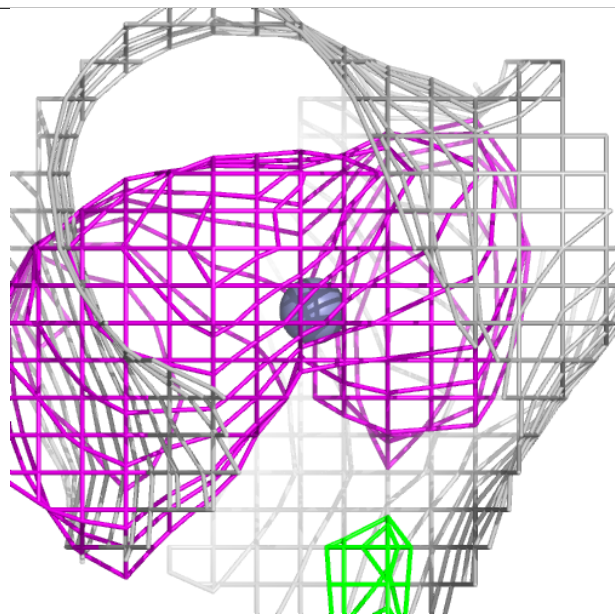
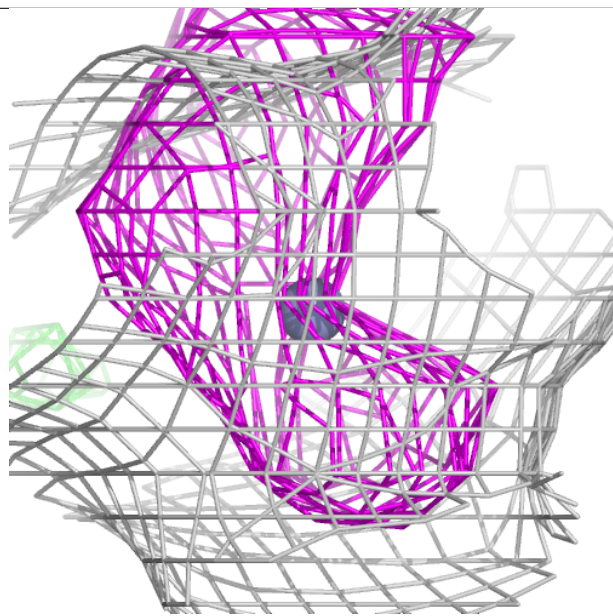
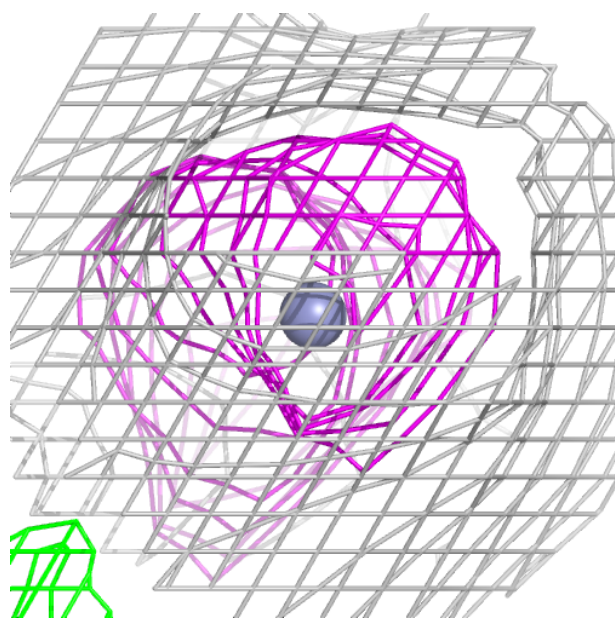
Electron density around XDU A 7102:

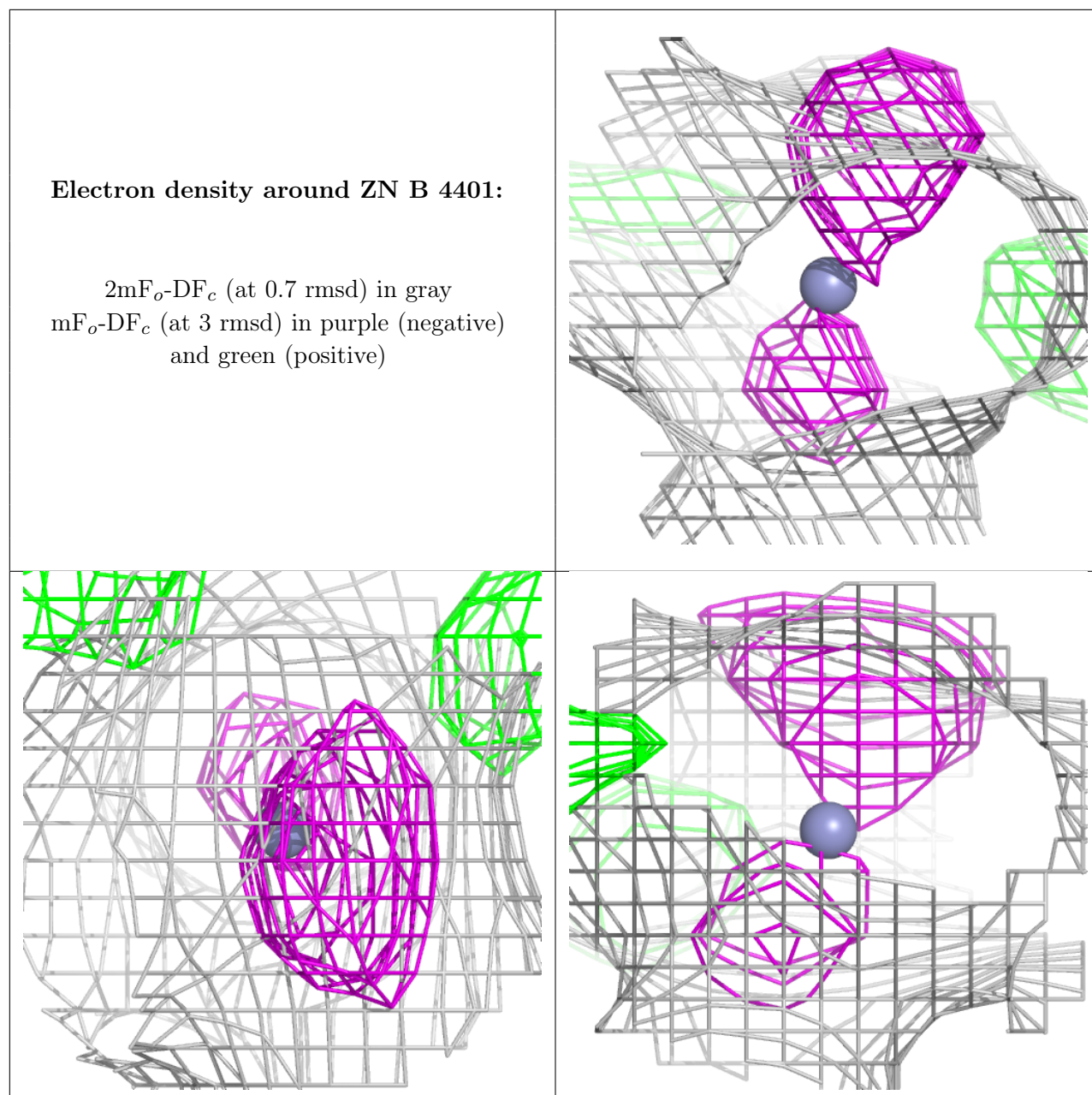
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.