



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:57 AM UTC

PDB ID : 8F4S / pdb_00008f4s
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	:	4-5-2 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

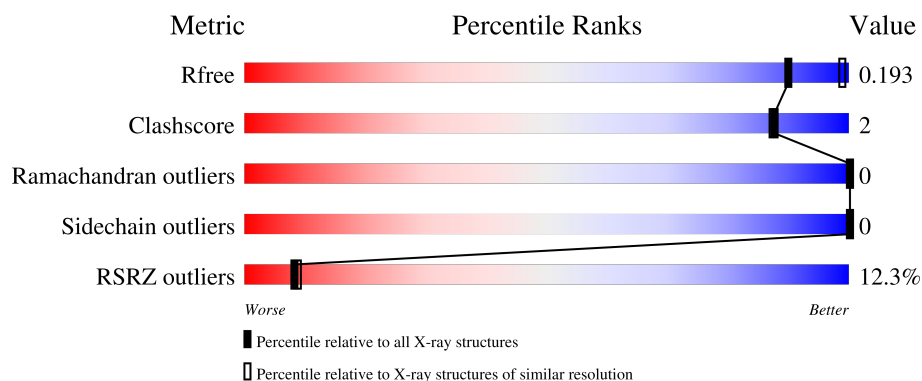
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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	8% 93% 6%
2	B	142	19% 75% 23%

2 Entry composition

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
1	A	298	Total	C	N	O	S	0	7	0
			2401	1531	404	447	19			

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
2	B	109	Total	C	N	O	S	0	2	0
			817	506	138	157	16			

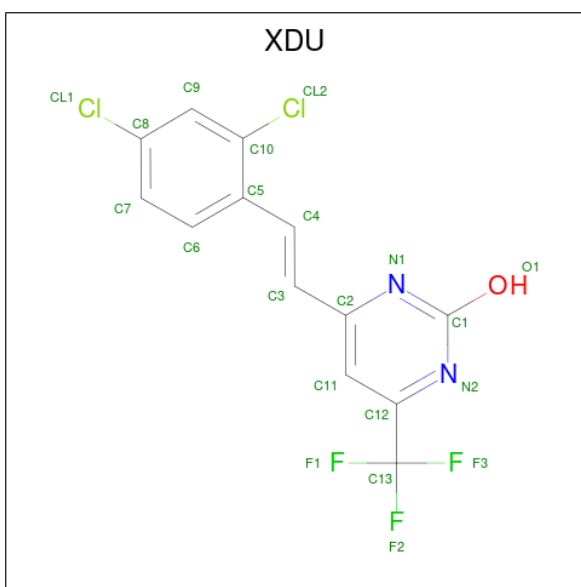
There are 3 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 (CCD ID: XDU) (formula: C₁₃H₇Cl₂F₃N₂O) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is FORMIC ACID (CCD ID: 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		

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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		

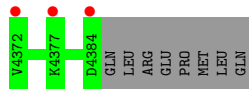
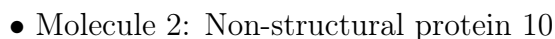
- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 7 is water.

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

- Molecule 1: 2'-O-methyltransferase



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)	Xtriage
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 (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
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

Xtriage'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, FMT, NA

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	0.46	0/2453	0.87	0/3324
2	B	0.47	0/835	0.91	0/1131
All	All	0.46	0/3288	0.88	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:6884:ARG:HH22	1:A:6906:ASP:CG	2.24	0.45
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: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%)	265 (100%)	0	100	100
2	B	91/115 (79%)	91 (100%)	0	100	100
All	All	356/375 (95%)	356 (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. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6827	ASN
1	A	7033	ASN
2	B	4293	ASN

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 oligosaccharides 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	7105	-	2,2,2	0.21	0	1,1,1	0.29	0
5	FMT	A	7107	-	2,2,2	0.35	0	1,1,1	0.22	0
4	XDU	A	7102	-	21,22,22	1.08	2 (9%)	30,32,32	2.90	15 (50%)
5	FMT	A	7104	-	2,2,2	0.20	0	1,1,1	0.25	0
5	FMT	A	7106	-	2,2,2	0.32	0	1,1,1	0.22	0
5	FMT	A	7103	-	2,2,2	0.28	0	1,1,1	0.23	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	3.02	1.80	1.73
4	A	7102	XDU	C8-CL1	2.25	1.79	1.74

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7102	XDU	C13-C12-N2	7.39	123.39	114.60
4	A	7102	XDU	C5-C10-CL2	6.04	125.39	120.17
4	A	7102	XDU	C2-C11-C12	4.39	119.14	116.95
4	A	7102	XDU	C11-C2-C3	-4.37	110.60	121.29
4	A	7102	XDU	C5-C4-C3	-4.08	114.49	126.47
4	A	7102	XDU	C3-C2-N1	3.80	128.21	117.87
4	A	7102	XDU	C9-C10-C5	-3.70	119.67	122.45
4	A	7102	XDU	C6-C5-C10	3.51	119.94	116.70
4	A	7102	XDU	C10-C5-C4	3.48	125.01	121.87
4	A	7102	XDU	C6-C5-C4	-3.32	114.51	121.13
4	A	7102	XDU	F3-C13-C12	-2.23	108.50	112.43
4	A	7102	XDU	C11-C12-N2	-2.21	119.77	123.34
4	A	7102	XDU	F1-C13-C12	-2.19	108.57	112.43
4	A	7102	XDU	C9-C10-CL2	-2.16	114.91	118.45
4	A	7102	XDU	C11-C12-C13	-2.14	116.84	120.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

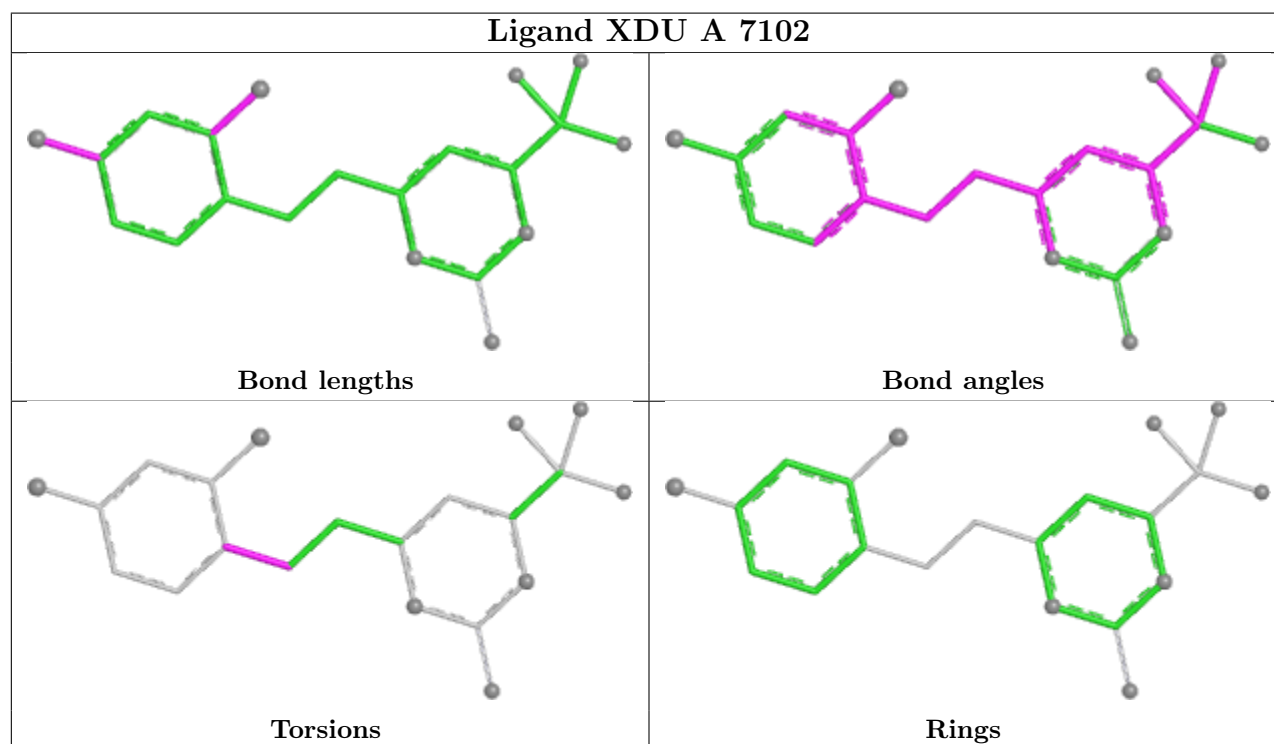
Mol	Chain	Res	Type	Atoms
4	A	7102	XDU	C3-C4-C5-C10
4	A	7102	XDU	C3-C4-C5-C6

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%)	0.25	23 (7%)	19 22	24, 50, 96, 159	7 (2%)
2	B	109/142 (76%)	1.18	27 (24%)	2 2	36, 81, 168, 184	2 (1%)
All	All	407/443 (91%)	0.50	50 (12%)	8 9	24, 55, 144, 184	9 (2%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4276	ALA	6.2
2	B	4342	PHE	5.9
2	B	4316[A]	MET	4.6
1	A	6799	SER	4.4
2	B	4339	PRO	4.2
2	B	4284	LEU	4.1
1	A	6862[A]	ASN	4.0
2	B	4278	LYS	3.7
2	B	4281	LYS	3.6
2	B	4280	TYR	3.6
2	B	4277	ALA	3.5
2	B	4279	ALA	3.4
2	B	4377	LYS	3.3
1	A	7061	LYS	3.3
1	A	6932	PRO	3.2
2	B	4285	ALA	3.0
1	A	7093	LEU	2.9
1	A	6828	TYR	2.9
2	B	4286[A]	SER	2.9
2	B	4384	ASP	2.8
2	B	4368	THR	2.8
1	A	6913	CYS	2.8
1	A	7065[A]	ILE	2.8
2	B	4366	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	6934	THR	2.8
2	B	4340	LYS	2.7
1	A	7058	MET	2.7
2	B	4287	GLY	2.7
1	A	6833	THR	2.6
2	B	4372	VAL	2.6
1	A	7092	VAL	2.6
1	A	6839[A]	MET	2.6
1	A	7096	ASN	2.6
2	B	4290	PRO	2.4
2	B	4333	HIS	2.4
1	A	6817[A]	ARG	2.4
1	A	6939	LYS	2.4
1	A	6938	THR	2.3
2	B	4291	ILE	2.3
2	B	4371	THR	2.3
1	A	6935	LYS	2.3
2	B	4344	ASP	2.3
1	A	6945	GLU	2.2
1	A	6937	VAL	2.2
1	A	6824	ASP	2.2
1	A	7052	LEU	2.1
2	B	4365	LEU	2.1
2	B	4334	ILE	2.1
1	A	6900	ASP	2.0
2	B	4337	PRO	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](#)

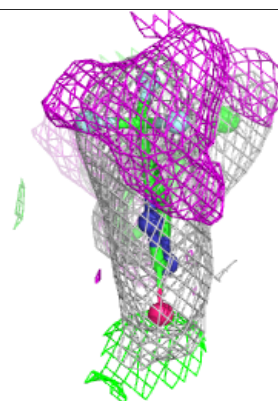
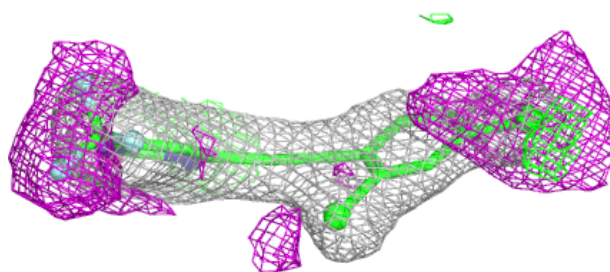
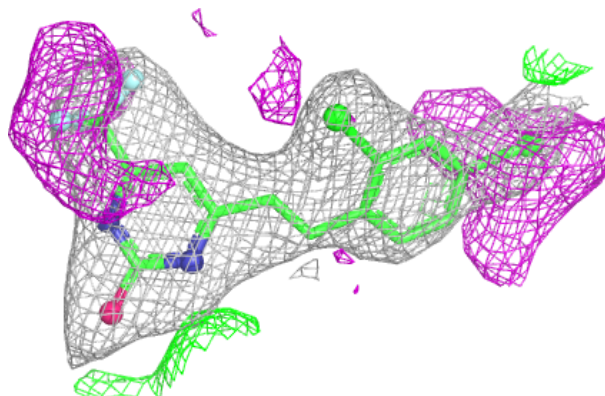
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	FMT	A	7106	3/3	0.78	0.30	78,78,98,101	0
5	FMT	A	7103	3/3	0.79	0.19	84,84,102,110	0
5	FMT	A	7107	3/3	0.84	0.23	71,71,84,91	0
4	XDU	A	7102	21/21	0.90	0.14	60,80,91,104	0
3	NA	A	7101	1/1	0.90	0.15	58,58,58,58	0
5	FMT	A	7105	3/3	0.94	0.22	58,58,58,60	0
5	FMT	A	7104	3/3	0.95	0.14	60,60,64,64	0
6	ZN	B	4402	1/1	0.97	0.10	115,115,115,115	0
6	ZN	B	4401	1/1	0.98	0.04	73,73,73,73	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.

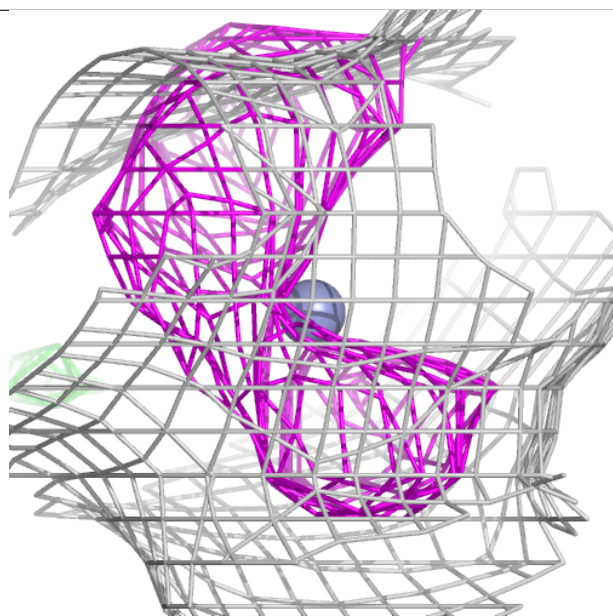
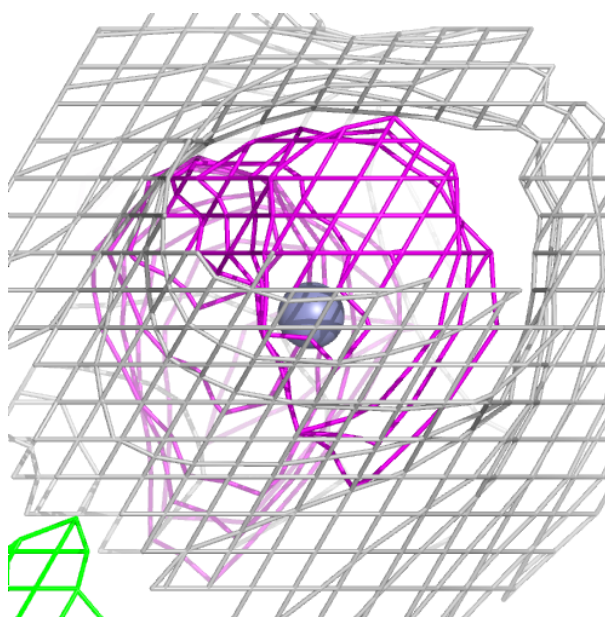
Electron density around XDU A 7102:

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



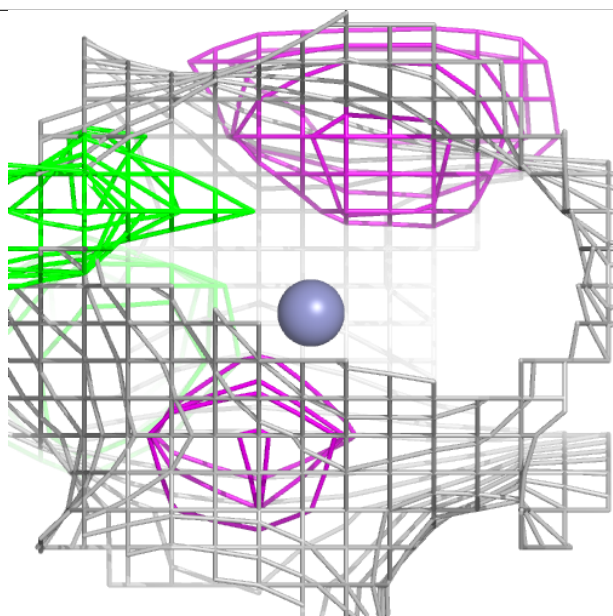
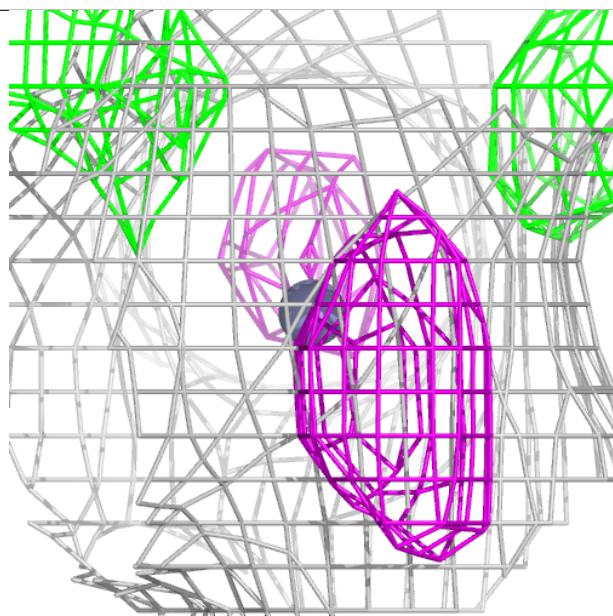
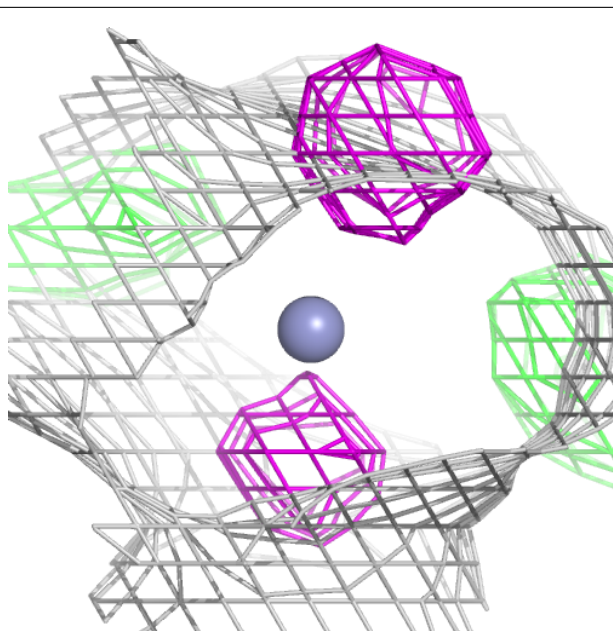
Electron density around ZN B 4402:

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



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.