Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 03:09 PM JST

PDB ID	:	7VB6
Title	:	Crystal structure of hydroxynitrile lyase from Linum usitatissium complexed with (R)-2-hydroxy-2-methylbutanenitrile
Authors	:	Zheng, D.; Nakabayashi, M.; Asano, Y.
Deposited on	:	2021-08-30
Resolution	:	1.74 Å(reported)

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

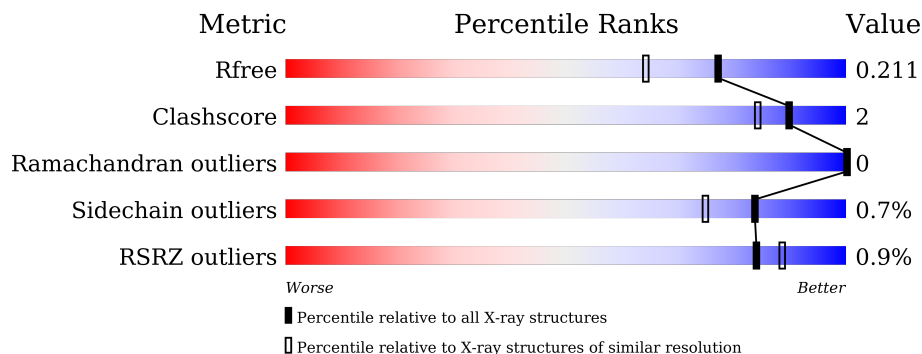|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.74 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.

	Worse	Better	Value
Rfree			0.211
Clashscore			2
Ramachandran outliers			0
Sidechain outliers			0.7%
RSRZ outliers			0.9%

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	443	87% 5% 8%
1	B	443	91% · 7%
1	C	443	87% 5% 8%
1	D	443	87% 5% 8%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 14242 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 Aliphatic (R)-hydroxynitrile lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	2	0
			3121	1977	522	598	24			
1	B	414	Total	C	N	O	S	0	1	0
			3153	1994	527	608	24			
1	C	408	Total	C	N	O	S	0	1	0
			3110	1971	518	597	24			
1	D	408	Total	C	N	O	S	0	1	0
			3108	1967	518	599	24			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P93243
A	-19	GLY	-	expression tag	UNP P93243
A	-18	SER	-	expression tag	UNP P93243
A	-17	SER	-	expression tag	UNP P93243
A	-16	HIS	-	expression tag	UNP P93243
A	-15	HIS	-	expression tag	UNP P93243
A	-14	HIS	-	expression tag	UNP P93243
A	-13	HIS	-	expression tag	UNP P93243
A	-12	HIS	-	expression tag	UNP P93243
A	-11	HIS	-	expression tag	UNP P93243
A	-10	SER	-	expression tag	UNP P93243
A	-9	SER	-	expression tag	UNP P93243
A	-8	GLY	-	expression tag	UNP P93243
A	-7	LEU	-	expression tag	UNP P93243
A	-6	VAL	-	expression tag	UNP P93243
A	-5	PRO	-	expression tag	UNP P93243
A	-4	ARG	-	expression tag	UNP P93243
A	-3	GLY	-	expression tag	UNP P93243
A	-2	SER	-	expression tag	UNP P93243
A	-1	HIS	-	expression tag	UNP P93243
A	0	MET	-	expression tag	UNP P93243

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Chain	Residue	Modelled	Actual	Comment	Reference
A	117	THR	VAL	conflict	UNP P93243
B	-20	MET	-	initiating methionine	UNP P93243
B	-19	GLY	-	expression tag	UNP P93243
B	-18	SER	-	expression tag	UNP P93243
B	-17	SER	-	expression tag	UNP P93243
B	-16	HIS	-	expression tag	UNP P93243
B	-15	HIS	-	expression tag	UNP P93243
B	-14	HIS	-	expression tag	UNP P93243
B	-13	HIS	-	expression tag	UNP P93243
B	-12	HIS	-	expression tag	UNP P93243
B	-11	HIS	-	expression tag	UNP P93243
B	-10	SER	-	expression tag	UNP P93243
B	-9	SER	-	expression tag	UNP P93243
B	-8	GLY	-	expression tag	UNP P93243
B	-7	LEU	-	expression tag	UNP P93243
B	-6	VAL	-	expression tag	UNP P93243
B	-5	PRO	-	expression tag	UNP P93243
B	-4	ARG	-	expression tag	UNP P93243
B	-3	GLY	-	expression tag	UNP P93243
B	-2	SER	-	expression tag	UNP P93243
B	-1	HIS	-	expression tag	UNP P93243
B	0	MET	-	expression tag	UNP P93243
B	117	THR	VAL	conflict	UNP P93243
C	-20	MET	-	initiating methionine	UNP P93243
C	-19	GLY	-	expression tag	UNP P93243
C	-18	SER	-	expression tag	UNP P93243
C	-17	SER	-	expression tag	UNP P93243
C	-16	HIS	-	expression tag	UNP P93243
C	-15	HIS	-	expression tag	UNP P93243
C	-14	HIS	-	expression tag	UNP P93243
C	-13	HIS	-	expression tag	UNP P93243
C	-12	HIS	-	expression tag	UNP P93243
C	-11	HIS	-	expression tag	UNP P93243
C	-10	SER	-	expression tag	UNP P93243
C	-9	SER	-	expression tag	UNP P93243
C	-8	GLY	-	expression tag	UNP P93243
C	-7	LEU	-	expression tag	UNP P93243
C	-6	VAL	-	expression tag	UNP P93243
C	-5	PRO	-	expression tag	UNP P93243
C	-4	ARG	-	expression tag	UNP P93243
C	-3	GLY	-	expression tag	UNP P93243
C	-2	SER	-	expression tag	UNP P93243

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	HIS	-	expression tag	UNP P93243
C	0	MET	-	expression tag	UNP P93243
C	117	THR	VAL	conflict	UNP P93243
D	-20	MET	-	initiating methionine	UNP P93243
D	-19	GLY	-	expression tag	UNP P93243
D	-18	SER	-	expression tag	UNP P93243
D	-17	SER	-	expression tag	UNP P93243
D	-16	HIS	-	expression tag	UNP P93243
D	-15	HIS	-	expression tag	UNP P93243
D	-14	HIS	-	expression tag	UNP P93243
D	-13	HIS	-	expression tag	UNP P93243
D	-12	HIS	-	expression tag	UNP P93243
D	-11	HIS	-	expression tag	UNP P93243
D	-10	SER	-	expression tag	UNP P93243
D	-9	SER	-	expression tag	UNP P93243
D	-8	GLY	-	expression tag	UNP P93243
D	-7	LEU	-	expression tag	UNP P93243
D	-6	VAL	-	expression tag	UNP P93243
D	-5	PRO	-	expression tag	UNP P93243
D	-4	ARG	-	expression tag	UNP P93243
D	-3	GLY	-	expression tag	UNP P93243
D	-2	SER	-	expression tag	UNP P93243
D	-1	HIS	-	expression tag	UNP P93243
D	0	MET	-	expression tag	UNP P93243
D	117	THR	VAL	conflict	UNP P93243

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).
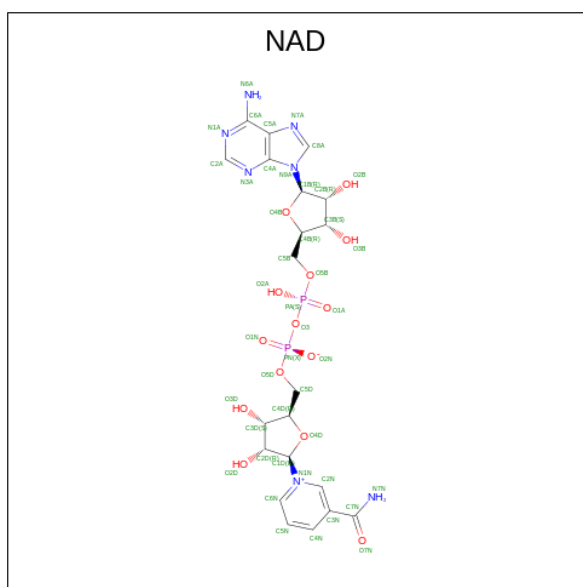
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0

- Molecule 5 is (2R)-2-methyl-2-oxidanyl-butanenitrile (three-letter code: 5Z9) (formula: C_5H_9NO) (labeled as "Ligand of Interest" by depositor).
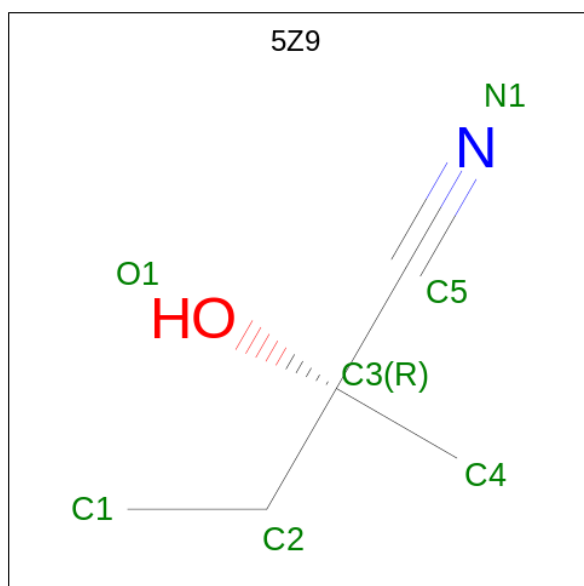
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 7	C 5	N 1	O 1	0	0
5	B	1	Total 7	C 5	N 1	O 1	0	0
5	C	1	Total 7	C 5	N 1	O 1	0	0
5	D	1	Total 7	C 5	N 1	O 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
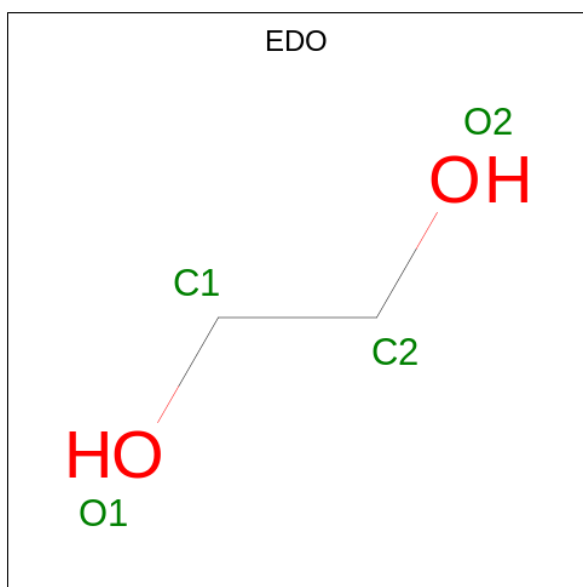
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total C O 4 2 2			0	0
6	A	1	Total C O 4 2 2			0	0
6	A	1	Total C O 4 2 2			0	0
6	A	1	Total C O 4 2 2			0	0
6	A	1	Total C O 4 2 2			0	0
6	B	1	Total C O 4 2 2			0	0
6	B	1	Total C O 4 2 2			0	0
6	D	1	Total C O 4 2 2			0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
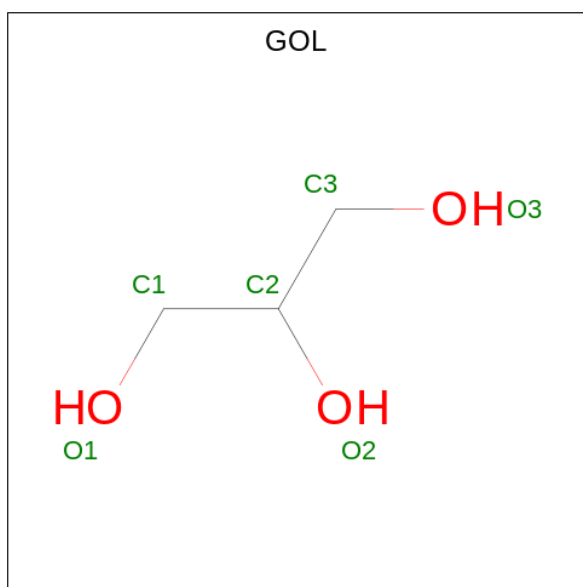
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0

- Molecule 8 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN
  E-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).

BTB
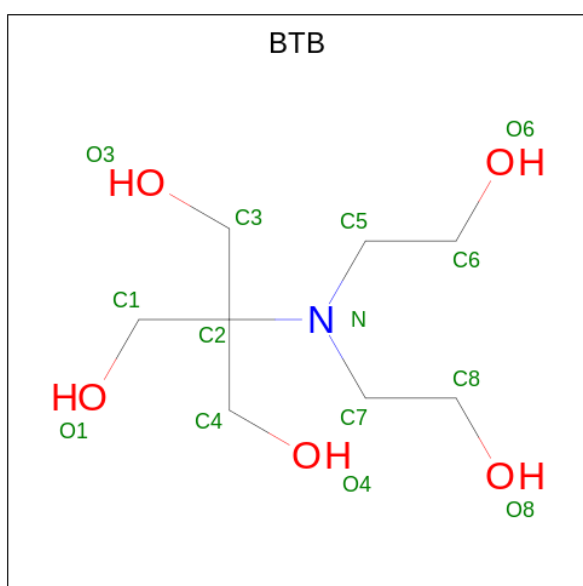
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total 14	C 8	N 1	O 5	0	0
8	A	1	Total 14	C 8	N 1	O 5	0	0
8	A	1	Total 14	C 8	N 1	O 5	0	0
8	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	463	Total 463	O 463	0	0
9	B	481	Total 481	O 481	0	0
9	C	226	Total 226	O 226	0	0
9	D	252	Total 252	O 252	0	0

3 Residue-property plots ⓘ
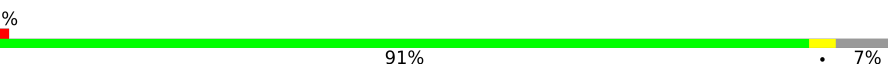
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Aliphatic (R)-hydroxynitrile lyase

Chain A:
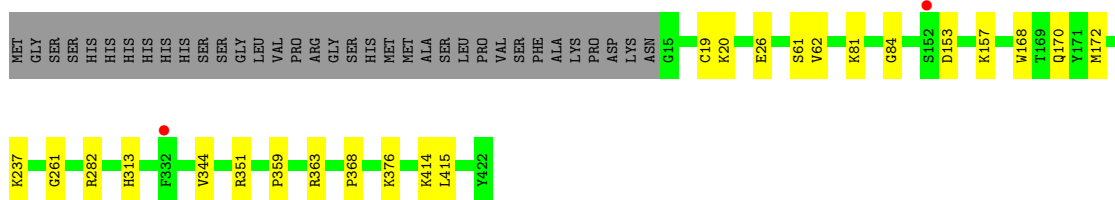
• Molecule 1: Aliphatic (R)-hydroxynitrile lyase

Chain B:
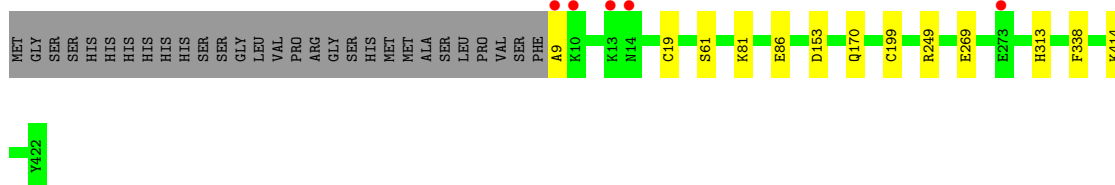
• Molecule 1: Aliphatic (R)-hydroxynitrile lyase

Chain C:

• Molecule 1: Aliphatic (R)-hydroxynitrile lyase

Chain D:

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET MET ALA SER LEU PRO VAL SER PHE ALA LYS PRO ASP LYS ASN G15 S61 K81 I82 F101 A138 K155 L159 L163 L182 A186 T203 R282

S294 H313 T318 E323 R330 I331 F332 F338 G350 Q366 T397 P398 K414 Y422
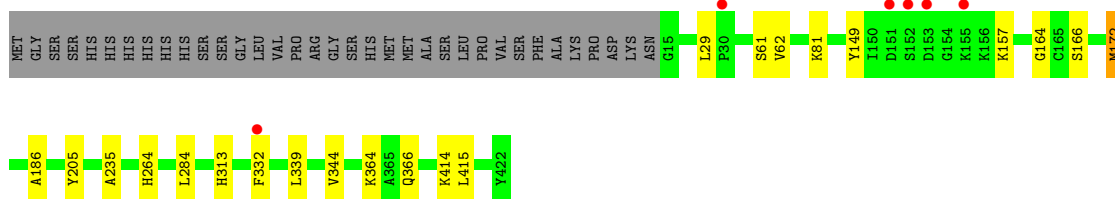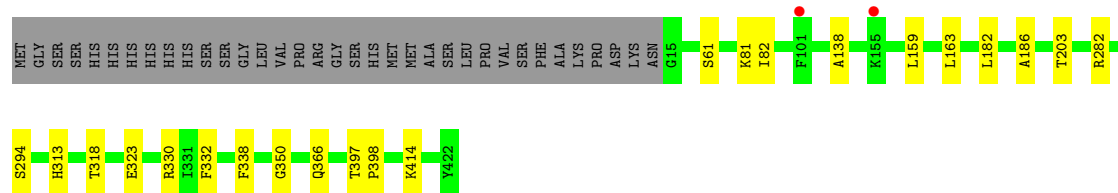
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.18Å 52.10Å 169.85Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	49.85 – 1.74 49.80 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.85-1.74) 98.6 (49.80-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.163 , 0.206 0.174 , 0.211	Depositor DCC
R_{free} test set	8653 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.3	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14242	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAD, GOL, ZN, SNC, BTB, EDO, MG, 5Z9

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	0.78	1/3170 (0.0%)	0.87	3/4284 (0.1%)
1	B	0.77	0/3202	0.87	0/4328
1	C	0.71	0/3159	0.82	0/4270
1	D	0.72	0/3156	0.83	2/4266 (0.0%)
All	All	0.75	1/12687 (0.0%)	0.85	5/17148 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	GLU	CD-OE2	-5.27	1.19	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
1	D	282	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	282	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	282	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	282	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	351	ARG	NE-CZ-NH1	5.32	122.96	120.30

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3121	0	3136	12	0
1	B	3153	0	3167	8	0
1	C	3110	0	3124	16	0
1	D	3108	0	3121	16	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	0	0	0
5	B	7	0	0	0	0
5	C	7	0	0	0	0
5	D	7	0	0	0	0
6	A	20	0	30	0	0
6	B	8	0	12	0	0
6	D	4	0	6	0	0
7	A	6	0	8	2	0
7	B	18	0	24	0	0
8	A	42	0	57	3	0
8	D	14	0	19	0	0
9	A	463	0	0	4	0
9	B	481	0	0	3	0
9	C	226	0	0	2	0
9	D	252	0	0	2	0
All	All	14242	0	12808	47	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 (47) 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)
8:A:514:BTB:H51	9:A:942:HOH:O	1.80	0.82
1:B:313:HIS:HD2	9:B:858:HOH:O	1.70	0.74
1:C:313:HIS:HD2	9:C:733:HOH:O	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:HG12	1:D:338:PHE:HZ	1.67	0.60
1:D:61:SER:HB2	1:D:414:LYS:HD2	1.84	0.58
1:A:344:VAL:HG12	1:B:338:PHE:HZ	1.70	0.56
1:C:149:TYR:CE1	1:C:157:LYS:HB2	2.40	0.56
1:B:313:HIS:HE1	9:B:974:HOH:O	1.88	0.55
1:D:313:HIS:HE1	9:D:821:HOH:O	1.88	0.55
1:A:61:SER:HB2	1:A:414:LYS:HD2	1.91	0.53
1:B:9:ALA:HB2	9:B:727:HOH:O	2.09	0.52
1:B:249:ARG:HB2	1:B:269:GLU:HG3	1.91	0.51
1:C:344:VAL:HG12	1:D:338:PHE:CZ	2.46	0.51
1:C:62:VAL:HG21	1:C:415:LEU:HD23	1.92	0.50
1:A:20:LYS:HE3	9:A:669:HOH:O	2.10	0.50
1:A:237:LYS:HD3	7:A:511:GOL:H12	1.94	0.49
1:D:182:LEU:HD12	1:D:182:LEU:N	2.28	0.48
1:C:332[B]:PHE:CD1	1:D:330:ARG:NH2	2.81	0.48
1:C:186:ALA:HA	1:C:366:GLN:NE2	2.29	0.48
1:A:157:LYS:HE2	9:A:614:HOH:O	2.13	0.47
1:B:19:CYS:HB2	1:B:170:GLN:HB2	1.96	0.47
1:B:61:SER:HB2	1:B:414:LYS:HD2	1.97	0.47
1:A:19:CYS:HB2	1:A:170:GLN:HB2	1.97	0.46
1:A:62:VAL:HG21	1:A:415:LEU:HD23	1.98	0.46
1:D:313:HIS:HD2	9:D:713:HOH:O	1.98	0.44
1:A:359:PRO:O	1:A:363[B]:ARG:HG3	2.17	0.44
1:D:186:ALA:HA	1:D:366:GLN:NE2	2.33	0.43
1:A:368:PRO:HD2	1:C:29:LEU:HD12	2.00	0.43
1:D:138:ALA:HA	1:D:163:LEU:O	2.18	0.43
1:A:313:HIS:HE1	9:A:990:HOH:O	2.01	0.43
1:B:86:GLU:OE2	1:B:199:CYS:HB3	2.18	0.43
1:C:61:SER:HB2	1:C:414:LYS:HD2	2.00	0.43
1:C:332[B]:PHE:CD1	1:D:330:ARG:CZ	3.02	0.42
1:C:339:LEU:HD22	1:D:323:GLU:HG2	2.00	0.42
1:C:166:SER:O	1:C:172:MET:HB2	2.19	0.42
1:C:264:HIS:CD2	1:C:284:LEU:HD22	2.54	0.42
1:C:332[A]:PHE:CE2	1:D:332:PHE:HB3	2.55	0.42
8:A:514:BTB:O8	8:A:514:BTB:H61	2.20	0.42
1:D:294:SER:O	1:D:318:THR:HA	2.20	0.41
1:A:84:GLY:HA3	1:A:168:TRP:CD1	2.55	0.41
8:A:514:BTB:H41	8:A:514:BTB:H52	1.98	0.41
1:C:205:TYR:CD2	1:C:235:ALA:HB2	2.56	0.41
1:A:261:GLY:O	7:A:511:GOL:C1	2.69	0.41
1:C:164:GLY:HA3	9:C:809:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:397:THR:N	1:D:398:PRO:CD	2.85	0.40
1:D:82:ILE:HD11	1:D:159:LEU:HD13	2.04	0.40
1:D:203:THR:HA	1:D:350:GLY:N	2.36	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	407/443 (92%)	397 (98%)	10 (2%)	0	100	100
1	B	412/443 (93%)	401 (97%)	11 (3%)	0	100	100
1	C	406/443 (92%)	391 (96%)	15 (4%)	0	100	100
1	D	406/443 (92%)	393 (97%)	13 (3%)	0	100	100
All	All	1631/1772 (92%)	1582 (97%)	49 (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	339/367 (92%)	335 (99%)	4 (1%)	71	56
1	B	343/367 (94%)	341 (99%)	2 (1%)	86	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	338/367 (92%)	335 (99%)	3 (1%)	78	67
1	D	338/367 (92%)	337 (100%)	1 (0%)	92	89
All	All	1358/1468 (92%)	1348 (99%)	10 (1%)	84	75

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LYS
1	A	153	ASP
1	A	172	MET
1	A	376	LYS
1	B	81	LYS
1	B	153	ASP
1	C	81	LYS
1	C	172	MET
1	C	364	LYS
1	D	81	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	215	GLN
1	A	366	GLN
1	B	130	GLN
1	B	131	ASN
1	B	215	GLN
1	B	313	HIS
1	B	366	GLN
1	C	130	GLN
1	C	131	ASN
1	C	183	ASN
1	C	313	HIS
1	C	366	GLN
1	D	130	GLN
1	D	131	ASN
1	D	313	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are 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	$\#|Z| > 2$
1	SNC	B	265	1	4,7,8	0.87	0	1,7,9	0.13	0
1	SNC	C	265	1	4,7,8	0.71	0	1,7,9	1.73	0
1	SNC	D	265	1	4,7,8	0.86	0	1,7,9	1.09	0
1	SNC	A	265	1	4,7,8	0.84	0	1,7,9	0.57	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
1	SNC	B	265	1	-	0/0/6/8	-
1	SNC	C	265	1	-	0/0/6/8	-
1	SNC	D	265	1	-	0/0/6/8	-
1	SNC	A	265	1	-	0/0/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	#$|Z| > 2$
6	EDO	B	507	-	3,3,3	0.45	0	2,2,2	0.51	0
6	EDO	A	510	-	3,3,3	0.30	0	2,2,2	0.20	0
2	NAD	D	501	-	42,48,48	0.61	1 (2%)	50,73,73	0.95	3 (6%)
6	EDO	A	507	-	3,3,3	0.14	0	2,2,2	0.46	0
8	BTB	A	512	-	13,13,13	1.45	3 (23%)	7,16,16	0.52	0
7	GOL	B	510	-	5,5,5	0.13	0	5,5,5	0.44	0
6	EDO	A	509	-	3,3,3	0.40	0	2,2,2	0.49	0
2	NAD	A	501	-	42,48,48	0.75	1 (2%)	50,73,73	0.83	1 (2%)
5	5Z9	B	505	3	3,6,6	1.76	1 (33%)	4,8,8	1.13	1 (25%)
6	EDO	B	506	-	3,3,3	0.58	0	2,2,2	0.46	0
6	EDO	A	506	-	3,3,3	0.15	0	2,2,2	0.14	0
8	BTB	A	513	-	13,13,13	1.74	3 (23%)	7,16,16	0.53	0
2	NAD	C	501	-	42,48,48	0.66	1 (2%)	50,73,73	0.82	2 (4%)
7	GOL	B	508	-	5,5,5	0.14	0	5,5,5	0.14	0
5	5Z9	D	505	3	3,6,6	0.28	0	4,8,8	0.37	0
7	GOL	A	511	-	5,5,5	0.22	0	5,5,5	0.51	0
2	NAD	B	501	-	42,48,48	0.68	0	50,73,73	0.87	2 (4%)
8	BTB	D	507	-	13,13,13	1.22	3 (23%)	7,16,16	0.50	0
8	BTB	A	514	-	13,13,13	1.57	3 (23%)	7,16,16	1.10	0
5	5Z9	A	505	3	3,6,6	0.72	0	4,8,8	0.90	0
5	5Z9	C	505	3	3,6,6	0.17	0	4,8,8	1.35	0
6	EDO	D	506	-	3,3,3	0.47	0	2,2,2	0.74	0
6	EDO	A	508	-	3,3,3	0.05	0	2,2,2	0.02	0
7	GOL	B	509	-	5,5,5	0.14	0	5,5,5	0.30	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
6	EDO	B	507	-	-	1/1/1/1	-
6	EDO	A	510	-	-	0/1/1/1	-
2	NAD	D	501	-	-	5/26/62/62	0/5/5/5
6	EDO	A	507	-	-	0/1/1/1	-
8	BTB	A	512	-	-	3/21/21/21	-
7	GOL	B	510	-	-	3/4/4/4	-
6	EDO	A	509	-	-	1/1/1/1	-
2	NAD	A	501	-	-	5/26/62/62	0/5/5/5
5	5Z9	B	505	3	-	0/3/6/6	-
6	EDO	B	506	-	-	1/1/1/1	-
6	EDO	A	506	-	-	1/1/1/1	-
8	BTB	A	513	-	-	1/21/21/21	-
2	NAD	C	501	-	-	4/26/62/62	0/5/5/5
7	GOL	B	508	-	-	4/4/4/4	-
5	5Z9	D	505	3	-	0/3/6/6	-
7	GOL	A	511	-	-	4/4/4/4	-
2	NAD	B	501	-	-	5/26/62/62	0/5/5/5
8	BTB	D	507	-	-	6/21/21/21	-
8	BTB	A	514	-	-	4/21/21/21	-
5	5Z9	A	505	3	-	0/3/6/6	-
5	5Z9	C	505	3	-	0/3/6/6	-
6	EDO	D	506	-	-	1/1/1/1	-
6	EDO	A	508	-	-	1/1/1/1	-
7	GOL	B	509	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	513	BTB	C2-N	4.69	1.57	1.48
8	A	514	BTB	C2-N	4.14	1.56	1.48
8	A	512	BTB	C2-N	3.55	1.55	1.48
8	D	507	BTB	C2-N	2.95	1.54	1.48
8	A	514	BTB	C5-N	2.74	1.51	1.48
8	A	513	BTB	C5-N	2.71	1.51	1.48
2	A	501	NAD	C2N-N1N	2.70	1.38	1.35
8	A	512	BTB	C5-N	2.69	1.51	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	505	5Z9	C5-N1	2.66	1.18	1.14
8	D	507	BTB	C5-N	2.36	1.51	1.48
8	A	513	BTB	C7-N	2.34	1.51	1.48
8	A	512	BTB	C7-N	2.23	1.51	1.48
2	C	501	NAD	C8A-N7A	-2.15	1.30	1.34
2	D	501	NAD	C8A-N7A	-2.08	1.31	1.34
8	D	507	BTB	C7-N	2.04	1.50	1.48
8	A	514	BTB	C7-N	2.01	1.50	1.48

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAD	C6N-N1N-C2N	-3.32	118.94	121.97
2	B	501	NAD	C6N-N1N-C2N	-2.74	119.47	121.97
2	C	501	NAD	C6N-N1N-C2N	-2.58	119.63	121.97
2	A	501	NAD	C6N-N1N-C2N	-2.34	119.84	121.97
2	C	501	NAD	C5A-C6A-N6A	2.25	123.78	120.35
5	B	505	5Z9	O1-C3-C5	2.17	113.03	108.91
2	D	501	NAD	O2A-PA-O1A	2.14	122.81	112.24
2	D	501	NAD	O7N-C7N-C3N	-2.11	117.10	119.63
2	B	501	NAD	O7N-C7N-C3N	2.02	122.05	119.63

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAD	O4D-C1D-N1N-C2N
2	A	501	NAD	O4D-C1D-N1N-C6N
2	A	501	NAD	C2D-C1D-N1N-C2N
2	A	501	NAD	C2D-C1D-N1N-C6N
2	B	501	NAD	O4D-C1D-N1N-C2N
2	B	501	NAD	O4D-C1D-N1N-C6N
2	B	501	NAD	C2D-C1D-N1N-C2N
2	B	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4D-C1D-N1N-C2N
2	C	501	NAD	O4D-C1D-N1N-C6N
2	C	501	NAD	C2D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C2N
2	D	501	NAD	O4D-C1D-N1N-C6N
2	D	501	NAD	C2D-C1D-N1N-C2N
7	A	511	GOL	C1-C2-C3-O3
7	A	511	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	B	508	GOL	O1-C1-C2-O2
7	B	508	GOL	O1-C1-C2-C3
7	B	509	GOL	O1-C1-C2-C3
8	A	512	BTB	C1-C2-C3-O3
8	A	512	BTB	C4-C2-C3-O3
8	A	512	BTB	N-C2-C3-O3
8	A	514	BTB	O1-C1-C2-C3
8	A	514	BTB	O1-C1-C2-C4
8	D	507	BTB	C1-C2-N-C5
8	D	507	BTB	C3-C2-N-C5
8	D	507	BTB	C4-C2-N-C5
8	D	507	BTB	C4-C2-N-C7
6	B	506	EDO	O1-C1-C2-O2
7	A	511	GOL	O1-C1-C2-C3
7	B	508	GOL	C1-C2-C3-O3
7	B	510	GOL	C1-C2-C3-O3
6	A	506	EDO	O1-C1-C2-O2
6	B	507	EDO	O1-C1-C2-O2
6	D	506	EDO	O1-C1-C2-O2
7	B	509	GOL	O1-C1-C2-O2
7	B	510	GOL	O1-C1-C2-C3
8	A	514	BTB	N-C7-C8-O8
7	B	510	GOL	O2-C2-C3-O3
8	D	507	BTB	C6-C5-N-C7
6	A	509	EDO	O1-C1-C2-O2
8	A	513	BTB	N-C2-C4-O4
8	A	514	BTB	O1-C1-C2-N
8	D	507	BTB	C1-C2-N-C7
7	A	511	GOL	O1-C1-C2-O2
2	A	501	NAD	O4B-C4B-C5B-O5B
7	B	508	GOL	O2-C2-C3-O3
6	A	508	EDO	O1-C1-C2-O2
2	D	501	NAD	C2D-C1D-N1N-C6N
2	C	501	NAD	O4B-C4B-C5B-O5B
2	D	501	NAD	O4B-C4B-C5B-O5B
2	B	501	NAD	O4B-C4B-C5B-O5B

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	511	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	514	BTB	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 then 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.

Ligand NAD D 501

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD A 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 5Z9 B 505

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD C 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 5Z9 D 505

Bond lengths

Bond angles

Torsions

Rings

Ligand NAD B 501

Bond lengths

Bond angles

Torsions

Rings

Ligand 5Z9 A 505

Bond lengths

Bond angles

Torsions

Rings

Ligand 5Z9 C 505

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	407/443 (91%)	-0.21	2 (0%)	91	93	10, 15, 26, 54	0
1	B	413/443 (93%)	-0.17	5 (1%)	79	84	10, 15, 30, 63	0
1	C	407/443 (91%)	0.12	6 (1%)	73	80	18, 29, 45, 75	0
1	D	407/443 (91%)	-0.04	2 (0%)	91	93	16, 26, 42, 70	0
All	All	1634/1772 (92%)	-0.07	15 (0%)	84	88	10, 21, 40, 75	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	SER	4.3
1	B	9	ALA	3.4
1	B	273	GLU	3.4
1	C	153	ASP	2.9
1	A	332[A]	PHE	2.7
1	D	101	PHE	2.6
1	C	332[A]	PHE	2.5
1	D	155	LYS	2.4
1	C	151	ASP	2.4
1	B	10	LYS	2.3
1	C	155	LYS	2.2
1	A	152	SER	2.1
1	B	13	LYS	2.1
1	C	30	PRO	2.1
1	B	14	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SNC	C	265	8/9	0.89	0.12	26,30,37,42	0
1	SNC	D	265	8/9	0.94	0.09	17,22,24,31	0
1	SNC	A	265	8/9	0.96	0.07	15,16,21,32	0
1	SNC	B	265	8/9	0.96	0.08	12,15,22,25	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	511	6/6	0.65	0.26	41,44,44,46	0
8	BTB	A	514	14/14	0.68	0.24	40,55,65,66	0
8	BTB	A	513	14/14	0.70	0.21	26,36,40,41	0
6	EDO	A	509	4/4	0.70	0.16	33,40,41,46	0
6	EDO	D	506	4/4	0.72	0.26	43,43,47,47	0
6	EDO	B	506	4/4	0.75	0.18	33,37,38,41	0
6	EDO	B	507	4/4	0.79	0.19	43,45,47,49	0
7	GOL	B	510	6/6	0.79	0.13	39,45,45,50	0
6	EDO	A	506	4/4	0.80	0.12	42,46,47,47	0
8	BTB	D	507	14/14	0.81	0.25	40,60,65,69	0
7	GOL	B	509	6/6	0.83	0.21	32,38,43,51	0
8	BTB	A	512	14/14	0.85	0.14	25,30,36,37	0
6	EDO	A	508	4/4	0.85	0.15	50,52,54,55	0
7	GOL	B	508	6/6	0.88	0.17	34,38,41,44	0
6	EDO	A	510	4/4	0.90	0.16	34,38,39,40	0
5	5Z9	C	505	7/7	0.93	0.10	19,23,24,25	0
6	EDO	A	507	4/4	0.94	0.10	24,33,35,38	0
5	5Z9	D	505	7/7	0.94	0.12	21,24,27,27	0
5	5Z9	B	505	7/7	0.94	0.10	11,14,16,17	0
5	5Z9	A	505	7/7	0.96	0.10	14,14,15,15	0
2	NAD	C	501	44/44	0.96	0.07	16,24,27,28	0
4	MG	D	504	1/1	0.97	0.07	34,34,34,34	0
2	NAD	A	501	44/44	0.97	0.08	10,13,15,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAD	D	501	44/44	0.97	0.07	17,21,23,25	0
2	NAD	B	501	44/44	0.98	0.07	10,13,16,19	0
3	ZN	D	502	1/1	0.99	0.03	21,21,21,21	1
3	ZN	D	503	1/1	0.99	0.03	23,23,23,23	0
4	MG	B	504	1/1	0.99	0.07	16,16,16,16	0
4	MG	C	504	1/1	0.99	0.11	31,31,31,31	0
3	ZN	A	502	1/1	0.99	0.05	14,14,14,14	0
4	MG	A	504	1/1	1.00	0.08	14,14,14,14	0
3	ZN	B	503	1/1	1.00	0.05	12,12,12,12	0
3	ZN	C	502	1/1	1.00	0.03	23,23,23,23	0
3	ZN	C	503	1/1	1.00	0.03	23,23,23,23	0
3	ZN	A	503	1/1	1.00	0.04	14,14,14,14	0
3	ZN	B	502	1/1	1.00	0.04	15,15,15,15	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 5Z9 C 505:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
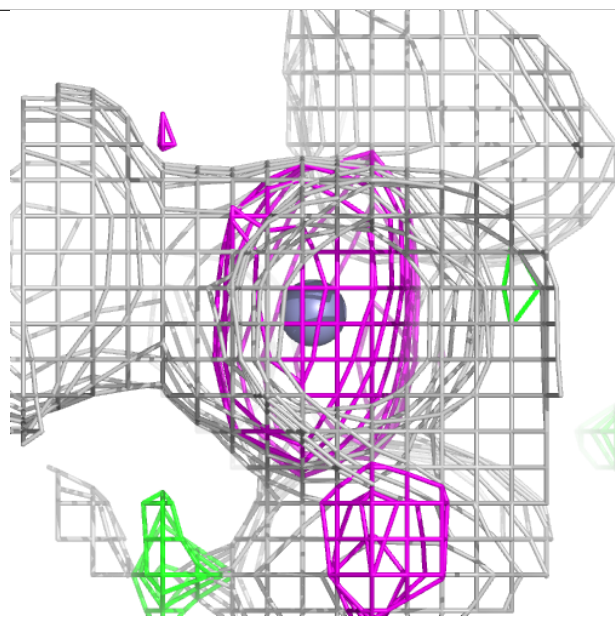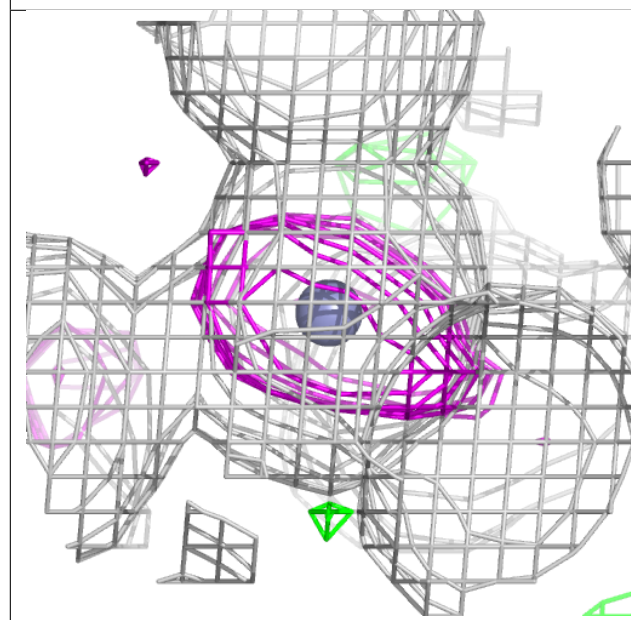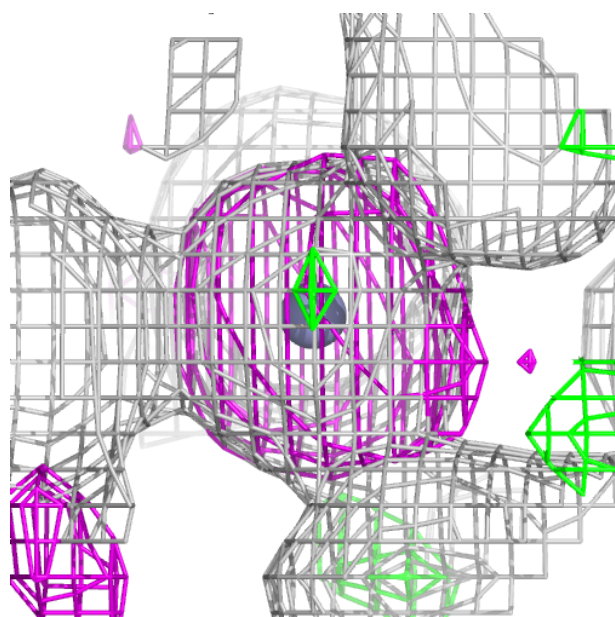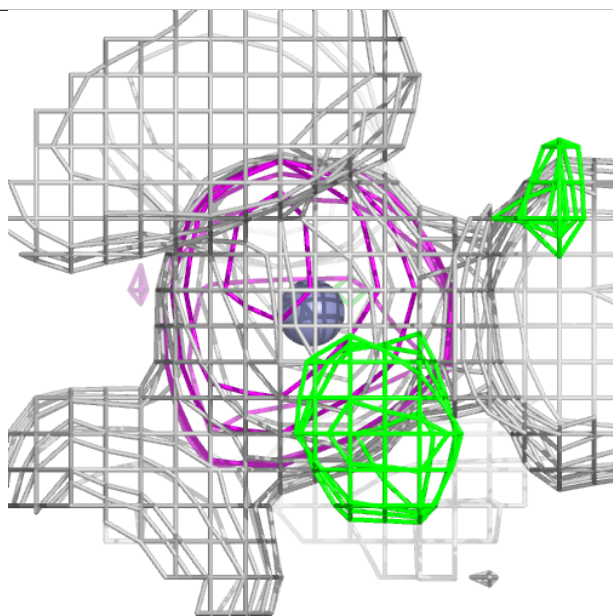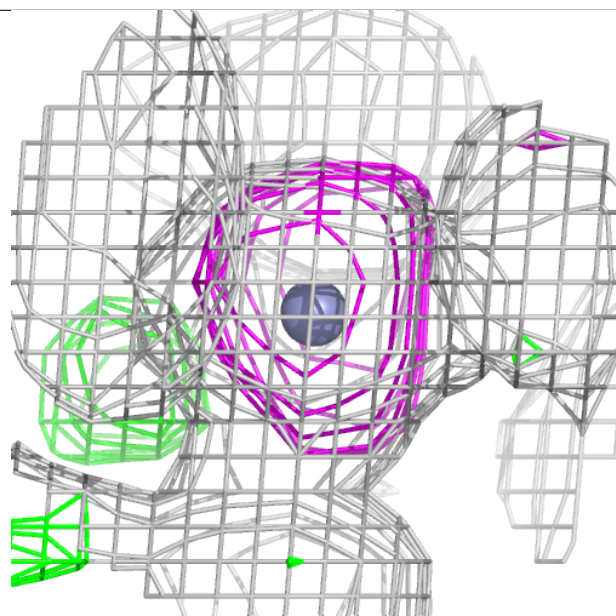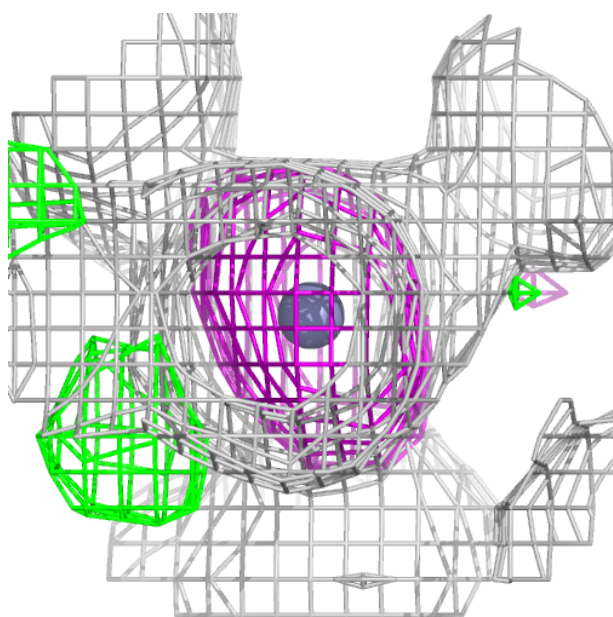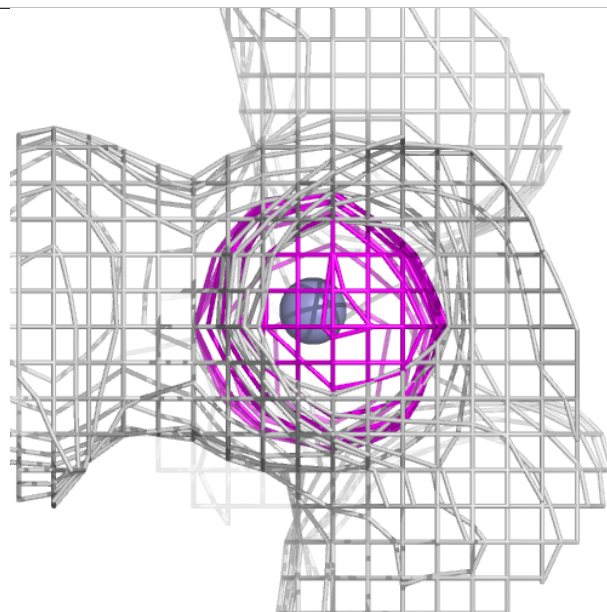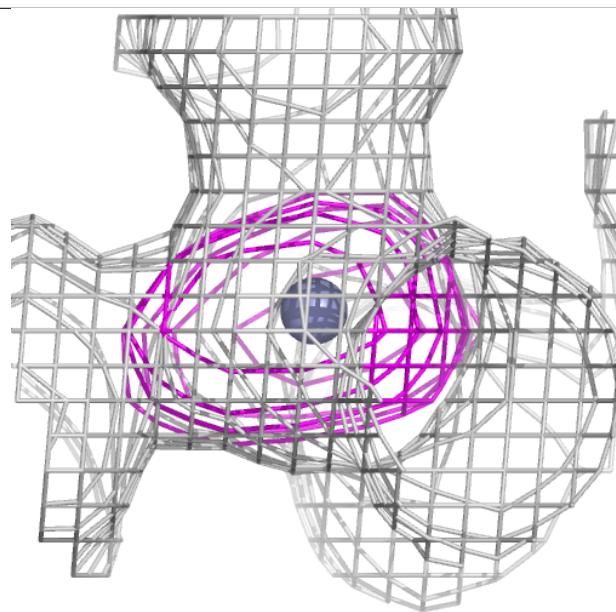and green (positive)
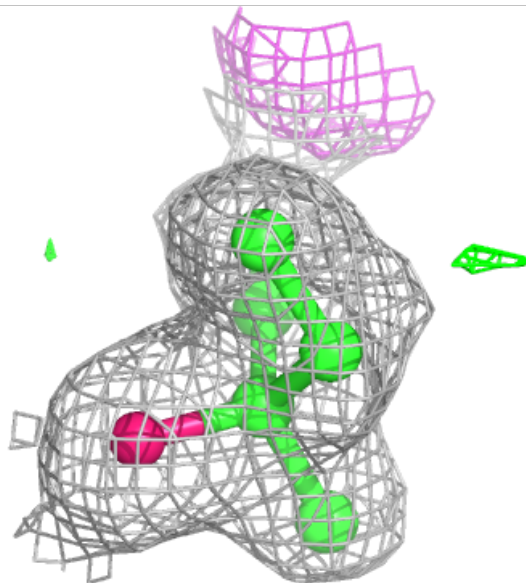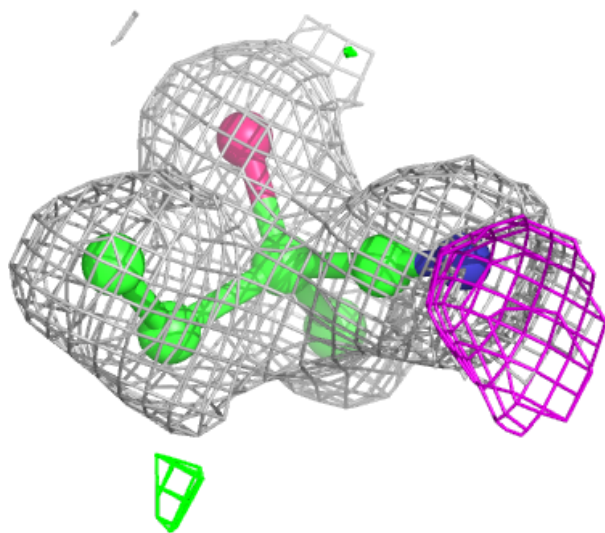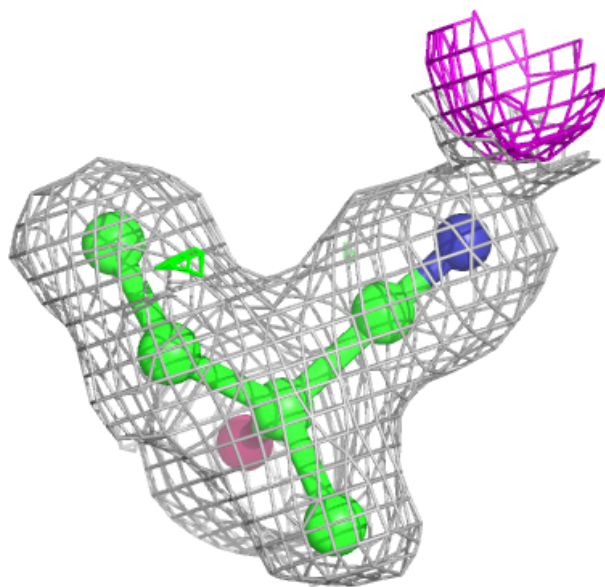
Electron density around 5Z9 D 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
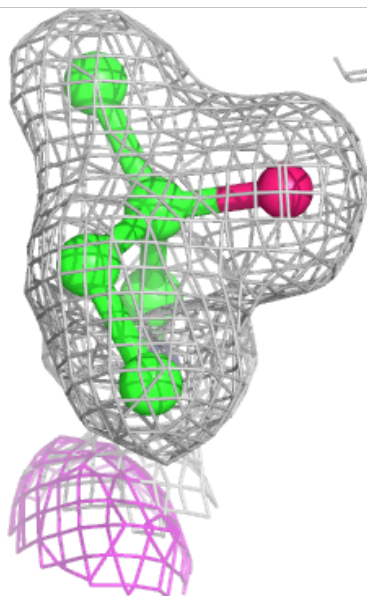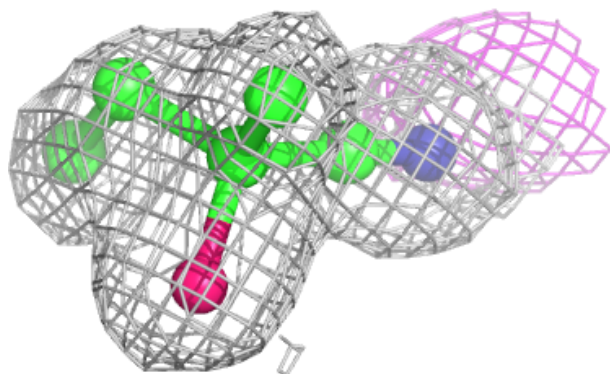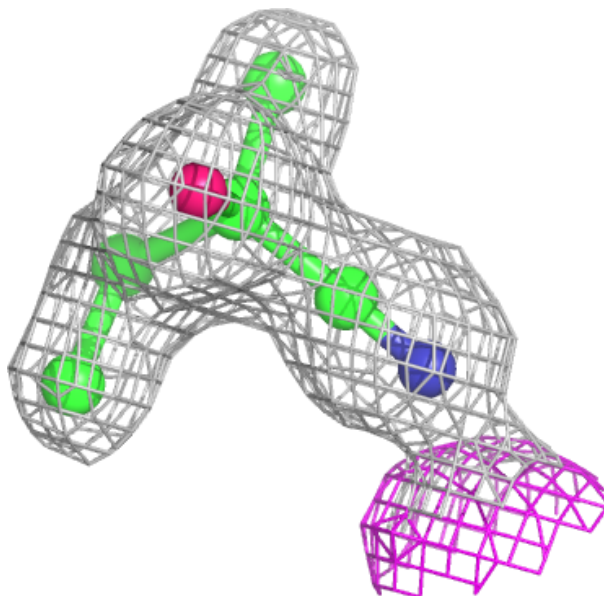
Electron density around 5Z9 B 505:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
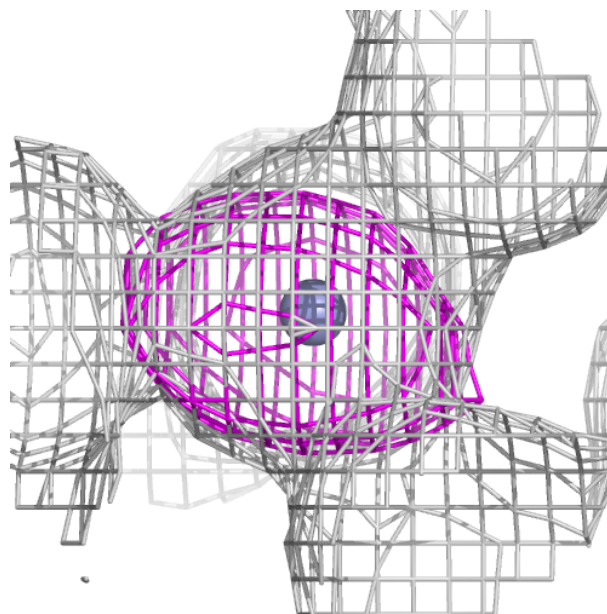and green (positive)
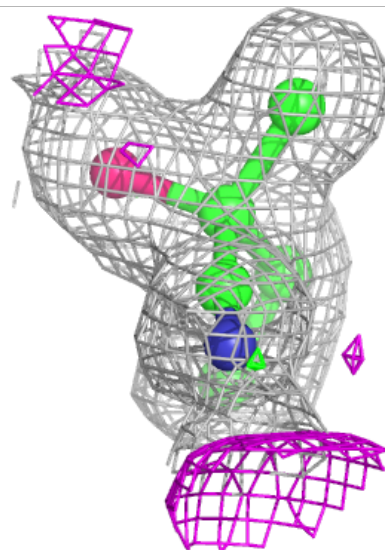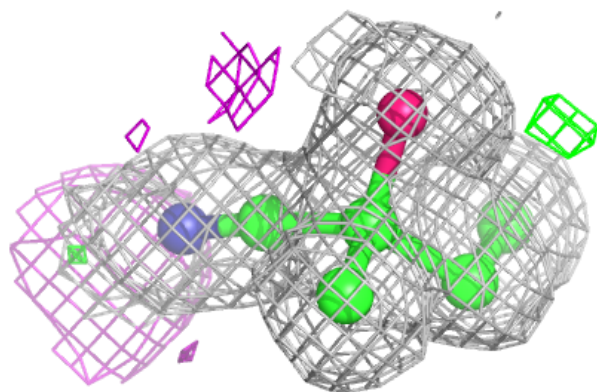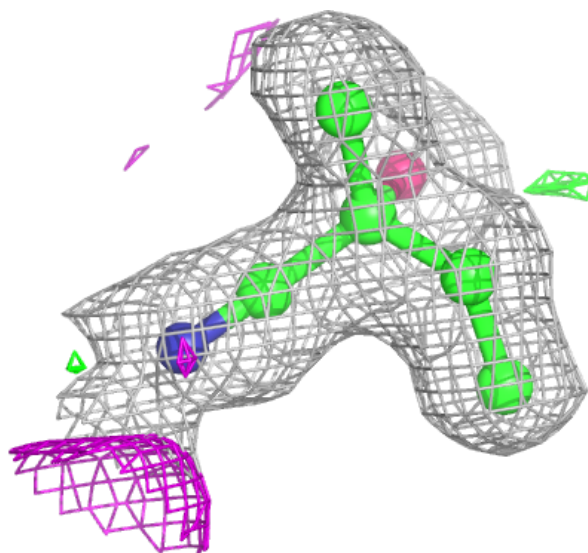
Electron density around 5Z9 A 505:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
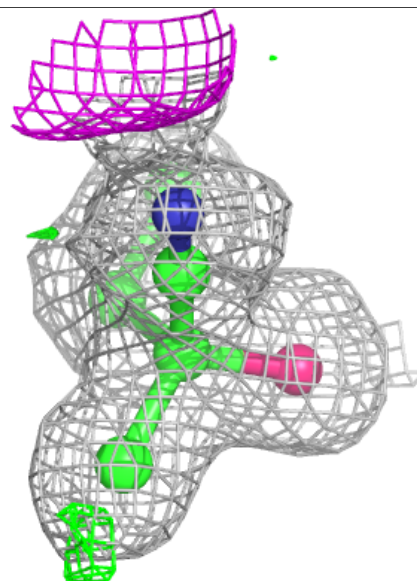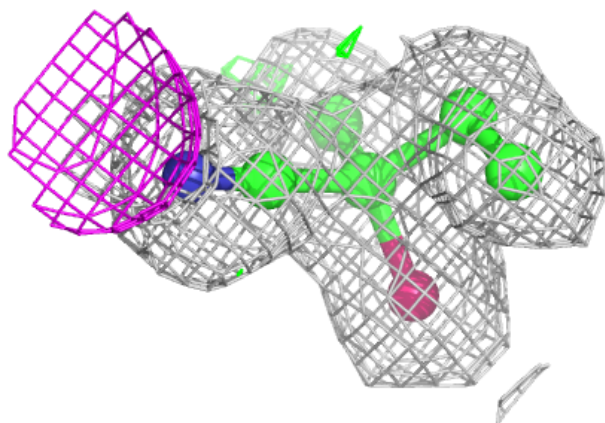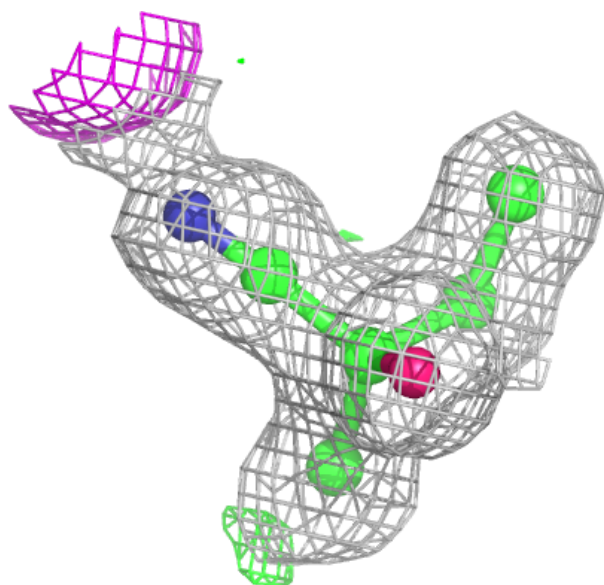
Electron density around NAD C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
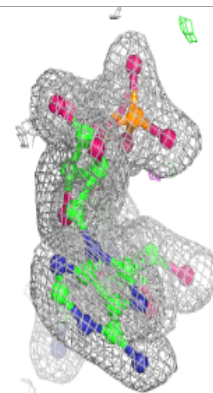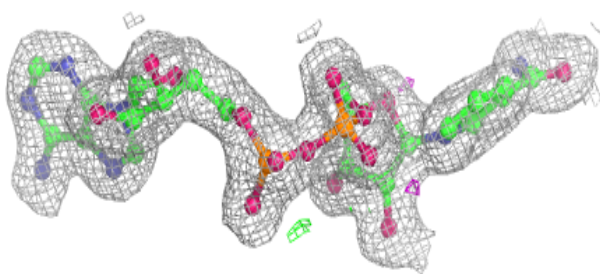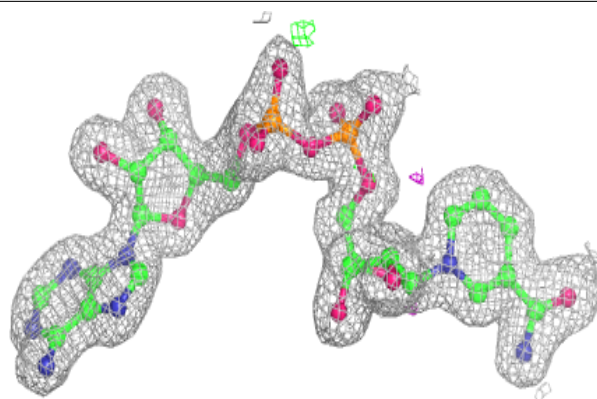
Electron density around NAD A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
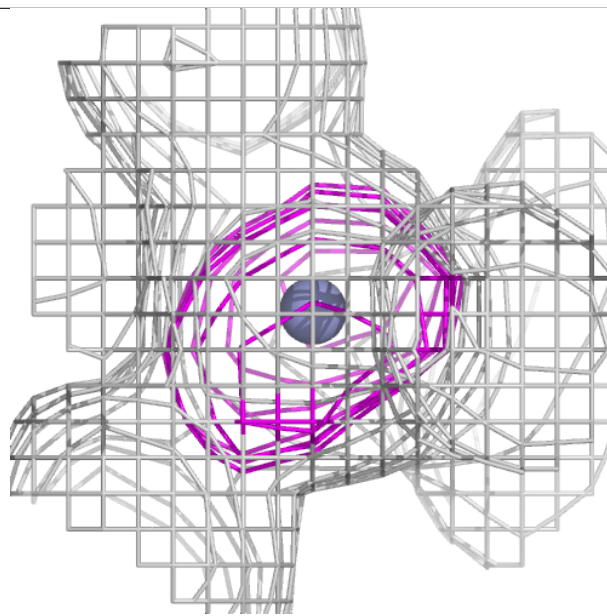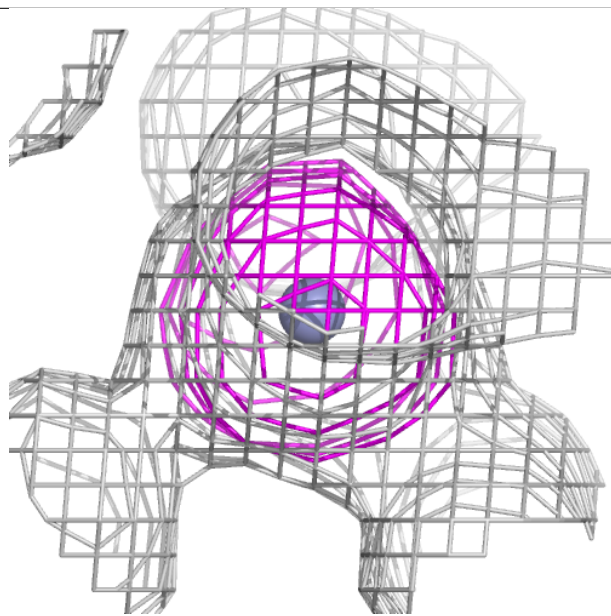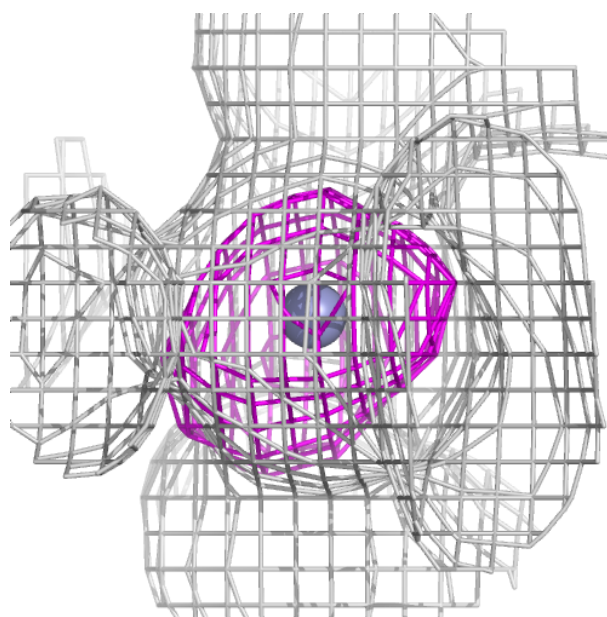and green (positive)
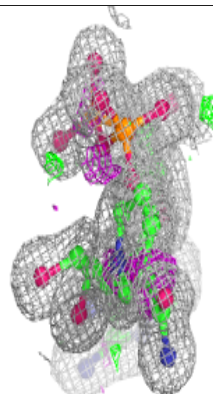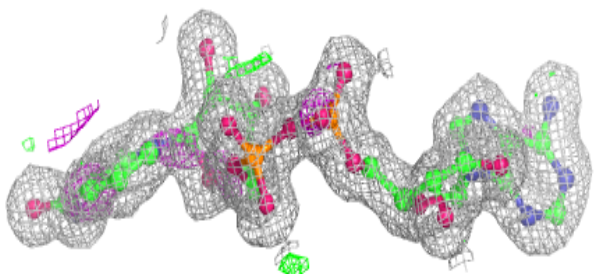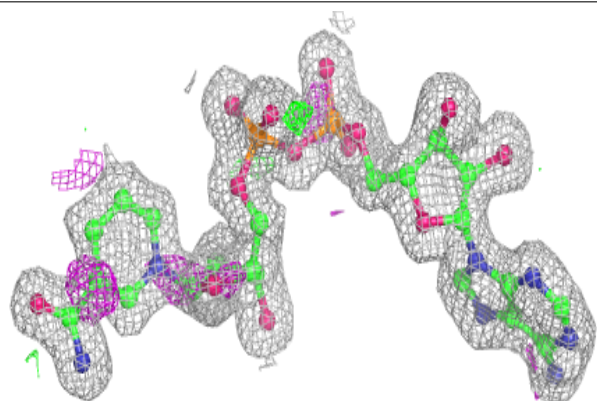
Electron density around NAD D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
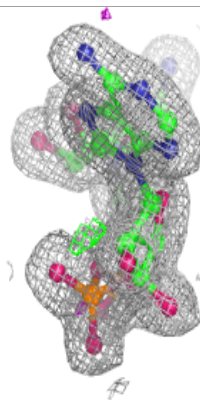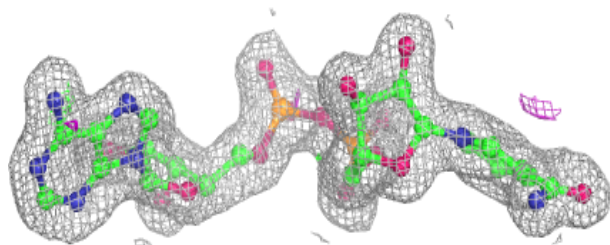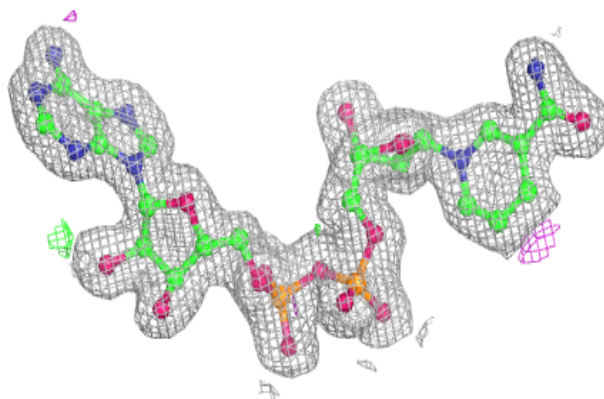
Electron density around NAD B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
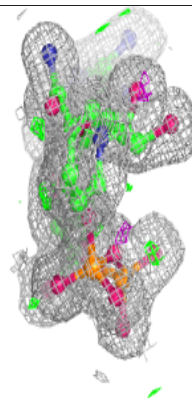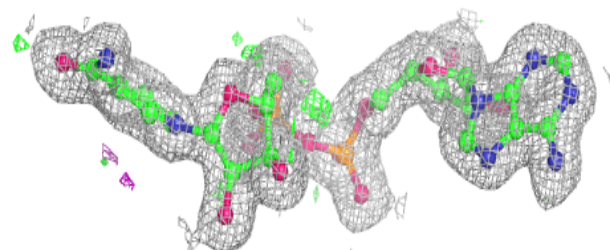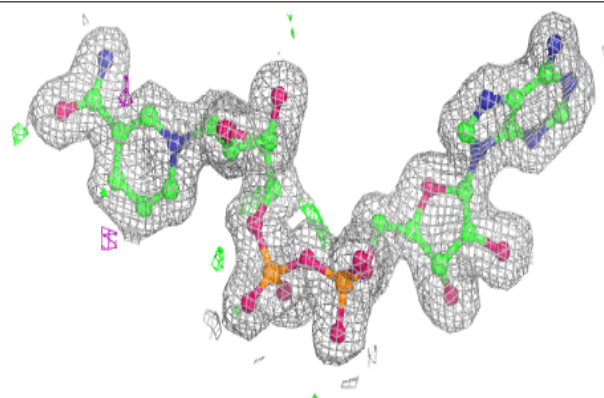
Electron density around ZN D 502:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
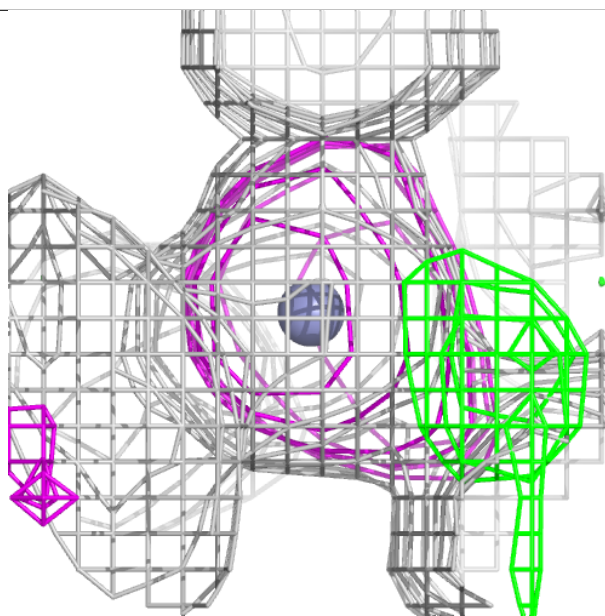and green (positive)
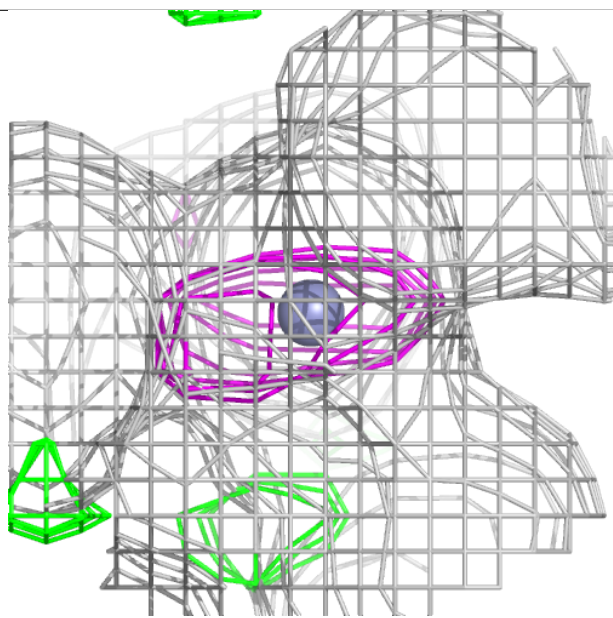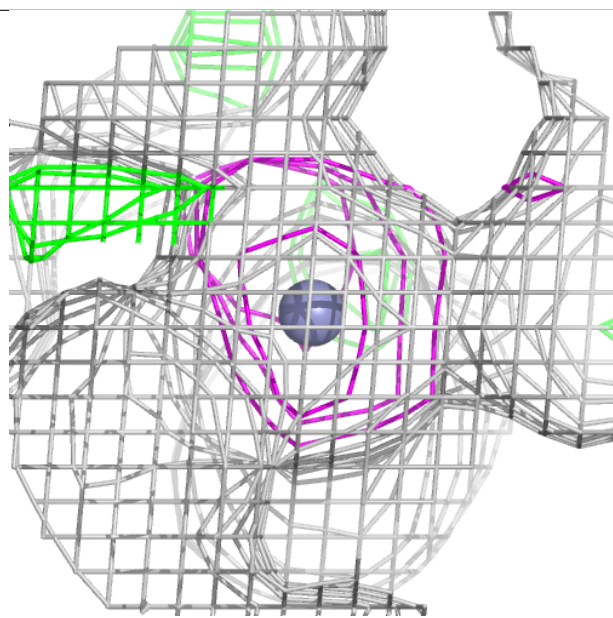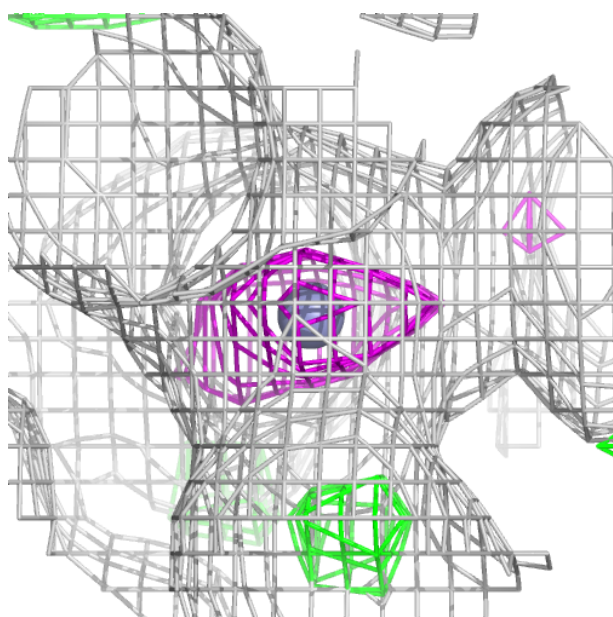
Electron density around ZN D 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
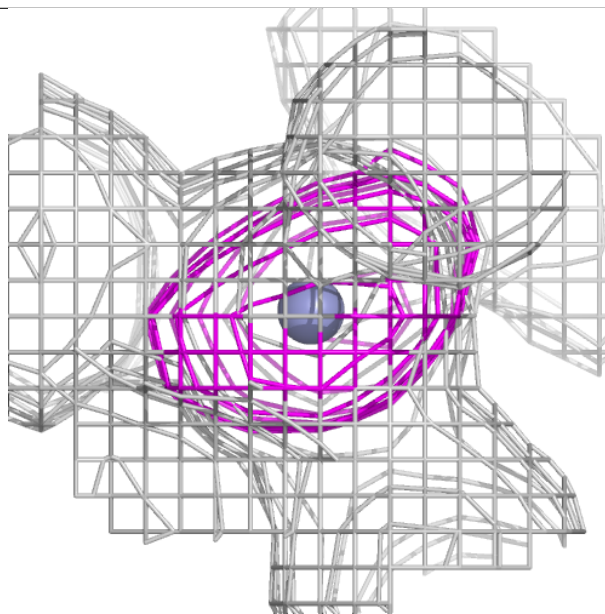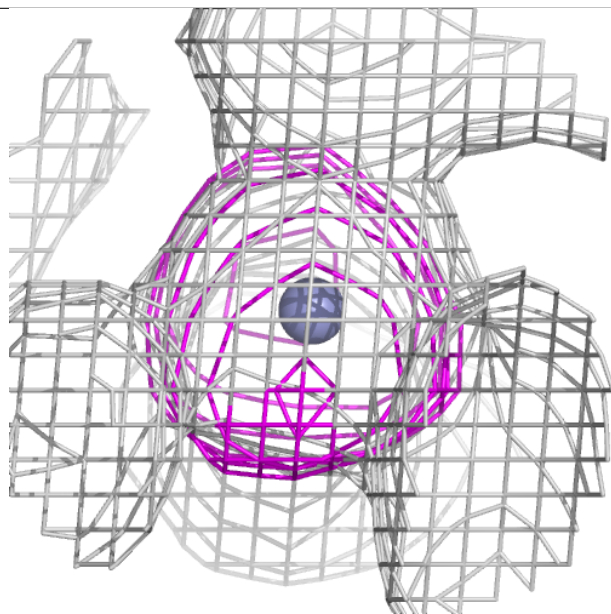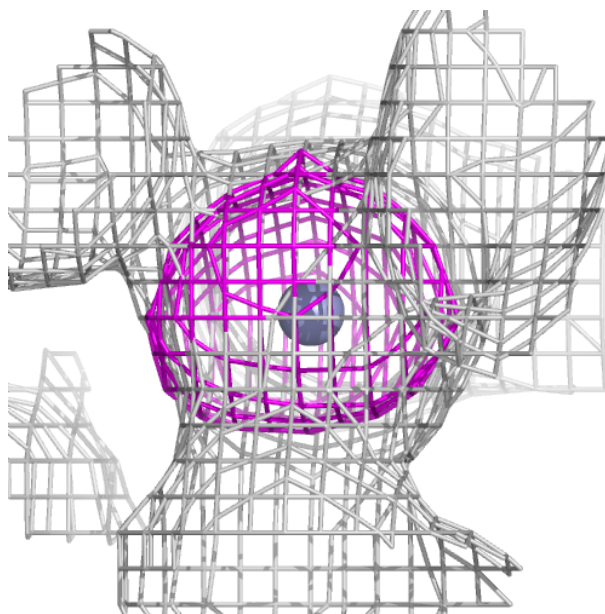
Electron density around ZN A 502:

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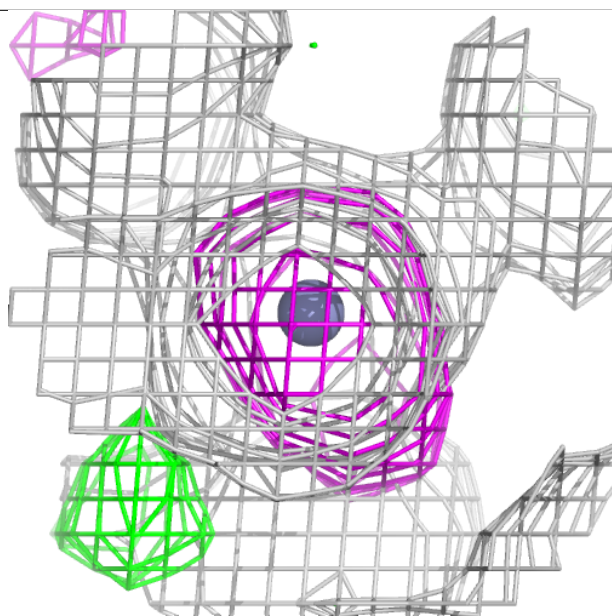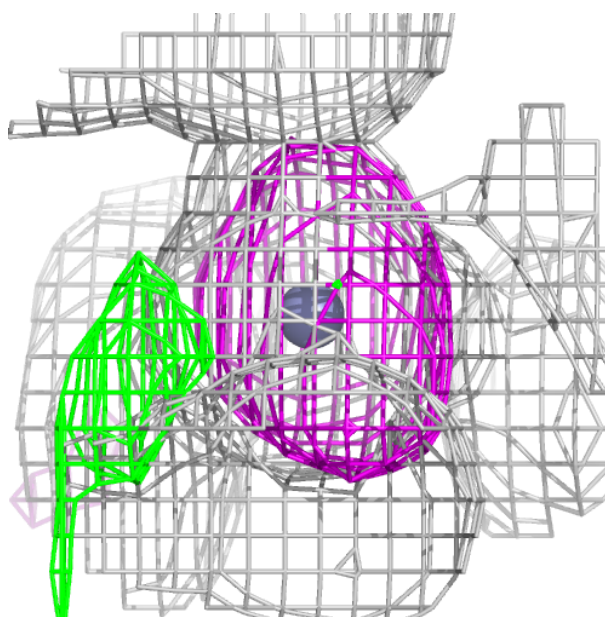and green (positive)

Electron density around ZN B 503:

$2mF_o$-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 C 502:

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

Electron density around ZN C 503:
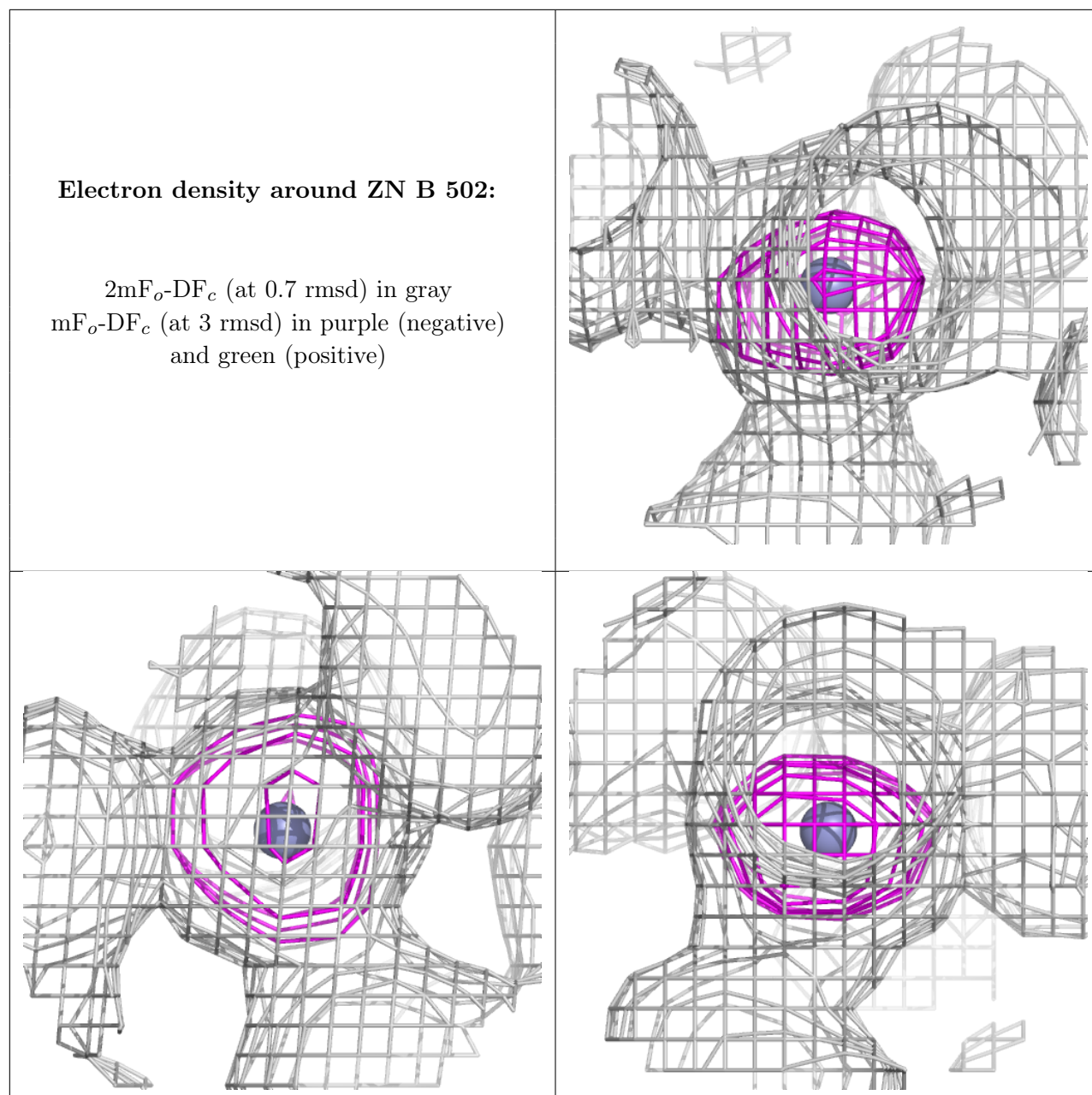
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ZN A 503:

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

Electron density around ZN B 502:

$2mF_o$-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.