



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:50 AM UTC

PDB ID : 6YI1 / pdb_00006yi1
Title : Crystal structure of human glutaminy cyclase in complex with Glu(gamma-hydrazide)-Phe-Ala
Authors : Kupski, O.; Sautner, V.; Tittmann, K.
Deposited on : 2020-03-31
Resolution : 1.92 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
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

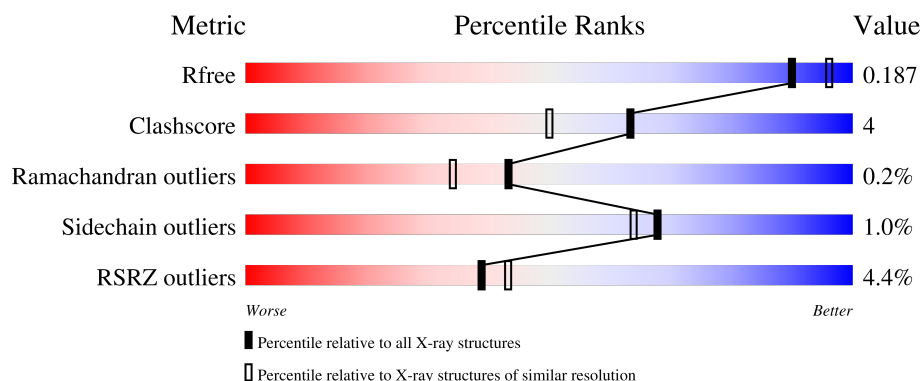
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	329	3% 92% 8%
1	B	329	5% 92% 7%
2	C	4	75% 25%
2	D	4	50% 50%
2	E	4	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	PEG	A	417	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6178 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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	6	0
			2699	1724	465	501	9			
1	B	329	Total	C	N	O	S	0	14	0
			2745	1752	479	505	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	expression tag	UNP Q16769
A	34	PRO	-	expression tag	UNP Q16769
B	33	GLY	-	expression tag	UNP Q16769
B	34	PRO	-	expression tag	UNP Q16769

- Molecule 2 is a protein called Glu(gamma-hydrazide)-Phe-Ala.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	1
			27	17	6	4			
2	D	4	Total	C	N	O	0	0	1
			27	17	6	4			
2	E	4	Total	C	N	O	0	2	1
			33	20	8	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

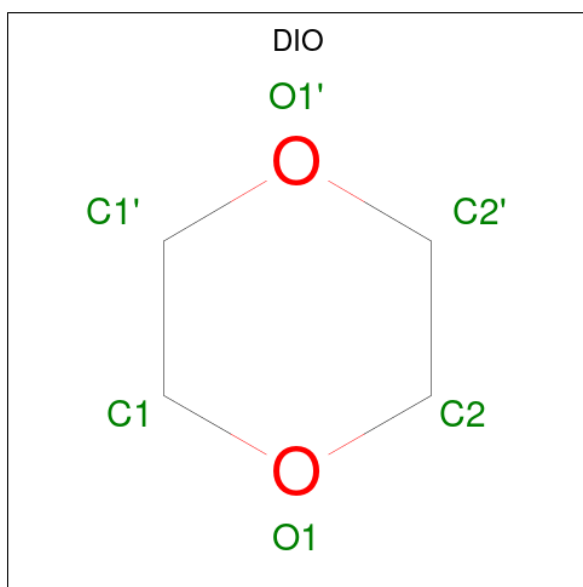
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Zn	0	0
			5	5		
4	B	5	Total	Zn	0	0
			5	5		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



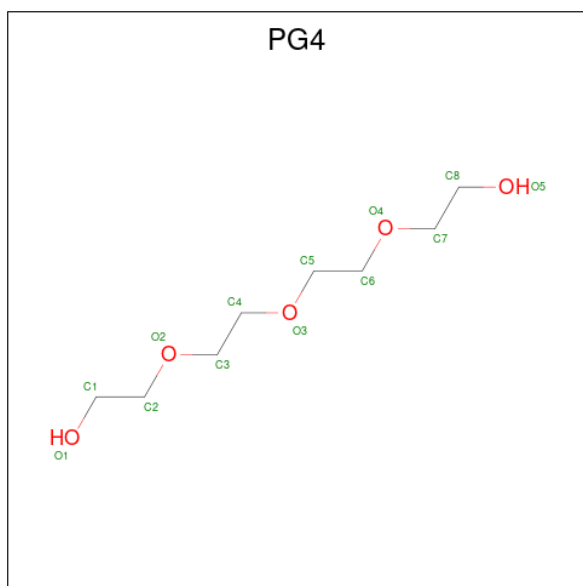
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	1
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



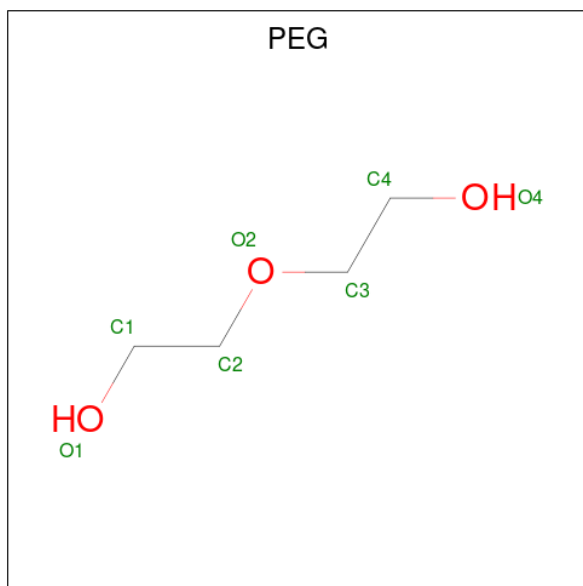
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	4	2		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



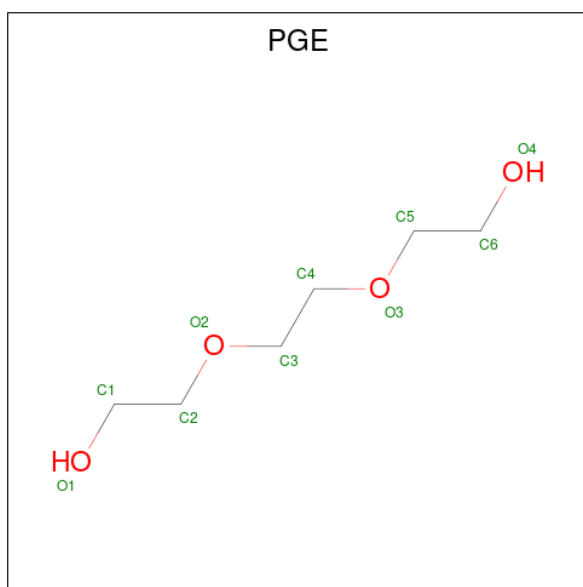
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



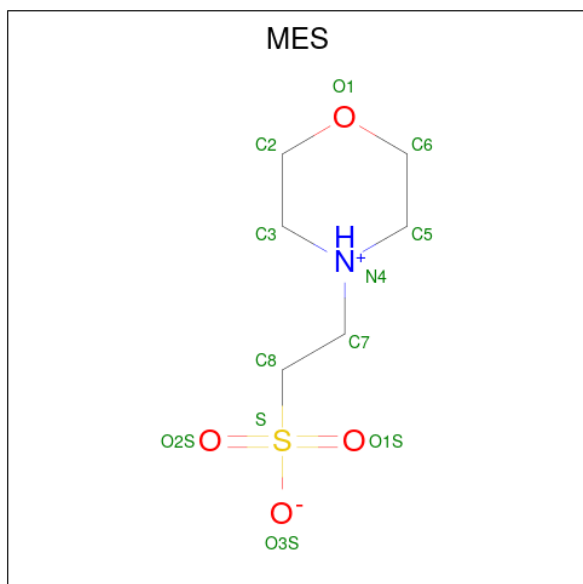
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

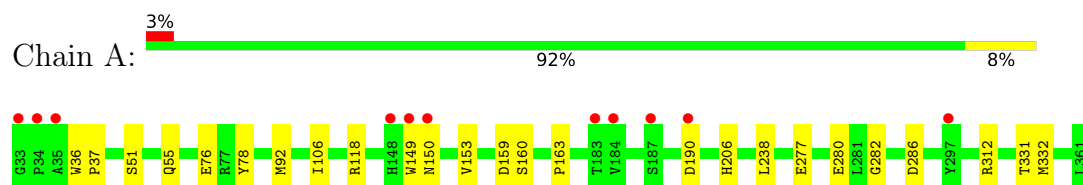
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	231	Total	O	0	3
			234	234		
11	B	192	Total	O	0	5
			194	194		

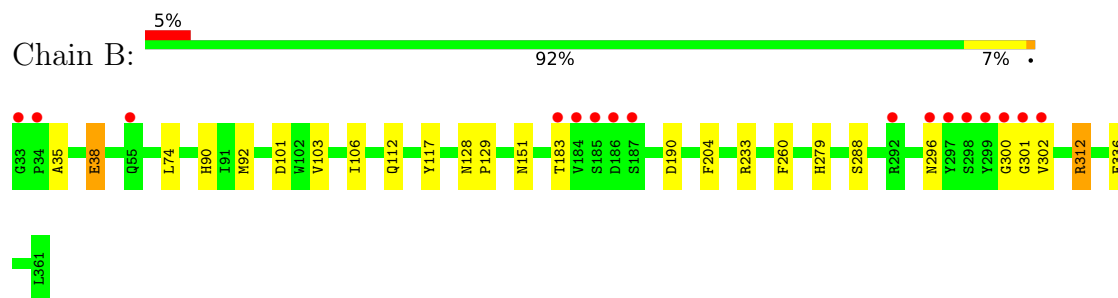
3 Residue-property plots

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.

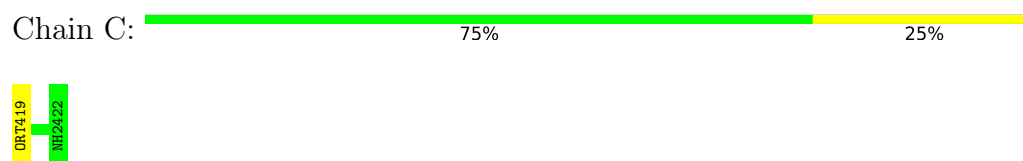
- Molecule 1: Glutaminyl-peptide cyclotransferase



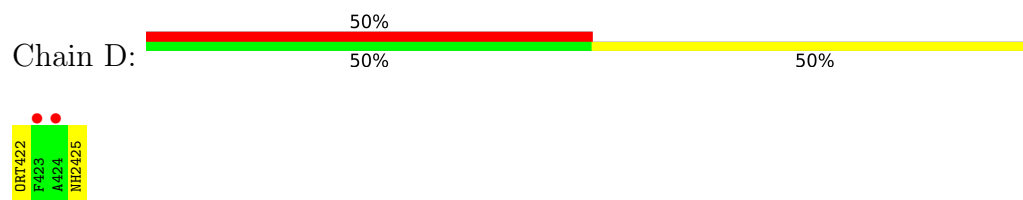
- Molecule 1: Glutaminyl-peptide cyclotransferase



- Molecule 2: Glu(gamma-hydrazide)-Phe-Ala



- Molecule 2: Glu(gamma-hydrazide)-Phe-Ala



- Molecule 2: Glu(gamma-hydrazide)-Phe-Ala



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	120.38Å 120.38Å 331.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.28 – 1.92 88.28 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.4 (88.28-1.92) 94.2 (88.28-1.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.92Å)	Xtriage
Refinement program	PHENIX dev_2940	Depositor
R, R_{free}	0.159 , 0.186 0.160 , 0.187	Depositor DCC
R_{free} test set	3497 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6178	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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: ZN, DIO, ORT, NH2, MES, PGE, PG4, GOL, SO4, PEG

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	0.43	0/2778	0.58	0/3782
1	B	0.39	0/2831	0.53	0/3854
2	C	0.36	0/16	0.45	0/20
2	D	0.24	0/16	0.37	0/20
2	E	0.40	0/20	0.35	0/24
All	All	0.41	0/5661	0.55	0/7700

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	2699	0	2605	20	0
1	B	2745	0	2651	20	0
2	C	27	0	14	1	0
2	D	27	0	14	2	0
2	E	33	0	19	0	0
3	A	20	0	0	0	0
3	B	35	0	0	2	0
4	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	0	0	0
5	A	12	0	16	0	0
5	B	18	0	24	0	0
6	A	6	0	8	0	0
7	A	39	0	54	5	0
8	A	21	0	30	7	0
8	B	14	0	20	2	0
9	B	20	0	28	1	0
10	B	24	0	24	7	0
11	A	234	0	0	3	0
11	B	194	0	0	4	0
All	All	6178	0	5507	45	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 4.

All (45) 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)
11:A:502:HOH:O	2:D:425:NH2:N	2.20	0.74
1:A:118:ARG:HH12	8:A:418:PEG:H22	1.61	0.65
1:B:183:THR:HG22	11:B:638:HOH:O	1.99	0.63
1:A:312:ARG:HA	7:A:415:PG4:H41	1.81	0.63
1:A:277:GLU:HA	7:A:413:PG4:H52	1.82	0.62
1:A:331:THR:HB	8:A:417:PEG:H31	1.83	0.60
1:A:118:ARG:NH1	8:A:418:PEG:H22	2.18	0.59
1:B:90:HIS:HD2	11:B:683:HOH:O	1.85	0.59
1:B:296[A]:ASN:N	3:B:421[A]:SO4:O2	2.34	0.57
1:A:332:MET:HB2	8:A:417:PEG:H42	1.86	0.56
1:B:35:ALA:O	1:B:38:GLU:HG3	2.04	0.55
1:A:92:MET:SD	1:A:106:ILE:HD11	2.47	0.55
1:B:151:ASN:ND2	11:B:502:HOH:O	2.31	0.54
1:A:149:TRP:CE3	1:A:150:ASN:HB3	2.44	0.53
1:B:233:ARG:N	3:B:418:SO4:O1	2.40	0.52
1:B:103:VAL:HG21	10:B:420:MES:H32	1.92	0.52
1:A:280:GLU:OE1	11:A:501:HOH:O	2.19	0.51
1:A:331:THR:HA	8:A:417:PEG:H21	1.93	0.51
1:B:101:ASP:OD2	10:B:420:MES:H52	2.12	0.50
9:B:415:PGE:H5	9:B:415:PGE:O2	2.11	0.50
1:B:279:HIS:NE2	10:B:419:MES:N4	2.60	0.49
1:B:190[A]:ASP:N	1:B:190[A]:ASP:OD1	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASN:HA	10:B:420:MES:O3S	2.13	0.48
1:A:332:MET:H	8:A:417:PEG:H31	1.79	0.47
1:A:277:GLU:HG2	7:A:413:PG4:H51	1.96	0.47
1:A:76:GLU:HB2	1:A:153:VAL:HG11	1.97	0.47
1:B:288:SER:HA	10:B:419:MES:H82	1.97	0.47
1:A:190:ASP:OD1	1:A:190:ASP:N	2.47	0.46
1:B:312:ARG:HH21	8:B:416:PEG:H22	1.80	0.46
1:A:51[B]:SER:O	1:A:55[B]:GLN:HG3	2.17	0.45
7:A:414:PG4:H82	11:A:642:HOH:O	2.18	0.44
1:A:282:GLY:O	2:D:422:ORT:N	2.51	0.44
1:A:159:ASP:OD1	2:C:419:ORT:N2	2.51	0.44
1:B:74:LEU:HD13	1:B:336:GLU:HB2	2.01	0.43
1:A:36:TRP:CG	1:A:37:PRO:HD3	2.53	0.43
1:A:160:SER:C	1:A:163:PRO:HD2	2.44	0.43
1:B:129:PRO:HD2	10:B:420:MES:H71	2.01	0.43
8:B:417:PEG:H42	11:B:576:HOH:O	2.17	0.43
1:B:279:HIS:CD2	10:B:419:MES:H62	2.55	0.42
7:A:413:PG4:H51	7:A:413:PG4:H72	1.84	0.42
1:B:260:PHE:CE1	1:B:300[A]:GLY:HA2	2.56	0.41
1:B:112:GLN:HG3	1:B:117:TYR:CE1	2.56	0.41
1:B:300[B]:GLY:HA3	1:B:301[B]:GLY:HA2	1.63	0.40
1:B:92:MET:SD	1:B:106:ILE:HD11	2.62	0.40
1:A:78:TYR:HE1	8:A:418:PEG:H21	1.87	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	333/329 (101%)	324 (97%)	9 (3%)	0	100	100
1	B	341/329 (104%)	325 (95%)	14 (4%)	2 (1%)	21	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	2/4 (50%)	2 (100%)	0	0	100	100
2	D	2/4 (50%)	2 (100%)	0	0	100	100
2	E	3/4 (75%)	3 (100%)	0	0	100	100
All	All	681/670 (102%)	656 (96%)	23 (3%)	2 (0%)	43	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	302[A]	VAL
1	B	302[B]	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/290 (102%)	293 (99%)	3 (1%)	68	64
1	B	298/290 (103%)	295 (99%)	3 (1%)	68	64
2	C	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
2	E	1/1 (100%)	1 (100%)	0	100	100
All	All	597/583 (102%)	591 (99%)	6 (1%)	68	64

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	HIS
1	A	238	LEU
1	A	286	ASP
1	B	38	GLU
1	B	204	PHE
1	B	312	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	194	GLN
1	B	67	GLN
1	B	90	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 10 are monoatomic - leaving 29 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	PEG	B	417	-	6,6,6	0.57	0	5,5,5	0.48	0
8	PEG	A	417	-	6,6,6	0.40	0	5,5,5	0.91	0
3	SO4	B	409	4	4,4,4	0.35	0	6,6,6	0.23	0
3	SO4	B	408	-	4,4,4	0.25	0	6,6,6	0.12	0
3	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.06	0
8	PEG	A	418	-	6,6,6	0.52	0	5,5,5	0.66	0
3	SO4	B	407	-	4,4,4	0.25	0	6,6,6	0.17	0
7	PG4	A	415	-	12,12,12	0.49	0	11,11,11	0.53	0
9	PGE	B	415	-	9,9,9	0.49	0	8,8,8	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	418	-	4,4,4	0.18	0	6,6,6	0.25	0
3	SO4	A	407	-	4,4,4	0.22	0	6,6,6	0.43	0
5	GOL	B	411	-	5,5,5	0.73	0	5,5,5	1.39	0
10	MES	B	419	-	12,12,12	2.32	1 (8%)	15,16,16	1.94	2 (13%)
5	GOL	A	410	-	5,5,5	1.07	0	5,5,5	0.80	0
10	MES	B	420	-	12,12,12	2.28	1 (8%)	15,16,16	2.06	2 (13%)
3	SO4	B	410	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	B	401	-	4,4,4	0.27	0	6,6,6	0.38	0
8	PEG	B	416	-	6,6,6	0.65	0	5,5,5	0.72	0
8	PEG	A	416	-	6,6,6	0.65	0	5,5,5	0.93	0
3	SO4	B	421[A]	-	4,4,4	0.25	0	6,6,6	0.17	0
5	GOL	B	412[A]	-	5,5,5	1.00	0	5,5,5	1.45	1 (20%)
3	SO4	A	408	-	4,4,4	0.22	0	6,6,6	0.13	0
7	PG4	A	414	-	12,12,12	0.65	0	11,11,11	0.42	0
3	SO4	A	409	-	4,4,4	0.34	0	6,6,6	0.30	0
5	GOL	A	411	-	5,5,5	1.34	1 (20%)	5,5,5	1.08	0
6	DIO	A	412	-	6,6,6	0.60	0	6,6,6	0.28	0
5	GOL	B	413	-	5,5,5	0.83	0	5,5,5	0.95	0
7	PG4	A	413	-	12,12,12	0.59	0	11,11,11	0.82	0
9	PGE	B	414	-	9,9,9	0.39	0	8,8,8	0.59	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
5	GOL	A	411	-	-	0/4/4/4	-
8	PEG	B	416	-	-	1/4/4/4	-
5	GOL	B	413	-	-	0/4/4/4	-
8	PEG	B	417	-	-	0/4/4/4	-
8	PEG	A	417	-	-	0/4/4/4	-
6	DIO	A	412	-	-	-	0/1/1/1
7	PG4	A	415	-	-	0/10/10/10	-
8	PEG	A	416	-	-	0/4/4/4	-
8	PEG	A	418	-	-	0/4/4/4	-
7	PG4	A	413	-	-	2/10/10/10	-
9	PGE	B	415	-	-	0/7/7/7	-
9	PGE	B	414	-	-	0/7/7/7	-
5	GOL	B	411	-	-	2/4/4/4	-
5	GOL	B	412[A]	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	420	-	-	4/6/14/14	0/1/1/1
10	MES	B	419	-	-	4/6/14/14	0/1/1/1
5	GOL	A	410	-	-	0/4/4/4	-
7	PG4	A	414	-	-	1/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	419	MES	C8-S	-7.76	1.66	1.77
10	B	420	MES	C8-S	-7.71	1.66	1.77
5	A	411	GOL	C1-C2	2.17	1.60	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	420	MES	C5-N4-C3	6.21	122.22	108.84
10	B	419	MES	C5-N4-C3	4.71	118.98	108.84
10	B	419	MES	O1S-S-C8	3.45	111.94	106.73
10	B	420	MES	C7-N4-C3	2.48	117.85	111.24
5	B	412[A]	GOL	O3-C3-C2	-2.12	100.81	110.38

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	411	GOL	C1-C2-C3-O3
5	B	411	GOL	O2-C2-C3-O3
5	B	412[A]	GOL	C1-C2-C3-O3
5	B	412[A]	GOL	O2-C2-C3-O3
10	B	420	MES	C7-C8-S-O1S
10	B	420	MES	C7-C8-S-O3S
10	B	420	MES	C8-C7-N4-C5
10	B	419	MES	C7-C8-S-O2S
10	B	420	MES	C7-C8-S-O2S
10	B	419	MES	N4-C7-C8-S
7	A	413	PG4	C3-C4-O3-C5
10	B	419	MES	C7-C8-S-O3S
10	B	419	MES	C7-C8-S-O1S
8	B	416	PEG	C4-C3-O2-C2
7	A	414	PG4	C5-C6-O4-C7
7	A	413	PG4	O3-C5-C6-O4

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	417	PEG	1	0
8	A	417	PEG	4	0
8	A	418	PEG	3	0
7	A	415	PG4	1	0
9	B	415	PGE	1	0
3	B	418	SO4	1	0
10	B	419	MES	3	0
10	B	420	MES	4	0
8	B	416	PEG	1	0
3	B	421[A]	SO4	1	0
7	A	414	PG4	1	0
7	A	413	PG4	3	0

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	329/329 (100%)	-0.32	11 (3%)	49	54	11, 23, 47, 102	6 (1%)
1	B	329/329 (100%)	-0.11	16 (4%)	35	39	11, 27, 51, 95	14 (4%)
2	C	2/4 (50%)	-0.60	0	100	100	20, 20, 20, 22	0
2	D	2/4 (50%)	2.48	2 (100%)	0	0	55, 55, 55, 59	0
2	E	2/4 (50%)	0.72	0	100	100	14, 14, 14, 26	1 (50%)
All	All	664/670 (99%)	-0.21	29 (4%)	39	43	11, 24, 50, 102	21 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299[A]	TYR	19.3
1	A	34	PRO	7.3
1	A	33	GLY	6.5
1	B	300[A]	GLY	6.1
1	B	301[A]	GLY	6.0
1	A	149	TRP	5.7
1	B	297[A]	TYR	5.3
1	B	302[A]	VAL	5.2
1	B	298[A]	SER	4.6
1	B	33	GLY	3.9
1	A	183	THR	3.6
1	A	190	ASP	3.4
1	B	186	ASP	3.3
1	B	183	THR	3.0
1	B	296[A]	ASN	2.9
1	B	55[A]	GLN	2.9
1	A	297	TYR	2.8
1	A	35	ALA	2.8
2	D	423	PHE	2.8
1	B	184	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	187	SER	2.7
1	A	187	SER	2.4
1	A	184	VAL	2.4
1	B	292[A]	ARG	2.3
1	B	185	SER	2.3
2	D	424	ALA	2.2
1	A	150	ASN	2.2
1	A	148	HIS	2.1
1	B	34	PRO	2.1

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(Å ²)	Q<0.9
3	SO4	B	421[A]	5/5	0.71	0.17	36,41,43,46	5
3	SO4	B	418	5/5	0.72	0.20	80,82,82,85	0
10	MES	B	419	12/12	0.74	0.18	52,58,73,74	0
8	PEG	A	417	7/7	0.75	0.25	59,59,62,62	0
3	SO4	A	409	5/5	0.76	0.15	61,61,70,70	0
8	PEG	B	416	7/7	0.79	0.22	54,57,58,58	0
3	SO4	B	407	5/5	0.80	0.16	93,94,95,95	0
5	GOL	B	413	6/6	0.81	0.20	52,55,57,59	0
10	MES	B	420	12/12	0.81	0.26	68,81,89,90	0
9	PGE	B	415	10/10	0.82	0.25	46,58,61,63	0
5	GOL	B	412[A]	6/6	0.84	0.18	24,25,27,28	6
8	PEG	A	418	7/7	0.84	0.18	51,59,64,67	0
3	SO4	A	408	5/5	0.85	0.14	76,76,79,79	0
3	SO4	B	410	5/5	0.87	0.16	79,80,81,82	5

Continued on next page...

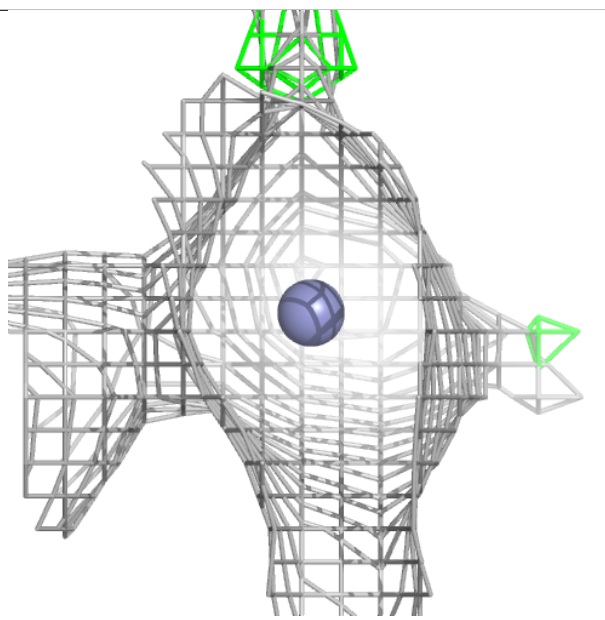
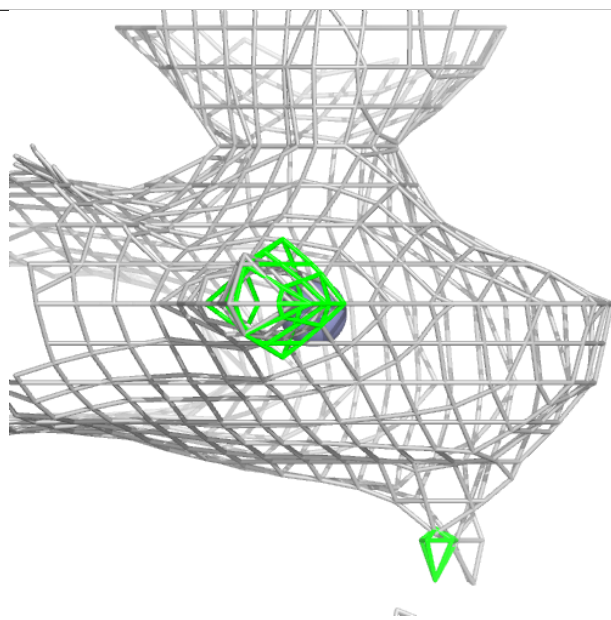
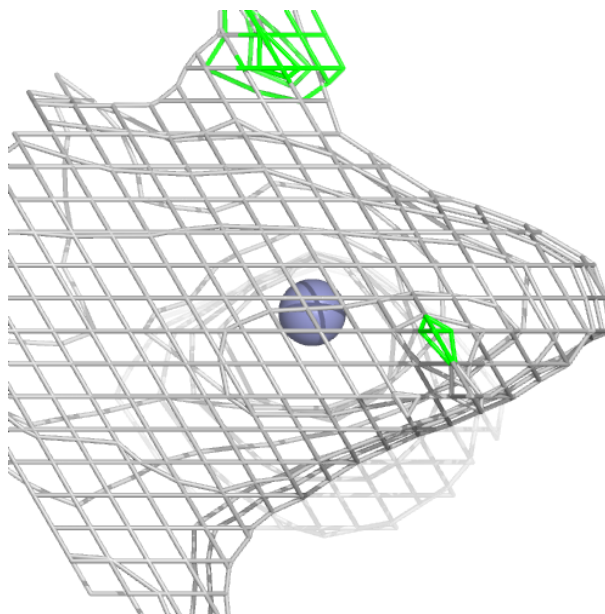
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PG4	A	414	13/13	0.88	0.15	41,46,55,60	0
8	PEG	B	417	7/7	0.88	0.18	58,58,60,60	0
9	PGE	B	414	10/10	0.88	0.16	41,43,50,55	0
7	PG4	A	415	13/13	0.89	0.16	47,50,59,60	0
5	GOL	A	411	6/6	0.90	0.13	24,38,39,40	0
7	PG4	A	413	13/13	0.90	0.13	43,49,53,53	0
3	SO4	B	408	5/5	0.90	0.12	68,70,72,72	0
6	DIO	A	412	6/6	0.91	0.13	44,45,45,45	0
3	SO4	A	407	5/5	0.91	0.11	40,42,49,50	5
8	PEG	A	416	7/7	0.92	0.12	43,46,49,50	0
5	GOL	B	411	6/6	0.93	0.11	25,34,36,36	0
3	SO4	A	401	5/5	0.94	0.08	65,65,66,66	5
5	GOL	A	410	6/6	0.96	0.08	40,42,42,43	0
4	ZN	B	406	1/1	0.96	0.05	48,48,48,48	1
4	ZN	A	405	1/1	0.98	0.04	32,32,32,32	0
3	SO4	B	401	5/5	0.98	0.13	32,32,33,33	5
4	ZN	A	406	1/1	0.99	0.03	26,26,26,26	1
4	ZN	B	404	1/1	0.99	0.02	24,24,24,24	1
3	SO4	B	409	5/5	0.99	0.04	28,28,29,30	0
4	ZN	A	403	1/1	1.00	0.01	20,20,20,20	1
4	ZN	B	402	1/1	1.00	0.01	20,20,20,20	0
4	ZN	B	403	1/1	1.00	0.04	21,21,21,21	0
4	ZN	A	404	1/1	1.00	0.03	26,26,26,26	1
4	ZN	B	405	1/1	1.00	0.01	21,21,21,21	1
4	ZN	A	402	1/1	1.00	0.01	18,18,18,18	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.

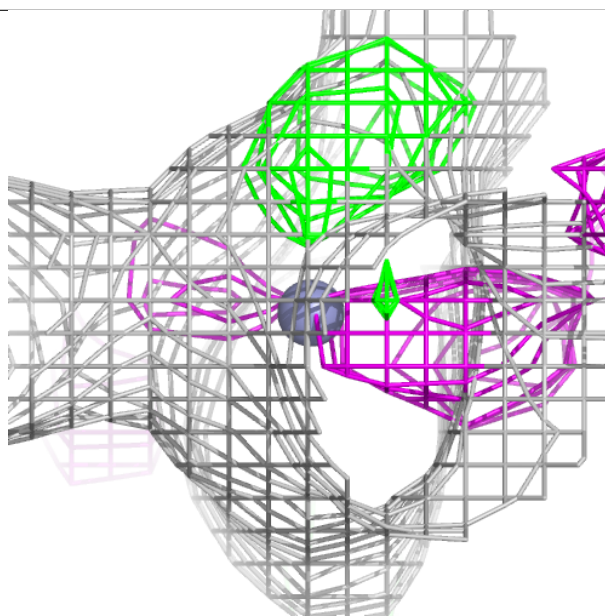
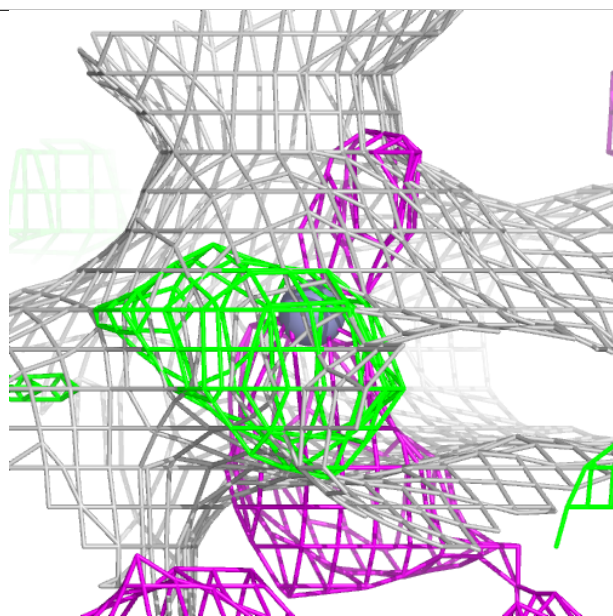
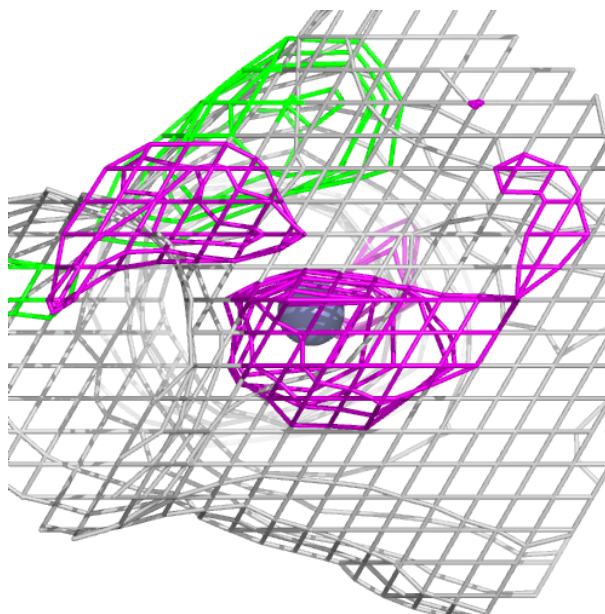
Electron density around ZN B 406:

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



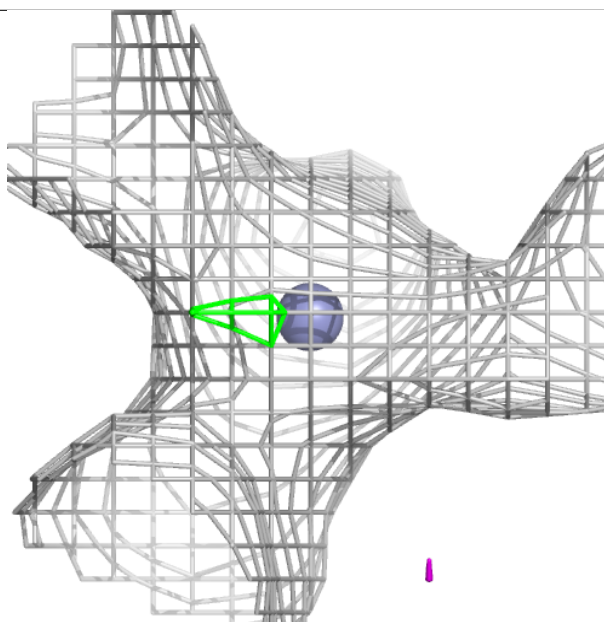
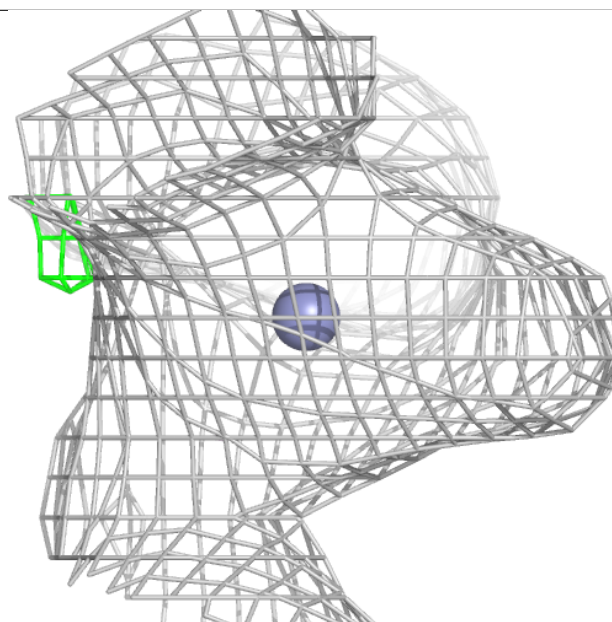
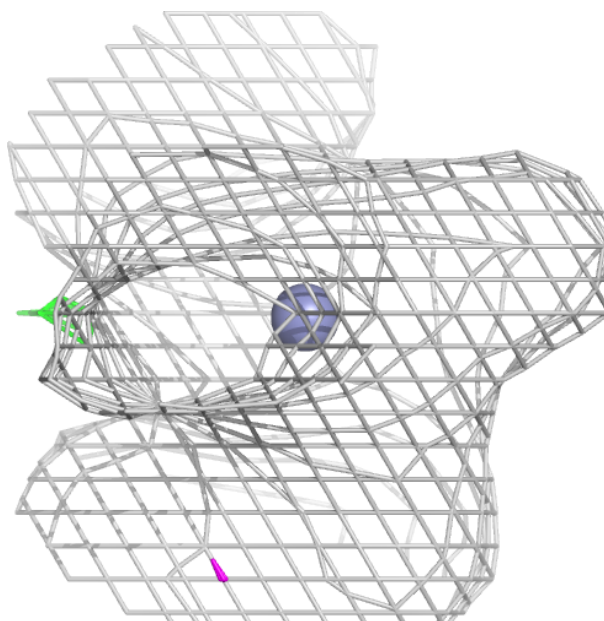
Electron density around ZN A 405:

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



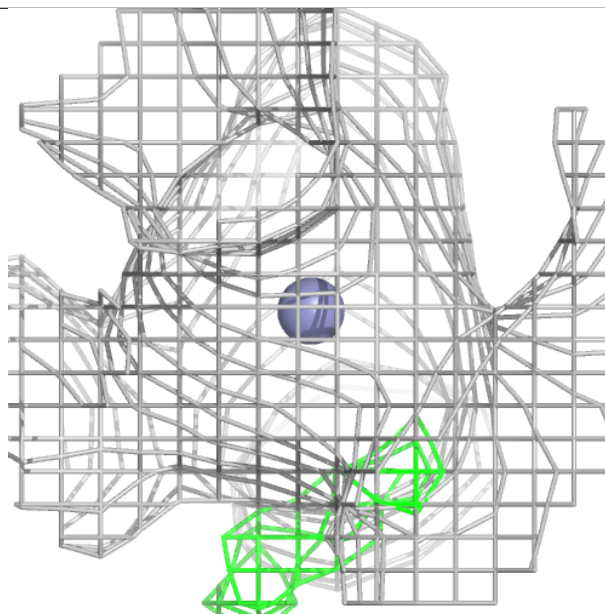
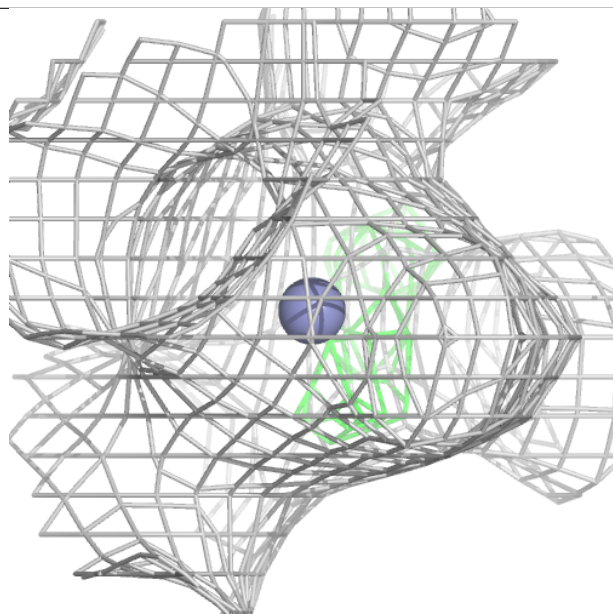
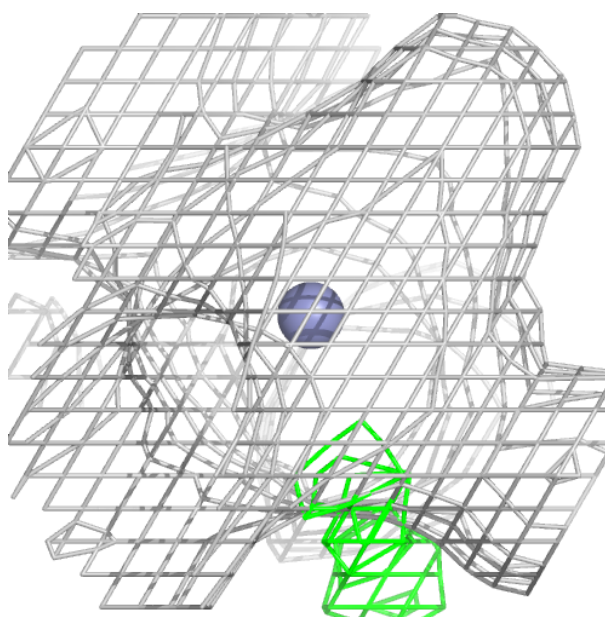
Electron density around ZN A 406:

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



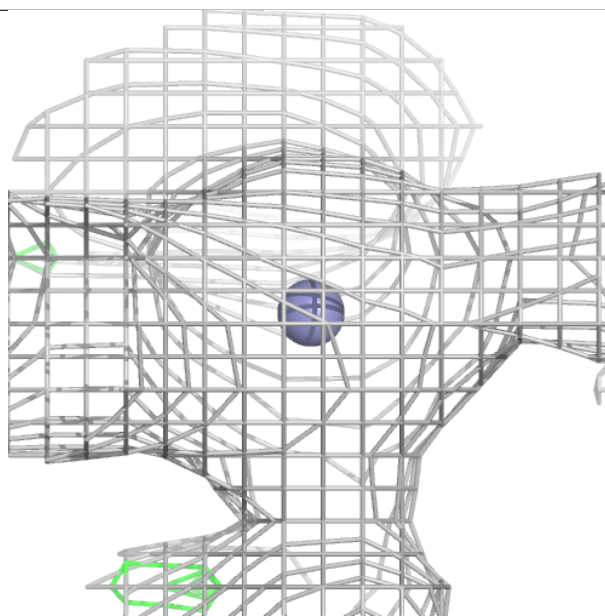
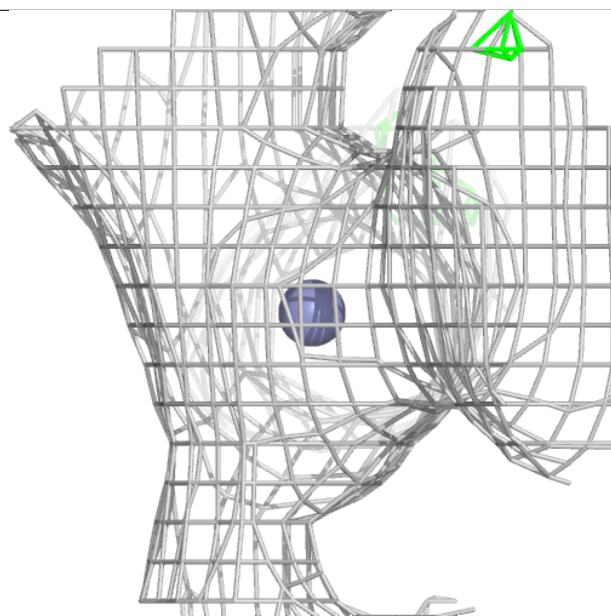
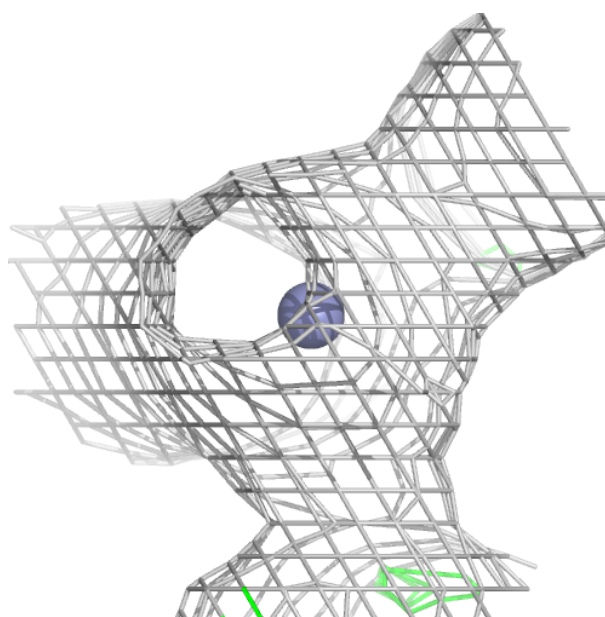
Electron density around ZN B 404:

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



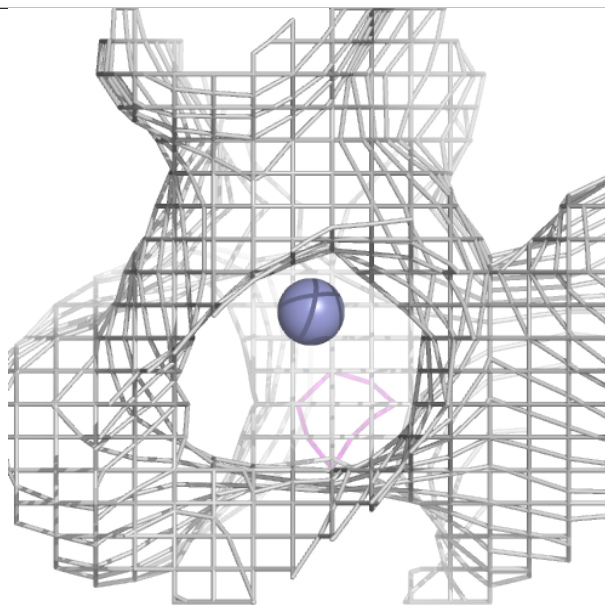
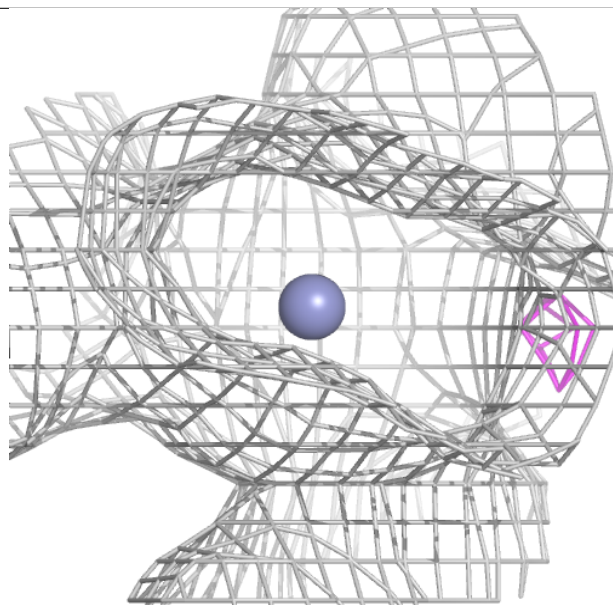
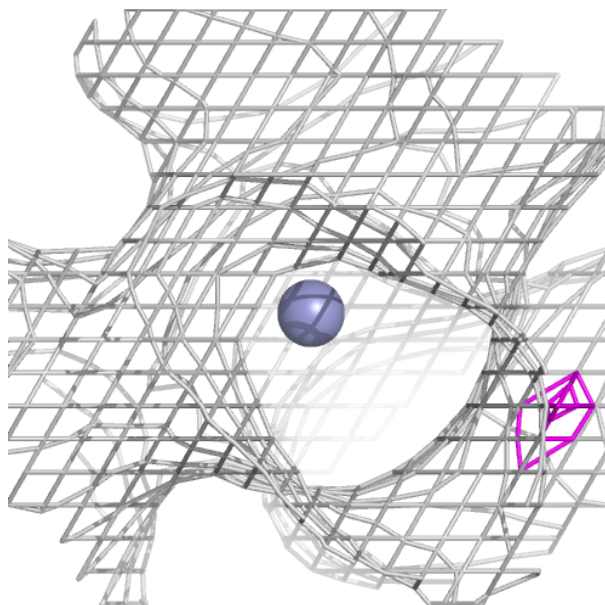
Electron density around ZN A 403:

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



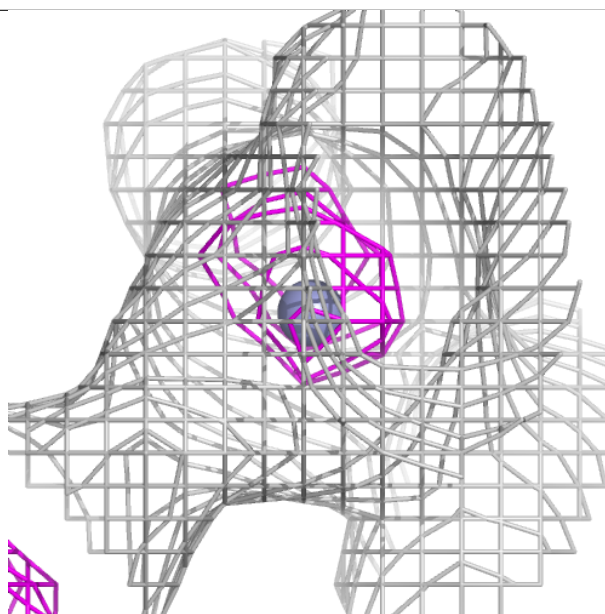
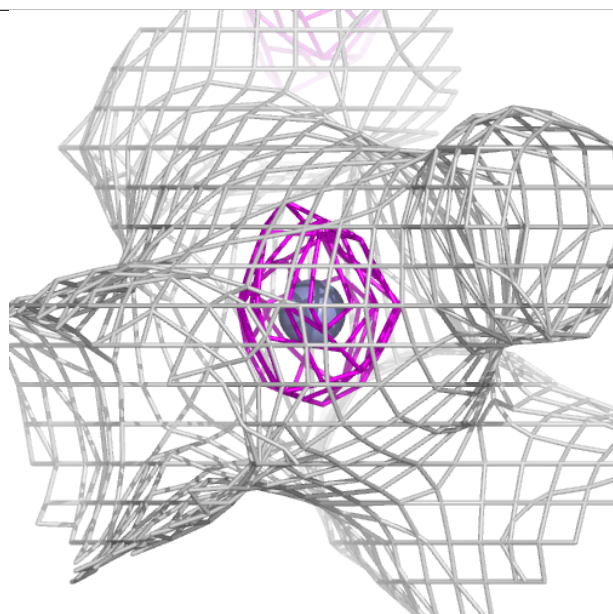
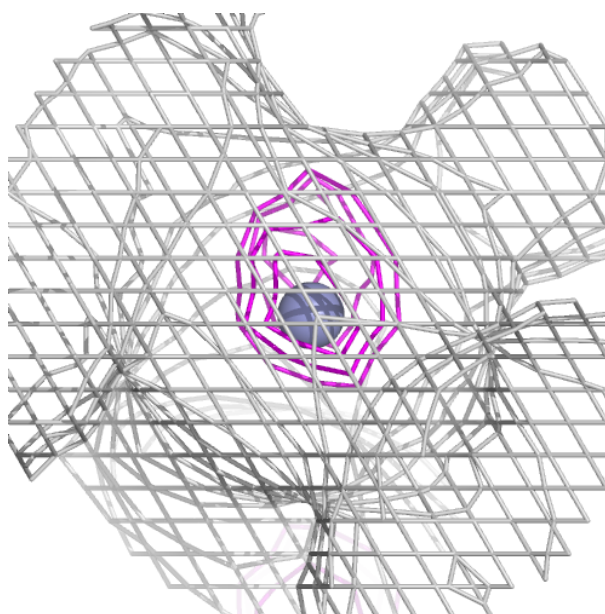
Electron density around ZN B 402:

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



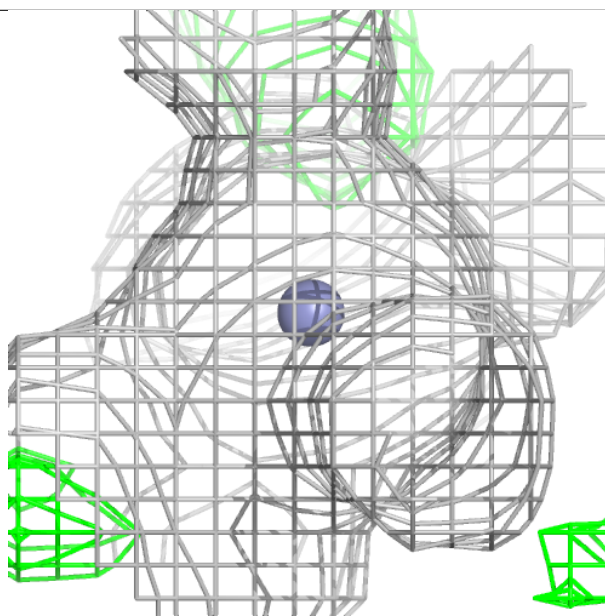
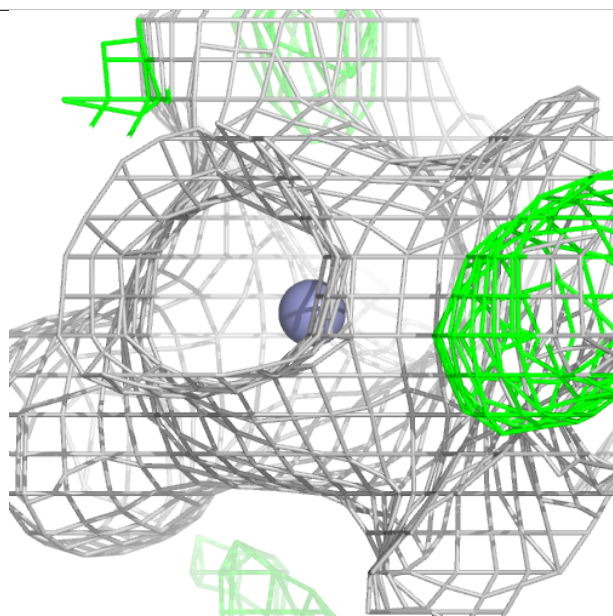
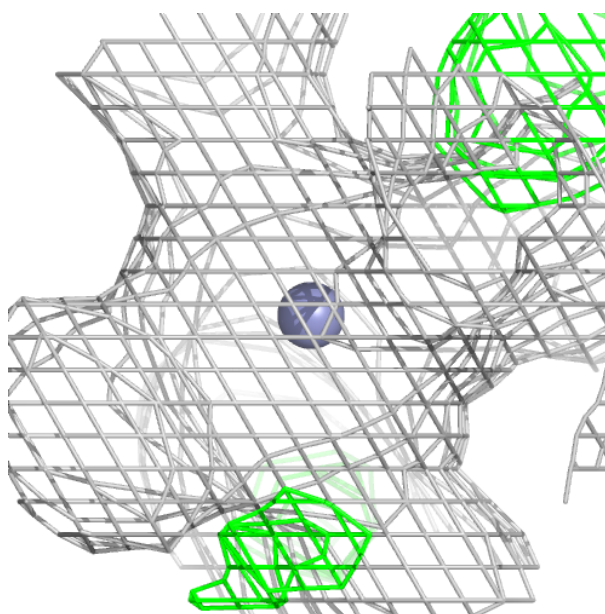
Electron density around ZN B 403:

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



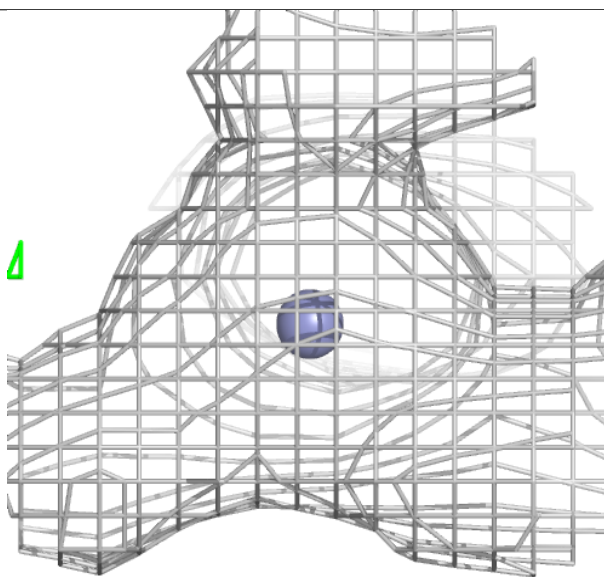
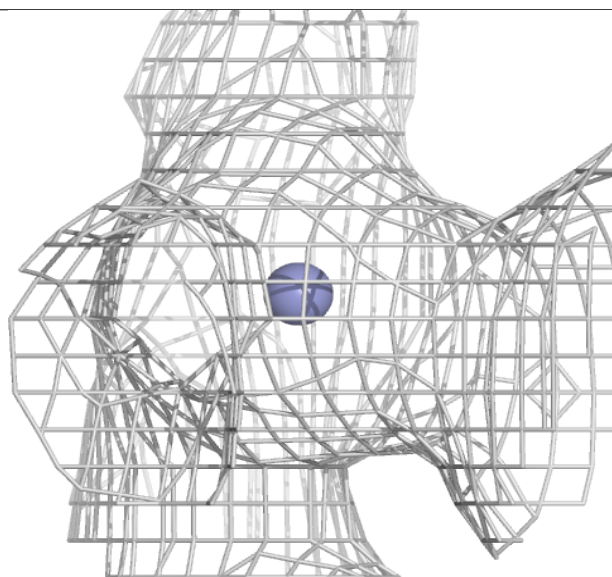
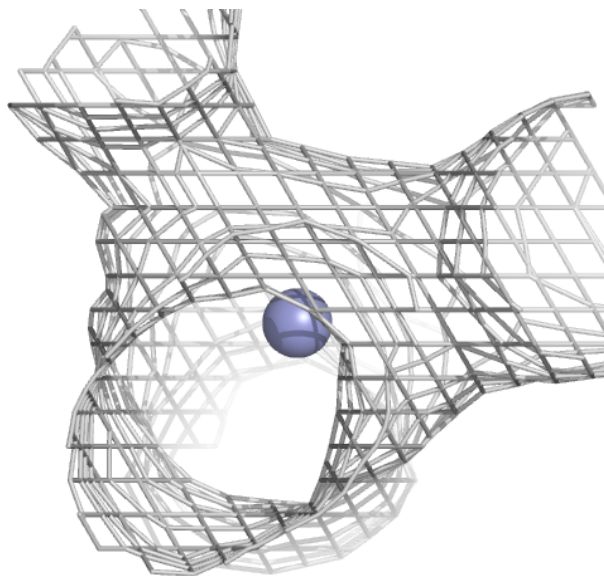
Electron density around ZN A 404:

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



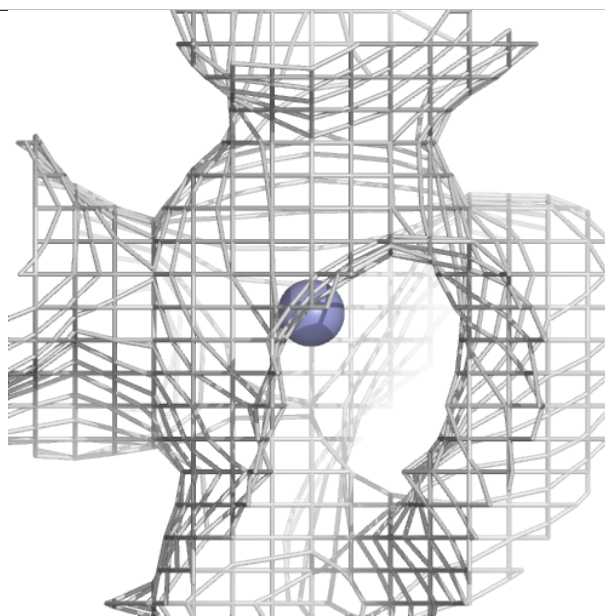
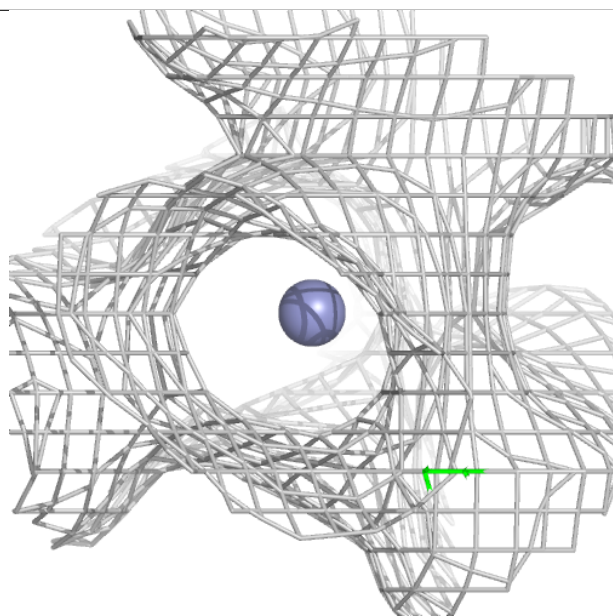
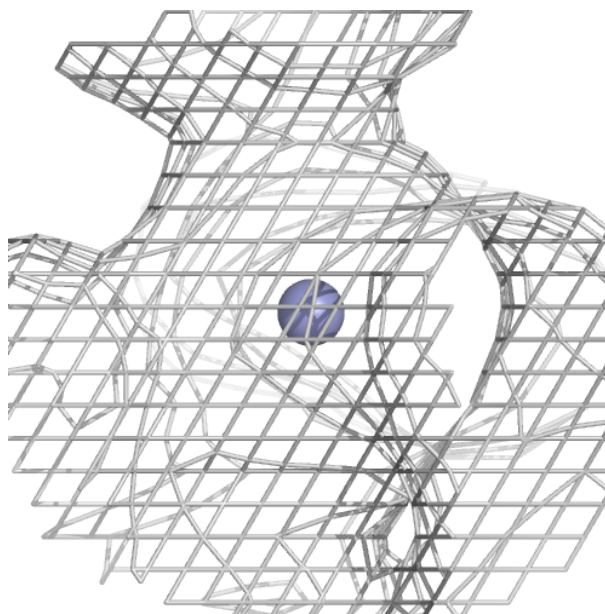
Electron density around ZN B 405:

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



Electron density around ZN A 402:

$2mF_o-DF_c$ (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.