



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:16 pm BST

PDB ID : 6NW5
Title : Crystal structure of TmPep1050 aminopeptidase with its metal cofactors
Authors : Dutoit, R.
Deposited on : 2019-02-06
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

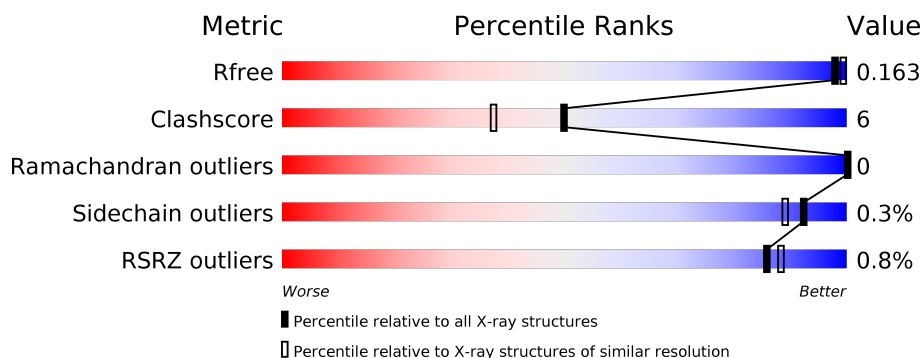
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 on 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	331	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 88%; width: 12%; height: 10px; background-color: yellow;"></div> </div> <div>88%12%</div> </div>
1	B	331	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 91%; width: 9%; height: 10px; background-color: yellow;"></div> </div> <div>91%9%</div> </div>
1	C	331	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 91%; width: 9%; height: 10px; background-color: yellow;"></div> </div> <div>91%9%</div> </div>
1	D	331	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 0; left: 93%; width: 7%; height: 10px; background-color: yellow;"></div> </div> <div>93%7%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	408	-	-	-	X
4	SO4	D	408	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12367 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 Aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	38	0
			2727	1744	455	514	14			
1	B	331	Total	C	N	O	S	0	39	0
			2706	1738	440	514	14			
1	C	331	Total	C	N	O	S	0	27	0
			2653	1692	441	507	13			
1	D	331	Total	C	N	O	S	0	30	0
			2673	1705	437	517	14			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Co	0	0
			1	1		
3	A	1	Total	Co	0	0
			1	1		
3	D	1	Total	Co	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Co	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



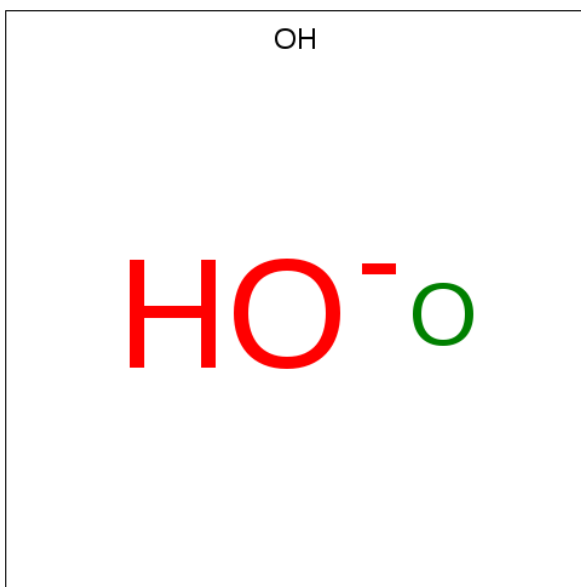
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is HYDROXIDE ION (three-letter code: OH) (formula: HO) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O 1 1	0	0

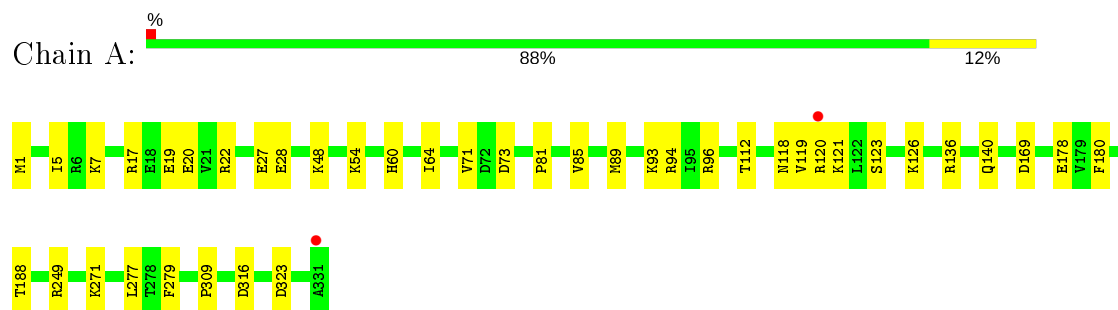
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	374	Total O 374 374	0	0
6	B	382	Total O 382 382	0	0
6	C	338	Total O 338 338	0	0
6	D	380	Total O 380 380	0	0

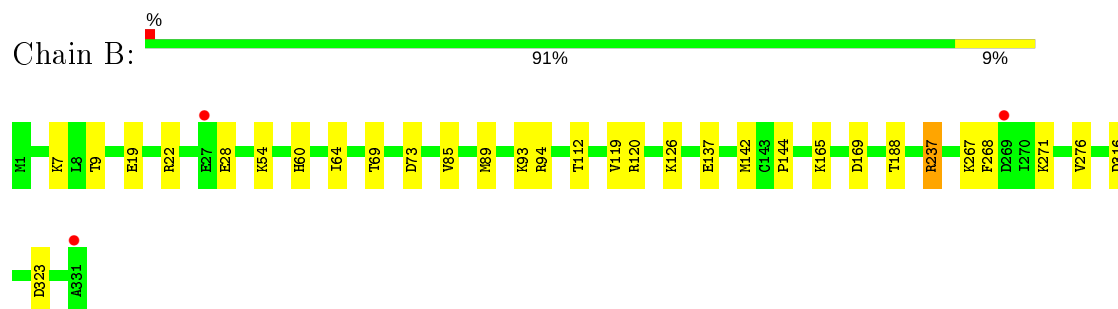
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

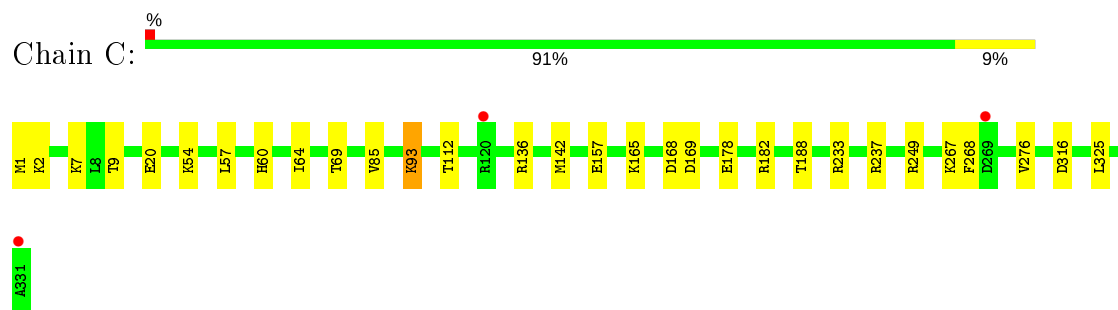
• Molecule 1: Aminopeptidase



• Molecule 1: Aminopeptidase

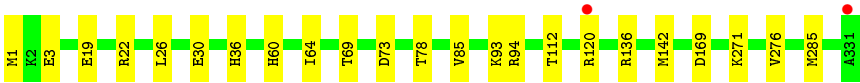


• Molecule 1: Aminopeptidase



• Molecule 1: Aminopeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	131.15Å 131.15Å 285.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.60 – 1.70 47.60 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.60-1.70) 99.8 (47.60-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.14-3260-00	Depositor
R, R_{free}	0.143 , 0.164 0.142 , 0.163	Depositor DCC
R_{free} test set	9715 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12367	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, CO, SO₄, OH

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	0.90	0/2882	0.86	0/3880
1	B	0.90	2/2861 (0.1%)	0.87	0/3855
1	C	0.85	0/2775	0.83	0/3742
1	D	0.90	0/2801	0.85	0/3776
All	All	0.89	2/11319 (0.0%)	0.85	0/15253

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237[A]	ARG	C-O	5.22	1.33	1.23
1	B	237[B]	ARG	C-O	5.22	1.33	1.23

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	2727	0	2870	45	0
1	B	2706	0	2830	39	0
1	C	2653	0	2731	26	0
1	D	2673	0	2752	24	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	30	0	0	1	0
4	B	40	0	0	1	0
4	C	25	0	0	2	0
4	D	30	0	0	3	0
5	D	1	0	0	0	0
6	A	374	0	0	15	0
6	B	382	0	0	16	0
6	C	338	0	0	11	2
6	D	380	0	0	7	2
All	All	12367	0	11183	129	2

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 6.

All (129) 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:B:7[B]:LYS:HE2	6:B:559:HOH:O	1.11	1.28
1:C:316[B]:ASP:OD2	6:C:501:HOH:O	1.73	1.04
1:B:73[B]:ASP:OD1	6:B:501:HOH:O	1.81	0.99
1:D:73:ASP:OD1	1:D:136:ARG:NH1	2.03	0.91
1:B:271:LYS:HB2	6:B:770:HOH:O	1.72	0.88
1:A:316[B]:ASP:OD2	6:A:501:HOH:O	1.93	0.86
1:B:137:GLU:OE1	6:B:502:HOH:O	1.93	0.85
1:C:316[B]:ASP:OD2	6:C:502:HOH:O	1.97	0.81
1:A:73[A]:ASP:OD1	1:A:136[A]:ARG:NH1	2.13	0.80
1:A:19[B]:GLU:HG2	1:A:22[B]:ARG:NH2	1.98	0.79
1:A:19[A]:GLU:HG3	1:A:22[A]:ARG:NH2	1.99	0.77
1:D:142[B]:MET:SD	6:D:664:HOH:O	2.42	0.77
1:B:142[B]:MET:SD	6:B:723:HOH:O	2.41	0.77
1:C:237[B]:ARG:NH1	6:C:504:HOH:O	2.21	0.74
1:B:237[B]:ARG:NH1	6:B:508:HOH:O	2.22	0.71
1:B:64:ILE:HD12	1:B:85[B]:VAL:HG12	1.73	0.70
1:A:19[A]:GLU:HG3	1:A:22[A]:ARG:HH22	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323[B]:ASP:OD2	6:A:502:HOH:O	2.08	0.70
1:A:64:ILE:HD12	1:A:85[B]:VAL:HG12	1.75	0.68
1:B:19[A]:GLU:HG3	1:B:22[A]:ARG:NH2	2.09	0.68
1:B:316[B]:ASP:OD2	6:B:503:HOH:O	2.11	0.68
1:C:142[B]:MET:SD	6:C:696:HOH:O	2.51	0.68
1:A:17[B]:ARG:NH2	6:A:507:HOH:O	2.26	0.66
6:C:610:HOH:O	1:D:78:THR:HG21	1.96	0.65
1:B:323[B]:ASP:OD2	6:B:504:HOH:O	2.15	0.65
1:A:7[B]:LYS:NZ	1:A:28:GLU:OE2	2.32	0.63
1:A:136[B]:ARG:NH2	6:A:508:HOH:O	2.30	0.63
1:A:121:LYS:O	1:A:126[B]:LYS:NZ	2.30	0.63
1:A:178[B]:GLU:OE2	6:A:503:HOH:O	2.15	0.62
1:C:316[B]:ASP:CG	6:C:501:HOH:O	2.28	0.61
1:C:20:GLU:OE2	6:C:503:HOH:O	2.16	0.61
1:A:120:ARG:HG3	1:B:120[A]:ARG:HG3	1.83	0.61
1:A:71:VAL:O	1:A:136[B]:ARG:NH1	2.34	0.60
1:C:267:LYS:HE2	1:C:268:PHE:CZ	2.37	0.59
1:A:112[B]:THR:HG22	6:A:758:HOH:O	2.02	0.59
1:B:126[A]:LYS:HG3	6:B:776:HOH:O	2.05	0.57
4:A:404:SO4:O3	6:A:504:HOH:O	2.16	0.56
1:A:27[A]:GLU:HG3	6:A:704:HOH:O	2.05	0.56
1:B:112[A]:THR:HG22	6:B:727:HOH:O	2.06	0.56
1:B:19[B]:GLU:HG2	1:B:22[B]:ARG:NH2	2.20	0.56
1:A:64:ILE:HB	1:A:85[B]:VAL:HG13	1.87	0.56
1:A:118:ASN:CG	1:A:126[B]:LYS:HD2	2.26	0.56
1:B:267:LYS:HE2	1:B:268:PHE:CZ	2.42	0.55
1:D:3[B]:GLU:HG3	6:D:759:HOH:O	2.07	0.55
1:B:19[B]:GLU:HG2	1:B:22[B]:ARG:HH21	1.71	0.55
1:A:93[B]:LYS:HZ2	1:B:93[B]:LYS:NZ	2.04	0.55
1:B:89:MET:O	1:B:93[B]:LYS:HG3	2.07	0.54
1:B:7[A]:LYS:NZ	1:B:28:GLU:OE2	2.29	0.54
1:B:276:VAL:HG11	1:C:69[A]:THR:HG22	1.89	0.54
1:C:20:GLU:CD	6:C:503:HOH:O	2.46	0.54
1:B:64:ILE:HB	1:B:85[B]:VAL:HG13	1.88	0.54
1:C:233:ARG:HB3	1:D:69[B]:THR:HG21	1.89	0.54
1:D:136:ARG:NH2	4:D:404:SO4:O4	2.41	0.54
1:A:93[B]:LYS:HE2	1:A:309:PRO:HG2	1.89	0.53
1:B:126[B]:LYS:HG3	6:B:776:HOH:O	2.09	0.53
1:C:1:MET:N	4:C:407:SO4:O4	2.41	0.53
1:D:285[B]:MET:HG3	6:D:725:HOH:O	2.09	0.53
1:A:136[B]:ARG:NH2	6:A:505:HOH:O	2.17	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:LYS:HB3	6:D:763:HOH:O	2.09	0.52
1:B:54:LYS:NZ	6:B:520:HOH:O	2.43	0.52
1:A:93[A]:LYS:NZ	6:A:513:HOH:O	2.34	0.51
1:B:54:LYS:HG3	1:B:188:THR:HB	1.93	0.51
1:C:136:ARG:NH2	4:C:406:SO4:O3	2.44	0.51
1:C:64:ILE:HD12	1:C:85:VAL:HG22	1.92	0.50
1:D:78:THR:HG23	6:D:697:HOH:O	2.10	0.50
1:A:89:MET:O	1:A:93[B]:LYS:HG3	2.10	0.50
4:D:408:SO4:O3	6:D:501:HOH:O	2.19	0.50
1:A:96:ARG:NH2	6:A:520:HOH:O	2.45	0.50
1:A:20:GLU:CD	6:A:506:HOH:O	2.49	0.50
1:D:1:MET:N	4:D:408:SO4:O2	2.39	0.49
1:A:93[B]:LYS:HZ2	1:B:93[B]:LYS:HZ2	1.60	0.49
1:A:81:PRO:HB3	1:A:85[B]:VAL:HG23	1.95	0.49
1:A:93[B]:LYS:NZ	1:B:93[B]:LYS:HZ2	2.11	0.49
1:B:19[A]:GLU:HG3	1:B:22[A]:ARG:HH22	1.77	0.48
1:A:136[B]:ARG:NE	1:A:140:GLN:OE1	2.46	0.48
1:C:57[B]:LEU:HD21	1:C:325:LEU:HD13	1.95	0.48
1:A:1[B]:MET:HG2	1:A:5:ILE:HD11	1.96	0.47
1:B:64:ILE:HD12	1:B:85[A]:VAL:HG22	1.96	0.46
1:A:271:LYS:NZ	6:A:514:HOH:O	2.49	0.46
1:A:126[B]:LYS:HD3	6:A:522:HOH:O	2.14	0.46
1:C:93[B]:LYS:HB3	1:C:93[B]:LYS:HE3	1.70	0.46
1:B:69[A]:THR:HG22	1:D:276:VAL:HG11	1.98	0.46
1:B:7[B]:LYS:HA	1:B:7[B]:LYS:HD3	1.75	0.46
1:A:136[B]:ARG:NH2	6:A:516:HOH:O	2.49	0.45
1:C:54:LYS:HG3	1:C:188:THR:HB	1.99	0.45
1:D:93[A]:LYS:HG3	1:D:94:ARG:N	2.31	0.45
1:B:7[B]:LYS:CE	6:B:559:HOH:O	1.99	0.45
1:B:126[A]:LYS:CG	6:B:776:HOH:O	2.64	0.45
1:D:64:ILE:HD12	1:D:85[B]:VAL:HG22	1.98	0.44
1:A:22[B]:ARG:HH11	1:A:22[B]:ARG:HG2	1.81	0.44
1:A:64:ILE:HD12	1:A:85[B]:VAL:CG1	2.43	0.44
1:C:276:VAL:HG11	1:D:69[A]:THR:HG22	2.00	0.44
1:A:1[A]:MET:HE2	1:A:5:ILE:HD11	2.00	0.44
4:B:406:SO4:O4	6:B:507:HOH:O	2.21	0.43
1:C:178:GLU:OE2	1:C:182[A]:ARG:NE	2.44	0.43
1:C:60:HIS:NE2	1:C:169:ASP:HB2	2.33	0.43
1:A:277:LEU:HG	1:A:279:PHE:O	2.18	0.43
1:B:93[A]:LYS:HG3	1:B:94:ARG:N	2.33	0.43
1:D:1:MET:HG3	1:D:1:MET:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112[B]:THR:HG22	6:C:713:HOH:O	2.19	0.43
1:D:19[A]:GLU:HG3	1:D:22[A]:ARG:NH2	2.34	0.43
1:A:48[A]:LYS:NZ	1:A:180:PHE:O	2.51	0.42
1:A:93[B]:LYS:CE	1:A:309:PRO:HG2	2.49	0.42
1:B:144:PRO:HB2	6:B:701:HOH:O	2.19	0.42
1:A:1[B]:MET:CE	1:A:178[B]:GLU:HG3	2.49	0.42
1:A:123:SER:H	1:A:126[B]:LYS:HE2	1.84	0.42
1:B:64:ILE:HD12	1:B:85[B]:VAL:CG1	2.47	0.41
1:B:60:HIS:NE2	1:B:169:ASP:HB2	2.34	0.41
1:D:136:ARG:HH11	1:D:136:ARG:HD2	1.68	0.41
1:A:93[A]:LYS:HG3	1:A:94:ARG:N	2.36	0.41
1:C:2:LYS:NZ	1:C:157:GLU:OE1	2.41	0.41
1:C:168:ASP:HA	1:C:169:ASP:HA	1.89	0.41
1:C:7:LYS:NZ	6:C:518:HOH:O	2.53	0.41
1:C:9:THR:HB	1:C:165:LYS:O	2.20	0.41
1:D:120[B]:ARG:HD3	1:D:120[B]:ARG:HA	1.81	0.41
1:D:26[A]:LEU:HD23	1:D:26[A]:LEU:HA	1.94	0.41
1:B:22[A]:ARG:HH11	1:B:22[A]:ARG:HD3	1.71	0.41
1:A:60:HIS:NE2	1:A:169:ASP:HB2	2.35	0.41
1:D:26[B]:LEU:HD21	1:D:36:HIS:CE1	2.56	0.41
1:A:54:LYS:HG3	1:A:188:THR:HB	2.02	0.41
1:D:60:HIS:NE2	1:D:169:ASP:HB2	2.35	0.41
1:B:9:THR:HB	1:B:165:LYS:O	2.21	0.41
1:C:249:ARG:HD3	1:C:249:ARG:HA	1.89	0.40
1:D:112[B]:THR:HG22	6:D:683:HOH:O	2.20	0.40
1:A:249:ARG:HA	1:A:249:ARG:HD3	1.88	0.40
1:C:20:GLU:CG	6:C:503:HOH:O	2.69	0.40
1:D:22[A]:ARG:HD3	1:D:22[A]:ARG:HH11	1.70	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:762:HOH:O	6:D:857:HOH:O[2_655]	1.92	0.28
6:C:520:HOH:O	6:D:522:HOH:O[2_655]	2.03	0.17

5.3 Torsion angles

5.3.1 Protein backbone

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	367/331 (111%)	357 (97%)	10 (3%)	0	100	100
1	B	367/331 (111%)	356 (97%)	11 (3%)	0	100	100
1	C	357/331 (108%)	346 (97%)	11 (3%)	0	100	100
1	D	360/331 (109%)	349 (97%)	11 (3%)	0	100	100
All	All	1451/1324 (110%)	1408 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	305/273 (112%)	303 (99%)	2 (1%)	84	77
1	B	300/273 (110%)	298 (99%)	2 (1%)	84	77
1	C	289/273 (106%)	287 (99%)	2 (1%)	84	77
1	D	295/273 (108%)	295 (100%)	0	100	100
All	All	1189/1092 (109%)	1183 (100%)	6 (0%)	92	83

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

Mol	Chain	Res	Type
1	A	119[A]	VAL
1	A	119[B]	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	119[A]	VAL
1	B	119[B]	VAL
1	C	93[A]	LYS
1	C	93[B]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	116	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 1 is modelled with single atom and 8 are monoatomic - leaving 25 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	$\# Z > 2$
4	SO4	D	406	-	4,4,4	0.50	0	6,6,6	0.56	0
4	SO4	B	408	-	4,4,4	0.14	0	6,6,6	0.17	0
4	SO4	C	406	-	4,4,4	0.19	0	6,6,6	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	407	-	4,4,4	0.11	0	6,6,6	0.42	0
4	SO4	D	403	-	4,4,4	0.40	0	6,6,6	0.83	0
4	SO4	D	404	-	4,4,4	0.15	0	6,6,6	0.21	0
4	SO4	C	404	-	4,4,4	0.34	0	6,6,6	0.26	0
4	SO4	A	404	-	4,4,4	0.49	0	6,6,6	0.63	0
4	SO4	D	408	-	4,4,4	0.64	0	6,6,6	1.18	1 (16%)
4	SO4	D	405	-	4,4,4	0.32	0	6,6,6	0.29	0
4	SO4	B	403	-	4,4,4	0.37	0	6,6,6	0.66	0
4	SO4	A	405	-	4,4,4	0.22	0	6,6,6	0.49	0
4	SO4	A	408	-	4,4,4	0.38	0	6,6,6	0.99	1 (16%)
4	SO4	C	405	-	4,4,4	0.46	0	6,6,6	0.54	0
4	SO4	A	403	-	4,4,4	0.23	0	6,6,6	1.05	0
4	SO4	A	407	-	4,4,4	0.17	0	6,6,6	0.46	0
4	SO4	B	406	-	4,4,4	0.18	0	6,6,6	0.39	0
4	SO4	C	403	-	4,4,4	0.43	0	6,6,6	0.75	0
4	SO4	B	405	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	A	406	-	4,4,4	0.17	0	6,6,6	0.29	0
4	SO4	B	404	-	4,4,4	0.49	0	6,6,6	0.82	0
4	SO4	C	407	-	4,4,4	0.63	0	6,6,6	0.62	0
4	SO4	B	410	-	4,4,4	0.69	0	6,6,6	1.26	1 (16%)
4	SO4	B	407	-	4,4,4	0.16	0	6,6,6	0.46	0
4	SO4	B	409	-	4,4,4	0.25	0	6,6,6	0.64	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	410	SO4	O3-S-O1	2.71	123.48	109.31
4	D	408	SO4	O3-S-O1	2.57	122.73	109.31
4	A	408	SO4	O4-S-O3	2.24	118.61	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	406	SO4	1	0
4	D	404	SO4	1	0
4	A	404	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	408	SO4	2	0
4	B	406	SO4	1	0
4	C	407	SO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	331/331 (100%)	-0.41	2 (0%) 89 91	14, 19, 32, 47	0
1	B	331/331 (100%)	-0.32	3 (0%) 84 87	15, 21, 34, 60	0
1	C	331/331 (100%)	-0.40	3 (0%) 84 87	17, 22, 35, 53	0
1	D	331/331 (100%)	-0.41	2 (0%) 89 91	15, 20, 32, 46	0
All	All	1324/1324 (100%)	-0.39	10 (0%) 86 88	14, 21, 33, 60	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	331	ALA	4.9
1	A	331	ALA	3.8
1	C	331	ALA	3.5
1	D	331	ALA	2.9
1	B	27[A]	GLU	2.4
1	D	120[A]	ARG	2.4
1	B	269[A]	ASP	2.3
1	A	120	ARG	2.3
1	C	120[A]	ARG	2.2
1	C	269[A]	ASP	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 carbohydrates 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.

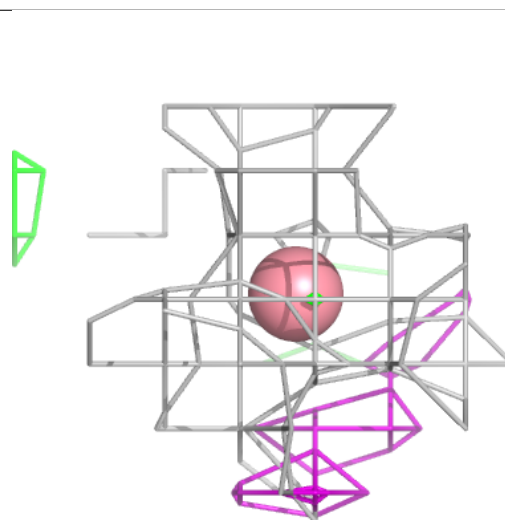
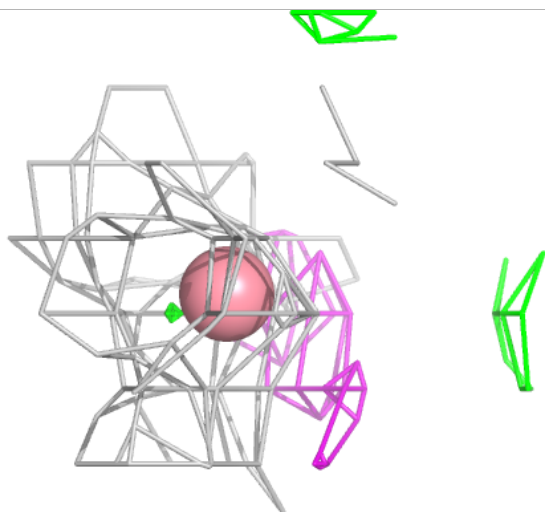
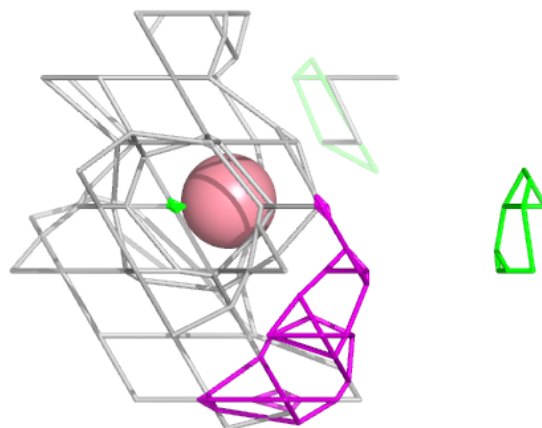
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	405	5/5	-0.08	0.36	24,30,49,54	5
4	SO4	C	407	5/5	0.68	0.23	29,31,56,59	5
4	SO4	D	408	5/5	0.69	0.20	21,24,55,59	5
4	SO4	B	408	5/5	0.71	0.41	67,80,83,93	5
4	SO4	A	408	5/5	0.73	0.20	24,28,45,51	5
4	SO4	A	406	5/5	0.74	0.24	55,56,65,69	5
4	SO4	B	410	5/5	0.74	0.22	25,27,51,57	5
4	SO4	B	409	5/5	0.77	0.15	47,51,57,69	5
3	CO	A	402	1/1	0.82	0.27	59,59,59,59	1
4	SO4	C	404	5/5	0.83	0.21	29,39,44,45	5
4	SO4	A	407	5/5	0.83	0.20	25,29,33,46	5
4	SO4	A	405	5/5	0.85	0.19	25,41,43,44	5
4	SO4	D	407	5/5	0.86	0.45	43,45,47,50	5
4	SO4	B	407	5/5	0.86	0.23	27,41,48,55	5
4	SO4	D	405	5/5	0.86	0.22	23,31,36,38	5
4	SO4	C	406	5/5	0.89	0.19	30,43,46,47	5
3	CO	C	402	1/1	0.91	0.17	49,49,49,49	1
4	SO4	C	405	5/5	0.92	0.15	23,24,44,50	5
3	CO	B	402	1/1	0.92	0.14	44,44,44,44	1
4	SO4	D	406	5/5	0.92	0.13	22,24,38,38	5
5	OH	D	409	1/1	0.92	0.10	29,29,29,29	0
4	SO4	C	403	5/5	0.92	0.19	28,34,40,54	5
4	SO4	B	403	5/5	0.92	0.13	23,25,37,41	5
4	SO4	D	404	5/5	0.93	0.14	34,43,47,56	5
4	SO4	A	404	5/5	0.94	0.09	20,22,35,41	5
4	SO4	B	404	5/5	0.94	0.11	27,35,37,52	5
4	SO4	A	403	5/5	0.96	0.09	25,33,39,51	5
3	CO	D	402	1/1	0.96	0.23	42,42,42,42	1
4	SO4	B	406	5/5	0.96	0.15	33,33,40,44	5
4	SO4	D	403	5/5	0.97	0.07	29,30,38,45	5
2	ZN	A	401	1/1	1.00	0.07	17,17,17,17	1
2	ZN	C	401	1/1	1.00	0.05	20,20,20,20	0
2	ZN	D	401	1/1	1.00	0.05	18,18,18,18	1
2	ZN	B	401	1/1	1.00	0.06	18,18,18,18	1

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.

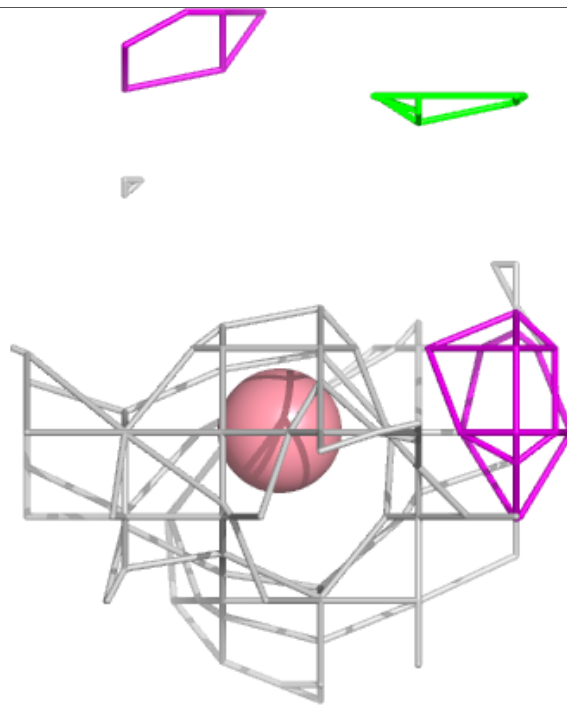
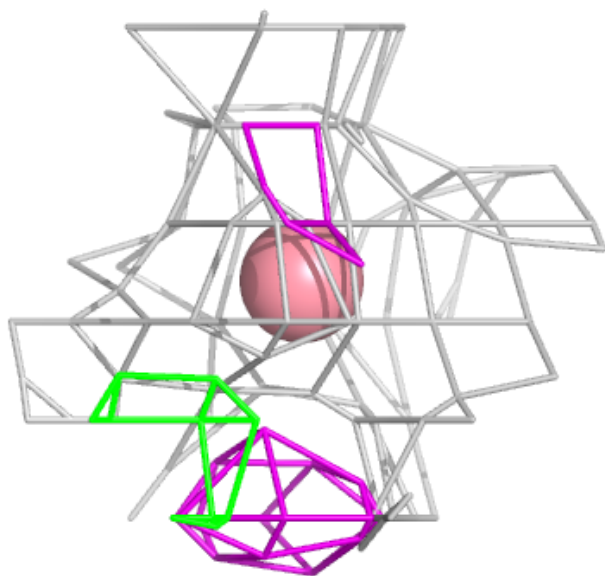
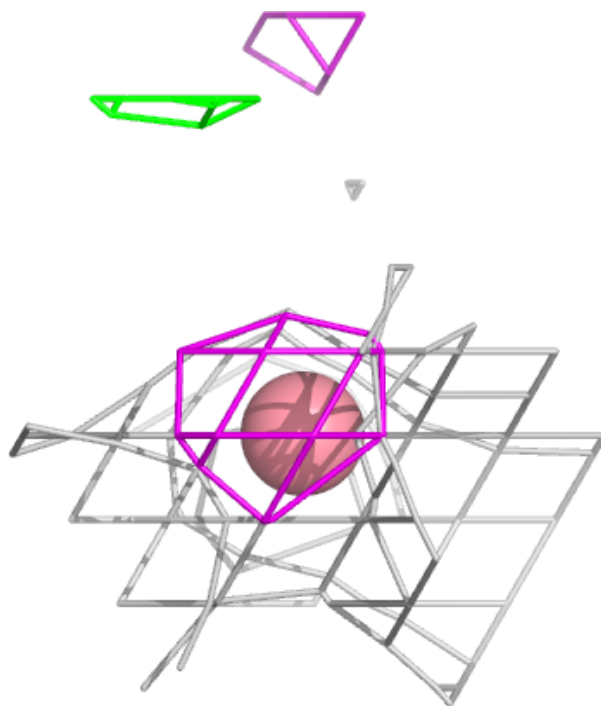
Electron density around CO A 402:

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



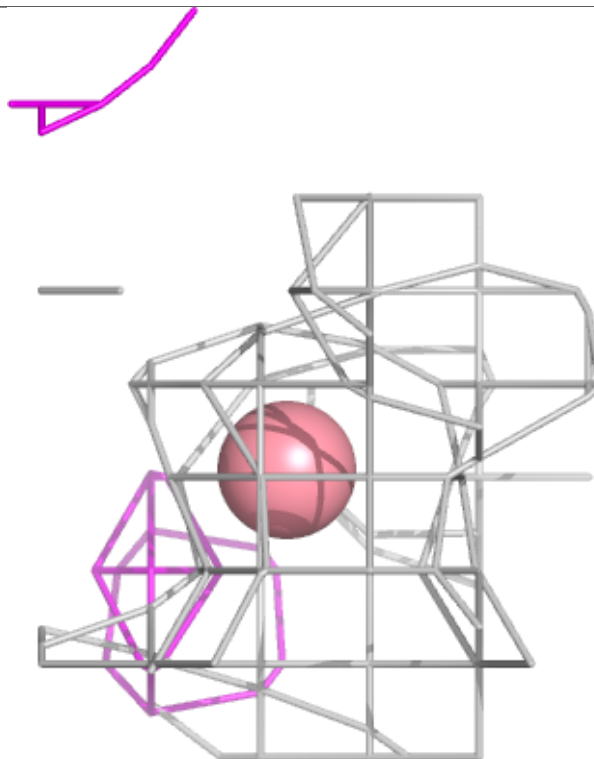
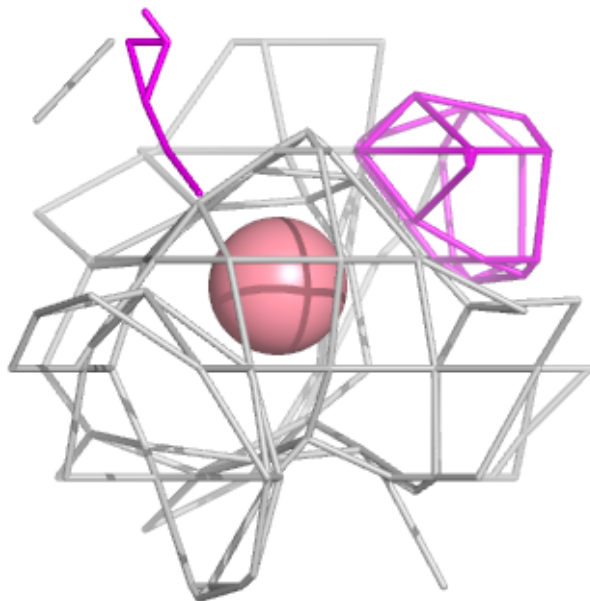
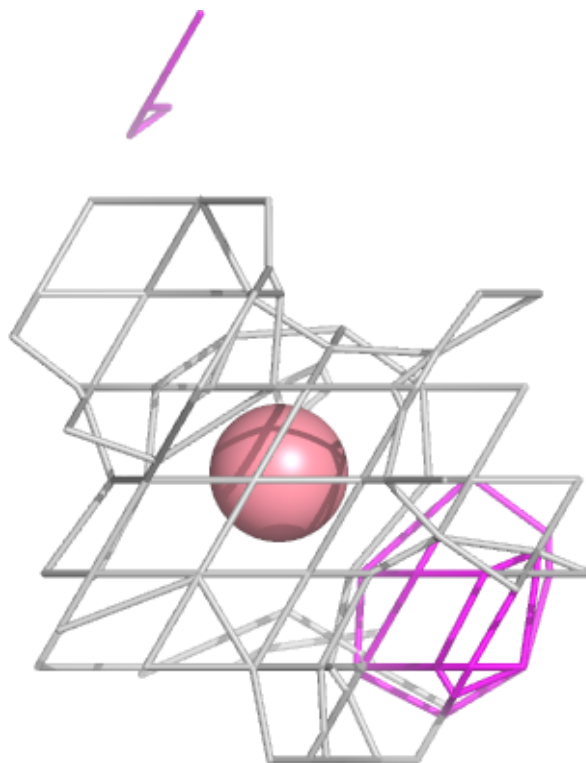
Electron density around CO C 402:

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



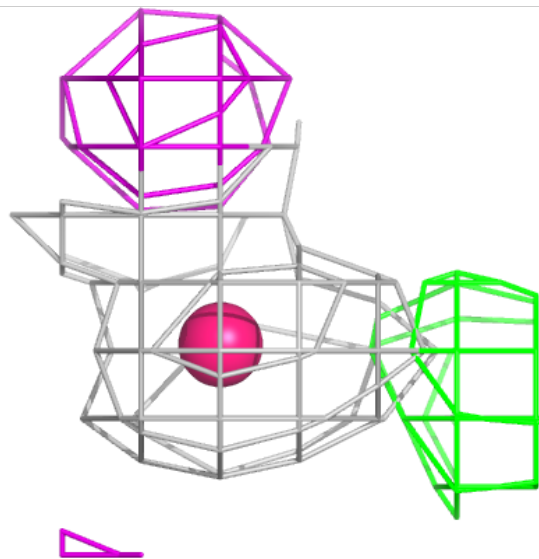
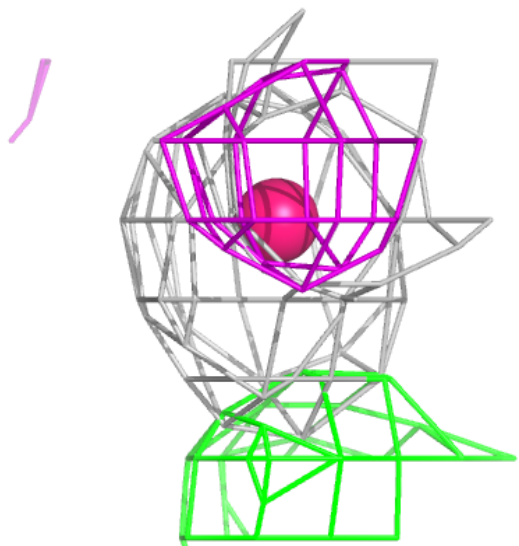
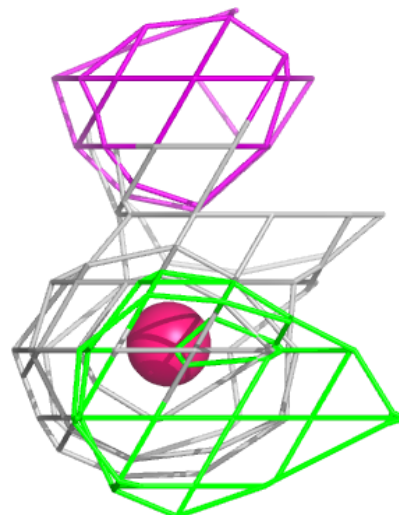
Electron density around CO B 402:

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



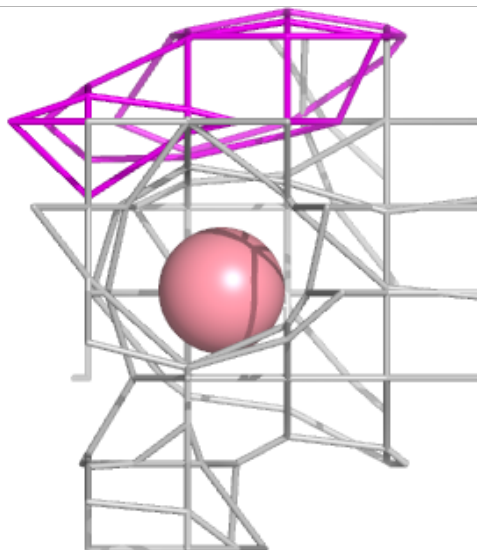
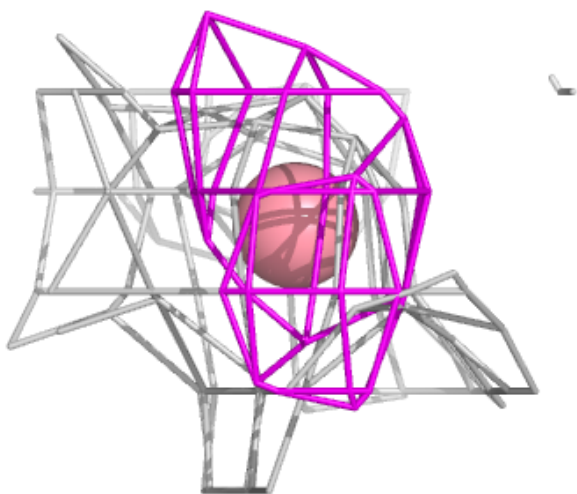
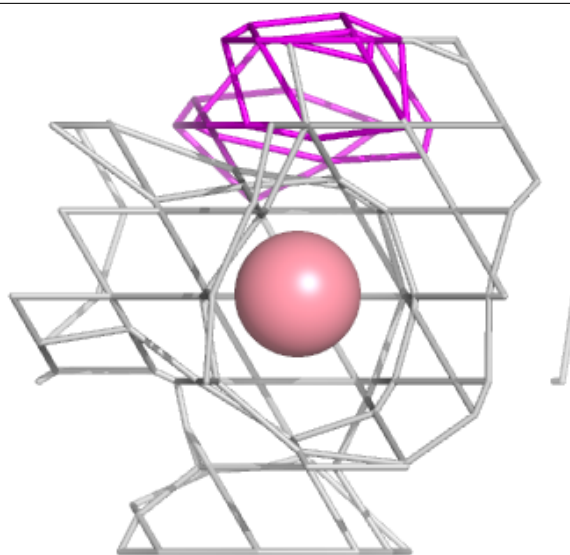
Electron density around OH D 409:

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



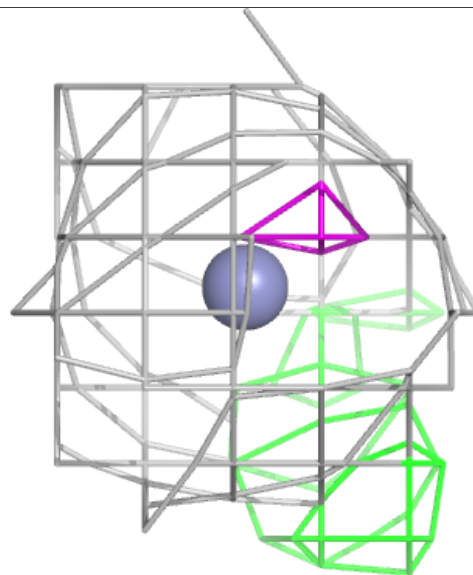
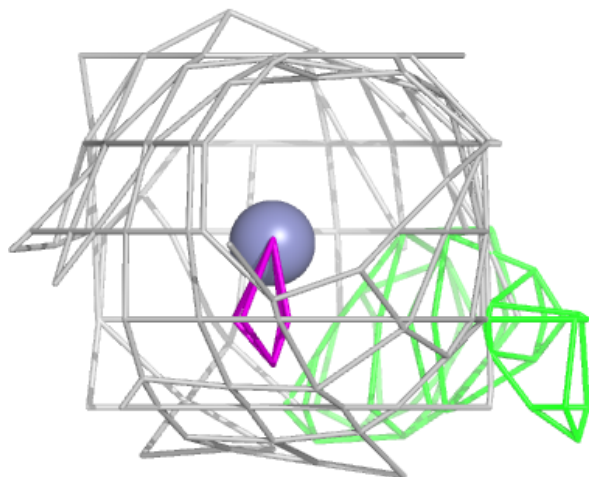
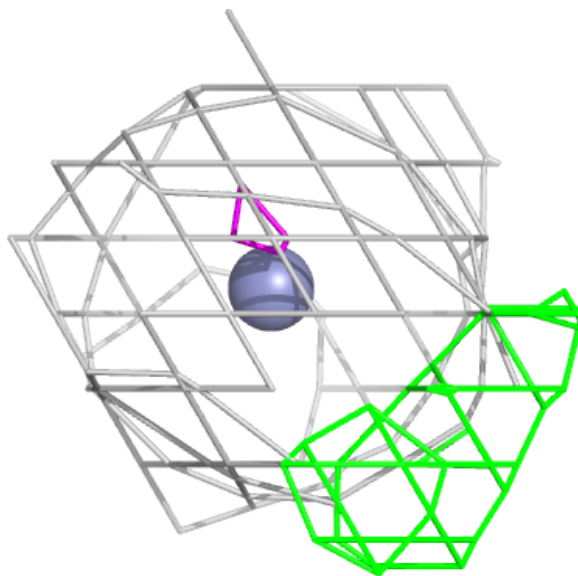
Electron density around CO D 402:

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



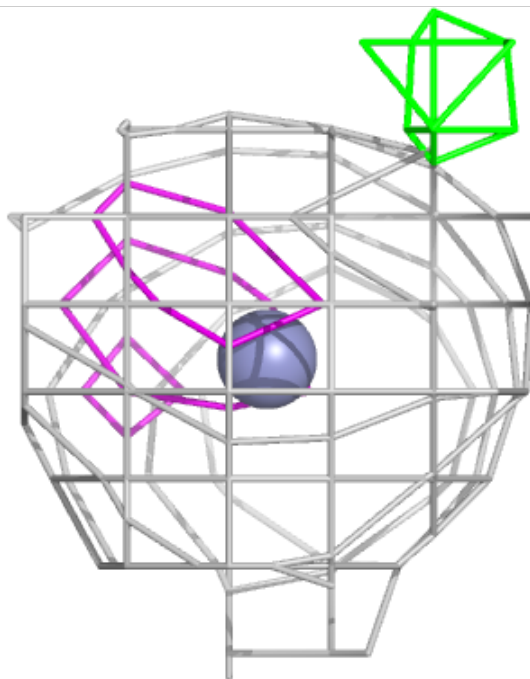
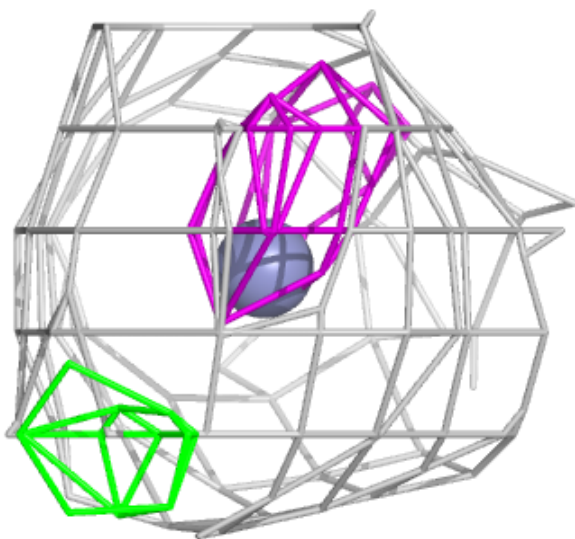
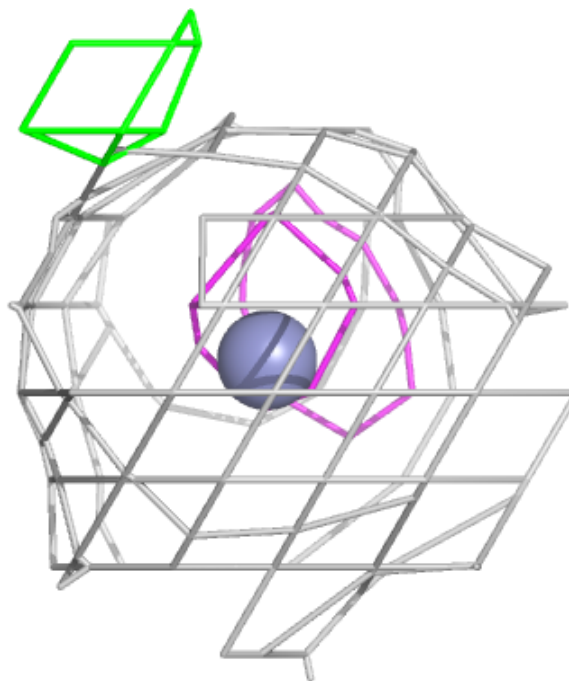
Electron density around ZN A 401:

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



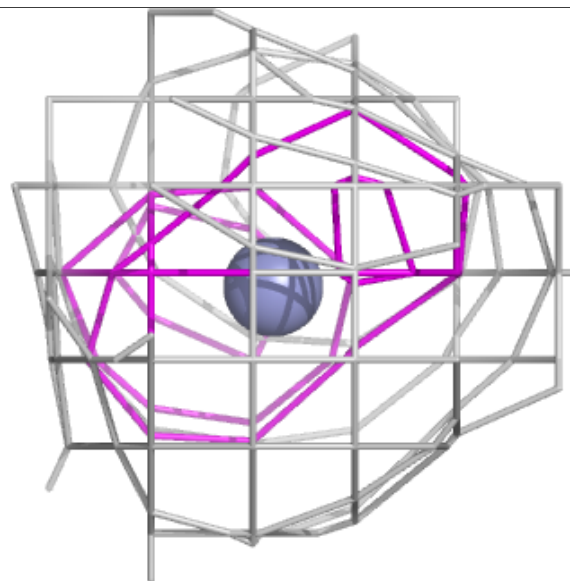
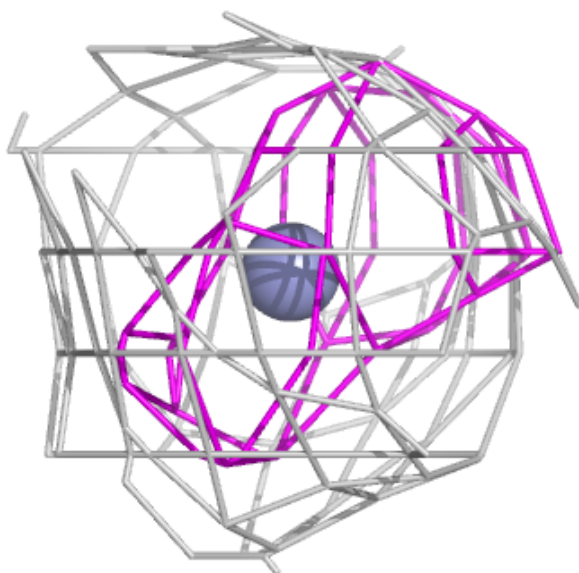
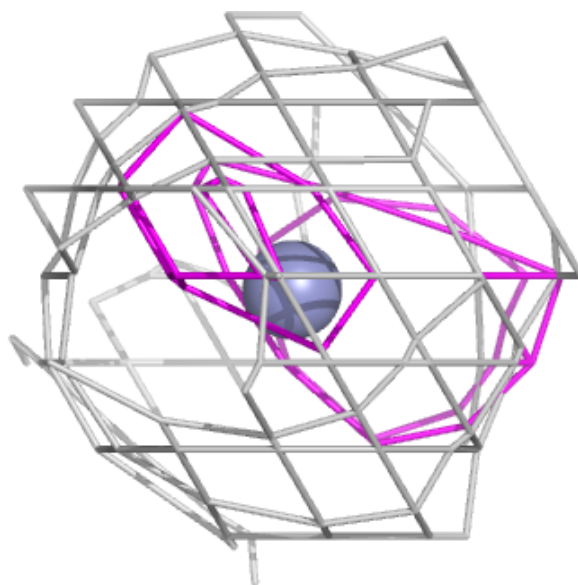
Electron density around ZN C 401:

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



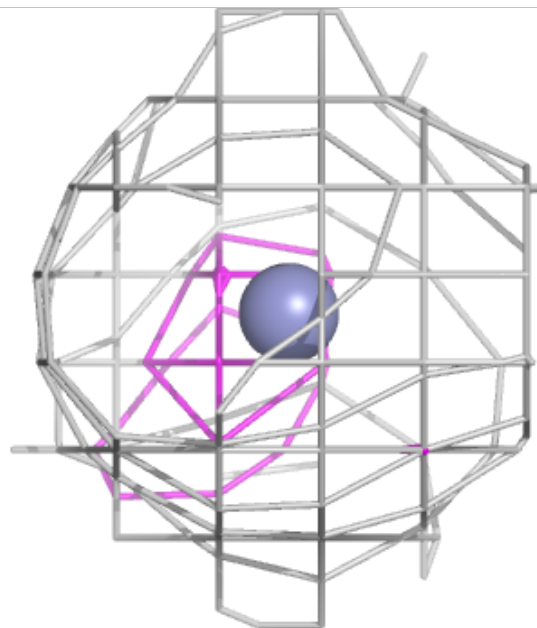
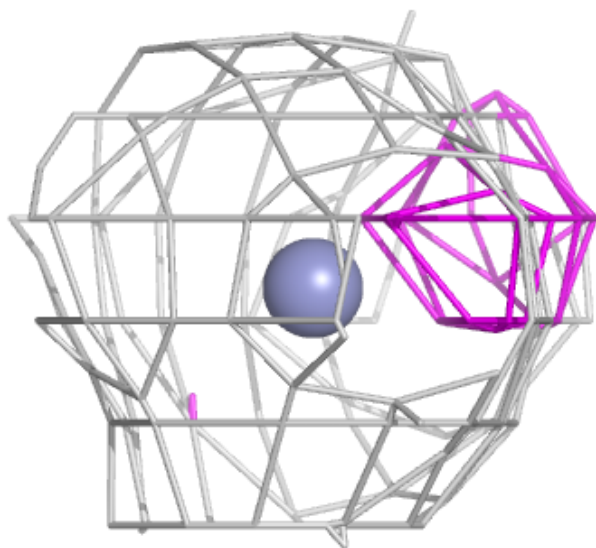
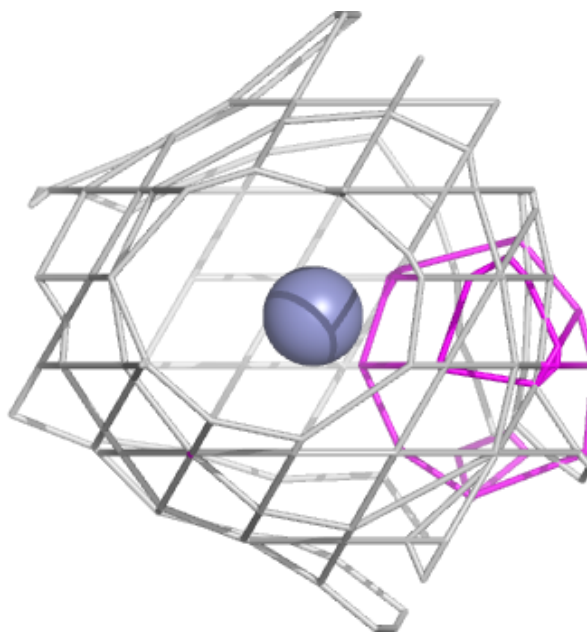
Electron density around ZN D 401:

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



Electron density around ZN B 401:

$2mF_o-DF_c$ (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.