Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2023 – 03:22 pm GMT

PDB ID : 8BQH

Title : W-formate dehydrogenase from Desulfovibrio vulgaris - Soaking with Formate 1.5 min

Authors : Vilela-Alves, G.; Mota, C.; Oliveira, A.R.; Manuel, R.R.; Pereira, I.C.; Romao, M.J.

Deposited on : 2022-11-21

Resolution : 1.61 Å(reported)

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

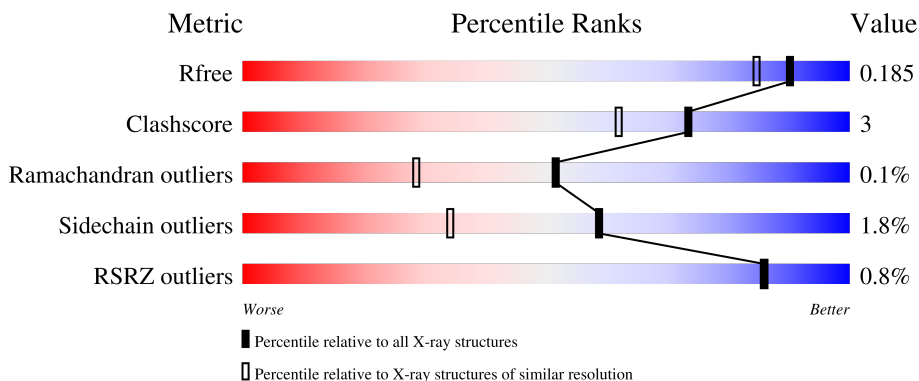|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 1.61 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	Percentile Ranks	Value
Rfree		0.185
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		1.8%
RSRZ outliers		0.8%

Worse ——— *Better*

▮ 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	1013	87% 7% 6%
2	B	236	84% 6% 9%

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
10	EDO	A	1112	-	-	X	-
10	EDO	A	1113	-	-	X	-
11	FMT	A	1120	-	-	X	-

2 Entry composition ⓘ

There are 13 unique types of molecules in this entry. The entry contains 9927 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 Formate dehydrogenase, alpha subunit, selenocysteine-contai ning.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	955	7476	4762	1303	1368	42	1	0	2	0

There are 43 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q72EJ1
A	2	THR	-	expression tag	UNP Q72EJ1
A	3	VAL	-	expression tag	UNP Q72EJ1
A	4	THR	-	expression tag	UNP Q72EJ1
A	5	ARG	-	expression tag	UNP Q72EJ1
A	6	ARG	-	expression tag	UNP Q72EJ1
A	7	HIS	-	expression tag	UNP Q72EJ1
A	8	PHE	-	expression tag	UNP Q72EJ1
A	9	LEU	-	expression tag	UNP Q72EJ1
A	10	LYS	-	expression tag	UNP Q72EJ1
A	11	LEU	-	expression tag	UNP Q72EJ1
A	12	SER	-	expression tag	UNP Q72EJ1
A	13	ALA	-	expression tag	UNP Q72EJ1
A	14	GLY	-	expression tag	UNP Q72EJ1
A	15	ALA	-	expression tag	UNP Q72EJ1
A	16	ALA	-	expression tag	UNP Q72EJ1
A	17	VAL	-	expression tag	UNP Q72EJ1
A	18	ALA	-	expression tag	UNP Q72EJ1
A	19	GLY	-	expression tag	UNP Q72EJ1
A	20	ALA	-	expression tag	UNP Q72EJ1
A	21	PHE	-	expression tag	UNP Q72EJ1
A	22	THR	-	expression tag	UNP Q72EJ1
A	23	GLY	-	expression tag	UNP Q72EJ1
A	24	LEU	-	expression tag	UNP Q72EJ1
A	25	GLY	-	expression tag	UNP Q72EJ1
A	26	LEU	-	expression tag	UNP Q72EJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	SER	-	expression tag	UNP Q72EJ1
A	28	LEU	-	expression tag	UNP Q72EJ1
A	29	ALA	-	expression tag	UNP Q72EJ1
A	30	PRO	-	expression tag	UNP Q72EJ1
A	31	THR	-	expression tag	UNP Q72EJ1
A	32	VAL	-	expression tag	UNP Q72EJ1
A	33	ALA	-	expression tag	UNP Q72EJ1
A	34	ARG	-	expression tag	UNP Q72EJ1
A	35	ALA	-	expression tag	UNP Q72EJ1
A	1006	TRP	-	expression tag	UNP Q72EJ1
A	1007	SER	-	expression tag	UNP Q72EJ1
A	1008	HIS	-	expression tag	UNP Q72EJ1
A	1009	PRO	-	expression tag	UNP Q72EJ1
A	1010	GLN	-	expression tag	UNP Q72EJ1
A	1011	PHE	-	expression tag	UNP Q72EJ1
A	1012	GLU	-	expression tag	UNP Q72EJ1
A	1013	LYS	-	expression tag	UNP Q72EJ1

- Molecule 2 is a protein called Formate dehydrogenase, beta subunit, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	214	1664	1041	291	316	16	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q72EJ0
B	216	ASP	-	expression tag	UNP Q72EJ0
B	217	LEU	-	expression tag	UNP Q72EJ0
B	218	ALA	-	expression tag	UNP Q72EJ0
B	219	PRO	-	expression tag	UNP Q72EJ0
B	220	SER	-	expression tag	UNP Q72EJ0
B	221	MET	-	expression tag	UNP Q72EJ0
B	222	MET	-	expression tag	UNP Q72EJ0
B	223	THR	-	expression tag	UNP Q72EJ0
B	224	ARG	-	expression tag	UNP Q72EJ0
B	225	GLN	-	expression tag	UNP Q72EJ0
B	226	GLN	-	expression tag	UNP Q72EJ0
B	227	LEU	-	expression tag	UNP Q72EJ0
B	228	PHE	-	expression tag	UNP Q72EJ0
B	229	ALA	-	expression tag	UNP Q72EJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	230	ARG	-	expression tag	UNP Q72EJ0
B	231	LEU	-	expression tag	UNP Q72EJ0
B	232	PHE	-	expression tag	UNP Q72EJ0
B	233	ARG	-	expression tag	UNP Q72EJ0
B	234	PRO	-	expression tag	UNP Q72EJ0
B	235	ARG	-	expression tag	UNP Q72EJ0
B	236	ALA	-	expression tag	UNP Q72EJ0

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$) (labeled as "Ligand of Interest" by depositor).
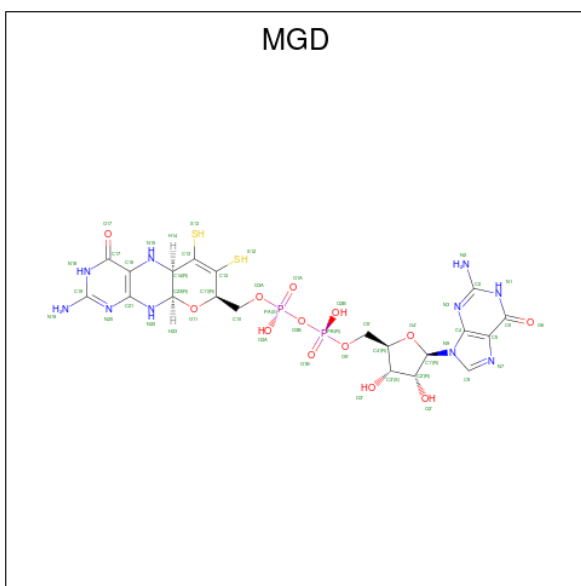
MGD

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
3	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is HYDROSULFURIC ACID (three-letter code: H2S) (formula: H_2S) (labeled as "Ligand of Interest" by depositor).
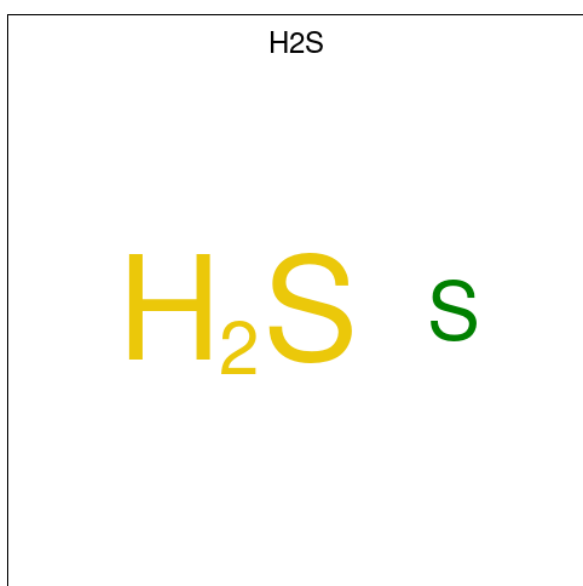
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	S 1	0	0

- Molecule 6 is TUNGSTEN ION (three-letter code: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	W 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
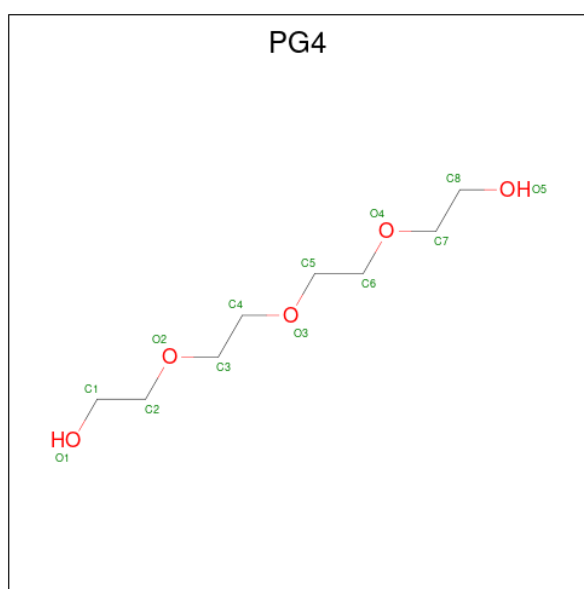
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 13	C 8	O 5	0	0
7	A	1	Total 13	C 8	O 5	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

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

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

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
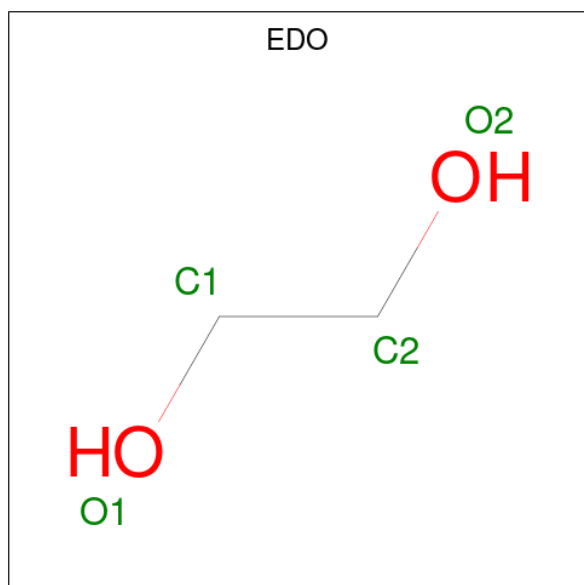
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0
10	A	1	Total 4	C 2	O 2	0	0

- Molecule 11 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2) (labeled as "Ligand of Interest" by depositor).

FMT
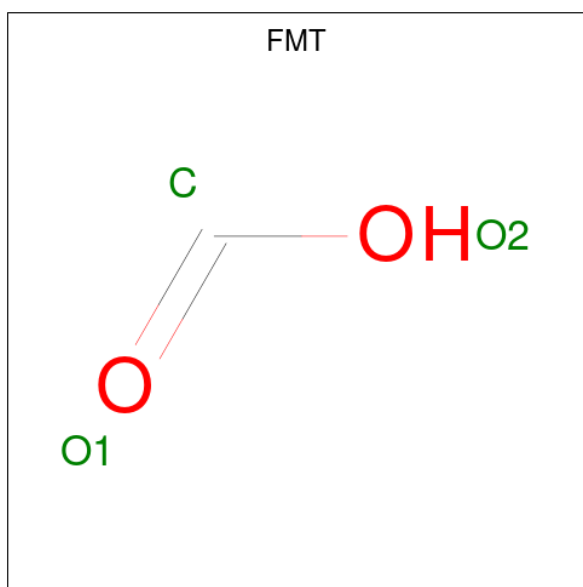
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total 3	C 1	O 2	0	0
11	A	1	Total 3	C 1	O 2	0	0
11	A	1	Total 3	C 1	O 2	0	0
11	A	1	Total 3	C 1	O 2	0	0
11	B	1	Total 3	C 1	O 2	0	0

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	5	Total 5	Cl 5	0	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	464	Total 464	O 464	0	0
13	B	93	Total 93	O 93	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: Formate dehydrogenase, alpha subunit, selenocysteine-containing

Chain A:
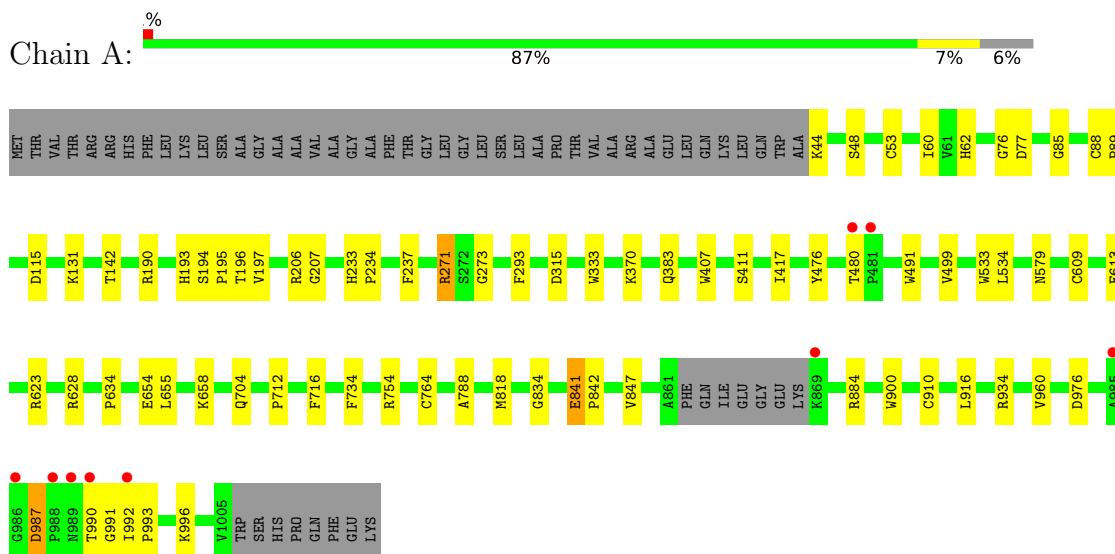
• Molecule 2: Formate dehydrogenase, beta subunit, putative

Chain B:
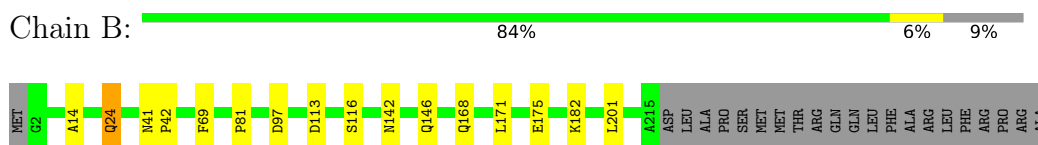
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.36Å 127.46Å 128.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.65 – 1.61 90.65 – 1.61	Depositor EDS
% Data completeness (in resolution range)	68.5 (90.65-1.61) 68.5 (90.65-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.151 , 0.175 0.163 , 0.185	Depositor DCC
R_{free} test set	4778 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	14.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9927	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: PEG, CL, PG4, W, MGD, EDO, FMT, SEC, SF4, GOL, H2S

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	0.71	0/7674	0.80	3/10410 (0.0%)
2	B	0.69	0/1699	0.79	0/2302
All	All	0.71	0/9373	0.80	3/12712 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	271	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	976	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	271	ARG	NE-CZ-NH1	5.39	123.00	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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7476	0	7308	47	0
2	B	1664	0	1633	9	0
3	A	94	0	44	2	0
4	A	8	0	0	0	0
4	B	24	0	0	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
7	A	26	0	36	5	0
8	A	12	0	16	0	0
9	A	28	0	40	1	0
10	A	16	0	23	6	0
11	A	12	0	4	2	0
11	B	3	0	1	0	0
12	A	5	0	0	0	0
13	A	464	0	0	2	0
13	B	93	0	0	0	0
All	All	9927	0	9105	61	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 3.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:GLU:HG3	1:A:847:VAL:HG21	1.34	1.06
1:A:370:LYS:HE3	13:A:1241:HOH:O	1.63	0.95
1:A:579:ASN:OD1	3:A:1102:MGD:O2'	1.92	0.87
1:A:841:GLU:CG	1:A:847:VAL:HG21	2.14	0.74
1:A:206:ARG:HH21	7:A:1106:PG4:H11	1.52	0.72
1:A:195:PRO:HG3	1:A:992:ILE:HG13	1.72	0.70
1:A:206:ARG:HH21	7:A:1106:PG4:C1	2.05	0.69
1:A:754:ARG:HD2	1:A:788:ALA:O	1.94	0.67
1:A:315:ASP:HA	13:A:1360:HOH:O	1.98	0.63
2:B:97:ASP:OD2	2:B:146:GLN:NE2	2.32	0.63
1:A:992:ILE:HG23	1:A:993:PRO:HD2	1.81	0.62
10:A:1112:EDO:O1	10:A:1113:EDO:H11	2.00	0.61
2:B:113:ASP:OD2	2:B:116:SER:OG	2.19	0.61
10:A:1112:EDO:H11	9:A:1117:PEG:H21	1.82	0.60
1:A:62:HIS:CE1	10:A:1114:EDO:H22	2.39	0.57
1:A:190:ARG:O	1:A:992:ILE:HD12	2.06	0.56
1:A:197:VAL:CG2	11:A:1120:FMT:H	2.38	0.54
1:A:233:HIS:N	1:A:234:PRO:HD3	2.23	0.54
1:A:88:CYS:HB2	1:A:89:PRO:HD2	1.90	0.53
1:A:206:ARG:HD3	7:A:1106:PG4:H42	1.91	0.53
10:A:1112:EDO:C1	10:A:1113:EDO:H12	2.39	0.53
2:B:171:LEU:O	2:B:175:GLU:HG2	2.09	0.52
1:A:609[B]:CYS:SG	1:A:634:PRO:HB3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1112:EDO:O1	10:A:1113:EDO:C1	2.59	0.51
1:A:411:SER:HB3	1:A:987:ASP:OD2	2.12	0.49
1:A:534:LEU:HD12	1:A:991:GLY:C	2.31	0.49
1:A:712:PRO:HG2	1:A:716:PHE:CD2	2.47	0.49
1:A:916:LEU:C	1:A:916:LEU:HD23	2.32	0.49
1:A:992:ILE:CG2	1:A:993:PRO:HD2	2.43	0.49
1:A:609[A]:CYS:HB2	1:A:613:GLU:OE1	2.13	0.48
1:A:910:CYS:SG	1:A:960:VAL:HG13	2.54	0.48
10:A:1112:EDO:H12	10:A:1113:EDO:H12	1.95	0.48
2:B:41:ASN:HA	2:B:42:PRO:C	2.35	0.47
1:A:916:LEU:HD23	1:A:916:LEU:O	2.13	0.47
1:A:754:ARG:CD	1:A:788:ALA:O	2.62	0.47
1:A:60[B]:ILE:HG12	1:A:77:ASP:HA	1.97	0.47
1:A:884:ARG:HH22	3:A:1102:MGD:H15	1.63	0.46
2:B:201:LEU:C	2:B:201:LEU:HD23	2.36	0.46
1:A:491:TRP:HB3	1:A:818:MET:SD	2.55	0.46
1:A:990:THR:OG1	1:A:992:ILE:HB	2.16	0.46
1:A:407:TRP:CD1	1:A:996:LYS:HB2	2.51	0.45
1:A:534:LEU:HD12	1:A:991:GLY:O	2.17	0.45
1:A:273:GLY:HA3	1:A:842:PRO:HG2	1.99	0.45
1:A:654:GLU:O	1:A:658:LYS:HG2	2.18	0.44
1:A:194:SER:N	1:A:195:PRO:CD	2.81	0.44
1:A:476:TYR:HE1	1:A:499:VAL:HG21	1.83	0.44
1:A:196:THR:HB	1:A:417:ILE:HG13	2.01	0.43
1:A:207:GLY:H	7:A:1106:PG4:H72	1.84	0.43
2:B:81:PRO:HD2	4:B:302:SF4:S3	2.59	0.43
1:A:193:HIS:O	1:A:197:VAL:HG13	2.19	0.42
2:B:142:ASN:O	2:B:146:GLN:HG2	2.20	0.42
1:A:88:CYS:CB	1:A:89:PRO:HD2	2.49	0.42
1:A:131:LYS:HG3	1:A:655:LEU:HD11	2.01	0.42
2:B:14:ALA:HB2	2:B:69:PHE:CG	2.55	0.42
1:A:623:ARG:O	1:A:764:CYS:HA	2.20	0.41
1:A:48:SER:HA	1:A:628:ARG:HB2	2.02	0.41
1:A:900:TRP:CH2	2:B:24:GLN:HA	2.55	0.41
11:A:1120:FMT:C	11:A:1121:FMT:H	2.51	0.41
1:A:76:GLY:HA3	1:A:85:GLY:O	2.21	0.40
1:A:206:ARG:CD	7:A:1106:PG4:H42	2.51	0.40
1:A:333:TRP:CH2	1:A:834:GLY:HA2	2.56	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	952/1013 (94%)	925 (97%)	26 (3%)	1 (0%)	51	28
2	B	212/236 (90%)	204 (96%)	8 (4%)	0	100	100
All	All	1164/1249 (93%)	1129 (97%)	34 (3%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	TRP

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	777/819 (95%)	763 (98%)	14 (2%)	59	34
2	B	185/204 (91%)	182 (98%)	3 (2%)	62	40
All	All	962/1023 (94%)	945 (98%)	17 (2%)	59	34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	53	CYS
1	A	115	ASP
1	A	142	THR
1	A	237	PHE

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Mol	Chain	Res	Type
1	A	271	ARG
1	A	293	PHE
1	A	383	GLN
1	A	480	THR
1	A	704	GLN
1	A	734	PHE
1	A	841	GLU
1	A	934	ARG
1	A	987	ASP
2	B	24	GLN
2	B	168	GLN
2	B	182	LYS

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

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 1 is modelled with single atom and 6 are monoatomic - leaving 23 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	GOL	A	1108	-	5,5,5	0.22	0	5,5,5	0.25	0
11	FMT	B	304	-	2,2,2	0.19	0	1,1,1	0.09	0
3	MGD	A	1101	6	41,52,52	0.98	2 (4%)	40,81,81	1.17	3 (7%)
9	PEG	A	1110	-	6,6,6	0.17	0	5,5,5	0.12	0
10	EDO	A	1114	-	3,3,3	0.18	0	2,2,2	0.38	0
9	PEG	A	1115	-	6,6,6	0.29	0	5,5,5	0.25	0
10	EDO	A	1112	-	3,3,3	0.12	0	2,2,2	0.26	0
4	SF4	B	301	2	0,12,12	-	-	-		
4	SF4	B	302	2	0,12,12	-	-	-		
11	FMT	A	1119	-	2,2,2	0.36	0	1,1,1	0.16	0
11	FMT	A	1120	-	2,2,2	0.41	0	1,1,1	0.05	0
11	FMT	A	1121	-	2,2,2	0.66	0	1,1,1	0.13	0
10	EDO	A	1113	-	3,3,3	0.16	0	2,2,2	0.45	0
4	SF4	B	303	2	0,12,12	-	-	-		
9	PEG	A	1117	-	6,6,6	0.39	0	5,5,5	0.18	0
3	MGD	A	1102	6	41,52,52	0.90	2 (4%)	40,81,81	1.24	5 (12%)
7	PG4	A	1106	-	12,12,12	0.34	0	11,11,11	0.39	0
9	PEG	A	1111	-	6,6,6	0.19	0	5,5,5	0.22	0
11	FMT	A	1118	-	2,2,2	0.44	0	1,1,1	0.11	0
8	GOL	A	1109	-	5,5,5	0.31	0	5,5,5	0.64	0
10	EDO	A	1116	-	3,3,3	1.81	1 (33%)	2,2,2	0.16	0
7	PG4	A	1107	-	12,12,12	0.25	0	11,11,11	0.30	0
4	SF4	A	1103	1	0,12,12	-	-	-		

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
8	GOL	A	1108	-	-	0/4/4/4	-
10	EDO	A	1112	-	-	1/1/1/1	-
3	MGD	A	1101	6	-	1/18/66/66	0/6/6/6
9	PEG	A	1117	-	-	1/4/4/4	-
4	SF4	B	301	2	-	-	0/6/5/5
10	EDO	A	1114	-	-	1/1/1/1	-
7	PG4	A	1106	-	-	4/10/10/10	-
3	MGD	A	1102	6	-	4/18/66/66	0/6/6/6
9	PEG	A	1110	-	-	2/4/4/4	-
4	SF4	B	303	2	-	-	0/6/5/5
9	PEG	A	1111	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	302	2	-	-	0/6/5/5
9	PEG	A	1115	-	-	1/4/4/4	-
8	GOL	A	1109	-	-	2/4/4/4	-
10	EDO	A	1113	-	-	1/1/1/1	-
10	EDO	A	1116	-	-	0/1/1/1	-
7	PG4	A	1107	-	-	3/10/10/10	-
4	SF4	A	1103	1	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1116	EDO	O1-C1	-2.90	1.27	1.42
3	A	1101	MGD	C5-C6	-2.68	1.42	1.47
3	A	1102	MGD	C5-C6	-2.67	1.42	1.47
3	A	1101	MGD	C5-C4	-2.30	1.37	1.43
3	A	1102	MGD	C8-N7	-2.05	1.31	1.35

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MGD	O11-C23-C14	3.60	111.36	108.96
3	A	1102	MGD	O11-C23-C14	3.17	111.08	108.96
3	A	1102	MGD	O4'-C1'-C2'	-2.98	102.56	106.93
3	A	1102	MGD	C19-N20-C21	2.79	118.47	113.43
3	A	1101	MGD	C19-N20-C21	2.63	118.18	113.43
3	A	1102	MGD	C17-C16-N15	2.50	123.46	116.76
3	A	1101	MGD	PA-O3B-PB	2.32	140.77	132.83
3	A	1102	MGD	O6-C6-C5	2.13	128.53	124.37

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	MGD	C4'-C5'-O5'-PB
3	A	1102	MGD	O4'-C4'-C5'-O5'
3	A	1102	MGD	C3'-C4'-C5'-O5'
7	A	1106	PG4	O3-C5-C6-O4
9	A	1110	PEG	O2-C3-C4-O4
9	A	1117	PEG	O1-C1-C2-O2
7	A	1106	PG4	O4-C7-C8-O5
9	A	1111	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
8	A	1109	GOL	C1-C2-C3-O3
10	A	1113	EDO	O1-C1-C2-O2
9	A	1111	PEG	C1-C2-O2-C3
9	A	1110	PEG	O1-C1-C2-O2
10	A	1112	EDO	O1-C1-C2-O2
7	A	1106	PG4	O2-C3-C4-O3
8	A	1109	GOL	O2-C2-C3-O3
10	A	1114	EDO	O1-C1-C2-O2
3	A	1101	MGD	PA-O3B-PB-O5'
7	A	1107	PG4	C4-C3-O2-C2
9	A	1111	PEG	C4-C3-O2-C2
7	A	1107	PG4	C6-C5-O3-C4
9	A	1115	PEG	C4-C3-O2-C2
7	A	1107	PG4	O1-C1-C2-O2
9	A	1111	PEG	O2-C3-C4-O4
7	A	1106	PG4	C4-C3-O2-C2
3	A	1102	MGD	C5'-O5'-PB-O1B

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1114	EDO	1	0
10	A	1112	EDO	5	0
4	B	302	SF4	1	0
11	A	1120	FMT	2	0
11	A	1121	FMT	1	0
10	A	1113	EDO	4	0
9	A	1117	PEG	1	0
3	A	1102	MGD	2	0
7	A	1106	PG4	5	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 FMT B 304	
Bond lengths	Bond angles
Torsions	Rings

Ligand MGD A 1101	
Bond lengths	Bond angles
Torsions	Rings

Ligand SF4 B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand FMT A 1119

Bond lengths

Bond angles

Torsions

Rings

Ligand FMT A 1120

Bond lengths

Bond angles

Torsions

Rings

Ligand FMT A 1121

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand MGD A 1102

Bond lengths

Bond angles

Torsions

Rings

Ligand FMT A 1118

Bond lengths

Bond angles

Torsions

Rings

Ligand SF4 A 1103

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	954/1013 (94%)	-0.61	9 (0%)	84	84	9, 16, 38, 101	0
2	B	214/236 (90%)	-0.57	0	100	100	11, 19, 42, 57	0
All	All	1168/1249 (93%)	-0.61	9 (0%)	86	86	9, 17, 39, 101	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	988	PRO	5.4
1	A	481	PRO	4.7
1	A	985	ALA	4.6
1	A	986	GLY	4.2
1	A	989	ASN	4.0
1	A	480	THR	3.5
1	A	990	THR	3.0
1	A	869	LYS	2.6
1	A	992	ILE	2.2

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

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

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
10	EDO	A	1113	4/4	0.79	0.15	42,49,53,56	0
9	PEG	A	1117	7/7	0.82	0.15	34,39,42,46	0
11	FMT	A	1120	3/3	0.85	0.12	36,36,40,48	0
9	PEG	A	1111	7/7	0.87	0.09	38,43,45,46	0
9	PEG	A	1115	7/7	0.88	0.12	33,38,43,46	0
10	EDO	A	1112	4/4	0.89	0.11	40,44,45,50	0
12	CL	A	1126	1/1	0.89	0.05	44,44,44,44	0
10	EDO	A	1114	4/4	0.91	0.09	34,37,40,43	0
9	PEG	A	1110	7/7	0.91	0.09	37,43,56,61	0
7	PG4	A	1106	13/13	0.91	0.11	28,37,51,54	0
12	CL	A	1125	1/1	0.92	0.07	42,42,42,42	0
7	PG4	A	1107	13/13	0.93	0.08	24,27,36,40	0
11	FMT	A	1121	3/3	0.93	0.12	26,26,27,37	0
11	FMT	A	1119	3/3	0.94	0.06	34,34,37,47	0
12	CL	A	1124	1/1	0.94	0.07	43,43,43,43	0
11	FMT	A	1118	3/3	0.96	0.18	22,22,31,35	0
8	GOL	A	1109	6/6	0.96	0.06	16,22,25,25	0
11	FMT	B	304	3/3	0.96	0.10	21,21,30,32	0
8	GOL	A	1108	6/6	0.97	0.06	11,14,14,15	0
10	EDO	A	1116	4/4	0.97	0.14	10,17,20,24	0
12	CL	A	1122	1/1	0.98	0.12	34,34,34,34	0
12	CL	A	1123	1/1	0.99	0.03	26,26,26,26	0
3	MGD	A	1101	47/47	0.99	0.05	8,11,13,14	0
3	MGD	A	1102	47/47	0.99	0.05	10,12,16,18	0
5	H2S	A	1104	1/1	0.99	0.04	17,17,17,17	0
4	SF4	B	303	8/8	1.00	0.04	12,13,14,14	0
4	SF4	A	1103	8/8	1.00	0.04	10,10,11,12	0
6	W	A	1105	1/1	1.00	0.03	12,12,12,12	0
4	SF4	B	301	8/8	1.00	0.04	11,11,12,13	0
4	SF4	B	302	8/8	1.00	0.04	14,15,16,16	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 FMT A 1120:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
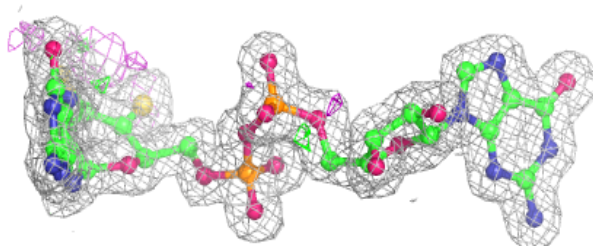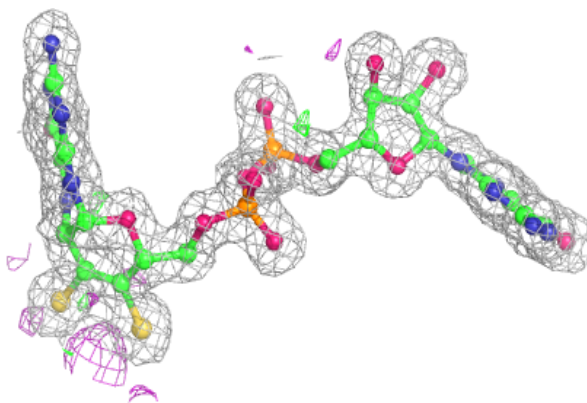$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
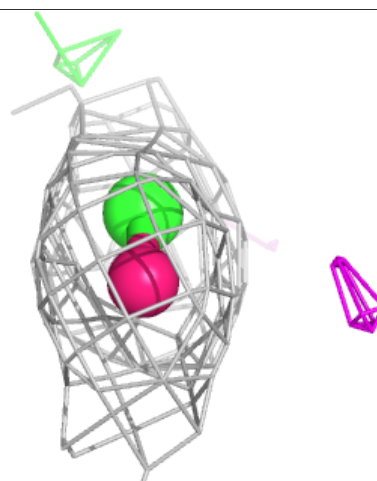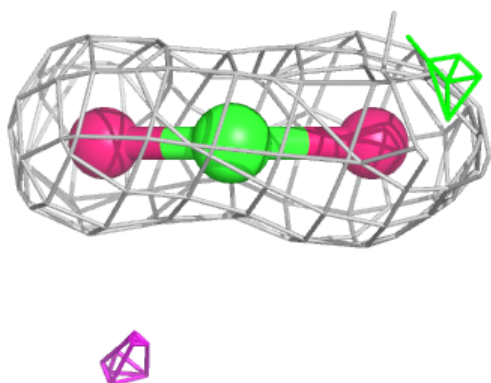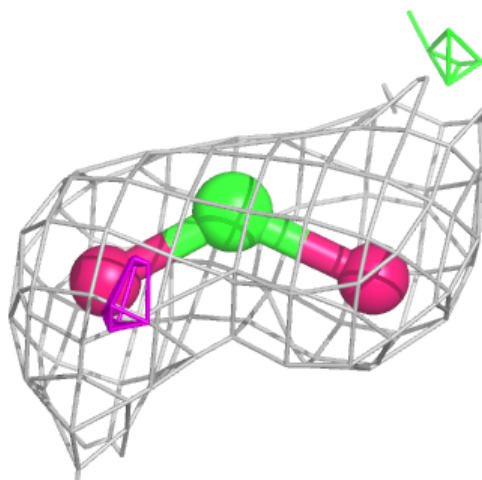
Electron density around FMT A 1121:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
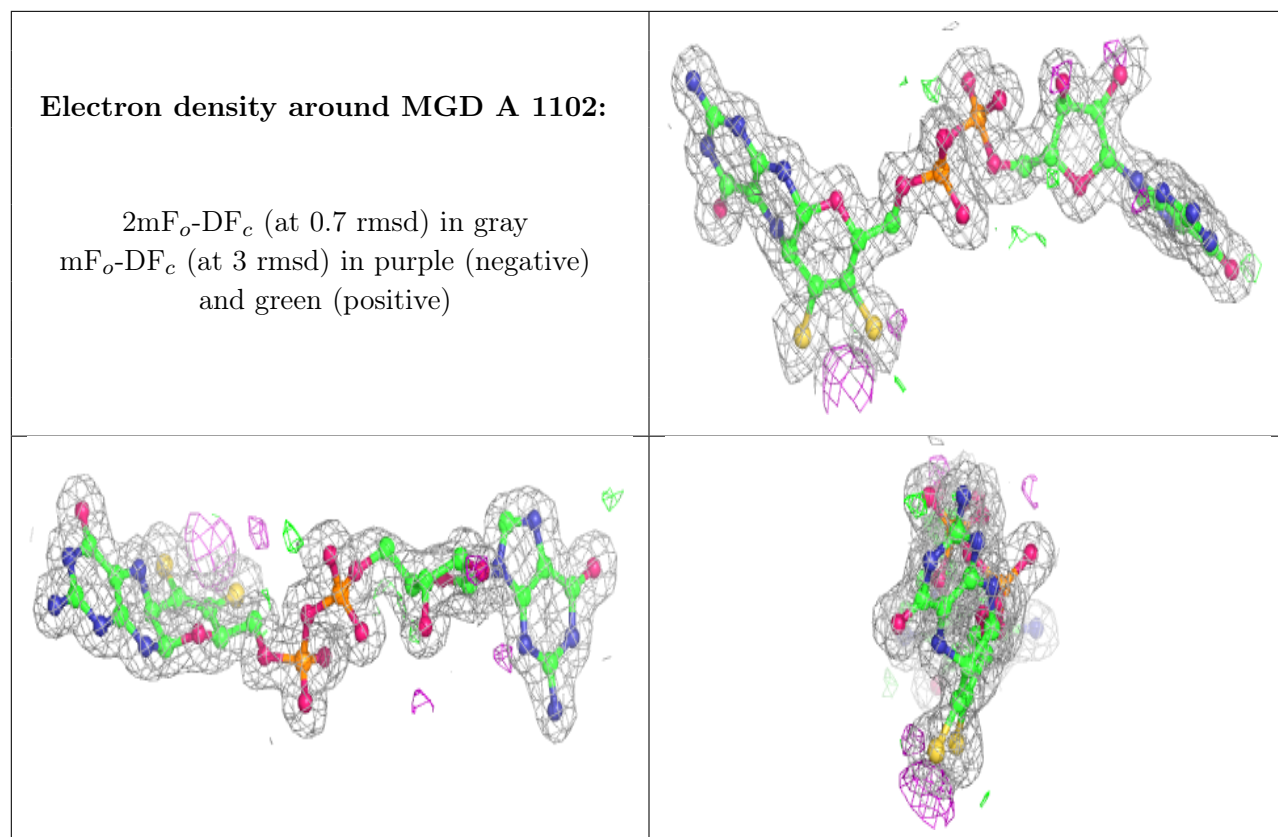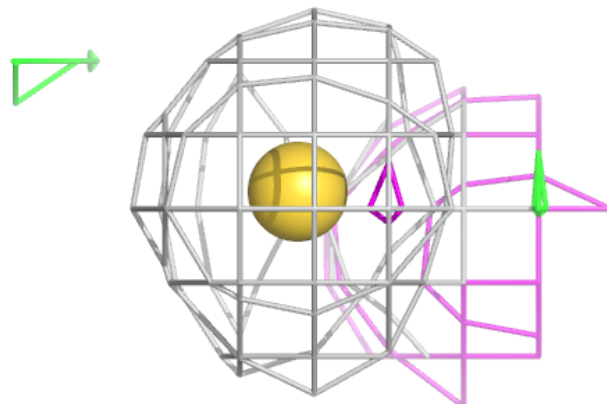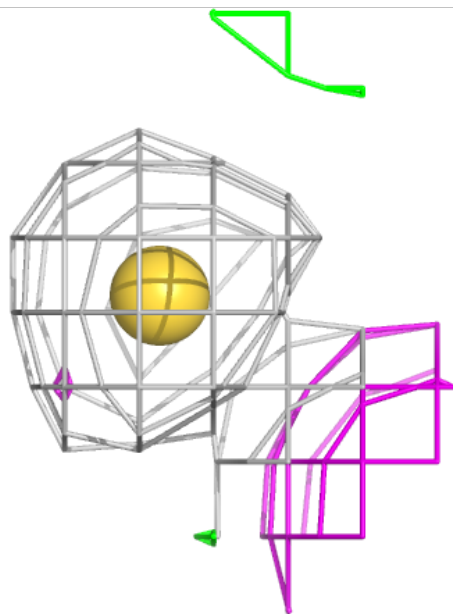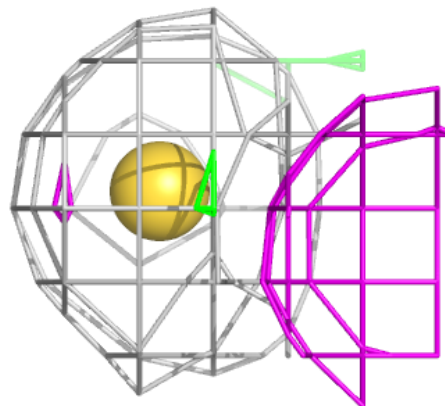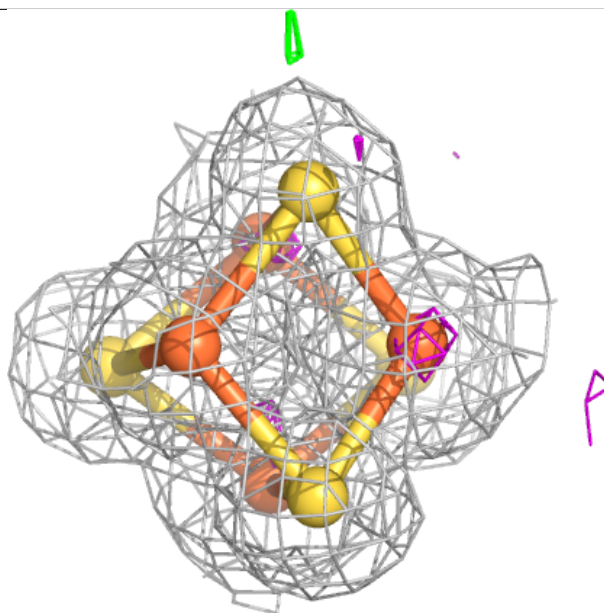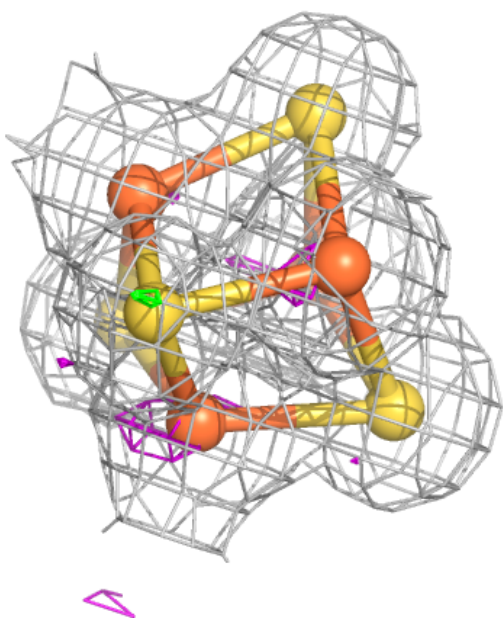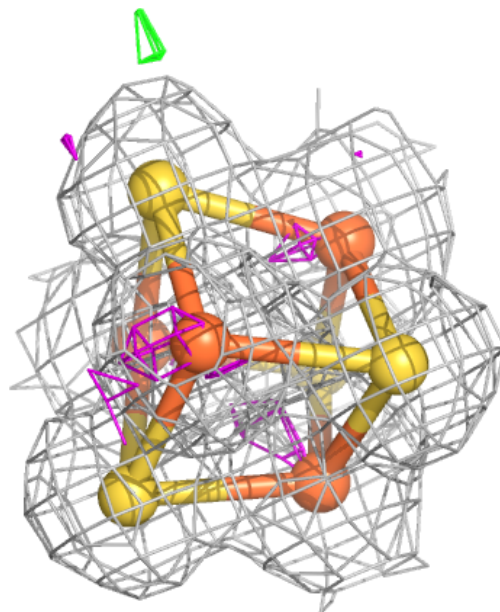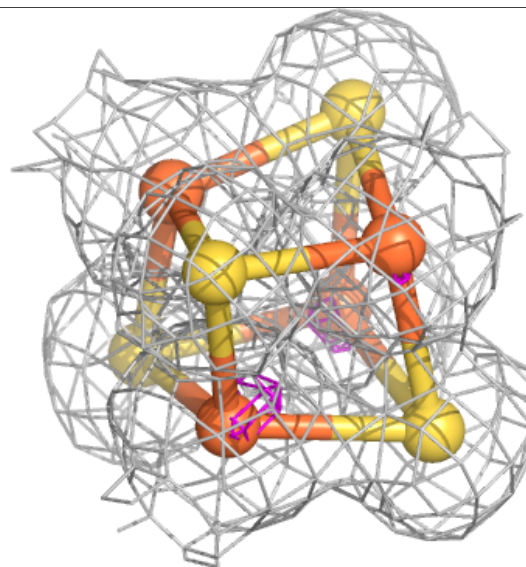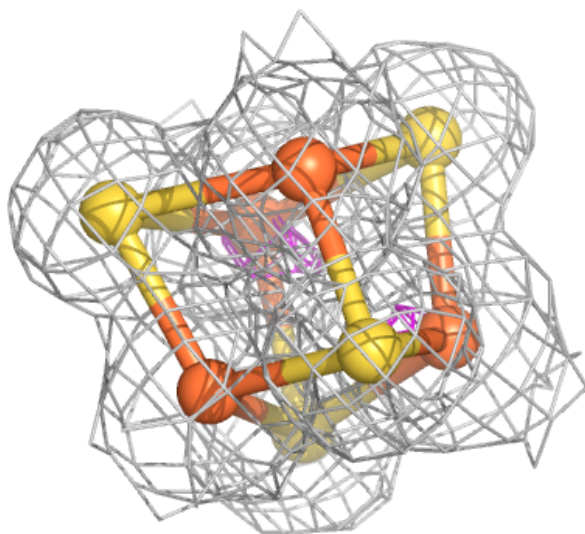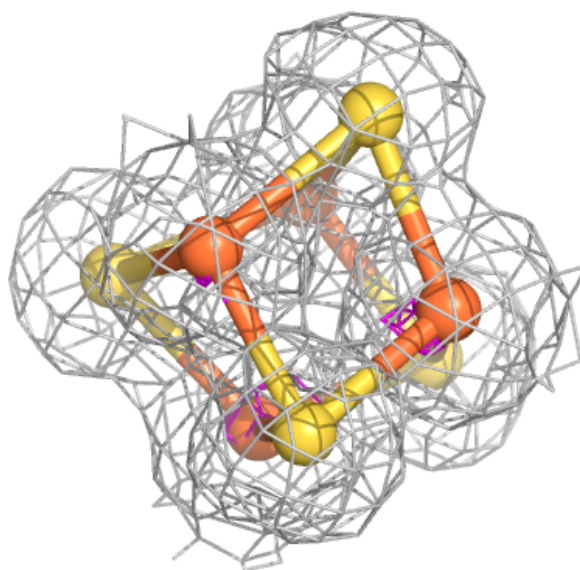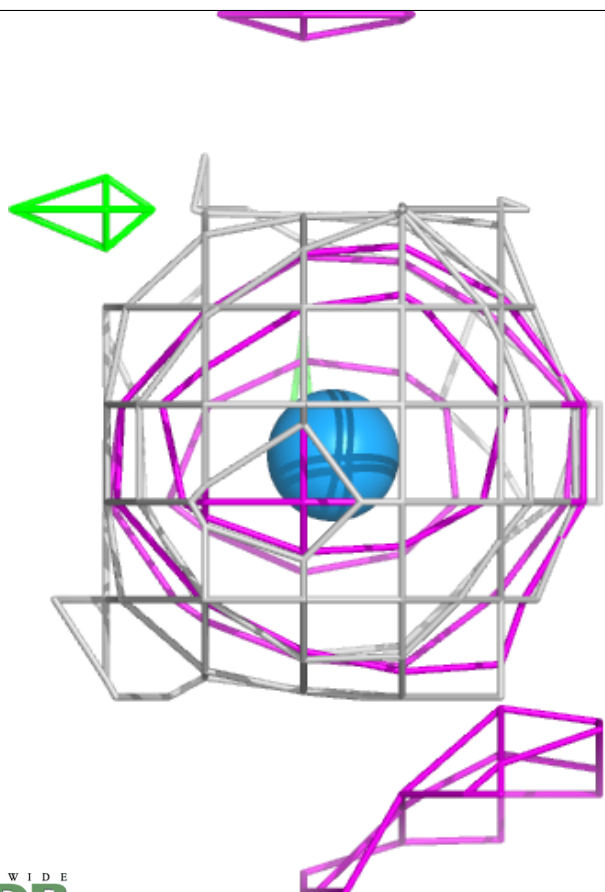mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
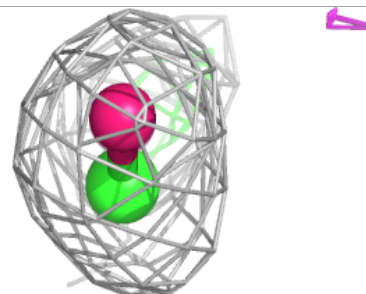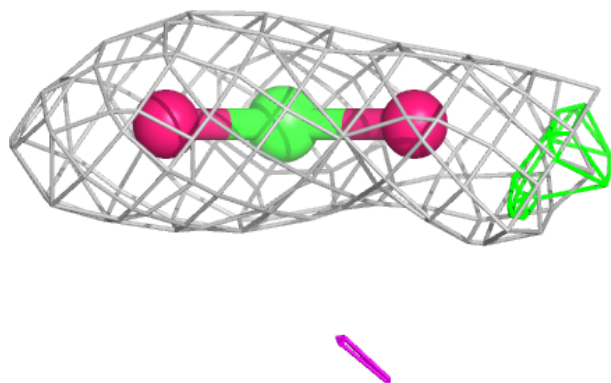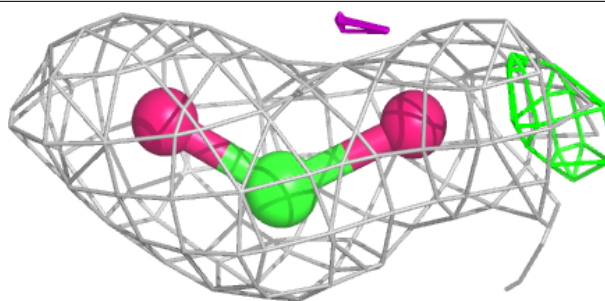
Electron density around FMT A 1119:

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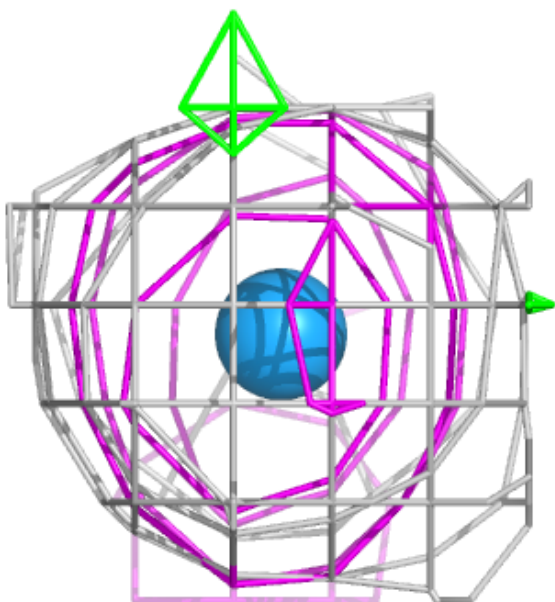and green (positive)

Electron density around FMT A 1118:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
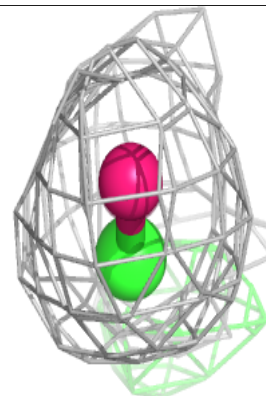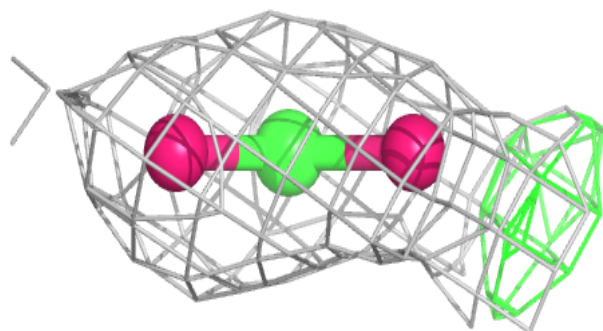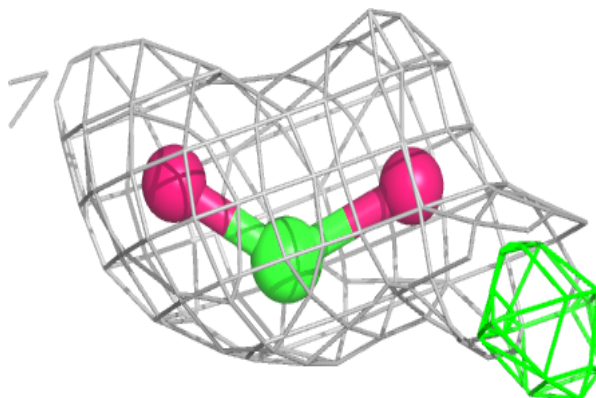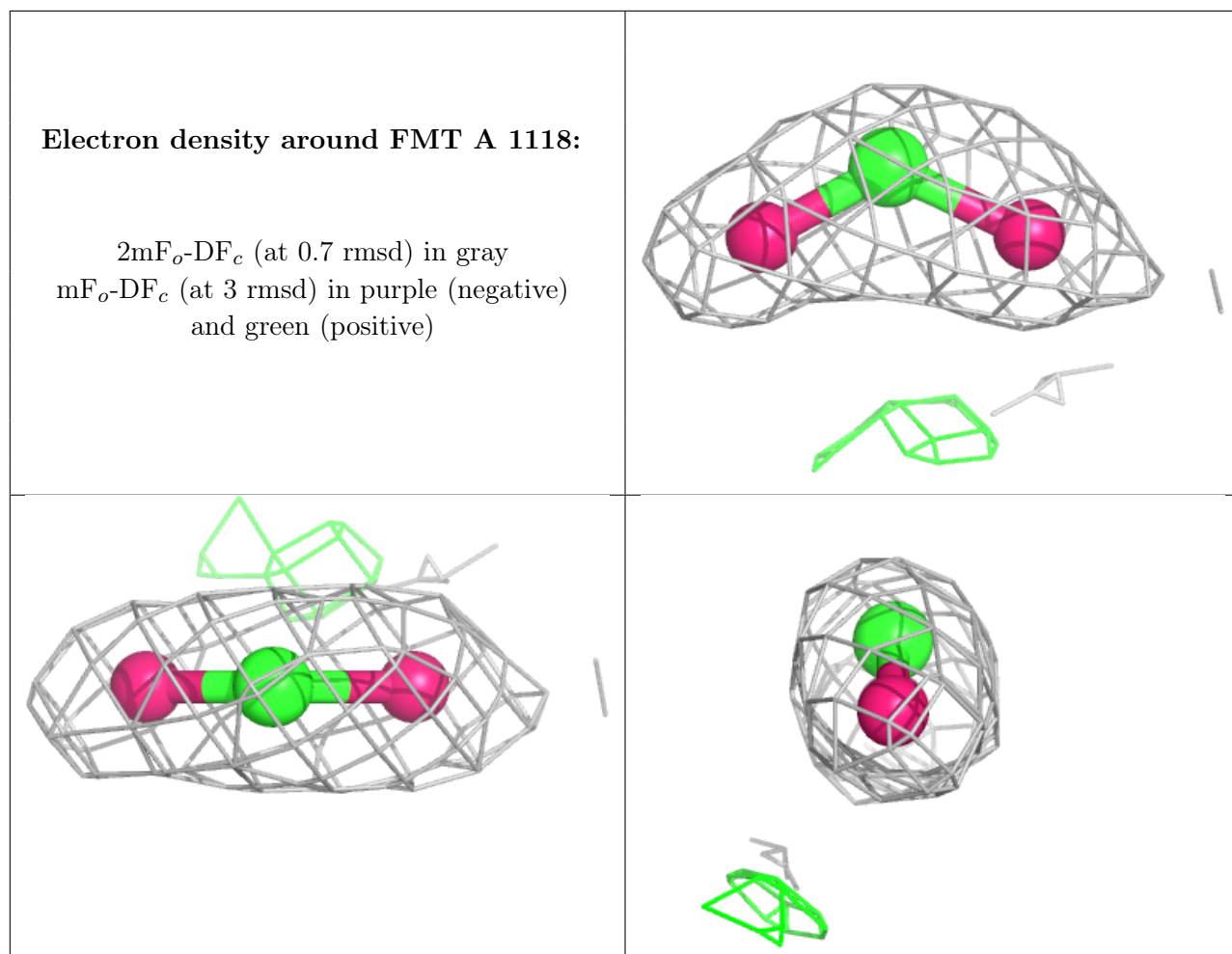
Electron density around FMT B 304:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
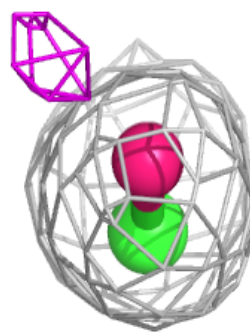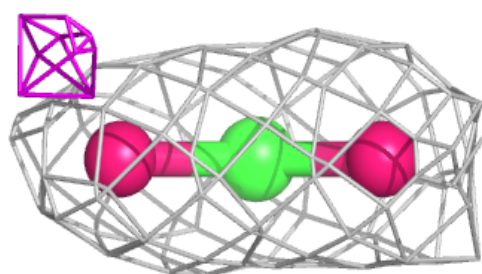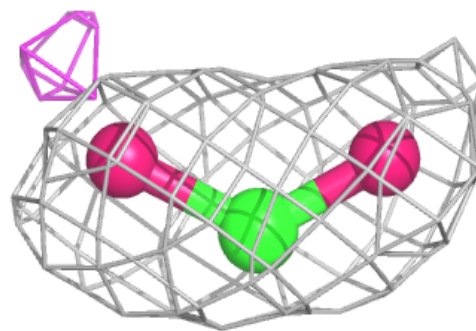
Electron density around MGD A 1101:

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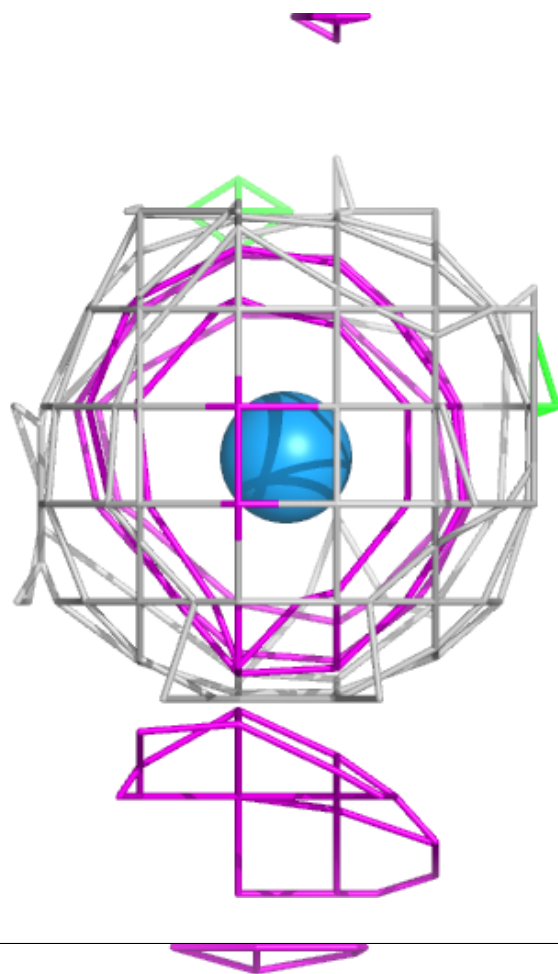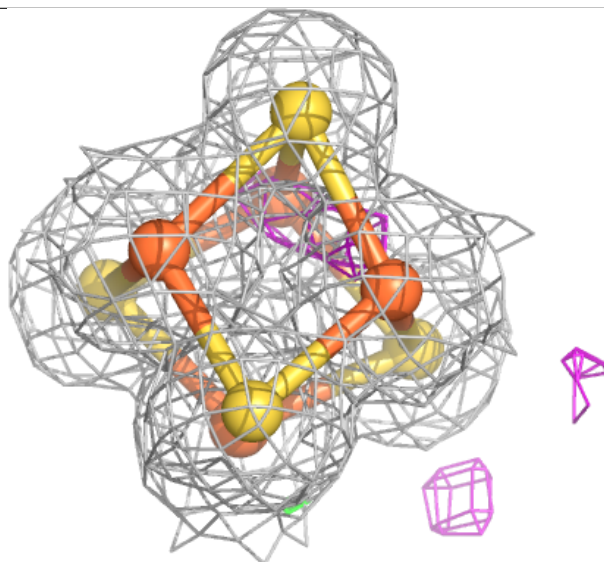and green (positive)

Electron density around MGD A 1102:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
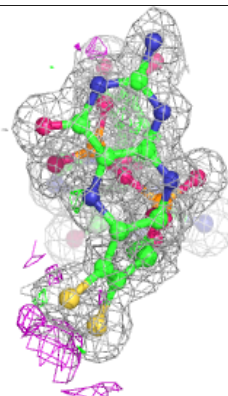
Electron density around H2S A 1104:

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

Electron density around SF4 B 303:

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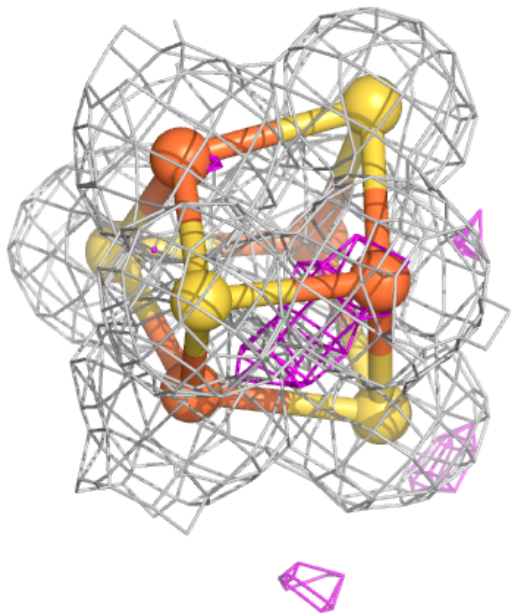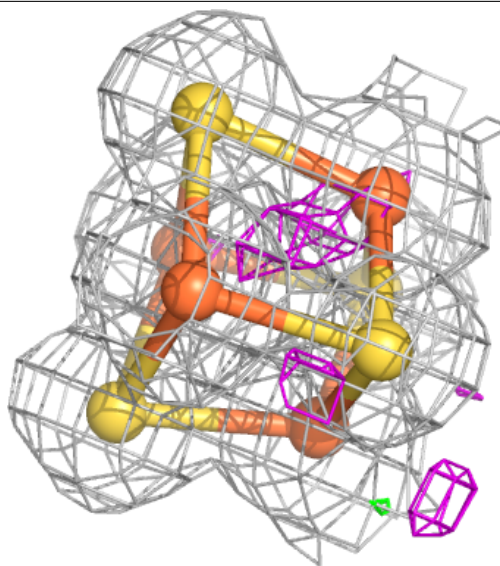and green (positive)

Electron density around SF4 A 1103:

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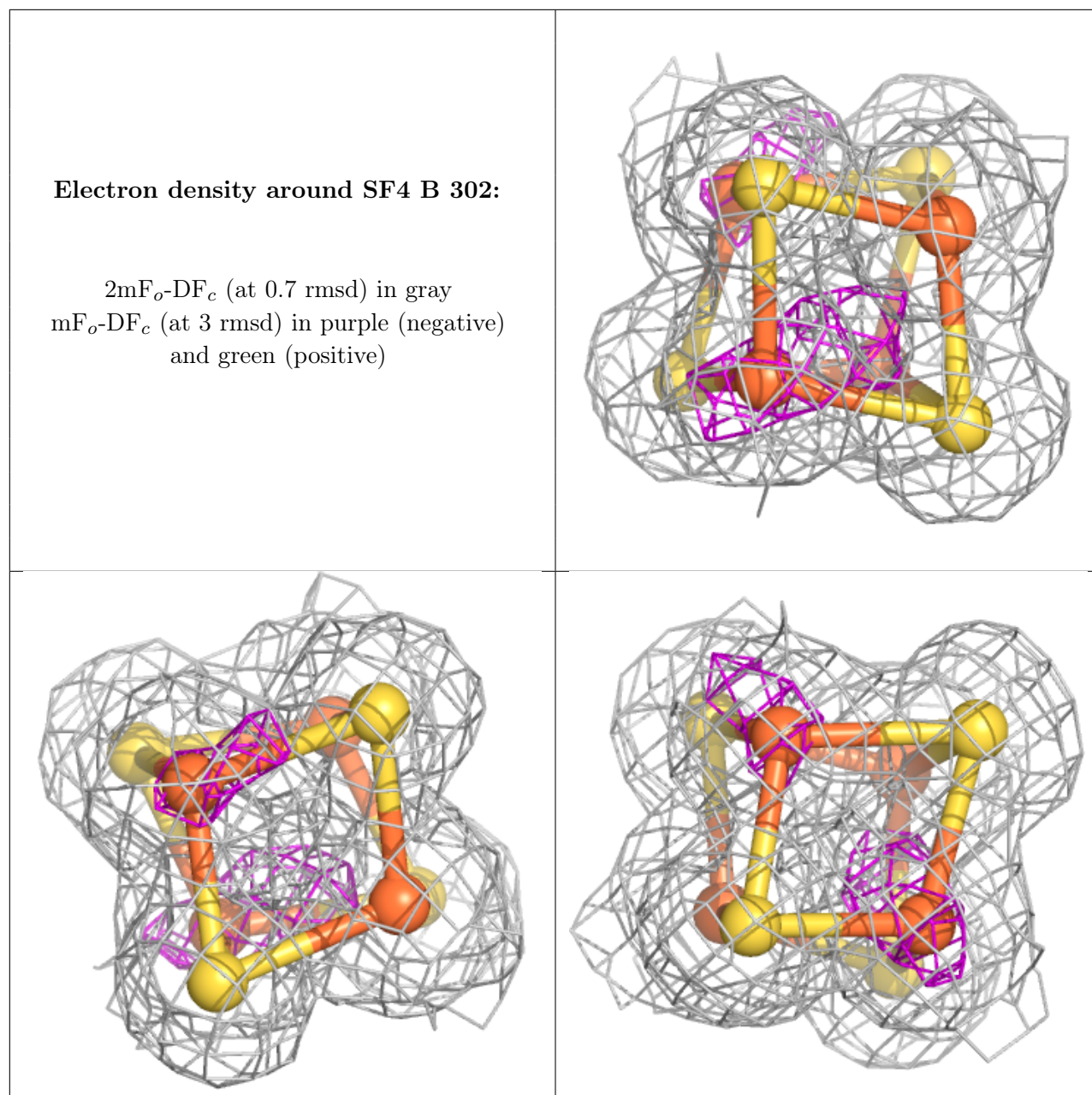and green (positive)

Electron density around W A 1105:

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 SF4 B 301:

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

Electron density around SF4 B 302:

$2mF_o$-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.