



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:59 AM UTC

PDB ID : 9FVT / pdb_00009fvt
Title : Crystal structure of marine sulfatase (OpSulf1) from Ochrovirga pacifica
Authors : Solanki, V.A.; Krull, J.; Hehemann, J.H.
Deposited on : 2024-06-28
Resolution : 1.49 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
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

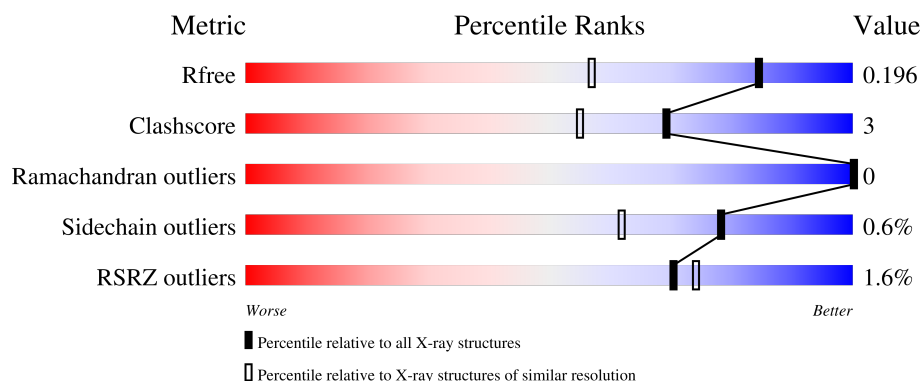
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.49 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	519	2% 92% 8%
1	B	519	2% 92% 7%
1	C	519	% 92% 8%
1	D	519	2% 90% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34828 atoms, of which 16570 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 Sulfatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	519	Total	C	H	N	O	S	115	0	0
			8353	2695	4144	724	781	9			
1	B	519	Total	C	H	N	O	S	115	0	0
			8353	2695	4144	724	781	9			
1	C	519	Total	C	H	N	O	S	115	0	0
			8353	2695	4144	724	781	9			
1	D	519	Total	C	H	N	O	S	115	0	0
			8347	2695	4138	724	781	9			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

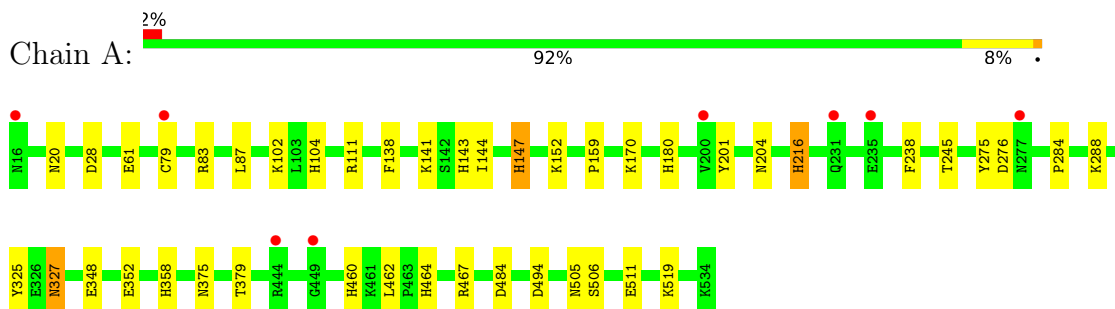
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	379	Total	O	0	0
			379	379		
3	B	345	Total	O	0	0
			345	345		
3	C	366	Total	O	0	0
			366	366		
3	D	328	Total	O	0	0
			328	328		

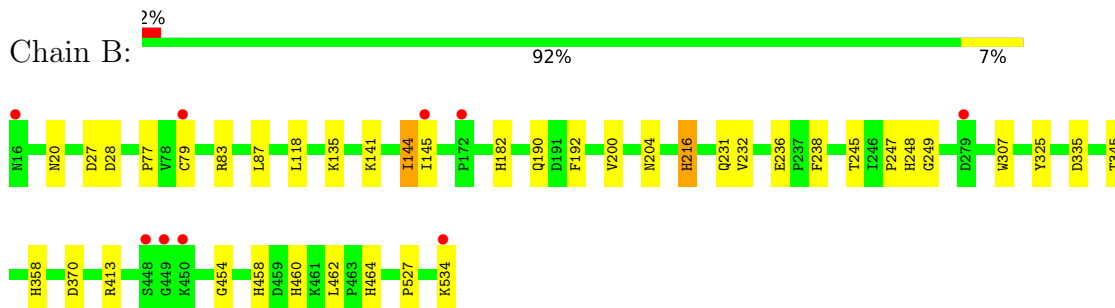
3 Residue-property plots [i](#)

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.

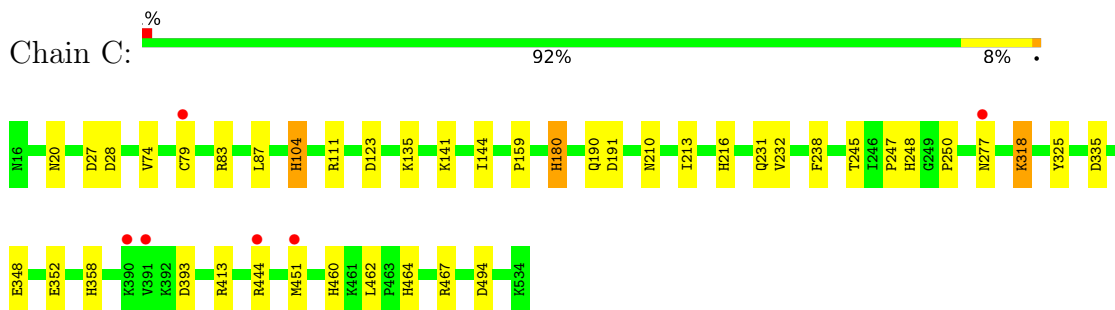
• Molecule 1: Sulfatase



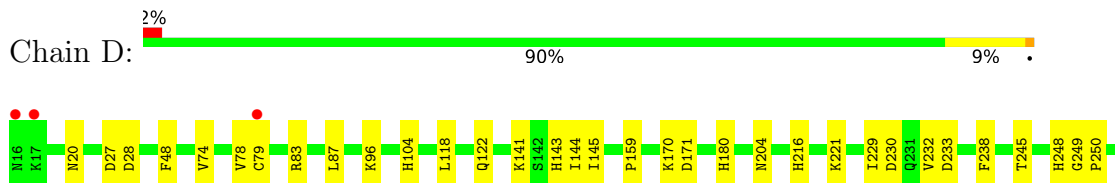
• Molecule 1: Sulfatase

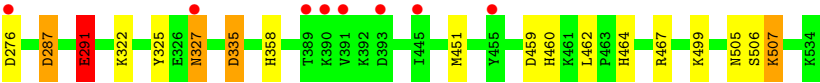


• Molecule 1: Sulfatase



• Molecule 1: Sulfatase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	115.27Å 115.27Å 169.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.33 – 1.49 49.33 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.33-1.49) 100.0 (49.33-1.49)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.166 , 0.196 0.175 , 0.196	Depositor DCC
R_{free} test set	18250 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34828	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5256e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MG

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	0.83	3/4322 (0.1%)	1.16	10/5839 (0.2%)
1	B	0.81	1/4322 (0.0%)	1.16	7/5839 (0.1%)
1	C	0.79	0/4322	1.15	10/5839 (0.2%)
1	D	0.78	1/4322 (0.0%)	1.14	8/5839 (0.1%)
All	All	0.80	5/17288 (0.0%)	1.15	35/23356 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	THR	C-O	-6.87	1.18	1.24
1	A	519	LYS	C-O	-6.38	1.16	1.24
1	A	201	TYR	C-O	-5.48	1.17	1.24
1	D	78	VAL	C-O	-5.20	1.18	1.23
1	B	144	ILE	C-O	-5.10	1.18	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	216	HIS	CB-CG-CD2	-7.95	120.86	131.20
1	C	28	ASP	CA-CB-CG	7.18	119.78	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ASP	CA-CB-CG	6.94	119.54	112.60
1	C	104	HIS	CB-CG-CD2	-6.89	122.25	131.20
1	A	216	HIS	CB-CG-CD2	-6.77	122.39	131.20
1	D	276	ASP	CA-CB-CG	6.71	119.31	112.60
1	B	216	HIS	CB-CG-ND1	6.59	132.59	122.70
1	A	147	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	D	233	ASP	CB-CA-C	6.43	120.36	109.75
1	D	335	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	494	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	291	GLU	N-CA-CB	6.00	119.04	110.16
1	D	28	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	494	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	484	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	335	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	171	ASP	CA-CB-CG	5.78	118.38	112.60
1	C	393	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	236	GLU	CB-CA-C	5.68	116.18	109.47
1	C	191	ASP	CA-CB-CG	5.68	118.28	112.60
1	C	248	HIS	CA-CB-CG	5.64	119.44	113.80
1	C	104	HIS	CB-CG-ND1	5.56	131.04	122.70
1	A	375	ASN	CA-CB-CG	5.47	118.07	112.60
1	B	370	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	147	HIS	CB-CG-ND1	5.38	130.77	122.70
1	B	28	ASP	CA-CB-CG	5.26	117.86	112.60
1	D	27	ASP	CA-CB-CG	5.25	117.86	112.60
1	C	123	ASP	CB-CA-C	-5.20	100.31	109.62
1	A	327	ASN	CA-CB-CG	-5.15	107.45	112.60
1	C	123	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	511	GLU	N-CA-CB	5.12	117.64	110.12
1	C	180	HIS	CB-CG-CD2	-5.10	124.57	131.20
1	D	48	PHE	CA-CB-CG	5.03	118.83	113.80
1	B	307	TRP	CA-CB-CG	5.01	123.13	113.60
1	A	276	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	413	ARG	Sidechain
1	C	444	ARG	Sidechain

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	4209	4144	4124	30	0
1	B	4209	4144	4124	28	0
1	C	4209	4144	4124	29	0
1	D	4209	4138	4124	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	379	0	0	5	0
3	B	345	0	0	1	0
3	C	366	0	0	2	0
3	D	328	0	0	3	0
All	All	18258	16570	16496	116	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 (116) 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:C:231:GLN:HE22	1:D:505:ASN:HD21	1.22	0.84
1:C:190:GLN:HE22	1:D:506:SER:H	1.23	0.83
1:A:506:SER:H	1:B:190:GLN:HE22	1.27	0.81
1:A:505:ASN:HD21	1:B:231:GLN:HE22	1.33	0.75
1:D:104:HIS:CE1	1:D:467:ARG:HH22	2.09	0.70
1:A:460:HIS:HD2	1:A:462:LEU:O	1.75	0.68
1:A:104:HIS:CE1	1:A:467:ARG:HH22	2.11	0.68
1:A:104:HIS:HE1	1:A:467:ARG:HH22	1.41	0.66
1:C:135:LYS:HD3	1:C:232:VAL:HG22	1.77	0.66
1:C:460:HIS:HD2	1:C:462:LEU:O	1.78	0.65
1:B:182:HIS:HE1	1:B:200:VAL:H	1.42	0.65
1:B:460:HIS:HD2	1:B:462:LEU:O	1.81	0.64
1:D:460:HIS:HD2	1:D:462:LEU:O	1.79	0.64
1:D:325:TYR:OH	1:D:358:HIS:HE1	1.81	0.64
1:D:104:HIS:HE1	1:D:467:ARG:HH22	1.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:HIS:CE1	1:C:467:ARG:HH22	2.17	0.63
1:D:216:HIS:HD2	1:D:245:THR:OG1	1.81	0.62
1:B:135:LYS:HD2	1:B:232:VAL:HG22	1.82	0.62
1:C:104:HIS:HE1	1:C:467:ARG:HH22	1.49	0.61
1:C:79:CYS:SG	1:C:83:ARG:NE	2.74	0.60
1:B:87:LEU:HD12	1:B:144:ILE:HD11	1.83	0.60
1:B:216:HIS:HD2	1:B:245:THR:OG1	1.84	0.60
1:C:79:CYS:SG	1:C:83:ARG:HD2	2.41	0.60
1:C:190:GLN:NE2	1:D:506:SER:H	1.98	0.60
1:A:325:TYR:OH	1:A:358:HIS:HE1	1.84	0.60
1:C:216:HIS:HD2	1:C:245:THR:OG1	1.85	0.60
1:A:141:LYS:HZ1	1:A:204:ASN:HD21	1.48	0.59
1:A:216:HIS:HD2	1:A:245:THR:OG1	1.84	0.59
1:B:79:CYS:SG	1:B:141:LYS:HE2	2.42	0.59
1:C:79:CYS:SG	1:C:141:LYS:NZ	2.76	0.58
1:B:20:ASN:HD22	1:B:238:PHE:H	1.51	0.58
1:A:141:LYS:NZ	1:A:204:ASN:HD21	2.01	0.58
1:B:79:CYS:SG	1:B:141:LYS:NZ	2.77	0.58
1:D:287:ASP:O	1:D:291:GLU:HG2	2.02	0.58
1:A:464:HIS:HE1	3:A:1031:HOH:O	1.87	0.57
1:D:141:LYS:NZ	1:D:204:ASN:HD21	2.01	0.57
1:D:248:HIS:HD2	1:D:249:GLY:O	1.87	0.57
1:A:79:CYS:SG	1:A:141:LYS:HE2	2.45	0.57
1:A:348:GLU:OE1	1:A:352:GLU:OE2	2.23	0.56
1:A:460:HIS:HE1	3:A:1028:HOH:O	1.88	0.55
1:B:248:HIS:HD2	1:B:249:GLY:O	1.89	0.55
1:A:79:CYS:SG	1:A:141:LYS:NZ	2.80	0.55
1:D:141:LYS:HZ1	1:D:204:ASN:HD21	1.52	0.55
1:A:20:ASN:HD22	1:A:238:PHE:H	1.55	0.54
1:A:288:LYS:HE2	3:A:1033:HOH:O	2.07	0.54
1:B:79:CYS:SG	1:B:141:LYS:CE	2.96	0.54
1:B:79:CYS:SG	1:B:83:ARG:NE	2.81	0.54
1:A:79:CYS:SG	1:A:83:ARG:NE	2.82	0.53
1:A:152:LYS:HE2	3:A:1040:HOH:O	2.08	0.53
1:C:325:TYR:OH	1:C:358:HIS:HE1	1.92	0.53
1:A:79:CYS:SG	1:A:141:LYS:CE	2.98	0.52
1:C:20:ASN:HD22	1:C:238:PHE:H	1.58	0.52
1:C:79:CYS:SG	1:C:141:LYS:HE2	2.50	0.52
1:C:348:GLU:OE1	1:C:352:GLU:OE2	2.27	0.52
1:B:118:LEU:HD12	1:B:145:ILE:HD11	1.92	0.52
1:C:79:CYS:SG	1:C:83:ARG:CD	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ASN:HD22	1:D:238:PHE:H	1.58	0.52
1:A:288:LYS:CE	3:A:1033:HOH:O	2.57	0.52
1:B:141:LYS:HZ1	1:B:204:ASN:HD21	1.59	0.51
1:D:464:HIS:HE1	3:D:990:HOH:O	1.94	0.51
1:C:464:HIS:HE1	3:C:1016:HOH:O	1.94	0.50
1:D:79:CYS:SG	1:D:83:ARG:NE	2.84	0.49
1:B:325:TYR:OH	1:B:358:HIS:HE1	1.96	0.49
1:A:284:PRO:HB3	1:A:288:LYS:HE2	1.95	0.49
1:A:325:TYR:OH	1:A:358:HIS:CE1	2.65	0.49
1:B:182:HIS:CE1	1:B:200:VAL:H	2.26	0.48
1:D:79:CYS:SG	1:D:141:LYS:HE2	2.53	0.48
1:D:87:LEU:HD12	1:D:144:ILE:CD1	2.44	0.48
1:D:170:LYS:HE3	3:D:855:HOH:O	2.13	0.48
1:C:104:HIS:CE1	1:C:111:ARG:H	2.33	0.47
1:D:79:CYS:SG	1:D:141:LYS:NZ	2.88	0.47
1:D:118:LEU:HD12	1:D:145:ILE:HD11	1.96	0.47
1:A:143:HIS:O	1:A:147:HIS:HE1	1.99	0.46
1:B:141:LYS:NZ	1:B:204:ASN:HD21	2.13	0.46
1:D:159:PRO:O	1:D:180:HIS:HE1	1.98	0.46
1:A:87:LEU:HD12	1:A:144:ILE:HD11	1.97	0.46
1:B:325:TYR:OH	1:B:358:HIS:CE1	2.69	0.46
1:C:79:CYS:SG	1:C:141:LYS:CE	3.04	0.46
1:C:74:VAL:HG11	1:C:335:ASP:O	2.15	0.45
1:A:159:PRO:O	1:A:180:HIS:HE1	1.98	0.45
1:C:451:MET:HE2	1:C:460:HIS:CA	2.46	0.45
1:B:464:HIS:HE1	3:B:1003:HOH:O	1.98	0.45
1:D:229:ILE:O	1:D:232:VAL:HG22	2.17	0.45
1:B:27:ASP:O	1:B:247:PRO:HD2	2.17	0.45
1:D:74:VAL:HG11	1:D:335:ASP:O	2.17	0.44
1:C:87:LEU:HD12	1:C:144:ILE:HD11	1.97	0.44
1:D:216:HIS:HE1	1:D:250:PRO:O	2.00	0.44
1:C:325:TYR:OH	1:C:358:HIS:CE1	2.68	0.44
1:D:451:MET:HE2	1:D:459:ASP:C	2.42	0.44
1:C:159:PRO:O	1:C:180:HIS:HE1	2.00	0.43
1:D:87:LEU:HD12	1:D:144:ILE:HD11	2.00	0.43
1:D:327:ASN:HD22	1:D:327:ASN:HA	1.69	0.43
1:C:216:HIS:HE1	1:C:250:PRO:O	2.00	0.43
1:B:77:PRO:HG3	1:B:345:THR:O	2.19	0.43
1:A:505:ASN:ND2	1:B:231:GLN:HE22	2.10	0.43
1:C:210:ASN:HD22	1:C:213:ILE:H	1.67	0.43
1:D:230:ASP:HA	1:D:322:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:LYS:HD2	1:D:507:LYS:HA	1.76	0.41
1:A:138:PHE:C	1:A:138:PHE:CD1	2.98	0.41
1:C:27:ASP:O	1:C:247:PRO:HD2	2.20	0.41
1:D:79:CYS:SG	1:D:141:LYS:CE	3.09	0.41
1:A:170:LYS:HE2	1:A:275:TYR:CE1	2.56	0.41
1:B:454:GLY:HA3	1:B:458:HIS:O	2.21	0.41
1:D:325:TYR:OH	1:D:358:HIS:CE1	2.69	0.41
1:B:325:TYR:CZ	1:B:358:HIS:HE1	2.38	0.41
1:D:221:LYS:NZ	1:D:245:THR:OG1	2.53	0.41
1:B:145:ILE:HD12	1:B:192:PHE:CG	2.56	0.41
1:B:527:PRO:HG2	1:B:534:LYS:HE3	2.02	0.41
1:C:210:ASN:HB3	1:C:213:ILE:HG12	2.03	0.40
1:A:87:LEU:HD12	1:A:144:ILE:CD1	2.51	0.40
1:D:96:LYS:HB2	1:D:122:GLN:HE22	1.87	0.40
1:A:104:HIS:CE1	1:A:111:ARG:H	2.40	0.40
1:B:87:LEU:HD12	1:B:144:ILE:CD1	2.51	0.40
1:C:318:LYS:HE2	1:C:318:LYS:HB2	1.95	0.40
3:C:892:HOH:O	1:D:499:LYS:HE2	2.22	0.40
1:D:464:HIS:HD2	3:D:927:HOH:O	2.04	0.40

There are no symmetry-related clashes.

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	517/519 (100%)	497 (96%)	20 (4%)	0	100	100
1	B	517/519 (100%)	497 (96%)	20 (4%)	0	100	100
1	C	517/519 (100%)	503 (97%)	14 (3%)	0	100	100
1	D	517/519 (100%)	499 (96%)	18 (4%)	0	100	100
All	All	2068/2076 (100%)	1996 (96%)	72 (4%)	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	454/454 (100%)	451 (99%)	3 (1%)	76	57
1	B	454/454 (100%)	454 (100%)	0	100	100
1	C	454/454 (100%)	451 (99%)	3 (1%)	76	57
1	D	454/454 (100%)	449 (99%)	5 (1%)	65	41
All	All	1816/1816 (100%)	1805 (99%)	11 (1%)	78	62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLU
1	A	102	LYS
1	A	327	ASN
1	C	277	ASN
1	C	318	LYS
1	C	413	ARG
1	D	143	HIS
1	D	287	ASP
1	D	291	GLU
1	D	327	ASN
1	D	507	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	35	ASN
1	A	104	HIS
1	A	122	GLN
1	A	147	HIS
1	A	151	HIS

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Mol	Chain	Res	Type
1	A	156	GLN
1	A	180	HIS
1	A	190	GLN
1	A	204	ASN
1	A	210	ASN
1	A	216	HIS
1	A	231	GLN
1	A	277	ASN
1	A	327	ASN
1	A	358	HIS
1	A	460	HIS
1	A	464	HIS
1	A	470	HIS
1	A	487	GLN
1	A	503	ASN
1	B	20	ASN
1	B	38	HIS
1	B	65	ASN
1	B	122	GLN
1	B	182	HIS
1	B	190	GLN
1	B	204	ASN
1	B	210	ASN
1	B	216	HIS
1	B	231	GLN
1	B	248	HIS
1	B	358	HIS
1	B	361	ASN
1	B	460	HIS
1	B	464	HIS
1	B	487	GLN
1	B	533	ASN
1	C	16	ASN
1	C	20	ASN
1	C	38	HIS
1	C	65	ASN
1	C	104	HIS
1	C	156	GLN
1	C	180	HIS
1	C	190	GLN
1	C	204	ASN
1	C	210	ASN

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Mol	Chain	Res	Type
1	C	216	HIS
1	C	231	GLN
1	C	277	ASN
1	C	338	ASN
1	C	358	HIS
1	C	460	HIS
1	C	464	HIS
1	C	487	GLN
1	D	20	ASN
1	D	65	ASN
1	D	104	HIS
1	D	122	GLN
1	D	180	HIS
1	D	204	ASN
1	D	210	ASN
1	D	216	HIS
1	D	248	HIS
1	D	327	ASN
1	D	358	HIS
1	D	460	HIS
1	D	464	HIS
1	D	470	HIS
1	D	487	GLN
1	D	533	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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	519/519 (100%)	-0.21	8 (1%) 72 75	11, 19, 41, 62	0
1	B	519/519 (100%)	-0.10	9 (1%) 69 72	11, 20, 43, 60	0
1	C	519/519 (100%)	-0.17	6 (1%) 76 80	11, 20, 41, 62	0
1	D	519/519 (100%)	-0.03	11 (2%) 63 67	12, 21, 45, 70	0
All	All	2076/2076 (100%)	-0.13	34 (1%) 70 74	11, 20, 43, 70	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	534	LYS	5.1
1	D	17	LYS	3.6
1	B	145	ILE	3.5
1	C	79	CYS	3.3
1	B	448	SER	3.2
1	D	276	ASP	3.0
1	C	277	ASN	3.0
1	D	79	CYS	3.0
1	D	16	ASN	2.9
1	A	79	CYS	2.8
1	A	231	GLN	2.8
1	B	450	LYS	2.8
1	D	455	TYR	2.8
1	D	327	ASN	2.7
1	B	79	CYS	2.6
1	A	235	GLU	2.5
1	A	16	ASN	2.5
1	C	444	ARG	2.5
1	D	391	VAL	2.5
1	B	449	GLY	2.4
1	C	391	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	172	PRO	2.4
1	D	390	LYS	2.3
1	A	449	GLY	2.3
1	C	390	LYS	2.3
1	A	277	ASN	2.2
1	B	16	ASN	2.2
1	A	200	VAL	2.2
1	A	444	ARG	2.2
1	D	445	ILE	2.1
1	D	389	THR	2.1
1	D	393	ASP	2.1
1	B	279	ASP	2.1
1	C	451	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

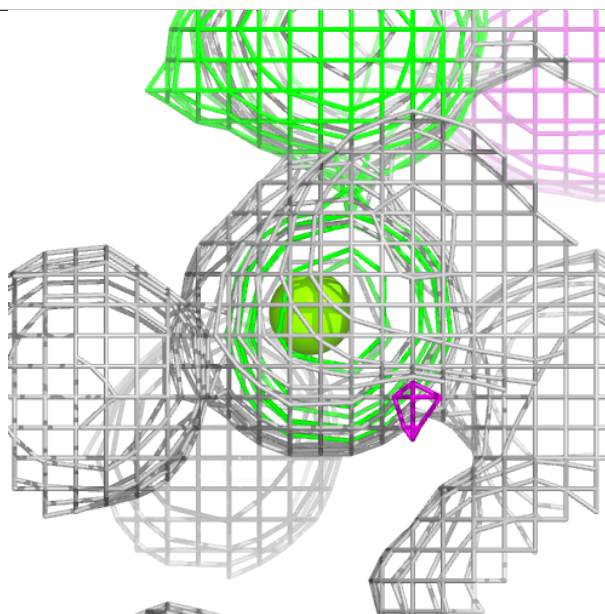
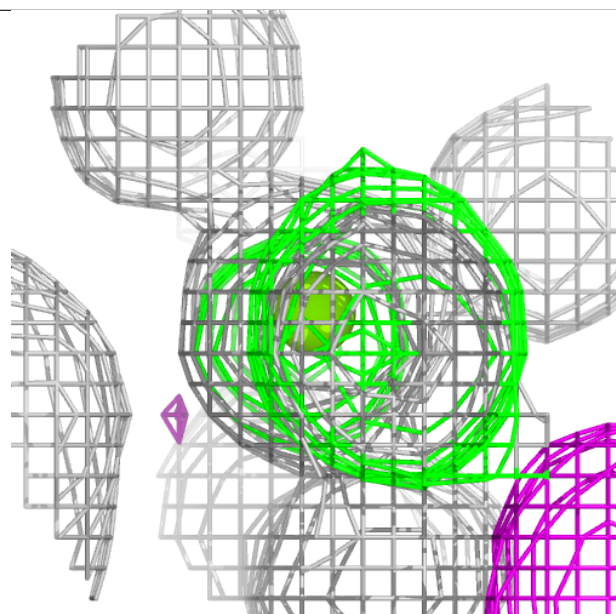
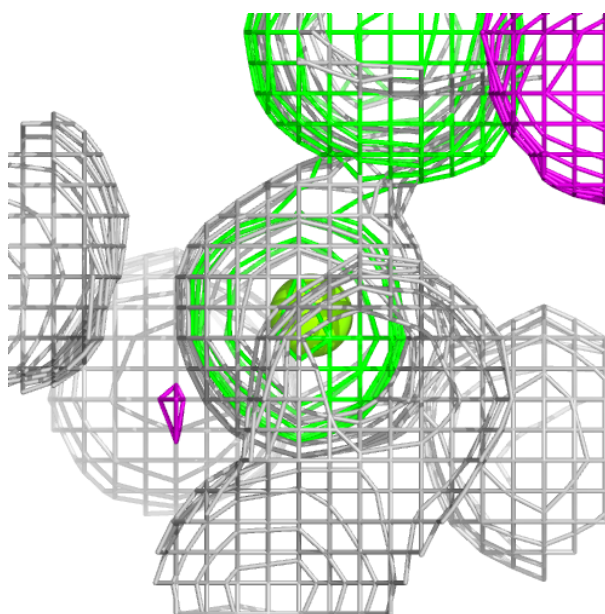
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	601	1/1	0.95	0.22	30,30,30,30	0
2	MG	B	601	1/1	0.99	0.02	15,15,15,15	0
2	MG	D	601	1/1	0.99	0.17	30,30,30,30	0
2	MG	C	601	1/1	1.00	0.01	14,14,14,14	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.

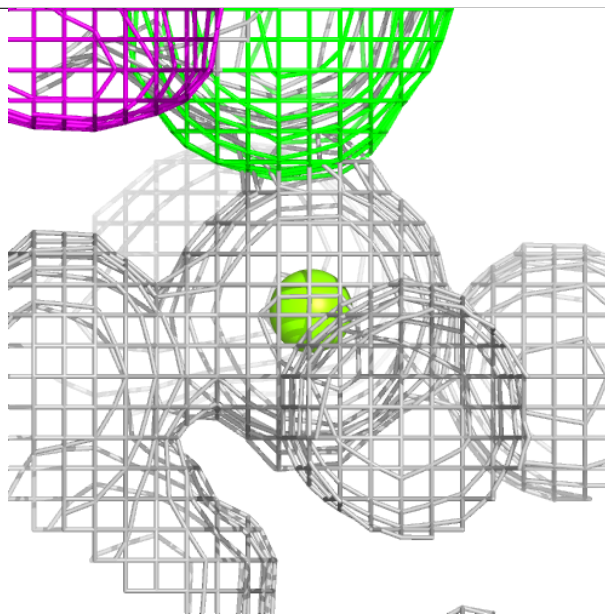
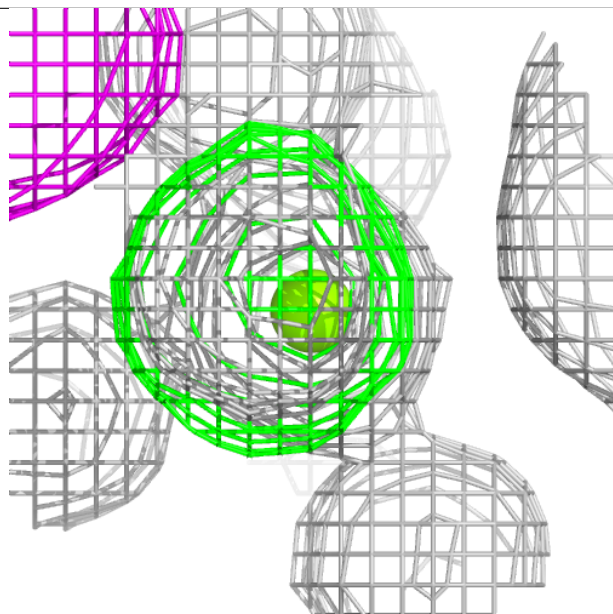
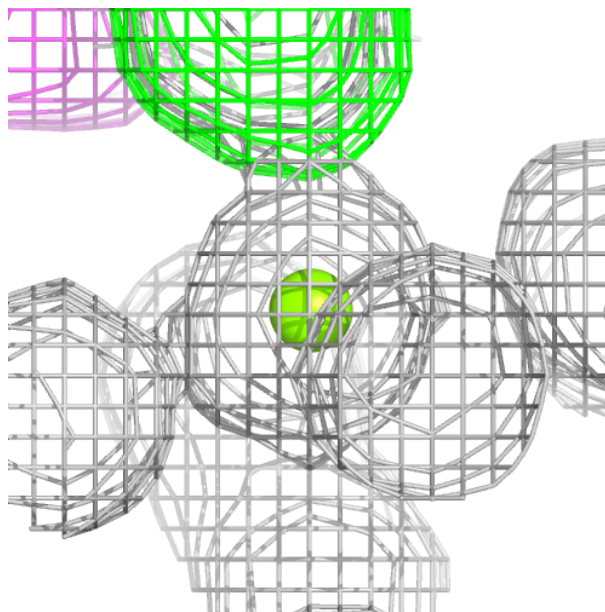
Electron density around MG A 601:

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



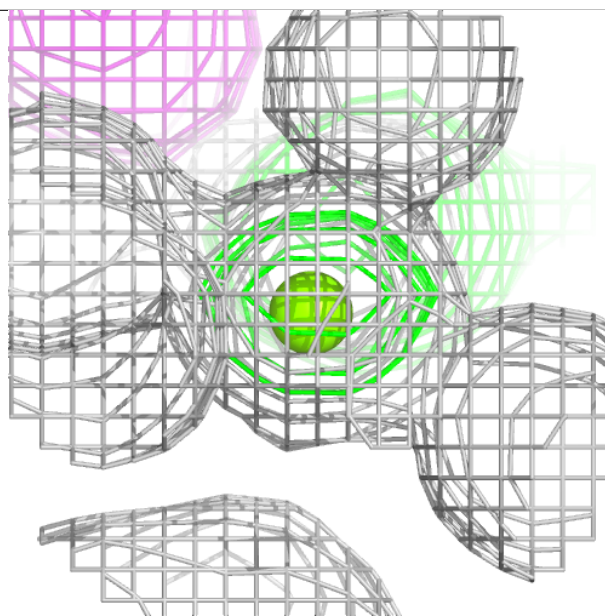
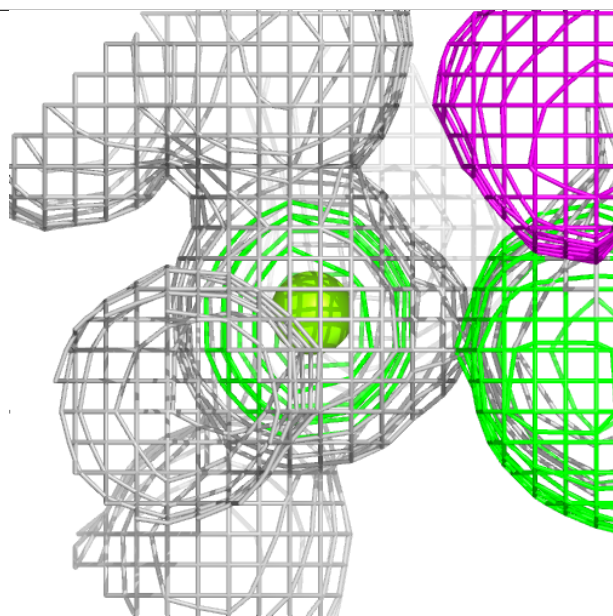
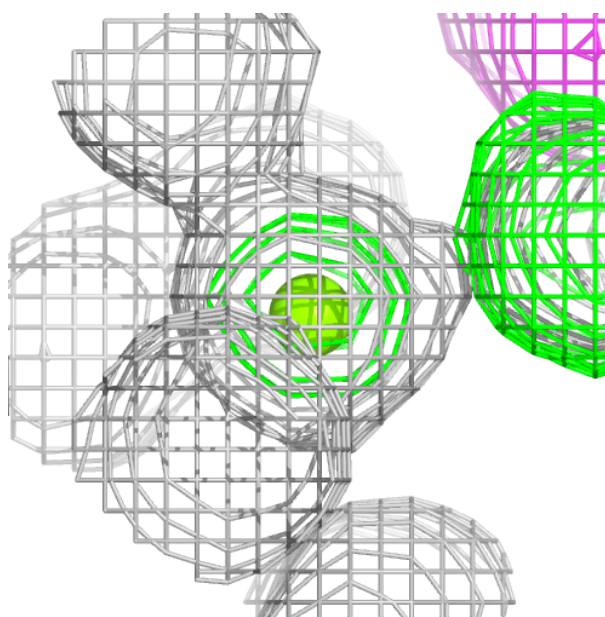
Electron density around MG B 601:

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and green (positive)



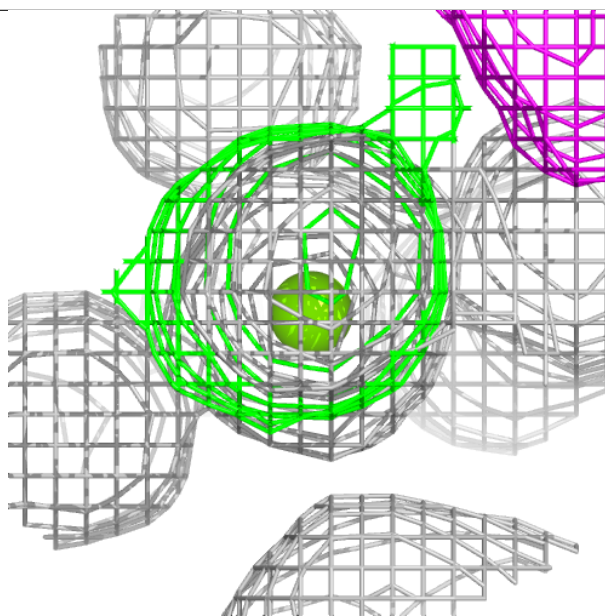
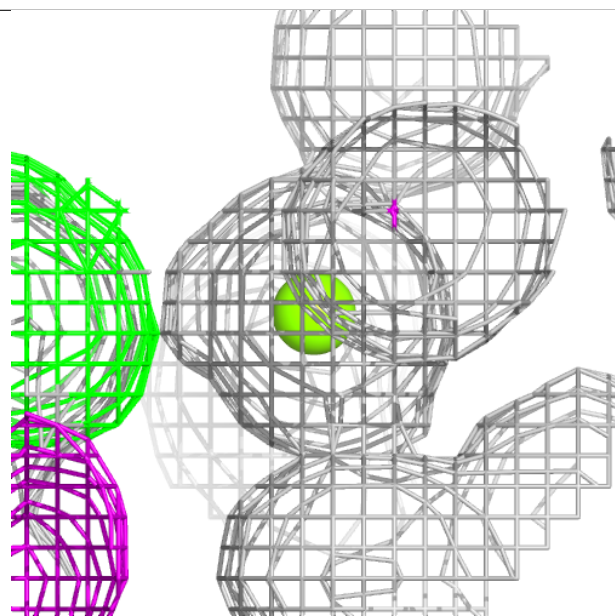
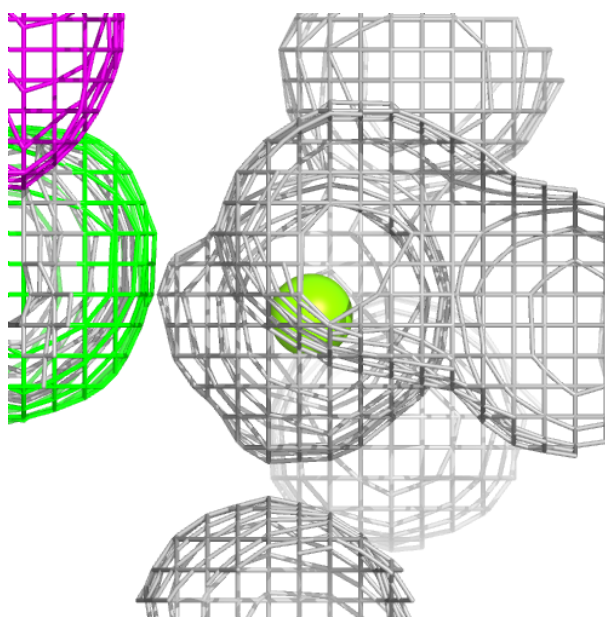
Electron density around MG D 601:

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



Electron density around MG C 601:

$2mF_o-DF_c$ (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.