



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:35 PM UTC

PDB ID : 6VD2 / pdb_00006vd2
Title : Crystal structure of Arabidopsis thaliana S-adenosylmethionine Synthase 2 (AtMAT2) in complex with S-adenosylmethionine
Authors : Sekula, B.; Ruszkowski, M.; Dauter, Z.
Deposited on : 2019-12-23
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

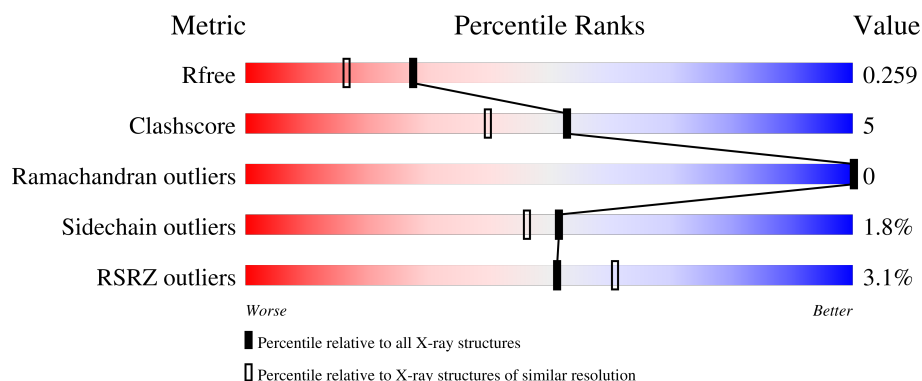
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

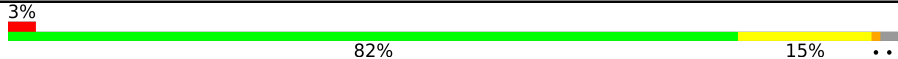
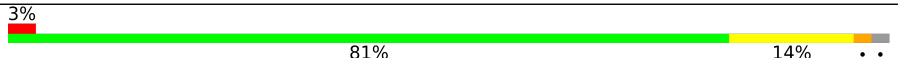
The reported resolution of this entry is 1.97 Å.

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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	402	
1	B	402	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6882 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.

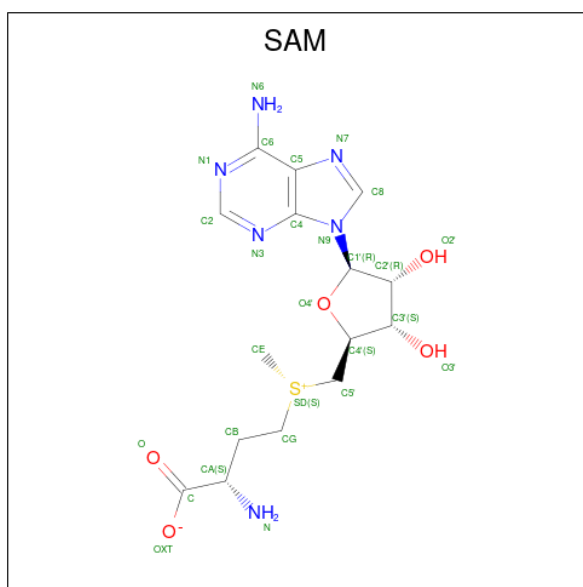
- Molecule 1 is a protein called S-adenosylmethionine synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	2	0
			3063	1931	530	586	16			
1	B	392	Total	C	N	O	S	0	2	0
			3043	1919	526	582	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P17562
A	-1	ASN	-	expression tag	UNP P17562
A	0	ALA	-	expression tag	UNP P17562
A	393	LEU	-	expression tag	UNP P17562
A	394	ASN	-	expression tag	UNP P17562
A	395	ASN	-	expression tag	UNP P17562
A	396	ILE	-	expression tag	UNP P17562
A	397	GLY	-	expression tag	UNP P17562
A	398	SER	-	expression tag	UNP P17562
A	399	GLY	-	expression tag	UNP P17562
B	-2	SER	-	expression tag	UNP P17562
B	-1	ASN	-	expression tag	UNP P17562
B	0	ALA	-	expression tag	UNP P17562
B	393	LEU	-	expression tag	UNP P17562
B	394	ASN	-	expression tag	UNP P17562
B	395	ASN	-	expression tag	UNP P17562
B	396	ILE	-	expression tag	UNP P17562
B	397	GLY	-	expression tag	UNP P17562
B	398	SER	-	expression tag	UNP P17562
B	399	GLY	-	expression tag	UNP P17562

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

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

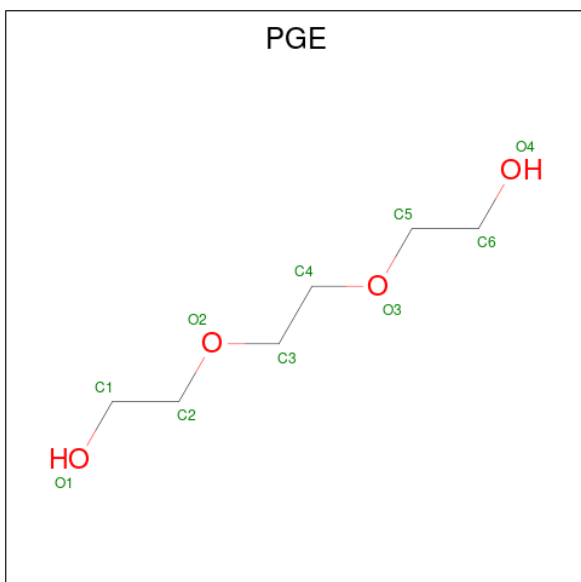
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



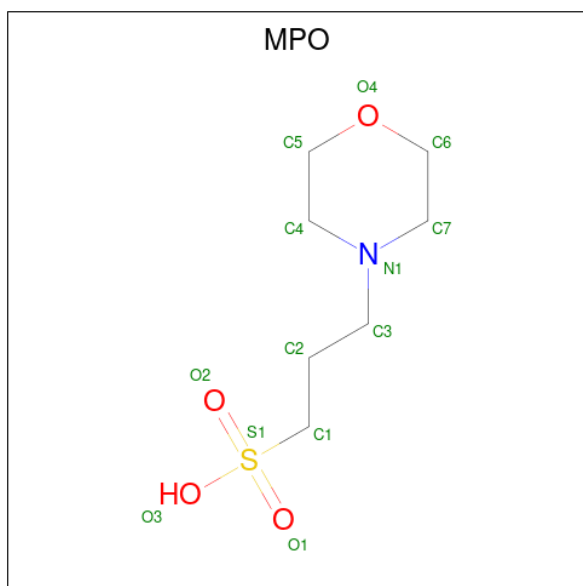
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



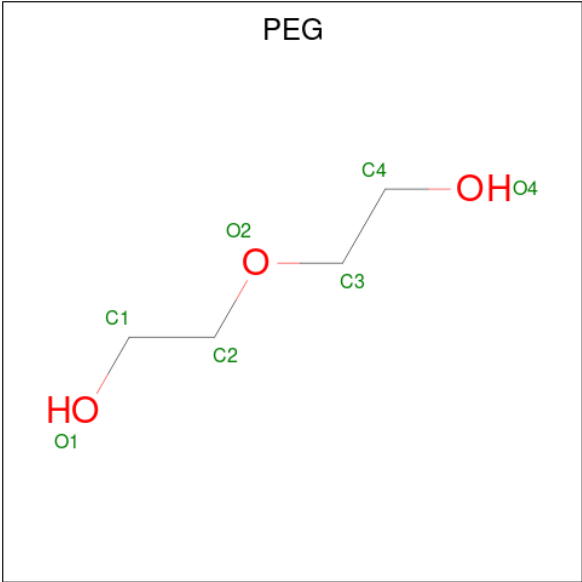
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



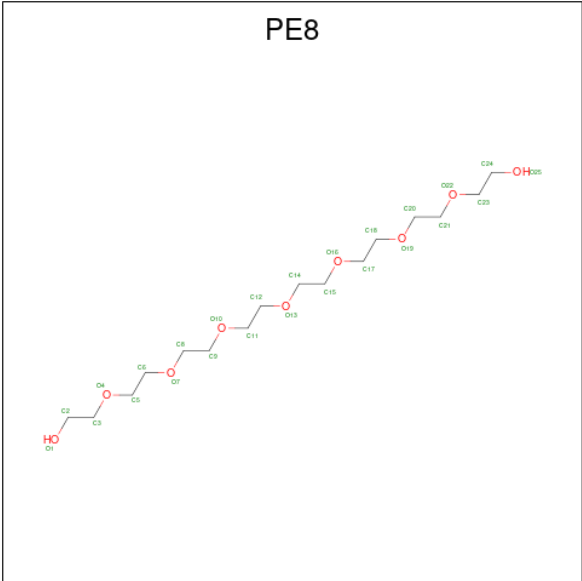
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

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



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

- Molecule 9 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			25	16	9		

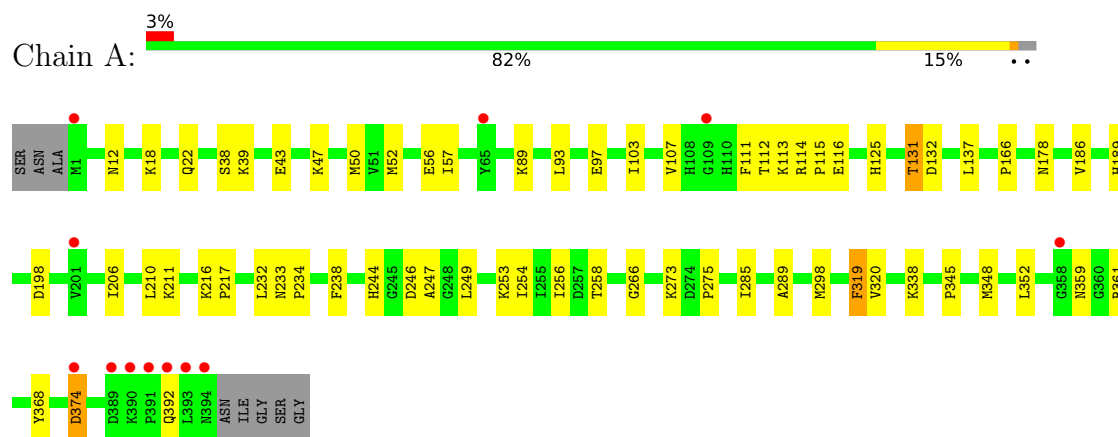
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	302	Total 302	O 302	0	0
10	B	314	Total 314	O 314	0	0

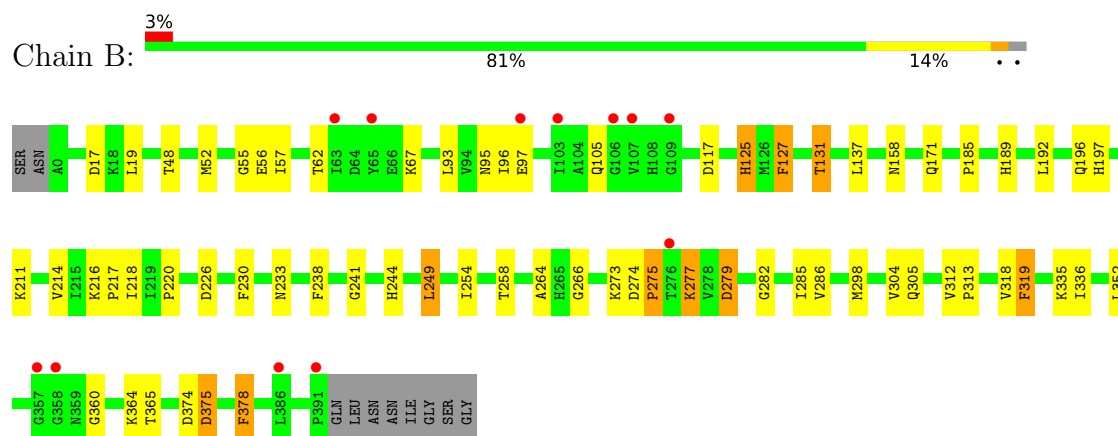
3 Residue-property plots [i](#)

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: S-adenosylmethionine synthase 2



• Molecule 1: S-adenosylmethionine synthase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.98Å 101.35Å 84.71Å 90.00° 99.80° 90.00°	Depositor
Resolution (Å)	45.72 – 1.97 45.72 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.72-1.97) 98.0 (45.72-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.191 , 0.240 0.208 , 0.259	Depositor DCC
R_{free} test set	1075 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6882	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.58% 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: K, MPO, PO4, MG, PGE, PEG, SAM, PE8

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	1.30	10/3134 (0.3%)	1.51	15/4246 (0.4%)
1	B	1.30	11/3114 (0.4%)	1.53	22/4219 (0.5%)
All	All	1.30	21/6248 (0.3%)	1.52	37/8465 (0.4%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	THR	CA-C	7.36	1.55	1.52
1	B	125	HIS	C-O	7.11	1.32	1.23
1	A	273	LYS	C-O	6.77	1.32	1.24
1	A	189	HIS	CE1-NE2	6.65	1.39	1.32
1	A	38	SER	C-O	6.51	1.31	1.23
1	B	249	LEU	C-O	6.39	1.31	1.23
1	A	210	LEU	C-O	6.36	1.31	1.24
1	A	361	ARG	C-O	6.19	1.31	1.24
1	B	378	PHE	C-O	6.16	1.32	1.23
1	A	320	VAL	C-O	6.15	1.30	1.24
1	B	55	GLY	C-O	-6.09	1.19	1.24
1	B	95	ASN	C-O	5.66	1.30	1.23
1	B	241	GLY	C-O	5.61	1.29	1.23
1	B	279	ASP	C-O	5.44	1.30	1.24
1	A	289	ALA	C-O	5.42	1.30	1.24
1	B	125	HIS	CE1-NE2	5.34	1.37	1.32
1	A	232	LEU	C-O	-5.22	1.18	1.24
1	B	189	HIS	CE1-NE2	5.18	1.37	1.32
1	B	185	PRO	C-O	-5.13	1.18	1.23
1	A	12	ASN	C-O	5.03	1.30	1.23
1	B	17	ASP	C-O	5.03	1.30	1.24

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ILE	N-CA-C	-11.17	102.80	111.62
1	B	258	THR	CA-C-O	-9.16	114.55	119.77
1	B	304	VAL	CA-C-O	-8.04	112.15	120.27
1	B	375	ASP	CB-CA-C	6.65	119.67	109.50
1	A	246	ASP	CA-CB-CG	6.47	119.07	112.60
1	B	233	ASN	CB-CA-C	6.42	116.59	111.00
1	B	230	PHE	CA-C-O	-6.38	113.48	120.24
1	A	233	ASN	CB-CA-C	6.32	115.69	111.20
1	A	234	PRO	CB-CA-C	-6.07	103.23	111.85
1	B	62	THR	CA-CB-OG1	-6.04	100.53	109.60
1	A	275	PRO	N-CA-C	6.04	120.96	114.68
1	B	214	VAL	CA-C-O	-5.96	115.63	120.70
1	B	226	ASP	CA-CB-CG	5.86	118.46	112.60
1	B	127	PHE	CA-C-N	5.84	126.59	122.33
1	B	127	PHE	C-N-CA	5.84	126.59	122.33
1	A	113	LYS	CA-C-N	5.77	129.46	120.68
1	A	113	LYS	C-N-CA	5.77	129.46	120.68
1	A	186	VAL	N-CA-C	-5.61	106.20	111.48
1	B	275	PRO	N-CA-C	5.58	120.89	114.03
1	A	132	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	277	LYS	CB-CA-C	5.41	120.19	111.05
1	B	105	GLN	CA-C-N	5.35	125.89	120.00
1	B	105	GLN	C-N-CA	5.35	125.89	120.00
1	A	244	HIS	N-CA-C	-5.35	105.45	111.28
1	B	258	THR	O-C-N	5.26	124.72	120.83
1	A	166	PRO	N-CA-C	5.25	120.74	113.65
1	B	117	ASP	N-CA-C	-5.20	106.34	113.30
1	A	112	THR	N-CA-CB	5.19	117.88	110.67
1	A	43	GLU	CB-CG-CD	5.18	121.40	112.60
1	A	234	PRO	N-CA-C	5.17	120.56	113.84
1	A	238	PHE	CB-CA-C	5.08	119.82	111.74
1	B	220	PRO	CA-C-N	5.08	127.40	120.54
1	B	220	PRO	C-N-CA	5.08	127.40	120.54
1	B	19	LEU	CA-C-N	5.08	127.39	120.54
1	B	19	LEU	C-N-CA	5.08	127.39	120.54
1	A	22	GLN	CA-C-O	-5.07	115.05	120.42
1	B	244	HIS	CB-CA-C	5.04	119.15	110.79

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	3063	0	3032	30	0
1	B	3043	0	3012	35	0
2	A	27	0	22	0	0
2	B	27	0	22	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	10	0	0	0	0
5	B	15	0	0	0	0
6	A	10	0	14	1	0
7	A	13	0	15	2	0
7	B	13	0	14	0	0
8	A	7	0	10	2	0
8	B	7	0	10	0	0
9	A	25	0	34	1	0
10	A	302	0	0	5	0
10	B	314	0	0	3	0
All	All	6882	0	6185	62	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 5.

All (62) 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:97:GLU:OE1	1:B:48:THR:HB	1.80	0.82
1:A:97:GLU:OE1	1:B:48:THR:CB	2.45	0.64
1:B:56:GLU:HA	1:B:97:GLU:O	1.97	0.63
1:A:285[B]:ILE:HG12	1:A:352:LEU:HD11	1.85	0.58
1:B:274:ASP:HB2	1:B:275:PRO:HD2	1.85	0.58
1:A:125:HIS:CE1	1:A:266:GLY:HA2	2.42	0.55
1:B:282:GLY:O	1:B:286:VAL:HG22	2.06	0.55
1:A:178:ASN:ND2	9:A:411:PE8:H172	2.22	0.55
1:B:67:LYS:NZ	10:B:508:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HD2	1:A:256:ILE:HD12	1.90	0.54
1:A:216:LYS:N	1:A:217:PRO:CD	2.73	0.52
1:A:56:GLU:HA	1:A:97:GLU:O	2.11	0.51
1:B:374:ASP:OD1	1:B:374:ASP:N	2.44	0.51
1:A:131:THR:O	1:A:137:LEU:HA	2.10	0.51
1:A:111:PHE:O	7:A:409:MPO:H22	2.10	0.51
1:A:47:LYS:HD3	1:A:247:ALA:HB2	1.93	0.50
8:A:410:PEG:H12	10:A:568:HOH:O	2.10	0.50
1:A:368:TYR:CD2	6:A:408:PGE:H52	2.47	0.50
1:B:57:ILE:HD12	1:B:96:ILE:HG21	1.95	0.49
1:B:365:THR:HG22	1:B:378:PHE:CE2	2.48	0.49
1:B:131:THR:O	1:B:137:LEU:HA	2.13	0.49
1:A:211:LYS:NZ	10:A:515:HOH:O	2.45	0.49
1:B:285[A]:ILE:CD1	1:B:352:LEU:HD11	2.43	0.48
1:B:364:LYS:NZ	1:B:375:ASP:OD2	2.37	0.48
1:A:345:PRO:HA	1:A:348:MET:HE2	1.96	0.47
1:A:39:LYS:O	1:A:57:ILE:HA	2.15	0.47
1:B:171:GLN:HB3	1:B:192:LEU:HD23	1.96	0.46
1:A:254:ILE:HD11	1:B:254:ILE:HD11	1.97	0.46
1:A:125:HIS:O	1:A:266:GLY:HA3	2.16	0.46
1:B:298:MET:HE1	1:B:336:ILE:HD13	1.98	0.46
1:A:359:ASN:CB	10:A:671:HOH:O	2.64	0.46
8:A:410:PEG:C1	10:A:568:HOH:O	2.64	0.45
1:A:114:ARG:O	1:A:115:PRO:C	2.59	0.45
1:A:374:ASP:OD1	1:A:374:ASP:N	2.38	0.45
1:A:206:ILE:HD13	1:A:206:ILE:HG21	1.75	0.45
1:B:125:HIS:O	1:B:266:GLY:HA3	2.17	0.45
1:B:197:HIS:HE2	1:B:238:PHE:H	1.64	0.45
1:A:50:MET:HE1	1:B:52:MET:HE1	1.99	0.45
1:B:375:ASP:N	10:B:524:HOH:O	2.50	0.44
1:A:103:ILE:O	1:A:107:VAL:HG23	2.17	0.44
1:B:211:LYS:HE3	10:B:696:HOH:O	2.16	0.44
1:B:158:ASN:C	1:B:158:ASN:OD1	2.59	0.44
1:B:285[A]:ILE:HD13	1:B:352:LEU:HD11	1.99	0.44
1:B:305:GLN:HB2	1:B:319[B]:PHE:CE2	2.53	0.43
1:B:312:VAL:HA	1:B:313:PRO:HD3	1.92	0.43
1:A:285[A]:ILE:HD12	1:A:285[A]:ILE:HA	1.78	0.42
1:B:127:PHE:CG	1:B:264:ALA:HB3	2.54	0.42
1:B:360:GLY:O	1:B:364:LYS:HD3	2.19	0.42
1:B:273:LYS:NZ	1:B:279:ASP:OD2	2.52	0.42
1:B:216:LYS:N	1:B:217:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:MET:HG3	1:B:93:LEU:HB2	2.01	0.42
1:A:249:LEU:HB3	1:B:249:LEU:HD23	2.02	0.41
1:A:198:ASP:OD1	1:A:198:ASP:C	2.62	0.41
1:B:196:GLN:HA	1:B:238:PHE:O	2.21	0.41
1:B:305:GLN:O	1:B:318:VAL:HA	2.20	0.41
1:A:52:MET:HA	1:A:93:LEU:O	2.21	0.41
1:A:111:PHE:HA	7:A:409:MPO:O3	2.20	0.41
1:B:125:HIS:CE1	1:B:266:GLY:HA2	2.56	0.41
1:B:375:ASP:HB3	1:B:378:PHE:CD1	2.56	0.40
1:A:359:ASN:HB2	10:A:671:HOH:O	2.21	0.40
1:B:274:ASP:O	1:B:277:LYS:HB2	2.20	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	394/402 (98%)	383 (97%)	11 (3%)	0	100	100
1	B	392/402 (98%)	379 (97%)	13 (3%)	0	100	100
All	All	786/804 (98%)	762 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/337 (99%)	324 (97%)	10 (3%)	36	27
1	B	331/337 (98%)	327 (99%)	4 (1%)	63	58
All	All	665/674 (99%)	651 (98%)	14 (2%)	51	40

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	89	LYS
1	A	116	GLU
1	A	131	THR
1	A	298	MET
1	A	319[A]	PHE
1	A	319[B]	PHE
1	A	338	LYS
1	A	374	ASP
1	A	392	GLN
1	B	131	THR
1	B	319[A]	PHE
1	B	319[B]	PHE
1	B	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	B	288	GLN
1	B	363	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 6 are monoatomic - leaving 13 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
2	SAM	B	401	-	27,29,29	0.51	0	34,42,42	1.05	2 (5%)
5	PO4	B	406	-	4,4,4	0.83	0	6,6,6	0.50	0
7	MPO	A	409	-	13,13,13	0.91	1 (7%)	17,17,17	1.24	2 (11%)
8	PEG	B	408	-	6,6,6	0.28	0	5,5,5	0.16	0
7	MPO	B	407	-	13,13,13	0.87	1 (7%)	17,17,17	1.13	2 (11%)
5	PO4	B	404	3	4,4,4	0.51	0	6,6,6	0.48	0
9	PE8	A	411	-	24,24,24	0.33	0	23,23,23	0.17	0
6	PGE	A	408	-	9,9,9	0.34	0	8,8,8	0.20	0
5	PO4	A	405	3	4,4,4	1.25	1 (25%)	6,6,6	0.59	0
2	SAM	A	401	-	27,29,29	0.55	0	34,42,42	1.15	1 (2%)
8	PEG	A	410	-	6,6,6	0.29	0	5,5,5	0.30	0
5	PO4	B	405	3	4,4,4	0.72	0	6,6,6	0.55	0
5	PO4	A	406	3	4,4,4	1.31	1 (25%)	6,6,6	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAM	B	401	-	-	5/17/33/33	0/3/3/3
7	MPO	A	409	-	-	5/7/15/15	0/1/1/1
8	PEG	B	408	-	-	1/4/4/4	-
7	MPO	B	407	-	-	5/7/15/15	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PE8	A	411	-	-	9/22/22/22	-
6	PGE	A	408	-	-	5/7/7/7	-
2	SAM	A	401	-	-	5/17/33/33	0/3/3/3
8	PEG	A	410	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	407	MPO	O2-S1	2.94	1.53	1.45
5	A	406	PO4	P-O3	-2.56	1.47	1.54
7	A	409	MPO	O3-S1	2.49	1.56	1.47
5	A	405	PO4	P-O4	-2.32	1.47	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAM	CG-SD-C5'	-5.50	89.99	103.43
2	B	401	SAM	CG-SD-C5'	-5.40	90.24	103.43
7	B	407	MPO	O2-S1-C1	-3.12	102.01	106.73
7	A	409	MPO	C3-N1-C7	2.85	118.83	111.24
7	A	409	MPO	C3-N1-C4	2.70	118.42	111.24
7	B	407	MPO	O3-S1-O1	2.62	117.96	111.40
2	B	401	SAM	C2'-C3'-C4'	-2.04	98.67	102.61

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	MPO	C2-C1-S1-O1
7	A	409	MPO	C2-C1-S1-O2
7	A	409	MPO	C1-C2-C3-N1
7	B	407	MPO	C2-C1-S1-O2
7	B	407	MPO	C1-C2-C3-N1
9	A	411	PE8	O4-C5-C6-O7
7	A	409	MPO	C2-C1-S1-O3
9	A	411	PE8	O7-C8-C9-O10
9	A	411	PE8	O10-C11-C12-O13
7	B	407	MPO	C2-C3-N1-C4
7	B	407	MPO	C2-C3-N1-C7
9	A	411	PE8	O19-C20-C21-O22

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Mol	Chain	Res	Type	Atoms
2	A	401	SAM	O-C-CA-CB
7	B	407	MPO	C2-C1-S1-O3
2	A	401	SAM	OXT-C-CA-CB
6	A	408	PGE	O1-C1-C2-O2
2	A	401	SAM	C2'-C1'-N9-C8
6	A	408	PGE	C6-C5-O3-C4
2	B	401	SAM	O-C-CA-CB
2	B	401	SAM	OXT-C-CA-CB
9	A	411	PE8	C8-C9-O10-C11
9	A	411	PE8	C20-C21-O22-C23
8	A	410	PEG	C1-C2-O2-C3
9	A	411	PE8	C14-C15-O16-C17
2	B	401	SAM	C2'-C1'-N9-C8
6	A	408	PGE	C4-C3-O2-C2
7	A	409	MPO	C2-C3-N1-C4
9	A	411	PE8	C21-C20-O19-C18
2	B	401	SAM	O4'-C1'-N9-C8
2	A	401	SAM	OXT-C-CA-N
2	A	401	SAM	O4'-C1'-N9-C8
8	A	410	PEG	C4-C3-O2-C2
6	A	408	PGE	O3-C5-C6-O4
8	B	408	PEG	O2-C3-C4-O4
6	A	408	PGE	O2-C3-C4-O3
9	A	411	PE8	O16-C17-C18-O19
8	A	410	PEG	O2-C3-C4-O4
2	B	401	SAM	OXT-C-CA-N

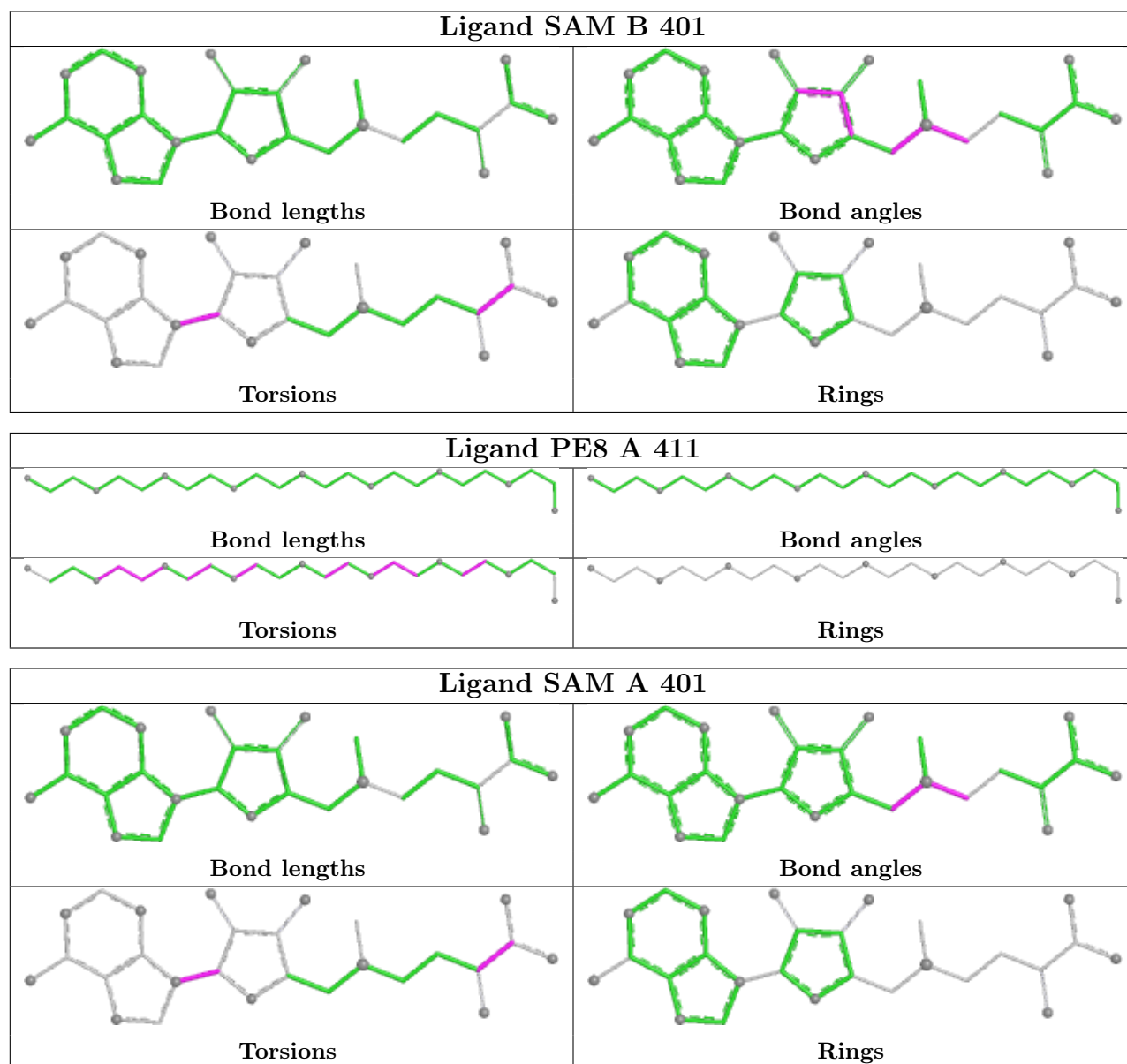
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	409	MPO	2	0
9	A	411	PE8	1	0
6	A	408	PGE	1	0
8	A	410	PEG	2	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 than 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.



5.7 Other polymers [i](#)

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	394/402 (98%)	0.48	12 (3%)	52	62	18, 36, 55, 84	2 (0%)
1	B	392/402 (97%)	0.45	12 (3%)	51	61	17, 35, 53, 84	2 (0%)
All	All	786/804 (97%)	0.47	24 (3%)	51	61	17, 36, 54, 84	4 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	PRO	4.3
1	A	393	LEU	3.5
1	B	107	VAL	3.1
1	B	358	GLY	3.1
1	B	106	GLY	3.0
1	B	357	GLY	3.0
1	A	1	MET	3.0
1	A	392	GLN	2.9
1	A	109	GLY	2.8
1	B	386	LEU	2.8
1	B	103	ILE	2.8
1	B	65	TYR	2.7
1	A	358	GLY	2.5
1	A	389	ASP	2.5
1	A	65	TYR	2.4
1	B	391	PRO	2.4
1	A	390	LYS	2.3
1	B	109	GLY	2.3
1	A	394	ASN	2.2
1	B	97	GLU	2.2
1	B	63	ILE	2.2
1	A	374	ASP	2.1
1	B	276	THR	2.0
1	A	201	VAL	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](#)

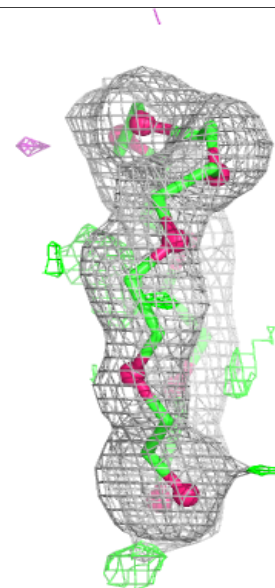
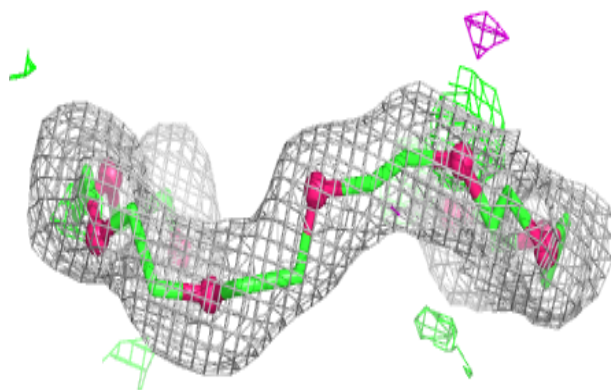
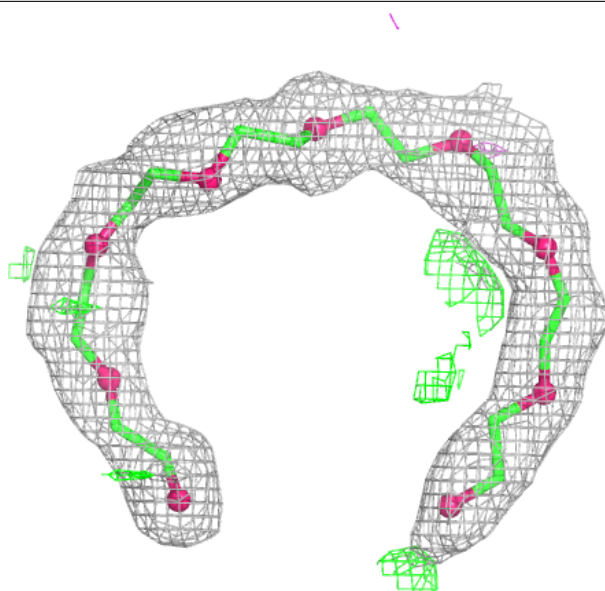
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	MPO	B	407	13/13	0.81	0.24	34,40,48,51	13
8	PEG	B	408	7/7	0.81	0.18	51,58,59,62	0
5	PO4	B	406	5/5	0.82	0.20	40,43,47,47	5
6	PGE	A	408	10/10	0.84	0.19	53,68,69,69	0
9	PE8	A	411	25/25	0.87	0.15	51,64,67,69	0
7	MPO	A	409	13/13	0.88	0.15	42,47,56,61	0
8	PEG	A	410	7/7	0.89	0.15	53,59,66,66	0
2	SAM	A	401	27/27	0.91	0.11	27,37,50,54	0
2	SAM	B	401	27/27	0.94	0.10	29,35,48,51	0
5	PO4	A	405	5/5	0.96	0.07	32,36,42,44	0
5	PO4	A	406	5/5	0.96	0.07	30,30,35,36	0
4	K	A	404	1/1	0.96	0.11	46,46,46,46	0
5	PO4	B	405	5/5	0.97	0.07	30,31,37,39	0
3	MG	A	402	1/1	0.97	0.04	30,30,30,30	0
4	K	B	403	1/1	0.98	0.07	40,40,40,40	0
3	MG	B	402	1/1	0.98	0.03	30,30,30,30	0
3	MG	A	403	1/1	0.98	0.03	36,36,36,36	0
5	PO4	B	404	5/5	0.98	0.05	27,28,29,31	0
3	MG	A	407	1/1	0.99	0.04	32,32,32,32	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.

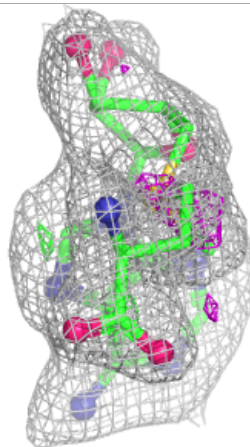
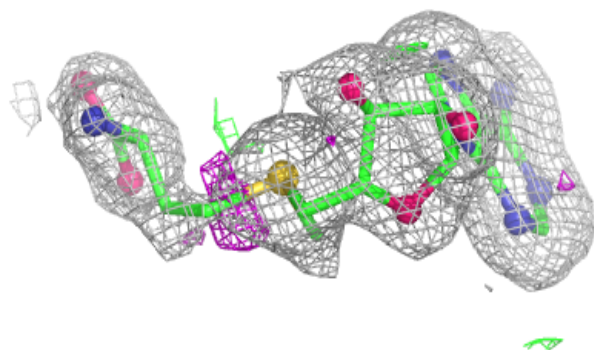
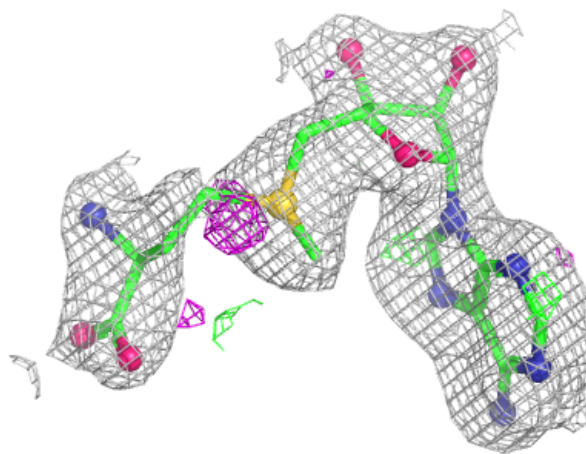
Electron density around PE8 A 411:

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



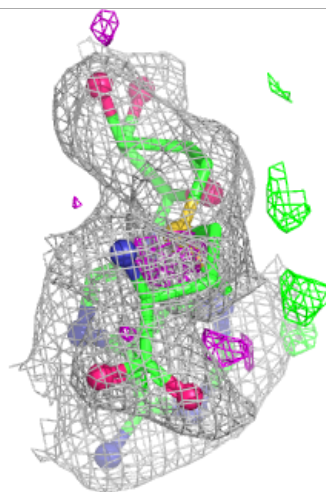
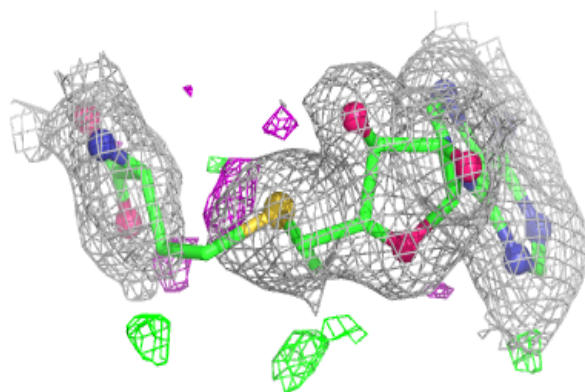
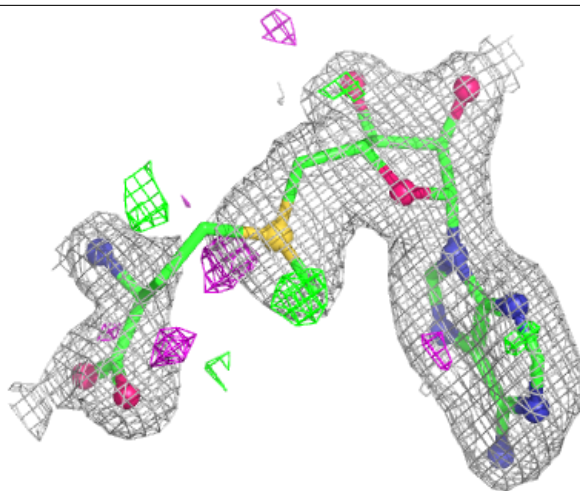
Electron density around SAM A 401:

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and green (positive)



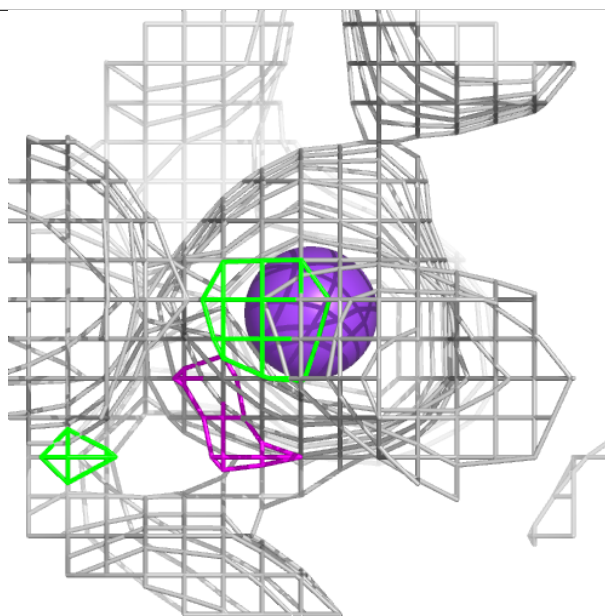
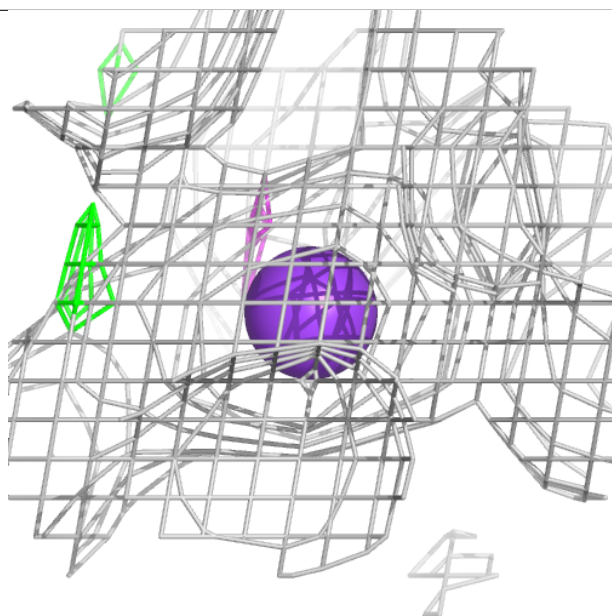
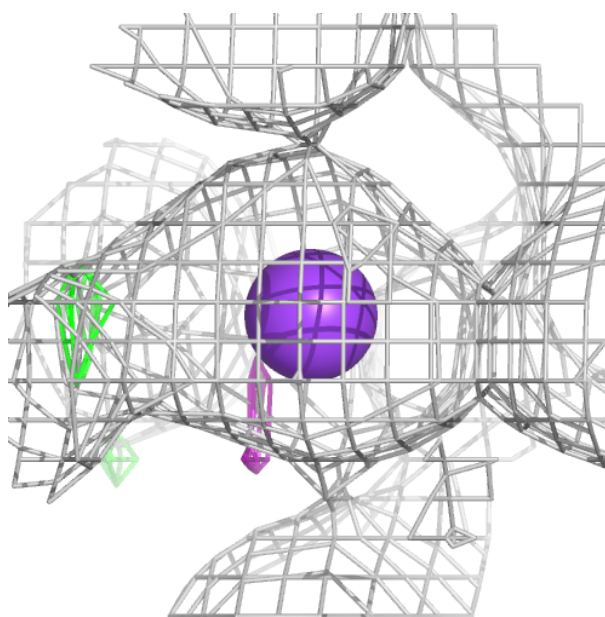
Electron density around SAM B 401:

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and green (positive)



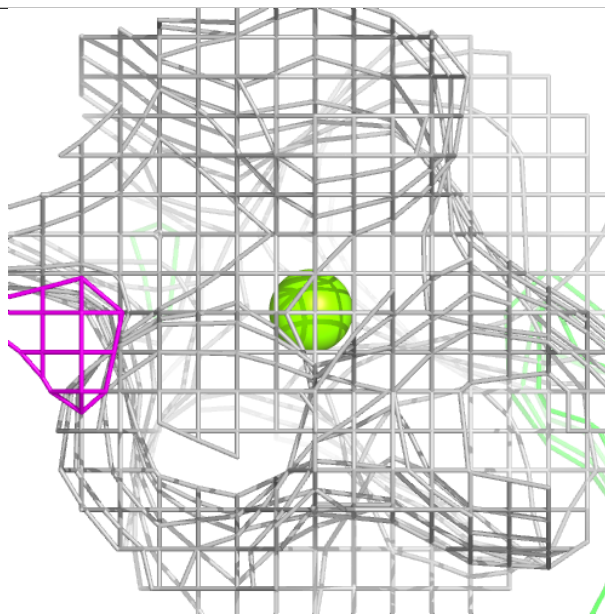
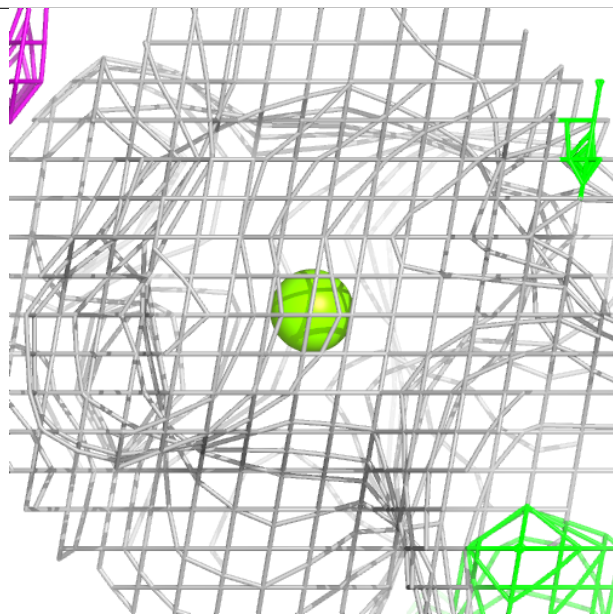
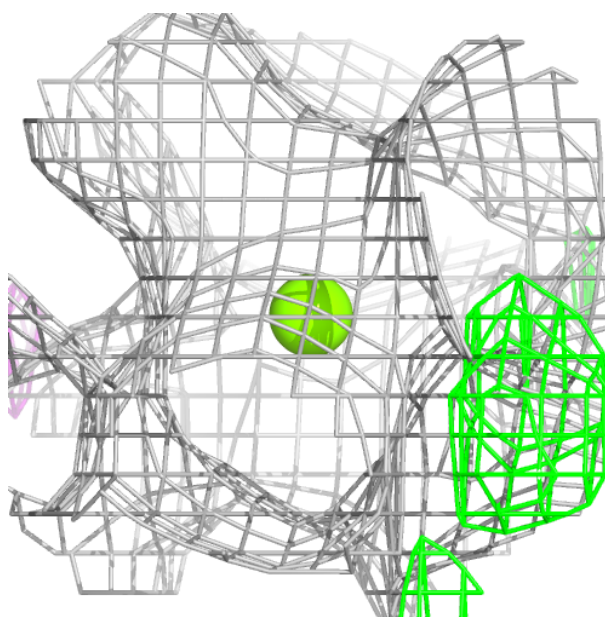
Electron density around K A 404:

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and green (positive)



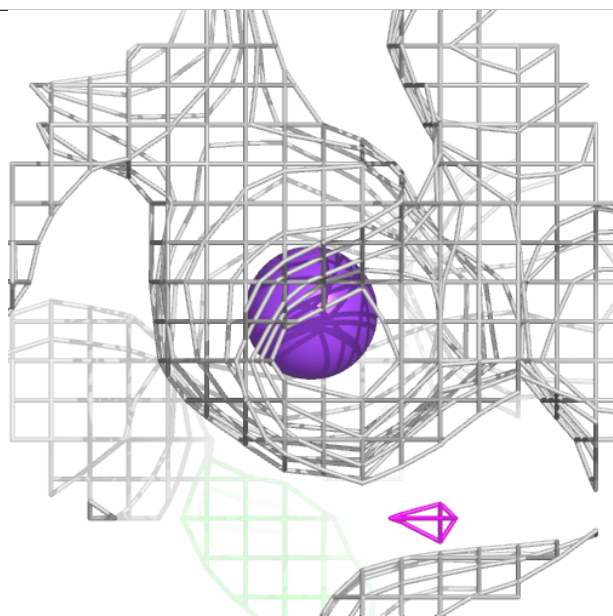
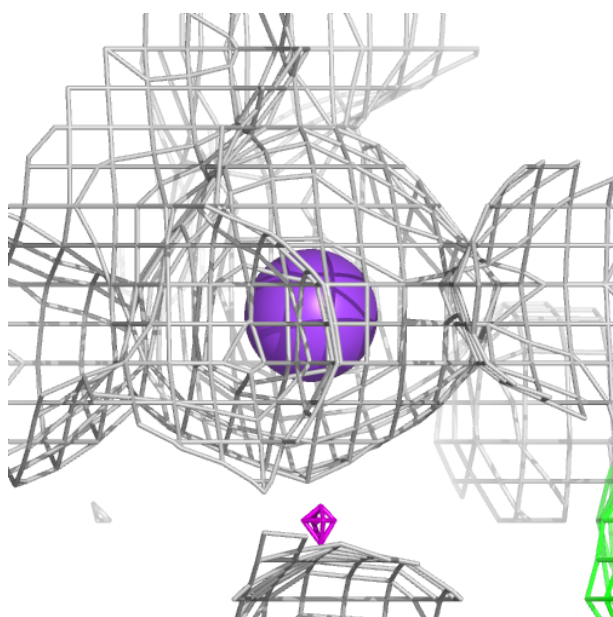
Electron density around MG A 402:

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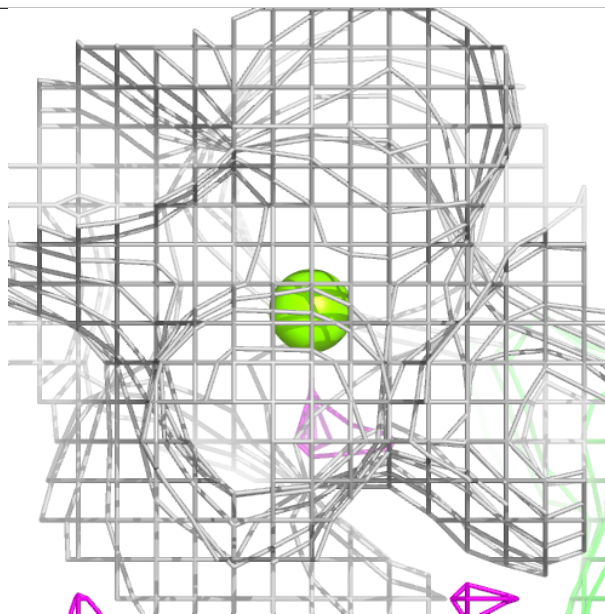
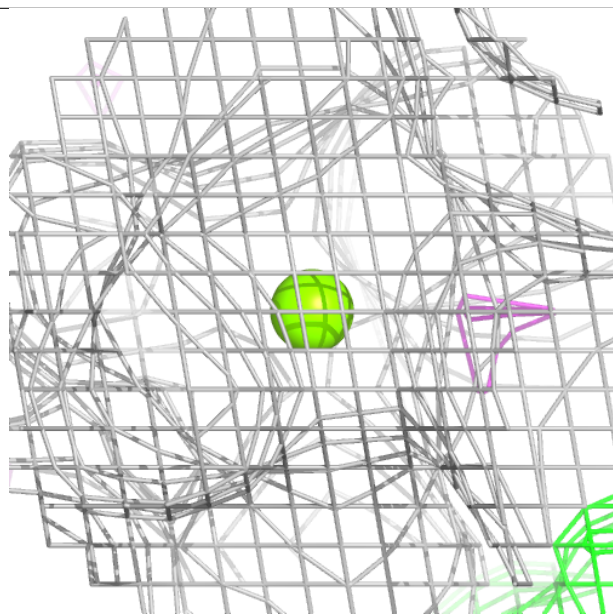
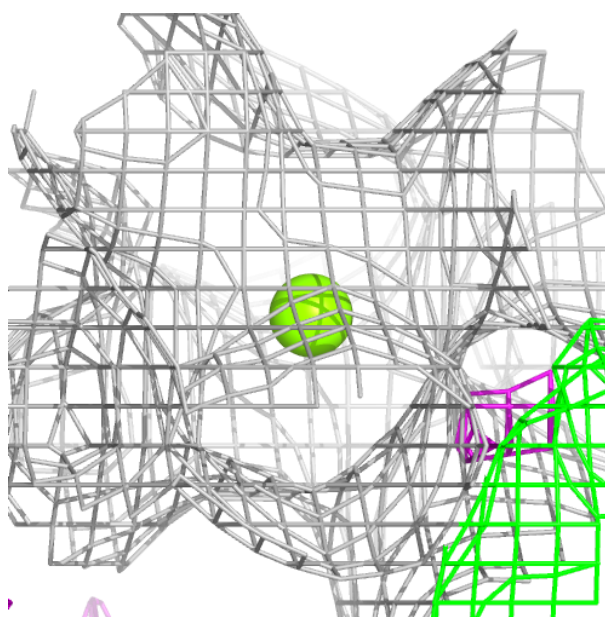
Electron density around K B 403:

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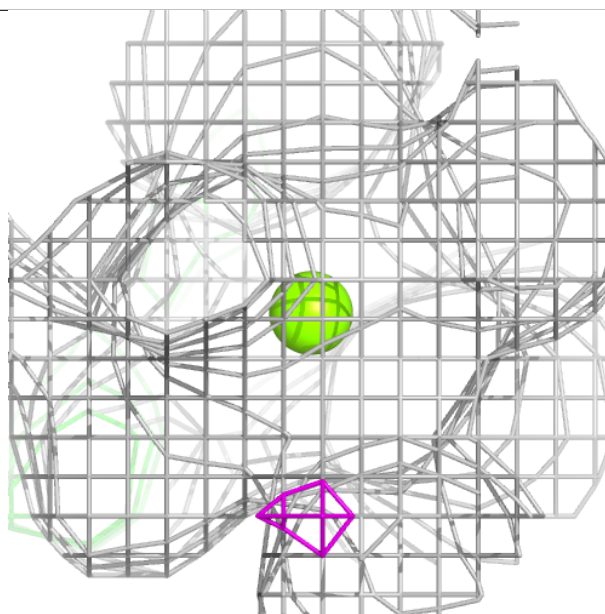
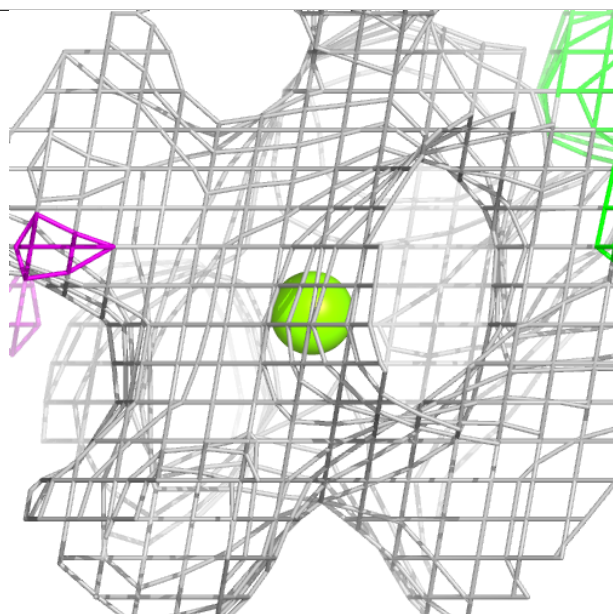
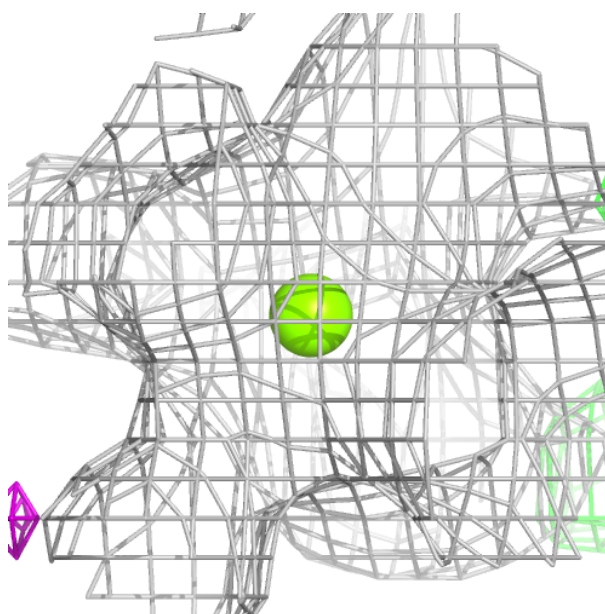
Electron density around MG B 402:

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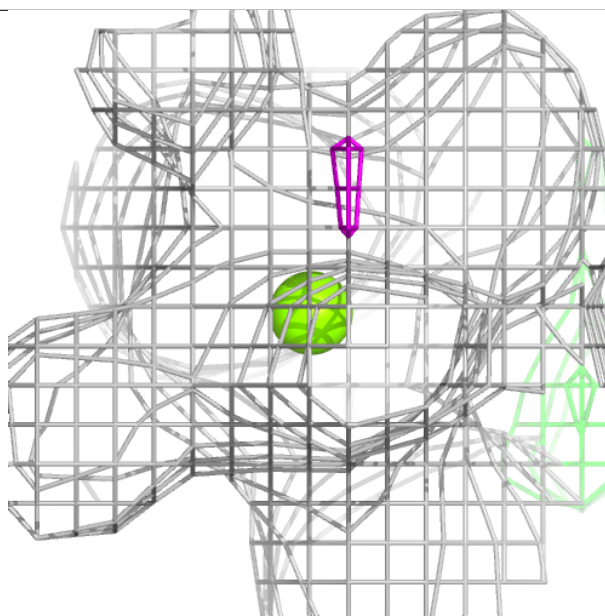
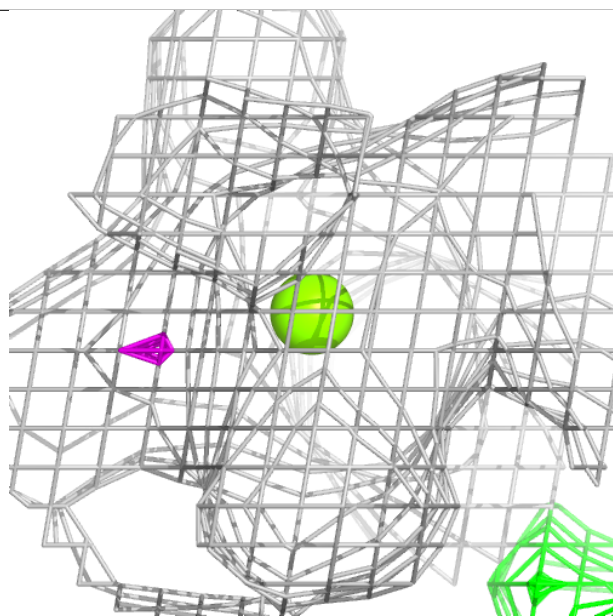
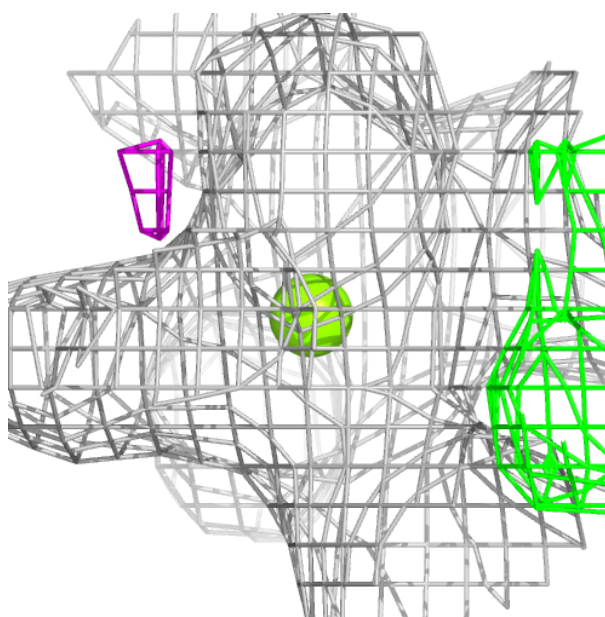
Electron density around MG A 403:

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



Electron density around MG A 407:

$2mF_o-DF_c$ (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.