



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:40 PM UTC

PDB ID : 6VD1 / pdb_00006vd1
Title : Crystal structure of Arabidopsis thaliana S-adenosylmethionine Synthase 2 (AtMAT2) in complex with S-adenosylmethionine and PPNP
Authors : Sekula, B.; Ruszkowski, M.; Dauter, Z.
Deposited on : 2019-12-23
Resolution : 1.32 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

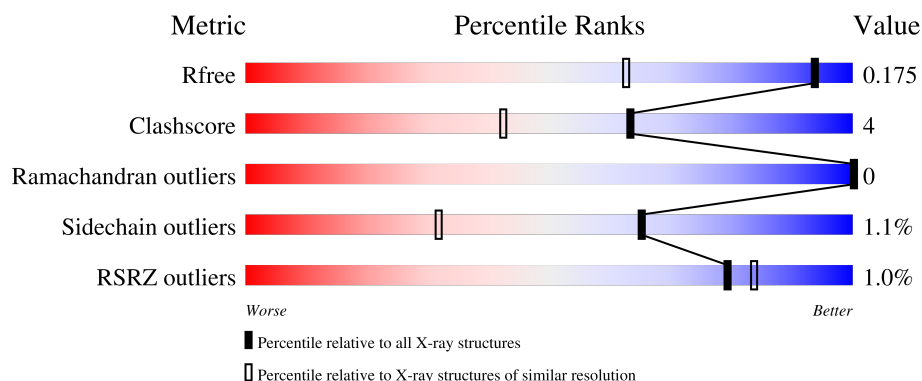
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.32 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	2531 (1.34-1.30)
Clashscore	190562	2585 (1.34-1.30)
Ramachandran outliers	187476	2528 (1.34-1.30)
Sidechain outliers	187428	2528 (1.34-1.30)
RSRZ outliers	180081	2528 (1.34-1.30)

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	

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	PDO	B	402	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 7665 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.

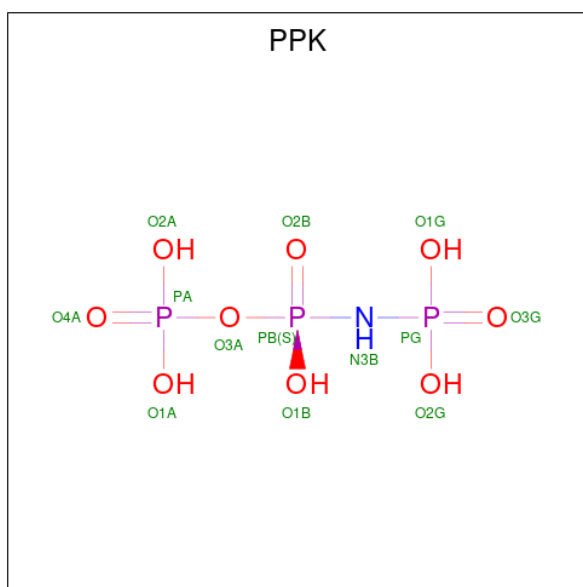
- Molecule 1 is a protein called S-adenosylmethionine synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	11	0
			3124	1975	537	594	18			
1	B	392	Total	C	N	O	S	0	16	0
			3130	1982	536	593	19			

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 (DIPHOSPHONO)AMINOPHOSPHONIC ACID (CCD ID: PPK) (formula: $\text{H}_6\text{NO}_9\text{P}_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	N	O	P	0	0
			13	1	9	3		
2	B	1	Total	N	O	P	0	0
			13	1	9	3		

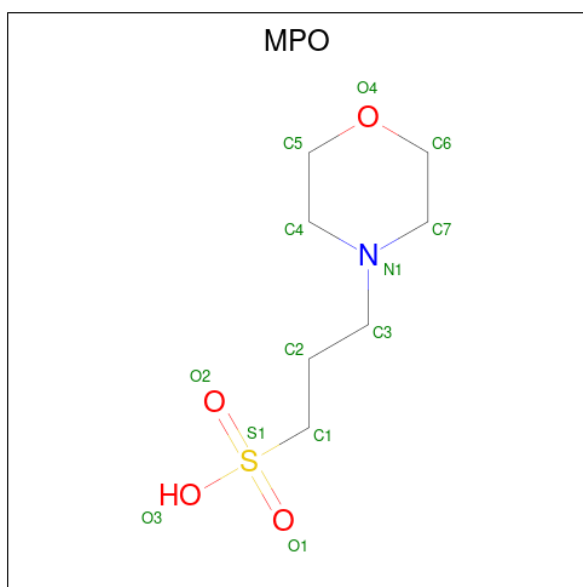
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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).

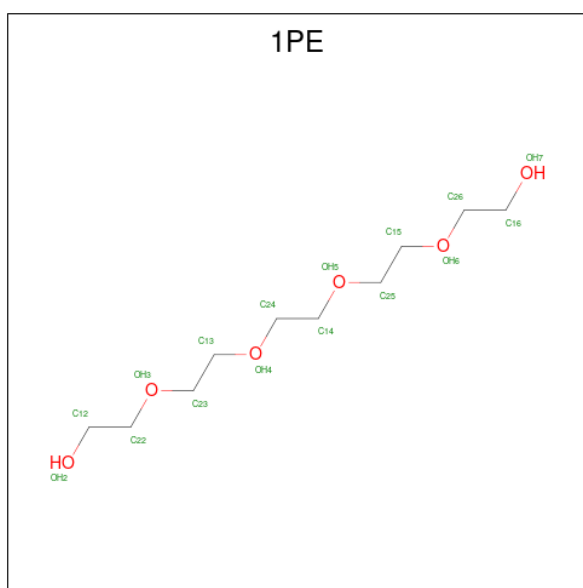
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		

- Molecule 5 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: C₇H₁₅NO₄S).



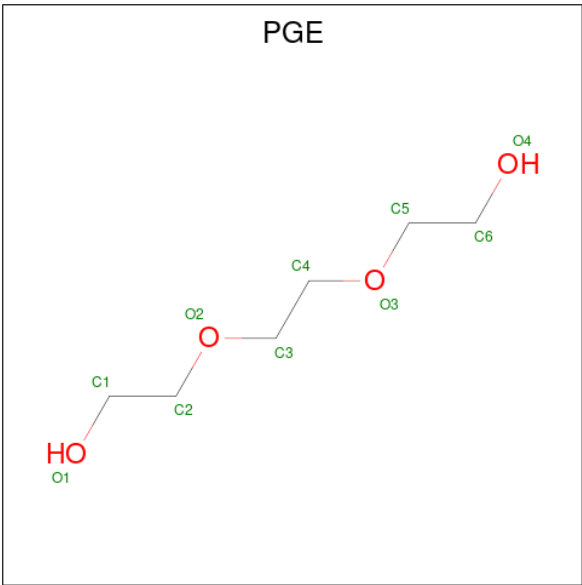
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



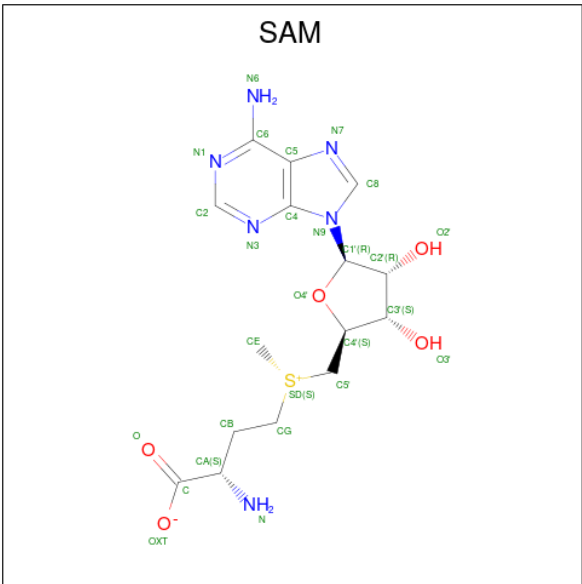
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 8 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



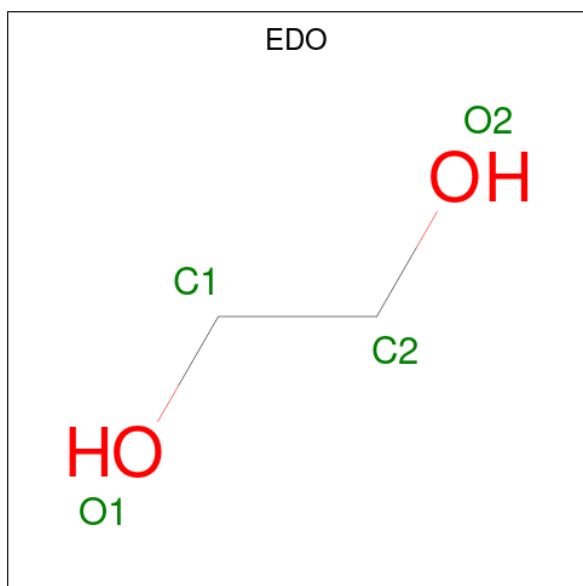
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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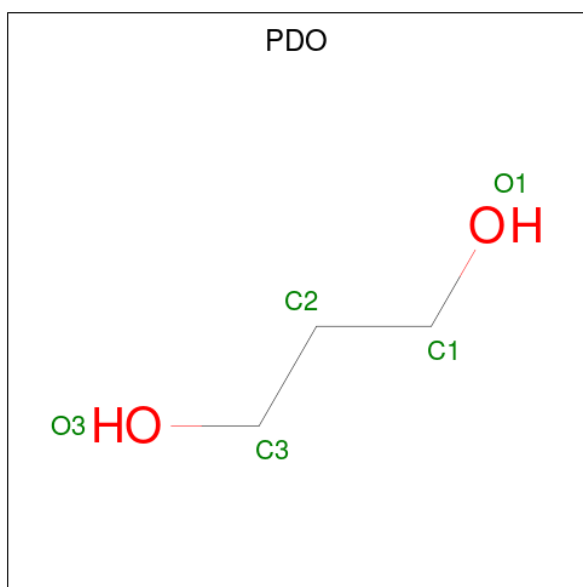
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



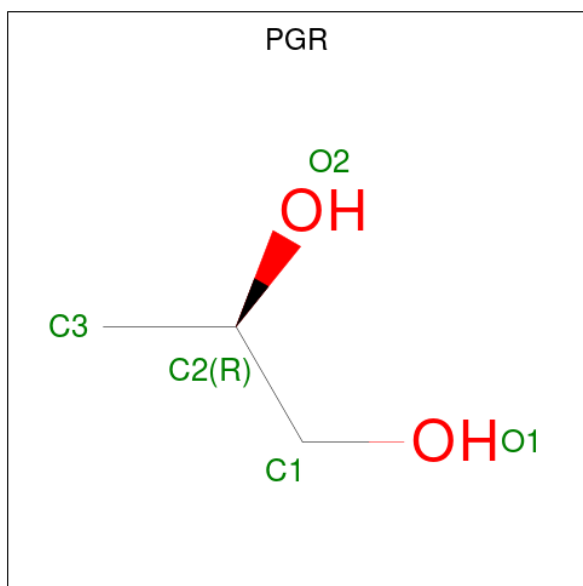
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is 1,3-PROPANDIOL (CCD ID: PDO) (formula: $C_3H_8O_2$).



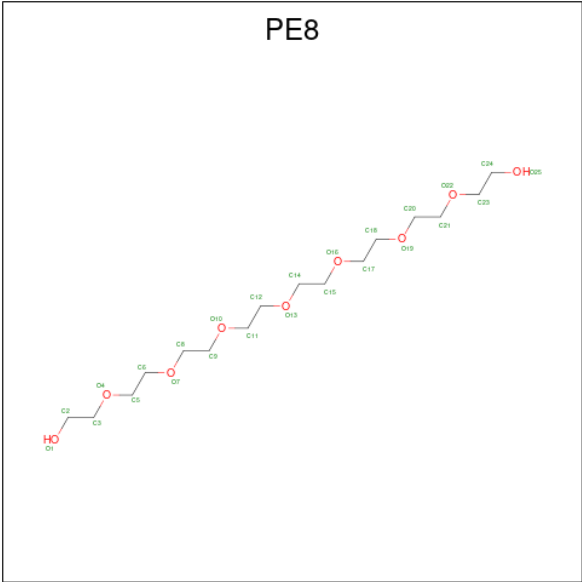
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 11 is R-1,2-PROPANEDIOL (CCD ID: PGR) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 12 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: $C_{16}H_{34}O_9$).



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

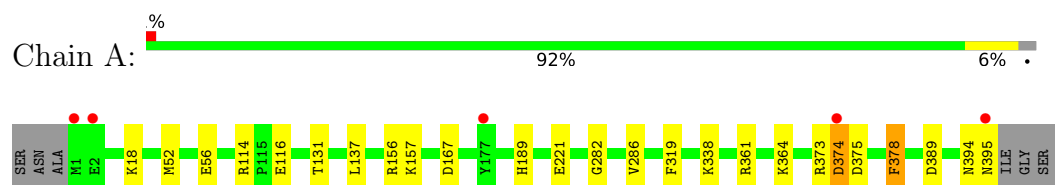
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	587	Total	O	0	10
			596	596		
13	B	611	Total	O	0	14
			624	624		

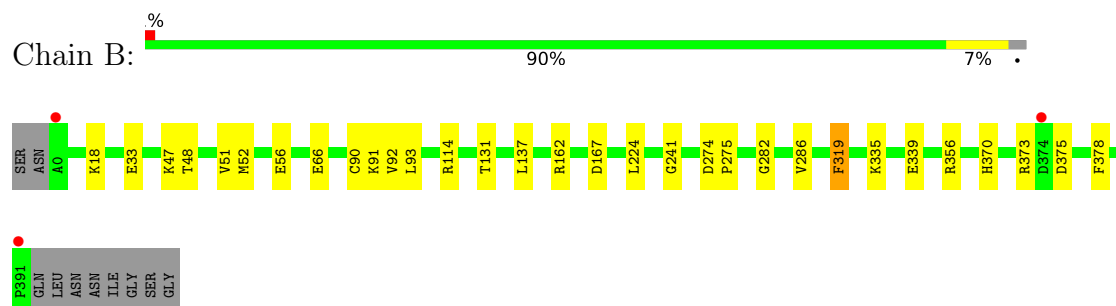
3 Residue-property plots [i](#)

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	61.20Å 101.48Å 84.33Å 90.00° 99.37° 90.00°	Depositor
Resolution (Å)	47.09 – 1.32 47.09 – 1.32	Depositor EDS
% Data completeness (in resolution range)	97.8 (47.09-1.32) 97.8 (47.09-1.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.142 , 0.173 0.142 , 0.175	Depositor DCC
R_{free} test set	1163 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	9.6	Xtriage
Anisotropy	1.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7665	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.23% 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: 1PE, SAM, PGE, PPK, K, EDO, PGR, MPO, PE8, PDO, 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	1.01	3/3222 (0.1%)	1.09	1/4360 (0.0%)
1	B	1.02	3/3234 (0.1%)	1.13	1/4374 (0.0%)
All	All	1.01	6/6456 (0.1%)	1.11	2/8734 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	394	ASN	C-O	5.61	1.30	1.24
1	A	189	HIS	CE1-NE2	5.61	1.38	1.32
1	A	378	PHE	C-O	5.29	1.29	1.23
1	B	356	ARG	C-O	-5.19	1.17	1.24
1	B	241	GLY	C-O	5.06	1.28	1.23
1	B	370	HIS	CE1-NE2	5.01	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	167	ASP	CA-CB-CG	6.69	119.29	112.60
1	B	167	ASP	CA-CB-CG	6.63	119.23	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3124	0	3124	22	0
1	B	3130	0	3141	24	0
2	A	13	0	1	0	0
2	B	13	0	1	1	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	13	0	14	0	0
5	B	13	0	15	0	0
6	A	16	0	22	0	0
7	A	10	0	14	0	0
7	B	10	0	14	4	0
8	A	27	0	22	0	0
8	B	27	0	22	1	0
9	A	4	0	6	0	0
9	B	4	0	6	0	0
10	B	5	0	8	6	0
11	B	5	0	8	1	0
12	B	25	0	34	4	0
13	A	596	0	0	8	0
13	B	624	0	0	11	0
All	All	7665	0	6452	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (51) 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)
12:B:405:PE8:H182	13:B:774:HOH:O	1.52	1.09
12:B:405:PE8:H81	13:B:820:HOH:O	1.61	0.98
1:B:162:ARG:HH21	7:B:408:PGE:C4	2.00	0.74
1:A:52[B]:MET:HE3	1:B:52[B]:MET:CE	2.19	0.73
1:A:374:ASP:C	13:A:502:HOH:O	2.32	0.72
7:B:408:PGE:H22	13:B:879:HOH:O	1.91	0.71
1:A:52[B]:MET:CE	1:B:52[B]:MET:HE3	2.21	0.71
1:A:375:ASP:N	13:A:502:HOH:O	2.23	0.70
1:A:157:LYS:NZ	13:A:504:HOH:O	2.25	0.67
1:A:52[B]:MET:HE3	1:B:52[B]:MET:HE3	1.77	0.67
1:B:91:LYS:HD3	1:B:93:LEU:HD21	1.78	0.65
12:B:405:PE8:H151	13:B:850:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52[B]:MET:HE3	1:B:52[B]:MET:HE1	1.85	0.58
1:A:156:ARG:NH2	13:A:503:HOH:O	2.23	0.57
1:B:224:LEU:HD12	10:B:402:PDO:C1	2.36	0.56
1:B:162:ARG:HH21	7:B:408:PGE:H42	1.71	0.55
1:A:52[B]:MET:HE1	1:B:52[B]:MET:HE3	1.89	0.54
1:B:224:LEU:HD12	10:B:402:PDO:H12	1.88	0.54
12:B:405:PE8:H122	13:B:871:HOH:O	2.07	0.53
1:B:375:ASP:N	13:B:508:HOH:O	2.43	0.51
1:A:374:ASP:OD1	1:A:374:ASP:N	2.40	0.51
1:B:131:THR:O	1:B:137:LEU:HA	2.11	0.50
1:B:51:VAL:HG23	1:B:90[B]:CYS:SG	2.52	0.50
1:A:373[B]:ARG:HG3	1:A:378:PHE:CE2	2.47	0.50
10:B:402:PDO:H32	13:B:618:HOH:O	2.12	0.49
11:B:403:PGR:H31	13:B:991:HOH:O	2.13	0.49
1:B:335:LYS:O	1:B:339:GLU:HG3	2.14	0.48
1:A:338:LYS:NZ	13:A:510:HOH:O	2.42	0.47
1:B:47:LYS:O	1:B:48:THR:C	2.56	0.47
1:A:131:THR:O	1:A:137:LEU:HA	2.14	0.46
1:A:114:ARG:NH2	13:A:516:HOH:O	2.49	0.46
1:A:389:ASP:HB3	13:A:871:HOH:O	2.15	0.46
1:B:114:ARG:NH2	13:B:512:HOH:O	2.47	0.46
1:B:66:GLU:HG2	1:B:92:VAL:HB	1.98	0.45
1:A:282:GLY:O	1:A:286:VAL:HG22	2.16	0.45
1:B:282:GLY:O	1:B:286:VAL:HG22	2.17	0.44
1:A:116[B]:GLU:OE1	13:A:501:HOH:O	2.21	0.44
1:B:373[A]:ARG:HG3	1:B:378:PHE:CE2	2.54	0.43
7:B:408:PGE:H42	7:B:408:PGE:H62	1.69	0.43
10:B:402:PDO:C3	13:B:618:HOH:O	2.67	0.43
1:A:364[B]:LYS:HD3	1:A:375:ASP:OD2	2.19	0.42
1:B:274:ASP:HB2	1:B:275:PRO:HD2	2.01	0.42
1:B:224:LEU:HD12	10:B:402:PDO:H11	2.01	0.42
1:A:52[A]:MET:HE2	1:B:52[A]:MET:HE2	2.01	0.42
2:B:401:PPK:O2A	8:B:409:SAM:H4'	2.19	0.42
1:A:361:ARG:O	1:A:364[B]:LYS:HG2	2.19	0.41
10:B:402:PDO:H21	13:B:888:HOH:O	2.20	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	404/402 (100%)	397 (98%)	7 (2%)	0	100	100
1	B	406/402 (101%)	399 (98%)	7 (2%)	0	100	100
All	All	810/804 (101%)	796 (98%)	14 (2%)	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	344/337 (102%)	340 (99%)	4 (1%)	63	28
1	B	345/337 (102%)	340 (99%)	5 (1%)	59	22
All	All	689/674 (102%)	680 (99%)	9 (1%)	65	24

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	221	GLU
1	A	374	ASP
1	A	395	ASN
1	B	18	LYS
1	B	33[A]	GLU
1	B	33[B]	GLU
1	B	319[A]	PHE

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Mol	Chain	Res	Type
1	B	319[B]	PHE

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

Mol	Chain	Res	Type
1	A	395	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 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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
12	PE8	B	405	-	24,24,24	0.70	0	23,23,23	0.70	0
7	PGE	B	408	-	9,9,9	0.22	0	8,8,8	0.17	0
8	SAM	A	409	-	27,29,29	0.53	0	34,42,42	1.22	1 (2%)
9	EDO	B	410	-	3,3,3	0.14	0	2,2,2	0.26	0
5	MPO	B	407	-	13,13,13	0.50	0	17,17,17	0.75	1 (5%)
10	PDO	B	402	-	4,4,4	0.37	0	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	PGR	B	403	-	4,4,4	0.59	0	4,4,4	0.66	0
2	PPK	B	401	3,4	11,12,12	1.69	5 (45%)	14,20,20	2.19	5 (35%)
8	SAM	B	409	-	27,29,29	0.68	1 (3%)	34,42,42	1.23	1 (2%)
7	PGE	A	408	-	9,9,9	0.19	0	8,8,8	0.25	0
6	1PE	A	407	-	15,15,15	0.60	0	14,14,14	0.66	0
9	EDO	A	410	-	3,3,3	0.09	0	2,2,2	0.13	0
5	MPO	A	406	-	13,13,13	1.40	1 (7%)	17,17,17	1.16	2 (11%)
2	PPK	A	401	3,4	11,12,12	2.68	5 (45%)	14,20,20	1.66	4 (28%)

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
12	PE8	B	405	-	-	11/22/22/22	-
7	PGE	B	408	-	-	6/7/7/7	-
8	SAM	A	409	-	-	4/17/33/33	0/3/3/3
9	EDO	B	410	-	-	1/1/1/1	-
5	MPO	B	407	-	-	0/7/15/15	0/1/1/1
10	PDO	B	402	-	-	1/2/2/2	-
11	PGR	B	403	-	-	2/2/2/2	-
2	PPK	B	401	3,4	-	2/8/12/12	-
8	SAM	B	409	-	-	5/17/33/33	0/3/3/3
7	PGE	A	408	-	-	1/7/7/7	-
6	1PE	A	407	-	-	4/13/13/13	-
9	EDO	A	410	-	-	1/1/1/1	-
5	MPO	A	406	-	-	1/7/15/15	0/1/1/1
2	PPK	A	401	3,4	-	2/8/12/12	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PPK	PG-O3G	5.65	1.54	1.46
5	A	406	MPO	O2-S1	4.61	1.58	1.45
2	A	401	PPK	PG-O1G	-3.63	1.47	1.56
2	A	401	PPK	PB-O2B	3.36	1.51	1.46
2	A	401	PPK	PB-O1B	-2.91	1.49	1.56
2	A	401	PPK	PB-O3A	2.88	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PPK	PG-O3G	2.66	1.50	1.46
2	B	401	PPK	PB-O3A	2.27	1.61	1.59
2	B	401	PPK	PG-O2G	-2.22	1.50	1.56
2	B	401	PPK	PB-O1B	-2.20	1.51	1.56
8	B	409	SAM	OXT-C	-2.14	1.23	1.30
2	B	401	PPK	PB-O2B	2.06	1.49	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	409	SAM	CG-SD-C5'	-6.27	88.10	103.43
8	B	409	SAM	CG-SD-C5'	-6.01	88.73	103.43
2	B	401	PPK	O3G-PG-N3B	-4.83	104.66	111.77
2	A	401	PPK	O1B-PB-O2B	4.03	118.51	109.87
2	B	401	PPK	O1G-PG-O2G	3.83	117.89	107.59
2	B	401	PPK	O1B-PB-O2B	3.64	117.67	109.87
2	A	401	PPK	O3G-PG-N3B	-2.59	107.96	111.77
2	B	401	PPK	O1G-PG-O3G	-2.28	107.75	113.45
2	A	401	PPK	O1G-PG-O3G	-2.25	107.81	113.45
2	B	401	PPK	O2B-PB-N3B	-2.21	108.52	111.77
5	A	406	MPO	O3-S1-O1	2.18	116.85	111.40
5	A	406	MPO	C6-C7-N1	2.14	113.37	110.12
2	A	401	PPK	O1G-PG-O2G	2.04	113.07	107.59
5	B	407	MPO	C6-C7-N1	2.02	113.19	110.12

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PPK	PG-N3B-PB-O3A
2	B	401	PPK	PB-N3B-PG-O3G
2	B	401	PPK	PG-N3B-PB-O3A
10	B	402	PDO	O1-C1-C2-C3
11	B	403	PGR	O1-C1-C2-O2
12	B	405	PE8	O7-C8-C9-O10
6	A	407	1PE	OH6-C15-C25-OH5
7	B	408	PGE	O1-C1-C2-O2
6	A	407	1PE	OH7-C16-C26-OH6
12	B	405	PE8	O13-C14-C15-O16
12	B	405	PE8	O16-C17-C18-O19
7	A	408	PGE	O3-C5-C6-O4
9	A	410	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	B	408	PGE	O3-C5-C6-O4
7	B	408	PGE	C6-C5-O3-C4
11	B	403	PGR	O1-C1-C2-C3
8	B	409	SAM	O-C-CA-CB
8	A	409	SAM	C2'-C1'-N9-C8
8	B	409	SAM	C2'-C1'-N9-C8
8	A	409	SAM	O-C-CA-CB
6	A	407	1PE	C15-C25-OH5-C14
12	B	405	PE8	C8-C9-O10-C11
8	A	409	SAM	OXT-C-CA-CB
8	B	409	SAM	OXT-C-CA-CB
12	B	405	PE8	C15-C14-O13-C12
12	B	405	PE8	C12-C11-O10-C9
6	A	407	1PE	C12-C22-OH3-C23
9	B	410	EDO	O1-C1-C2-O2
12	B	405	PE8	C11-C12-O13-C14
7	B	408	PGE	C3-C4-O3-C5
12	B	405	PE8	C2-C3-O4-C5
5	A	406	MPO	C1-C2-C3-N1
8	A	409	SAM	O4'-C1'-N9-C8
12	B	405	PE8	O10-C11-C12-O13
8	B	409	SAM	O4'-C1'-N9-C8
7	B	408	PGE	C4-C3-O2-C2
7	B	408	PGE	O2-C3-C4-O3
8	B	409	SAM	CA-CB-CG-SD
2	A	401	PPK	PA-O3A-PB-O2B
12	B	405	PE8	C14-C15-O16-C17
12	B	405	PE8	C24-C23-O22-C21

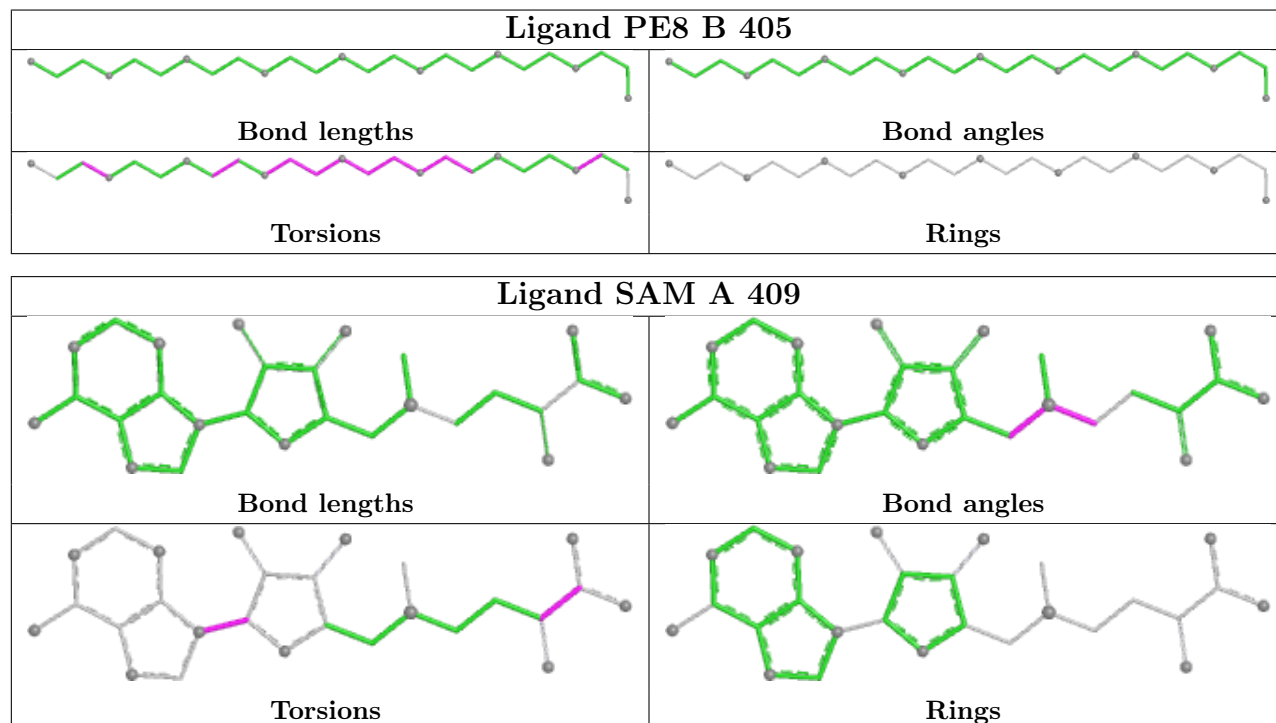
There are no ring outliers.

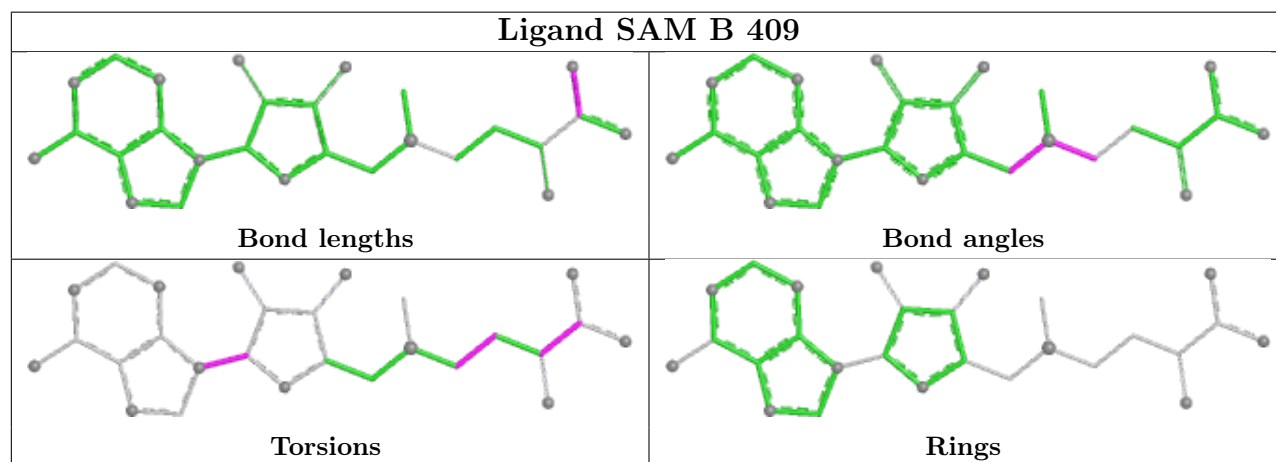
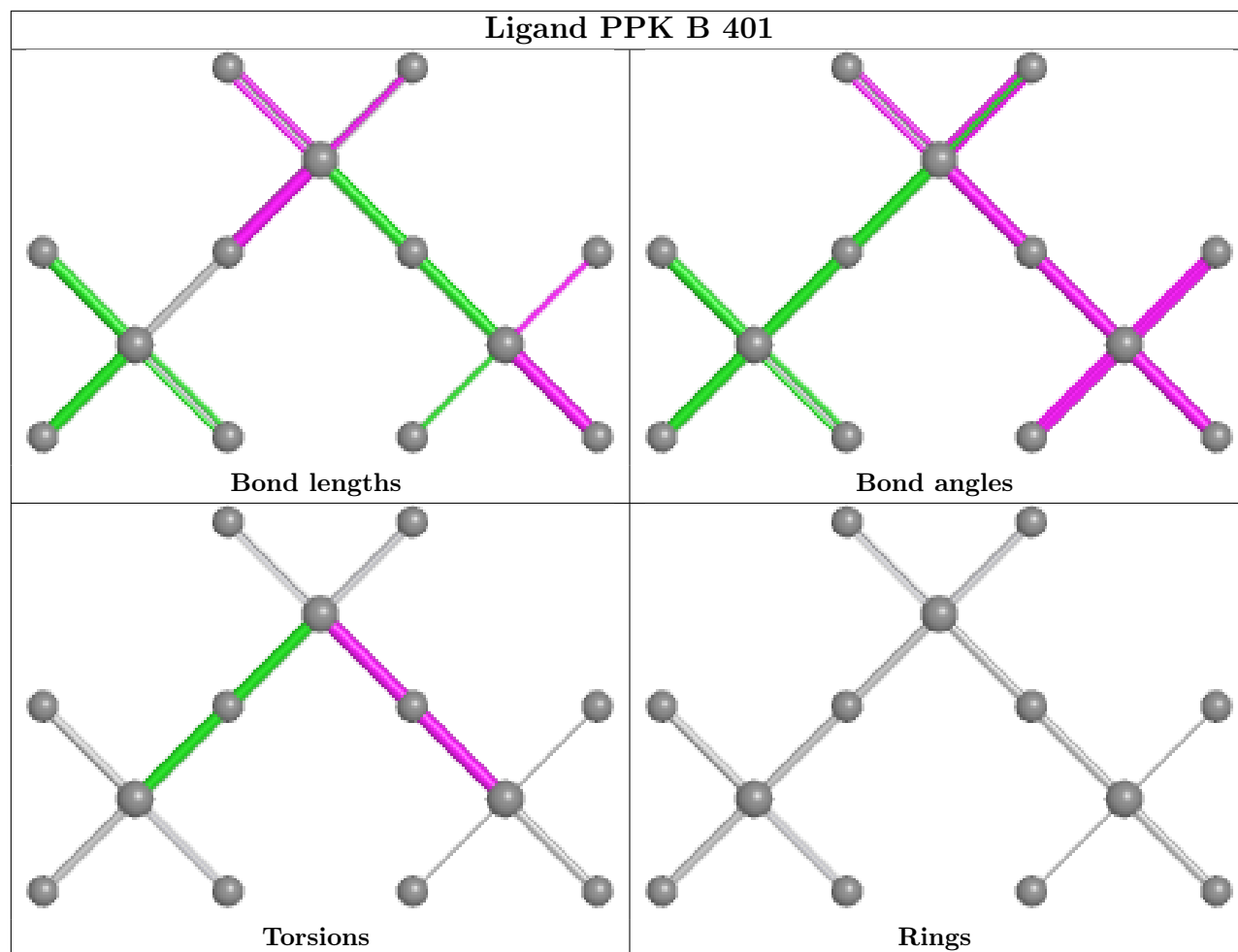
6 monomers are involved in 16 short contacts:

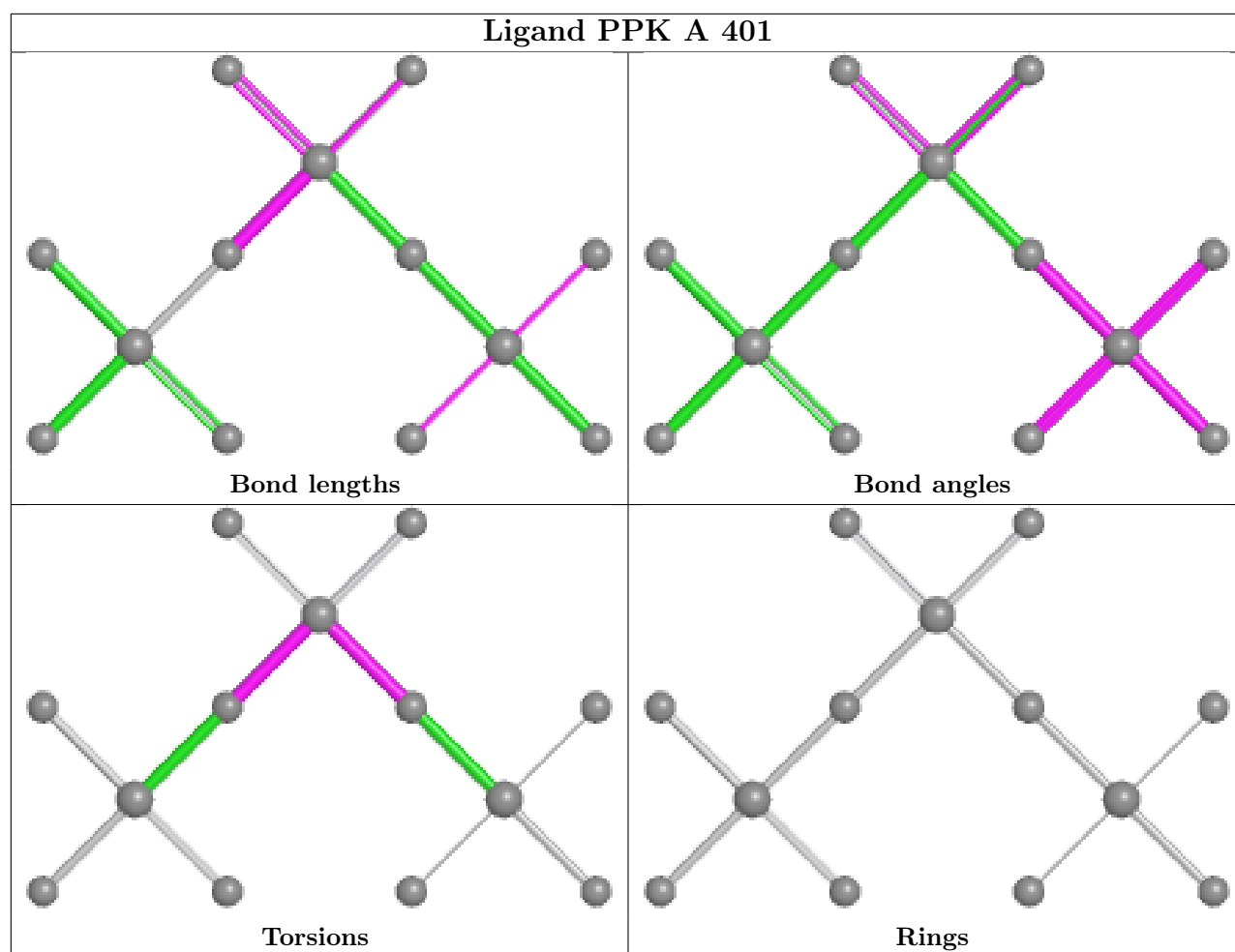
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	405	PE8	4	0
7	B	408	PGE	4	0
10	B	402	PDO	6	0
11	B	403	PGR	1	0
2	B	401	PPK	1	0
8	B	409	SAM	1	0

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	395/402 (98%)	-0.19	5 (1%) 75 80	7, 13, 22, 46	11 (2%)
1	B	392/402 (97%)	-0.24	3 (0%) 82 87	7, 12, 21, 38	16 (4%)
All	All	787/804 (97%)	-0.22	8 (1%) 79 84	7, 12, 22, 46	27 (3%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	395	ASN	4.9
1	A	374	ASP	3.2
1	B	391	PRO	2.9
1	B	374	ASP	2.6
1	A	1	MET	2.6
1	B	0	ALA	2.2
1	A	2	GLU	2.1
1	A	177	TYR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

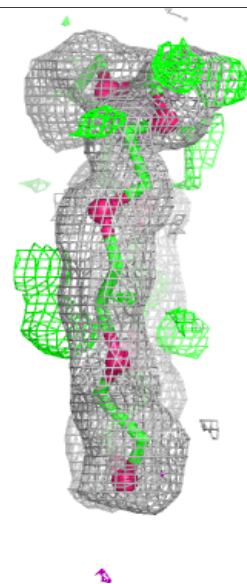
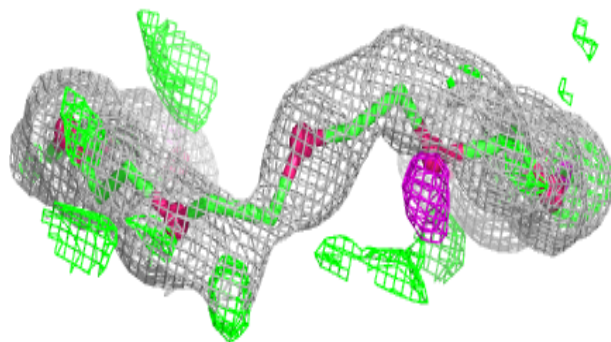
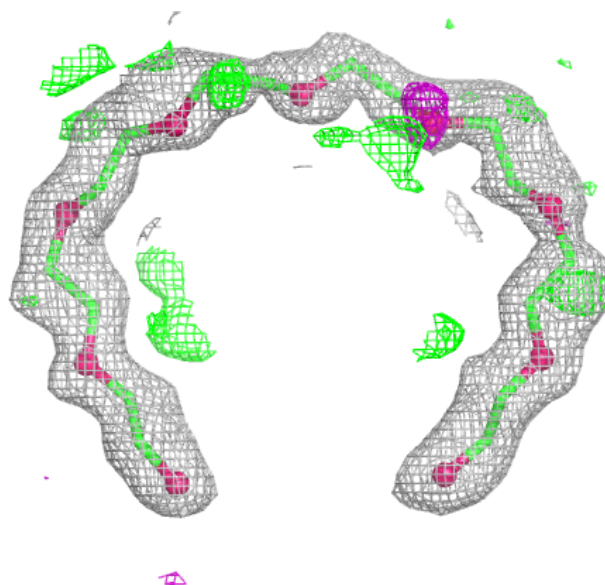
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	EDO	A	410	4/4	0.78	0.17	39,44,48,48	0
7	PGE	A	408	10/10	0.82	0.19	33,39,48,77	0
6	1PE	A	407	16/16	0.83	0.18	36,42,48,49	0
11	PGR	B	403	5/5	0.83	0.16	23,27,30,34	5
12	PE8	B	405	25/25	0.85	0.15	26,34,45,49	0
7	PGE	B	408	10/10	0.86	0.14	35,38,41,51	0
9	EDO	B	410	4/4	0.92	0.11	36,40,42,44	0
10	PDO	B	402	5/5	0.92	0.11	29,30,31,31	0
5	MPO	A	406	13/13	0.93	0.11	20,24,28,29	0
5	MPO	B	407	13/13	0.95	0.10	17,20,22,22	0
8	SAM	A	409	27/27	0.97	0.06	11,13,18,24	0
8	SAM	B	409	27/27	0.98	0.06	9,12,17,22	0
2	PPK	B	401	13/13	0.98	0.04	9,11,11,12	0
2	PPK	A	401	13/13	0.99	0.04	9,11,11,12	0
3	MG	A	402	1/1	1.00	0.01	12,12,12,12	0
3	MG	A	403	1/1	1.00	0.01	11,11,11,11	0
3	MG	A	404	1/1	1.00	0.01	11,11,11,11	0
3	MG	B	404	1/1	1.00	0.03	13,13,13,13	0
4	K	A	405	1/1	1.00	0.01	13,13,13,13	0
4	K	B	406	1/1	1.00	0.02	13,13,13,13	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.

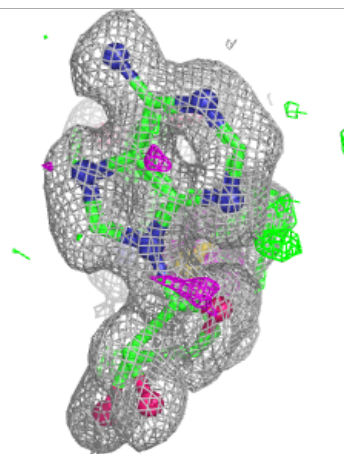
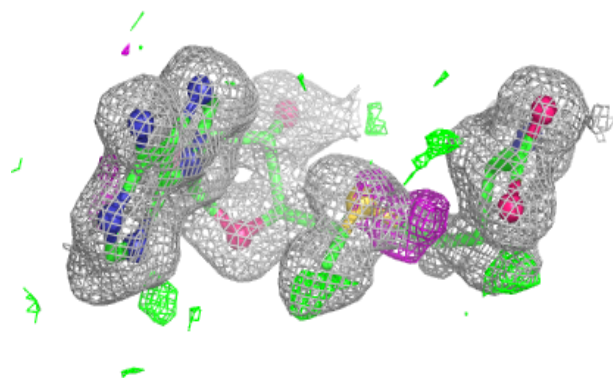
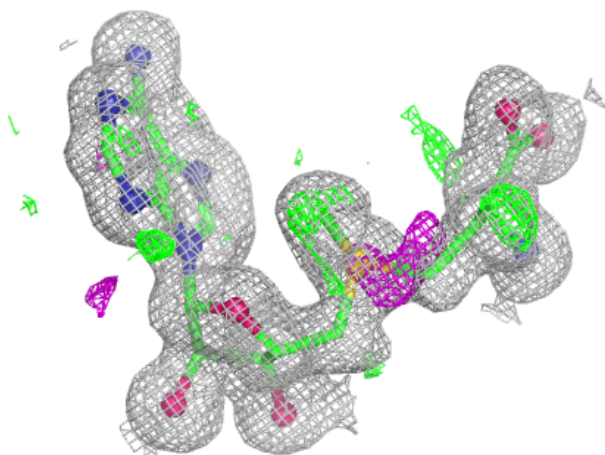
Electron density around PE8 B 405:

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



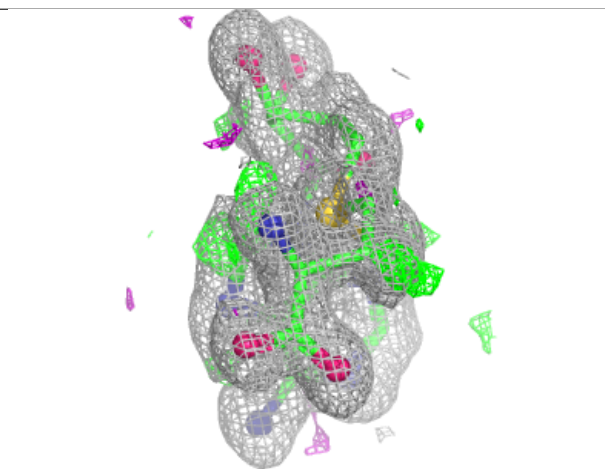
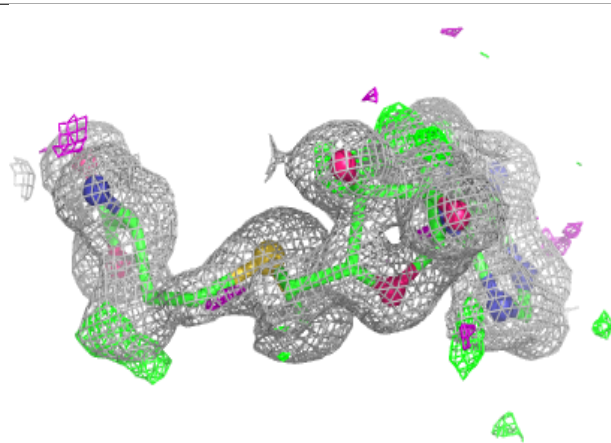
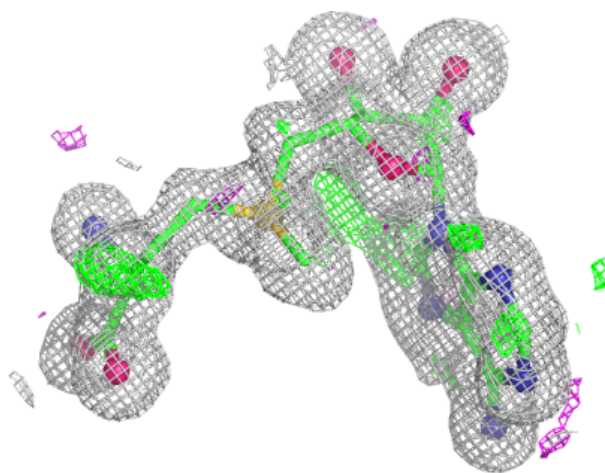
Electron density around SAM A 409:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



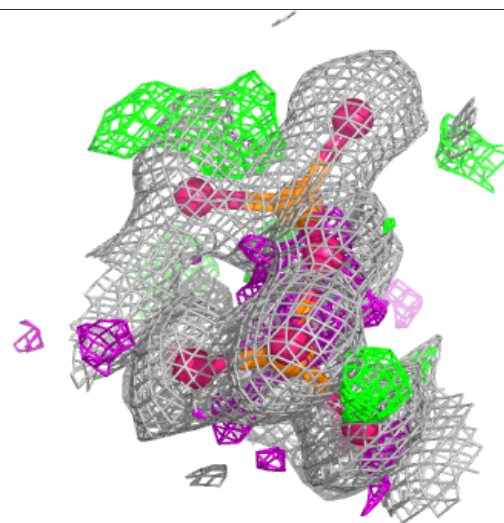
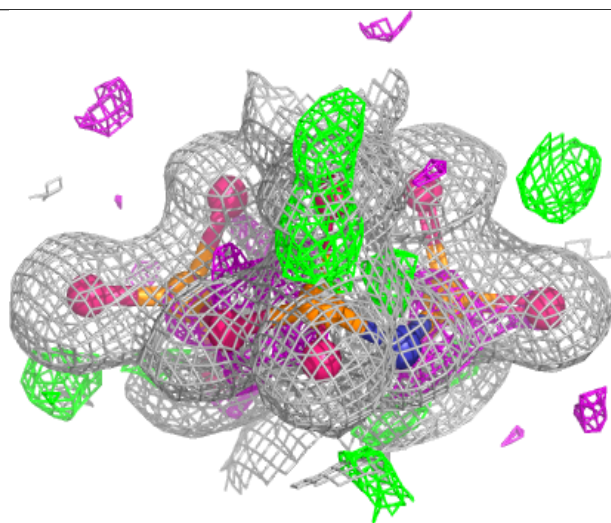
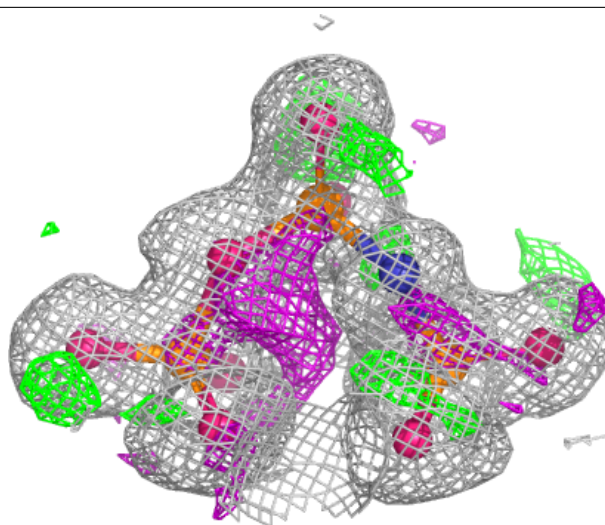
Electron density around SAM B 409:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



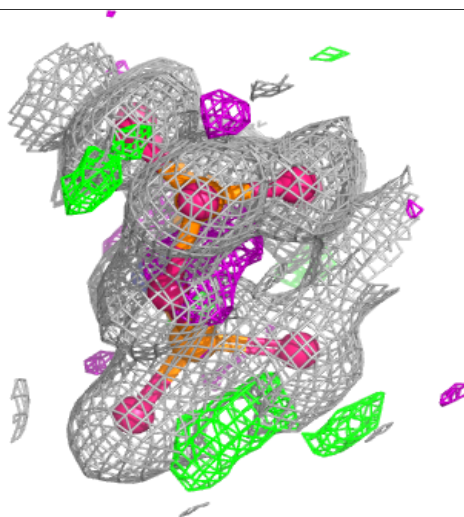
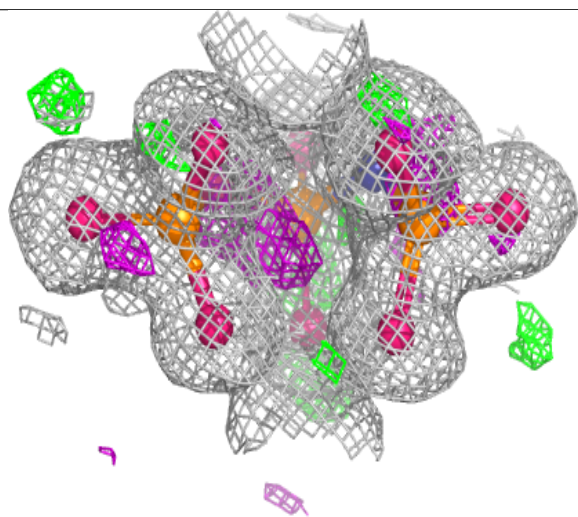
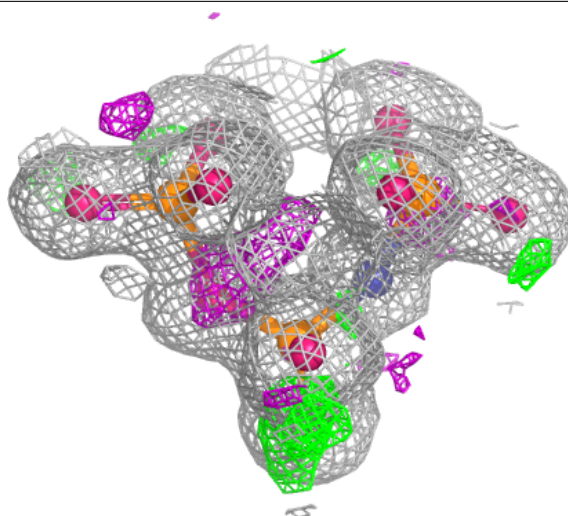
Electron density around PPK B 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



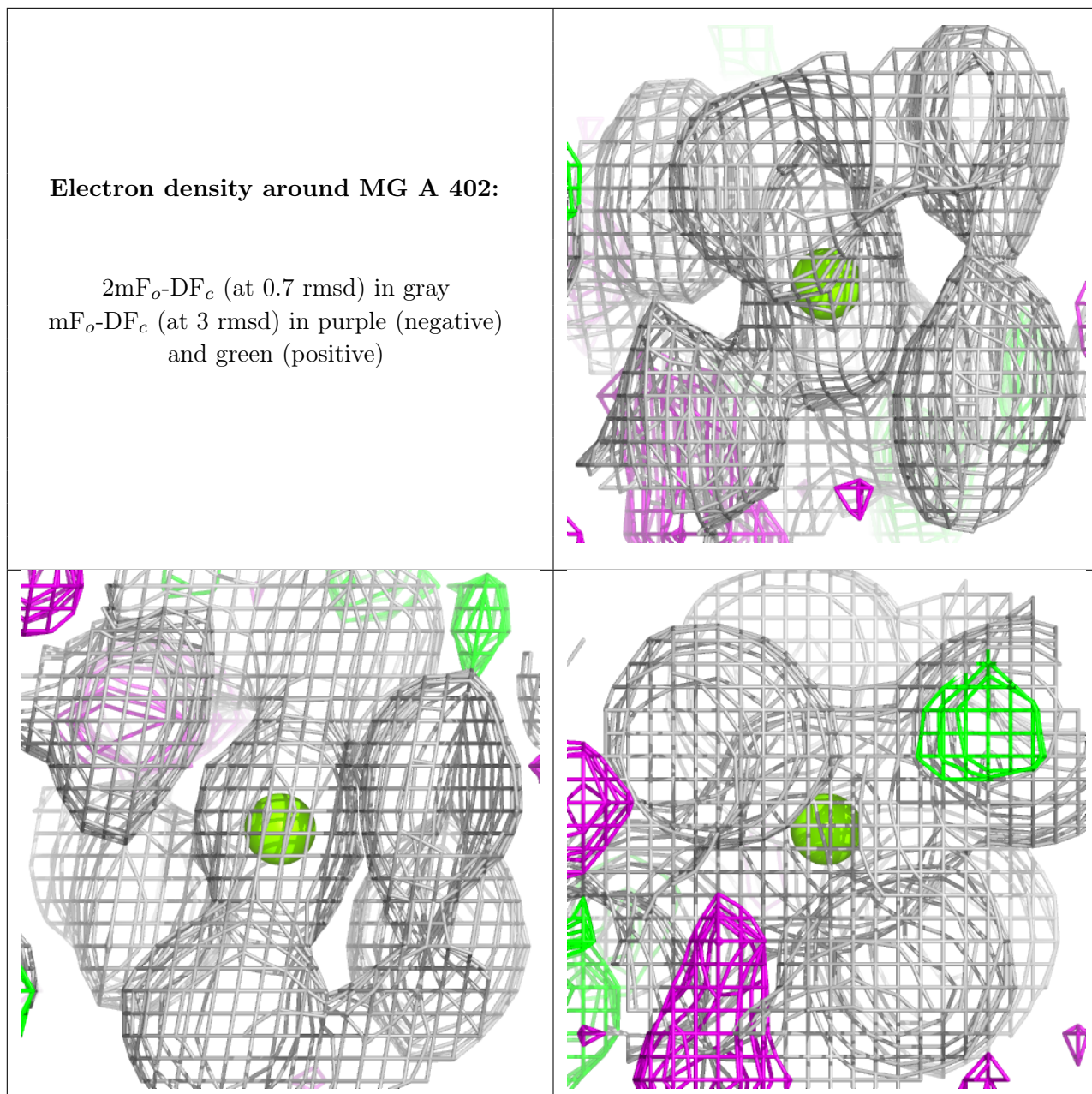
Electron density around PPK A 401:

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and green (positive)



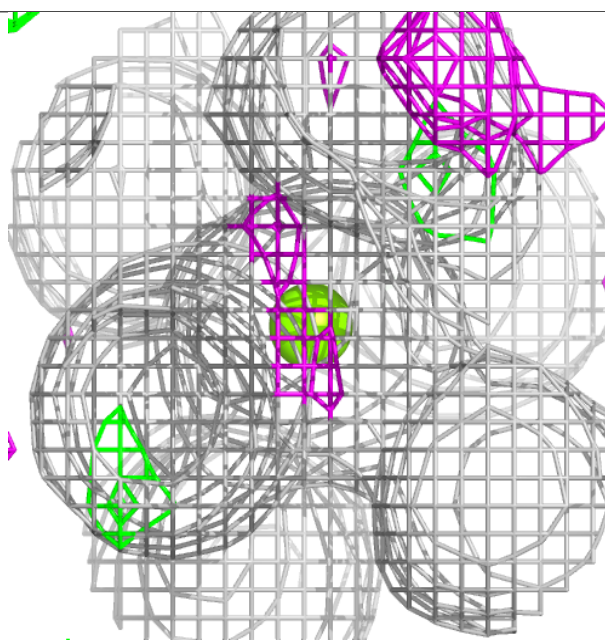
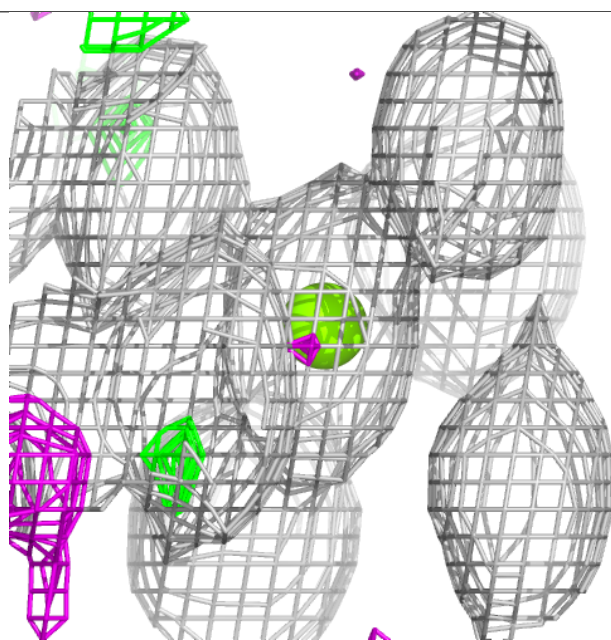
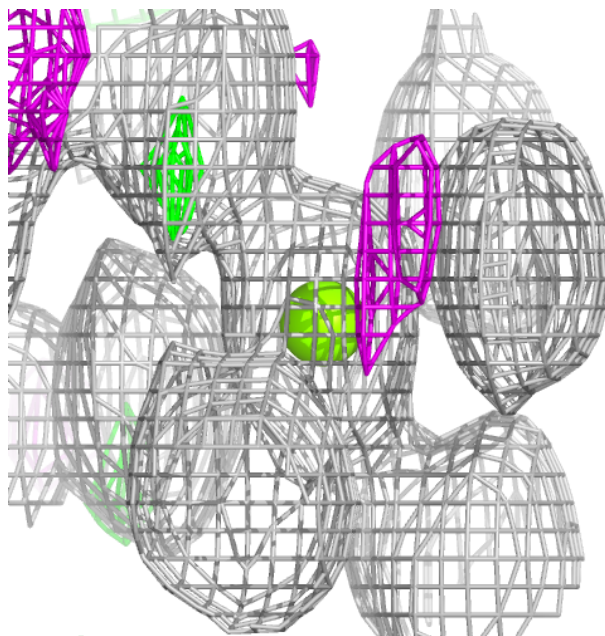
Electron density around MG A 402:

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and green (positive)



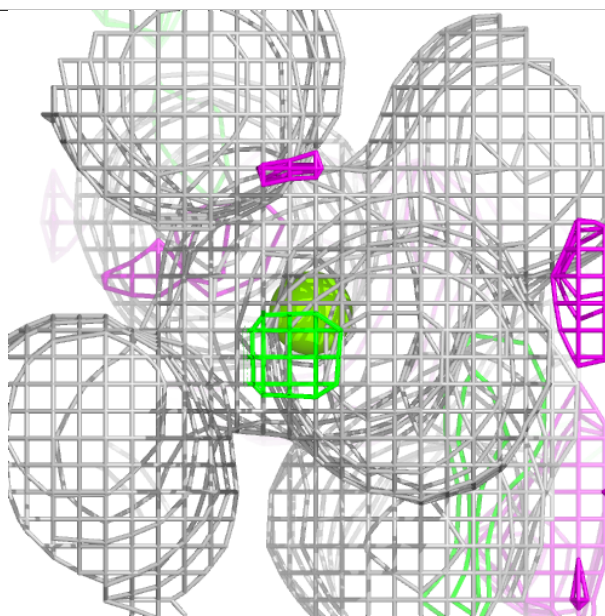
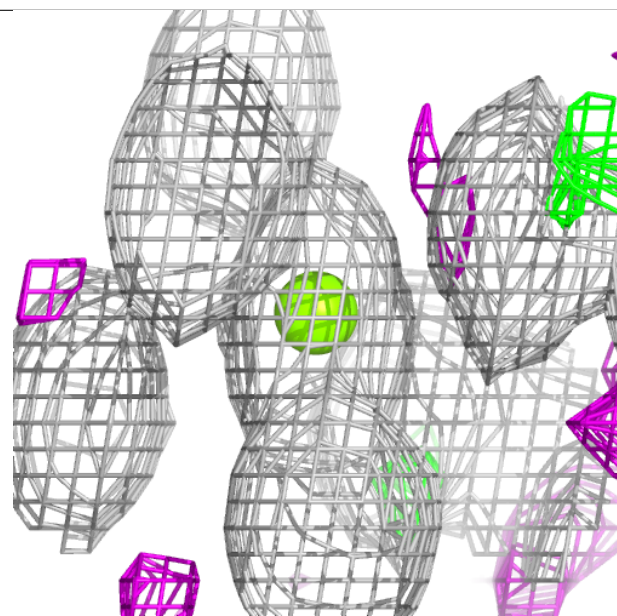
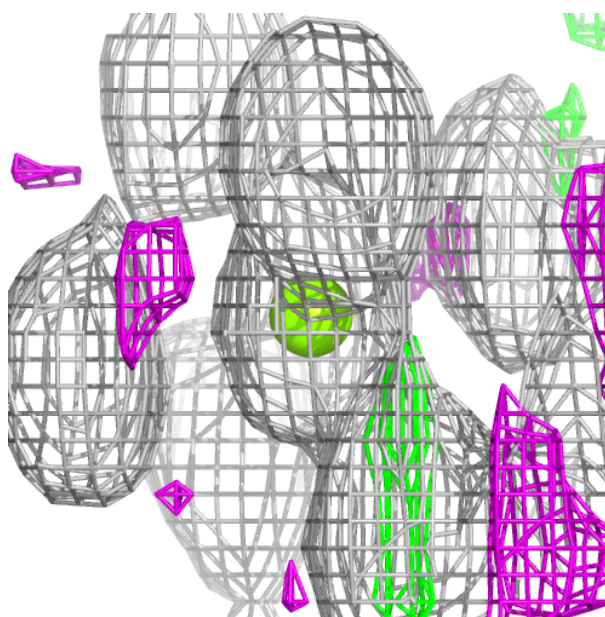
Electron density around MG A 403:

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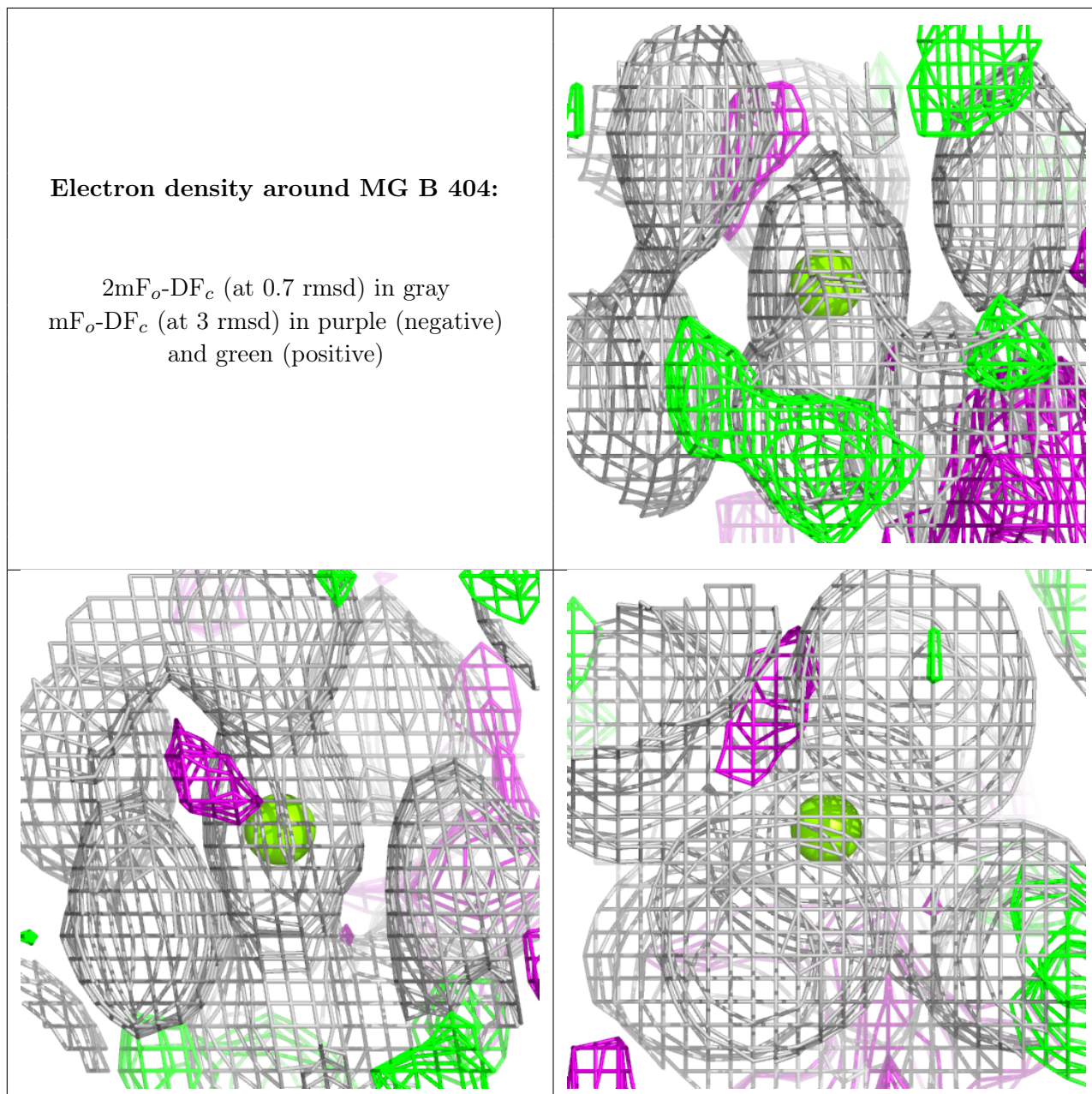
Electron density around MG A 404:

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and green (positive)



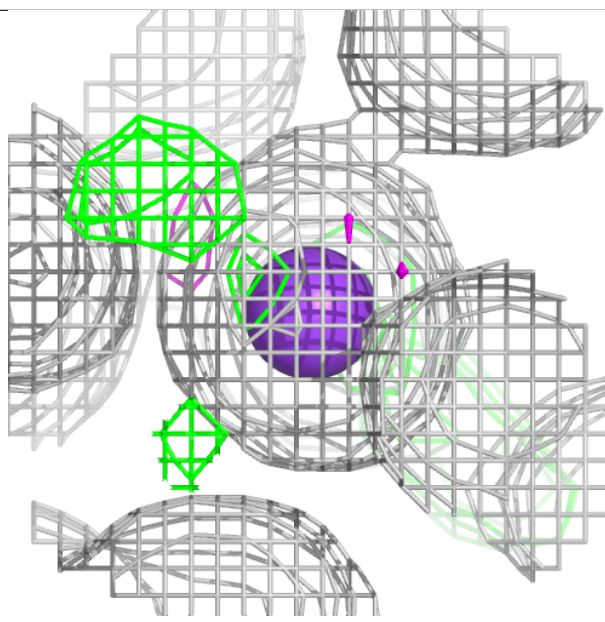
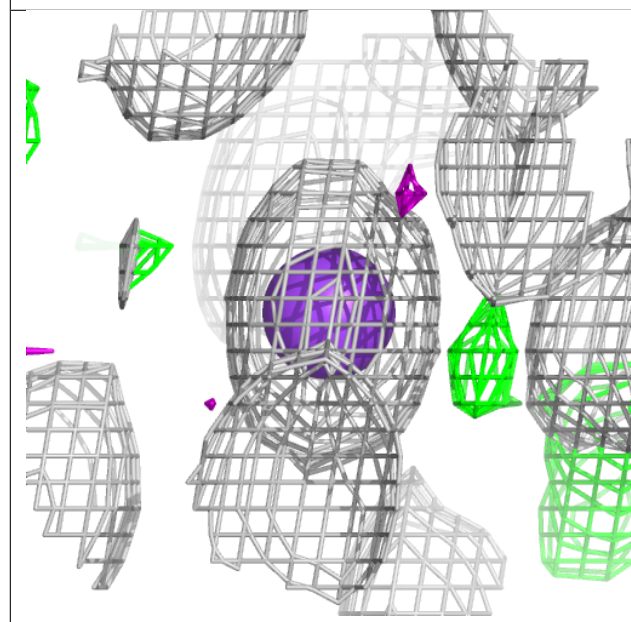
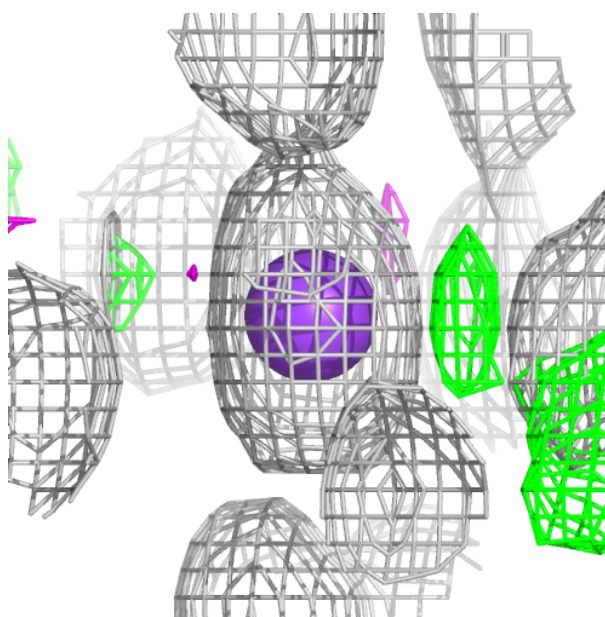
Electron density around MG B 404:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



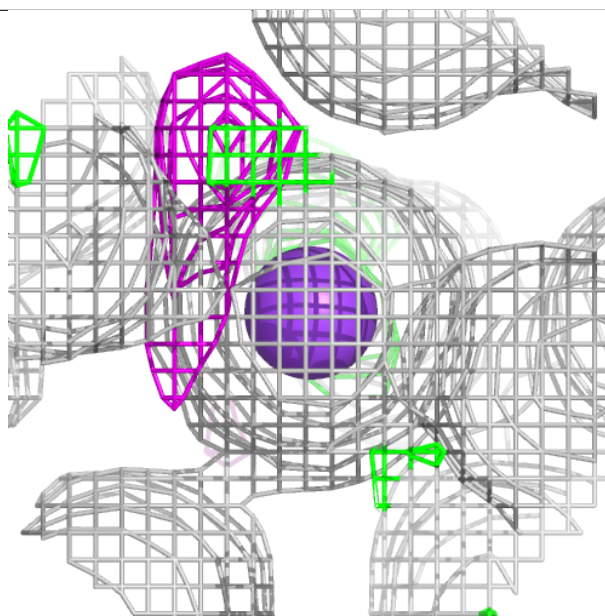
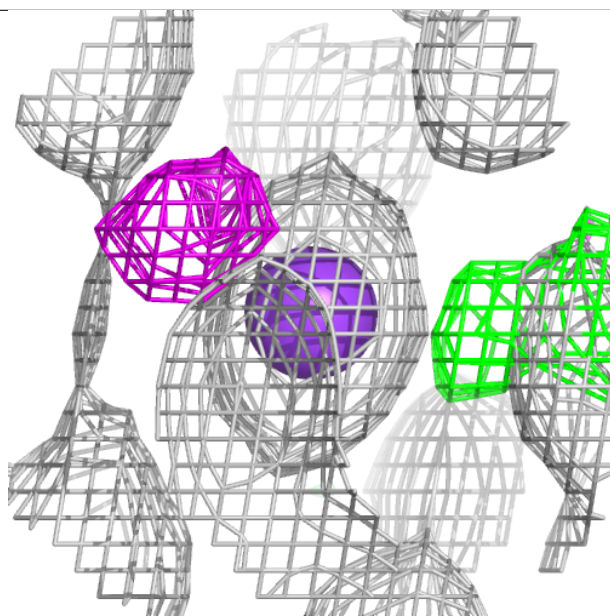
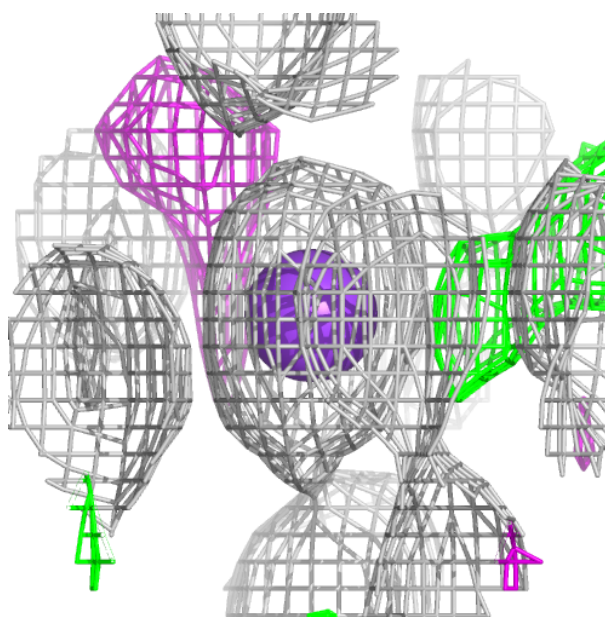
Electron density around K A 405:

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



Electron density around K B 406:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.