



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:30 PM UTC

PDB ID : 4NDN / pdb_00004ndn
Title : Structural insights of MAT enzymes: MATa2b complexed with SAM and PPNP
Authors : Murray, B.; Antonyuk, S.V.; Marina, A.; Lu, S.C.; Mato, J.M.; Hasnain, S.S.; Rojas, A.L.
Deposited on : 2013-10-27
Resolution : 2.34 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

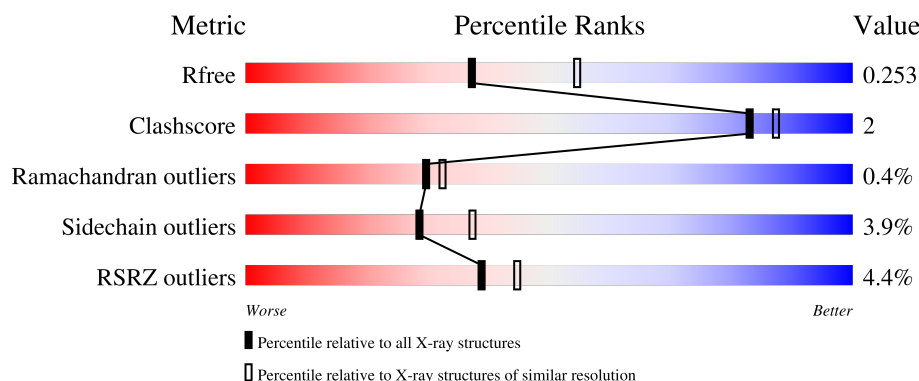
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	395	
1	B	395	
1	C	395	
1	D	395	

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Mol	Chain	Length	Quality of chain
2	E	323	6% 92% . . .
2	F	323	15% 82% 11% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17113 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 isoform type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2822	1790	492	529	11			
1	B	383	Total	C	N	O	S	0	0	0
			2980	1883	520	566	11			
1	C	360	Total	C	N	O	S	0	0	0
			2809	1782	490	526	11			
1	D	382	Total	C	N	O	S	0	1	0
			2980	1882	522	565	11			

- Molecule 2 is a protein called Methionine adenosyltransferase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	309	Total	C	N	O	S	0	1	0
			2456	1551	449	446	10			
2	F	304	Total	C	N	O	S	0	1	0
			2416	1527	442	437	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



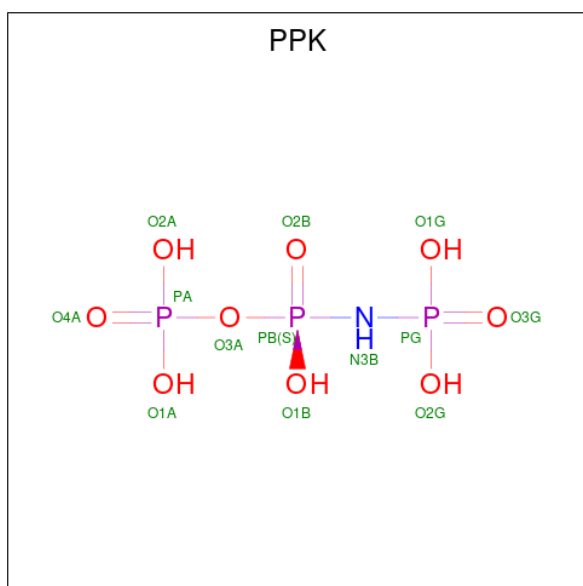
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

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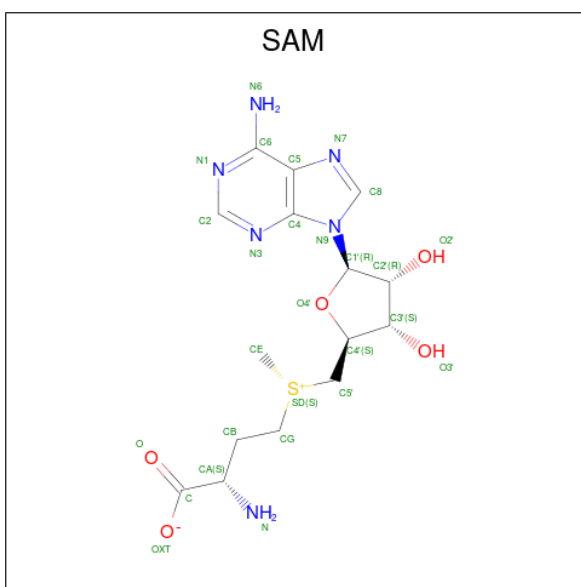
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (CCD ID: PPK) (formula: $\text{H}_6\text{NO}_9\text{P}_3$).



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

- Molecule 6 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $\text{C}_{15}\text{H}_{22}\text{N}_6\text{O}_5\text{S}$).



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

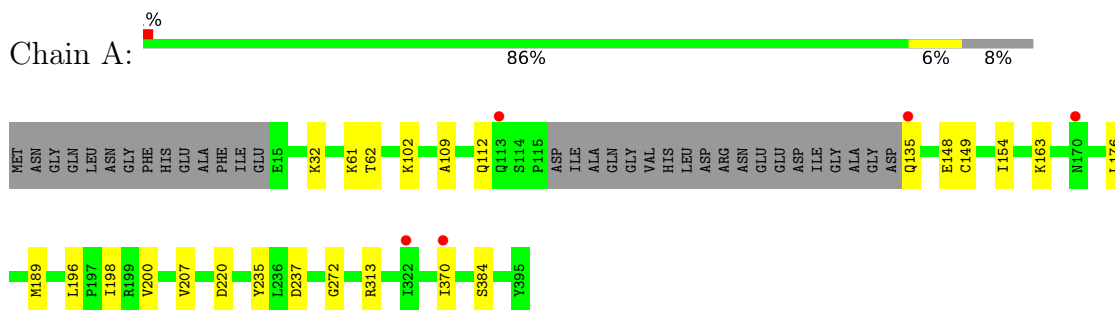
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	109	Total O 109 109	0	0
7	B	97	Total O 97 97	0	0
7	C	91	Total O 91 91	0	0
7	D	116	Total O 116 116	0	0
7	E	67	Total O 67 67	0	0
7	F	18	Total O 18 18	0	0

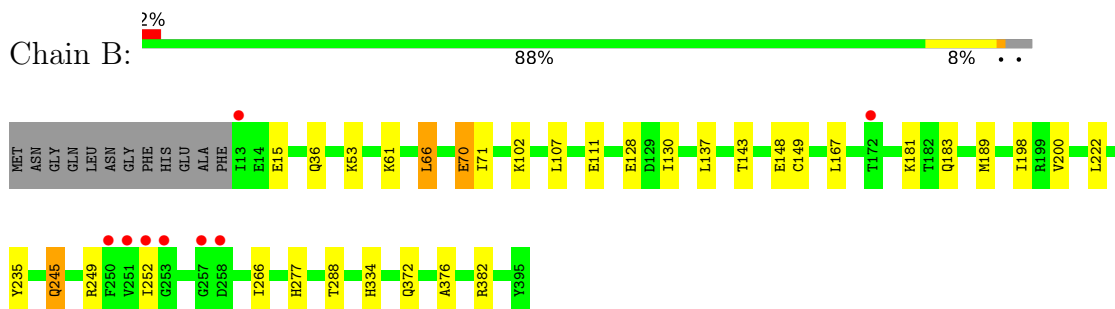
3 Residue-property plots [i](#)

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.

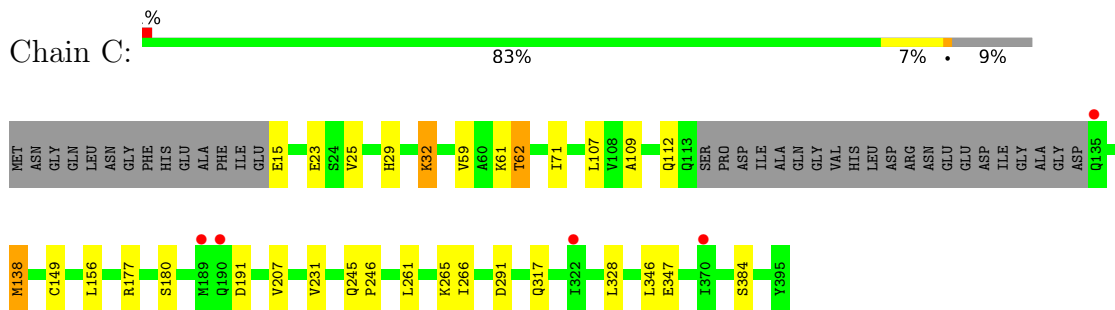
- Molecule 1: S-adenosylmethionine synthase isoform type-2



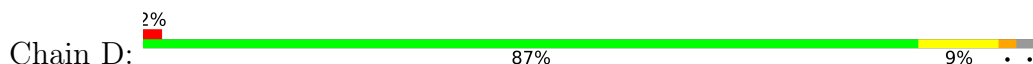
- Molecule 1: S-adenosylmethionine synthase isoform type-2

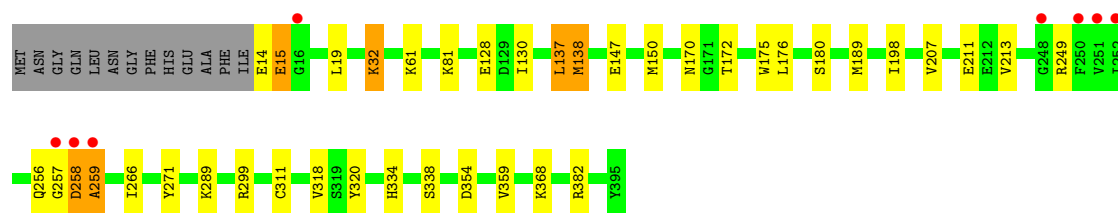


- Molecule 1: S-adenosylmethionine synthase isoform type-2

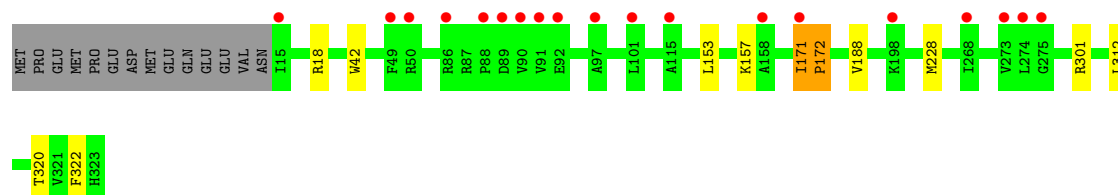
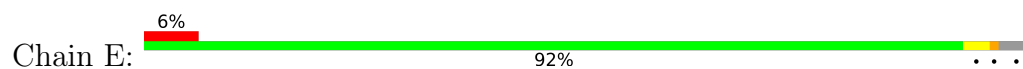


- Molecule 1: S-adenosylmethionine synthase isoform type-2

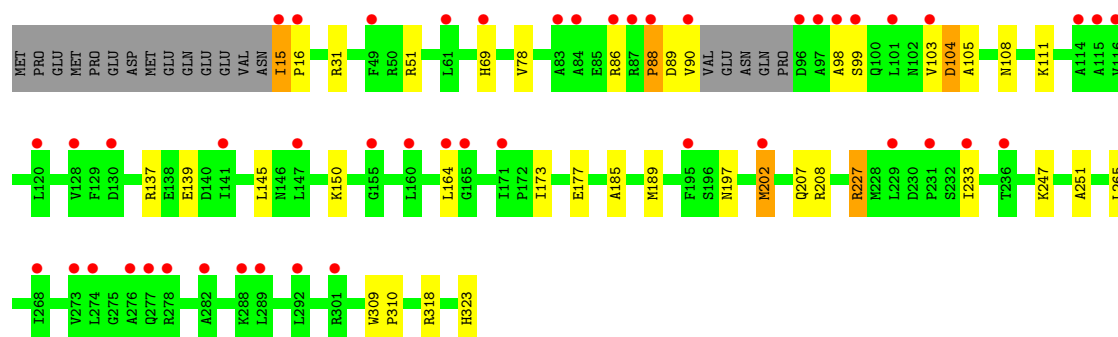
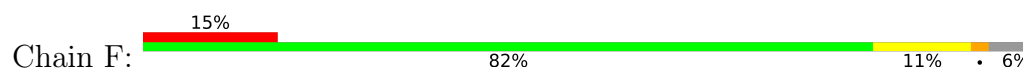




• Molecule 2: Methionine adenosyltransferase 2 subunit beta



• Molecule 2: Methionine adenosyltransferase 2 subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.14Å 122.18Å 298.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.78 – 2.34 47.78 – 2.34	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.78-2.34) 96.9 (47.78-2.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.34Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.211 , 0.251 0.212 , 0.253	Depositor DCC
R_{free} test set	5409 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17113	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: MG, SAM, EDO, PPK

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	0.46	0/2879	0.69	0/3893
1	B	0.46	0/3039	0.69	0/4111
1	C	0.43	0/2865	0.68	0/3873
1	D	0.47	0/3042	0.70	0/4114
2	E	0.44	0/2518	0.71	0/3415
2	F	0.45	0/2476	0.73	0/3355
All	All	0.45	0/16819	0.70	0/22761

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
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	88	PRO	Peptide

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	2822	0	2832	12	0
1	B	2980	0	2973	17	0
1	C	2809	0	2820	14	0
1	D	2980	0	2975	29	0
2	E	2456	0	2431	5	0
2	F	2416	0	2394	12	0
3	A	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	18	0	0
4	B	20	0	30	0	0
4	C	8	0	12	0	0
4	D	24	0	36	0	0
4	E	4	0	6	0	0
5	A	13	0	1	0	0
5	C	13	0	1	0	0
6	A	27	0	22	0	0
6	C	27	0	22	1	0
7	A	109	0	0	0	0
7	B	97	0	0	0	0
7	C	91	0	0	0	0
7	D	116	0	0	0	0
7	E	67	0	0	0	0
7	F	18	0	0	0	0
All	All	17113	0	16573	80	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 2.

All (80) 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:D:150:MET:HE3	1:D:299:ARG:NH1	2.07	0.69
1:D:189:MET:HB2	1:D:198:ILE:HD11	1.77	0.66
1:D:150:MET:HA	1:D:150:MET:HE2	1.80	0.64
1:D:150:MET:HE1	1:D:271:TYR:CE1	2.34	0.62
2:F:202:MET:HE1	2:F:265:LEU:HD22	1.82	0.62
1:B:36:GLN:HE21	1:B:372:GLN:HE21	1.52	0.56
1:D:150:MET:HE3	1:D:299:ARG:CZ	2.36	0.56
1:A:313:ARG:NH2	2:F:323:HIS:O	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:VAL:HG13	1:C:261:LEU:HD23	1.88	0.55
1:A:109:ALA:HB1	1:B:61:LYS:CE	2.37	0.54
1:B:376:ALA:O	1:B:382:ARG:NH2	2.41	0.53
2:E:301[A]:ARG:HH11	2:E:301[A]:ARG:HG2	1.73	0.53
1:D:150:MET:HE1	1:D:271:TYR:HE1	1.71	0.53
1:A:189:MET:HB2	1:A:198:ILE:HD11	1.89	0.53
1:B:245:GLN:HE21	1:B:245:GLN:HA	1.74	0.52
1:C:138:MET:HE2	1:C:291:ASP:HA	1.90	0.52
1:D:138:MET:HE3	1:D:318:VAL:HG23	1.91	0.52
1:C:71:ILE:O	1:C:112:GLN:HA	2.11	0.51
1:C:61:LYS:O	1:C:62:THR:C	2.53	0.51
2:F:31[B]:ARG:NH2	2:F:177:GLU:O	2.43	0.51
1:B:15:GLU:HB2	1:B:189:MET:HE1	1.93	0.51
1:D:15:GLU:N	1:D:15:GLU:OE1	2.44	0.50
1:D:138:MET:CE	1:D:318:VAL:HG23	2.42	0.49
1:A:109:ALA:HB1	1:B:61:LYS:HE3	1.94	0.49
2:E:228:MET:HA	2:E:228:MET:HE2	1.94	0.49
1:D:176:LEU:HD22	1:D:207:VAL:HG21	1.95	0.49
1:C:109:ALA:HB1	1:D:61:LYS:HE2	1.94	0.48
1:B:66:LEU:HD12	1:B:107:LEU:HB2	1.95	0.48
1:D:175:TRP:CG	1:D:213:VAL:HG11	2.48	0.48
1:D:170:ASN:OD1	1:D:172:THR:HG23	2.13	0.48
2:F:227:ARG:HG2	2:F:233:ILE:HB	1.95	0.47
1:B:200:VAL:HG23	1:B:235:TYR:HB3	1.96	0.47
1:D:311:CYS:HB3	1:D:338:SER:HB2	1.96	0.47
1:A:176:LEU:HD22	1:A:207:VAL:HG21	1.97	0.47
1:B:143:THR:O	1:B:149:CYS:HA	2.14	0.47
1:B:266:ILE:HD12	1:B:277:HIS:CE1	2.50	0.47
1:C:29:HIS:CE1	1:C:265:LYS:HE2	2.50	0.47
1:C:156:LEU:HD22	1:C:231:VAL:HG22	1.98	0.46
1:C:317:GLN:NE2	1:D:19:LEU:O	2.48	0.46
1:D:213:VAL:O	1:D:249:ARG:NH2	2.49	0.46
6:C:405:SAM:N	1:D:289:LYS:HE3	2.31	0.46
1:A:237:ASP:OD1	1:A:237:ASP:C	2.60	0.45
1:C:23:GLU:HG2	1:D:137:LEU:HD21	1.98	0.45
1:A:109:ALA:HB2	1:C:107:LEU:HD23	1.99	0.44
2:E:18:ARG:HB3	2:E:42:TRP:CE3	2.52	0.44
1:D:180:SER:HB3	1:D:207:VAL:HG23	1.99	0.44
1:A:109:ALA:HB1	1:B:61:LYS:HE2	1.99	0.44
1:A:154:ILE:HD12	1:A:272:GLY:HA3	2.00	0.44
2:F:103:VAL:HA	2:F:105:ALA:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:ILE:HD11	2:F:185:ALA:HB3	2.00	0.43
1:B:130:ILE:CD1	1:B:288:THR:HG22	2.48	0.43
1:A:154:ILE:HD12	1:A:272:GLY:CA	2.48	0.43
2:E:320:THR:HG23	2:E:322:PHE:O	2.18	0.43
1:A:61:LYS:O	1:A:62:THR:C	2.61	0.43
1:B:70:GLU:HA	1:B:111:GLU:O	2.19	0.43
1:C:180:SER:HB3	1:C:207:VAL:HG23	1.99	0.43
2:F:90:VAL:HG13	2:F:208:ARG:NH1	2.34	0.42
1:D:258:ASP:O	1:D:259:ALA:CB	2.67	0.42
1:D:354:ASP:HB3	1:D:359:VAL:HG11	2.00	0.42
2:E:171:ILE:HA	2:E:172:PRO:HD3	1.92	0.42
1:A:200:VAL:HG23	1:A:235:TYR:HB3	2.02	0.42
1:D:175:TRP:CD1	1:D:213:VAL:HG11	2.54	0.42
1:B:252:ILE:HG23	1:B:252:ILE:O	2.20	0.41
1:D:258:ASP:O	1:D:259:ALA:HB3	2.20	0.41
1:C:245:GLN:N	1:C:246:PRO:CD	2.83	0.41
2:F:15:ILE:N	2:F:16:PRO:HD2	2.35	0.41
2:F:103:VAL:HA	2:F:104:ASP:CB	2.50	0.41
2:F:189:MET:HE3	2:F:251:ALA:HB2	2.03	0.41
1:B:181:LYS:HE3	1:B:183:GLN:HE21	1.86	0.41
1:D:32:LYS:HA	1:D:32:LYS:HE2	2.02	0.41
1:D:138:MET:HE1	1:D:320:TYR:CD1	2.55	0.41
1:D:256:GLN:HA	1:D:257:GLY:HA2	1.81	0.41
2:F:309:TRP:CG	2:F:310:PRO:HD3	2.56	0.41
1:C:266:ILE:HD11	1:D:266:ILE:HD11	2.03	0.41
1:B:53:LYS:O	1:B:71:ILE:HA	2.22	0.40
1:C:25:VAL:CG2	1:C:32:LYS:HD3	2.51	0.40
1:D:150:MET:HE1	1:D:271:TYR:CD1	2.56	0.40
1:D:14:GLU:N	1:D:14:GLU:OE2	2.55	0.40
2:F:90:VAL:HG13	2:F:208:ARG:HH12	1.85	0.40
1:B:189:MET:HB2	1:B:198:ILE:HD11	2.02	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	358/395 (91%)	345 (96%)	13 (4%)	0	100	100
1	B	381/395 (96%)	365 (96%)	16 (4%)	0	100	100
1	C	356/395 (90%)	343 (96%)	12 (3%)	1 (0%)	36	41
1	D	381/395 (96%)	370 (97%)	10 (3%)	1 (0%)	36	41
2	E	308/323 (95%)	294 (96%)	13 (4%)	1 (0%)	36	41
2	F	301/323 (93%)	284 (94%)	12 (4%)	5 (2%)	7	5
All	All	2085/2226 (94%)	2001 (96%)	76 (4%)	8 (0%)	30	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	89	ASP
2	F	104	ASP
1	D	259	ALA
2	F	88	PRO
1	C	62	THR
2	F	98	ALA
2	F	86	ARG
2	E	172	PRO

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	302/327 (92%)	291 (96%)	11 (4%)	31	40
1	B	318/327 (97%)	307 (96%)	11 (4%)	32	41
1	C	300/327 (92%)	290 (97%)	10 (3%)	33	43
1	D	318/327 (97%)	305 (96%)	13 (4%)	27	35
2	E	263/276 (95%)	258 (98%)	5 (2%)	50	63
2	F	258/276 (94%)	240 (93%)	18 (7%)	14	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1759/1860 (95%)	1691 (96%)	68 (4%)	28	37

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	102	LYS
1	A	112	GLN
1	A	135	GLN
1	A	148	GLU
1	A	149	CYS
1	A	163	LYS
1	A	196	LEU
1	A	220	ASP
1	A	370	ILE
1	A	384	SER
1	B	66	LEU
1	B	70	GLU
1	B	102	LYS
1	B	128	GLU
1	B	137	LEU
1	B	148	GLU
1	B	167	LEU
1	B	222	LEU
1	B	245	GLN
1	B	249	ARG
1	B	334	HIS
1	C	15	GLU
1	C	32	LYS
1	C	138	MET
1	C	149	CYS
1	C	177	ARG
1	C	191	ASP
1	C	328	LEU
1	C	346	LEU
1	C	347	GLU
1	C	384	SER
1	D	15	GLU
1	D	32	LYS
1	D	81	LYS
1	D	128	GLU
1	D	130	ILE

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Mol	Chain	Res	Type
1	D	137	LEU
1	D	138	MET
1	D	147	GLU
1	D	211	GLU
1	D	258	ASP
1	D	334	HIS
1	D	368	LYS
1	D	382	ARG
2	E	153	LEU
2	E	157	LYS
2	E	171	ILE
2	E	188	VAL
2	E	312	LEU
2	F	15	ILE
2	F	51	ARG
2	F	69	HIS
2	F	78	VAL
2	F	99	SER
2	F	108	ASN
2	F	111	LYS
2	F	137	ARG
2	F	139	GLU
2	F	145	LEU
2	F	150	LYS
2	F	164	LEU
2	F	197	ASN
2	F	202	MET
2	F	207	GLN
2	F	227	ARG
2	F	247	LYS
2	F	318	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	243	HIS
1	B	36	GLN
1	B	89	HIS
1	B	105	ASN
1	B	183	GLN
1	B	245	GLN

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Mol	Chain	Res	Type
1	B	326	HIS
1	C	36	GLN
1	C	48	GLN
1	C	105	ASN
1	C	317	GLN
1	C	334	HIS
1	C	352	ASN
1	D	89	HIS
1	D	135	GLN
2	F	60	ASN
2	F	100	GLN
2	F	102	ASN
2	F	207	GLN
2	F	296	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	402	-	3,3,3	0.45	0	2,2,2	0.30	0
5	PPK	A	406	3	11,12,12	2.68	4 (36%)	14,20,20	1.01	0
6	SAM	C	405	-	27,29,29	1.48	4 (14%)	34,42,42	2.01	8 (23%)
6	SAM	A	407	-	27,29,29	1.46	4 (14%)	34,42,42	1.95	10 (29%)
4	EDO	D	403	-	3,3,3	0.45	0	2,2,2	0.35	0
4	EDO	B	402	-	3,3,3	0.64	0	2,2,2	0.07	0
4	EDO	A	403	-	3,3,3	0.44	0	2,2,2	0.26	0
4	EDO	A	405	-	3,3,3	0.43	0	2,2,2	0.34	0
5	PPK	C	404	3	11,12,12	2.65	4 (36%)	14,20,20	1.00	1 (7%)
4	EDO	B	404	-	3,3,3	0.47	0	2,2,2	0.29	0
4	EDO	A	404	-	3,3,3	0.41	0	2,2,2	0.36	0
4	EDO	B	405	-	3,3,3	0.42	0	2,2,2	0.34	0
4	EDO	D	404	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	C	402	-	3,3,3	0.39	0	2,2,2	0.38	0
4	EDO	D	407	-	3,3,3	0.46	0	2,2,2	0.20	0
4	EDO	E	401	-	3,3,3	0.44	0	2,2,2	0.37	0
4	EDO	B	403	-	3,3,3	0.44	0	2,2,2	0.34	0
4	EDO	D	406	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	D	405	-	3,3,3	0.56	0	2,2,2	0.22	0
4	EDO	B	401	-	3,3,3	0.43	0	2,2,2	0.36	0
4	EDO	C	403	-	3,3,3	0.52	0	2,2,2	0.16	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
4	EDO	D	402	-	-	1/1/1/1	-
5	PPK	A	406	3	-	2/8/12/12	-
6	SAM	C	405	-	-	6/17/33/33	0/3/3/3
6	SAM	A	407	-	-	6/17/33/33	0/3/3/3
4	EDO	D	403	-	-	1/1/1/1	-
4	EDO	B	402	-	-	0/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	A	405	-	-	1/1/1/1	-
5	PPK	C	404	3	-	4/8/12/12	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	D	404	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	402	-	-	1/1/1/1	-
4	EDO	D	407	-	-	1/1/1/1	-
4	EDO	E	401	-	-	0/1/1/1	-
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	D	406	-	-	1/1/1/1	-
4	EDO	D	405	-	-	1/1/1/1	-
4	EDO	B	401	-	-	1/1/1/1	-
4	EDO	C	403	-	-	1/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	406	PPK	PB-N3B	5.08	1.76	1.63
5	A	406	PPK	PG-N3B	4.94	1.76	1.63
5	C	404	PPK	PB-N3B	4.87	1.76	1.63
5	C	404	PPK	PG-N3B	4.67	1.75	1.63
6	C	405	SAM	C5-C4	4.35	1.46	1.39
6	A	407	SAM	C5-C4	4.19	1.46	1.39
5	C	404	PPK	PB-O3A	3.23	1.63	1.59
5	A	406	PPK	PB-O3A	3.03	1.62	1.59
6	A	407	SAM	C5-N7	-2.94	1.33	1.39
6	A	407	SAM	C4-N9	-2.70	1.32	1.37
6	C	405	SAM	C5-N7	-2.68	1.34	1.39
6	C	405	SAM	C5-C6	2.61	1.48	1.41
5	C	404	PPK	PB-O2B	2.26	1.49	1.46
6	C	405	SAM	C8-N7	2.26	1.36	1.31
6	A	407	SAM	C5-C6	2.24	1.47	1.41
5	A	406	PPK	PB-O1B	2.05	1.62	1.56

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	405	SAM	C5-C4-N3	-5.90	118.60	126.72
6	A	407	SAM	C5-C4-N3	-4.82	120.08	126.72
6	C	405	SAM	N3-C4-N9	4.57	134.93	127.17
6	A	407	SAM	N3-C4-N9	4.21	134.33	127.17
6	A	407	SAM	N3-C2-N1	-3.87	122.72	128.58
6	C	405	SAM	C2-N3-C4	3.85	121.22	111.83
6	C	405	SAM	N3-C2-N1	-3.67	123.03	128.58
6	C	405	SAM	C4-C5-N7	-3.57	106.50	110.58
6	A	407	SAM	C2-N3-C4	3.35	120.02	111.83
6	A	407	SAM	C4-N9-C8	3.21	109.10	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	407	SAM	C2-N1-C6	2.79	123.31	118.73
6	C	405	SAM	C5-N7-C8	2.73	107.73	103.45
6	C	405	SAM	C4-N9-C8	2.60	108.47	105.74
6	A	407	SAM	C4-C5-N7	-2.58	107.64	110.58
6	A	407	SAM	N9-C8-N7	-2.30	110.67	113.94
6	A	407	SAM	N6-C6-N1	2.29	123.47	118.38
6	A	407	SAM	C5-N7-C8	2.26	107.01	103.45
6	C	405	SAM	N9-C8-N7	-2.19	110.83	113.94
5	C	404	PPK	O1G-PG-O3G	-2.14	108.07	113.45

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406	PPK	PB-N3B-PG-O3G
5	A	406	PPK	PG-N3B-PB-O2B
5	C	404	PPK	PB-N3B-PG-O3G
5	C	404	PPK	PG-N3B-PB-O2B
5	C	404	PPK	PB-O3A-PA-O2A
6	C	405	SAM	N-CA-CB-CG
6	C	405	SAM	CA-CB-CG-SD
4	A	403	EDO	O1-C1-C2-O2
4	A	405	EDO	O1-C1-C2-O2
4	C	403	EDO	O1-C1-C2-O2
4	D	406	EDO	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2
4	B	401	EDO	O1-C1-C2-O2
4	D	402	EDO	O1-C1-C2-O2
4	D	405	EDO	O1-C1-C2-O2
6	A	407	SAM	C2'-C1'-N9-C8
6	C	405	SAM	C2'-C1'-N9-C8
6	C	405	SAM	C-CA-CB-CG
6	A	407	SAM	OXT-C-CA-CB
4	D	407	EDO	O1-C1-C2-O2
6	A	407	SAM	O-C-CA-CB
6	C	405	SAM	O4'-C1'-N9-C8
4	B	405	EDO	O1-C1-C2-O2
4	D	403	EDO	O1-C1-C2-O2
4	D	404	EDO	O1-C1-C2-O2
4	C	402	EDO	O1-C1-C2-O2
6	A	407	SAM	O4'-C1'-N9-C8
6	A	407	SAM	OXT-C-CA-N

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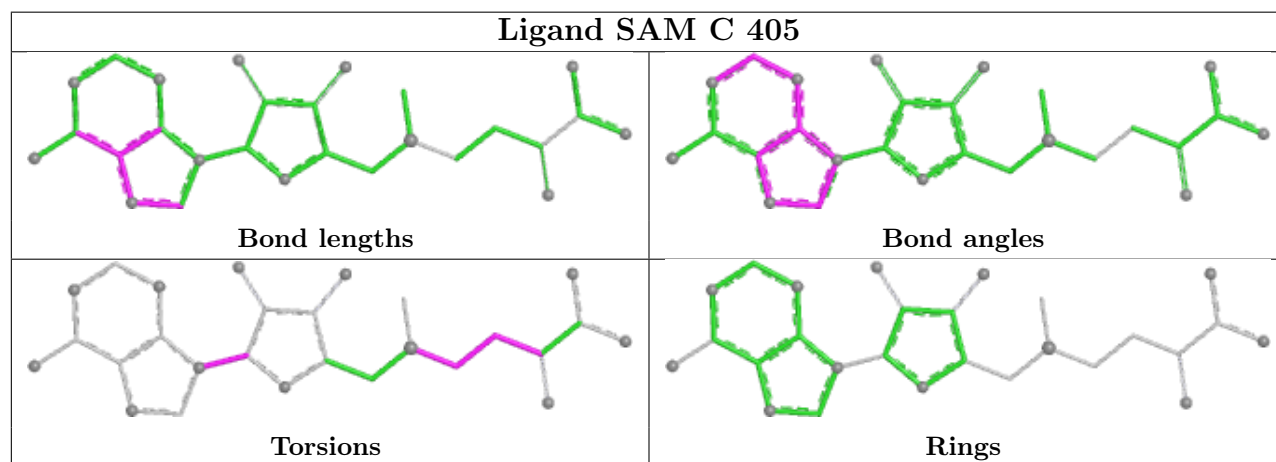
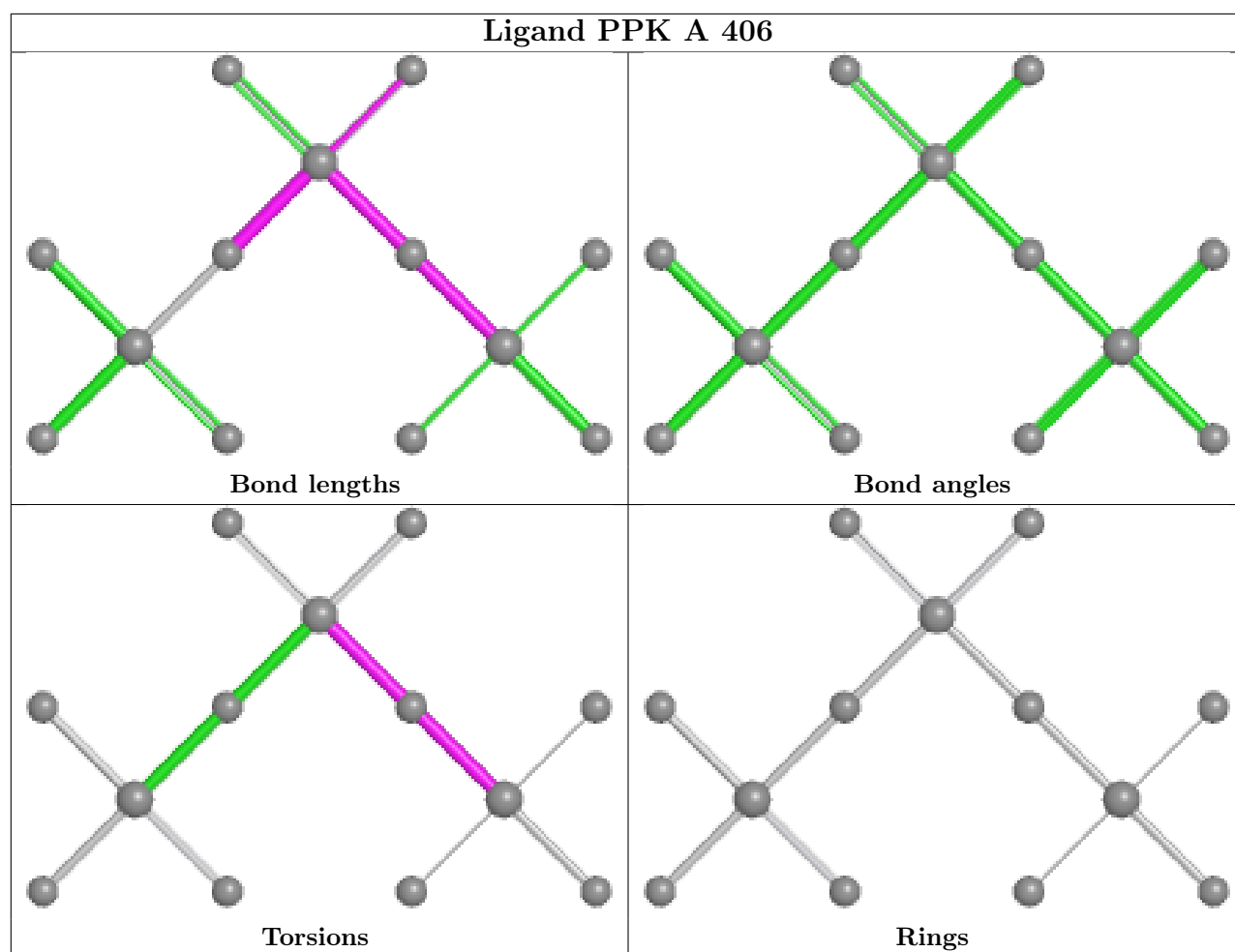
Mol	Chain	Res	Type	Atoms
5	C	404	PPK	PB-O3A-PA-O4A
6	C	405	SAM	CB-CG-SD-C5'
6	A	407	SAM	O-C-CA-N

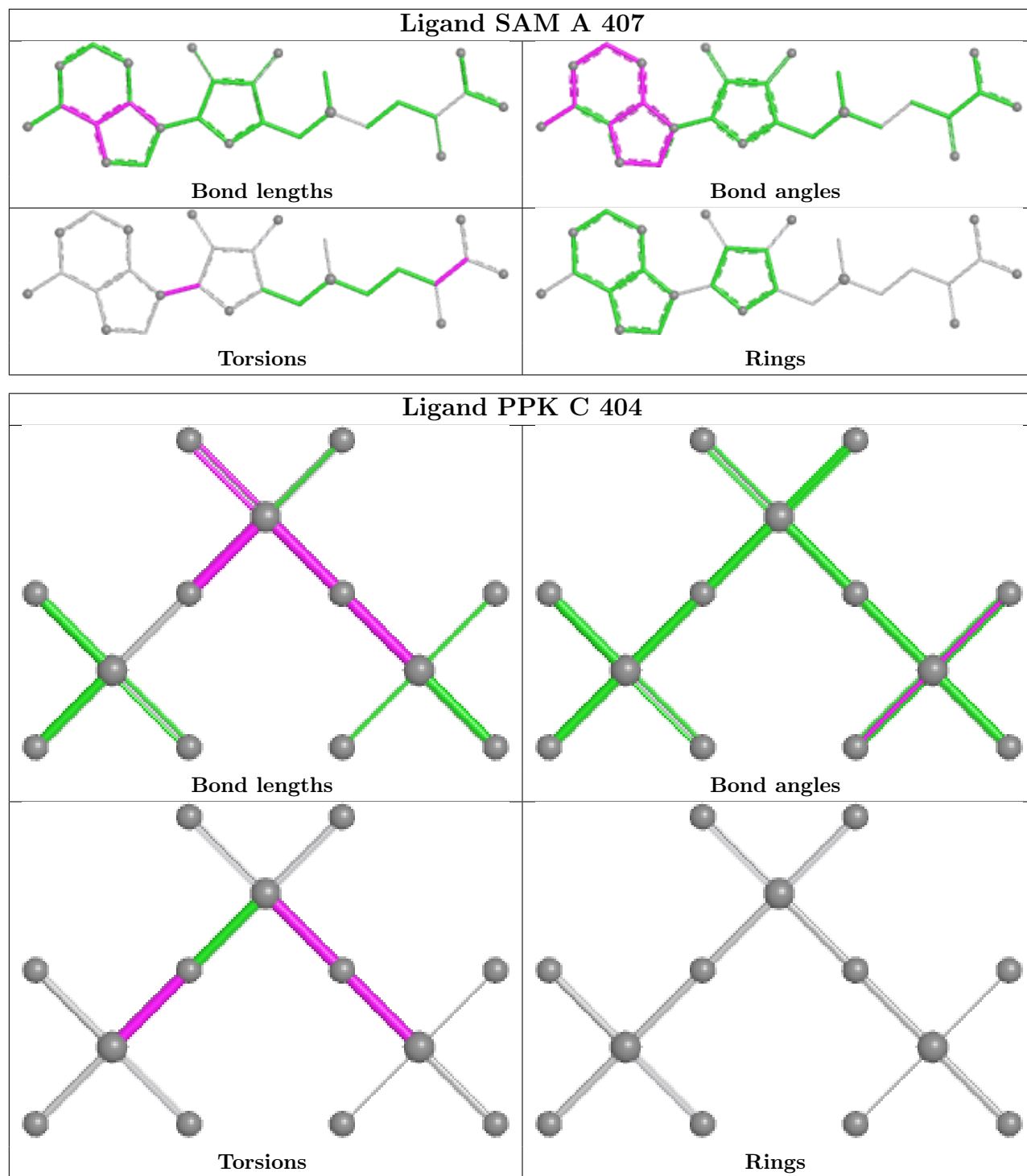
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	405	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 ⓘ

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	362/395 (91%)	0.07	5 (1%) 73 77	32, 47, 71, 109	0
1	B	383/395 (96%)	0.12	8 (2%) 63 68	34, 48, 74, 120	0
1	C	360/395 (91%)	0.30	5 (1%) 73 77	36, 56, 81, 93	0
1	D	382/395 (96%)	-0.05	8 (2%) 63 68	28, 44, 69, 104	1 (0%)
2	E	309/323 (95%)	0.41	19 (6%) 27 32	31, 57, 83, 106	1 (0%)
2	F	304/323 (94%)	1.21	47 (15%) 5 5	35, 83, 111, 130	1 (0%)
All	All	2100/2226 (94%)	0.31	92 (4%) 39 45	28, 52, 92, 130	3 (0%)

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	13	ILE	6.5
2	F	101	LEU	6.1
2	F	98	ALA	5.9
1	B	251	VAL	5.9
1	B	252	ILE	4.8
2	F	84	ALA	4.7
1	D	252	ILE	4.6
2	F	273	VAL	4.4
1	B	250	PHE	4.4
1	D	251	VAL	4.4
2	F	97	ALA	4.3
2	F	274	LEU	4.3
2	F	99	SER	4.1
2	F	103	VAL	4.1
2	F	15	ILE	4.1
1	D	257	GLY	4.0
2	F	87	ARG	3.9
1	D	250	PHE	3.9
2	F	268	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	F	88	PRO	3.8
2	E	49	PHE	3.7
2	E	268	ILE	3.6
1	C	370	ILE	3.5
1	D	259	ALA	3.5
1	B	253	GLY	3.5
2	F	96	ASP	3.4
2	F	164	LEU	3.3
2	F	90	VAL	3.3
2	F	61	LEU	3.2
2	F	292	LEU	3.2
2	F	115	ALA	3.1
2	F	202	MET	3.1
1	A	135	GLN	3.1
1	B	258	ASP	3.0
2	F	83	ALA	3.0
2	F	289	LEU	3.0
2	E	88	PRO	3.0
2	F	229	LEU	2.9
2	F	69	HIS	2.9
2	F	147	LEU	2.9
1	C	135	GLN	2.9
2	E	97	ALA	2.8
2	F	233	ILE	2.8
2	F	282	ALA	2.8
1	B	257	GLY	2.7
2	E	86	ARG	2.7
2	E	90	VAL	2.7
1	D	258	ASP	2.6
2	E	89	ASP	2.6
1	A	113	GLN	2.6
2	F	276	ALA	2.5
1	D	16	GLY	2.5
2	F	116	VAL	2.5
2	E	92	GLU	2.5
2	F	301	ARG	2.5
1	A	370	ILE	2.5
2	E	274	LEU	2.5
2	F	160	LEU	2.4
2	F	236	THR	2.4
2	F	165	GLY	2.4
2	F	155	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	172	THR	2.3
2	E	273	VAL	2.3
2	F	195	PHE	2.3
2	E	91	VAL	2.3
1	C	190	GLN	2.3
1	C	322	ILE	2.2
2	E	15	ILE	2.2
2	E	171	ILE	2.2
2	F	120	LEU	2.2
2	F	277	GLN	2.2
2	F	49	PHE	2.2
1	C	189	MET	2.2
2	F	86	ARG	2.1
2	F	16	PRO	2.1
1	D	248	GLY	2.1
2	E	50	ARG	2.1
2	F	278	ARG	2.1
1	A	322	ILE	2.1
2	F	128	VAL	2.1
2	E	115	ALA	2.1
2	F	130	ASP	2.1
2	F	288	LYS	2.1
2	E	101	LEU	2.1
2	F	141	ILE	2.1
2	E	198	LYS	2.0
2	E	158	ALA	2.0
2	F	231	PRO	2.0
2	E	275	GLY	2.0
2	F	114	ALA	2.0
1	A	170	ASN	2.0
2	F	171	ILE	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 ⓘ

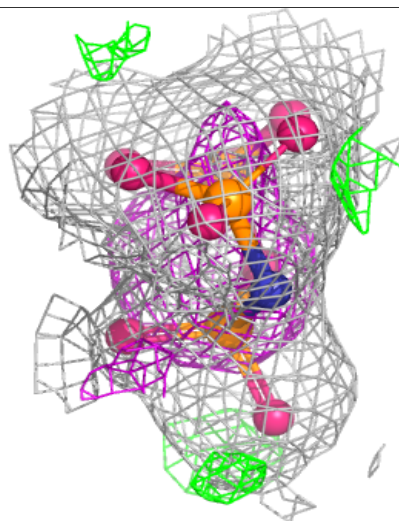
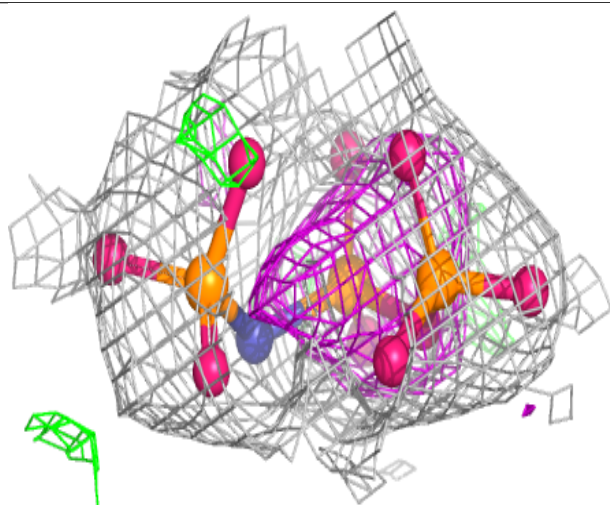
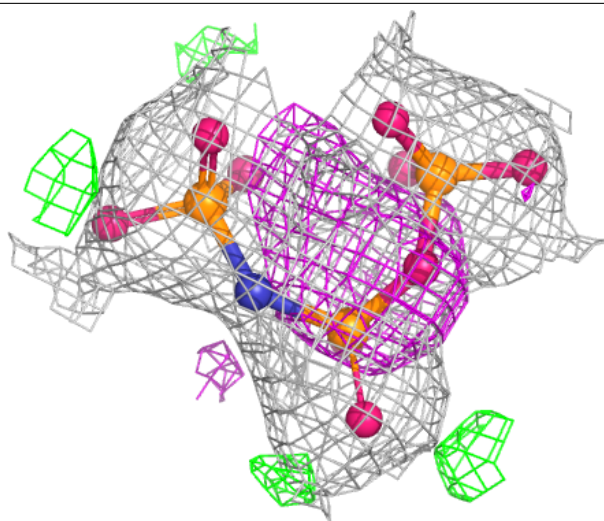
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	C	403	4/4	0.74	0.22	65,68,68,70	0
4	EDO	A	405	4/4	0.76	0.19	75,77,77,79	0
4	EDO	D	404	4/4	0.78	0.25	69,69,70,70	0
4	EDO	B	404	4/4	0.82	0.16	73,75,75,76	0
4	EDO	D	405	4/4	0.82	0.21	57,57,58,60	0
4	EDO	D	403	4/4	0.84	0.21	66,67,67,68	0
4	EDO	A	404	4/4	0.84	0.20	65,67,68,71	0
4	EDO	B	402	4/4	0.84	0.17	46,47,47,48	0
4	EDO	D	402	4/4	0.88	0.11	69,70,71,71	0
4	EDO	B	403	4/4	0.88	0.13	55,56,56,57	0
4	EDO	B	401	4/4	0.88	0.21	75,76,78,81	0
4	EDO	A	403	4/4	0.88	0.17	63,65,67,71	0
4	EDO	D	406	4/4	0.88	0.21	68,68,70,75	0
5	PPK	A	406	13/13	0.89	0.11	56,63,72,74	0
4	EDO	D	407	4/4	0.90	0.12	70,71,72,73	0
4	EDO	C	402	4/4	0.90	0.20	70,70,71,72	0
5	PPK	C	404	13/13	0.92	0.10	52,61,67,73	0
6	SAM	A	407	27/27	0.93	0.10	38,43,56,57	0
4	EDO	E	401	4/4	0.94	0.08	45,45,45,45	0
6	SAM	C	405	27/27	0.95	0.10	41,48,56,57	0
4	EDO	B	405	4/4	0.96	0.09	56,59,59,61	0
3	MG	D	401	1/1	0.97	0.04	32,32,32,32	0
3	MG	A	401	1/1	0.97	0.11	44,44,44,44	0
3	MG	A	402	1/1	0.98	0.05	37,37,37,37	0
3	MG	C	401	1/1	0.98	0.05	43,43,43,43	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.

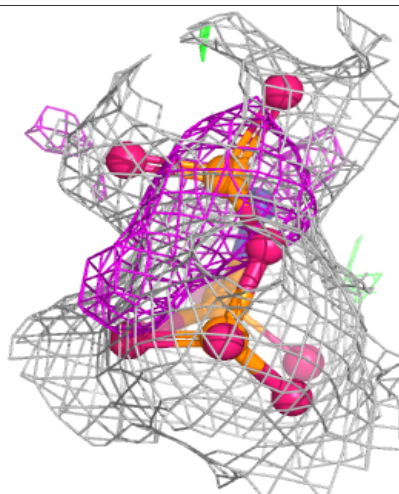
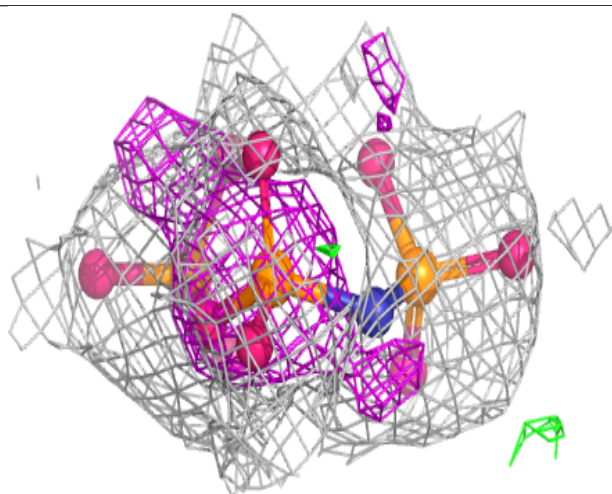
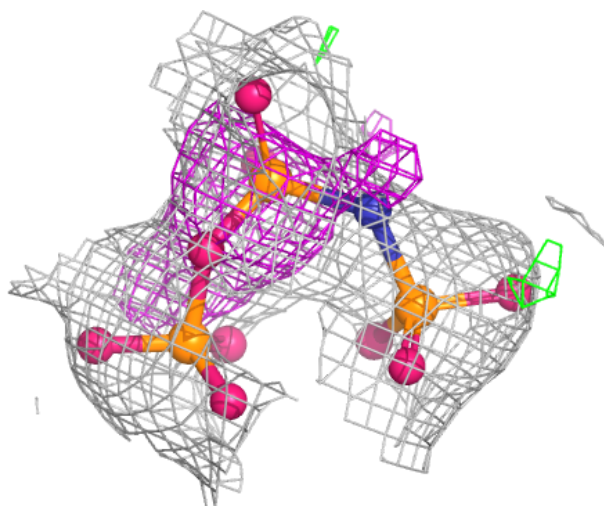
Electron density around PPK A 406:

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



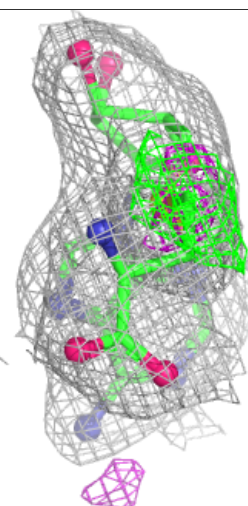
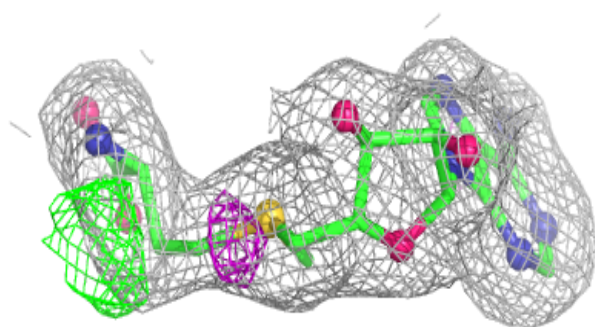
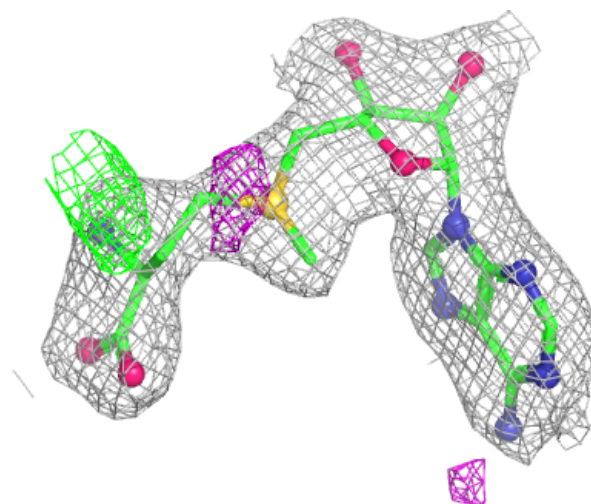
Electron density around PPK C 404:

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



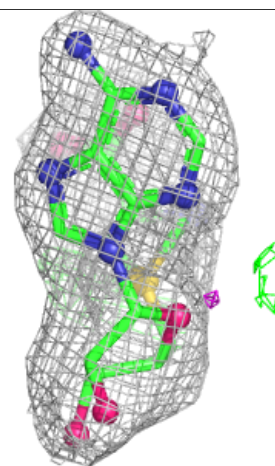
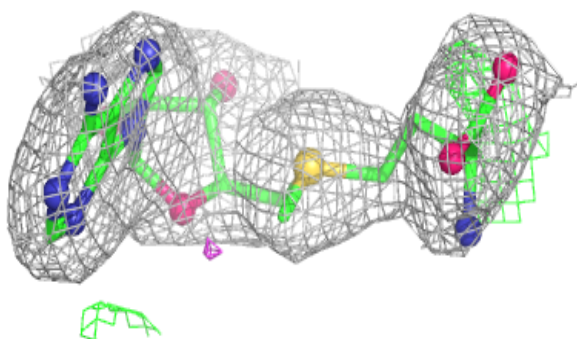
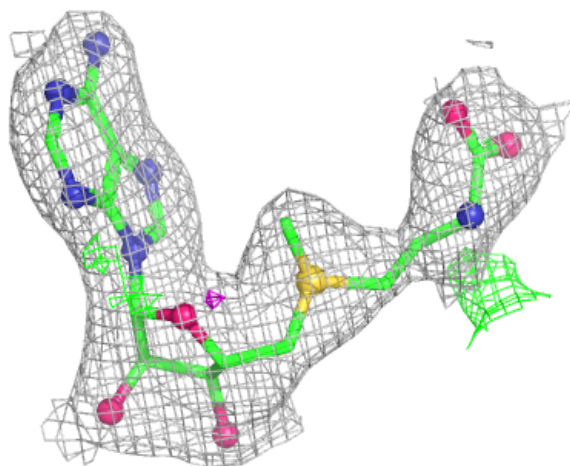
Electron density around SAM A 407:

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



Electron density around SAM C 405:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.