



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2021 – 10:07 AM EDT

PDB ID : 7LOO
Title : S-adenosyl methionine transferase cocrystallized with ATP
Authors : Jackson, C.J.; Tan, L.L.; Laurino, P.
Deposited on : 2021-02-10
Resolution : 1.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

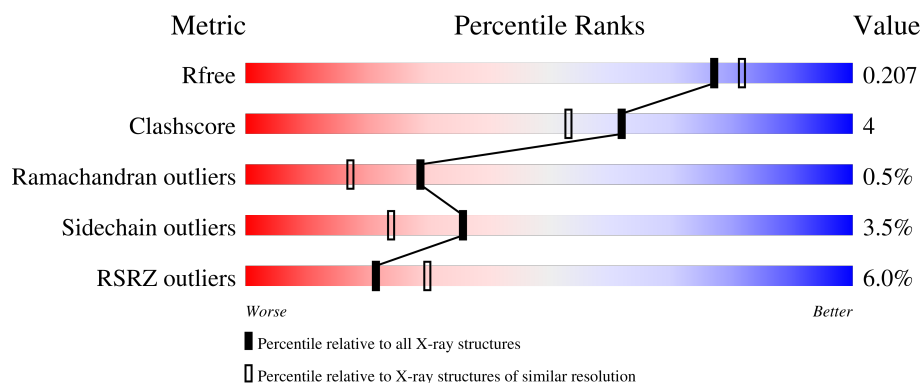
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	384	
1	B	384	
1	Q	384	
1	R	384	

2 Entry composition [i](#)

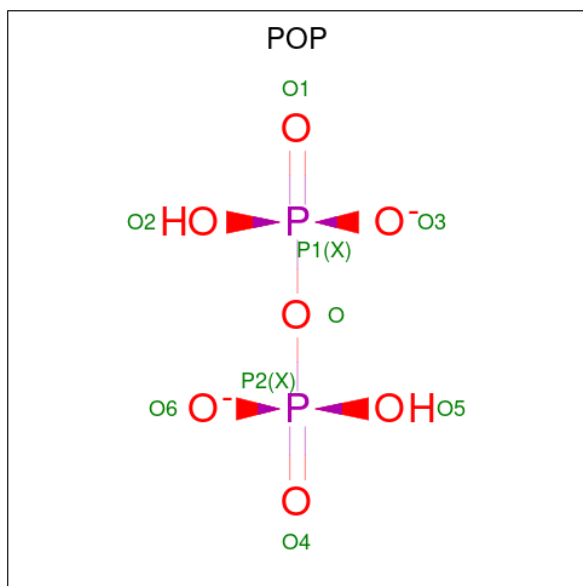
There are 8 unique types of molecules in this entry. The entry contains 12593 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	2	0
			2927	1844	502	567	14			
1	B	378	Total	C	N	O	S	0	1	0
			2917	1842	497	565	13			
1	Q	378	Total	C	N	O	S	0	3	0
			2930	1847	502	567	14			
1	R	377	Total	C	N	O	S	0	2	0
			2918	1839	500	565	14			

- Molecule 2 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			9	7	2		
2	B	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	Q	1	Total	O	P	0	0
			9	7	2		
2	R	1	Total	O	P	0	0
			9	7	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	Q	2	Total	Mg	0	0
			2	2		

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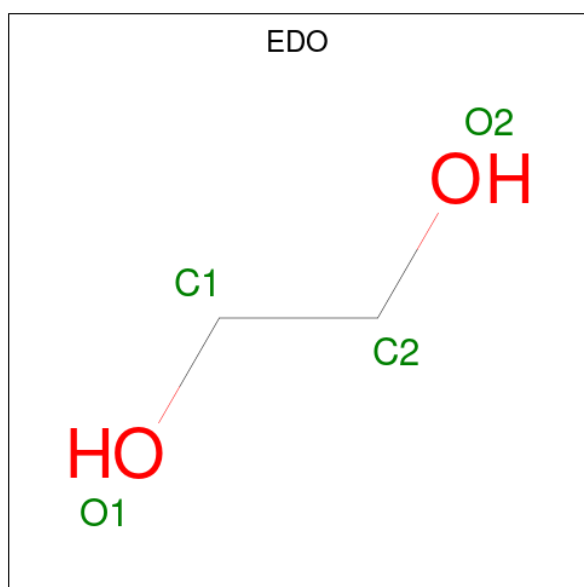
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	R	2	Total	Mg	0	0
			2	2		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	K	0	0
			2	2		
5	Q	2	Total	K	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



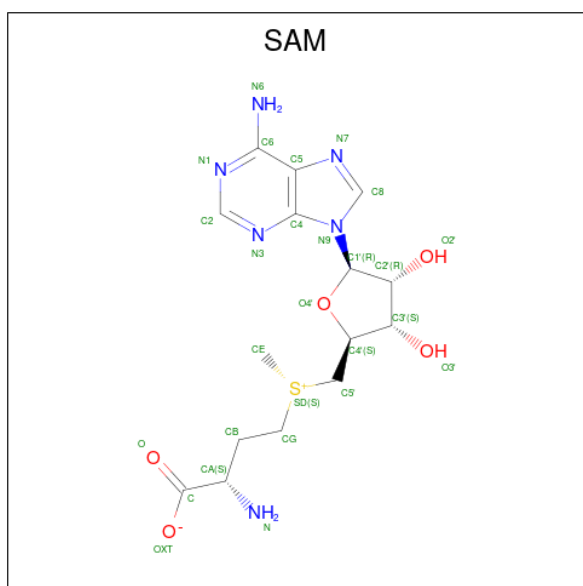
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	Q	1	Total	C	O	0	0
			4	2	2		
6	Q	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	Q	1	Total	C	O	0	0
			4	2	2		
6	Q	1	Total	C	O	0	0
			4	2	2		
6	R	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	244	Total 244	O 244	0	0
8	B	73	Total 73	O 73	0	0
8	Q	245	Total 245	O 245	0	0
8	R	73	Total 73	O 73	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.

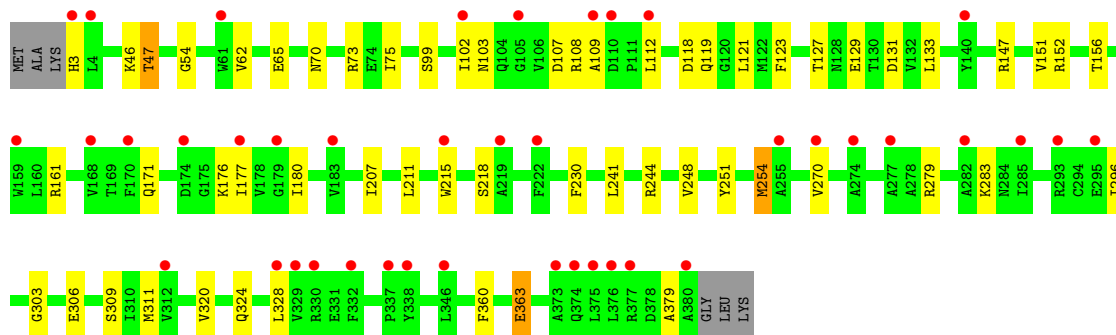
• Molecule 1: S-adenosylmethionine synthase

Chain A:  92% 7% .




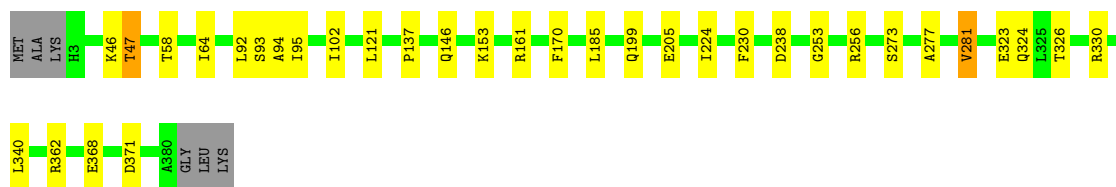
• Molecule 1: S-adenosylmethionine synthase

Chain B:  11% 84% 14% ..




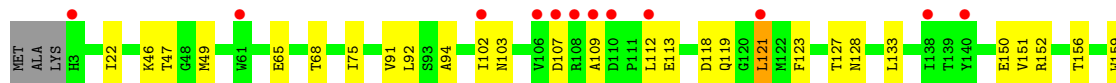
• Molecule 1: S-adenosylmethionine synthase

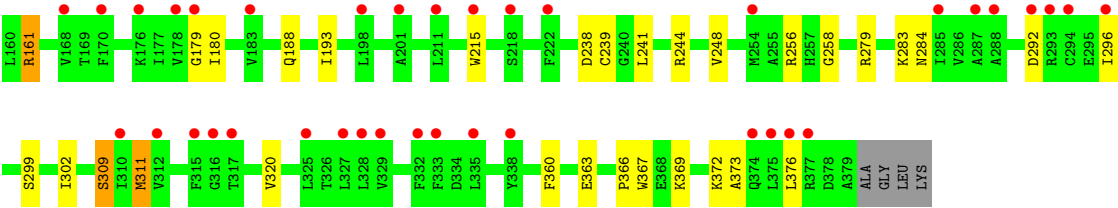
Chain Q:  90% 8% ..



• Molecule 1: S-adenosylmethionine synthase

Chain R:  13% 83% 14% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.92Å 117.78Å 113.21Å 90.00° 107.52° 90.00°	Depositor
Resolution (Å)	35.99 – 1.95 35.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.99-1.95) 99.6 (35.99-1.95)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.207 0.170 , 0.207	Depositor DCC
R_{free} test set	6216 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12593	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.39% 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, POP, K, PO4, EDO

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	0.43	0/2986	0.60	0/4050
1	B	0.29	0/2977	0.49	0/4039
1	Q	0.44	0/2989	0.60	0/4055
1	R	0.29	0/2977	0.49	0/4039
All	All	0.37	0/11929	0.55	0/16183

There are no bond length outliers.

There are no bond angle outliers.

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	2927	0	2879	20	0
1	B	2917	0	2868	27	0
1	Q	2930	0	2883	23	0
1	R	2918	0	2872	32	0
2	A	9	0	0	0	0
2	B	9	0	0	0	0
2	Q	9	0	0	0	0
2	R	9	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	Q	10	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	Q	2	0	0	0	0
4	R	2	0	0	0	0
5	A	2	0	0	0	0
5	Q	2	0	0	0	0
6	A	8	0	12	2	0
6	B	8	0	12	1	0
6	Q	16	0	24	3	0
6	R	4	0	6	0	0
7	A	54	0	43	11	0
7	B	27	0	21	1	0
7	Q	54	0	42	9	0
7	R	27	0	21	2	0
8	A	244	0	0	0	0
8	B	73	0	0	1	0
8	Q	245	0	0	3	0
8	R	73	0	0	0	0
All	All	12593	0	11683	103	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 (103) 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)
7:Q:411:SAM:C1'	7:Q:411:SAM:O4'	1.63	1.16
7:A:408:SAM:HE2	1:Q:102:ILE:HD11	1.61	0.81
1:A:91:VAL:H	6:A:406:EDO:H12	1.44	0.81
7:Q:410:SAM:HE1	7:Q:410:SAM:H3'	1.63	0.81
7:A:408:SAM:HE3	7:A:408:SAM:H3'	1.66	0.77
7:A:408:SAM:HE2	1:Q:102:ILE:CD1	2.21	0.70
7:Q:410:SAM:HA	7:Q:410:SAM:HE2	1.75	0.68
1:A:238:ASP:HB2	7:A:408:SAM:HE1	1.75	0.68
1:A:102:ILE:HD11	7:Q:410:SAM:HE3	1.75	0.67
1:R:284:ASN:HB3	1:R:376:LEU:HD11	1.76	0.66
1:B:151:VAL:HG23	1:B:156:THR:HB	1.79	0.63
1:R:373:ALA:HA	1:R:376:LEU:HD12	1.80	0.61
1:B:103:ASN:ND2	1:B:107:ASP:OD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:161[B]:ARG:HB2	1:R:188:GLN:HB3	1.84	0.59
1:Q:95:ILE:H	6:Q:413:EDO:H22	1.67	0.59
7:Q:411:SAM:H5'2	7:Q:411:SAM:N3	2.18	0.58
1:B:70:ASN:OD1	1:B:73:ARG:NH1	2.37	0.57
1:A:99:SER:HB3	1:A:102:ILE:HD12	1.87	0.56
7:A:409:SAM:H5'1	7:A:409:SAM:N3	2.20	0.56
1:A:238:ASP:HB2	7:A:408:SAM:CE	2.36	0.55
1:A:253:GLY:O	1:Q:256:ARG:HD2	2.07	0.54
1:B:218:SER:O	8:B:501:HOH:O	2.19	0.54
1:Q:146:GLN:NE2	8:Q:508:HOH:O	2.40	0.54
1:R:180:ILE:HG13	1:R:215:TRP:HB3	1.90	0.54
1:A:330[A]:ARG:HA	1:A:330[A]:ARG:NH2	2.24	0.53
1:B:54:GLY:HA2	1:R:239[B]:CYS:SG	2.49	0.52
7:B:407:SAM:HE1	1:R:102:ILE:HD13	1.91	0.52
1:B:62:VAL:HG22	6:B:406:EDO:H11	1.91	0.52
1:Q:205:GLU:OE2	8:Q:501:HOH:O	2.19	0.52
1:A:46:LYS:HD3	1:A:239[B]:CYS:SG	2.49	0.52
1:Q:64:ILE:HG12	7:Q:411:SAM:N6	2.25	0.52
7:R:404:SAM:HE3	7:R:404:SAM:H3'	1.91	0.51
1:B:75:ILE:O	1:B:152:ARG:NH1	2.43	0.51
1:B:363:GLU:H	1:B:363:GLU:CD	2.12	0.50
1:B:108:ARG:NH1	1:B:303:GLY:O	2.43	0.50
7:A:408:SAM:CE	7:A:408:SAM:HA	2.42	0.50
1:R:119:GLN:N	1:R:302:ILE:HG12	2.25	0.50
1:B:133:LEU:HD12	1:B:283:LYS:HG2	1.93	0.50
1:B:241:LEU:HB2	1:B:244:ARG:HG3	1.93	0.50
1:Q:94:ALA:HB2	1:R:92:LEU:HD22	1.94	0.50
1:Q:153:LYS:HZ2	6:Q:408:EDO:H11	1.76	0.50
1:A:133:LEU:HD12	1:A:283:LYS:HG3	1.95	0.49
1:Q:273:SER:HB2	1:Q:340:LEU:HD11	1.94	0.49
1:Q:92:LEU:HD22	1:R:94:ALA:HB2	1.95	0.49
1:A:256:ARG:HD2	1:Q:253:GLY:O	2.12	0.48
1:B:279:ARG:HG2	1:B:360:PHE:CD1	2.47	0.48
1:R:241:LEU:HB2	1:R:244:ARG:HG3	1.95	0.48
1:R:299:SER:OG	1:R:309:SER:HB3	2.13	0.48
1:B:180:ILE:HG13	1:B:215:TRP:HB3	1.95	0.48
1:R:159:TRP:CE2	1:R:193:ILE:HD13	2.49	0.48
1:Q:326:THR:O	1:Q:330:ARG:HG2	2.14	0.47
1:R:75:ILE:O	1:R:152:ARG:NH1	2.47	0.47
1:R:128:ASN:ND2	1:R:292:ASP:OD1	2.44	0.47
1:R:279:ARG:HH12	1:R:283:LYS:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:103:ASN:ND2	1:R:107:ASP:OD2	2.43	0.47
1:Q:58:THR:O	7:Q:411:SAM:H5'1	2.15	0.46
1:A:281:VAL:HG22	1:A:296:ILE:HG13	1.97	0.46
1:B:3:HIS:HB2	1:R:311:MET:HG3	1.98	0.46
1:Q:153:LYS:NZ	6:Q:408:EDO:H11	2.31	0.45
1:A:102:ILE:CD1	7:Q:410:SAM:HE3	2.43	0.45
1:B:99:SER:HB3	1:B:102:ILE:HD12	1.96	0.45
1:A:330[A]:ARG:HA	1:A:330[A]:ARG:HH21	1.81	0.45
1:B:279:ARG:HH12	1:B:283:LYS:HD2	1.81	0.45
1:R:133:LEU:HD12	1:R:283:LYS:HG2	1.98	0.45
1:A:137:PRO:HA	1:A:170:PHE:CE1	2.51	0.45
1:R:22:ILE:HD13	1:R:68:THR:HG23	1.99	0.45
1:B:147:ARG:O	1:B:151:VAL:HG12	2.17	0.44
1:R:279:ARG:HG3	1:R:279:ARG:HH11	1.83	0.44
1:R:238:ASP:HB2	7:R:404:SAM:HE1	1.98	0.44
1:R:46:LYS:HD3	1:R:239[B]:CYS:SG	2.58	0.44
1:A:64:ILE:HG12	7:A:409:SAM:N6	2.33	0.44
1:A:238:ASP:CB	7:A:408:SAM:HE1	2.47	0.43
1:R:121:LEU:O	1:R:258:GLY:HA3	2.18	0.43
1:B:251:TYR:OH	1:B:279:ARG:HD3	2.18	0.43
1:R:151:VAL:HG13	1:R:156:THR:HB	2.00	0.43
7:A:408:SAM:H3'	7:A:408:SAM:CE	2.42	0.43
1:B:254:MET:HE3	1:B:254:MET:HA	2.01	0.42
1:B:129:GLU:OE1	1:B:177:ILE:HD11	2.20	0.42
1:Q:46:LYS:O	1:Q:47:THR:C	2.57	0.42
1:B:207:ILE:HG23	1:B:211:LEU:HD22	2.00	0.42
1:Q:137:PRO:HA	1:Q:170:PHE:CE1	2.54	0.42
1:B:118:ASP:OD1	1:B:119:GLN:N	2.52	0.42
1:B:123:PHE:HA	1:B:296:ILE:O	2.19	0.42
1:R:279:ARG:HG2	1:R:360:PHE:CD1	2.54	0.42
1:Q:371:ASP:OD1	1:Q:371:ASP:N	2.53	0.42
1:A:49:MET:SD	1:R:92:LEU:HD21	2.59	0.41
1:A:92:LEU:HD11	1:R:49:MET:SD	2.61	0.41
1:A:127:THR:O	1:A:133:LEU:HA	2.21	0.41
6:A:407:EDO:H12	1:B:65:GLU:HB2	2.03	0.41
1:B:279:ARG:HH11	1:B:279:ARG:HG3	1.86	0.41
1:R:123:PHE:HA	1:R:296:ILE:O	2.21	0.41
1:Q:161:ARG:NE	8:Q:502:HOH:O	2.26	0.41
1:Q:362:ARG:O	1:Q:368:GLU:HG3	2.21	0.41
1:B:328:LEU:HD21	1:B:379:ALA:HB3	2.03	0.41
1:Q:199:GLN:HG2	1:Q:224:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:238:ASP:HB2	7:Q:410:SAM:HE1	2.03	0.40
1:Q:277:ALA:O	1:Q:281:VAL:HG13	2.21	0.40
1:R:179:GLY:HA2	1:R:215:TRP:CD1	2.56	0.40
1:R:65:GLU:HA	1:R:91:VAL:HG11	2.03	0.40
1:R:118:ASP:OD1	1:R:119:GLN:N	2.54	0.40
1:R:366:PRO:HD2	1:R:367:TRP:CZ3	2.56	0.40
1:A:59:SER:HA	7:A:409:SAM:HB1	2.02	0.40
1:B:46:LYS:HD2	1:B:47:THR:H	1.87	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	379/384 (99%)	369 (97%)	10 (3%)	0	100	100
1	B	377/384 (98%)	363 (96%)	11 (3%)	3 (1%)	19	9
1	Q	379/384 (99%)	367 (97%)	11 (3%)	1 (0%)	41	30
1	R	377/384 (98%)	364 (97%)	10 (3%)	3 (1%)	19	9
All	All	1512/1536 (98%)	1463 (97%)	42 (3%)	7 (0%)	29	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	109	ALA
1	R	363	GLU
1	B	109	ALA
1	B	47	THR
1	B	363	GLU
1	Q	47	THR
1	R	47	THR

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	310/312 (99%)	303 (98%)	7 (2%)	50	42
1	B	309/312 (99%)	293 (95%)	16 (5%)	23	10
1	Q	311/312 (100%)	304 (98%)	7 (2%)	50	42
1	R	310/312 (99%)	296 (96%)	14 (4%)	27	15
All	All	1240/1248 (99%)	1196 (96%)	44 (4%)	36	24

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	161	ARG
1	A	211	LEU
1	A	230	PHE
1	A	281	VAL
1	A	322	SER
1	A	377	ARG
1	B	112	LEU
1	B	121	LEU
1	B	127	THR
1	B	131	ASP
1	B	161	ARG
1	B	171	GLN
1	B	176	LYS
1	B	230	PHE
1	B	248	VAL
1	B	254	MET
1	B	270	VAL
1	B	306	GLU
1	B	309	SER
1	B	311	MET
1	B	320	VAL
1	B	324	GLN
1	Q	93	SER

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Mol	Chain	Res	Type
1	Q	121	LEU
1	Q	185	LEU
1	Q	230	PHE
1	Q	281	VAL
1	Q	323	GLU
1	Q	324	GLN
1	R	112	LEU
1	R	113	GLU
1	R	121	LEU
1	R	127	THR
1	R	150	GLU
1	R	161[A]	ARG
1	R	161[B]	ARG
1	R	248	VAL
1	R	256	ARG
1	R	309	SER
1	R	311	MET
1	R	320	VAL
1	R	369	LYS
1	R	372	LYS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 35 ligands modelled in this entry, 12 are monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	EDO	Q	413	-	3,3,3	0.39	0	2,2,2	0.62	0
6	EDO	B	405	-	3,3,3	0.47	0	2,2,2	0.46	0
7	SAM	R	404	-	21,29,29	5.19	8 (38%)	18,42,42	2.60	4 (22%)
6	EDO	Q	409	-	3,3,3	0.42	0	2,2,2	0.52	0
3	PO4	Q	403	-	4,4,4	0.97	0	6,6,6	0.31	0
3	PO4	Q	402	4	4,4,4	0.71	0	6,6,6	0.53	0
2	POP	Q	401	5,4	6,8,8	1.15	0	13,13,13	1.41	2 (15%)
7	SAM	A	409	-	21,29,29	5.24	8 (38%)	18,42,42	2.81	5 (27%)
7	SAM	B	407	-	21,29,29	5.21	8 (38%)	18,42,42	2.79	5 (27%)
7	SAM	A	408	-	21,29,29	4.56	8 (38%)	18,42,42	2.41	5 (27%)
2	POP	R	401	4	6,8,8	0.80	0	13,13,13	1.26	2 (15%)
6	EDO	A	407	-	3,3,3	0.37	0	2,2,2	0.68	0
6	EDO	R	405	-	3,3,3	0.40	0	2,2,2	0.42	0
6	EDO	Q	407	-	3,3,3	0.38	0	2,2,2	0.37	0
7	SAM	Q	411	-	21,29,29	5.30	8 (38%)	18,42,42	2.93	7 (38%)
6	EDO	A	406	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	Q	408	-	3,3,3	0.38	0	2,2,2	0.69	0
2	POP	A	401	5,4	6,8,8	1.15	0	13,13,13	1.22	1 (7%)
3	PO4	A	402	4	4,4,4	0.87	0	6,6,6	0.22	0
6	EDO	B	406	-	3,3,3	0.54	0	2,2,2	0.28	0
2	POP	B	401	4	6,8,8	0.77	0	13,13,13	1.18	2 (15%)
3	PO4	B	402	-	4,4,4	0.91	0	6,6,6	0.41	0
7	SAM	Q	410	-	21,29,29	4.57	8 (38%)	18,42,42	2.24	5 (27%)

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
6	EDO	Q	413	-	-	1/1/1/1	-
6	EDO	B	405	-	-	0/1/1/1	-
7	SAM	R	404	-	-	2/8/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	Q	409	-	-	0/1/1/1	-
2	POP	Q	401	5,4	-	0/6/6/6	-
7	SAM	A	409	-	-	3/8/33/33	0/3/3/3
7	SAM	B	407	-	-	3/8/33/33	0/3/3/3
7	SAM	A	408	-	-	0/8/33/33	0/3/3/3
2	POP	R	401	4	-	0/6/6/6	-
6	EDO	A	407	-	-	1/1/1/1	-
6	EDO	R	405	-	-	0/1/1/1	-
6	EDO	Q	407	-	-	0/1/1/1	-
7	SAM	Q	411	-	-	3/8/33/33	0/3/3/3
6	EDO	A	406	-	-	1/1/1/1	-
6	EDO	Q	408	-	-	1/1/1/1	-
2	POP	A	401	5,4	-	0/6/6/6	-
6	EDO	B	406	-	-	1/1/1/1	-
2	POP	B	401	4	-	0/6/6/6	-
7	SAM	Q	410	-	-	1/8/33/33	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	411	SAM	O4'-C1'	16.29	1.63	1.41
7	A	409	SAM	O4'-C1'	15.78	1.63	1.41
7	B	407	SAM	C2'-C1'	-15.53	1.30	1.53
7	A	409	SAM	C2'-C1'	-15.45	1.30	1.53
7	R	404	SAM	O4'-C1'	15.44	1.62	1.41
7	B	407	SAM	O4'-C1'	15.43	1.62	1.41
7	Q	411	SAM	C2'-C1'	-15.36	1.30	1.53
7	R	404	SAM	C2'-C1'	-15.25	1.30	1.53
7	A	408	SAM	C2'-C1'	-14.30	1.32	1.53
7	Q	410	SAM	C2'-C1'	-14.10	1.32	1.53
7	A	408	SAM	O4'-C1'	12.31	1.58	1.41
7	Q	410	SAM	O4'-C1'	12.22	1.58	1.41
7	R	404	SAM	O4'-C4'	-6.19	1.31	1.45
7	A	409	SAM	O4'-C4'	-6.04	1.31	1.45
7	Q	410	SAM	O4'-C4'	-6.02	1.31	1.45
7	B	407	SAM	O4'-C4'	-5.91	1.31	1.45
7	Q	411	SAM	O4'-C4'	-5.76	1.32	1.45
7	A	408	SAM	O4'-C4'	-5.19	1.33	1.45
7	B	407	SAM	C6-N6	3.65	1.47	1.34
7	R	404	SAM	C6-N6	3.63	1.47	1.34
7	Q	410	SAM	C5-C4	-3.57	1.31	1.40
7	A	409	SAM	C6-N6	3.56	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	411	SAM	C6-N6	3.45	1.46	1.34
7	Q	410	SAM	C2-N3	3.30	1.37	1.32
7	Q	411	SAM	O3'-C3'	-3.10	1.35	1.43
7	A	408	SAM	C6-N6	3.00	1.45	1.34
7	A	408	SAM	C5-C4	-2.95	1.33	1.40
7	A	408	SAM	C2-N3	2.94	1.36	1.32
7	B	407	SAM	O3'-C3'	-2.93	1.36	1.43
7	R	404	SAM	O3'-C3'	-2.93	1.36	1.43
7	B	407	SAM	O2'-C2'	2.88	1.49	1.43
7	R	404	SAM	O2'-C2'	2.82	1.49	1.43
7	A	409	SAM	O2'-C2'	2.79	1.49	1.43
7	Q	411	SAM	O2'-C2'	2.77	1.49	1.43
7	A	408	SAM	O2'-C2'	2.70	1.49	1.43
7	Q	410	SAM	C6-N6	2.68	1.43	1.34
7	R	404	SAM	C5-C4	-2.56	1.34	1.40
7	Q	411	SAM	C5-C4	-2.54	1.34	1.40
7	B	407	SAM	C2-N3	2.54	1.36	1.32
7	B	407	SAM	C5-C4	-2.48	1.34	1.40
7	A	409	SAM	C5-C4	-2.45	1.34	1.40
7	A	408	SAM	O3'-C3'	-2.45	1.37	1.43
7	R	404	SAM	C2-N3	2.44	1.36	1.32
7	A	409	SAM	O3'-C3'	-2.40	1.37	1.43
7	Q	410	SAM	O2'-C2'	2.40	1.48	1.43
7	Q	411	SAM	C2-N3	2.39	1.35	1.32
7	A	409	SAM	C2-N3	2.37	1.35	1.32
7	Q	410	SAM	O3'-C3'	-2.22	1.37	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	407	SAM	C5-C6-N6	7.69	132.04	120.35
7	R	404	SAM	C5-C6-N6	7.43	131.64	120.35
7	Q	411	SAM	C5-C6-N6	7.33	131.49	120.35
7	A	409	SAM	C5-C6-N6	7.12	131.17	120.35
7	Q	410	SAM	N3-C2-N1	-6.43	118.63	128.68
7	Q	411	SAM	N3-C2-N1	-6.16	119.05	128.68
7	A	408	SAM	N3-C2-N1	-6.11	119.14	128.68
7	A	409	SAM	N3-C2-N1	-6.02	119.27	128.68
7	R	404	SAM	N3-C2-N1	-5.38	120.27	128.68
7	Q	411	SAM	N6-C6-N1	-5.27	107.63	118.57
7	B	407	SAM	N3-C2-N1	-5.25	120.48	128.68
7	B	407	SAM	N6-C6-N1	-5.09	108.01	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	409	SAM	N6-C6-N1	-4.89	108.43	118.57
7	R	404	SAM	N6-C6-N1	-4.86	108.49	118.57
7	A	408	SAM	C5-C6-N6	4.48	127.17	120.35
7	A	408	SAM	C5'-SD-CG	-3.93	93.38	103.40
7	B	407	SAM	C3'-C2'-C1'	3.47	106.21	100.98
7	A	409	SAM	C3'-C2'-C1'	3.42	106.13	100.98
7	Q	411	SAM	C3'-C2'-C1'	3.39	106.08	100.98
7	A	408	SAM	N6-C6-N1	-3.36	111.59	118.57
7	A	409	SAM	C5'-SD-CG	3.23	111.65	103.40
7	Q	410	SAM	C5'-SD-CG	-3.23	95.17	103.40
2	Q	401	POP	O2-P1-O	3.15	115.19	104.64
2	A	401	POP	P2-O-P1	-3.13	122.09	132.83
7	Q	410	SAM	C5-C6-N6	2.87	124.71	120.35
2	R	401	POP	P2-O-P1	-2.86	123.01	132.83
7	Q	410	SAM	N6-C6-N1	-2.82	112.71	118.57
7	B	407	SAM	C5'-SD-CG	2.74	110.39	103.40
2	Q	401	POP	P2-O-P1	-2.72	123.51	132.83
7	R	404	SAM	C3'-C2'-C1'	2.66	104.98	100.98
2	B	401	POP	P2-O-P1	-2.51	124.20	132.83
7	Q	410	SAM	C3'-C2'-C1'	2.41	104.61	100.98
7	A	408	SAM	C3'-C2'-C1'	2.35	104.52	100.98
2	B	401	POP	O2-P1-O	2.35	112.50	104.64
7	Q	411	SAM	O4'-C4'-C5'	2.28	114.64	108.88
7	Q	411	SAM	C2'-C3'-C4'	2.19	106.89	102.64
7	Q	411	SAM	C5'-SD-CG	2.14	108.86	103.40
2	R	401	POP	O3-P1-O	2.12	111.73	104.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	SAM	N-CA-CB-CG
7	A	409	SAM	C-CA-CB-CG
7	B	407	SAM	CA-CB-CG-SD
7	B	407	SAM	CB-CG-SD-CE
7	Q	410	SAM	O4'-C4'-C5'-SD
7	R	404	SAM	O4'-C4'-C5'-SD
6	A	406	EDO	O1-C1-C2-O2
6	Q	413	EDO	O1-C1-C2-O2
6	Q	408	EDO	O1-C1-C2-O2
7	B	407	SAM	CB-CG-SD-C5'
7	A	409	SAM	CA-CB-CG-SD

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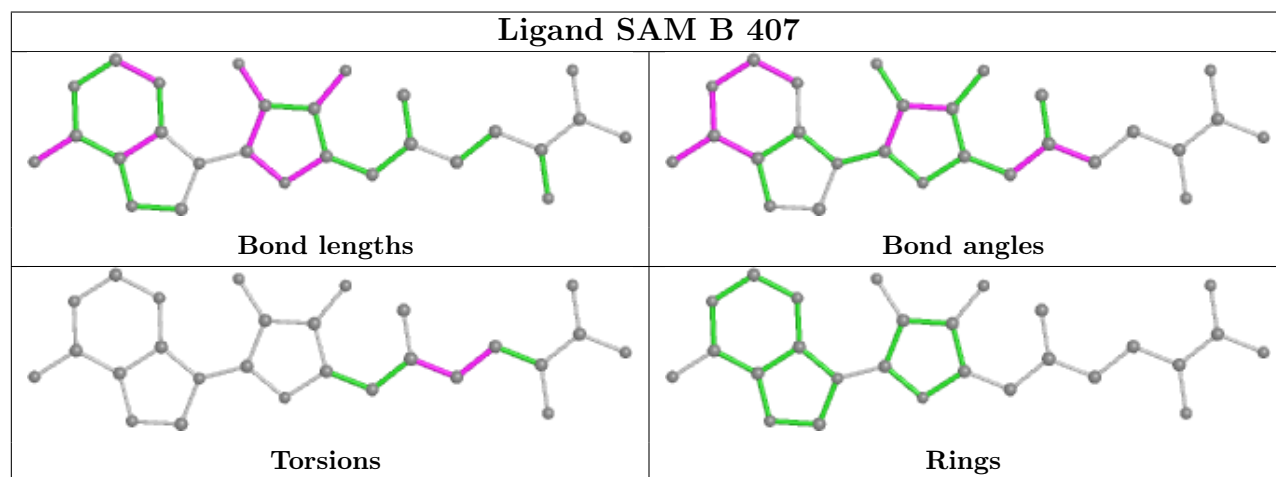
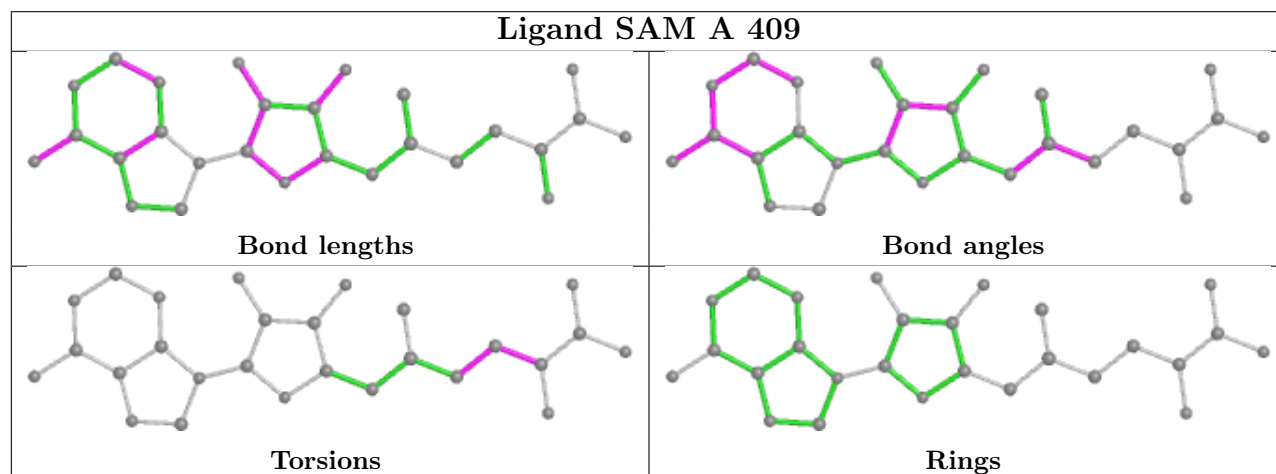
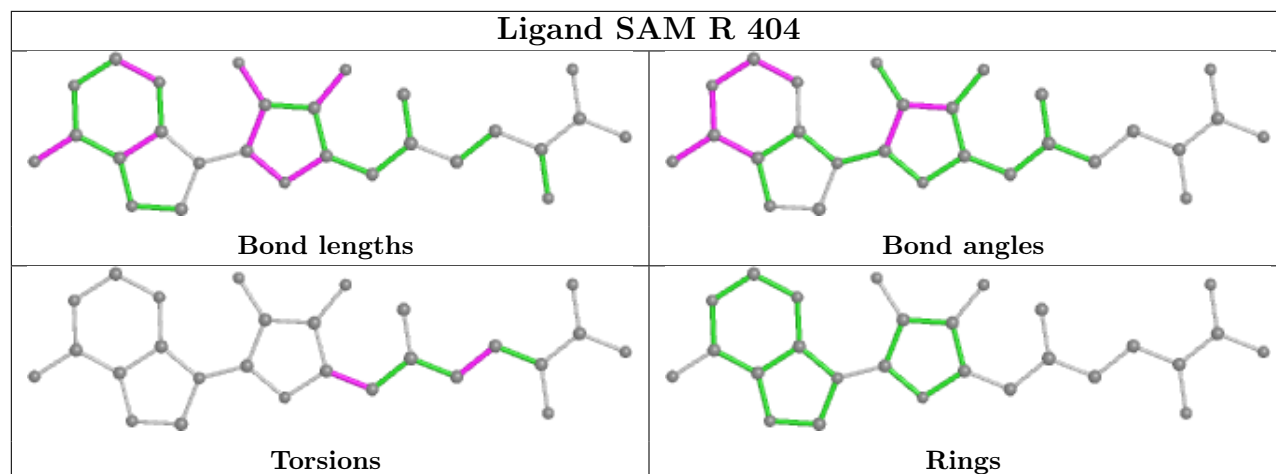
Mol	Chain	Res	Type	Atoms
7	Q	411	SAM	CA-CB-CG-SD
7	R	404	SAM	CA-CB-CG-SD
6	B	406	EDO	O1-C1-C2-O2
6	A	407	EDO	O1-C1-C2-O2
7	Q	411	SAM	CB-CG-SD-C5'
7	Q	411	SAM	C4'-C5'-SD-CG

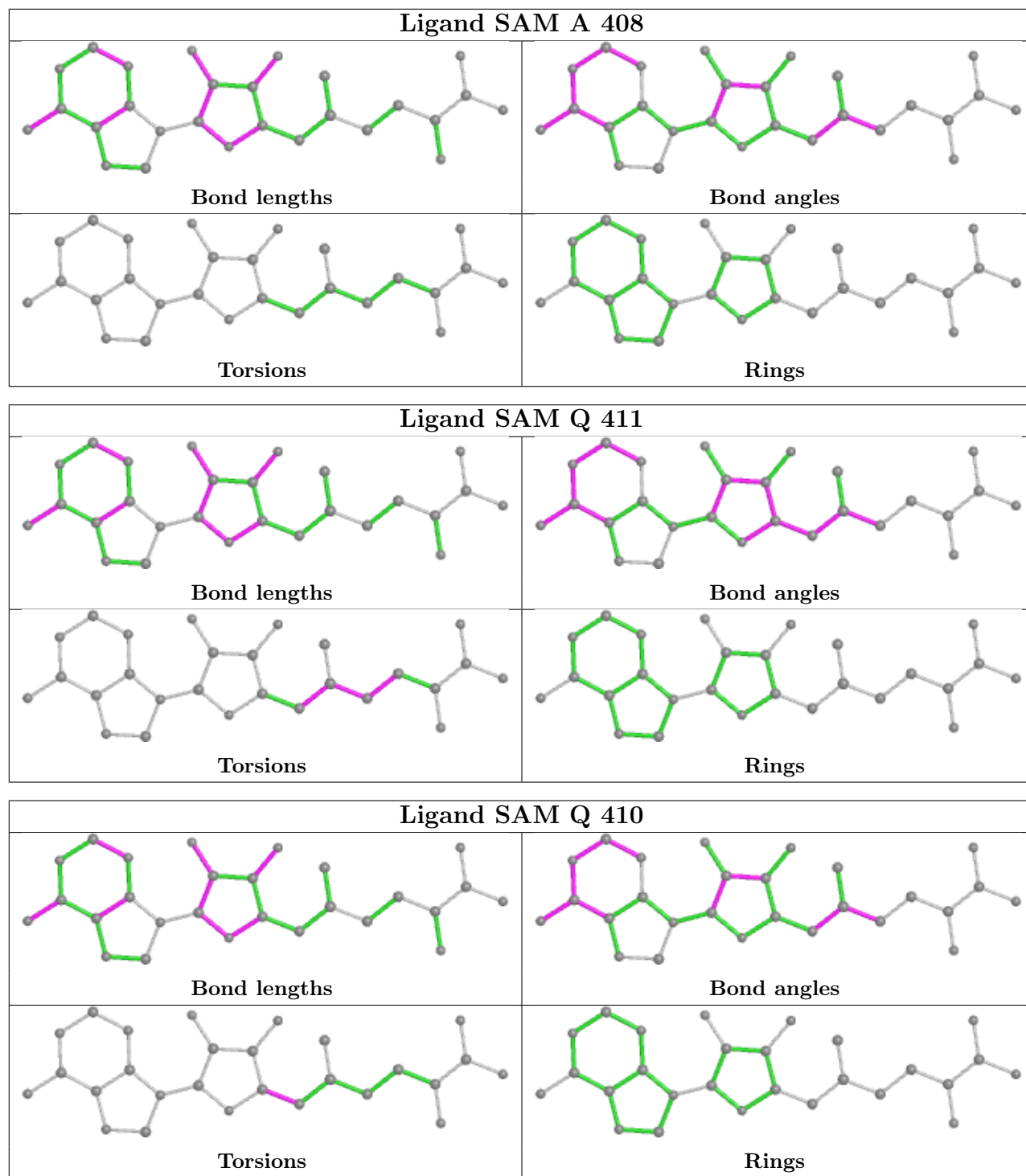
There are no ring outliers.

11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	413	EDO	1	0
7	R	404	SAM	2	0
7	A	409	SAM	3	0
7	B	407	SAM	1	0
7	A	408	SAM	8	0
6	A	407	EDO	1	0
7	Q	411	SAM	4	0
6	A	406	EDO	1	0
6	Q	408	EDO	2	0
6	B	406	EDO	1	0
7	Q	410	SAM	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

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 [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	379/384 (98%)	-0.30	0 100 100	21, 33, 68, 106	0
1	B	378/384 (98%)	0.60	41 (10%) 5 9	32, 87, 127, 159	0
1	Q	378/384 (98%)	-0.31	0 100 100	19, 33, 64, 97	0
1	R	377/384 (98%)	0.65	49 (12%) 3 5	33, 86, 129, 151	0
All	All	1512/1536 (98%)	0.16	90 (5%) 21 30	19, 53, 121, 159	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	ILE	7.1
1	R	376	LEU	6.8
1	B	168	VAL	6.6
1	B	376	LEU	6.6
1	R	179	GLY	6.1
1	R	285	ILE	5.9
1	R	325	LEU	5.7
1	R	332	PHE	5.5
1	R	377	ARG	5.5
1	B	179	GLY	4.7
1	B	332[A]	PHE	4.6
1	B	140	TYR	4.6
1	R	333	PHE	4.4
1	R	327	LEU	4.3
1	B	102	ILE	4.2
1	R	170	PHE	4.1
1	R	222	PHE	4.0
1	B	337	PRO	4.0
1	B	215	TRP	3.9
1	B	170	PHE	3.8
1	R	178	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	R	140	TYR	3.8
1	R	310	ILE	3.7
1	R	288	ALA	3.5
1	B	109	ALA	3.5
1	B	328	LEU	3.4
1	B	174	ASP	3.4
1	R	296	ILE	3.4
1	R	176	LYS	3.3
1	R	3	HIS	3.3
1	R	338	TYR	3.3
1	R	215	TRP	3.3
1	B	375	LEU	3.3
1	R	168	VAL	3.3
1	B	61	TRP	3.2
1	B	312	VAL	3.2
1	R	294	CYS	3.2
1	R	335	LEU	3.2
1	B	219	ALA	3.1
1	R	292	ASP	3.1
1	R	61	TRP	3.1
1	R	106	VAL	3.1
1	B	270	VAL	3.1
1	B	277	ALA	3.0
1	R	218	SER	3.0
1	R	317	THR	3.0
1	B	105	GLY	2.9
1	R	312	VAL	2.9
1	R	109	ALA	2.9
1	R	287	ALA	2.8
1	R	375	LEU	2.8
1	B	4	LEU	2.7
1	R	328	LEU	2.7
1	R	374	GLN	2.7
1	B	112	LEU	2.7
1	R	107	ASP	2.6
1	R	110	ASP	2.6
1	R	138	ILE	2.6
1	B	338	TYR	2.5
1	B	255	ALA	2.4
1	R	293	ARG	2.4
1	B	3	HIS	2.4
1	B	346	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	330	ARG	2.4
1	B	222	PHE	2.3
1	R	211	LEU	2.3
1	B	374	GLN	2.3
1	R	329	VAL	2.3
1	B	177	ILE	2.3
1	B	377	ARG	2.3
1	B	159	TRP	2.3
1	R	102	ILE	2.3
1	B	282	ALA	2.2
1	B	380	ALA	2.2
1	R	121	LEU	2.2
1	B	183	VAL	2.2
1	R	108	ARG	2.2
1	R	183	VAL	2.2
1	B	110	ASP	2.2
1	R	254	MET	2.2
1	R	198	LEU	2.2
1	B	293	ARG	2.2
1	B	295	GLU	2.1
1	R	316	GLY	2.1
1	B	274	ALA	2.1
1	B	329	VAL	2.1
1	R	201	ALA	2.1
1	R	315	PHE	2.1
1	B	373	ALA	2.1
1	R	112	LEU	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 monosaccharides 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,

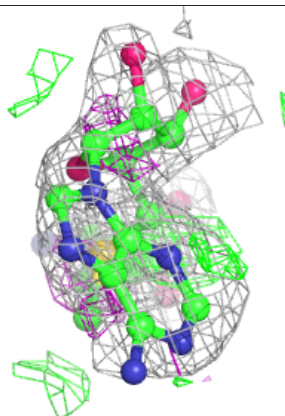
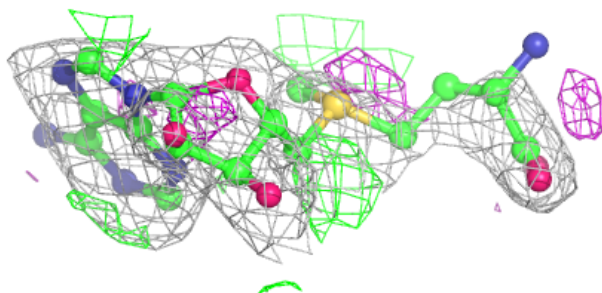
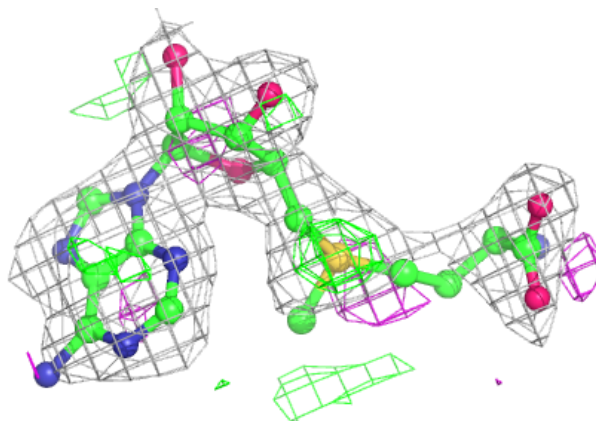
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MG	B	404	1/1	0.77	0.36	81,81,81,81	0
5	K	Q	406	1/1	0.77	0.13	116,116,116,116	0
5	K	A	405	1/1	0.80	0.12	109,109,109,109	0
4	MG	R	402	1/1	0.82	0.13	81,81,81,81	0
6	EDO	A	406	4/4	0.85	0.16	58,59,59,63	0
7	SAM	Q	411	27/27	0.85	0.24	43,73,104,105	0
7	SAM	A	409	27/27	0.86	0.19	49,70,96,98	0
6	EDO	B	406	4/4	0.87	0.15	65,66,66,66	0
6	EDO	Q	413	4/4	0.87	0.16	52,55,61,67	0
4	MG	R	403	1/1	0.88	0.04	45,45,45,45	0
5	K	A	404	1/1	0.90	0.09	85,85,85,85	0
6	EDO	B	405	4/4	0.90	0.14	47,51,53,58	0
6	EDO	Q	409	4/4	0.92	0.10	57,58,58,62	0
6	EDO	A	407	4/4	0.92	0.15	52,59,64,65	0
7	SAM	R	404	27/27	0.93	0.13	70,79,89,90	0
7	SAM	B	407	27/27	0.94	0.12	68,76,97,98	0
3	PO4	B	402	5/5	0.94	0.21	103,104,107,107	0
5	K	Q	405	1/1	0.94	0.08	76,76,76,76	0
3	PO4	Q	402	5/5	0.95	0.08	29,29,48,50	0
6	EDO	R	405	4/4	0.95	0.11	45,50,55,59	0
3	PO4	Q	403	5/5	0.95	0.19	91,95,97,100	0
6	EDO	Q	407	4/4	0.95	0.23	48,50,50,51	0
6	EDO	Q	408	4/4	0.95	0.11	58,59,61,62	0
4	MG	B	403	1/1	0.95	0.06	47,47,47,47	0
7	SAM	A	408	27/27	0.96	0.11	18,25,35,43	0
7	SAM	Q	410	27/27	0.96	0.08	18,28,36,45	0
4	MG	A	410	1/1	0.97	0.06	28,28,28,28	0
2	POP	R	401	9/9	0.98	0.08	51,56,65,68	0
3	PO4	A	402	5/5	0.98	0.05	27,29,49,51	0
4	MG	Q	404	1/1	0.98	0.06	31,31,31,31	0
2	POP	B	401	9/9	0.98	0.08	52,60,66,69	0
4	MG	A	403	1/1	0.99	0.08	20,20,20,20	0
2	POP	Q	401	9/9	0.99	0.12	18,23,26,31	0
4	MG	Q	412	1/1	0.99	0.14	22,22,22,22	0
2	POP	A	401	9/9	0.99	0.12	18,24,28,31	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.

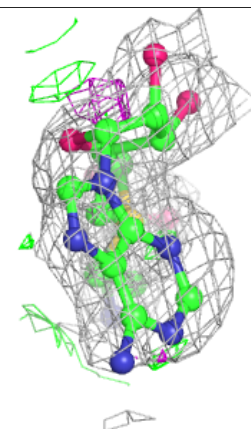
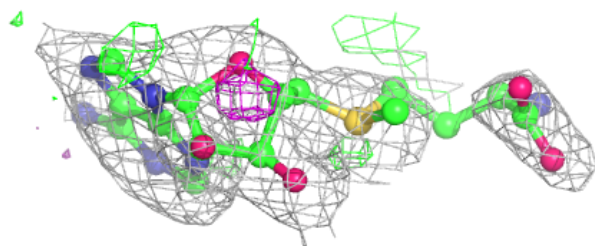
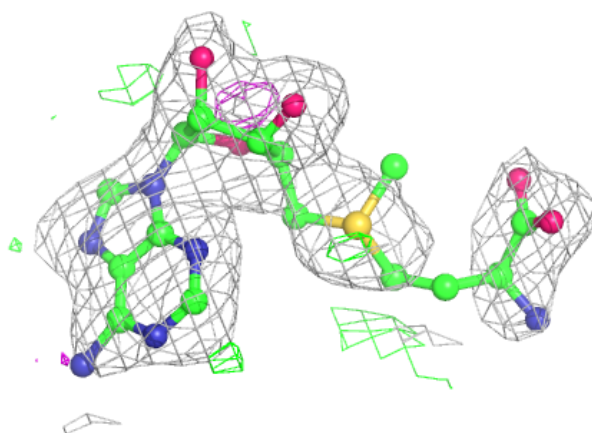
Electron density around SAM Q 411:

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



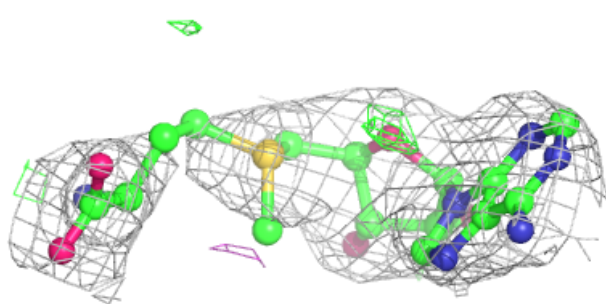
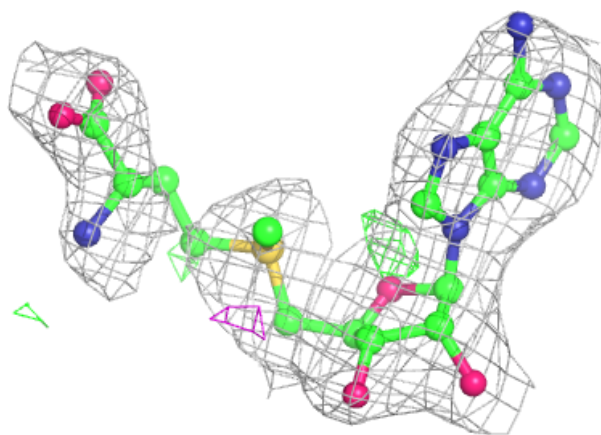
Electron density around SAM A 409:

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



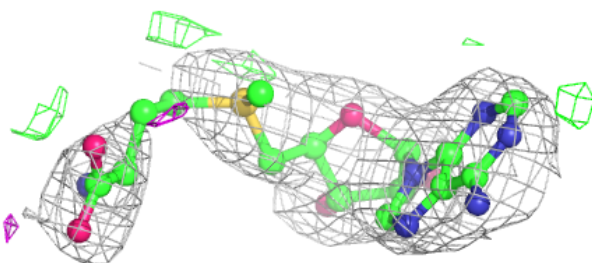
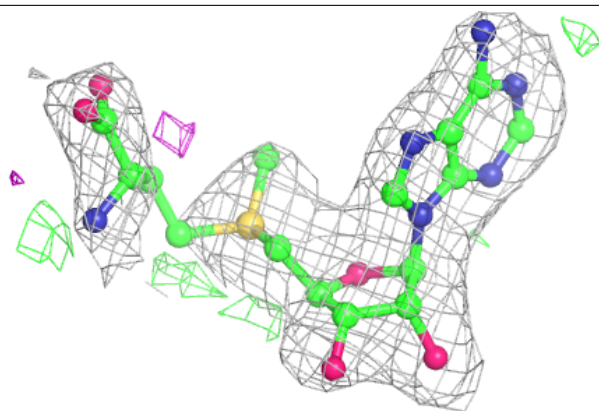
Electron density around SAM R 404:

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

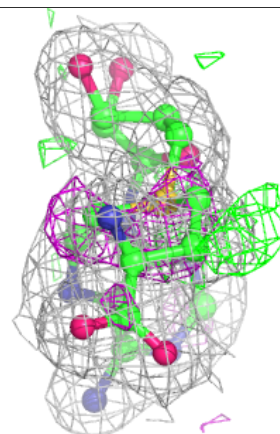
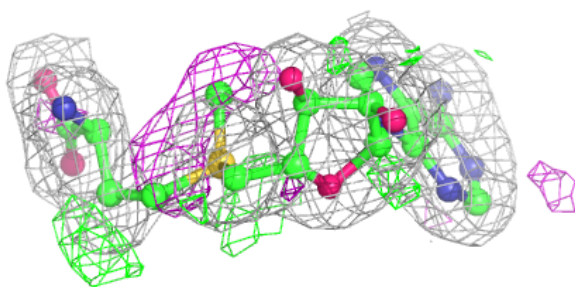
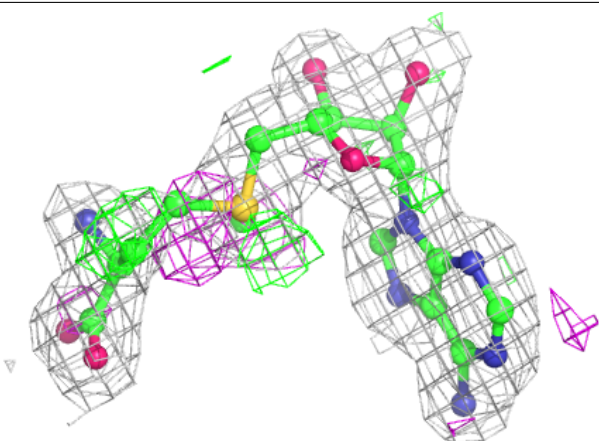


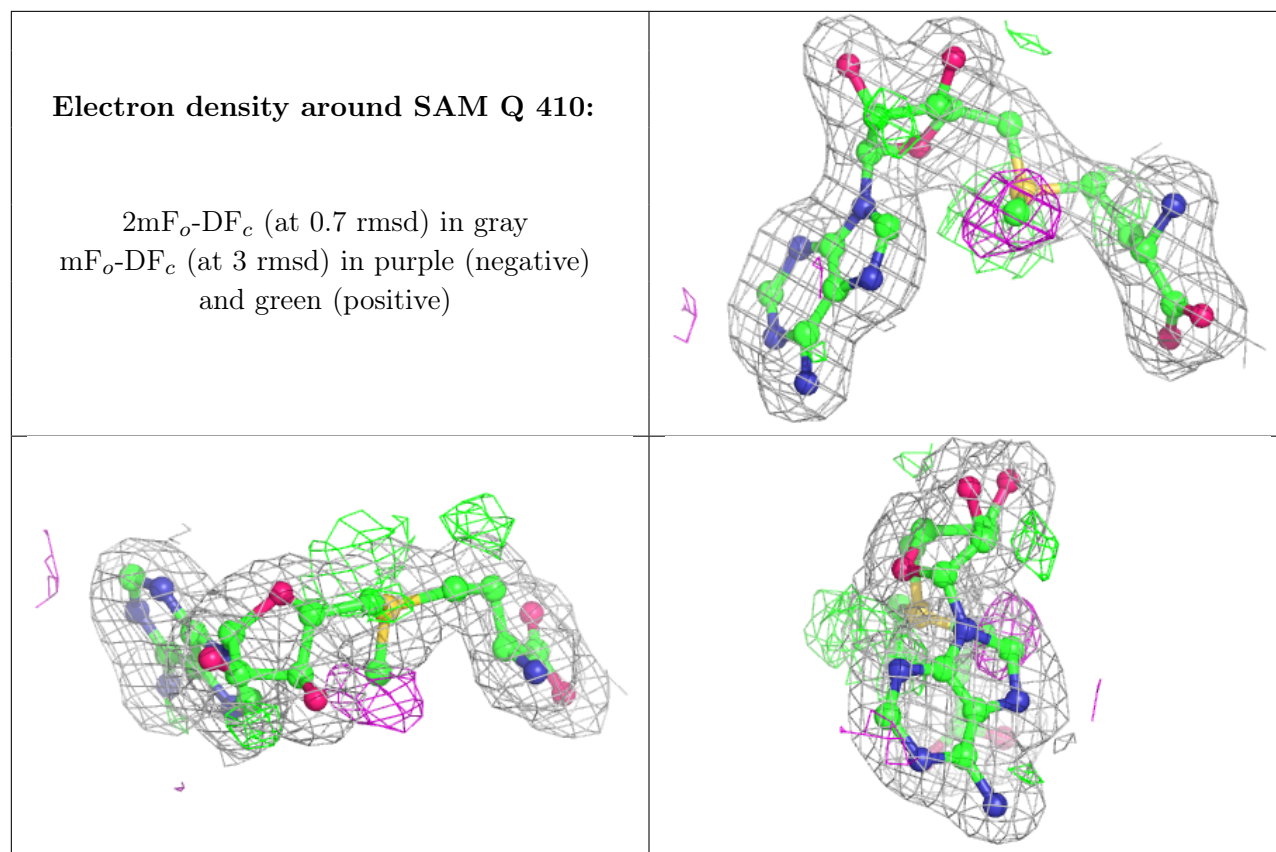
Electron density around SAM B 407:

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

**Electron density around SAM A 408:**

$2mF_o-DF_c$ (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.