



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:36 PM UTC

PDB ID : 7LOO / pdb_00007loo
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 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

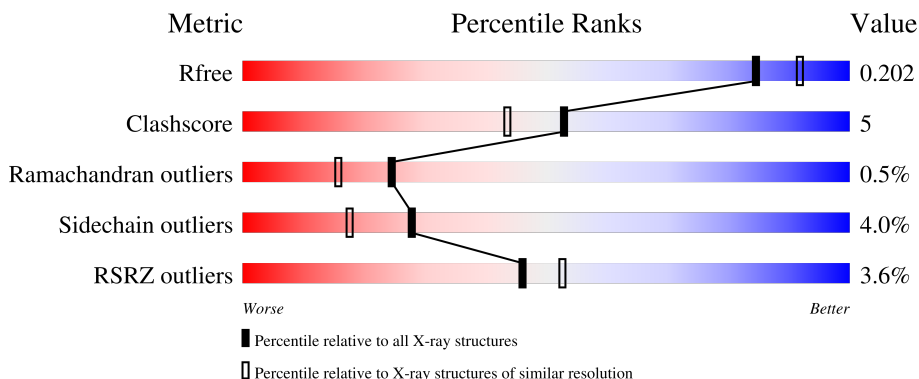
1 Overall quality at a glance i

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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	91% 7% ..
1	B	384	7% 83% 14% ..
1	Q	384	89% 9% ..
1	R	384	7% 82% 15% ..

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
7	SAM	A	408	-	-	X	-

2 Entry composition [i](#)

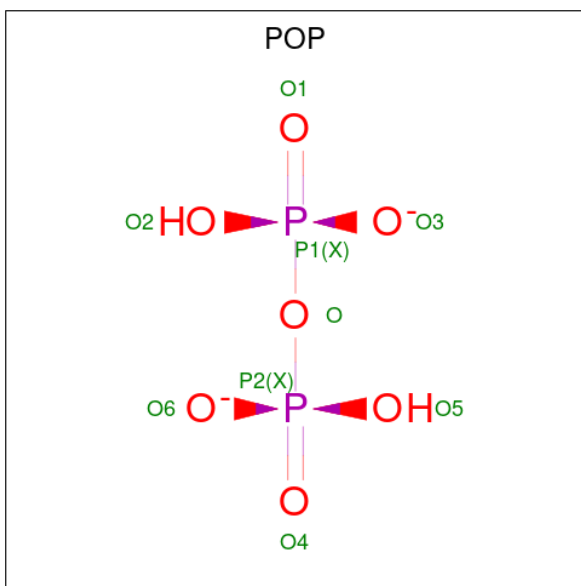
There are 8 unique types of molecules in this entry. The entry contains 12593 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



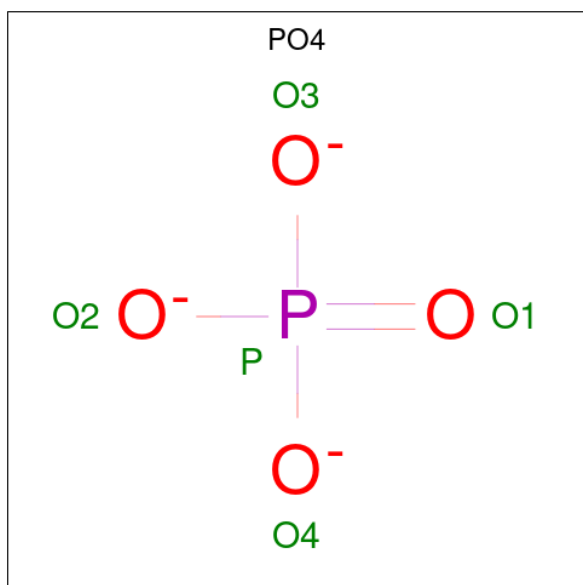
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	Total 9	O 7	P 2	0	0
2	B	1	Total 9	O 7	P 2	0	0

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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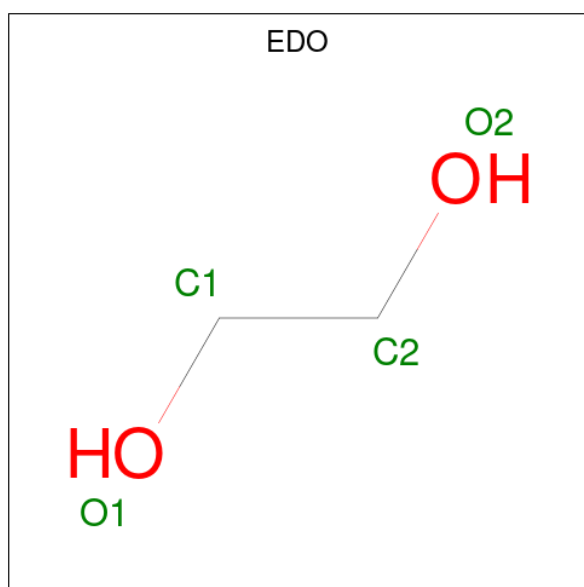
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	R	2	Total Mg 2 2	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



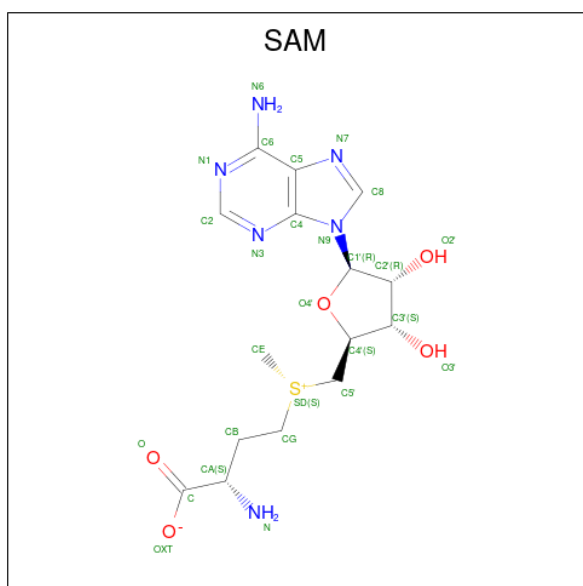
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	Q	1	Total C O 4 2 2	0	0
6	Q	1	Total C O 4 2 2	0	0

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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 (CCD ID: 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.

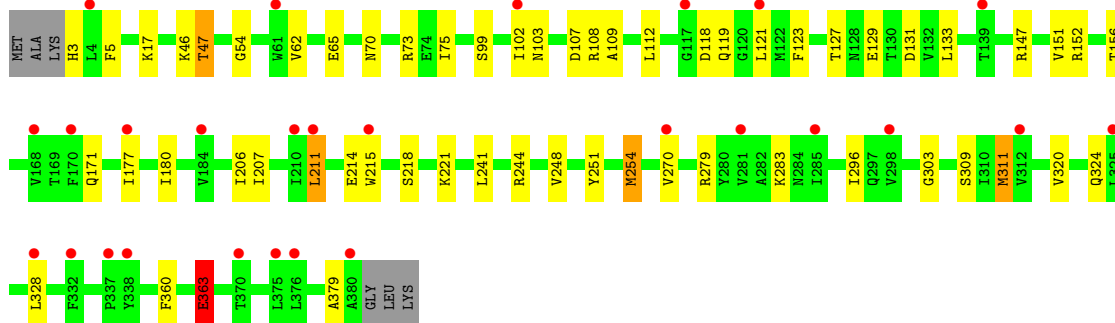
- Molecule 1: S-adenosylmethionine synthase

Chain A:  91% 7% ..




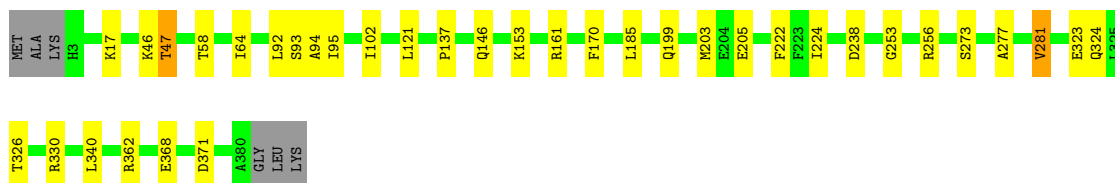
- Molecule 1: S-adenosylmethionine synthase

Chain B:  7% 83% 14% ..




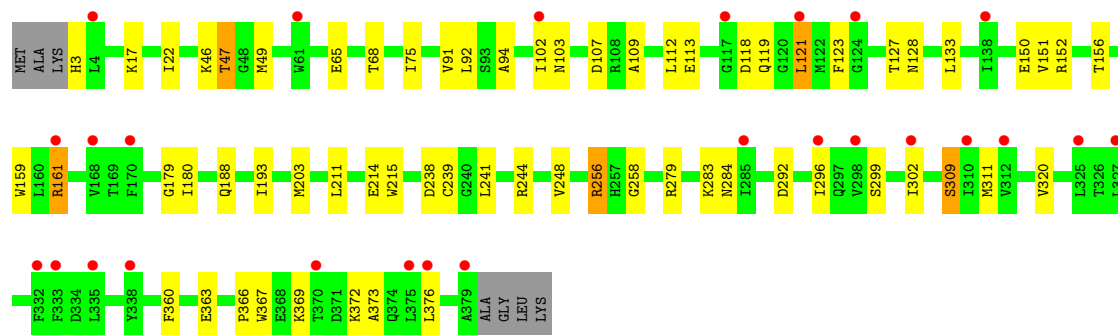
- Molecule 1: S-adenosylmethionine synthase

Chain Q:  89% 9% ..



- Molecule 1: S-adenosylmethionine synthase

Chain R:  7% 82% 15% ..



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) 98.5 (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)	Xtrriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.170 , 0.207 (Not available) , 0.202	Depositor DCC
R_{free} test set	6216 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.467 for h,-k,-h-l	Xtrriage
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

Xtrriage'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: POP, PO4, SAM, MG, K, 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	0.37	0/2986	0.56	0/4050
1	B	0.18	0/2977	0.41	0/4039
1	Q	0.38	0/2989	0.56	0/4055
1	R	0.18	0/2977	0.40	0/4039
All	All	0.29	0/11929	0.49	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	25	0
1	B	2917	0	2868	29	0
1	Q	2930	0	2883	25	0
1	R	2918	0	2872	35	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	2	0
6	R	4	0	6	0	0
7	A	54	0	43	16	0
7	B	27	0	21	1	0
7	Q	54	0	42	12	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	118	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (118) 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
1:A:238:ASP:HB2	7:A:408:SAM:HE2	1.56	0.85
1:A:91:VAL:H	6:A:406:EDO:H12	1.44	0.81
1:Q:238:ASP:HB2	7:Q:410:SAM:HE2	1.65	0.78
1:R:284:ASN:HB3	1:R:376:LEU:HD11	1.76	0.66
7:A:408:SAM:HE3	7:A:408:SAM:HA	1.78	0.65
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:A:102:ILE:HD11	7:Q:410:SAM:HE3	1.82	0.61
7:Q:410:SAM:HE1	7:Q:410:SAM:C8	2.31	0.60
1:B:103:ASN:ND2	1:B:107:ASP:OD2	2.35	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:203:MET:HE1	1:Q:222:PHE:CE1	2.37	0.59
1:A:238:ASP:CB	7:A:408:SAM:HE2	2.30	0.59
1:A:102:ILE:CD1	7:Q:410:SAM:HE3	2.33	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:408:SAM:HE3	1:Q:102:ILE:HD11	1.88	0.56
7:A:409:SAM:H5'1	7:A:409:SAM:N3	2.20	0.56
1:B:363:GLU:H	1:B:363:GLU:CD	2.12	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
7:A:408:SAM:HE3	1:Q:102:ILE:CD1	2.39	0.53
1:B:54:GLY:HA2	1:R:239[B]:CYS:SG	2.49	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
1:Q:203:MET:HE1	1:Q:222:PHE:CZ	2.45	0.51
7:Q:410:SAM:HE3	7:Q:410:SAM:HA	1.92	0.51
1:B:75:ILE:O	1:B:152:ARG:NH1	2.43	0.51
1:B:108:ARG:NH1	1:B:303:GLY:O	2.43	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
7:A:408:SAM:H3'	7:A:408:SAM:HE1	1.93	0.49
7:A:408:SAM:H3'	7:A:408:SAM:CE	2.42	0.49
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
7:B:407:SAM:HE2	1:R:102:ILE:HD13	1.94	0.49
1:A:238:ASP:HB2	7:A:408:SAM:CE	2.36	0.49
7:R:404:SAM:HE1	7:R:404:SAM:H3'	1.93	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:Q:410:SAM:HE1	7:Q:410:SAM:H8	1.96	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
1:Q:46:LYS:O	1:Q:47:THR:C	2.57	0.47
1:R:103:ASN:ND2	1:R:107:ASP:OD2	2.43	0.47
7:A:408:SAM:HA	7:A:408:SAM:CE	2.42	0.46
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
7:A:408:SAM:CE	1:Q:102:ILE:HD11	2.45	0.46
1:B:3:HIS:HB2	1:R:311:MET:HG3	1.98	0.46
1:R:238:ASP:HB2	7:R:404:SAM:HE2	1.96	0.46
1:Q:153:LYS:NZ	6:Q:408:EDO:H11	2.31	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:A:340:LEU:HD12	1:A:340:LEU:C	2.42	0.44
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: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:46:LYS:O	1:A:47:THR:C	2.60	0.43
1:R:121:LEU:O	1:R:258:GLY:HA3	2.18	0.43
1:A:102:ILE:HD11	7:Q:410:SAM:CE	2.48	0.43
1:B:251:TYR:OH	1:B:279:ARG:HD3	2.18	0.43
1:A:240:GLY:C	1:A:241:LEU:HD12	2.43	0.43
1:R:151:VAL:HG13	1:R:156:THR:HB	2.00	0.43
1:B:5:PHE:CZ	1:B:254:MET:HE3	2.54	0.43
1:B:129:GLU:OE1	1:B:177:ILE:HD11	2.20	0.42
1:B:311:MET:HE3	1:R:3:HIS:ND1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:MET:SD	1:R:92:LEU:HD21	2.59	0.41
1:R:46:LYS:O	1:R:47:THR:C	2.62	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
7:A:409:SAM:HE1	7:A:409:SAM:H4'	1.83	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:A:238:ASP:CG	7:A:408:SAM:HE2	2.46	0.40
1:Q:199:GLN:HG2	1:Q:224:ILE:HB	2.03	0.40
7:A:408:SAM:HE1	7:A:408:SAM:H8	2.03	0.40
1:B:254:MET:HE2	1:R:256:ARG:NH2	2.36	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
7:Q:410:SAM:CE	7:Q:410:SAM:H3'	2.52	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	379/384 (99%)	369 (97%)	10 (3%)	0	100 100
1	B	377/384 (98%)	363 (96%)	11 (3%)	3 (1%)	16 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Q	379/384 (99%)	367 (97%)	11 (3%)	1 (0%)	36 28
1	R	377/384 (98%)	364 (97%)	10 (3%)	3 (1%)	16 8
All	All	1512/1536 (98%)	1463 (97%)	42 (3%)	7 (0%)	24 16

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	310/312 (99%)	301 (97%)	9 (3%)	37 29
1	B	309/312 (99%)	291 (94%)	18 (6%)	18 7
1	Q	311/312 (100%)	304 (98%)	7 (2%)	44 38
1	R	310/312 (99%)	293 (94%)	17 (6%)	19 8
All	All	1240/1248 (99%)	1189 (96%)	51 (4%)	28 17

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	161	ARG
1	A	185	LEU
1	A	211	LEU
1	A	281	VAL

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Mol	Chain	Res	Type
1	A	322	SER
1	A	330[A]	ARG
1	A	330[B]	ARG
1	A	377	ARG
1	B	17	LYS
1	B	112	LEU
1	B	121	LEU
1	B	127	THR
1	B	131	ASP
1	B	171	GLN
1	B	206	ILE
1	B	211	LEU
1	B	214	GLU
1	B	221	LYS
1	B	248	VAL
1	B	254	MET
1	B	270	VAL
1	B	309	SER
1	B	311	MET
1	B	320	VAL
1	B	324	GLN
1	B	363	GLU
1	Q	17	LYS
1	Q	93	SER
1	Q	121	LEU
1	Q	185	LEU
1	Q	281	VAL
1	Q	323	GLU
1	Q	324	GLN
1	R	17	LYS
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	203	MET
1	R	211	LEU
1	R	214	GLU
1	R	248	VAL
1	R	256	ARG

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Mol	Chain	Res	Type
1	R	309	SER
1	R	320	VAL
1	R	369	LYS
1	R	372	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	374	GLN
1	B	171	GLN
1	Q	103	ASN
1	Q	374	GLN
1	R	171	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 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
2	POP	A	401	5,4	6,8,8	1.18	0	12,13,13	0.90	0
7	SAM	R	404	-	27,29,29	3.03	8 (29%)	34,42,42	2.21	11 (32%)
7	SAM	A	408	-	27,29,29	2.68	7 (25%)	34,42,42	2.18	9 (26%)
6	EDO	B	405	-	3,3,3	0.44	0	2,2,2	0.50	0
6	EDO	Q	407	-	3,3,3	0.35	0	2,2,2	0.41	0
6	EDO	A	406	-	3,3,3	0.43	0	2,2,2	0.35	0
7	SAM	A	409	-	27,29,29	3.02	8 (29%)	34,42,42	2.39	10 (29%)
3	PO4	Q	402	4	4,4,4	0.76	0	6,6,6	0.56	0
6	EDO	B	406	-	3,3,3	0.51	0	2,2,2	0.32	0
6	EDO	R	405	-	3,3,3	0.37	0	2,2,2	0.46	0
7	SAM	Q	411	-	27,29,29	3.04	7 (25%)	34,42,42	2.39	12 (35%)
2	POP	B	401	4	6,8,8	0.79	0	12,13,13	1.00	1 (8%)
2	POP	R	401	4	6,8,8	0.83	0	12,13,13	1.02	1 (8%)
6	EDO	Q	408	-	3,3,3	0.36	0	2,2,2	0.71	0
6	EDO	A	407	-	3,3,3	0.35	0	2,2,2	0.70	0
6	EDO	Q	409	-	3,3,3	0.40	0	2,2,2	0.55	0
2	POP	Q	401	5,4	6,8,8	1.19	0	12,13,13	1.25	1 (8%)
3	PO4	A	402	4	4,4,4	0.92	0	6,6,6	0.24	0
3	PO4	Q	403	-	4,4,4	1.02	0	6,6,6	0.34	0
7	SAM	B	407	-	27,29,29	3.02	8 (29%)	34,42,42	2.32	13 (38%)
6	EDO	Q	413	-	3,3,3	0.36	0	2,2,2	0.65	0
3	PO4	B	402	-	4,4,4	0.96	0	6,6,6	0.44	0
7	SAM	Q	410	-	27,29,29	2.70	7 (25%)	34,42,42	2.24	9 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POP	A	401	5,4	-	0/6/6/6	-
7	SAM	R	404	-	-	6/17/33/33	0/3/3/3
7	SAM	A	408	-	-	5/17/33/33	0/3/3/3
6	EDO	B	405	-	-	0/1/1/1	-
6	EDO	Q	407	-	-	0/1/1/1	-
6	EDO	A	406	-	-	1/1/1/1	-
7	SAM	A	409	-	-	7/17/33/33	0/3/3/3
6	EDO	B	406	-	-	1/1/1/1	-
6	EDO	R	405	-	-	0/1/1/1	-
7	SAM	Q	411	-	-	6/17/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POP	B	401	4	-	0/6/6/6	-
2	POP	R	401	4	-	0/6/6/6	-
6	EDO	Q	408	-	-	1/1/1/1	-
6	EDO	A	407	-	-	1/1/1/1	-
6	EDO	Q	409	-	-	0/1/1/1	-
2	POP	Q	401	5,4	-	0/6/6/6	-
7	SAM	B	407	-	-	8/17/33/33	0/3/3/3
6	EDO	Q	413	-	-	1/1/1/1	-
7	SAM	Q	410	-	-	6/17/33/33	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Q	411	SAM	O4'-C1'	9.44	1.63	1.42
7	A	409	SAM	O4'-C1'	9.13	1.63	1.42
7	R	404	SAM	O4'-C1'	8.93	1.62	1.42
7	B	407	SAM	O4'-C1'	8.91	1.62	1.42
7	B	407	SAM	C2'-C1'	-7.41	1.30	1.53
7	A	409	SAM	C2'-C1'	-7.37	1.30	1.53
7	Q	411	SAM	C2'-C1'	-7.33	1.30	1.53
7	R	404	SAM	C2'-C1'	-7.27	1.30	1.53
7	A	408	SAM	O4'-C1'	7.03	1.58	1.42
7	Q	410	SAM	O4'-C1'	6.98	1.58	1.42
7	A	408	SAM	C2'-C1'	-6.82	1.32	1.53
7	Q	410	SAM	C2'-C1'	-6.72	1.32	1.53
7	R	404	SAM	O4'-C4'	-6.22	1.31	1.45
7	A	409	SAM	O4'-C4'	-6.07	1.31	1.45
7	Q	410	SAM	O4'-C4'	-6.05	1.31	1.45
7	B	407	SAM	O4'-C4'	-5.94	1.31	1.45
7	Q	411	SAM	O4'-C4'	-5.79	1.32	1.45
7	A	408	SAM	O4'-C4'	-5.21	1.33	1.45
7	B	407	SAM	C6-N6	5.16	1.47	1.34
7	R	404	SAM	C6-N6	5.12	1.47	1.34
7	A	409	SAM	C6-N6	5.03	1.47	1.34
7	Q	411	SAM	C6-N6	4.87	1.46	1.34
7	Q	410	SAM	C5-C4	-4.25	1.31	1.39
7	A	408	SAM	C6-N6	4.22	1.45	1.34
7	Q	410	SAM	C6-N6	3.77	1.43	1.34
7	A	408	SAM	C5-C4	-3.34	1.33	1.39
7	Q	411	SAM	O3'-C3'	-2.94	1.35	1.43
7	R	404	SAM	O3'-C3'	-2.78	1.36	1.43
7	B	407	SAM	O3'-C3'	-2.78	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	404	SAM	C5-C4	-2.76	1.34	1.39
7	B	407	SAM	O2'-C2'	2.74	1.49	1.43
7	Q	411	SAM	C5-C4	-2.74	1.34	1.39
7	R	404	SAM	O2'-C2'	2.69	1.49	1.43
7	A	409	SAM	O2'-C2'	2.67	1.49	1.43
7	Q	411	SAM	O2'-C2'	2.64	1.49	1.43
7	B	407	SAM	C5-C4	-2.64	1.34	1.39
7	A	409	SAM	C5-C4	-2.61	1.34	1.39
7	A	408	SAM	O2'-C2'	2.58	1.49	1.43
7	A	408	SAM	O3'-C3'	-2.32	1.37	1.43
7	Q	410	SAM	O2'-C2'	2.30	1.48	1.43
7	A	409	SAM	O3'-C3'	-2.28	1.37	1.43
7	B	407	SAM	C5-N7	-2.21	1.35	1.39
7	Q	410	SAM	O3'-C3'	-2.11	1.37	1.43
7	R	404	SAM	C5-N7	-2.10	1.35	1.39
7	A	409	SAM	C5-N7	-2.05	1.35	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	410	SAM	N3-C2-N1	-6.58	118.63	128.58
7	Q	411	SAM	N3-C2-N1	-6.29	119.05	128.58
7	A	408	SAM	N3-C2-N1	-6.24	119.14	128.58
7	A	409	SAM	N3-C2-N1	-6.15	119.28	128.58
7	A	409	SAM	C5-C4-N3	-5.50	119.14	126.72
7	R	404	SAM	N3-C2-N1	-5.49	120.28	128.58
7	B	407	SAM	N3-C2-N1	-5.35	120.48	128.58
7	B	407	SAM	C5-C4-N3	-5.33	119.38	126.72
7	Q	411	SAM	C5-C4-N3	-5.26	119.47	126.72
7	R	404	SAM	C5-C4-N3	-4.89	119.98	126.72
7	Q	411	SAM	N6-C6-N1	-4.83	107.63	118.38
7	B	407	SAM	N6-C6-N1	-4.65	108.01	118.38
7	A	409	SAM	N6-C6-N1	-4.47	108.43	118.38
7	R	404	SAM	N6-C6-N1	-4.44	108.49	118.38
7	Q	410	SAM	C5-C4-N3	-4.35	120.72	126.72
7	A	408	SAM	C5-C4-N3	-4.32	120.77	126.72
7	Q	410	SAM	N9-C8-N7	-4.26	107.89	113.94
7	R	404	SAM	N9-C8-N7	-4.15	108.05	113.94
7	A	408	SAM	CG-SD-C5'	-4.11	93.38	103.43
7	Q	411	SAM	C2-N3-C4	3.90	121.36	111.83
7	A	409	SAM	C2-N3-C4	3.83	121.18	111.83
7	Q	411	SAM	N9-C8-N7	-3.82	108.52	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	407	SAM	N9-C8-N7	-3.81	108.53	113.94
7	Q	410	SAM	N3-C4-N9	3.74	133.52	127.17
7	A	409	SAM	N3-C4-N9	3.66	133.40	127.17
7	A	409	SAM	N9-C8-N7	-3.64	108.77	113.94
7	A	408	SAM	N9-C8-N7	-3.63	108.79	113.94
7	B	407	SAM	C5-C6-N6	3.54	132.04	123.29
7	A	408	SAM	N3-C4-N9	3.46	133.06	127.17
7	Q	410	SAM	C2-N3-C4	3.44	120.23	111.83
7	B	407	SAM	C2-N3-C4	3.40	120.15	111.83
7	Q	410	SAM	CG-SD-C5'	-3.38	95.18	103.43
7	R	404	SAM	C5-C6-N6	3.37	131.64	123.29
7	A	409	SAM	CG-SD-C5'	3.36	111.65	103.43
7	Q	411	SAM	C5-C6-N6	3.32	131.49	123.29
7	Q	410	SAM	C4-N9-C8	3.31	109.21	105.74
7	R	404	SAM	C2-N3-C4	3.27	119.82	111.83
7	A	408	SAM	C2-N3-C4	3.20	119.65	111.83
7	A	409	SAM	C5-C6-N6	3.18	131.17	123.29
7	Q	411	SAM	N3-C4-N9	3.18	132.57	127.17
2	Q	401	POP	O2-P1-O	3.15	115.19	104.64
7	B	407	SAM	N3-C4-N9	3.11	132.46	127.17
7	A	408	SAM	N6-C6-N1	-3.05	111.59	118.38
7	R	404	SAM	N3-C4-N9	3.02	132.30	127.17
7	B	407	SAM	C5-N7-C8	2.94	108.07	103.45
7	R	404	SAM	C5-N7-C8	2.89	107.99	103.45
7	B	407	SAM	CG-SD-C5'	2.85	110.39	103.43
7	A	408	SAM	C4-N9-C8	2.84	108.72	105.74
7	Q	411	SAM	C5-N7-C8	2.61	107.55	103.45
7	A	409	SAM	C5-N7-C8	2.57	107.49	103.45
7	Q	410	SAM	N6-C6-N1	-2.54	112.71	118.38
7	B	407	SAM	C3'-C2'-C1'	2.51	106.21	101.46
7	A	409	SAM	C3'-C2'-C1'	2.46	106.12	101.46
7	Q	411	SAM	C3'-C2'-C1'	2.44	106.08	101.46
7	B	407	SAM	C6-C5-C4	2.35	120.39	117.18
7	B	407	SAM	C4-C5-N7	-2.35	107.90	110.58
2	B	401	POP	O2-P1-O	2.35	112.50	104.64
7	Q	410	SAM	O4'-C1'-N9	2.29	112.49	108.09
7	Q	411	SAM	O4'-C4'-C5'	2.28	114.64	108.88
7	R	404	SAM	C4-N9-C8	2.24	108.09	105.74
7	Q	411	SAM	CG-SD-C5'	2.22	108.86	103.43
7	Q	411	SAM	C2'-C3'-C4'	2.22	106.89	102.61
7	B	407	SAM	C5-C4-N9	2.16	108.16	105.81
7	R	404	SAM	C6-C5-C4	2.14	120.10	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	404	SAM	C4-C5-N7	-2.13	108.15	110.58
2	R	401	POP	O3-P1-O	2.12	111.73	104.64
7	A	408	SAM	C4'-O4'-C1'	-2.04	104.96	109.47

There are no chirality outliers.

All (43) 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	A	409	SAM	C4'-C5'-SD-CE
7	B	407	SAM	CA-CB-CG-SD
7	B	407	SAM	CB-CG-SD-CE
7	B	407	SAM	C4'-C5'-SD-CE
7	Q	410	SAM	O4'-C4'-C5'-SD
7	Q	411	SAM	O-C-CA-N
7	R	404	SAM	O4'-C4'-C5'-SD
7	Q	411	SAM	OXT-C-CA-N
7	B	407	SAM	OXT-C-CA-N
7	R	404	SAM	OXT-C-CA-N
7	A	408	SAM	O-C-CA-CB
7	A	408	SAM	OXT-C-CA-CB
6	A	406	EDO	O1-C1-C2-O2
7	A	408	SAM	C2'-C1'-N9-C8
7	A	409	SAM	CA-CB-CG-SD
7	Q	411	SAM	CA-CB-CG-SD
7	R	404	SAM	CA-CB-CG-SD
7	R	404	SAM	O-C-CA-CB
7	B	407	SAM	CB-CG-SD-C5'
7	Q	411	SAM	O-C-CA-CB
7	R	404	SAM	OXT-C-CA-CB
7	Q	411	SAM	OXT-C-CA-CB
6	Q	408	EDO	O1-C1-C2-O2
6	Q	413	EDO	O1-C1-C2-O2
7	Q	410	SAM	C2'-C1'-N9-C8
7	B	407	SAM	O-C-CA-CB
7	B	407	SAM	OXT-C-CA-CB
7	Q	410	SAM	O-C-CA-CB
7	Q	410	SAM	OXT-C-CA-CB
6	B	406	EDO	O1-C1-C2-O2
7	A	408	SAM	O4'-C1'-N9-C8
7	A	409	SAM	O4'-C1'-N9-C8

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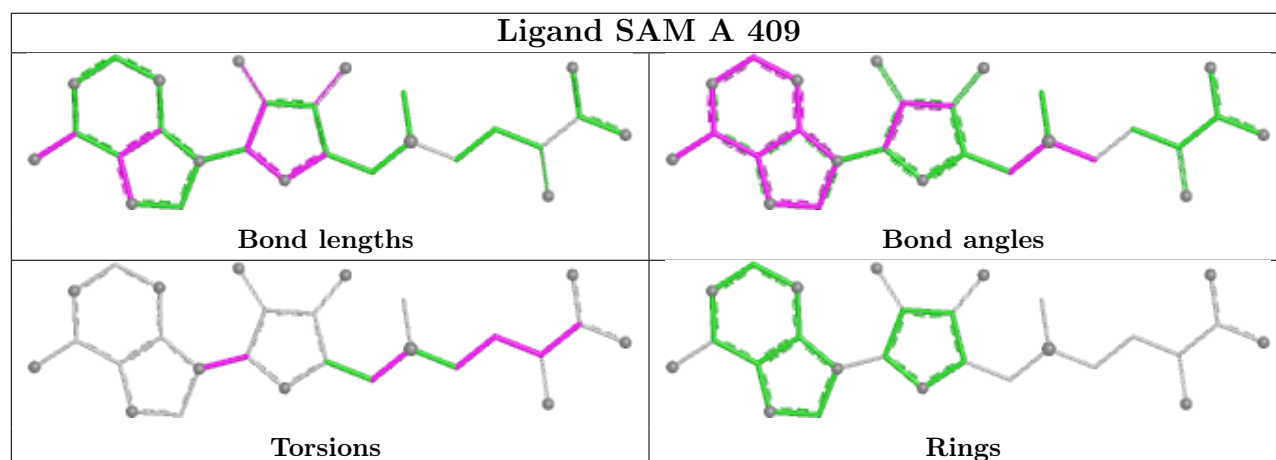
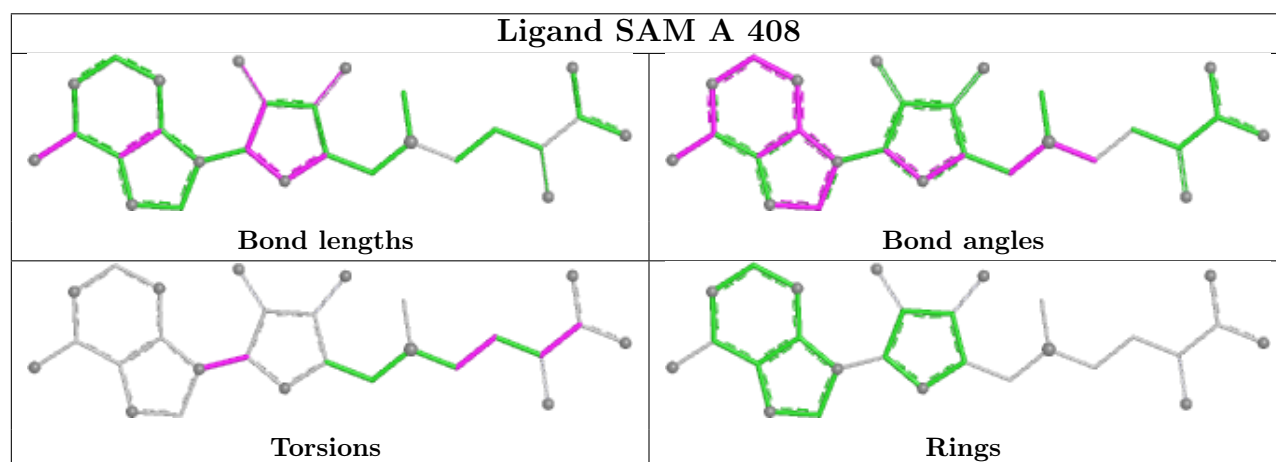
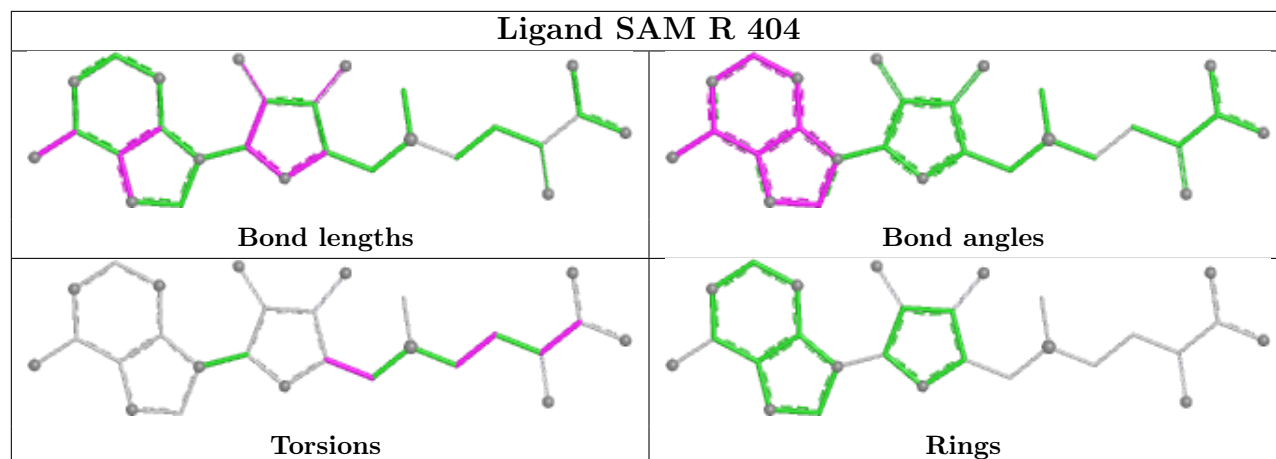
Mol	Chain	Res	Type	Atoms
6	A	407	EDO	O1-C1-C2-O2
7	A	409	SAM	C2'-C1'-N9-C8
7	A	408	SAM	CA-CB-CG-SD
7	Q	410	SAM	O4'-C1'-N9-C8
7	A	409	SAM	OXT-C-CA-N
7	Q	410	SAM	OXT-C-CA-N
7	Q	411	SAM	CB-CG-SD-C5'
7	B	407	SAM	O-C-CA-N
7	R	404	SAM	O-C-CA-N

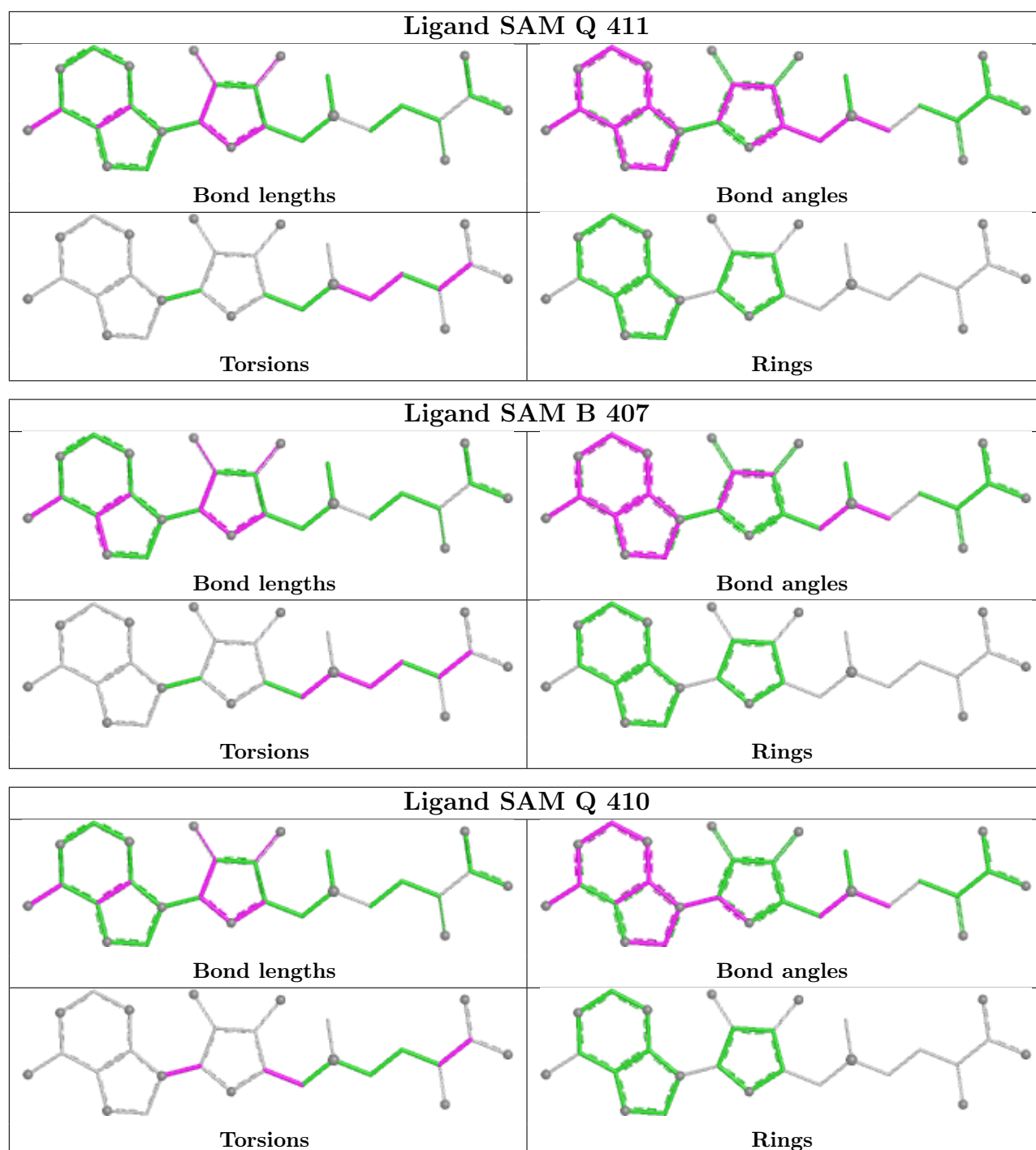
There are no ring outliers.

11 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	404	SAM	2	0
7	A	408	SAM	12	0
6	A	406	EDO	1	0
7	A	409	SAM	4	0
6	B	406	EDO	1	0
7	Q	411	SAM	4	0
6	Q	408	EDO	1	0
6	A	407	EDO	1	0
7	B	407	SAM	1	0
6	Q	413	EDO	1	0
7	Q	410	SAM	8	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	379/384 (98%)	-0.34	1 (0%) 90 92	13, 32, 68, 106	2 (0%)
1	B	378/384 (98%)	0.72	27 (7%) 22 25	32, 86, 127, 159	1 (0%)
1	Q	378/384 (98%)	-0.36	0 100 100	12, 32, 64, 97	3 (0%)
1	R	377/384 (98%)	0.71	26 (6%) 23 26	26, 86, 129, 151	2 (0%)
All	All	1512/1536 (98%)	0.18	54 (3%) 46 53	12, 53, 121, 159	8 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	285	ILE	4.0
1	B	61	TRP	3.9
1	B	285	ILE	3.8
1	R	61	TRP	3.7
1	R	376	LEU	3.6
1	R	302	ILE	3.3
1	B	376	LEU	3.2
1	B	380	ALA	3.2
1	R	375	LEU	3.1
1	B	102	ILE	3.0
1	B	375	LEU	2.9
1	R	332	PHE	2.9
1	R	338	TYR	2.7
1	R	4	LEU	2.7
1	R	102	ILE	2.7
1	B	332[A]	PHE	2.7
1	B	337	PRO	2.7
1	R	325	LEU	2.7
1	B	312	VAL	2.6
1	R	370	THR	2.5
1	B	328	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	R	333	PHE	2.5
1	R	379	ALA	2.5
1	B	168	VAL	2.5
1	R	327	LEU	2.4
1	B	177	ILE	2.4
1	B	210	ILE	2.4
1	B	121	LEU	2.3
1	R	117	GLY	2.3
1	B	338	TYR	2.2
1	R	310	ILE	2.2
1	R	312	VAL	2.2
1	B	139	THR	2.2
1	R	138	ILE	2.2
1	R	121	LEU	2.2
1	R	296	ILE	2.2
1	B	184	VAL	2.2
1	B	298	VAL	2.2
1	R	168	VAL	2.2
1	R	298	VAL	2.2
1	B	4	LEU	2.2
1	R	161[A]	ARG	2.2
1	R	170	PHE	2.1
1	B	215	TRP	2.1
1	A	330[A]	ARG	2.1
1	B	370	THR	2.1
1	B	170	PHE	2.0
1	R	124	GLY	2.0
1	B	211	LEU	2.0
1	B	325	LEU	2.0
1	R	335	LEU	2.0
1	B	117	GLY	2.0
1	B	270	VAL	2.0
1	B	281	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

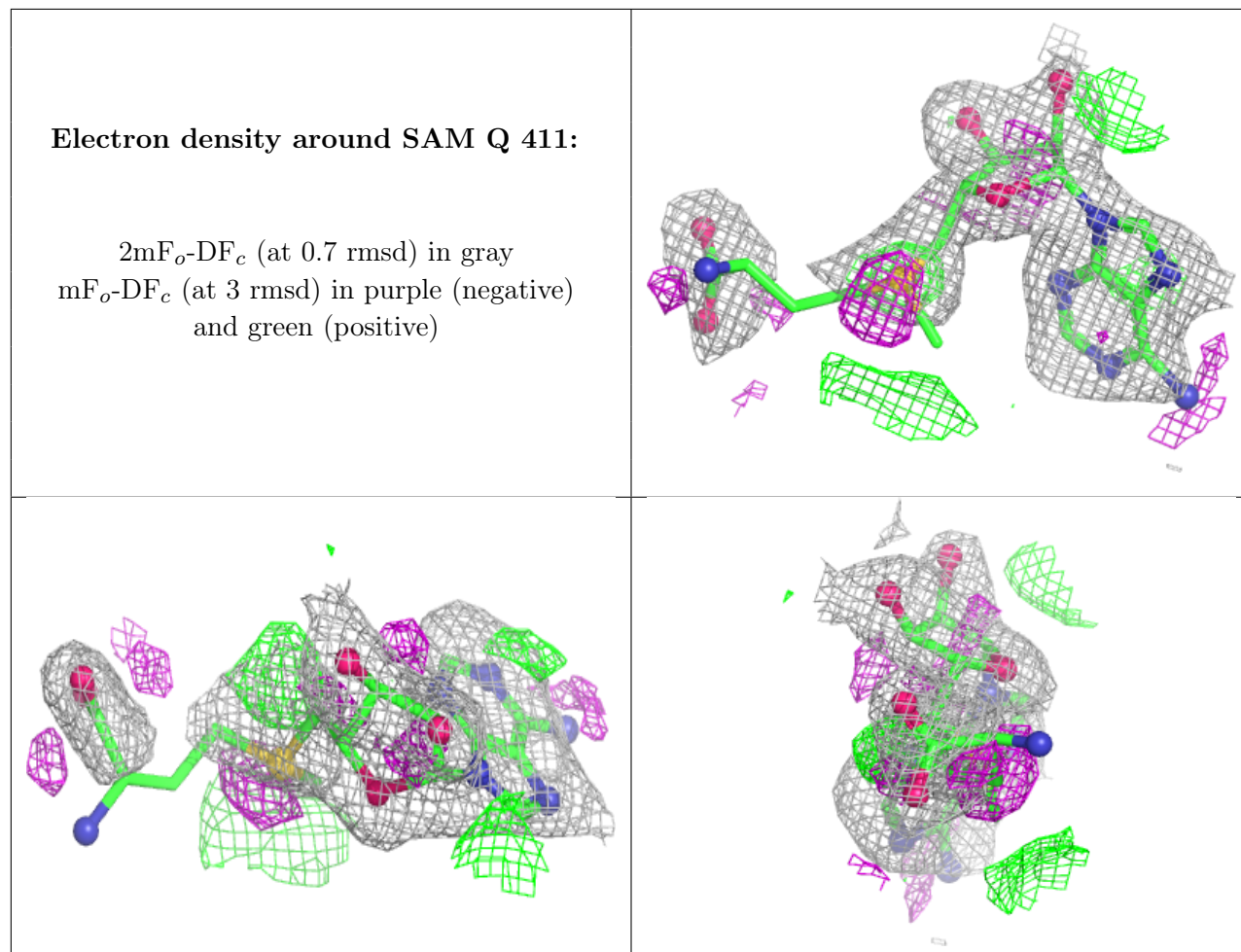
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	K	Q	406	1/1	0.69	0.20	116,116,116,116	0
5	K	A	405	1/1	0.74	0.20	109,109,109,109	0
4	MG	B	404	1/1	0.76	0.15	81,81,81,81	0
7	SAM	Q	411	27/27	0.77	0.15	43,73,104,105	0
7	SAM	A	409	27/27	0.83	0.13	49,70,96,98	0
6	EDO	Q	413	4/4	0.84	0.18	52,55,61,67	0
4	MG	R	402	1/1	0.84	0.11	81,81,81,81	0
6	EDO	Q	409	4/4	0.84	0.16	57,58,58,62	0
5	K	Q	405	1/1	0.85	0.15	76,76,76,76	0
3	PO4	B	402	5/5	0.86	0.14	103,104,107,107	0
6	EDO	A	406	4/4	0.87	0.17	58,59,59,63	0
6	EDO	B	406	4/4	0.87	0.13	65,66,66,66	0
3	PO4	Q	403	5/5	0.88	0.13	91,95,97,100	0
6	EDO	R	405	4/4	0.88	0.14	45,50,55,59	0
7	SAM	R	404	27/27	0.89	0.12	70,79,89,90	0
7	SAM	B	407	27/27	0.90	0.13	68,76,97,98	0
6	EDO	B	405	4/4	0.90	0.12	47,51,53,58	0
6	EDO	Q	408	4/4	0.90	0.14	58,59,61,62	0
5	K	A	404	1/1	0.91	0.13	85,85,85,85	0
2	POP	R	401	9/9	0.94	0.07	51,56,65,68	0
6	EDO	Q	407	4/4	0.94	0.18	48,50,50,51	0
2	POP	B	401	9/9	0.94	0.07	52,60,66,69	0
6	EDO	A	407	4/4	0.94	0.12	52,59,64,65	0
3	PO4	Q	402	5/5	0.94	0.10	29,29,48,50	0
7	SAM	Q	410	27/27	0.95	0.07	18,28,36,45	0
7	SAM	A	408	27/27	0.96	0.07	18,25,35,43	0
3	PO4	A	402	5/5	0.96	0.10	27,29,49,51	0
4	MG	Q	404	1/1	0.98	0.03	31,31,31,31	0
4	MG	B	403	1/1	0.98	0.04	47,47,47,47	0
4	MG	A	410	1/1	0.98	0.04	28,28,28,28	0
4	MG	R	403	1/1	0.99	0.05	45,45,45,45	0
4	MG	A	403	1/1	0.99	0.02	20,20,20,20	0
2	POP	Q	401	9/9	0.99	0.04	18,23,26,31	0
4	MG	Q	412	1/1	0.99	0.02	22,22,22,22	0
2	POP	A	401	9/9	0.99	0.04	18,24,28,31	0

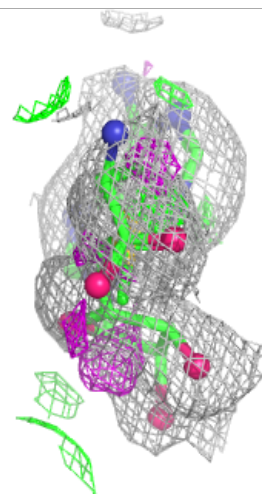
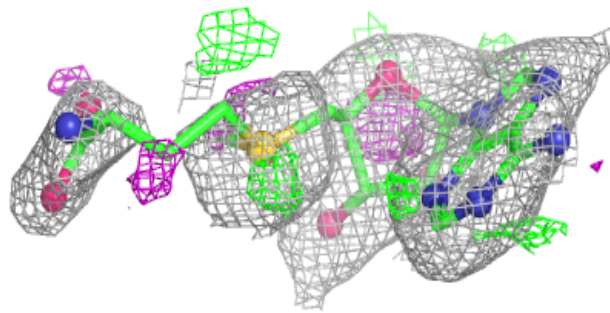
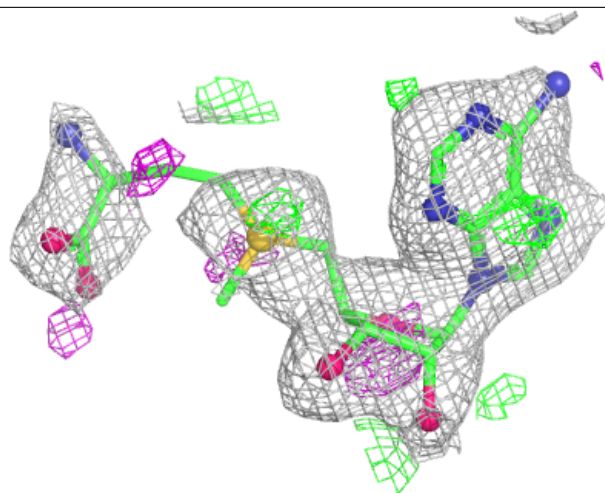
The following is a graphical depiction of the model fit to experimental electron density of all

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.



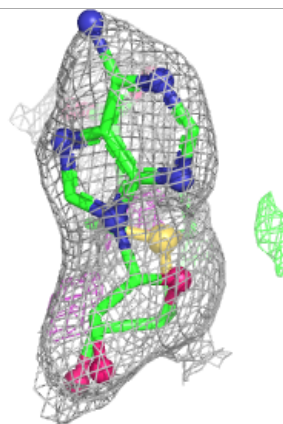
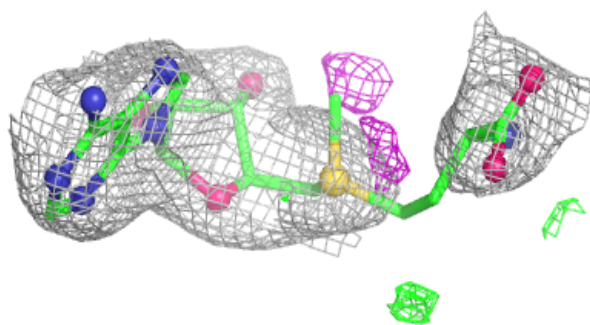
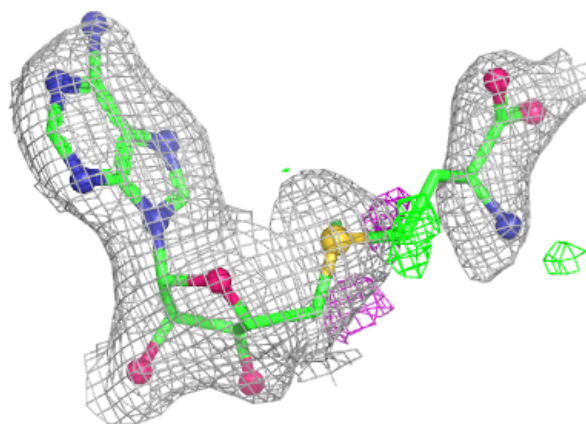
Electron density around SAM A 409:

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



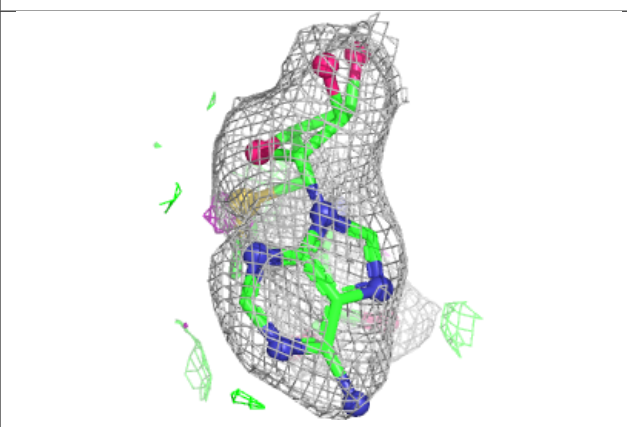
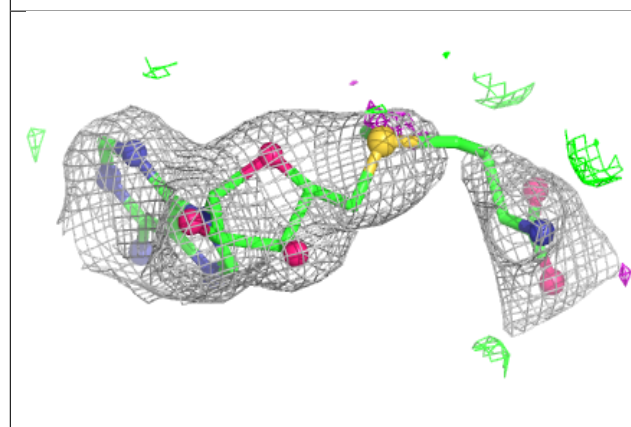
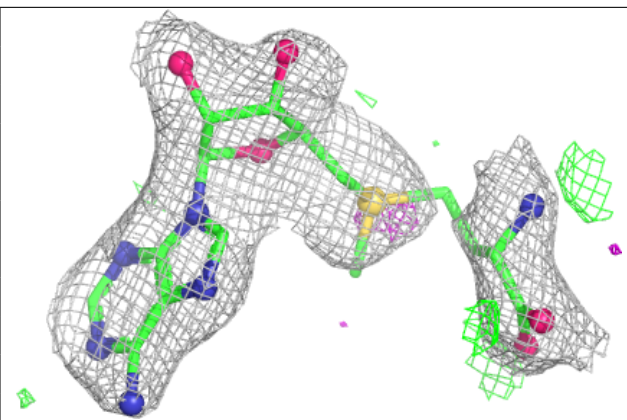
Electron density around SAM R 404:

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

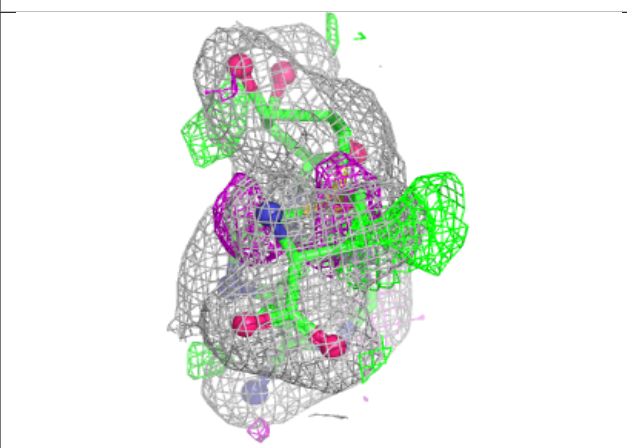
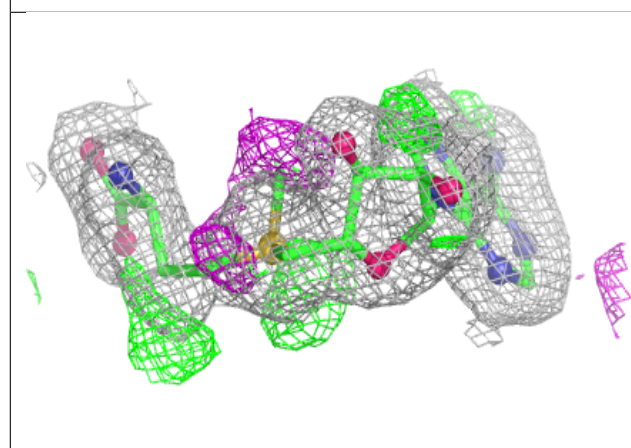
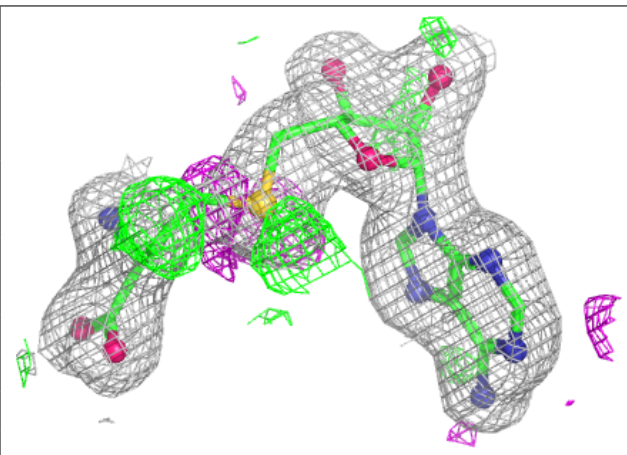


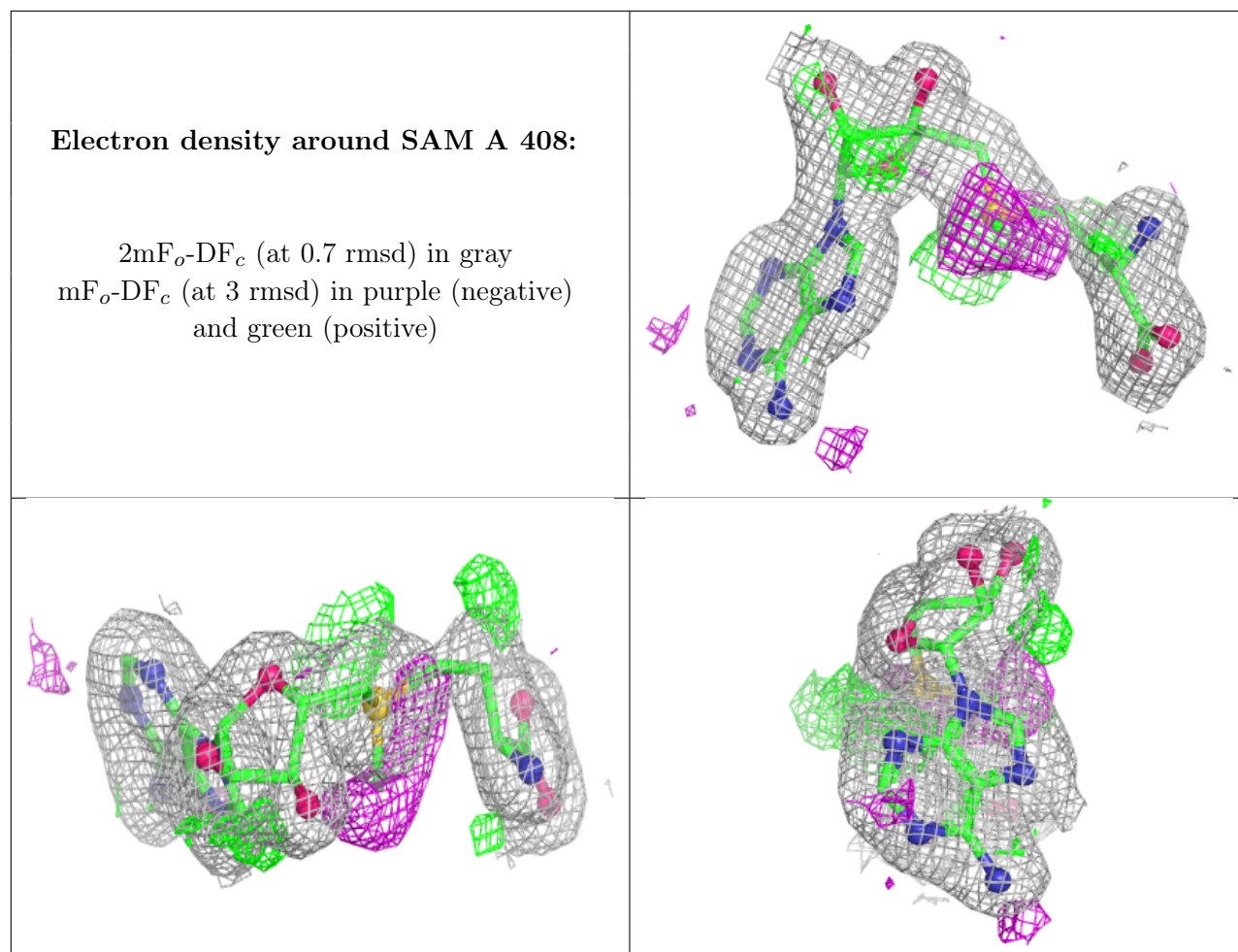
Electron density around SAM B 407:

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

**Electron density around SAM Q 410:**

$2mF_o-DF_c$ (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.