



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:07 AM UTC

PDB ID : 1N2X / pdb_00001n2x
Title : Crystal Structure Analysis of TM0872, a Putative SAM-dependent Methyltransferase, Complexed with SAM
Authors : Miller, D.J.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2002-10-24
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

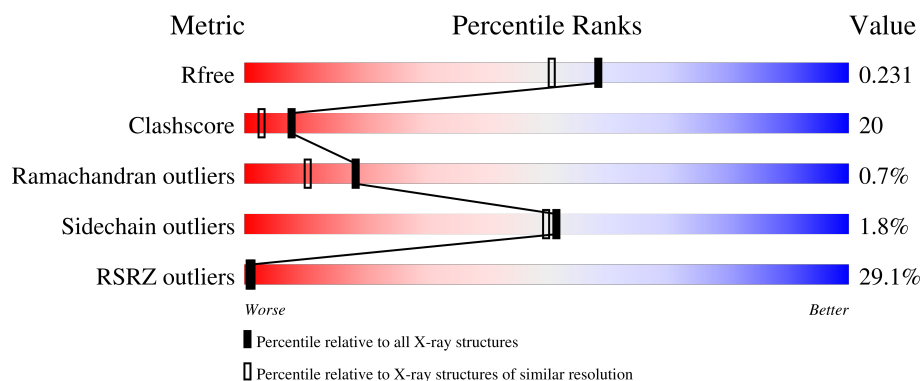
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	301	
1	B	301	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5009 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-adenosyl-methyltransferase mraW.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	Se	0	5	0
			2392	1509	436	440	3	4			
1	B	278	Total	C	N	O	S	Se	0	0	0
			2204	1398	395	404	3	4			

There are 14 discrepancies between the modelled and reference sequences:

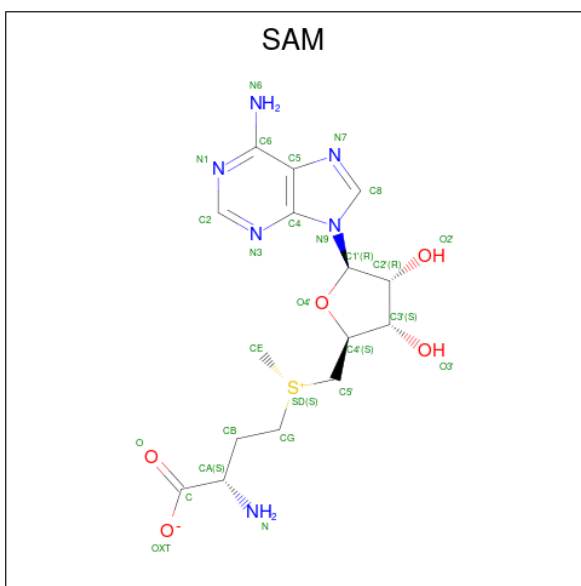
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q9WZX6
A	0	HIS	-	cloning artifact	UNP Q9WZX6
A	1	MSE	MET	modified residue	UNP Q9WZX6
A	12	MSE	MET	modified residue	UNP Q9WZX6
A	102	MSE	MET	modified residue	UNP Q9WZX6
A	128	MSE	MET	modified residue	UNP Q9WZX6
A	130	MSE	MET	modified residue	UNP Q9WZX6
B	-1	GLY	-	cloning artifact	UNP Q9WZX6
B	0	HIS	-	cloning artifact	UNP Q9WZX6
B	1	MSE	MET	modified residue	UNP Q9WZX6
B	12	MSE	MET	modified residue	UNP Q9WZX6
B	102	MSE	MET	modified residue	UNP Q9WZX6
B	128	MSE	MET	modified residue	UNP Q9WZX6
B	130	MSE	MET	modified residue	UNP Q9WZX6

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

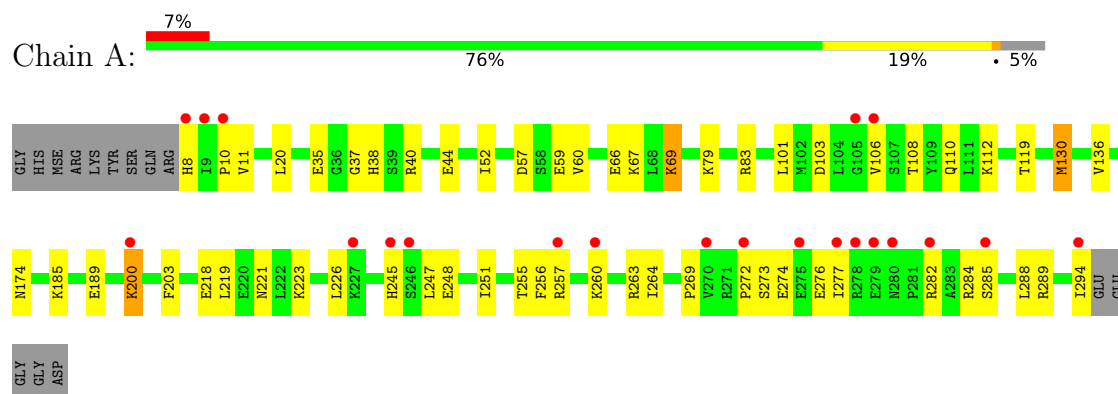
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	233	Total 233	O 233	0	0
4	B	116	Total 116	O 116	0	0

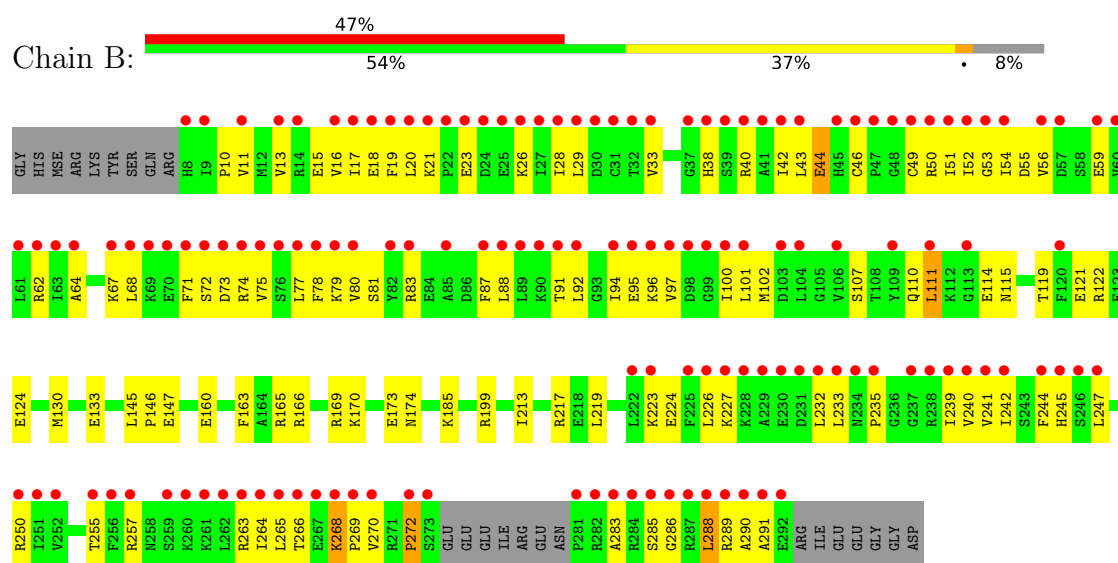
3 Residue-property plots

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-adenosyl-methyltransferase mraW



• Molecule 1: S-adenosyl-methyltransferase mraW



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	133.96Å 133.96Å 133.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 1.90 19.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.97-1.90) 99.9 (19.97-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.226 0.209 , 0.231	Depositor DCC
R_{free} test set	3187 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5009	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: SAM, SO4

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	0/2421	0.88	6/3239 (0.2%)
1	B	0.37	0/2231	0.83	4/2994 (0.1%)
All	All	0.42	0/4652	0.86	10/6233 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	PRO	N-CA-CB	6.25	109.81	103.25
1	A	218	GLU	N-CA-C	6.18	118.01	111.28
1	B	130	MSE	N-CA-C	-6.09	105.68	113.23
1	A	136	VAL	N-CA-C	5.67	116.37	108.89
1	A	203	PHE	N-CA-C	5.48	118.01	111.71
1	B	160	GLU	N-CA-C	-5.45	99.07	108.56
1	A	52	ILE	N-CA-C	-5.43	99.33	107.37
1	A	130	MSE	N-CA-C	-5.13	105.77	112.23
1	A	112	LYS	N-CA-C	5.11	119.79	113.50
1	B	199	ARG	N-CA-C	5.10	117.62	110.23

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	2392	0	2473	52	0
1	B	2204	0	2233	134	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	27	0	22	6	0
3	B	27	0	22	6	0
4	A	233	0	0	6	0
4	B	116	0	0	7	0
All	All	5009	0	4750	187	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 20.

All (187) 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:B:119:THR:OG1	1:B:121:GLU:HG2	1.69	0.92
1:B:257:ARG:HA	1:B:264:ILE:HD11	1.50	0.91
1:B:40:ARG:HA	1:B:40:ARG:NH2	1.89	0.85
1:B:270:VAL:HB	1:B:288:LEU:HB3	1.59	0.85
1:B:163:PHE:HE1	1:B:166:ARG:HH21	1.26	0.83
1:A:59:GLU:HG3	4:A:538:HOH:O	1.79	0.81
1:A:38:HIS:HD2	3:A:401:SAM:HN1	1.27	0.81
1:A:260:LYS:HA	1:A:260:LYS:HE2	1.64	0.78
1:B:80:VAL:HG11	1:B:88:LEU:HD22	1.68	0.76
1:A:269:PRO:HG3	1:A:289:ARG:CZ	2.17	0.75
1:B:226:LEU:HB3	1:B:255:THR:HG21	1.66	0.75
1:B:40:ARG:HH11	1:B:68:LEU:HA	1.50	0.74
1:B:245:HIS:CD2	1:B:247:LEU:HB3	2.23	0.74
1:A:35:GLU:O	1:A:67[A]:LYS:HE2	1.87	0.73
1:B:269:PRO:HG3	1:B:289:ARG:HH12	1.51	0.73
1:B:163:PHE:HE1	1:B:166:ARG:NH2	1.86	0.73
1:A:10:PRO:HA	4:A:733:HOH:O	1.89	0.72
1:A:245:HIS:CD2	1:A:247:LEU:HB3	2.25	0.71
1:B:265:LEU:HG	1:B:291:ALA:HA	1.73	0.70
1:B:110:GLN:HA	1:B:114:GLU:HG3	1.71	0.70
1:A:245:HIS:HB3	1:A:248:GLU:HG3	1.73	0.70
1:A:226:LEU:HB3	1:A:255:THR:HG21	1.73	0.70
1:B:269:PRO:HG3	1:B:289:ARG:HH22	1.57	0.69
1:B:245:HIS:NE2	1:B:247:LEU:HB3	2.07	0.69
1:A:269:PRO:HG3	1:A:289:ARG:NH2	2.08	0.69
1:B:213:ILE:CG2	1:B:219:LEU:HD23	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLU:O	1:B:96:LYS:HG3	1.94	0.68
1:B:13:VAL:O	1:B:16:VAL:HG12	1.94	0.68
1:A:119:THR:HG22	4:A:575:HOH:O	1.95	0.67
1:B:40:ARG:NH1	1:B:68:LEU:HA	2.10	0.67
1:B:268:LYS:HD2	1:B:268:LYS:H	1.59	0.67
1:B:288:LEU:HD13	1:B:289:ARG:N	2.09	0.67
1:B:50:ARG:HG2	1:B:51:ILE:H	1.60	0.66
1:B:40:ARG:HA	1:B:40:ARG:CZ	2.25	0.66
1:A:10:PRO:HG3	1:A:37:GLY:HA3	1.77	0.65
1:A:79[A]:LYS:HE2	4:A:515:HOH:O	1.97	0.65
1:B:119:THR:HG22	4:B:542:HOH:O	1.96	0.65
1:A:38:HIS:CD2	3:A:401:SAM:HN1	2.12	0.64
1:A:8:HIS:CE1	1:A:282:ARG:HH21	2.16	0.63
1:B:10:PRO:HB3	1:B:38:HIS:HD2	1.61	0.63
1:B:11:VAL:HG22	1:B:283:ALA:HB2	1.81	0.63
1:A:284:ARG:O	1:A:285:SER:HB2	1.99	0.63
1:B:42:ILE:HB	1:B:51:ILE:HD11	1.81	0.62
1:A:245:HIS:NE2	1:A:247:LEU:HB3	2.15	0.62
1:B:174:ASN:HD21	1:B:185:LYS:NZ	1.98	0.62
1:B:213:ILE:HG21	1:B:219:LEU:HD23	1.81	0.61
1:A:40:ARG:O	1:A:44:GLU:HG3	2.01	0.61
1:B:92:LEU:HD13	1:B:92:LEU:O	2.00	0.61
1:B:67:LYS:C	1:B:68:LEU:HD12	2.26	0.61
1:B:247:LEU:HD12	1:B:250:ARG:HH12	1.66	0.60
1:B:29:LEU:CG	1:B:97:VAL:HG11	2.32	0.60
1:B:107:SER:OG	1:B:110:GLN:HG3	2.01	0.60
1:A:8:HIS:HB2	1:A:108:THR:OG1	2.01	0.59
3:A:401:SAM:HB1	4:A:705:HOH:O	2.01	0.59
1:B:10:PRO:HB3	1:B:38:HIS:CD2	2.37	0.59
1:A:83:ARG:HD2	1:A:221:ASN:HA	1.85	0.59
1:B:29:LEU:HD21	1:B:97:VAL:HG11	1.84	0.59
1:B:264:ILE:HG22	1:B:266:THR:H	1.68	0.59
1:B:102:MSE:HB2	1:B:241:VAL:HG22	1.83	0.59
1:B:16:VAL:HG22	1:B:20:LEU:HD12	1.86	0.58
1:B:87:PHE:O	1:B:91:THR:HG23	2.04	0.57
1:A:38:HIS:HD2	3:A:401:SAM:N	2.01	0.57
1:A:272:PRO:HA	1:A:276:GLU:OE1	2.05	0.57
1:B:269:PRO:HG3	1:B:289:ARG:NH1	2.19	0.57
1:A:174:ASN:HD21	1:A:185:LYS:NZ	2.03	0.56
1:B:240:VAL:HG22	1:B:290:ALA:HB2	1.85	0.56
1:B:54:ILE:HG22	1:B:78:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:O	1:A:189:GLU:HG3	2.06	0.55
1:B:213:ILE:HG23	1:B:219:LEU:HD23	1.88	0.55
1:B:38:HIS:HD1	1:B:101:LEU:HD21	1.70	0.55
1:B:100:ILE:HD12	1:B:233:LEU:HD21	1.87	0.55
1:B:247:LEU:HD13	1:B:250:ARG:HH22	1.72	0.55
1:B:17:ILE:HG13	1:B:18:GLU:N	2.21	0.55
1:B:223:LYS:O	1:B:227:LYS:HG3	2.07	0.55
1:A:108:THR:HG21	4:A:730:HOH:O	2.07	0.54
1:B:28:ILE:HB	1:B:51:ILE:HG12	1.88	0.54
1:B:64:ALA:O	1:B:68:LEU:HD13	2.08	0.54
1:B:269:PRO:HG3	1:B:289:ARG:NH2	2.23	0.53
1:B:40:ARG:NH1	1:B:68:LEU:HG	2.23	0.53
1:B:163:PHE:CE1	1:B:166:ARG:NH2	2.67	0.53
1:B:38:HIS:ND1	1:B:101:LEU:HD21	2.24	0.53
1:B:11:VAL:HG21	1:B:244:PHE:HZ	1.73	0.52
1:B:26:LYS:O	1:B:49:CYS:HA	2.09	0.52
1:B:83:ARG:NE	1:B:224:GLU:OE1	2.42	0.52
1:B:50:ARG:HG2	1:B:51:ILE:N	2.25	0.52
1:B:165:ARG:NH1	4:B:575:HOH:O	2.29	0.51
1:B:288:LEU:HD13	1:B:288:LEU:C	2.35	0.51
1:A:263:ARG:HB2	1:A:294:ILE:HD13	1.92	0.50
1:B:122:ARG:HG2	1:B:122:ARG:HH11	1.76	0.50
1:B:29:LEU:CD2	1:B:97:VAL:HG11	2.41	0.50
1:A:277:ILE:HG21	1:A:284:ARG:NH1	2.27	0.50
1:B:242:ILE:HG12	1:B:288:LEU:CD2	2.41	0.50
1:B:240:VAL:HG22	1:B:290:ALA:CB	2.42	0.50
1:A:106:VAL:HG12	1:A:110:GLN:HB2	1.94	0.50
1:A:223:LYS:CG	1:A:251:ILE:HD13	2.41	0.49
1:B:53:GLY:O	1:B:77:LEU:HA	2.12	0.49
1:B:55:ASP:HA	3:B:402:SAM:N3	2.27	0.49
1:B:67:LYS:O	1:B:68:LEU:HD12	2.12	0.49
1:B:29:LEU:HG	1:B:97:VAL:HG11	1.95	0.49
1:B:169:ARG:O	1:B:173:GLU:HG3	2.12	0.49
1:A:257:ARG:HA	1:A:264:ILE:HD11	1.94	0.49
1:A:256:PHE:HB3	1:A:264:ILE:HG12	1.94	0.48
1:B:46:CYS:SG	1:B:46:CYS:O	2.71	0.48
1:B:29:LEU:HD23	1:B:52:ILE:HB	1.95	0.48
1:B:242:ILE:HG12	1:B:288:LEU:HD23	1.94	0.48
1:B:15:GLU:O	1:B:18:GLU:HB3	2.13	0.48
1:B:268:LYS:HD2	1:B:268:LYS:N	2.25	0.48
1:A:245:HIS:HB3	1:A:248:GLU:CG	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ASN:HD21	1:B:185:LYS:HZ3	1.61	0.48
1:B:244:PHE:HA	1:B:285:SER:O	2.13	0.48
1:A:284:ARG:O	1:A:285:SER:CB	2.61	0.48
1:A:11:VAL:O	1:A:38:HIS:HE1	1.97	0.47
1:A:10:PRO:HG3	1:A:37:GLY:CA	2.43	0.47
1:B:40:ARG:HA	1:B:40:ARG:HH21	1.78	0.47
1:B:50:ARG:HH21	1:B:52:ILE:HD11	1.80	0.47
1:B:81:SER:C	1:B:83:ARG:H	2.21	0.47
1:B:115:ASN:OD1	1:B:124:GLU:HG2	2.14	0.47
1:B:245:HIS:HE2	1:B:247:LEU:HB3	1.78	0.47
1:A:57:ASP:HB3	1:A:60[A]:VAL:HG22	1.96	0.47
1:B:71:PHE:HD2	1:B:74:ARG:HH21	1.62	0.47
1:B:94:ILE:HG22	1:B:96:LYS:H	1.79	0.47
1:B:38:HIS:O	1:B:42:ILE:HG13	2.15	0.46
1:B:55:ASP:OD2	3:B:402:SAM:H1'	2.16	0.46
1:A:277:ILE:HG21	1:A:284:ARG:HH11	1.81	0.46
1:B:59:GLU:HG2	1:B:62:ARG:HH21	1.81	0.46
1:B:247:LEU:CD1	1:B:250:ARG:HH22	2.29	0.46
1:A:288:LEU:HD23	1:A:288:LEU:C	2.41	0.46
1:B:40:ARG:HH22	1:B:43:LEU:HD12	1.80	0.45
1:B:110:GLN:HA	1:B:114:GLU:CG	2.42	0.45
1:B:16:VAL:HG13	1:B:17:ILE:N	2.31	0.45
1:B:29:LEU:CD2	1:B:52:ILE:HB	2.47	0.45
1:B:64:ALA:O	1:B:68:LEU:HB2	2.17	0.45
1:A:174:ASN:HD21	1:A:185:LYS:HZ3	1.64	0.45
1:A:273:SER:OG	1:A:276:GLU:HG3	2.17	0.45
1:B:269:PRO:CG	1:B:289:ARG:HH12	2.26	0.45
1:B:43:LEU:HD13	1:B:71:PHE:CB	2.46	0.45
1:B:233:LEU:HD22	1:B:233:LEU:N	2.31	0.45
1:B:269:PRO:CG	1:B:289:ARG:HH22	2.28	0.45
1:A:272:PRO:HB2	1:A:277:ILE:HD11	1.99	0.44
1:B:56:VAL:HG13	3:B:402:SAM:C2	2.47	0.44
1:B:111:LEU:HD13	1:B:111:LEU:O	2.17	0.44
1:B:174:ASN:ND2	4:B:609:HOH:O	2.50	0.44
1:A:223:LYS:HG3	1:A:251:ILE:HD13	1.99	0.44
1:A:8:HIS:CE1	1:A:282:ARG:HE	2.36	0.44
1:B:147:GLU:HG2	4:B:600:HOH:O	2.17	0.44
1:B:250:ARG:NH1	1:B:250:ARG:HB2	2.32	0.44
1:B:100:ILE:HB	1:B:239:ILE:HG13	1.99	0.44
1:B:111:LEU:HD13	1:B:111:LEU:C	2.43	0.44
1:B:72:SER:C	1:B:74:ARG:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:O	1:A:200:LYS:HE3	2.18	0.43
1:B:219:LEU:O	1:B:223:LYS:HG3	2.17	0.43
1:B:40:ARG:HD3	1:B:44:GLU:OE2	2.18	0.43
1:B:51:ILE:O	1:B:75:VAL:HG23	2.19	0.43
1:A:8:HIS:NE2	1:A:282:ARG:NH2	2.56	0.43
1:B:81:SER:HA	3:B:402:SAM:N1	2.33	0.43
1:A:66:GLU:OE2	1:A:69:LYS:HE3	2.19	0.43
1:B:250:ARG:HH11	1:B:250:ARG:CB	2.32	0.43
1:B:33:VAL:O	3:B:402:SAM:HA	2.18	0.42
1:B:288:LEU:C	1:B:288:LEU:CD1	2.93	0.42
1:B:72:SER:O	1:B:74:ARG:N	2.53	0.42
1:B:122:ARG:HG2	1:B:122:ARG:NH1	2.34	0.42
1:A:260:LYS:HE2	1:A:260:LYS:CA	2.42	0.42
1:B:244:PHE:CD1	1:B:286:GLY:HA2	2.54	0.42
1:B:166:ARG:NH1	4:B:580:HOH:O	2.53	0.42
1:B:174:ASN:HD21	1:B:185:LYS:HZ2	1.67	0.41
1:B:217:ARG:NH1	4:B:612:HOH:O	2.53	0.41
1:B:29:LEU:CD1	1:B:97:VAL:HG21	2.50	0.41
1:B:97:VAL:HG22	1:B:232:LEU:O	2.20	0.41
1:B:289:ARG:HH11	1:B:289:ARG:HG3	1.86	0.41
1:A:35:GLU:HG3	1:A:60[B]:VAL:CG2	2.50	0.41
1:B:55:ASP:O	1:B:79:LYS:HA	2.19	0.41
1:B:74:ARG:NH1	1:B:74:ARG:HB3	2.36	0.41
1:B:263:ARG:HH11	1:B:263:ARG:HG3	1.84	0.41
1:A:20[B]:LEU:HD11	1:A:101:LEU:HB2	2.02	0.41
1:A:272:PRO:HB2	1:A:277:ILE:CD1	2.51	0.41
1:B:54:ILE:HA	1:B:78:PHE:O	2.20	0.41
1:B:239:ILE:O	1:B:290:ALA:HA	2.21	0.41
1:A:103:ASP:O	3:A:401:SAM:H5'2	2.21	0.41
1:B:15:GLU:O	1:B:19:PHE:HD2	2.04	0.41
1:B:169:ARG:HA	1:B:169:ARG:HD2	1.96	0.41
1:B:122:ARG:CZ	4:B:615:HOH:O	2.69	0.40
1:B:55:ASP:CG	3:B:402:SAM:H1'	2.46	0.40
1:B:170:LYS:HA	1:B:170:LYS:HD3	1.91	0.40
1:B:145:LEU:HA	1:B:146:PRO:HD3	1.96	0.40
1:B:81:SER:C	1:B:83:ARG:N	2.79	0.40
1:A:130:MSE:SE	3:A:401:SAM:H8	2.71	0.40
1:B:19:PHE:O	1:B:21:LYS:HG3	2.21	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	290/301 (96%)	282 (97%)	8 (3%)	0	100	100
1	B	274/301 (91%)	249 (91%)	21 (8%)	4 (2%)	8	2
All	All	564/602 (94%)	531 (94%)	29 (5%)	4 (1%)	18	10

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	ASP
1	B	272	PRO
1	B	23	GLU
1	B	235	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	263/264 (100%)	259 (98%)	4 (2%)	57	56
1	B	234/264 (89%)	229 (98%)	5 (2%)	47	44
All	All	497/528 (94%)	488 (98%)	9 (2%)	51	50

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

Mol	Chain	Res	Type
1	A	69	LYS
1	A	200	LYS

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Mol	Chain	Res	Type
1	A	219	LEU
1	A	274	GLU
1	B	44	GLU
1	B	111	LEU
1	B	133	GLU
1	B	268	LYS
1	B	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	115	ASN
1	A	139	GLN
1	A	174	ASN
1	B	139	GLN
1	B	174	ASN
1	B	209	GLN
1	B	245	HIS

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](#)

4 ligands are modelled in this entry.

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	SO4	A	500	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	B	501	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SAM	B	402	-	27,29,29	0.47	0	34,42,42	0.45	0
3	SAM	A	401	-	27,29,29	0.56	0	34,42,42	0.49	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
3	SAM	B	402	-	-	1/17/33/33	0/3/3/3
3	SAM	A	401	-	-	1/17/33/33	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	SAM	CB-CG-SD-CE
3	A	401	SAM	C2'-C1'-N9-C8

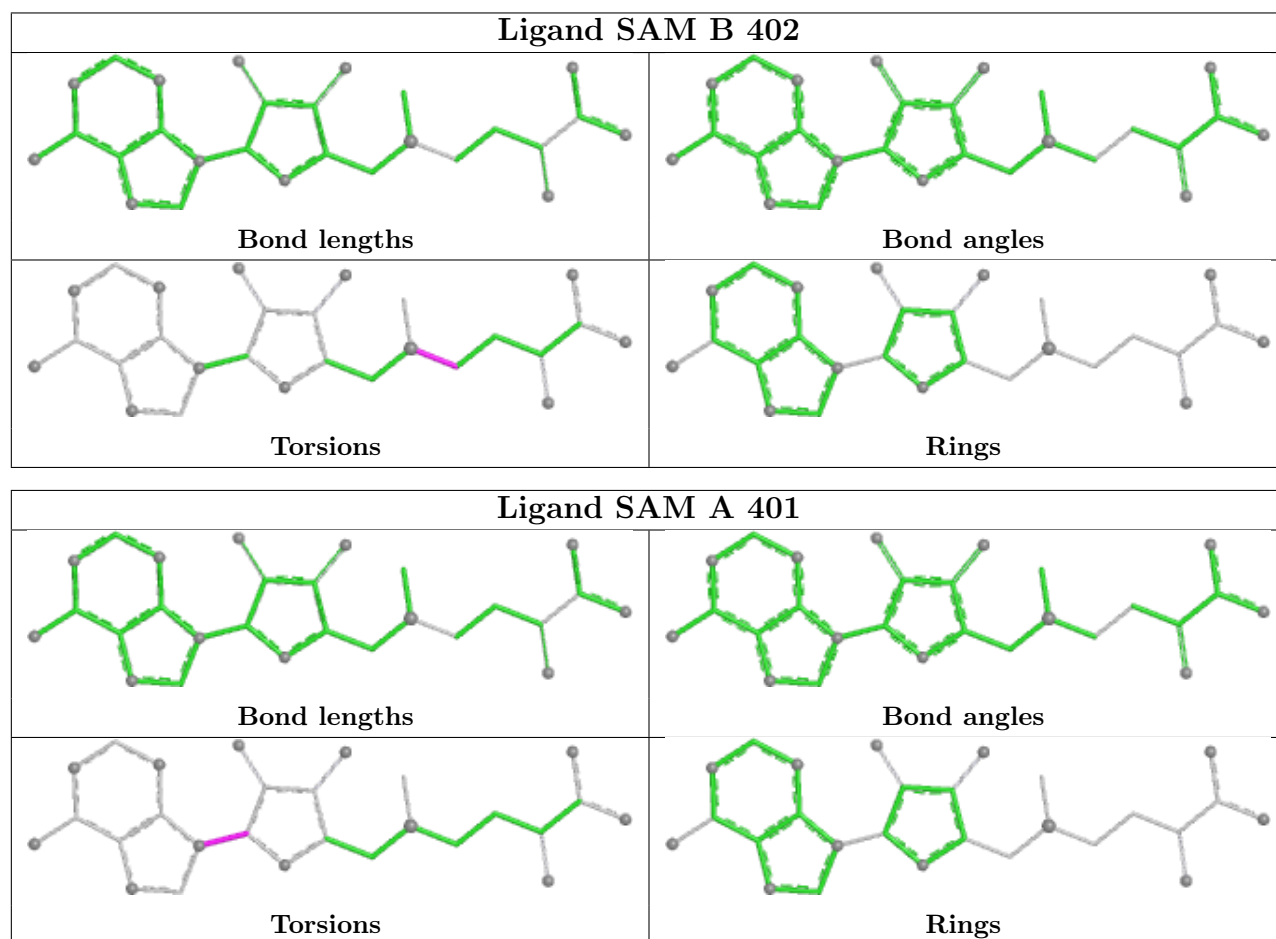
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	SAM	6	0
3	A	401	SAM	6	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

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	283/301 (94%)	0.16	21 (7%)	20 22	7, 22, 51, 70	5 (1%)
1	B	274/301 (91%)	2.04	141 (51%)	0 0	14, 70, 86, 88	0
All	All	557/602 (92%)	1.08	162 (29%)	1 1	7, 30, 84, 88	5 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	PHE	7.6
1	B	71	PHE	7.1
1	B	42	ILE	6.7
1	B	27	ILE	6.4
1	B	11	VAL	6.3
1	B	47	PRO	6.2
1	B	29	LEU	6.1
1	B	99	GLY	5.9
1	B	20	LEU	5.9
1	B	40	ARG	5.8
1	B	23	GLU	5.8
1	A	9	ILE	5.8
1	B	89	LEU	5.5
1	B	61	LEU	5.4
1	B	17	ILE	5.2
1	B	247	LEU	5.2
1	B	51	ILE	5.2
1	B	50	ARG	5.1
1	B	26	LYS	5.1
1	B	49	CYS	5.1
1	B	262	LEU	5.1
1	B	68	LEU	5.0
1	B	46	CYS	4.9
1	B	52	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	87	PHE	4.8
1	B	281	PRO	4.8
1	B	76	SER	4.7
1	B	13	VAL	4.7
1	B	270	VAL	4.7
1	A	279	GLU	4.7
1	B	56	VAL	4.6
1	B	97	VAL	4.6
1	B	72	SER	4.5
1	B	256	PHE	4.5
1	B	92	LEU	4.4
1	B	9	ILE	4.4
1	B	235	PRO	4.3
1	B	269	PRO	4.3
1	B	283	ALA	4.3
1	B	94	ILE	4.2
1	B	73	ASP	4.2
1	B	63	ILE	4.2
1	B	78	PHE	4.1
1	B	100	ILE	4.1
1	B	245	HIS	4.1
1	B	25	GLU	4.1
1	A	245	HIS	4.0
1	B	41	ALA	4.0
1	B	272	PRO	4.0
1	B	292	GLU	4.0
1	B	96	LYS	4.0
1	B	24	ASP	4.0
1	B	48	GLY	3.9
1	B	266	THR	3.9
1	B	39	SER	3.9
1	B	265	LEU	3.9
1	B	22	PRO	3.8
1	A	277	ILE	3.8
1	B	90	LYS	3.8
1	B	237	GLY	3.8
1	B	246	SER	3.8
1	B	229	ALA	3.7
1	B	33	VAL	3.7
1	B	43	LEU	3.6
1	B	273	SER	3.5
1	A	8	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	285	SER	3.5
1	B	28	ILE	3.5
1	B	60	VAL	3.5
1	B	242	ILE	3.5
1	A	272	PRO	3.4
1	B	234	ASN	3.4
1	A	294	ILE	3.4
1	B	264	ILE	3.4
1	B	257	ARG	3.4
1	B	239	ILE	3.4
1	B	241	VAL	3.4
1	B	244	PHE	3.4
1	B	38	HIS	3.4
1	B	69	LYS	3.4
1	B	250	ARG	3.4
1	B	62	ARG	3.3
1	B	59	GLU	3.3
1	B	8	HIS	3.3
1	B	85	ALA	3.3
1	B	14	ARG	3.2
1	B	77	LEU	3.2
1	B	88	LEU	3.2
1	B	226	LEU	3.2
1	B	288	LEU	3.2
1	B	290	ALA	3.2
1	B	291	ALA	3.2
1	A	280	ASN	3.2
1	B	111	LEU	3.2
1	B	251	ILE	3.1
1	B	225	PHE	3.1
1	B	232	LEU	3.1
1	B	233	LEU	3.1
1	B	268	LYS	3.1
1	B	284	ARG	3.1
1	B	98	ASP	3.0
1	B	104	LEU	3.0
1	B	230	GLU	3.0
1	B	54	ILE	3.0
1	B	227	LYS	2.9
1	B	106	VAL	2.9
1	A	227	LYS	2.9
1	B	37	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	278	ARG	2.8
1	B	282	ARG	2.8
1	B	101	LEU	2.8
1	A	285	SER	2.8
1	B	240	VAL	2.8
1	B	64	ALA	2.7
1	B	109	TYR	2.7
1	A	10	PRO	2.7
1	B	260	LYS	2.7
1	B	287	ARG	2.7
1	B	75	VAL	2.7
1	B	82	TYR	2.6
1	B	238	ARG	2.6
1	B	32	THR	2.6
1	B	267	GLU	2.6
1	B	80	VAL	2.6
1	B	57	ASP	2.6
1	A	106	VAL	2.6
1	B	91	THR	2.6
1	B	231	ASP	2.5
1	B	74	ARG	2.5
1	B	255	THR	2.5
1	B	95	GLU	2.5
1	B	16	VAL	2.5
1	A	275	GLU	2.4
1	B	31	CYS	2.4
1	B	113	GLY	2.4
1	B	103	ASP	2.4
1	B	286	GLY	2.4
1	B	30	ASP	2.3
1	B	79	LYS	2.3
1	B	45	HIS	2.3
1	A	105	GLY	2.3
1	B	259	SER	2.3
1	A	270	VAL	2.3
1	B	228	LYS	2.3
1	B	222	LEU	2.2
1	B	67	LYS	2.2
1	B	261	LYS	2.2
1	A	257	ARG	2.2
1	A	282	ARG	2.2
1	B	263	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	18	GLU	2.1
1	A	246	SER	2.1
1	A	260	LYS	2.1
1	B	21	LYS	2.1
1	B	289	ARG	2.1
1	A	200	LYS	2.1
1	B	223	LYS	2.1
1	B	53	GLY	2.1
1	B	70	GLU	2.0
1	B	252	VAL	2.0
1	B	120	PHE	2.0
1	B	83	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

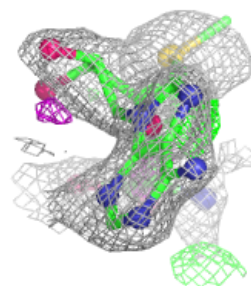
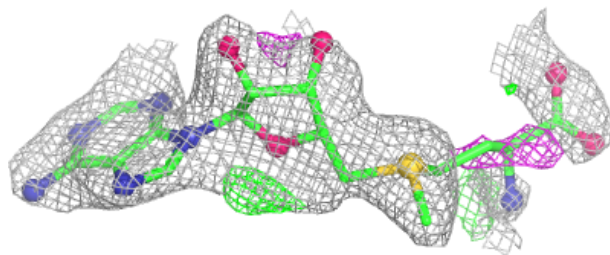
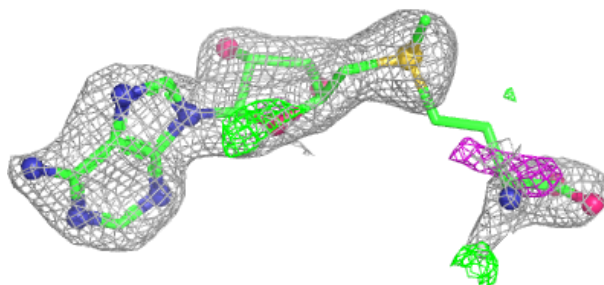
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SAM	B	402	27/27	0.78	0.16	60,62,67,67	0
2	SO4	A	500	5/5	0.95	0.07	40,41,43,45	0
3	SAM	A	401	27/27	0.97	0.06	16,20,26,29	0
2	SO4	B	501	5/5	0.97	0.07	38,40,41,41	0

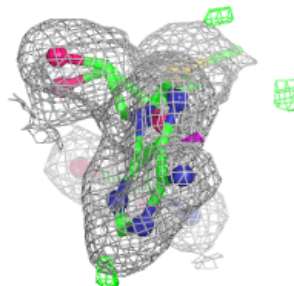
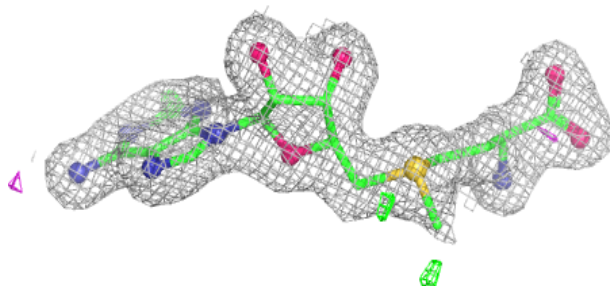
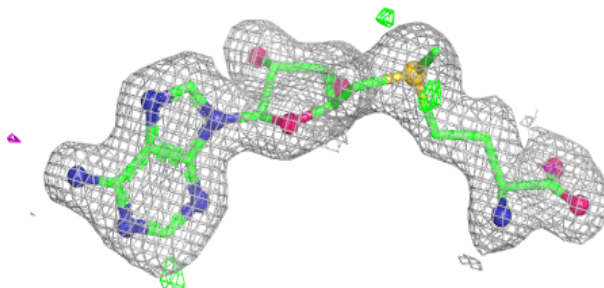
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAM B 402:

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

**Electron density around SAM A 401:**

$2mF_o-DF_c$ (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.