



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:17 AM UTC

PDB ID : 7F4P / pdb_00007f4p
Title : Crystal structure of SAM-bound MTA1-p2 complex
Authors : Chen, J.; Liu, L.
Deposited on : 2021-06-21
Resolution : 2.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

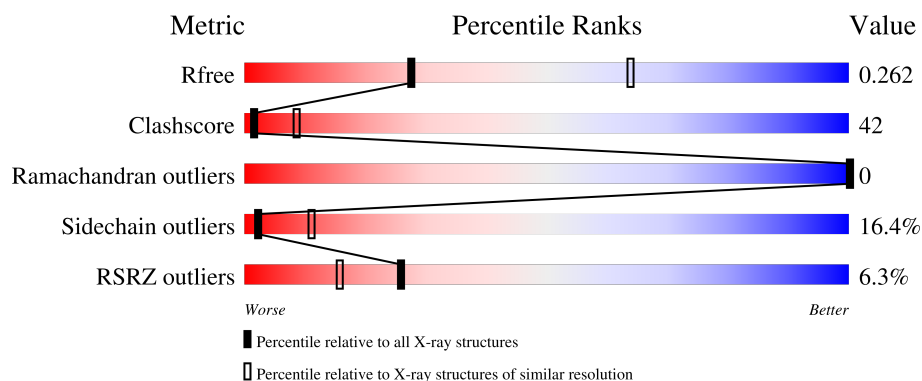
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	B	142	
2	A	247	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2821 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.

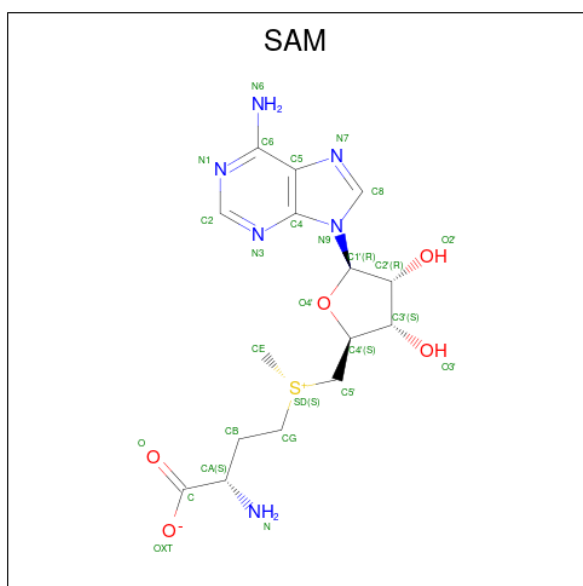
- Molecule 1 is a protein called Transmembrane protein, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	129	Total	C	N	O	S	0	0	0
			1026	649	172	201	4			

- Molecule 2 is a protein called MT-a70 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	218	Total	C	N	O	S	0	0	0
			1750	1113	306	321	10			

- Molecule 3 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
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

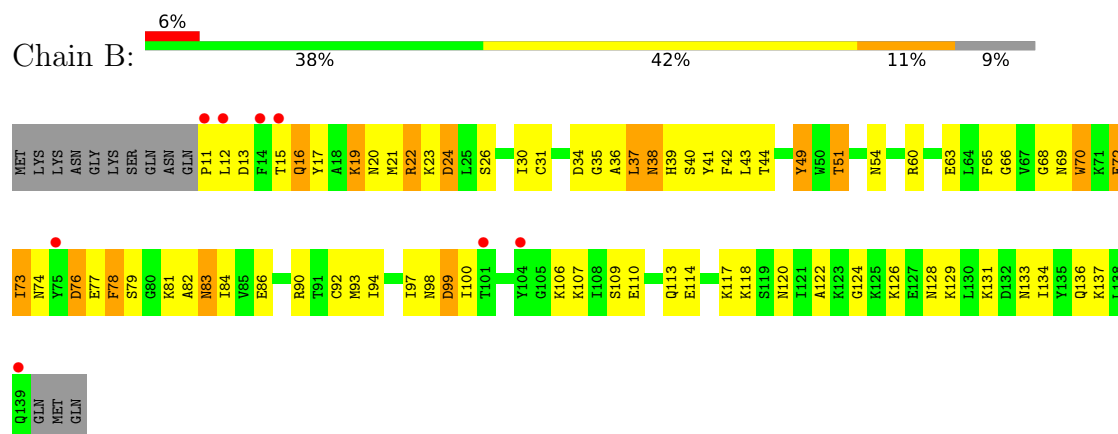
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total 5	O 5	0	0
4	A	13	Total 13	O 13	0	0

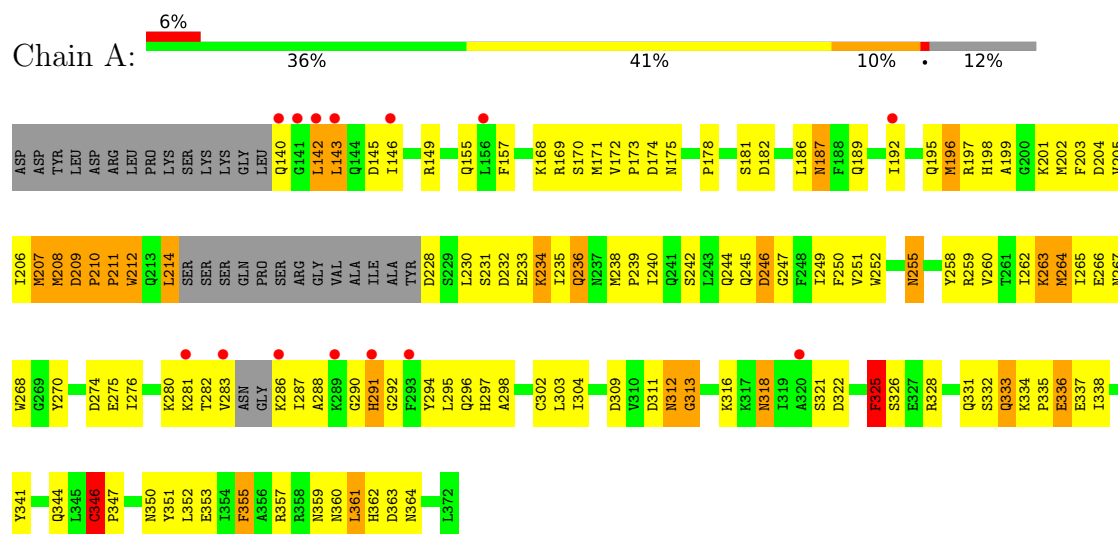
3 Residue-property plots [i](#)

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: Transmembrane protein, putative



- Molecule 2: MT-a70 family protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.03Å 137.03Å 61.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.83 – 2.98 29.83 – 2.98	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.83-2.98) 86.5 (29.83-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.249 , 0.265 0.247 , 0.262	Depositor DCC
R_{free} test set	626 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	2821	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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	B	1.04	1/1042 (0.1%)	1.12	10/1401 (0.7%)
2	A	1.05	4/1785 (0.2%)	1.05	13/2406 (0.5%)
All	All	1.05	5/2827 (0.2%)	1.08	23/3807 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	209	ASP	C-N	8.17	1.40	1.33
2	A	210	PRO	C-O	-5.78	1.20	1.25
1	B	51	THR	C-N	5.77	1.40	1.34
2	A	346	CYS	C-N	5.72	1.40	1.33
2	A	239	PRO	N-CD	5.08	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	209	ASP	CA-C-N	-8.39	113.54	119.66
2	A	209	ASP	C-N-CA	-8.39	113.54	119.66
1	B	12	LEU	CA-C-N	-7.42	112.67	123.05
1	B	12	LEU	C-N-CA	-7.42	112.67	123.05
2	A	210	PRO	N-CA-C	7.23	117.41	110.47
1	B	76	ASP	N-CA-C	6.99	118.68	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	11	PRO	N-CA-CB	6.73	110.41	103.00
2	A	346	CYS	CA-C-N	-6.68	113.38	120.66
2	A	346	CYS	C-N-CA	-6.68	113.38	120.66
2	A	247	GLY	N-CA-C	6.30	118.94	110.43
1	B	51	THR	CA-C-N	-6.23	113.39	119.87
1	B	51	THR	C-N-CA	-6.23	113.39	119.87
1	B	106	LYS	CA-C-N	6.12	131.21	121.66
1	B	106	LYS	C-N-CA	6.12	131.21	121.66
2	A	210	PRO	O-C-N	6.03	124.08	121.31
2	A	264	MET	N-CA-C	5.95	117.57	111.14
1	B	82	ALA	N-CA-C	-5.76	99.28	109.06
1	B	13	ASP	O-C-N	5.71	130.01	123.27
2	A	313	GLY	N-CA-C	-5.64	108.46	114.67
2	A	325	PHE	N-CA-C	5.59	119.68	112.41
2	A	212	TRP	N-CA-C	-5.20	103.18	110.50
2	A	347	PRO	CA-N-CD	-5.11	104.85	112.00
2	A	290	GLY	N-CA-C	-5.09	103.12	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	78	PHE	Peptide
1	B	81	LYS	Peptide

5.2 Too-close contacts

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	B	1026	0	983	105	1
2	A	1750	0	1706	142	4
3	A	27	0	22	6	0
4	A	13	0	0	0	0
4	B	5	0	0	0	0
All	All	2821	0	2711	232	4

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 42.

All (232) 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:65:PHE:CZ	1:B:76:ASP:OD2	1.80	1.33
2:A:281:LYS:CD	2:A:325:PHE:HD1	1.56	1.19
2:A:238:MET:HE2	2:A:240:ILE:HD11	1.19	1.18
2:A:282:THR:OG1	2:A:286:LYS:N	1.79	1.15
2:A:281:LYS:HD2	2:A:325:PHE:HD1	1.00	1.14
2:A:231:SER:HB3	2:A:234:LYS:HD3	1.31	1.10
2:A:244:GLN:NE2	2:A:270:TYR:OH	1.84	1.09
2:A:336:GLU:OE2	2:A:362:HIS:NE2	1.84	1.08
2:A:238:MET:CE	2:A:240:ILE:HD11	1.84	1.07
1:B:16:GLN:O	1:B:20:ASN:ND2	1.88	1.05
1:B:16:GLN:OE1	1:B:20:ASN:ND2	1.88	1.04
2:A:281:LYS:HD2	2:A:325:PHE:CD1	1.93	1.04
2:A:281:LYS:CD	2:A:325:PHE:CD1	2.41	1.03
1:B:19:LYS:HD3	1:B:36:ALA:N	1.72	1.02
1:B:21:MET:HE1	2:A:195:GLN:HG2	1.42	1.01
2:A:282:THR:HG1	2:A:286:LYS:N	1.54	1.01
1:B:60:ARG:NH1	1:B:77:GLU:OE2	1.94	1.00
2:A:246:ASP:OD1	2:A:309:ASP:N	1.94	0.99
1:B:22:ARG:O	1:B:26:SER:HB2	1.62	0.98
1:B:65:PHE:HZ	1:B:76:ASP:OD2	1.25	0.97
2:A:209:ASP:OD2	3:A:401:SAM:N	1.99	0.95
1:B:21:MET:CE	2:A:195:GLN:HG2	1.97	0.94
2:A:281:LYS:HG3	2:A:325:PHE:CE1	2.04	0.92
1:B:17:TYR:HE2	1:B:21:MET:HE2	1.33	0.91
1:B:19:LYS:HD3	1:B:35:GLY:C	1.98	0.89
1:B:83:ASN:H	1:B:83:ASN:HD22	1.14	0.89
1:B:17:TYR:CE2	1:B:21:MET:HE2	2.08	0.88
2:A:231:SER:HB2	2:A:234:LYS:NZ	1.88	0.88
1:B:109:SER:O	1:B:113:GLN:HG3	1.75	0.86
1:B:15:THR:HA	2:A:175:ASN:HD21	1.38	0.86
2:A:182:ASP:OD1	3:A:401:SAM:N6	2.09	0.86
2:A:281:LYS:CG	2:A:325:PHE:CE1	2.58	0.85
1:B:17:TYR:CE2	1:B:21:MET:HG3	2.12	0.85
2:A:309:ASP:OD2	2:A:311:ASP:OD2	1.95	0.84
2:A:231:SER:CB	2:A:234:LYS:HZ3	1.90	0.84
2:A:231:SER:HB3	2:A:234:LYS:CD	2.07	0.84
2:A:140:GLN:CB	2:A:142:LEU:HD23	2.09	0.83
2:A:231:SER:H	2:A:234:LYS:HZ3	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:SER:OG	2:A:186:LEU:HB2	1.78	0.83
2:A:231:SER:CB	2:A:234:LYS:HD3	2.07	0.82
2:A:173:PRO:HB2	2:A:363:ASP:OD2	1.80	0.82
2:A:281:LYS:HD2	2:A:325:PHE:O	1.81	0.81
1:B:38:ASN:OD1	1:B:40:SER:OG	1.99	0.81
2:A:231:SER:CB	2:A:234:LYS:NZ	2.44	0.81
2:A:357:ARG:N	2:A:360:ASN:OD1	2.13	0.80
2:A:281:LYS:HE3	2:A:325:PHE:CD1	2.17	0.79
2:A:214:LEU:HD12	2:A:214:LEU:H	1.45	0.79
2:A:281:LYS:CG	2:A:325:PHE:CD1	2.66	0.78
1:B:37:LEU:HD23	1:B:37:LEU:H	1.47	0.78
2:A:236:GLN:HG2	2:A:264:MET:HG3	1.64	0.78
1:B:68:GLY:HA2	1:B:70:TRP:CE2	2.18	0.77
2:A:281:LYS:CE	2:A:325:PHE:CD1	2.69	0.76
2:A:281:LYS:HG3	2:A:325:PHE:CD1	2.22	0.74
2:A:201:LYS:NZ	2:A:202:MET:O	2.21	0.74
1:B:51:THR:HG23	1:B:54:ASN:H	1.50	0.74
1:B:21:MET:HE1	2:A:195:GLN:CG	2.18	0.73
2:A:275:GLU:HG3	2:A:303:LEU:HD12	1.70	0.73
2:A:294:TYR:O	2:A:295:LEU:HD23	1.88	0.73
2:A:187:ASN:HD21	2:A:189:GLN:HB2	1.55	0.72
2:A:209:ASP:CB	3:A:401:SAM:HN2	2.02	0.72
1:B:15:THR:HA	2:A:175:ASN:ND2	2.05	0.70
1:B:37:LEU:H	1:B:37:LEU:CD2	2.03	0.70
2:A:212:TRP:HZ3	2:A:232:ASP:OD1	1.74	0.70
2:A:231:SER:HB2	2:A:234:LYS:HZ2	1.55	0.70
2:A:281:LYS:CG	2:A:325:PHE:HE1	2.02	0.70
1:B:70:TRP:O	1:B:74:ASN:HB2	1.91	0.69
2:A:214:LEU:HD12	2:A:214:LEU:N	2.06	0.69
2:A:281:LYS:HB3	2:A:283:VAL:HG23	1.73	0.68
2:A:244:GLN:NE2	2:A:270:TYR:CZ	2.61	0.68
2:A:231:SER:N	2:A:234:LYS:HZ3	1.91	0.68
1:B:51:THR:HG23	1:B:54:ASN:OD1	1.94	0.68
1:B:131:LYS:CB	1:B:136:GLN:NE2	2.58	0.66
2:A:201:LYS:NZ	2:A:201:LYS:HB3	2.10	0.66
1:B:65:PHE:HB2	1:B:73:ILE:HG22	1.78	0.66
2:A:238:MET:CE	2:A:240:ILE:CD1	2.70	0.66
1:B:70:TRP:O	1:B:74:ASN:N	2.28	0.66
1:B:69:ASN:O	1:B:72:GLU:N	2.29	0.65
1:B:65:PHE:O	1:B:69:ASN:ND2	2.29	0.65
2:A:332:SER:O	2:A:357:ARG:NH2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PHE:CD2	1:B:73:ILE:HG22	2.32	0.65
1:B:51:THR:CG2	1:B:54:ASN:OD1	2.45	0.64
1:B:136:GLN:HE22	2:A:155:GLN:NE2	1.94	0.64
2:A:192:ILE:HD11	2:A:242:SER:OG	1.98	0.64
2:A:334:LYS:HB3	2:A:335:PRO:HD2	1.79	0.63
1:B:131:LYS:CB	1:B:136:GLN:HE21	2.12	0.62
2:A:187:ASN:ND2	2:A:189:GLN:H	1.98	0.62
2:A:255:ASN:OD1	2:A:297:HIS:CE1	2.52	0.62
1:B:83:ASN:H	1:B:83:ASN:ND2	1.90	0.62
1:B:69:ASN:O	1:B:72:GLU:HB3	1.99	0.62
2:A:201:LYS:NZ	2:A:204:ASP:OD1	2.30	0.62
1:B:19:LYS:HD2	1:B:35:GLY:HA3	1.82	0.61
1:B:19:LYS:HD3	1:B:35:GLY:CA	2.29	0.61
2:A:209:ASP:CG	3:A:401:SAM:HN2	2.08	0.61
2:A:210:PRO:HB3	2:A:235:ILE:HD13	1.81	0.61
2:A:142:LEU:HD12	2:A:142:LEU:O	2.00	0.61
1:B:100:ILE:HG12	1:B:100:ILE:O	2.00	0.60
1:B:19:LYS:CD	1:B:35:GLY:HA3	2.31	0.60
2:A:208:MET:HE1	2:A:268:TRP:HH2	1.64	0.60
2:A:291:HIS:O	2:A:291:HIS:ND1	2.31	0.60
1:B:131:LYS:HB3	1:B:136:GLN:NE2	2.17	0.60
2:A:244:GLN:NE2	2:A:270:TYR:CE2	2.70	0.60
1:B:19:LYS:HD3	1:B:36:ALA:H	1.66	0.59
2:A:312:ASN:N	2:A:312:ASN:OD1	2.35	0.59
1:B:17:TYR:HE2	1:B:21:MET:CE	2.11	0.59
2:A:201:LYS:HB3	2:A:201:LYS:HZ2	1.67	0.59
1:B:17:TYR:CE2	1:B:21:MET:CG	2.86	0.58
2:A:331:GLN:HA	2:A:333:GLN:N	2.17	0.58
2:A:309:ASP:OD2	2:A:311:ASP:CG	2.45	0.58
1:B:17:TYR:CE2	1:B:21:MET:CE	2.86	0.58
2:A:262:ILE:O	2:A:266:GLU:HG3	2.04	0.57
1:B:131:LYS:HB2	1:B:136:GLN:NE2	2.20	0.57
1:B:42:PHE:CD2	2:A:172:VAL:HG21	2.40	0.57
2:A:169:ARG:NH2	2:A:174:ASP:OD2	2.38	0.57
1:B:30:ILE:HG12	1:B:41:TYR:CE1	2.40	0.56
2:A:211:PRO:HB2	2:A:228:ASP:N	2.21	0.56
1:B:68:GLY:HA2	1:B:70:TRP:CZ2	2.41	0.55
2:A:288:ALA:HB3	2:A:298:ALA:HA	1.87	0.55
1:B:92:CYS:HB3	1:B:97:ILE:O	2.06	0.55
2:A:209:ASP:OD2	2:A:334:LYS:CE	2.55	0.55
2:A:209:ASP:OD2	2:A:334:LYS:HE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:231:SER:H	2:A:234:LYS:NZ	2.01	0.54
2:A:276:ILE:HB	2:A:302:CYS:HB3	1.89	0.54
1:B:83:ASN:O	1:B:86:GLU:N	2.41	0.54
2:A:208:MET:HE1	2:A:268:TRP:CH2	2.42	0.53
1:B:44:THR:HG21	1:B:49:TYR:HA	1.91	0.53
1:B:133:ASN:C	1:B:134:ILE:HD12	2.34	0.53
2:A:206:ILE:HB	2:A:249:ILE:HG13	1.90	0.53
2:A:292:GLY:HA3	2:A:295:LEU:O	2.08	0.53
2:A:208:MET:HG2	2:A:355:PHE:HE2	1.74	0.53
1:B:51:THR:CG2	1:B:54:ASN:CG	2.82	0.52
1:B:131:LYS:HB2	1:B:136:GLN:HE21	1.72	0.52
1:B:133:ASN:O	1:B:134:ILE:HD12	2.10	0.52
1:B:19:LYS:CD	1:B:35:GLY:C	2.78	0.52
2:A:231:SER:HB2	2:A:234:LYS:HZ3	1.56	0.52
2:A:360:ASN:O	2:A:362:HIS:ND1	2.43	0.52
2:A:326:SER:HB2	2:A:335:PRO:HB3	1.91	0.52
1:B:69:ASN:O	1:B:72:GLU:CB	2.58	0.51
2:A:207:MET:HG2	2:A:250:PHE:HB2	1.91	0.51
1:B:21:MET:HE2	2:A:195:GLN:HG2	1.89	0.51
1:B:34:ASP:OD1	1:B:34:ASP:N	2.41	0.51
2:A:140:GLN:CB	2:A:142:LEU:CD2	2.85	0.50
2:A:212:TRP:CZ3	2:A:232:ASP:OD1	2.60	0.50
2:A:231:SER:HB3	2:A:234:LYS:CE	2.41	0.50
2:A:280:LYS:HB2	2:A:288:ALA:HB2	1.92	0.50
2:A:195:GLN:HE22	2:A:350:ASN:HD22	1.59	0.50
2:A:281:LYS:HG2	2:A:325:PHE:HE1	1.73	0.49
1:B:41:TYR:CD1	1:B:42:PHE:CE1	3.00	0.49
1:B:65:PHE:CE1	1:B:76:ASP:OD2	2.55	0.49
2:A:258:TYR:CE1	2:A:303:LEU:HD11	2.46	0.49
1:B:70:TRP:HA	1:B:73:ILE:HG12	1.95	0.49
2:A:309:ASP:OD2	2:A:311:ASP:CB	2.61	0.49
1:B:15:THR:CA	2:A:175:ASN:HD21	2.20	0.48
1:B:83:ASN:HD22	1:B:83:ASN:N	1.94	0.48
2:A:196:MET:O	2:A:199:ALA:O	2.31	0.48
2:A:276:ILE:HG12	2:A:304:ILE:HD11	1.96	0.48
2:A:309:ASP:OD2	2:A:311:ASP:HB2	2.13	0.48
2:A:211:PRO:HG2	2:A:211:PRO:O	2.14	0.47
1:B:19:LYS:CD	1:B:35:GLY:CA	2.89	0.47
2:A:211:PRO:HG2	2:A:230:LEU:HB2	1.96	0.47
2:A:291:HIS:ND1	2:A:291:HIS:C	2.72	0.47
2:A:313:GLY:O	2:A:316:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLY:HA2	1:B:70:TRP:NE1	2.29	0.47
2:A:197:ARG:HD2	2:A:198:HIS:NE2	2.30	0.47
1:B:30:ILE:HG21	2:A:178:PRO:HG2	1.96	0.47
1:B:69:ASN:O	1:B:73:ILE:N	2.43	0.47
2:A:211:PRO:HD3	2:A:355:PHE:CD1	2.50	0.47
2:A:143:LEU:O	2:A:146:ILE:HG23	2.16	0.46
1:B:124:GLY:O	1:B:129:LYS:N	2.47	0.46
1:B:93:MET:HE2	2:A:157:PHE:HE1	1.80	0.46
1:B:31:CYS:HA	1:B:37:LEU:HA	1.98	0.46
2:A:187:ASN:ND2	2:A:187:ASN:C	2.73	0.46
2:A:195:GLN:O	2:A:199:ALA:HB3	2.15	0.46
2:A:363:ASP:O	2:A:364:ASN:HB2	2.15	0.46
1:B:51:THR:HG22	1:B:54:ASN:OD1	2.16	0.46
1:B:136:GLN:HE22	2:A:155:GLN:HE22	1.62	0.46
1:B:39:HIS:O	1:B:43:LEU:HD12	2.16	0.46
1:B:54:ASN:HB2	1:B:78:PHE:CE1	2.51	0.46
2:A:231:SER:HB3	2:A:234:LYS:NZ	2.27	0.46
2:A:263:LYS:O	2:A:267:ASN:ND2	2.48	0.46
1:B:99:ASP:HB2	1:B:137:LYS:HB3	1.98	0.46
1:B:97:ILE:HG12	1:B:99:ASP:H	1.81	0.45
1:B:63:GLU:OE2	1:B:110:GLU:HG3	2.15	0.45
1:B:37:LEU:HD23	1:B:37:LEU:N	2.18	0.45
2:A:143:LEU:O	2:A:146:ILE:CG2	2.65	0.45
1:B:23:LYS:HG2	1:B:35:GLY:HA2	1.99	0.45
2:A:326:SER:OG	2:A:337:GLU:OE1	2.34	0.45
2:A:181:SER:HG	2:A:186:LEU:HB2	1.77	0.44
1:B:66:GLY:HA2	1:B:107:LYS:HA	1.99	0.44
2:A:205:VAL:HB	2:A:351:TYR:HD1	1.81	0.44
2:A:282:THR:HG23	2:A:287:ILE:O	2.18	0.44
2:A:352:LEU:HD23	2:A:353:GLU:N	2.32	0.44
2:A:252:TRP:HZ2	2:A:338:ILE:HG13	1.82	0.44
2:A:341:TYR:HD2	2:A:341:TYR:N	2.16	0.44
1:B:41:TYR:HA	1:B:49:TYR:CD1	2.53	0.43
1:B:98:ASN:ND2	1:B:136:GLN:OE1	2.51	0.43
1:B:49:TYR:CD2	1:B:49:TYR:C	2.96	0.43
1:B:97:ILE:HB	1:B:120:ASN:HD22	1.83	0.43
1:B:107:LYS:HE2	1:B:107:LYS:HB2	1.70	0.43
1:B:122:ALA:O	1:B:126:LYS:HG3	2.17	0.43
2:A:236:GLN:O	2:A:236:GLN:NE2	2.52	0.43
2:A:209:ASP:OD2	2:A:334:LYS:HE3	2.18	0.43
1:B:94:ILE:O	1:B:117:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLU:O	1:B:118:LYS:HG3	2.18	0.43
1:B:51:THR:HG22	1:B:54:ASN:CG	2.44	0.43
1:B:65:PHE:CB	1:B:73:ILE:HG22	2.46	0.43
2:A:341:TYR:N	2:A:341:TYR:CD2	2.85	0.43
2:A:195:GLN:HG3	2:A:203:PHE:CZ	2.54	0.43
1:B:129:LYS:O	1:B:136:GLN:HG2	2.19	0.42
1:B:97:ILE:HD13	1:B:99:ASP:O	2.19	0.42
2:A:240:ILE:HG13	2:A:268:TRP:CZ2	2.54	0.42
1:B:39:HIS:HB3	2:A:170:SER:HB2	2.01	0.42
2:A:357:ARG:HG3	3:A:401:SAM:O3'	2.20	0.42
1:B:41:TYR:HD1	1:B:42:PHE:CE1	2.37	0.42
1:B:90:ARG:O	1:B:93:MET:HB2	2.20	0.42
2:A:331:GLN:HA	2:A:332:SER:C	2.44	0.42
2:A:258:TYR:O	2:A:262:ILE:HG13	2.20	0.42
1:B:65:PHE:HD2	1:B:73:ILE:HG22	1.82	0.42
2:A:357:ARG:CG	3:A:401:SAM:O3'	2.68	0.41
1:B:24:ASP:OD2	2:A:198:HIS:HE1	2.02	0.41
2:A:231:SER:CA	2:A:234:LYS:HZ3	2.30	0.41
1:B:22:ARG:HG2	1:B:26:SER:OG	2.21	0.41
2:A:346:CYS:O	2:A:346:CYS:SG	2.78	0.41
1:B:93:MET:HE2	2:A:157:PHE:CE1	2.55	0.41
1:B:69:ASN:HB3	1:B:73:ILE:HG23	2.03	0.41
2:A:171:MET:O	2:A:172:VAL:C	2.64	0.41
2:A:181:SER:OG	2:A:182:ASP:N	2.53	0.41
2:A:208:MET:HB3	2:A:251:VAL:HG23	2.02	0.41
1:B:69:ASN:O	1:B:72:GLU:CA	2.69	0.41
2:A:145:ASP:CG	2:A:149:ARG:HH21	2.29	0.40
2:A:361:LEU:N	2:A:361:LEU:CD1	2.84	0.40
1:B:51:THR:O	1:B:54:ASN:OD1	2.39	0.40
1:B:69:ASN:OD1	1:B:72:GLU:HB2	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:258:TYR:OH	2:A:258:TYR:OH[5_675]	1.29	0.91
2:A:296:GLN:O	2:A:322:ASP:OD1[5_675]	1.83	0.37
1:B:107:LYS:NZ	2:A:311:ASP:OD2[6_655]	1.88	0.32
2:A:292:GLY:O	2:A:318:ASN:OD1[5_675]	1.95	0.25

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	B	127/142 (89%)	126 (99%)	1 (1%)	0	100	100
2	A	212/247 (86%)	205 (97%)	7 (3%)	0	100	100
All	All	339/389 (87%)	331 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	106/127 (84%)	91 (86%)	15 (14%)	3	14
2	A	187/219 (85%)	154 (82%)	33 (18%)	2	9
All	All	293/346 (85%)	245 (84%)	48 (16%)	2	11

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	19	LYS
1	B	22	ARG
1	B	24	ASP
1	B	37	LEU
1	B	38	ASN
1	B	49	TYR
1	B	70	TRP

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Mol	Chain	Res	Type
1	B	72	GLU
1	B	73	ILE
1	B	79	SER
1	B	83	ASN
1	B	84	ILE
1	B	99	ASP
1	B	128	ASN
2	A	142	LEU
2	A	143	LEU
2	A	168	LYS
2	A	187	ASN
2	A	196	MET
2	A	207	MET
2	A	208	MET
2	A	211	PRO
2	A	214	LEU
2	A	233	GLU
2	A	234	LYS
2	A	236	GLN
2	A	245	GLN
2	A	246	ASP
2	A	255	ASN
2	A	259	ARG
2	A	260	VAL
2	A	263	LYS
2	A	265	ILE
2	A	274	ASP
2	A	291	HIS
2	A	312	ASN
2	A	318	ASN
2	A	321	SER
2	A	325	PHE
2	A	328	ARG
2	A	333	GLN
2	A	336	GLU
2	A	344	GLN
2	A	346	CYS
2	A	355	PHE
2	A	359	ASN
2	A	361	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	59	GLN
1	B	83	ASN
1	B	128	ASN
1	B	133	ASN
2	A	155	GLN
2	A	175	ASN
2	A	187	ASN
2	A	195	GLN
2	A	237	ASN
2	A	244	GLN
2	A	267	ASN
2	A	297	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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
3	SAM	A	401	-	27,29,29	1.52	5 (18%)	34,42,42	2.03	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
3	SAM	A	401	-	-	9/17/33/33	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	SAM	C5-C4	4.08	1.46	1.39
3	A	401	SAM	C5-N7	-3.31	1.33	1.39
3	A	401	SAM	C4-N9	-2.28	1.32	1.37
3	A	401	SAM	CE-SD	-2.21	1.64	1.78
3	A	401	SAM	OXT-C	-2.20	1.23	1.30

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SAM	C5-C4-N3	-5.96	118.51	126.72
3	A	401	SAM	N3-C4-N9	4.74	135.23	127.17
3	A	401	SAM	C2-N3-C4	3.55	120.49	111.83
3	A	401	SAM	CG-SD-C5'	3.36	111.64	103.43
3	A	401	SAM	N3-C2-N1	-3.09	123.90	128.58
3	A	401	SAM	C4-C5-N7	-2.57	107.64	110.58
3	A	401	SAM	O2'-C2'-C3'	-2.54	103.66	111.82
3	A	401	SAM	O3'-C3'-C2'	-2.31	104.42	111.82
3	A	401	SAM	C2'-C3'-C4'	2.04	106.55	102.61

There are no chirality outliers.

All (9) torsion outliers are listed below:

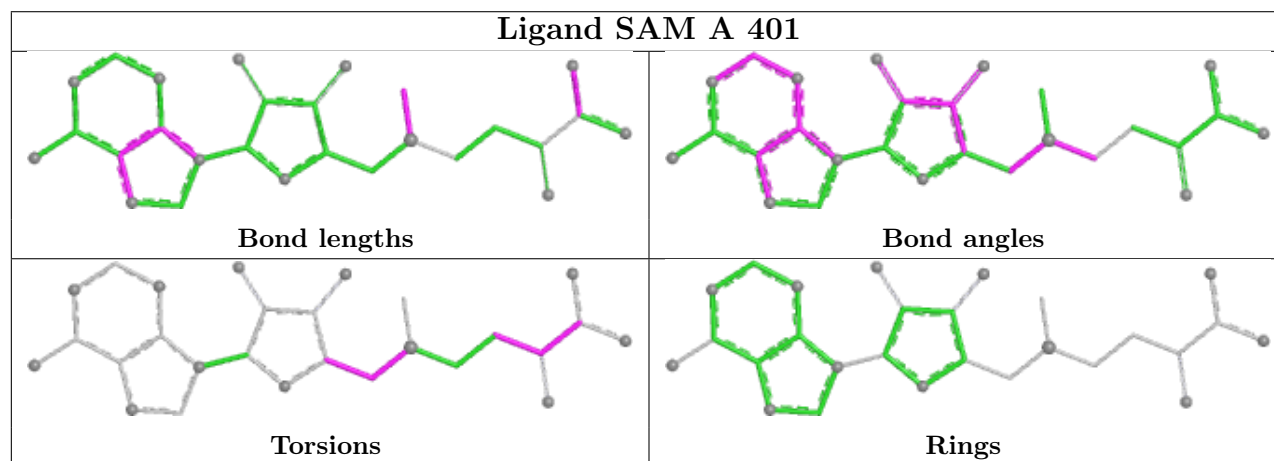
Mol	Chain	Res	Type	Atoms
3	A	401	SAM	C4'-C5'-SD-CG
3	A	401	SAM	C4'-C5'-SD-CE
3	A	401	SAM	O4'-C4'-C5'-SD
3	A	401	SAM	OXT-C-CA-CB
3	A	401	SAM	C3'-C4'-C5'-SD
3	A	401	SAM	O-C-CA-CB
3	A	401	SAM	C-CA-CB-CG
3	A	401	SAM	OXT-C-CA-N
3	A	401	SAM	O-C-CA-N

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	B	129/142 (90%)	0.61	8 (6%) 26 16	14, 45, 63, 77	0
2	A	218/247 (88%)	0.62	14 (6%) 25 15	9, 38, 69, 85	0
All	All	347/389 (89%)	0.62	22 (6%) 26 16	9, 41, 69, 85	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	286	LYS	5.0
1	B	11	PRO	3.5
2	A	140	GLN	3.4
2	A	283	VAL	3.0
2	A	291	HIS	2.7
1	B	104	TYR	2.7
1	B	15	THR	2.6
2	A	293	PHE	2.6
2	A	146	ILE	2.5
1	B	14	PHE	2.5
2	A	281	LYS	2.5
2	A	143	LEU	2.5
2	A	141	GLY	2.5
2	A	289	LYS	2.4
1	B	139	GLN	2.4
2	A	156	LEU	2.3
1	B	101	THR	2.2
2	A	142	LEU	2.2
2	A	320	ALA	2.2
1	B	12	LEU	2.2
2	A	192	ILE	2.0
1	B	75	TYR	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](#)

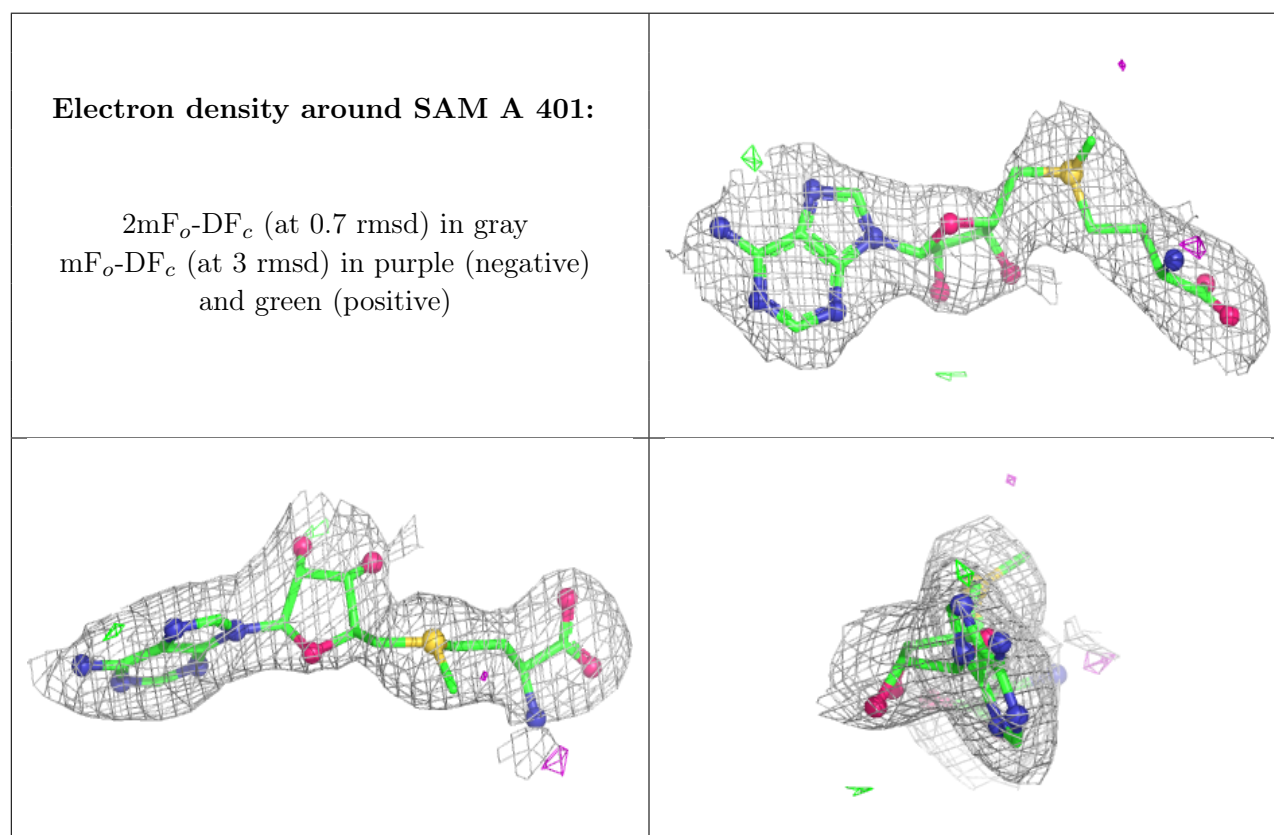
There are no oligosaccharides in this entry.

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	A	401	27/27	0.93	0.10	24,33,44,47	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.