



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:53 am BST

PDB ID : 4FP9  
Title : Human MTERF4-NSUN4 protein complex  
Authors : Spahr, H.; Hallberg, B.M.  
Deposited on : 2012-06-21  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

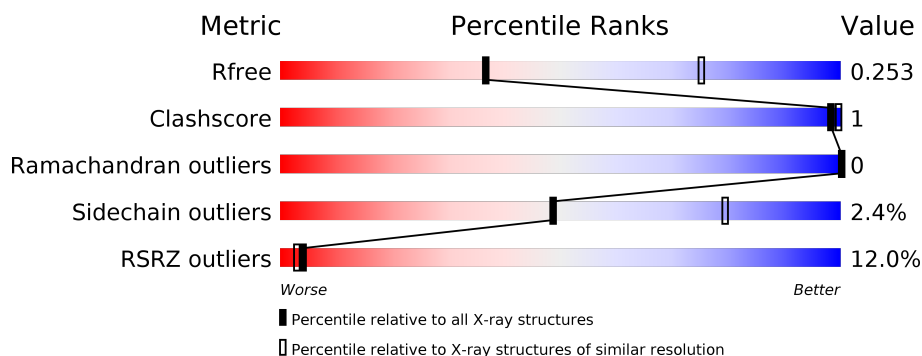
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	360	<div> <div></div> <div>89%</div> <div>6%</div> </div>
1	C	360	<div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	D	360	<div> <div></div> <div>88%</div> <div>8%</div> </div>
1	F	360	<div> <div>3%</div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
2	B	335	<div> <div>2%</div> <div>72%</div> <div>27%</div> </div>
2	E	335	<div> <div>2%</div> <div>71%</div> <div>27%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	335	<div><div><div></div><div></div><div></div></div><div>31%71%27%</div></div>
2	H	335	<div><div><div></div><div></div><div></div></div><div>42%72%27%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18717 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 methyltransferase NSUN4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2665	1694	466	488	17			
1	C	338	Total	C	N	O	S	0	0	0
			2665	1694	466	488	17			
1	D	333	Total	C	N	O	S	0	0	0
			2618	1662	459	480	17			
1	F	338	Total	C	N	O	S	0	0	0
			2665	1694	466	488	17			

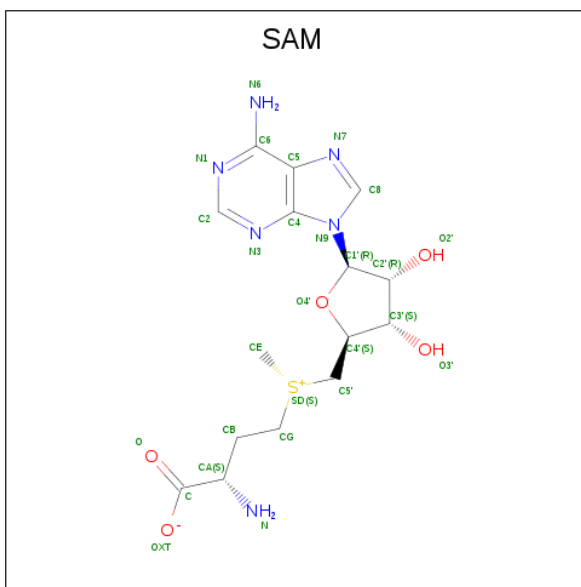
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	EXPRESSION TAG	UNP Q96CB9
C	25	MET	-	EXPRESSION TAG	UNP Q96CB9
D	25	MET	-	EXPRESSION TAG	UNP Q96CB9
F	25	MET	-	EXPRESSION TAG	UNP Q96CB9

- Molecule 2 is a protein called mTERF domain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	E	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	G	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	H	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

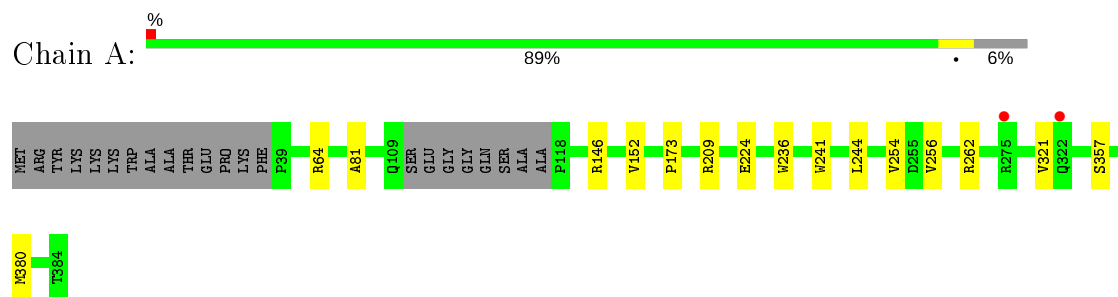


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

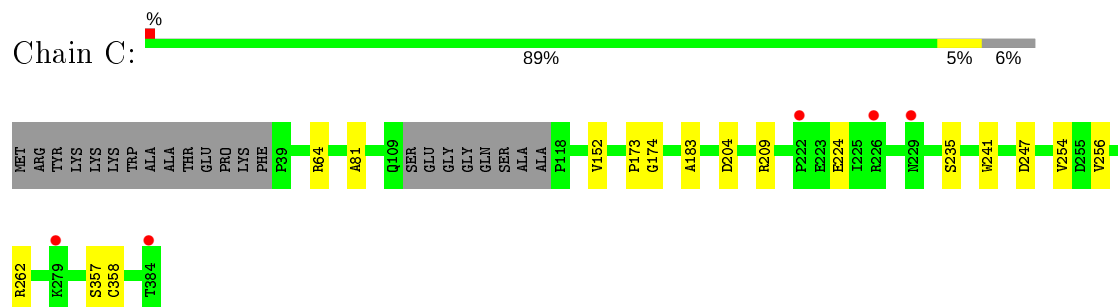
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

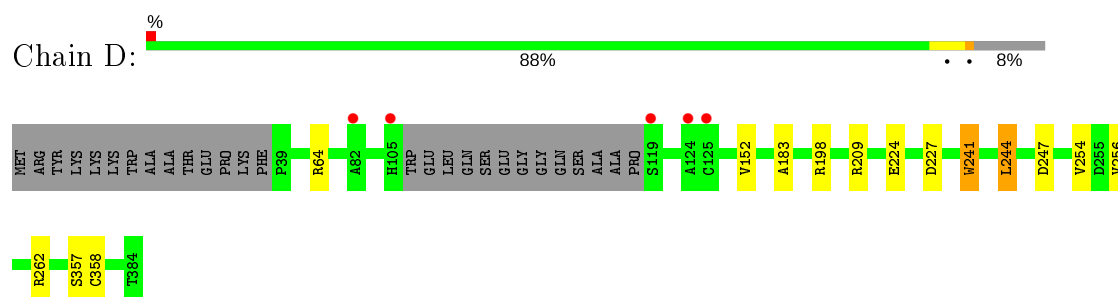
- Molecule 1: methyltransferase NSUN4



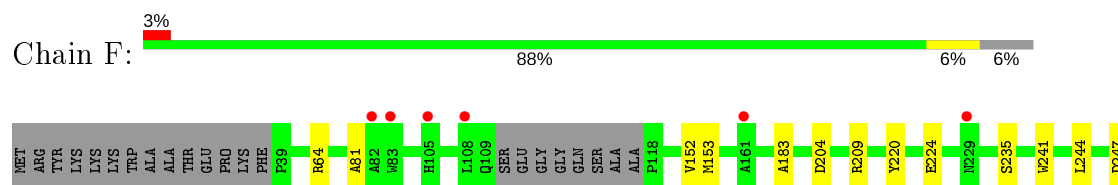
- Molecule 1: methyltransferase NSUN4

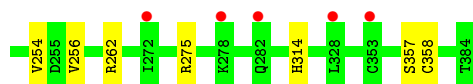


- Molecule 1: methyltransferase NSUN4

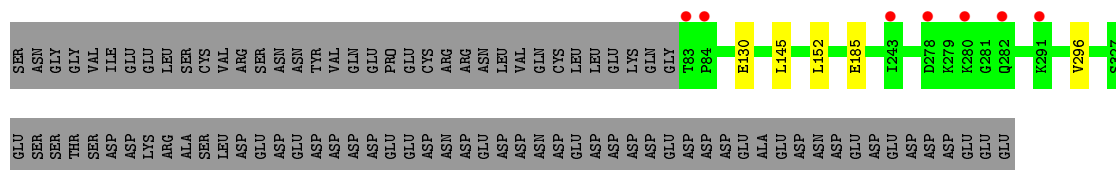
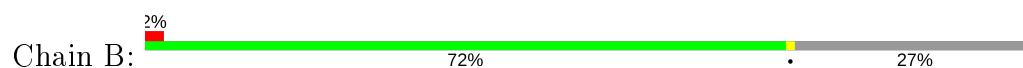


- Molecule 1: methyltransferase NSUN4

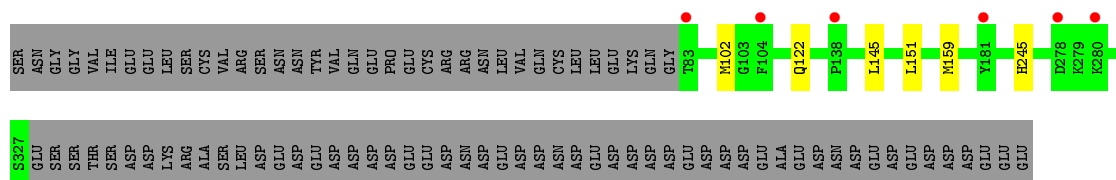




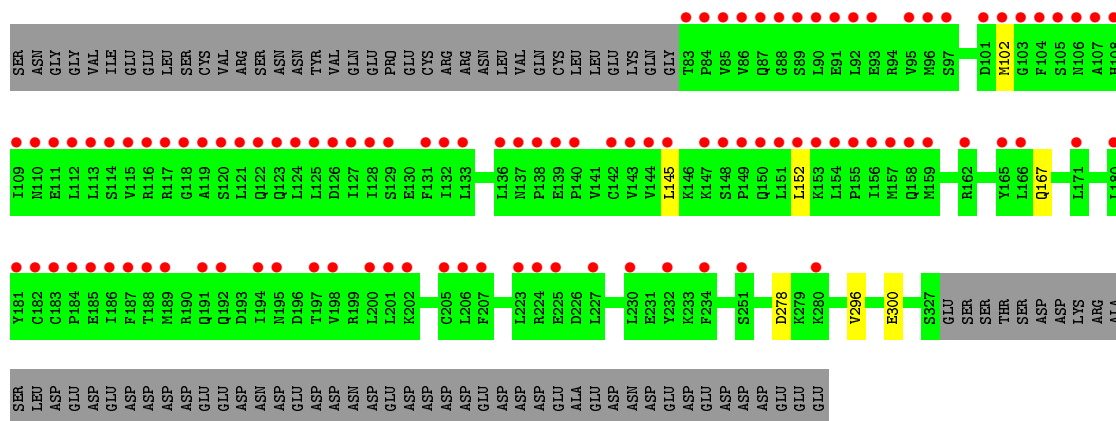
• Molecule 2: mTERF domain-containing protein 2



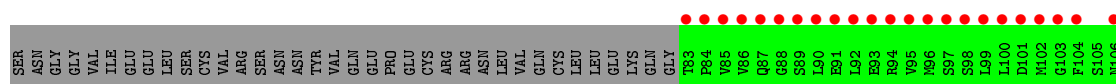
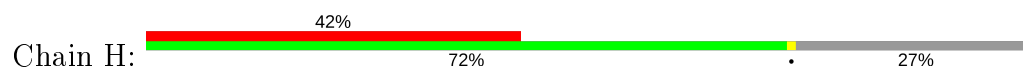
• Molecule 2: mTERF domain-containing protein 2



• Molecule 2: mTERF domain-containing protein 2



• Molecule 2: mTERF domain-containing protein 2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.76 Å 82.27 Å 507.57 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 39.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.90) 99.8 (39.97-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 2.90 Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.229 , 0.246 0.238 , 0.253	Depositor DCC
$R_{free}$ test set	3754 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 61.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18717	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SO4, 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	A	0.39	0/2726	0.58	0/3700
1	C	0.37	0/2726	0.57	0/3700
1	D	0.39	0/2676	0.58	0/3631
1	F	0.38	0/2726	0.57	0/3700
2	B	0.41	0/2021	0.52	0/2718
2	E	0.40	0/2021	0.51	0/2718
2	G	0.42	0/2021	0.50	0/2718
2	H	0.42	0/2021	0.49	0/2718
All	All	0.40	0/18938	0.55	0/25603

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	2665	0	2643	7	0
1	C	2665	0	2643	6	0
1	D	2618	0	2600	4	0
1	F	2665	0	2643	6	0
2	B	1989	0	2083	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1989	0	2083	1	0
2	G	1989	0	2083	1	0
2	H	1989	0	2083	0	0
3	A	27	0	22	1	0
3	C	27	0	22	0	0
3	D	27	0	22	0	0
3	F	27	0	22	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	15	0	0	0	0
4	E	5	0	0	1	0
4	F	5	0	0	0	0
All	All	18717	0	18949	23	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 1.

All (23) 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:A:173:PRO:HG3	1:F:244:LEU:HD13	1.86	0.57
1:A:209:ARG:NH1	3:A:401:SAM:O3'	2.42	0.52
2:B:145:LEU:HD22	2:B:152:LEU:CD1	2.40	0.52
2:G:145:LEU:HD22	2:G:152:LEU:CD1	2.40	0.51
1:A:244:LEU:HD13	1:C:173:PRO:HG3	1.93	0.51
1:A:321:VAL:HG13	1:A:380:MET:HE3	1.92	0.50
1:C:81:ALA:HB2	1:C:152:VAL:HG23	1.92	0.50
1:F:81:ALA:HB2	1:F:152:VAL:HG23	1.96	0.47
1:A:81:ALA:HB2	1:A:152:VAL:HG23	1.98	0.46
1:A:254:VAL:HG12	1:A:256:VAL:HG13	1.98	0.46
1:C:254:VAL:HG12	1:C:256:VAL:HG13	1.98	0.46
1:F:254:VAL:HG12	1:F:256:VAL:HG13	1.98	0.46
1:D:254:VAL:HG12	1:D:256:VAL:HG13	1.98	0.46
2:E:245:HIS:ND1	4:E:401:SO4:O1	2.42	0.45
1:C:183:ALA:HB1	1:C:209:ARG:HB3	2.00	0.44
1:A:236:TRP:CE3	1:C:174:GLY:HA2	2.53	0.44
1:F:183:ALA:HB1	1:F:209:ARG:HB3	2.01	0.43
1:D:183:ALA:HB1	1:D:209:ARG:HB3	2.00	0.43
1:D:241:TRP:HA	1:D:244:LEU:HD12	2.01	0.42
1:D:241:TRP:O	1:D:244:LEU:O	2.37	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:MET:HB2	1:F:220:TYR:CE1	2.55	0.41
1:C:204:ASP:O	1:C:235:SER:HA	2.21	0.40
1:F:204:ASP:O	1:F:235:SER:HA	2.22	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	334/360 (93%)	321 (96%)	13 (4%)	0	100	100
1	C	334/360 (93%)	321 (96%)	13 (4%)	0	100	100
1	D	329/360 (91%)	312 (95%)	17 (5%)	0	100	100
1	F	334/360 (93%)	320 (96%)	14 (4%)	0	100	100
2	B	243/335 (72%)	238 (98%)	5 (2%)	0	100	100
2	E	243/335 (72%)	237 (98%)	6 (2%)	0	100	100
2	G	243/335 (72%)	236 (97%)	7 (3%)	0	100	100
2	H	243/335 (72%)	238 (98%)	5 (2%)	0	100	100
All	All	2303/2780 (83%)	2223 (96%)	80 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	292/308 (95%)	286 (98%)	6 (2%)	53	81
1	C	292/308 (95%)	285 (98%)	7 (2%)	49	79
1	D	287/308 (93%)	276 (96%)	11 (4%)	33	67
1	F	292/308 (95%)	283 (97%)	9 (3%)	40	74
2	B	227/312 (73%)	224 (99%)	3 (1%)	69	90
2	E	227/312 (73%)	222 (98%)	5 (2%)	52	81
2	G	227/312 (73%)	222 (98%)	5 (2%)	52	81
2	H	227/312 (73%)	224 (99%)	3 (1%)	69	90
All	All	2071/2480 (84%)	2022 (98%)	49 (2%)	49	79

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	146	ARG
1	A	224	GLU
1	A	241	TRP
1	A	262	ARG
1	A	357	SER
2	B	130	GLU
2	B	185	GLU
2	B	296	VAL
1	C	64	ARG
1	C	224	GLU
1	C	241	TRP
1	C	247	ASP
1	C	262	ARG
1	C	357	SER
1	C	358	CYS
1	D	64	ARG
1	D	152	VAL
1	D	198	ARG
1	D	224	GLU
1	D	227	ASP
1	D	241	TRP
1	D	244	LEU
1	D	247	ASP
1	D	262	ARG
1	D	357	SER
1	D	358	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	102	MET
2	E	122	GLN
2	E	145	LEU
2	E	151	LEU
2	E	159	MET
1	F	64	ARG
1	F	224	GLU
1	F	241	TRP
1	F	247	ASP
1	F	262	ARG
1	F	275	ARG
1	F	314	HIS
1	F	357	SER
1	F	358	CYS
2	G	102	MET
2	G	167	GLN
2	G	278	ASP
2	G	296	VAL
2	G	300	GLU
2	H	192	GLN
2	H	196	ASP
2	H	296	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	55	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 carbohydrates in this entry.

## 5.6 Ligand geometry

12 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$
4	SO4	E	401	-	4,4,4	1.50	1 (25%)	6,6,6	0.25	0
4	SO4	A	402	-	4,4,4	0.28	0	6,6,6	0.31	0
3	SAM	C	401	-	21,29,29	0.77	0	18,42,42	1.03	1 (5%)
3	SAM	A	401	-	21,29,29	0.78	1 (4%)	18,42,42	1.03	1 (5%)
4	SO4	F	402	-	4,4,4	0.22	0	6,6,6	0.12	0
4	SO4	B	401	-	4,4,4	0.19	0	6,6,6	0.16	0
4	SO4	D	402	-	4,4,4	0.63	0	6,6,6	0.37	0
4	SO4	D	403	-	4,4,4	0.19	0	6,6,6	0.16	0
4	SO4	D	404	-	4,4,4	0.22	0	6,6,6	0.15	0
3	SAM	F	401	-	21,29,29	0.79	0	18,42,42	1.05	2 (11%)
4	SO4	C	402	-	4,4,4	0.37	0	6,6,6	0.21	0
3	SAM	D	401	-	21,29,29	0.76	0	18,42,42	1.05	2 (11%)

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	F	401	-	-	0/8/33/33	0/3/3/3
3	SAM	A	401	-	-	0/8/33/33	0/3/3/3
3	SAM	D	401	-	-	0/8/33/33	0/3/3/3
3	SAM	C	401	-	-	0/8/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	SO4	O2-S	2.21	1.58	1.46
3	A	401	SAM	CG-CB	2.02	1.57	1.51



All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	SAM	O4'-C1'-C2'	-2.31	103.54	106.93
3	C	401	SAM	C5-C6-N6	2.24	123.75	120.35
3	A	401	SAM	C5-C6-N6	2.18	123.67	120.35
3	D	401	SAM	C5-C6-N6	2.16	123.64	120.35
3	F	401	SAM	C5-C6-N6	2.12	123.58	120.35
3	D	401	SAM	O4'-C1'-C2'	-2.11	103.84	106.93

There are no chirality outliers.

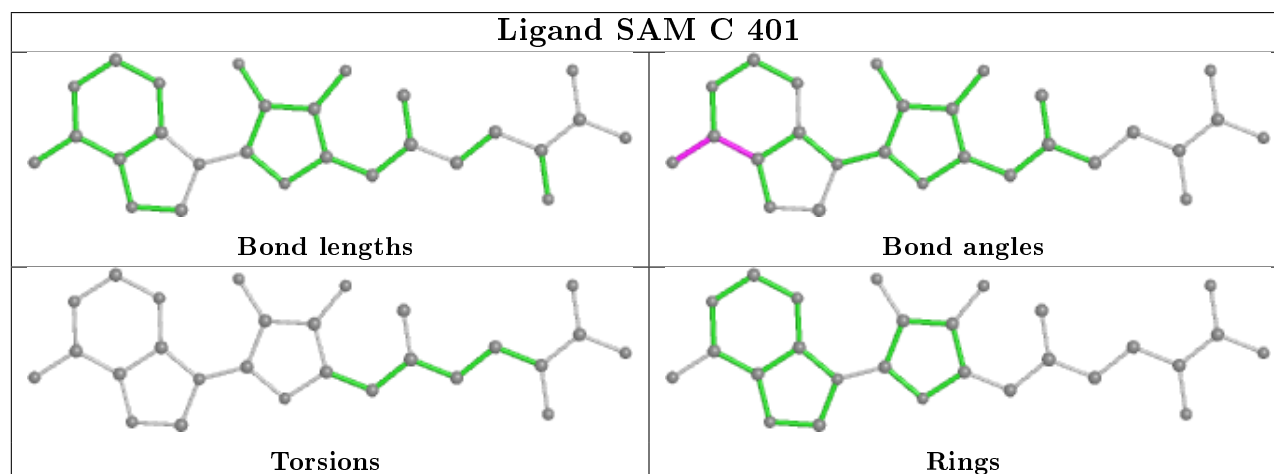
There are no torsion outliers.

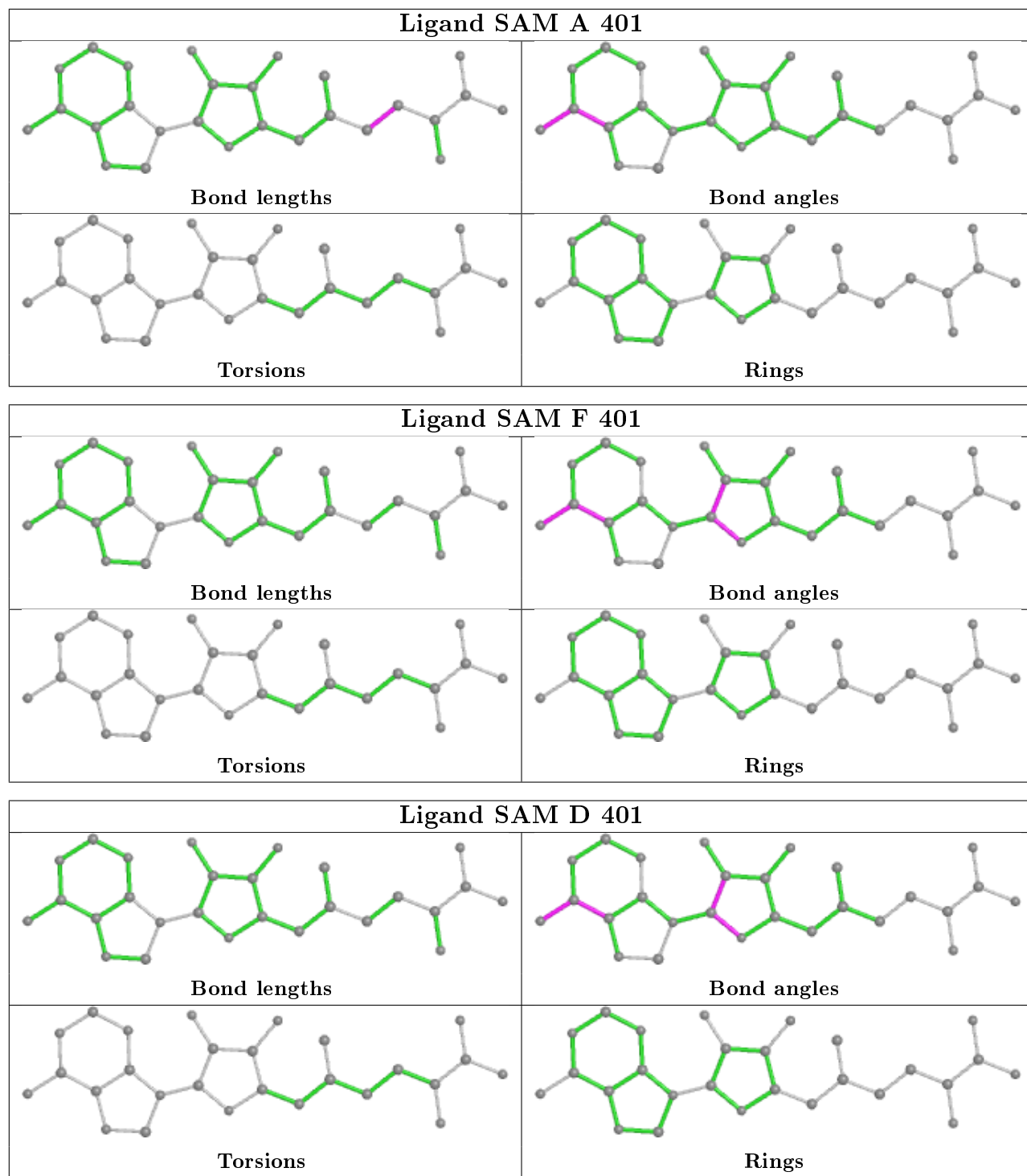
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	SO4	1	0
3	A	401	SAM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	338/360 (93%)	0.11	2 (0%) 89 89	17, 39, 97, 139	0
1	C	338/360 (93%)	0.12	5 (1%) 73 73	12, 51, 115, 157	0
1	D	333/360 (92%)	0.09	5 (1%) 73 73	13, 42, 101, 162	0
1	F	338/360 (93%)	0.29	11 (3%) 46 41	17, 53, 111, 160	0
2	B	245/335 (73%)	0.22	7 (2%) 51 47	27, 59, 106, 151	0
2	E	245/335 (73%)	0.22	6 (2%) 59 56	30, 65, 112, 155	0
2	G	245/335 (73%)	2.05	103 (42%) 0 0	27, 131, 222, 275	0
2	H	245/335 (73%)	2.78	140 (57%) 0 0	57, 139, 195, 220	0
All	All	2327/2780 (83%)	0.64	279 (11%) 4 3	12, 60, 169, 275	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	121	LEU	12.6
2	G	122	GLN	9.9
2	H	131	PHE	9.8
2	G	187	PHE	9.6
2	H	84	PRO	9.5
2	H	85	VAL	9.2
2	H	142	CYS	9.0
2	H	278	ASP	8.6
2	H	294	LEU	8.5
2	G	144	VAL	8.5
2	G	151	LEU	8.4
2	H	88	GLY	8.3
2	G	115	VAL	8.3
2	G	83	THR	8.1
2	H	136	LEU	8.1
2	H	86	VAL	8.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	145	LEU	7.8
2	H	113	LEU	7.8
2	H	90	LEU	7.8
2	G	129	SER	7.7
2	G	182	CYS	7.6
2	G	85	VAL	7.4
2	G	184	PRO	7.4
2	H	115	VAL	7.4
2	H	89	SER	7.3
2	H	157	MET	7.1
2	G	87	GLN	6.9
2	H	280	LYS	6.9
2	H	83	THR	6.8
2	G	118	GLY	6.7
2	H	119	ALA	6.6
2	H	293	ILE	6.6
2	H	87	GLN	6.6
2	G	152	LEU	6.6
2	G	84	PRO	6.5
2	G	112	LEU	6.4
2	H	171	LEU	6.4
2	H	243	ILE	6.3
2	H	112	LEU	6.3
2	H	253	TYR	6.3
2	H	151	LEU	6.2
2	H	242	GLY	6.1
2	G	108	HIS	6.0
2	H	191	GLN	6.0
2	H	176	LEU	5.9
2	G	90	LEU	5.9
2	G	114	SER	5.9
2	H	222	VAL	5.9
2	H	180	LEU	5.8
2	G	88	GLY	5.8
2	H	111	GLU	5.8
2	H	116	ARG	5.7
2	G	138	PRO	5.6
2	H	306	ALA	5.6
2	G	143	VAL	5.5
2	G	198	VAL	5.5
2	G	117	ARG	5.5
2	H	102	MET	5.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	86	VAL	5.4
2	H	121	LEU	5.4
2	H	104	PHE	5.4
2	H	277	PRO	5.3
2	G	92	LEU	5.3
2	H	124	LEU	5.2
2	H	120	SER	5.2
2	H	230	LEU	5.2
2	H	108	HIS	5.1
2	H	256	TYR	5.1
2	G	154	LEU	5.1
2	G	181	TYR	5.1
2	G	150	GLN	5.0
2	G	127	ILE	5.0
2	G	159	MET	5.0
2	H	179	VAL	5.0
2	H	248	ILE	5.0
2	H	279	LYS	4.9
2	G	183	CYS	4.9
2	H	165	TYR	4.9
2	H	305	THR	4.9
2	H	101	ASP	4.9
2	H	173	GLU	4.8
2	G	124	LEU	4.8
2	H	295	ARG	4.7
2	G	119	ALA	4.7
2	H	123	GLN	4.7
2	H	175	LYS	4.7
2	G	142	CYS	4.7
2	H	96	MET	4.7
2	H	122	GLN	4.7
2	H	138	PRO	4.6
2	H	254	LEU	4.6
2	G	111	GLU	4.6
2	H	227	LEU	4.6
2	G	126	ASP	4.6
2	G	139	GLU	4.6
2	H	97	SER	4.5
2	H	219	CYS	4.5
2	G	166	LEU	4.4
2	G	156	ILE	4.4
2	G	103	GLY	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	91	GLU	4.3
2	H	164	SER	4.3
2	H	133	LEU	4.2
2	G	147	LYS	4.2
2	H	178	ARG	4.2
2	G	116	ARG	4.2
2	G	202	LYS	4.2
2	G	162	ARG	4.2
2	H	92	LEU	4.2
2	H	103	GLY	4.2
2	H	234	PHE	4.1
2	G	223	LEU	4.1
2	G	104	PHE	4.1
2	B	83	THR	4.1
2	H	238	TYR	4.1
2	G	186	ILE	4.1
2	H	99	LEU	4.0
2	G	180	LEU	4.0
2	H	261	ILE	4.0
2	G	140	PRO	3.9
2	H	140	PRO	3.9
2	H	273	ARG	3.9
2	H	288	PRO	3.8
2	G	197	THR	3.8
2	G	207	PHE	3.8
1	C	226	ARG	3.8
2	H	137	ASN	3.8
2	H	147	LYS	3.8
2	G	191	GLN	3.7
2	H	215	ILE	3.7
2	H	114	SER	3.7
2	H	117	ARG	3.7
2	H	94	ARG	3.7
2	H	128	ILE	3.7
2	H	109	ILE	3.7
2	G	185	GLU	3.7
2	H	143	VAL	3.7
2	H	152	LEU	3.7
2	H	118	GLY	3.6
2	H	144	VAL	3.6
2	G	101	ASP	3.6
2	G	205	CYS	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	207	PHE	3.6
2	H	98	SER	3.5
2	G	96	MET	3.5
2	G	97	SER	3.5
2	G	194	ILE	3.5
2	G	120	SER	3.5
2	G	109	ILE	3.5
2	H	146	LYS	3.4
1	F	108	LEU	3.4
2	B	291	LYS	3.4
2	G	188	THR	3.4
1	A	275	ARG	3.4
2	H	107	ALA	3.4
2	B	278	ASP	3.4
2	G	107	ALA	3.4
2	H	281	GLY	3.4
2	H	202	LYS	3.3
1	F	272	ILE	3.3
2	G	125	LEU	3.3
2	H	200	LEU	3.3
1	F	83	TRP	3.3
2	H	290	LEU	3.3
2	H	282	GLN	3.3
2	H	174	GLY	3.3
2	G	149	PRO	3.3
2	B	280	LYS	3.3
2	H	229	GLN	3.3
1	D	105	HIS	3.3
2	H	169	LEU	3.2
2	H	159	MET	3.2
2	H	205	CYS	3.2
1	C	279	LYS	3.2
2	G	131	PHE	3.2
2	G	234	PHE	3.2
2	G	158	GLN	3.2
2	H	232	TYR	3.2
1	C	384	THR	3.1
2	G	165	TYR	3.1
2	G	102	MET	3.1
2	H	187	PHE	3.1
1	A	322	GLN	3.1
2	H	110	ASN	3.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	89	SER	3.0
1	D	124	ALA	3.0
2	E	138	PRO	3.0
2	H	145	LEU	3.0
2	G	232	TYR	3.0
2	G	93	GLU	3.0
2	G	128	ILE	3.0
2	G	200	LEU	3.0
2	G	189	MET	3.0
2	G	171	LEU	2.9
2	H	177	LYS	2.9
2	H	307	CYS	2.9
2	G	105	SER	2.9
2	H	141	VAL	2.9
2	G	153	LYS	2.9
2	G	95	VAL	2.9
2	H	150	GLN	2.9
2	H	213	THR	2.8
2	H	198	VAL	2.8
2	G	192	GLN	2.8
2	E	181	TYR	2.8
1	F	82	ALA	2.8
2	H	129	SER	2.8
2	H	203	GLU	2.8
2	G	230	LEU	2.7
2	H	95	VAL	2.7
2	G	201	LEU	2.7
2	G	227	LEU	2.7
2	H	149	PRO	2.7
2	G	91	GLU	2.7
2	H	153	LYS	2.7
2	E	278	ASP	2.6
2	G	206	LEU	2.6
2	G	113	LEU	2.6
2	G	123	GLN	2.6
2	G	148	SER	2.6
1	D	82	ALA	2.6
2	G	225	GLU	2.6
2	H	158	GLN	2.6
2	G	155	PRO	2.6
2	H	208	THR	2.6
2	H	276	THR	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	243	ILE	2.5
2	H	302	LEU	2.5
2	G	224	ARG	2.5
2	G	157	MET	2.5
2	H	161	LYS	2.5
2	H	284	GLN	2.5
2	H	289	LEU	2.5
2	H	93	GLU	2.5
1	D	119	SER	2.5
2	H	100	LEU	2.5
2	G	110	ASN	2.4
2	H	125	LEU	2.4
2	H	195	ASN	2.4
1	D	125	CYS	2.4
2	G	133	LEU	2.4
2	E	104	PHE	2.3
1	F	282	GLN	2.3
2	G	106	ASN	2.3
1	F	105	HIS	2.3
2	B	282	GLN	2.3
2	H	168	LYS	2.3
2	H	181	TYR	2.3
1	F	161	ALA	2.3
2	H	244	LYS	2.3
2	H	252	GLU	2.3
2	B	84	PRO	2.3
2	G	280	LYS	2.3
2	G	137	ASN	2.3
2	H	190	ARG	2.3
2	H	241	MET	2.3
1	F	229	ASN	2.2
2	H	216	LEU	2.2
2	H	156	ILE	2.2
2	E	83	THR	2.2
2	H	218	SER	2.2
2	H	274	TYR	2.2
2	H	166	LEU	2.2
2	H	204	LYS	2.2
2	H	239	PHE	2.1
2	H	148	SER	2.1
1	C	229	ASN	2.1
1	F	278	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	132	ILE	2.1
1	C	222	PRO	2.1
1	F	353	CYS	2.1
2	E	280	LYS	2.1
2	G	136	LEU	2.1
2	H	192	GLN	2.1
2	G	195	ASN	2.1
2	H	106	ASN	2.1
2	H	154	LEU	2.0
1	F	328	LEU	2.0
2	G	251	SER	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](#)

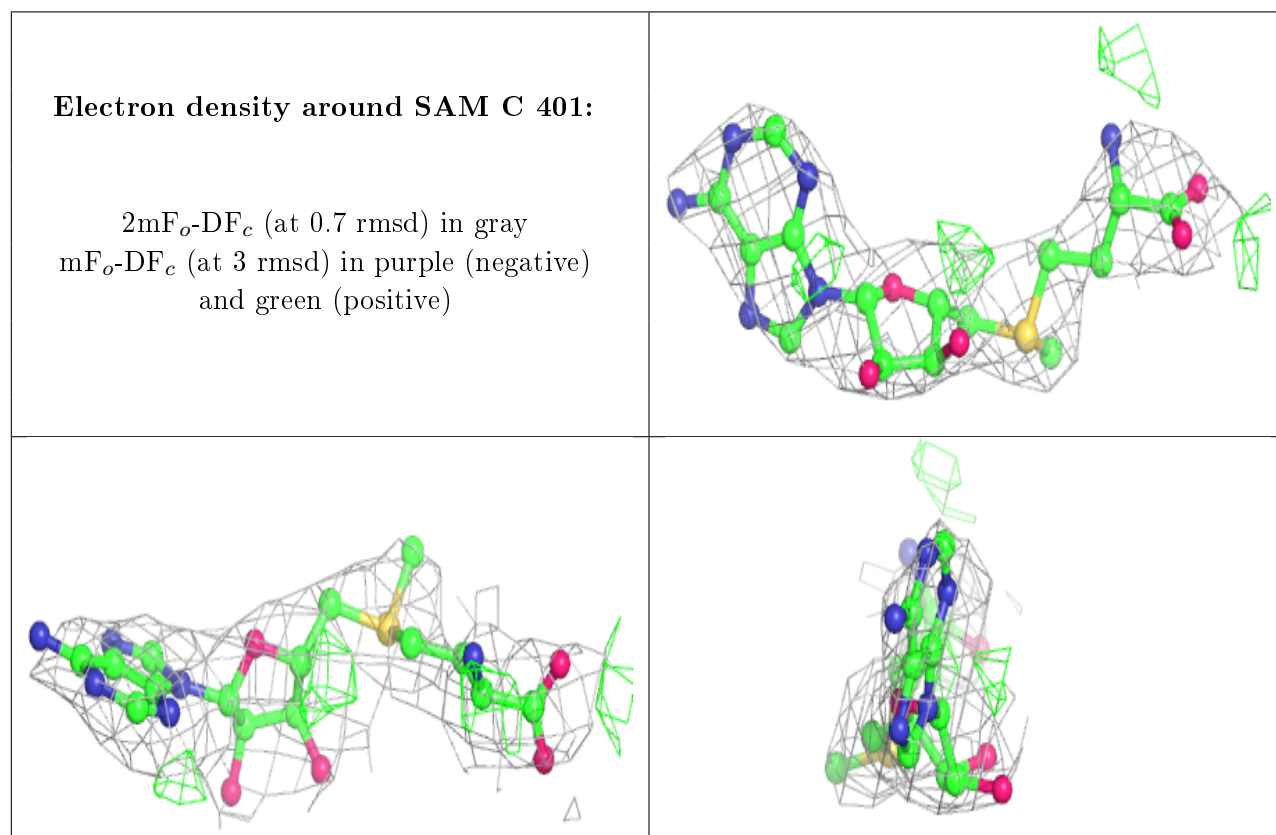
There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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.

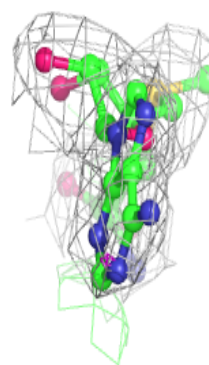
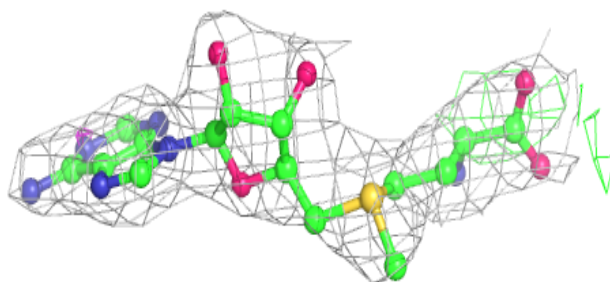
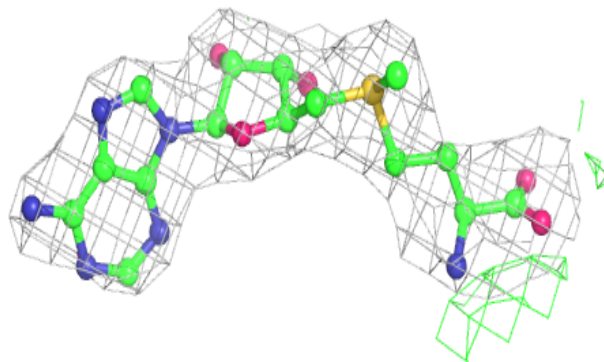
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	SAM	C	401	27/27	0.79	0.31	27,28,40,42	27
4	SO4	F	402	5/5	0.84	0.20	100,100,101,101	0
4	SO4	D	403	5/5	0.86	0.15	100,100,100,100	0
3	SAM	A	401	27/27	0.90	0.21	3,6,9,10	27
4	SO4	A	402	5/5	0.91	0.11	77,77,77,77	0
3	SAM	F	401	27/27	0.91	0.21	3,3,10,11	27
4	SO4	B	401	5/5	0.93	0.11	96,97,97,97	0
4	SO4	D	404	5/5	0.94	0.14	90,90,91,91	0
4	SO4	E	401	5/5	0.94	0.25	30,30,30,30	0
4	SO4	D	402	5/5	0.95	0.15	40,40,40,40	0
4	SO4	C	402	5/5	0.95	0.16	79,79,79,79	0
3	SAM	D	401	27/27	0.95	0.17	3,3,8,9	27

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.

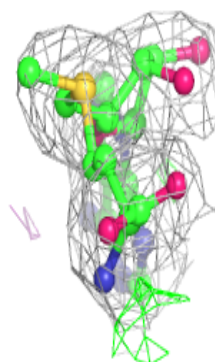
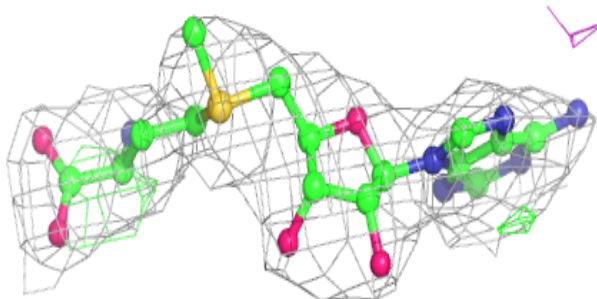
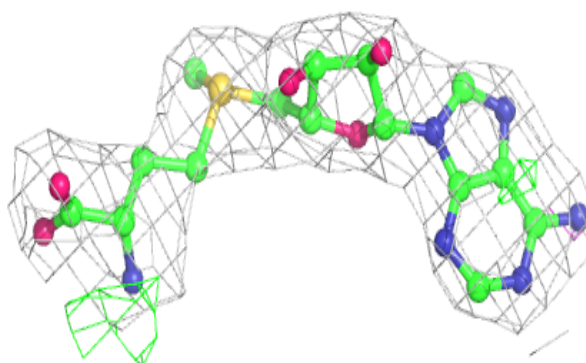


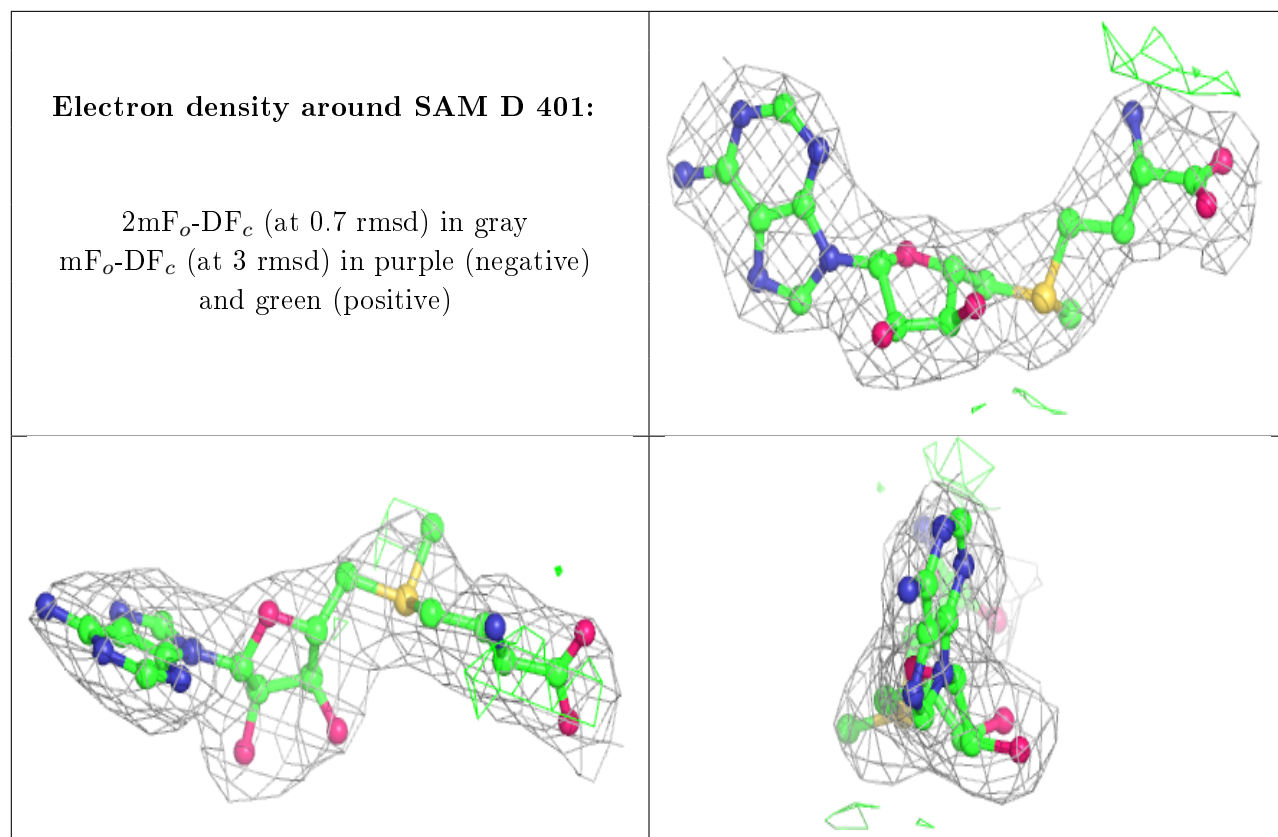
**Electron density around SAM A 401:**

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

**Electron density around SAM F 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.