



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:10 AM UTC

PDB ID : 4FP9 / pdb_00004fp9
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

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

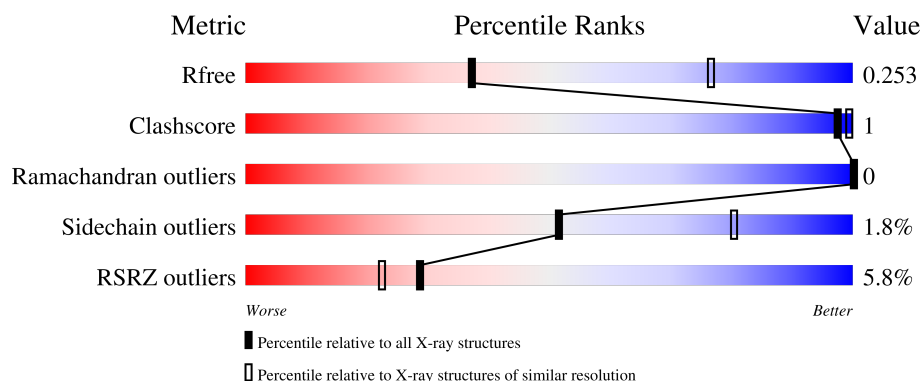
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



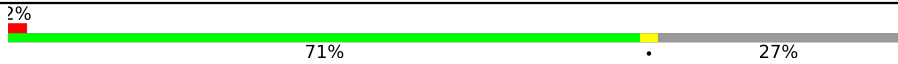
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 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	360	% 89% 5% 6%
1	C	360	2% 89% 5% 6%
1	D	360	3% 88% . . 8%
1	F	360	2% 89% 5% 6%
2	B	335	% 70% . 27%

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Mol	Chain	Length	Quality of chain
2	E	335	
2	G	335	
2	H	335	

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			

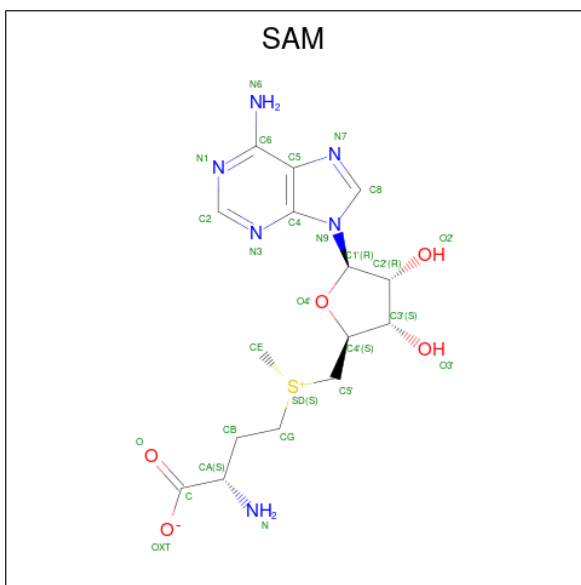
There are 4 discrepancies between the modelled and reference sequences:

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.

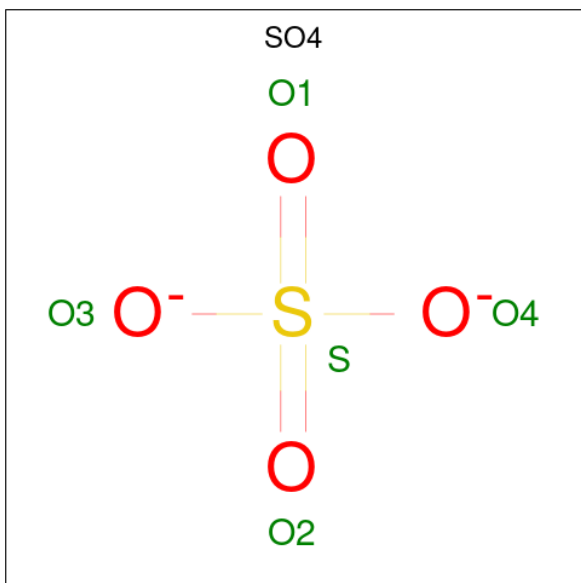
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	E	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	G	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	H	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

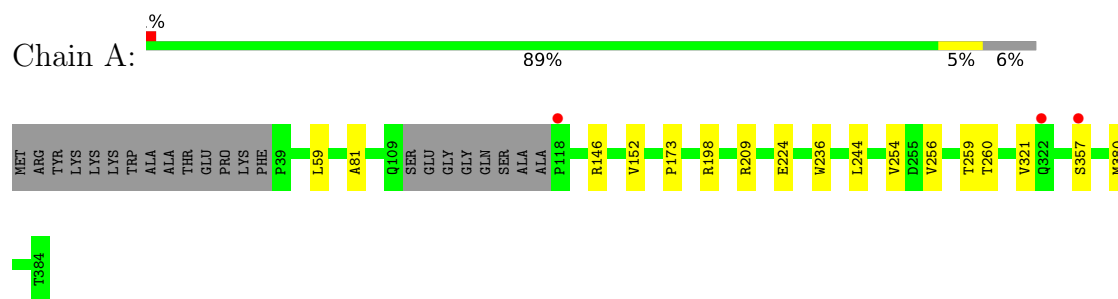


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

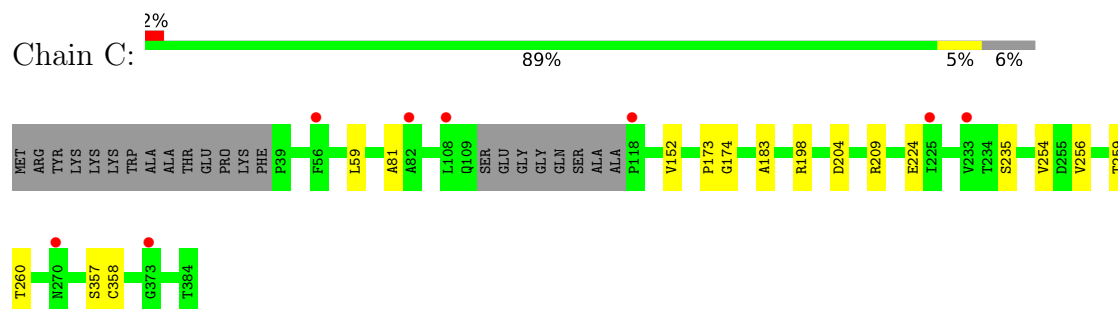
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

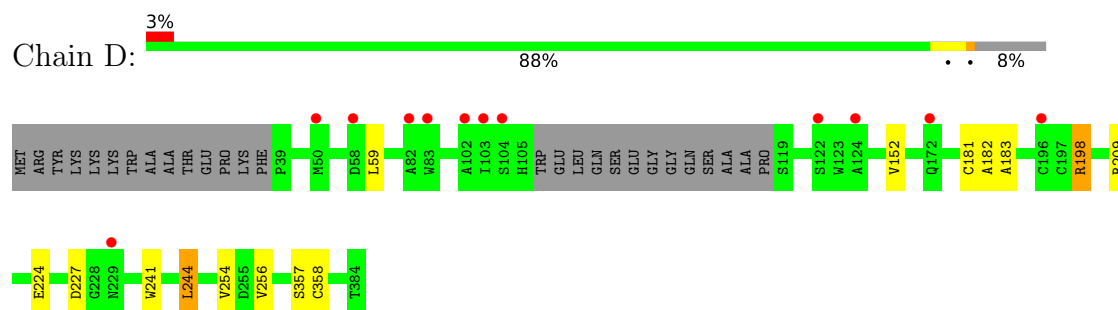
- Molecule 1: methyltransferase NSUN4



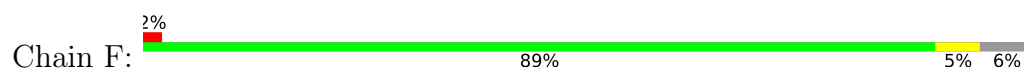
- Molecule 1: methyltransferase NSUN4



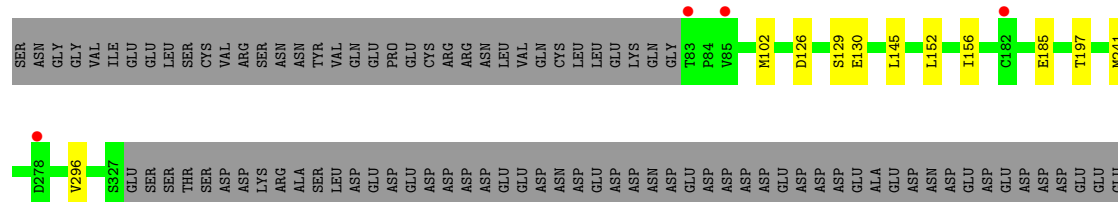
- Molecule 1: methyltransferase NSUN4



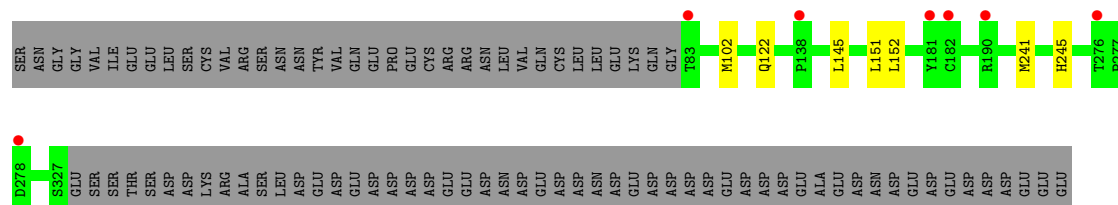
- Molecule 1: methyltransferase NSUN4



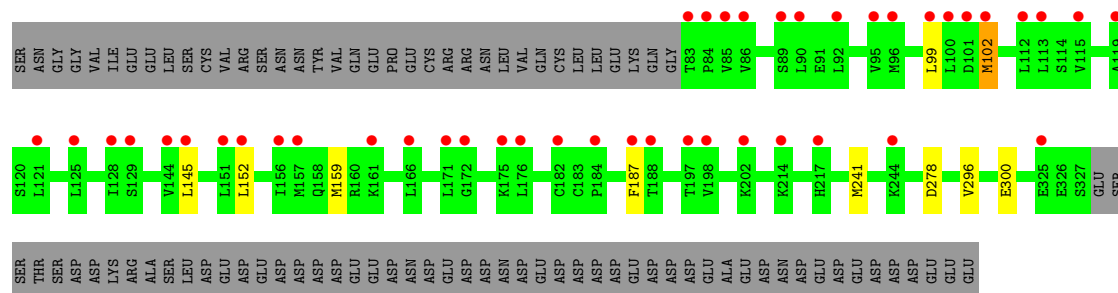
- Molecule 2: mTERF domain-containing protein 2



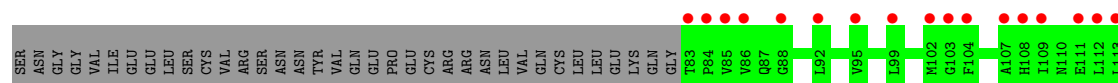
- Molecule 2: mTERF domain-containing protein 2

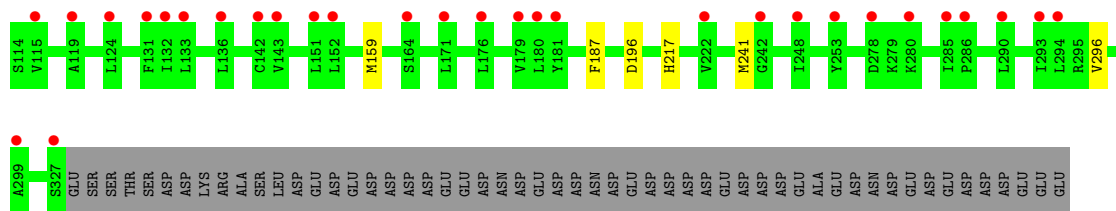


- Molecule 2: mTERF domain-containing protein 2



- 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, α , β , γ	78.76Å 82.27Å 507.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90 40.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-2.90) 99.8 (40.00-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.90Å)	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 ²)	64.1	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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	0.69	0/2726	1.02	1/3700 (0.0%)
1	C	0.68	0/2726	1.02	1/3700 (0.0%)
1	D	0.70	0/2676	1.05	4/3631 (0.1%)
1	F	0.69	0/2726	1.02	0/3700
2	B	0.75	1/2021 (0.0%)	1.03	2/2718 (0.1%)
2	E	0.74	1/2021 (0.0%)	1.01	0/2718
2	G	0.79	1/2021 (0.0%)	1.03	0/2718
2	H	0.78	1/2021 (0.0%)	1.02	0/2718
All	All	0.72	4/18938 (0.0%)	1.02	8/25603 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	241	MET	SD-CE	-8.40	1.58	1.79
2	B	241	MET	SD-CE	-7.58	1.60	1.79
2	G	241	MET	SD-CE	-7.25	1.61	1.79
2	H	241	MET	SD-CE	-7.12	1.61	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	182	ALA	N-CA-C	7.41	120.42	111.82
1	D	181	CYS	CA-C-N	5.60	128.82	120.31
1	D	181	CYS	C-N-CA	5.60	128.82	120.31
1	D	198	ARG	N-CA-C	-5.35	105.34	111.07
2	B	156	ILE	N-CA-C	5.24	115.97	110.62
1	C	198	ARG	N-CA-C	-5.11	105.62	111.14
1	A	198	ARG	N-CA-C	-5.06	105.68	111.14
2	B	126	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

There are no planarity outliers.

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	A	2665	0	2643	8	0
1	C	2665	0	2643	7	0
1	D	2618	0	2600	4	0
1	F	2665	0	2643	7	0
2	B	1989	0	2083	2	0
2	E	1989	0	2083	1	0
2	G	1989	0	2083	3	0
2	H	1989	0	2083	2	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	31	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 (31) 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
2:H:159:MET:HE2	2:H:187:PHE:CE1	2.43	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:HD13	1:C:173:PRO:HG3	1.93	0.51
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
1:A:321:VAL:HG13	1:A:380:MET:HE3	1.98	0.46
2:E:245:HIS:ND1	4:E:401:SO4:O1	2.42	0.45
2:B:102:MET:HE1	2:B:129:SER:OG	2.17	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
2:G:159:MET:HE2	2:G:187:PHE:CZ	2.53	0.42
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
1:F:153:MET:HB2	1:F:220:TYR:CE1	2.55	0.41
1:C:259:THR:O	1:C:260:THR:C	2.63	0.41
2:G:99:LEU:HA	2:G:102:MET:HE2	2.03	0.41
2:H:217:HIS:ND1	2:H:217:HIS:C	2.79	0.40
1:A:259:THR:O	1:A:260:THR:C	2.64	0.40
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
1:F:259:THR:O	1:F:260:THR:C	2.64	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	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 ⓘ

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%)	288 (99%)	4 (1%)	59	85
1	C	292/308 (95%)	288 (99%)	4 (1%)	59	85
1	D	287/308 (93%)	279 (97%)	8 (3%)	38	72
1	F	292/308 (95%)	286 (98%)	6 (2%)	47	77
2	B	227/312 (73%)	223 (98%)	4 (2%)	51	80
2	E	227/312 (73%)	222 (98%)	5 (2%)	45	77
2	G	227/312 (73%)	223 (98%)	4 (2%)	51	80
2	H	227/312 (73%)	225 (99%)	2 (1%)	70	90
All	All	2071/2480 (84%)	2034 (98%)	37 (2%)	51	80

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	146	ARG

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Mol	Chain	Res	Type
1	A	224	GLU
1	A	357	SER
2	B	130	GLU
2	B	185	GLU
2	B	197	THR
2	B	296	VAL
1	C	59	LEU
1	C	224	GLU
1	C	357	SER
1	C	358	CYS
1	D	59	LEU
1	D	152	VAL
1	D	198	ARG
1	D	224	GLU
1	D	227	ASP
1	D	244	LEU
1	D	357	SER
1	D	358	CYS
2	E	102	MET
2	E	122	GLN
2	E	145	LEU
2	E	151	LEU
2	E	152	LEU
1	F	59	LEU
1	F	224	GLU
1	F	275	ARG
1	F	314	HIS
1	F	357	SER
1	F	358	CYS
2	G	102	MET
2	G	278	ASP
2	G	296	VAL
2	G	300	GLU
2	H	196	ASP
2	H	296	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
2	B	106	ASN
2	B	229	GLN

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Mol	Chain	Res	Type
2	B	235	GLN
2	B	255	GLN
2	B	284	GLN
1	C	266	HIS
1	D	230	GLN
1	D	266	HIS
2	E	106	ASN
2	E	191	GLN
2	E	195	ASN
2	E	235	GLN
2	E	255	GLN
2	E	314	GLN
1	F	55	GLN
1	F	71	GLN
1	F	266	HIS
2	G	167	GLN
2	G	235	GLN
2	G	255	GLN
2	H	106	ASN
2	H	108	HIS
2	H	122	GLN
2	H	191	GLN
2	H	235	GLN
2	H	255	GLN

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 ⓘ

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	$\# Z > 2$
3	SAM	D	401	-	27,29,29	0.58	0	34,42,42	0.74	0
4	SO4	E	401	-	4,4,4	1.51	1 (25%)	6,6,6	0.24	0
3	SAM	C	401	-	27,29,29	0.63	0	34,42,42	0.72	0
3	SAM	F	401	-	27,29,29	0.63	0	34,42,42	0.73	0
4	SO4	A	402	-	4,4,4	0.39	0	6,6,6	0.32	0
4	SO4	D	403	-	4,4,4	0.30	0	6,6,6	0.15	0
4	SO4	F	402	-	4,4,4	0.32	0	6,6,6	0.14	0
4	SO4	D	402	-	4,4,4	0.71	0	6,6,6	0.38	0
4	SO4	D	404	-	4,4,4	0.33	0	6,6,6	0.12	0
3	SAM	A	401	-	27,29,29	0.64	1 (3%)	34,42,42	0.73	0
4	SO4	C	402	-	4,4,4	0.47	0	6,6,6	0.26	0
4	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.17	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. '1' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	D	401	-	-	0/17/33/33	0/3/3/3
3	SAM	C	401	-	-	0/17/33/33	0/3/3/3
3	SAM	A	401	-	-	1/17/33/33	0/3/3/3
3	SAM	F	401	-	-	0/17/33/33	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	1.44
3	A	401	SAM	CG-CB	2.02	1.57	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

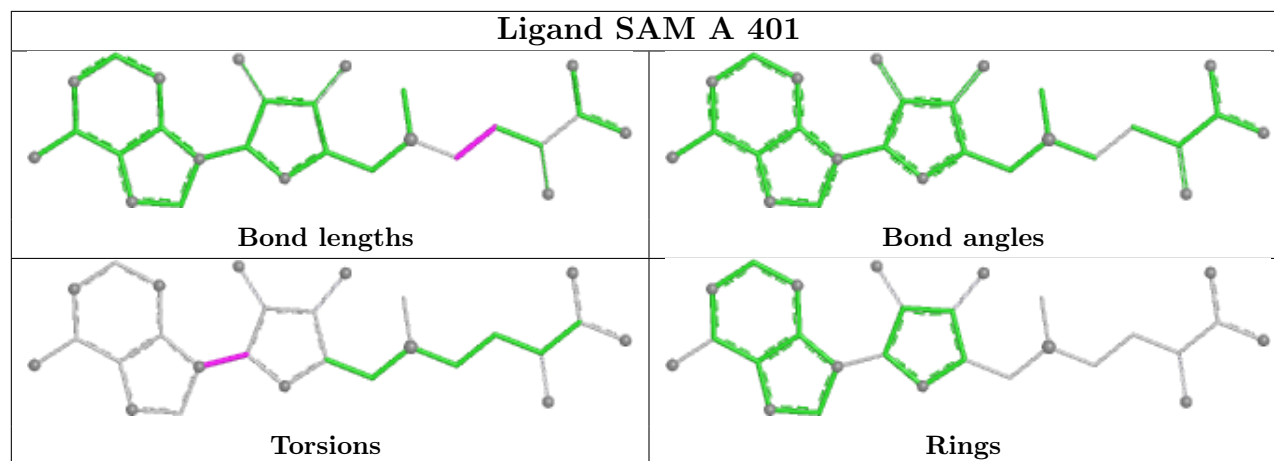
Mol	Chain	Res	Type	Atoms
3	A	401	SAM	C2'-C1'-N9-C8

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 [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	338/360 (93%)	-0.10	3 (0%) 81 75	17, 39, 97, 139	0
1	C	338/360 (93%)	0.08	8 (2%) 59 50	12, 51, 115, 157	0
1	D	333/360 (92%)	0.06	12 (3%) 46 38	13, 42, 101, 162	0
1	F	338/360 (93%)	0.21	9 (2%) 56 47	17, 53, 111, 160	0
2	B	245/335 (73%)	0.08	4 (1%) 70 62	27, 59, 106, 151	0
2	E	245/335 (73%)	0.12	7 (2%) 53 45	30, 65, 112, 155	0
2	G	245/335 (73%)	0.93	44 (17%) 3 3	27, 131, 222, 275	0
2	H	245/335 (73%)	1.07	47 (19%) 3 2	57, 139, 195, 220	0
All	All	2327/2780 (83%)	0.27	134 (5%) 29 22	12, 60, 169, 275	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	82	ALA	6.9
1	D	82	ALA	5.9
2	G	144	VAL	5.0
1	D	124	ALA	4.3
2	H	99	LEU	4.1
1	C	118	PRO	4.1
1	F	83	TRP	4.0
1	F	229	ASN	3.9
2	G	121	LEU	3.9
2	H	327	SER	3.6
2	H	131	PHE	3.6
2	G	85	VAL	3.4
2	H	152	LEU	3.3
2	H	294	LEU	3.3
2	G	95	VAL	3.3
2	G	129	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	G	92	LEU	3.2
2	G	100	LEU	3.2
2	H	104	PHE	3.2
2	G	90	LEU	3.1
2	E	278	ASP	3.1
2	H	112	LEU	3.1
2	H	136	LEU	3.1
1	C	82	ALA	3.0
1	D	122	SER	3.0
2	H	171	LEU	3.0
1	F	225	ILE	2.9
2	H	293	ILE	2.9
1	D	103	ILE	2.9
2	H	222	VAL	2.9
2	E	138	PRO	2.8
2	G	102	MET	2.8
2	E	181	TYR	2.8
2	H	113	LEU	2.8
2	H	176	LEU	2.8
1	A	118	PRO	2.8
2	H	179	VAL	2.7
2	H	88	GLY	2.7
1	A	322	GLN	2.7
2	G	151	LEU	2.7
1	D	102	ALA	2.7
2	H	119	ALA	2.7
2	H	181	TYR	2.7
2	G	125	LEU	2.7
2	H	180	LEU	2.7
2	H	85	VAL	2.6
2	H	115	VAL	2.6
2	G	99	LEU	2.6
1	D	83	TRP	2.6
2	G	184	PRO	2.6
2	B	85	VAL	2.6
2	G	86	VAL	2.6
2	G	176	LEU	2.6
2	G	187	PHE	2.6
1	A	357	SER	2.6
2	G	128	ILE	2.6
2	H	86	VAL	2.6
2	H	109	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	107	ALA	2.6
2	G	84	PRO	2.5
1	C	373	GLY	2.5
2	H	92	LEU	2.5
2	B	278	ASP	2.5
1	D	104	SER	2.5
2	H	102	MET	2.5
2	B	182	CYS	2.5
2	H	124	LEU	2.5
2	G	119	ALA	2.5
1	C	108	LEU	2.4
1	F	92	GLN	2.4
2	E	83	THR	2.4
1	D	58	ASP	2.4
2	H	290	LEU	2.4
1	C	270	ASN	2.4
1	C	225	ILE	2.4
2	G	175	LYS	2.4
2	H	133	LEU	2.4
2	H	111	GLU	2.3
1	F	109	GLN	2.3
2	G	96	MET	2.3
2	B	83	THR	2.3
2	G	145	LEU	2.3
2	G	244	LYS	2.3
1	D	229	ASN	2.3
2	G	325	GLU	2.3
1	D	196	CYS	2.3
1	F	368	LEU	2.3
2	G	152	LEU	2.3
2	G	171	LEU	2.3
2	G	182	CYS	2.3
2	G	161	LYS	2.3
2	G	188	THR	2.3
2	H	95	VAL	2.3
2	G	214	LYS	2.3
2	H	83	THR	2.3
2	H	84	PRO	2.3
2	H	299	ALA	2.2
2	G	89	SER	2.2
2	G	172	GLY	2.2
1	C	56	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	142	CYS	2.2
2	H	103	GLY	2.2
2	H	253	TYR	2.2
2	G	112	LEU	2.2
2	G	156	ILE	2.2
2	H	108	HIS	2.2
2	G	198	VAL	2.2
2	G	197	THR	2.2
2	H	286	PRO	2.1
2	E	182	CYS	2.1
1	F	272	ILE	2.1
2	H	285	ILE	2.1
2	G	217	HIS	2.1
2	G	115	VAL	2.1
2	H	143	VAL	2.1
2	G	202	LYS	2.1
2	G	101	ASP	2.1
2	G	83	THR	2.1
2	E	190	ARG	2.1
1	D	50	MET	2.1
2	G	113	LEU	2.1
2	H	248	ILE	2.1
2	G	157	MET	2.1
2	H	242	GLY	2.1
2	H	278	ASP	2.1
2	H	164	SER	2.0
1	D	172	GLN	2.0
2	G	166	LEU	2.0
2	H	280	LYS	2.0
1	C	233	VAL	2.0
1	F	205	LEU	2.0
2	H	151	LEU	2.0
2	H	132	ILE	2.0
2	E	276	THR	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

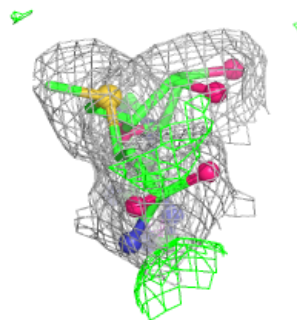
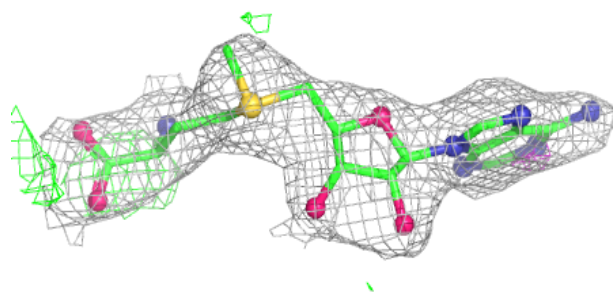
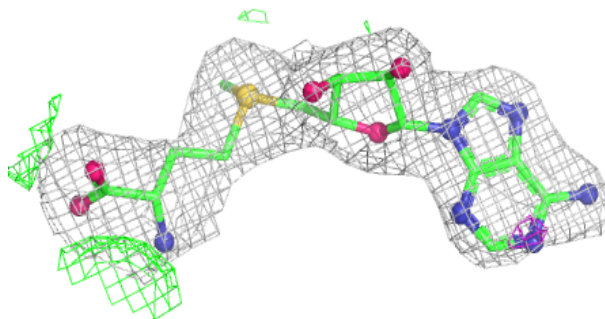
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	F	402	5/5	0.64	0.14	100,100,101,101	0
4	SO4	D	403	5/5	0.76	0.11	100,100,100,100	0
4	SO4	B	401	5/5	0.80	0.10	96,97,97,97	0
3	SAM	C	401	27/27	0.82	0.14	27,28,40,42	27
4	SO4	C	402	5/5	0.85	0.11	79,79,79,79	0
4	SO4	A	402	5/5	0.86	0.09	77,77,77,77	0
4	SO4	D	404	5/5	0.89	0.12	90,90,91,91	0
3	SAM	F	401	27/27	0.93	0.09	3,3,10,11	27
3	SAM	A	401	27/27	0.94	0.09	3,6,9,10	27
4	SO4	D	402	5/5	0.95	0.15	40,40,40,40	0
4	SO4	E	401	5/5	0.95	0.23	30,30,30,30	0
3	SAM	D	401	27/27	0.95	0.08	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)



6.5 Other polymers [i](#)

There are no such residues in this entry.