



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

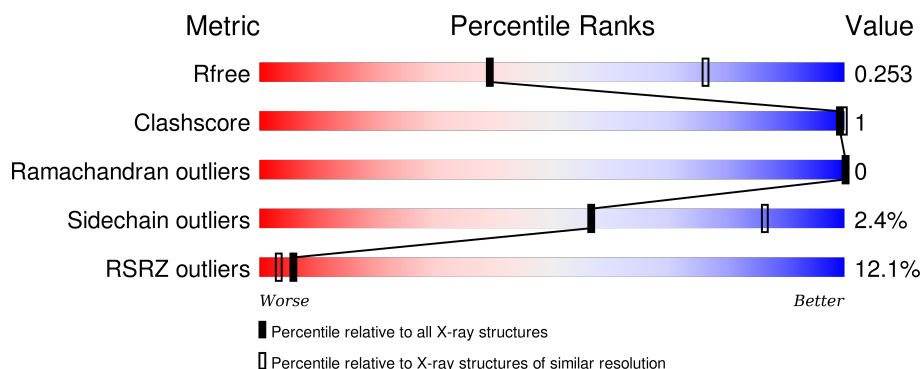
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>89%</div> <div>6%</div> </div>
1	C	360	<div> <div>89%</div> <div>5%</div> <div>6%</div> </div>
1	D	360	<div> <div>88%</div> <div>8%</div> </div>
1	F	360	<div> <div>88%</div> <div>6%</div> <div>6%</div> </div>
2	B	335	<div> <div>72%</div> <div>27%</div> </div>

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SAM	C	401	-	-	-	X

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			

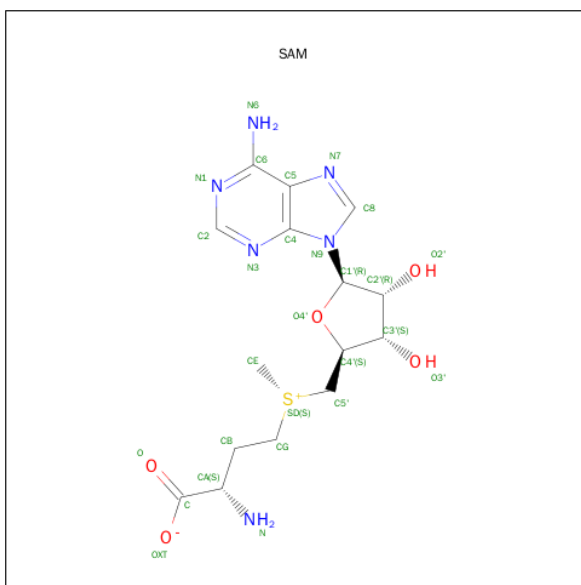
There are 4 discrepancies between the modelled and reference sequences:

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: C₁₅H₂₂N₆O₅S).



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: O₄S).

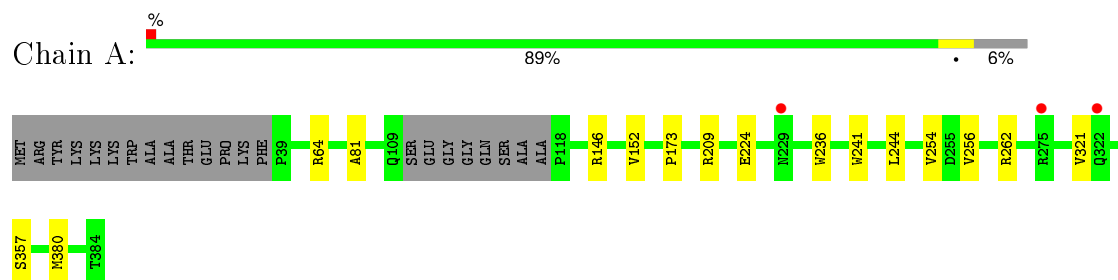


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

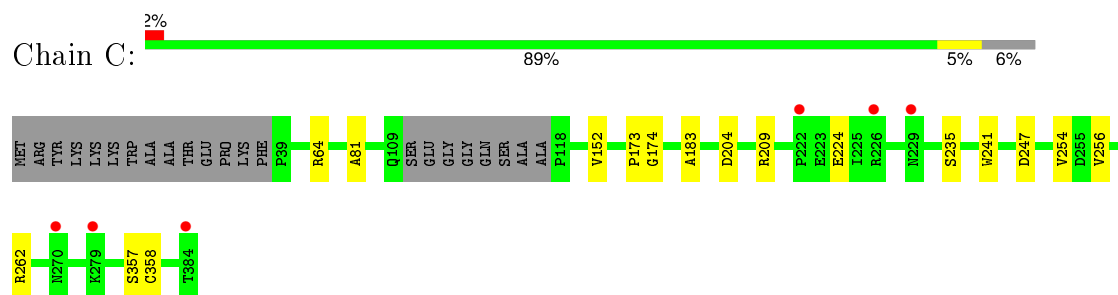
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

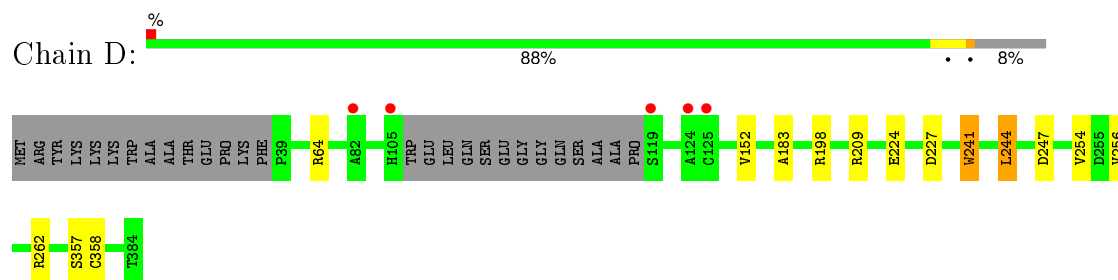
- Molecule 1: methyltransferase NSUN4



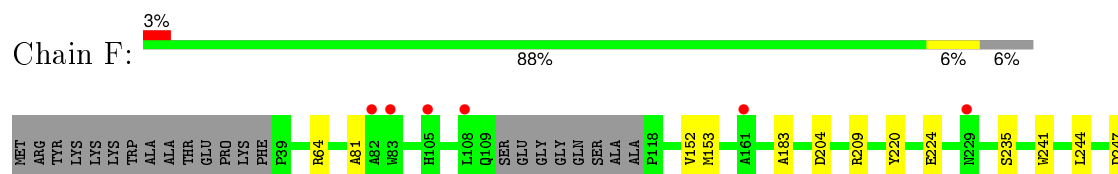
- Molecule 1: methyltransferase NSUN4

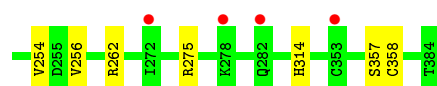


- Molecule 1: methyltransferase NSUN4



- Molecule 1: methyltransferase NSUN4

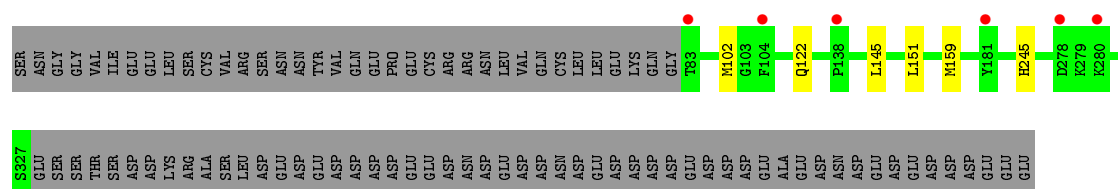




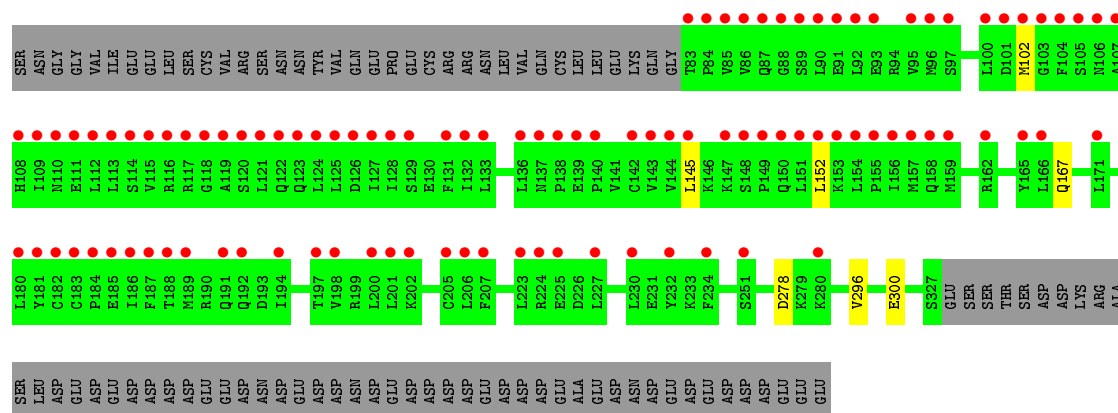
• Molecule 2: mTERF domain-containing protein 2



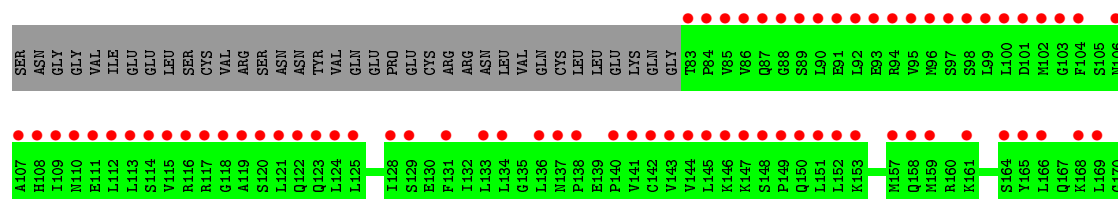
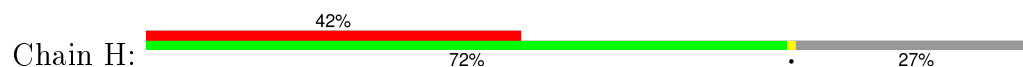
• Molecule 2: mTERF domain-containing protein 2

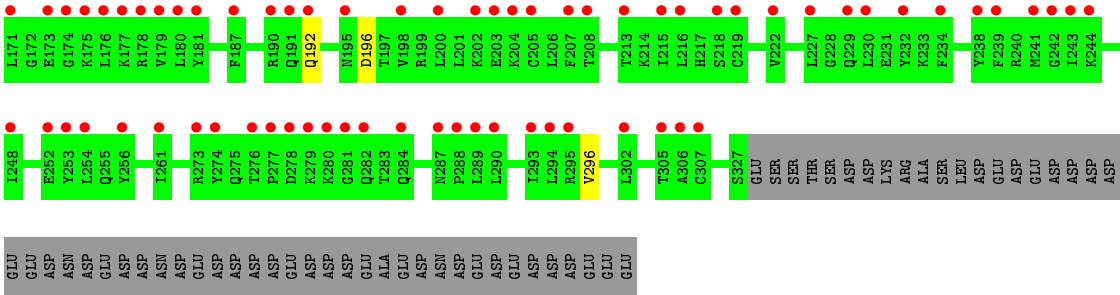


• Molecule 2: mTERF domain-containing protein 2



• 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	78.76 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
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.90 Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.229 , 0.246 0.238 , 0.253	Depositor DCC
R_{free} test set	3754 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.2	EDS
Estimated twinning fraction	0.026 for k,h,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 74501 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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

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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

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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%)	61	88
1	C	292/308 (95%)	285 (98%)	7 (2%)	57	86
1	D	287/308 (93%)	276 (96%)	11 (4%)	40	76
1	F	292/308 (95%)	283 (97%)	9 (3%)	47	82
2	B	227/312 (73%)	224 (99%)	3 (1%)	76	94
2	E	227/312 (73%)	222 (98%)	5 (2%)	60	88
2	G	227/312 (73%)	222 (98%)	5 (2%)	60	88
2	H	227/312 (73%)	224 (99%)	3 (1%)	76	94
All	All	2071/2480 (84%)	2022 (98%)	49 (2%)	57	86

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

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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 ⓘ

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 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$
3	SAM	A	401	-	21,29,29	1.12	1 (4%)	17,42,42	1.36	1 (5%)
4	SO4	A	402	-	4,4,4	0.27	0	6,6,6	0.36	0
4	SO4	B	401	-	4,4,4	0.08	0	6,6,6	0.12	0
3	SAM	C	401	-	21,29,29	1.04	1 (4%)	17,42,42	1.32	1 (5%)
4	SO4	C	402	-	4,4,4	0.35	0	6,6,6	0.40	0
3	SAM	D	401	-	21,29,29	1.01	1 (4%)	17,42,42	1.35	1 (5%)
4	SO4	D	402	-	4,4,4	0.91	0	6,6,6	0.23	0
4	SO4	D	403	-	4,4,4	0.17	0	6,6,6	0.23	0
4	SO4	D	404	-	4,4,4	0.12	0	6,6,6	0.11	0
4	SO4	E	401	-	4,4,4	2.68	3 (75%)	6,6,6	0.31	0
3	SAM	F	401	-	21,29,29	1.04	1 (4%)	17,42,42	1.30	1 (5%)
4	SO4	F	402	-	4,4,4	0.19	0	6,6,6	0.12	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	A	401	-	-	0/8/33/33	0/3/3/3
4	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	SO4	B	401	-	-	0/0/0/0	0/0/0/0
3	SAM	C	401	-	-	0/8/33/33	0/3/3/3
4	SO4	C	402	-	-	0/0/0/0	0/0/0/0
3	SAM	D	401	-	-	0/8/33/33	0/3/3/3
4	SO4	D	402	-	-	0/0/0/0	0/0/0/0
4	SO4	D	403	-	-	0/0/0/0	0/0/0/0
4	SO4	D	404	-	-	0/0/0/0	0/0/0/0
4	SO4	E	401	-	-	0/0/0/0	0/0/0/0
3	SAM	F	401	-	-	0/8/33/33	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	F	402	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	SO4	O3-S	2.52	1.56	1.47
4	E	401	SO4	O4-S	3.15	1.58	1.47
4	E	401	SO4	O2-S	3.16	1.58	1.47
3	D	401	SAM	CG-CB	3.86	1.57	1.52
3	C	401	SAM	CG-CB	3.97	1.57	1.52
3	F	401	SAM	CG-CB	4.01	1.57	1.52
3	A	401	SAM	CG-CB	4.44	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	SAM	C4'-O4'-C1'	-4.20	105.10	109.72
3	A	401	SAM	C4'-O4'-C1'	-4.19	105.12	109.72
3	C	401	SAM	C4'-O4'-C1'	-4.03	105.29	109.72
3	F	401	SAM	C4'-O4'-C1'	-3.94	105.39	109.72

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
3	A	401	SAM	1	0
4	E	401	SO4	1	0

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%)	0.12	3 (0%) 85 84	17, 39, 97, 139	0
1	C	338/360 (93%)	0.13	6 (1%) 71 68	12, 51, 115, 157	0
1	D	333/360 (92%)	0.10	5 (1%) 76 74	13, 42, 101, 162	0
1	F	338/360 (93%)	0.30	10 (2%) 54 47	17, 53, 111, 160	0
2	B	245/335 (73%)	0.22	8 (3%) 50 42	27, 59, 106, 151	0
2	E	245/335 (73%)	0.23	6 (2%) 62 57	30, 65, 112, 155	0
2	G	245/335 (73%)	2.02	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%)	0.65	281 (12%) 6 3	12, 60, 169, 275	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	121	LEU	12.0
2	H	84	PRO	10.0
2	G	122	GLN	9.8
2	H	131	PHE	9.5
2	H	85	VAL	9.5
2	G	187	PHE	9.2
2	H	142	CYS	9.1
2	H	278	ASP	8.9
2	G	144	VAL	8.5
2	G	151	LEU	8.5
2	H	294	LEU	8.4
2	H	136	LEU	8.4
2	G	115	VAL	8.3
2	G	83	THR	8.2
2	H	86	VAL	8.2
2	H	88	GLY	8.1

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Mol	Chain	Res	Type	RSRZ
2	G	184	PRO	8.0
2	G	182	CYS	8.0
2	H	113	LEU	7.9
2	G	129	SER	7.8
2	H	90	LEU	7.7
2	G	145	LEU	7.7
2	H	83	THR	7.4
2	H	280	LYS	7.3
2	H	89	SER	7.3
2	G	85	VAL	7.3
2	H	115	VAL	7.3
2	H	157	MET	6.9
2	G	118	GLY	6.8
2	H	87	GLN	6.7
2	G	152	LEU	6.7
2	G	87	GLN	6.6
2	H	243	ILE	6.6
2	H	119	ALA	6.5
2	H	293	ILE	6.5
2	H	242	GLY	6.5
2	H	171	LEU	6.4
2	G	84	PRO	6.4
2	H	112	LEU	6.3
2	G	112	LEU	6.2
2	H	191	GLN	6.2
2	H	253	TYR	6.2
2	H	102	MET	6.0
2	G	108	HIS	6.0
2	G	114	SER	6.0
2	G	138	PRO	5.9
2	H	151	LEU	5.9
2	H	222	VAL	5.8
2	G	90	LEU	5.8
2	H	111	GLU	5.7
2	H	277	PRO	5.7
2	H	176	LEU	5.7
2	H	180	LEU	5.6
2	G	150	GLN	5.6
2	H	104	PHE	5.5
2	G	88	GLY	5.5
2	G	143	VAL	5.5
2	H	116	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
2	G	86	VAL	5.4
2	H	230	LEU	5.3
2	H	306	ALA	5.3
2	H	279	LYS	5.3
2	G	117	ARG	5.3
2	G	181	TYR	5.2
2	G	183	CYS	5.2
2	H	121	LEU	5.2
2	H	120	SER	5.2
2	H	173	GLU	5.2
2	G	198	VAL	5.2
2	H	108	HIS	5.2
2	H	101	ASP	5.1
2	G	92	LEU	5.0
2	G	154	LEU	5.0
2	H	124	LEU	5.0
2	H	248	ILE	5.0
2	H	227	LEU	4.9
2	H	165	TYR	4.9
2	G	127	ILE	4.9
2	H	138	PRO	4.9
2	H	256	TYR	4.9
2	H	96	MET	4.9
2	H	179	VAL	4.8
2	H	305	THR	4.8
2	G	159	MET	4.7
2	H	175	LYS	4.7
2	H	97	SER	4.7
2	G	119	ALA	4.7
2	G	124	LEU	4.6
2	G	139	GLU	4.6
2	G	147	LYS	4.6
2	G	142	CYS	4.6
2	G	111	GLU	4.6
2	H	123	GLN	4.6
2	H	133	LEU	4.6
2	H	295	ARG	4.5
2	G	126	ASP	4.5
2	H	122	GLN	4.5
2	H	254	LEU	4.5
2	H	238	TYR	4.4
2	H	219	CYS	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	103	GLY	4.3
2	G	103	GLY	4.3
2	H	234	PHE	4.3
2	B	83	THR	4.2
2	H	164	SER	4.2
2	H	91	GLU	4.2
2	G	180	LEU	4.1
2	H	140	PRO	4.1
2	H	92	LEU	4.1
2	G	156	ILE	4.1
2	G	202	LYS	4.1
2	H	99	LEU	4.1
2	G	104	PHE	4.1
2	G	140	PRO	4.1
2	G	185	GLU	4.1
2	G	166	LEU	4.0
2	H	178	ARG	4.0
2	G	116	ARG	3.9
2	G	223	LEU	3.9
2	H	288	PRO	3.9
2	H	114	SER	3.9
2	G	186	ILE	3.8
2	H	137	ASN	3.8
2	G	101	ASP	3.8
2	H	118	GLY	3.7
2	H	261	ILE	3.7
2	H	147	LYS	3.7
2	H	273	ARG	3.7
2	H	109	ILE	3.6
2	G	207	PHE	3.6
2	B	278	ASP	3.6
2	G	97	SER	3.6
2	H	98	SER	3.6
2	G	188	THR	3.6
2	G	191	GLN	3.6
2	H	282	GLN	3.6
2	B	291	LYS	3.6
2	H	117	ARG	3.6
2	G	197	THR	3.5
2	G	162	ARG	3.5
2	H	207	PHE	3.5
2	H	229	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	83	TRP	3.5
2	H	143	VAL	3.5
1	C	226	ARG	3.5
1	F	108	LEU	3.5
2	H	281	GLY	3.5
1	F	272	ILE	3.5
2	H	215	ILE	3.5
2	B	280	LYS	3.5
2	H	144	VAL	3.5
1	A	275	ARG	3.4
2	H	128	ILE	3.4
2	H	200	LEU	3.4
2	H	152	LEU	3.4
2	G	205	CYS	3.4
2	G	149	PRO	3.4
1	D	105	HIS	3.4
2	H	107	ALA	3.4
2	H	174	GLY	3.4
2	H	205	CYS	3.3
2	H	146	LYS	3.3
2	G	96	MET	3.3
2	H	290	LEU	3.3
2	G	109	ILE	3.3
2	H	94	ARG	3.3
2	H	202	LYS	3.3
1	A	322	GLN	3.3
2	G	120	SER	3.3
2	H	169	LEU	3.3
2	H	232	TYR	3.3
2	G	107	ALA	3.2
2	G	125	LEU	3.2
2	H	110	ASN	3.2
1	C	384	THR	3.2
2	G	102	MET	3.2
2	G	194	ILE	3.2
1	C	279	LYS	3.2
2	E	138	PRO	3.2
2	G	234	PHE	3.1
2	G	232	TYR	3.1
2	G	131	PHE	3.0
2	G	153	LYS	3.0
2	H	307	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	G	89	SER	3.0
1	D	124	ALA	3.0
2	H	159	MET	3.0
2	G	105	SER	2.9
2	G	158	GLN	2.9
2	G	189	MET	2.9
2	H	177	LYS	2.9
2	G	128	ILE	2.9
2	H	276	THR	2.9
2	G	93	GLU	2.9
2	G	165	TYR	2.9
2	H	145	LEU	2.9
2	G	148	SER	2.9
2	H	198	VAL	2.8
2	G	171	LEU	2.8
2	H	187	PHE	2.8
2	H	203	GLU	2.8
2	G	192	GLN	2.8
2	G	200	LEU	2.8
2	H	150	GLN	2.8
2	E	181	TYR	2.8
2	E	278	ASP	2.8
1	F	82	ALA	2.7
2	H	213	THR	2.7
2	G	95	VAL	2.7
2	H	141	VAL	2.7
2	H	129	SER	2.7
2	H	284	GLN	2.7
2	G	227	LEU	2.6
2	H	149	PRO	2.6
2	G	123	GLN	2.6
1	D	82	ALA	2.6
2	H	95	VAL	2.6
2	H	208	THR	2.6
1	D	119	SER	2.6
2	G	230	LEU	2.6
2	G	155	PRO	2.5
2	H	93	GLU	2.5
2	H	153	LYS	2.5
2	H	168	LYS	2.5
2	B	282	GLN	2.5
2	H	100	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	280	LYS	2.5
2	G	225	GLU	2.5
2	G	113	LEU	2.5
2	G	133	LEU	2.5
2	G	206	LEU	2.5
2	G	137	ASN	2.5
2	G	224	ARG	2.5
2	H	239	PHE	2.5
2	G	110	ASN	2.5
1	F	282	GLN	2.5
2	H	158	GLN	2.5
1	F	105	HIS	2.5
2	H	161	LYS	2.5
2	B	243	ILE	2.4
2	E	104	PHE	2.4
1	D	125	CYS	2.4
2	G	106	ASN	2.4
2	H	241	MET	2.4
2	G	201	LEU	2.4
2	H	289	LEU	2.4
2	H	302	LEU	2.4
2	H	244	LYS	2.4
2	G	91	GLU	2.4
2	E	83	THR	2.4
2	H	195	ASN	2.4
2	G	157	MET	2.4
2	B	84	PRO	2.3
1	F	229	ASN	2.3
2	H	274	TYR	2.3
2	H	192	GLN	2.3
2	H	190	ARG	2.3
2	H	181	TYR	2.3
1	F	161	ALA	2.3
2	G	132	ILE	2.2
2	B	279	LYS	2.2
2	H	252	GLU	2.2
1	F	353	CYS	2.2
2	H	204	LYS	2.2
2	H	125	LEU	2.2
2	G	136	LEU	2.2
1	C	222	PRO	2.1
1	F	278	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	280	LYS	2.1
1	C	270	ASN	2.1
2	H	106	ASN	2.1
2	H	218	SER	2.1
1	C	229	ASN	2.1
2	H	148	SER	2.1
2	H	287	ASN	2.0
2	H	134	LEU	2.0
2	G	100	LEU	2.0
2	G	251	SER	2.0
2	H	166	LEU	2.0
2	H	216	LEU	2.0
1	A	229	ASN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	SAM	C	401	27/27	0.79	0.31	2.67	27,28,40,42	27
3	SAM	A	401	27/27	0.90	0.21	0.26	3,6,9,10	27
3	SAM	F	401	27/27	0.91	0.21	0.17	3,3,10,11	27
3	SAM	D	401	27/27	0.95	0.17	-0.29	3,3,8,9	27
4	SO4	D	402	5/5	0.95	0.15	-1.68	40,40,40,40	0
4	SO4	B	401	5/5	0.93	0.11	-1.86	96,97,97,97	0
4	SO4	A	402	5/5	0.92	0.11	-	77,77,77,77	0
4	SO4	D	403	5/5	0.86	0.14	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SO4	D	404	5/5	0.94	0.13	-	90,90,91,91	0
4	SO4	F	402	5/5	0.84	0.20	-	100,100,101,101	0
4	SO4	C	402	5/5	0.95	0.16	-	79,79,79,79	0
4	SO4	E	401	5/5	0.94	0.25	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.