



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:22 am 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

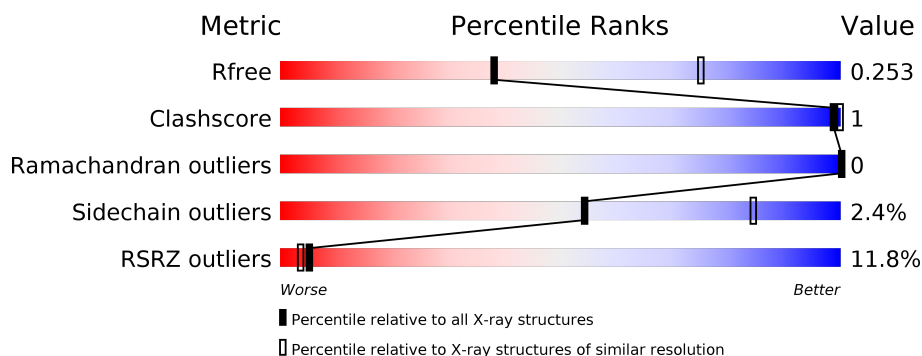
1 Overall quality at a glance

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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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 style="width: 89%;"></div> <div style="width: 6%;"></div> <div style="width: 5%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
1	C	360	<div> <div style="width: 89%;"></div> <div style="width: 6%;"></div> <div style="width: 5%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
1	D	360	<div> <div style="width: 88%;"></div> <div style="width: 8%;"></div> <div style="width: 4%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
1	F	360	<div> <div style="width: 88%;"></div> <div style="width: 6%;"></div> <div style="width: 6%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
2	B	335	<div> <div style="width: 72%;"></div> <div style="width: 27%;"></div> <div style="width: 1%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>
2	E	335	<div> <div style="width: 71%;"></div> <div style="width: 27%;"></div> <div style="width: 2%;"></div> <div style="width: 0%;"></div> <div style="width: 0%;"></div> </div>

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Mol	Chain	Length	Quality of chain
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			

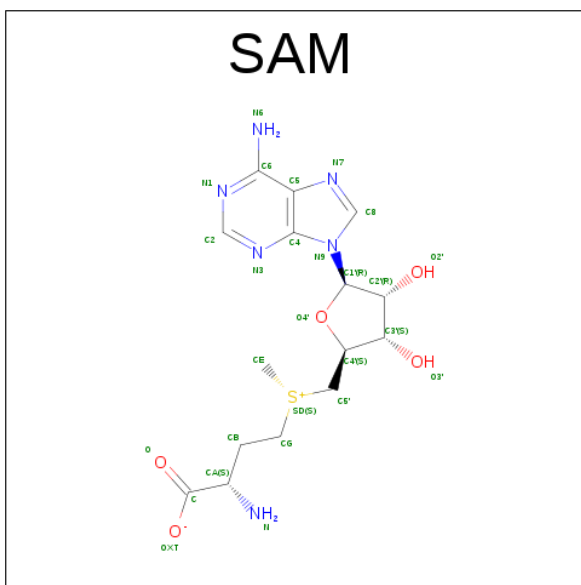
There are 4 discrepancies between the modelled and reference sequences:

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.

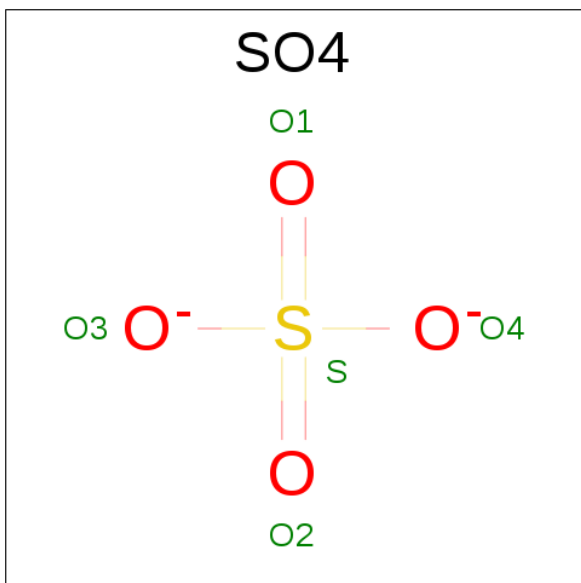
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	E	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	G	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			
2	H	245	Total	C	N	O	S	0	0	0
			1989	1273	344	360	12			

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 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 (three-letter code: SO4) (formula: O₄S).

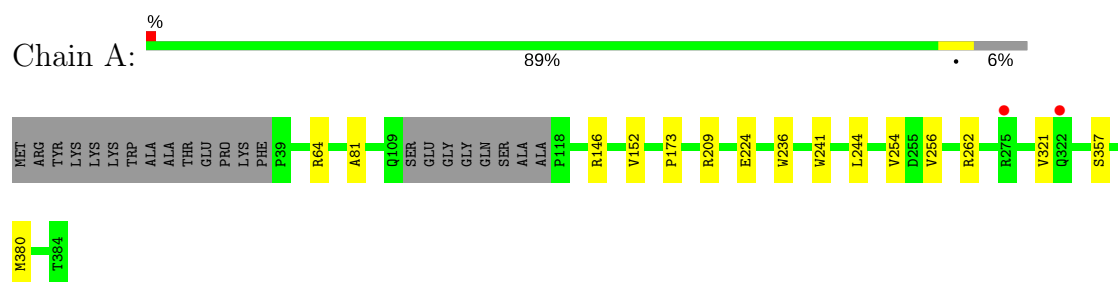


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

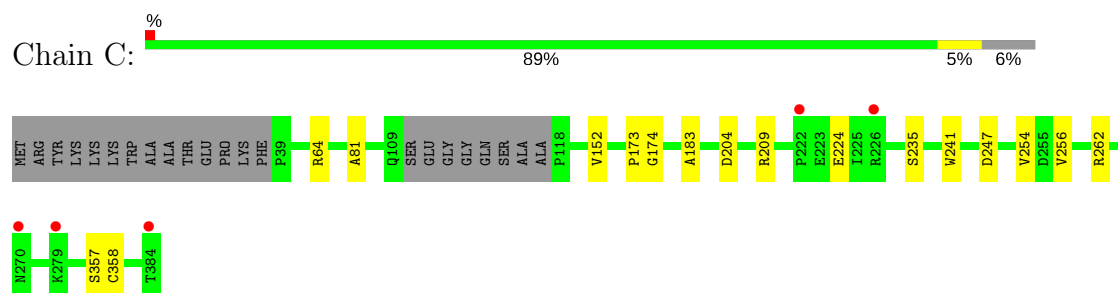
3 Residue-property plots [i](#)

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.

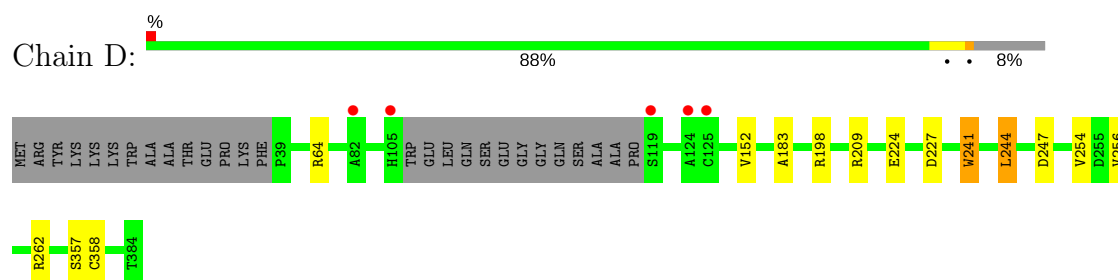
- Molecule 1: methyltransferase NSUN4



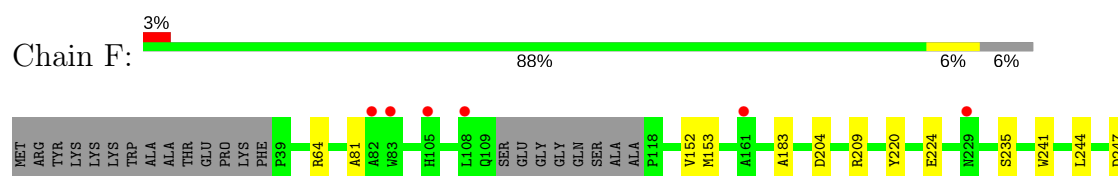
- Molecule 1: methyltransferase NSUN4

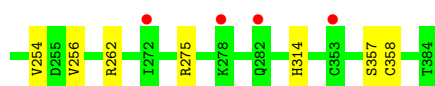


- Molecule 1: methyltransferase NSUN4

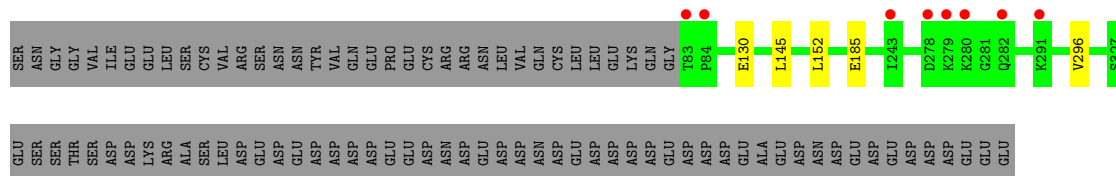
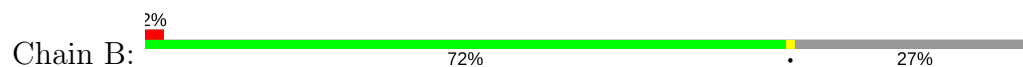


- Molecule 1: methyltransferase NSUN4

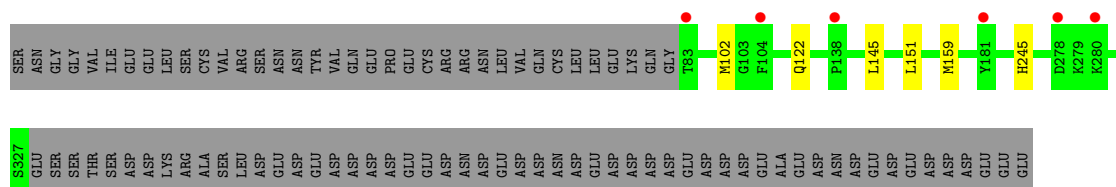




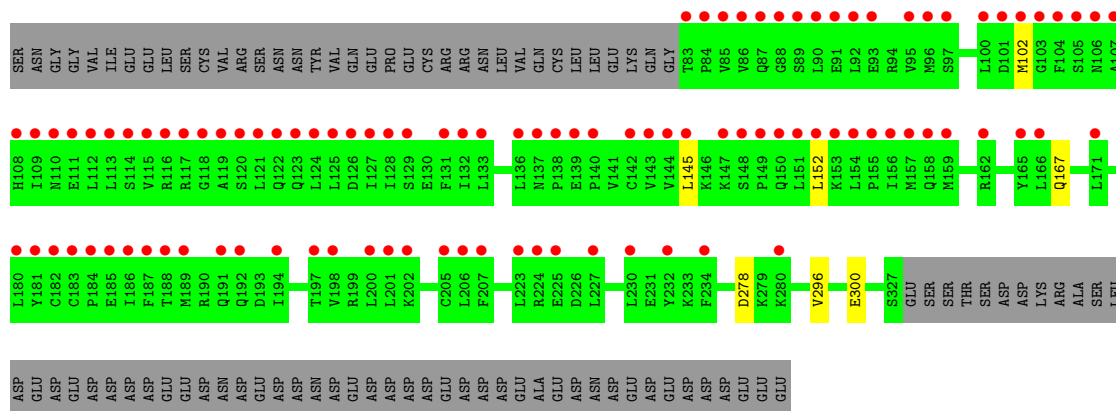
- Molecule 2: mTERF domain-containing protein 2



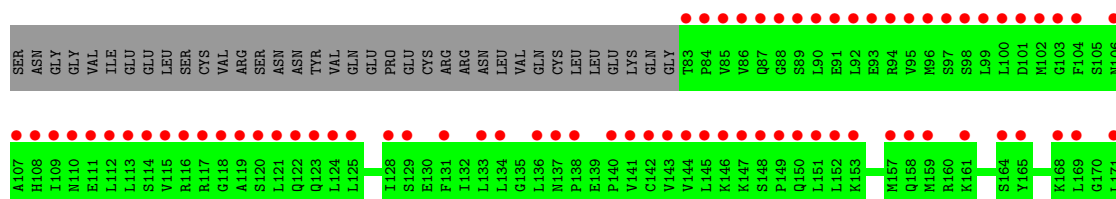
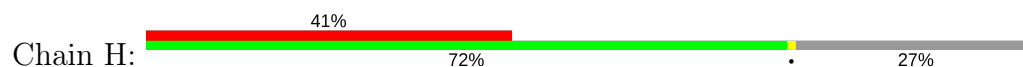
- Molecule 2: mTERF domain-containing protein 2

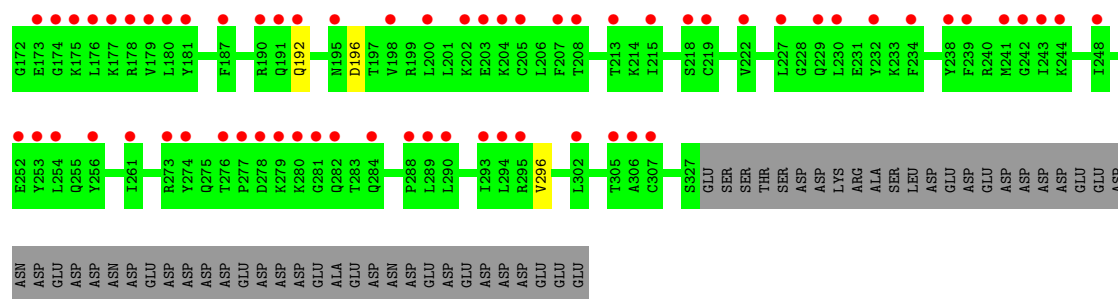


- Molecule 2: mTERF domain-containing protein 2



- 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, α , β , γ	78.76Å 82.27Å 507.57Å 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 2.90Å)	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
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: 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%)	59	86
1	C	292/308 (95%)	285 (98%)	7 (2%)	54	84
1	D	287/308 (93%)	276 (96%)	11 (4%)	38	73
1	F	292/308 (95%)	283 (97%)	9 (3%)	45	79
2	B	227/312 (73%)	224 (99%)	3 (1%)	73	93
2	E	227/312 (73%)	222 (98%)	5 (2%)	57	86
2	G	227/312 (73%)	222 (98%)	5 (2%)	57	86
2	H	227/312 (73%)	224 (99%)	3 (1%)	73	93
All	All	2071/2480 (84%)	2022 (98%)	49 (2%)	54	84

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 [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$
3	SAM	A	401	-	21,29,29	0.75	1 (4%)	17,42,42	1.36	1 (5%)
4	SO4	A	402	-	4,4,4	0.36	0	6,6,6	0.30	0
4	SO4	B	401	-	4,4,4	0.25	0	6,6,6	0.16	0
3	SAM	C	401	-	21,29,29	0.74	0	17,42,42	1.32	1 (5%)
4	SO4	C	402	-	4,4,4	0.44	0	6,6,6	0.20	0
3	SAM	D	401	-	21,29,29	0.72	0	17,42,42	1.34	1 (5%)
4	SO4	D	402	-	4,4,4	0.71	0	6,6,6	0.35	0
4	SO4	D	403	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	D	404	-	4,4,4	0.29	0	6,6,6	0.15	0
4	SO4	E	401	-	4,4,4	1.57	1 (25%)	6,6,6	0.25	0
3	SAM	F	401	-	21,29,29	0.76	0	17,42,42	1.28	1 (5%)
4	SO4	F	402	-	4,4,4	0.28	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	SAM	CG-CB	2.06	1.57	1.52
4	E	401	SO4	O2-S	2.28	1.58	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	SAM	C4'-O4'-C1'	-4.38	105.10	109.77
3	A	401	SAM	C4'-O4'-C1'	-4.37	105.12	109.77
3	C	401	SAM	C4'-O4'-C1'	-4.21	105.29	109.77
3	F	401	SAM	C4'-O4'-C1'	-4.12	105.39	109.77

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%)	0.11	2 (0%) 89 88	17, 39, 97, 139	0
1	C	338/360 (93%)	0.12	5 (1%) 74 72	12, 51, 115, 157	0
1	D	333/360 (92%)	0.08	5 (1%) 74 72	13, 42, 101, 162	0
1	F	338/360 (93%)	0.29	10 (2%) 51 44	17, 53, 111, 160	0
2	B	245/335 (73%)	0.21	8 (3%) 47 40	27, 59, 106, 151	0
2	E	245/335 (73%)	0.21	6 (2%) 59 55	30, 65, 112, 155	0
2	G	245/335 (73%)	1.98	102 (41%) 0 0	27, 131, 222, 275	0
2	H	245/335 (73%)	2.73	137 (55%) 0 0	57, 139, 195, 220	0
All	All	2327/2780 (83%)	0.63	275 (11%) 5 4	12, 60, 169, 275	0

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	121	LEU	11.8
2	H	84	PRO	9.7
2	G	122	GLN	9.5
2	H	85	VAL	9.4
2	H	131	PHE	9.3
2	G	187	PHE	9.1
2	H	142	CYS	8.8
2	H	278	ASP	8.7
2	G	144	VAL	8.4
2	G	151	LEU	8.3
2	H	294	LEU	8.3
2	H	136	LEU	8.2
2	G	115	VAL	8.2
2	H	86	VAL	8.1
2	H	88	GLY	8.1
2	G	83	THR	8.0

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Mol	Chain	Res	Type	RSRZ
2	H	113	LEU	7.8
2	G	184	PRO	7.8
2	G	182	CYS	7.7
2	H	90	LEU	7.6
2	G	129	SER	7.6
2	G	145	LEU	7.6
2	H	83	THR	7.2
2	H	280	LYS	7.2
2	G	85	VAL	7.2
2	H	115	VAL	7.2
2	H	89	SER	7.1
2	H	157	MET	6.7
2	G	118	GLY	6.7
2	G	152	LEU	6.5
2	H	119	ALA	6.5
2	H	87	GLN	6.5
2	H	243	ILE	6.5
2	G	87	GLN	6.4
2	H	242	GLY	6.4
2	H	293	ILE	6.4
2	H	171	LEU	6.3
2	H	112	LEU	6.2
2	G	84	PRO	6.2
2	G	112	LEU	6.1
2	H	253	TYR	6.0
2	H	191	GLN	6.0
2	G	108	HIS	5.9
2	H	102	MET	5.8
2	G	114	SER	5.8
2	H	151	LEU	5.8
2	H	222	VAL	5.8
2	G	138	PRO	5.7
2	G	90	LEU	5.7
2	H	116	ARG	5.7
2	H	176	LEU	5.6
2	H	111	GLU	5.6
2	H	277	PRO	5.5
2	H	180	LEU	5.5
2	G	117	ARG	5.5
2	G	88	GLY	5.4
2	H	104	PHE	5.4
2	G	143	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
2	G	150	GLN	5.4
2	G	86	VAL	5.3
2	H	306	ALA	5.3
2	H	230	LEU	5.3
2	H	279	LYS	5.2
2	H	121	LEU	5.1
2	G	198	VAL	5.1
2	G	181	TYR	5.1
2	H	108	HIS	5.1
2	H	120	SER	5.1
2	H	173	GLU	5.1
2	G	183	CYS	5.0
2	H	101	ASP	5.0
2	G	92	LEU	4.9
2	G	154	LEU	4.9
2	H	124	LEU	4.9
2	H	248	ILE	4.9
2	H	227	LEU	4.8
2	G	127	ILE	4.8
2	H	179	VAL	4.8
2	H	165	TYR	4.8
2	H	256	TYR	4.7
2	H	96	MET	4.7
2	G	119	ALA	4.7
2	H	138	PRO	4.7
2	H	295	ARG	4.7
2	H	305	THR	4.7
2	H	175	LYS	4.6
2	G	159	MET	4.6
2	H	97	SER	4.6
2	G	124	LEU	4.6
2	G	139	GLU	4.5
2	G	147	LYS	4.5
2	H	133	LEU	4.5
2	G	111	GLU	4.5
2	H	123	GLN	4.4
2	H	254	LEU	4.4
2	G	142	CYS	4.4
2	G	126	ASP	4.4
2	H	122	GLN	4.3
2	H	238	TYR	4.3
2	H	103	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	H	219	CYS	4.3
2	G	103	GLY	4.2
2	H	234	PHE	4.2
2	H	164	SER	4.1
2	H	178	ARG	4.1
2	B	83	THR	4.1
2	H	91	GLU	4.1
2	G	180	LEU	4.1
2	H	92	LEU	4.1
2	G	156	ILE	4.1
2	G	116	ARG	4.0
2	G	202	LYS	4.0
2	H	99	LEU	4.0
2	G	104	PHE	4.0
2	H	140	PRO	4.0
2	G	166	LEU	4.0
2	G	185	GLU	4.0
2	G	140	PRO	3.9
2	H	273	ARG	3.8
2	G	223	LEU	3.8
2	G	186	ILE	3.8
2	H	114	SER	3.8
2	H	288	PRO	3.7
2	H	117	ARG	3.7
2	G	162	ARG	3.7
2	H	137	ASN	3.7
2	H	118	GLY	3.7
2	G	101	ASP	3.6
1	C	226	ARG	3.6
2	H	261	ILE	3.6
2	H	147	LYS	3.6
2	H	109	ILE	3.6
1	A	275	ARG	3.6
2	G	207	PHE	3.6
2	G	97	SER	3.5
2	H	98	SER	3.5
2	G	188	THR	3.5
2	B	278	ASP	3.5
2	G	191	GLN	3.5
2	H	143	VAL	3.5
2	B	291	LYS	3.5
2	H	207	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	281	GLY	3.4
1	F	108	LEU	3.4
2	G	197	THR	3.4
2	H	94	ARG	3.4
2	H	282	GLN	3.4
1	F	272	ILE	3.4
2	H	144	VAL	3.4
2	H	107	ALA	3.4
2	H	215	ILE	3.4
2	H	229	GLN	3.4
1	F	83	TRP	3.4
2	B	280	LYS	3.4
2	H	128	ILE	3.4
2	H	200	LEU	3.4
2	H	152	LEU	3.4
2	H	174	GLY	3.3
1	D	105	HIS	3.3
2	G	149	PRO	3.3
2	H	290	LEU	3.3
2	G	205	CYS	3.3
2	G	109	ILE	3.3
2	G	107	ALA	3.3
2	H	146	LYS	3.3
2	G	96	MET	3.2
2	H	202	LYS	3.2
2	H	169	LEU	3.2
2	H	205	CYS	3.2
2	G	120	SER	3.2
2	H	232	TYR	3.2
2	G	125	LEU	3.2
1	A	322	GLN	3.2
2	G	194	ILE	3.1
1	C	384	THR	3.1
2	G	102	MET	3.1
2	H	110	ASN	3.1
1	C	279	LYS	3.1
2	E	138	PRO	3.1
2	G	234	PHE	3.0
2	G	131	PHE	3.0
1	D	124	ALA	3.0
2	G	232	TYR	3.0
2	G	153	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	G	89	SER	2.9
2	H	159	MET	2.9
2	G	128	ILE	2.9
2	H	307	CYS	2.9
2	G	105	SER	2.8
2	H	177	LYS	2.8
2	G	189	MET	2.8
2	H	145	LEU	2.8
2	G	158	GLN	2.8
2	G	93	GLU	2.8
2	H	276	THR	2.8
2	G	165	TYR	2.8
2	H	198	VAL	2.8
2	G	148	SER	2.8
2	G	171	LEU	2.8
2	H	187	PHE	2.8
1	F	82	ALA	2.8
2	G	200	LEU	2.8
2	H	203	GLU	2.7
2	G	192	GLN	2.7
2	G	95	VAL	2.7
2	H	141	VAL	2.7
2	E	181	TYR	2.7
2	H	150	GLN	2.7
2	E	278	ASP	2.7
2	H	213	THR	2.6
2	H	129	SER	2.6
1	D	82	ALA	2.6
2	G	227	LEU	2.6
2	H	284	GLN	2.6
2	H	95	VAL	2.6
2	G	224	ARG	2.6
2	G	230	LEU	2.5
2	H	149	PRO	2.5
2	G	123	GLN	2.5
2	H	208	THR	2.5
1	D	119	SER	2.5
2	H	153	LYS	2.5
2	H	100	LEU	2.5
2	H	93	GLU	2.5
2	H	168	LYS	2.5
2	G	113	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	G	133	LEU	2.5
2	G	155	PRO	2.4
2	G	206	LEU	2.5
2	G	280	LYS	2.4
2	H	239	PHE	2.4
2	B	282	GLN	2.4
1	F	105	HIS	2.4
2	G	225	GLU	2.4
2	B	243	ILE	2.4
2	E	104	PHE	2.4
2	H	161	LYS	2.4
2	G	137	ASN	2.4
2	G	201	LEU	2.4
2	H	289	LEU	2.4
2	H	302	LEU	2.4
1	F	282	GLN	2.4
2	H	158	GLN	2.4
2	G	110	ASN	2.4
2	H	190	ARG	2.4
2	H	241	MET	2.3
2	H	244	LYS	2.3
1	D	125	CYS	2.3
2	G	91	GLU	2.3
2	G	106	ASN	2.3
2	E	83	THR	2.3
2	G	157	MET	2.3
1	F	161	ALA	2.3
2	H	195	ASN	2.3
2	B	84	PRO	2.3
2	H	274	TYR	2.2
1	F	229	ASN	2.2
2	G	132	ILE	2.2
2	H	181	TYR	2.2
2	H	192	GLN	2.2
2	B	279	LYS	2.2
2	H	252	GLU	2.1
2	H	125	LEU	2.1
2	G	136	LEU	2.1
2	H	204	LYS	2.1
1	F	353	CYS	2.1
1	F	278	LYS	2.1
2	E	280	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	222	PRO	2.1
2	H	218	SER	2.0
1	C	270	ASN	2.0
2	H	106	ASN	2.0
2	H	134	LEU	2.0
2	H	148	SER	2.0
2	G	100	LEU	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
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.