



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:07 AM GMT

PDB ID : 3KU1
Title : Crystal structure of Streptococcus pneumoniae Sp1610, a putative tRNA (m1A22) methyltransferase, in complex with S-adenosyl-L-methionine
Authors : Ta, M.H.; Kim, K.K.
Deposited on : 2009-11-26
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

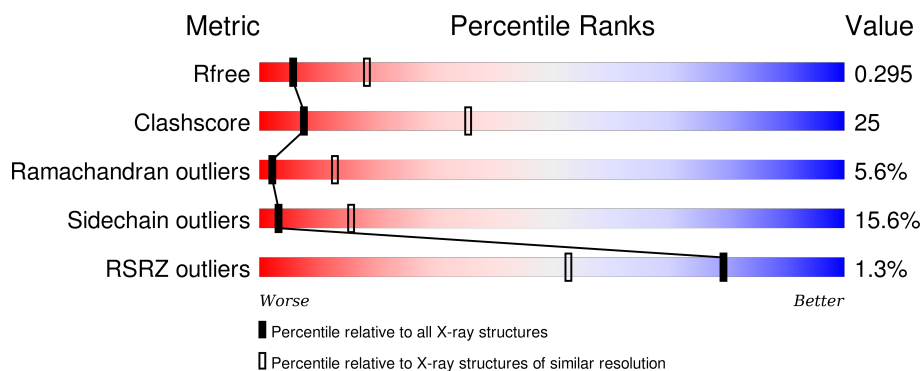
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	225	<div> <div>52%</div> <div>34%</div> <div>8%</div> <div>• 5%</div> </div>
1	B	225	<div> <div>2%</div> <div>46%</div> <div>36%</div> <div>11%</div> <div>• 5%</div> </div>
1	C	225	<div> <div>48%</div> <div>42%</div> <div>• 5%</div> </div>
1	D	225	<div> <div>2%</div> <div>46%</div> <div>35%</div> <div>13%</div> <div>• 5%</div> </div>
1	E	225	<div> <div>2%</div> <div>52%</div> <div>31%</div> <div>12%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	225	
1	G	225	
1	H	225	

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
2	SAM	C	226	-	-	X	-
2	SAM	G	226	-	-	X	-

2 Entry composition

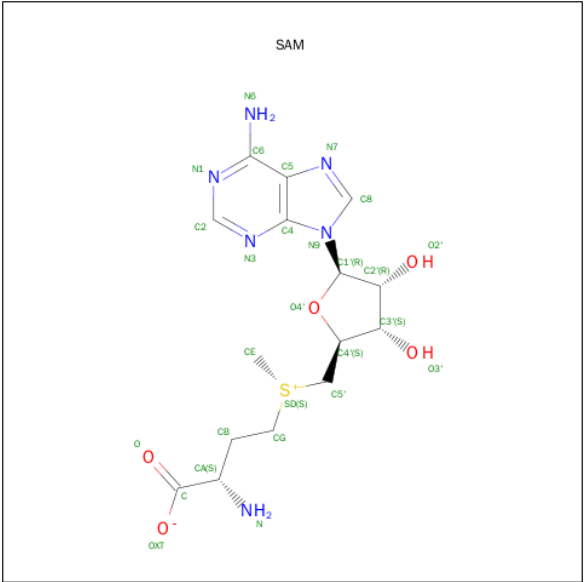
There are 2 unique types of molecules in this entry. The entry contains 13482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SAM-dependent methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1663	1064	283	313	3			
1	B	214	Total	C	N	O	S	0	0	0
			1673	1069	286	315	3			
1	C	214	Total	C	N	O	S	0	0	0
			1673	1069	286	315	3			
1	D	214	Total	C	N	O	S	0	0	0
			1673	1069	286	315	3			
1	E	214	Total	C	N	O	S	0	0	0
			1673	1069	286	315	3			
1	F	214	Total	C	N	O	S	0	0	0
			1673	1069	286	315	3			
1	G	214	Total	C	N	O	S	0	0	0
			1673	1069	286	315	3			
1	H	214	Total	C	N	O	S	0	0	0
			1673	1069	286	315	3			

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).

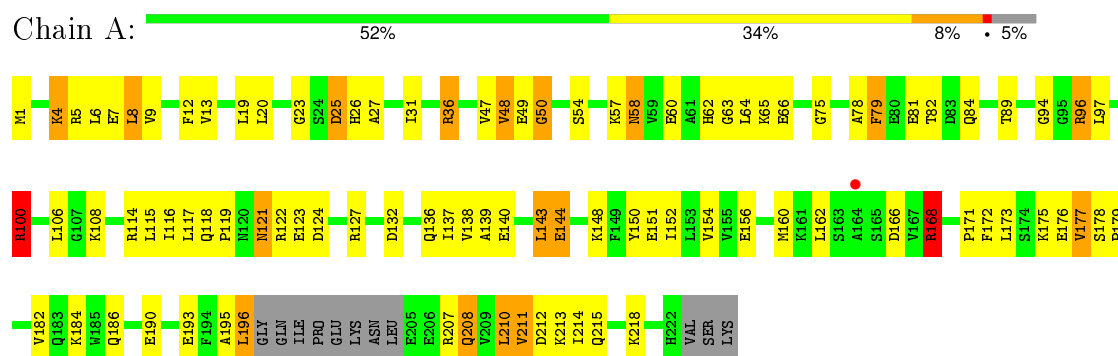


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

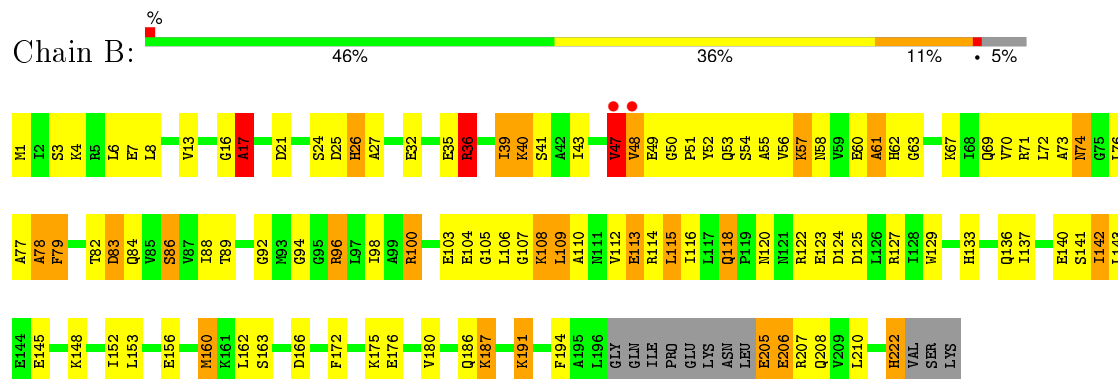
3 Residue-property plots

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: SAM-dependent methyltransferase



• Molecule 1: SAM-dependent methyltransferase



Chain D:

2% 46% 35% 13% 5%

Chain D: A horizontal stacked bar chart showing the distribution of amino acid types. The bar is divided into segments of green (46%), yellow (35%), orange (13%), and red (5%), with a small red segment at the beginning (2%).

Chain E:

52% 31% 12% 5%

M1 I2 S3 K4 E7 L8 Q15 G16 A17 T20 D25 H26 A27 F32 E35 R36 G37 Q38 I39 K40 S41 A42 G45 E46 V47 V48 E49 G50 S54 A55 V56 K57 E60 A61 H62 G63 L64 K65 E66 R71 L72 A73 V74 G75 L76 A77 A78 F79 E80 E81 T82 D83 Q84 H85 S86 E87 L88 T89 G92 A96 L97 R100 I101 I102 V112 E113 A114 L115 I116 I117 Q118 P119 N120 N121 R122 E123 D124 D125 V129 H133 Q136 A137 E140 S141 I142 E145 Y150 E151 I152 L153 E156 M160 L161 K162 L163 S165 D166 V167

Chain F:

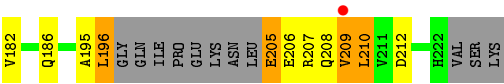
Amino Acid	Count
M1	1
I2	1
S3	1
E7	1
L8	1
S14	1
Q15	1
G16	1
A17	1
I18	1
L19	1
L20	1
D25	1
H26	1
A27	1
V34	1
E35	1
R36	1
I39	1
K40	1
S41	1
A42	1
A43	1
A44	1
G45	1
E46	1
V47	1
V48	1
E49	1
G50	1
P51	1
F52	1
Q53	1
S54	1
A55	1
V56	1
K57	1
M58	1
V59	1
E60	1
A61	1
H62	1
G63	1
L64	1
K65	1
E66	1
K67	1
L68	1
Q69	1
V70	1
R71	1
L72	1
A73	1
H74	1
G75	1
L76	1
A77	1
A78	1
F79	1
E80	1
E81	1
D83	1
K84	1
G85	1
S86	1
H87	1
I88	1
T89	1
G92	1
H93	1
G94	1
G95	1
R96	1
L97	1
I98	1
A99	1
I100	1
L101	1
L102	1
E103	1
E104	1
K108	1
L109	1
LYS	1
ASN	1
LEU	1
M111	1
V112	1
E113	1
R114	1
L115	1
I116	1
L117	1
Q118	1
P119	1
N120	1
N121	1
R122	1
E123	1
D124	1
D125	1
W129	1
D132	1
H133	1
G134	1
I137	1
E140	1
S141	1
I142	1
L143	1
Y150	1
E151	1
I152	1
L153	1
Q159	1
M160	1
K161	1
L162	1
S165	1
D166	1
V167	1
F172	1
K175	1
E176	1
K187	1
K191	1
L196	1
GLY	1
GLN	1
ILE	1
PRO	1
GLU	1
LYS	1
ASN	1
LEU	1
E205	1
E206	1
E207	1
Q208	1
V209	1
L210	1
K213	1
K218	1
L221	1
H222	1
VAL	1
SER	1
LYS	1

Chain G:

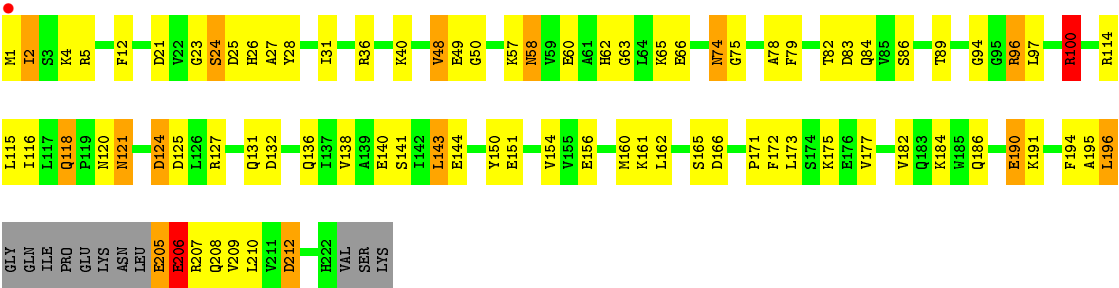
Category	Percentage
Green	55%
Yellow	34%
Red	6%
Grey	5%

Visual representation of Chain G's distribution across 32 nodes (M1 to M32). The nodes are color-coded: Green (55%), Yellow (34%), Red (6%), and Grey (5%).

Node	Color
M1	Yellow
I2	Yellow
S3	Green
K4	Yellow
R5	Yellow
L6	Yellow
E7	Yellow
F12	Yellow
V13	Yellow
G23	Yellow
S24	Yellow
D25	Yellow
H26	Yellow
A27	Yellow
Y28	Yellow
R36	Red
G37	Green
Q38	Yellow
A44	Yellow
G45	Green
E46	Yellow
V47	Yellow
V48	Yellow
A49	Green
G50	Yellow
P51	Yellow
A55	Yellow
V56	Yellow
K57	Yellow
M58	Yellow
V59	Green
E60	Yellow
A61	Green
H62	Yellow
E66	Yellow
G75	Yellow
A78	Yellow
F79	Yellow
E80	Green
H81	Yellow
T82	Yellow
T89	Yellow
G92	Yellow
R96	Red
L97	Yellow
R100	Red
L106	Yellow
L109	Green
A110	Yellow
M111	Yellow
R114	Yellow
L115	Green
L116	Yellow
L117	Yellow
L118	Yellow
P119	Yellow
R122	Yellow
E123	Yellow
D124	Yellow
L125	Green
L126	Green
A127	Yellow
I128	Green
V129	Yellow
L130	Yellow
Q131	Yellow
D132	Yellow
H133	Yellow
I137	Yellow
V138	Yellow
A139	Yellow
E140	Yellow
L143	Yellow
E144	Yellow
E145	Yellow
Y150	Yellow
E151	Yellow
L152	Yellow
L153	Yellow
V154	Yellow
V155	Yellow
E156	Yellow
K161	Yellow
L162	Yellow
S165	Yellow
D166	Yellow
V167	Yellow
R168	Yellow
F169	Yellow
G170	Yellow
P171	Yellow
F172	Yellow
L173	Yellow
S174	Yellow
K175	Yellow
E176	Yellow
V177	Yellow
S178	Yellow



● Molecule 1: SAM-dependent methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	142.75Å 142.75Å 148.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.46 – 3.00 46.73 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.46-3.00) 99.8 (46.73-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.296 0.242 , 0.295	Depositor DCC
R_{free} test set	3411 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
Estimated twinning fraction	0.479 for -h,-k,l 0.480 for h,-h-k,-l 0.479 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 67466 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13482	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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: 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	0.87	2/1685 (0.1%)	0.97	6/2271 (0.3%)
1	B	0.92	0/1695	0.96	2/2283 (0.1%)
1	C	0.88	2/1695 (0.1%)	1.00	6/2283 (0.3%)
1	D	0.94	4/1695 (0.2%)	0.98	2/2283 (0.1%)
1	E	0.91	1/1695 (0.1%)	0.94	0/2283
1	F	0.91	0/1695	0.93	0/2283
1	G	0.90	2/1695 (0.1%)	1.00	6/2283 (0.3%)
1	H	0.88	0/1695	0.98	1/2283 (0.0%)
All	All	0.90	11/13550 (0.1%)	0.97	23/18252 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	H	0	1
All	All	0	5

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	GLU	CG-CD	8.93	1.65	1.51
1	G	81	GLU	CB-CG	5.55	1.62	1.52
1	C	100	ARG	CG-CD	5.51	1.65	1.51
1	A	100	ARG	CG-CD	5.46	1.65	1.51
1	D	159	GLN	CG-CD	5.43	1.63	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	100	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	H	100	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	G	96	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	A	100	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	191	LYS	CD-CE-NZ	-6.73	96.23	111.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17	ALA	Peptide
1	D	206	GLU	Peptide
1	E	206	GLU	Peptide
1	F	17	ALA	Peptide
1	H	206	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1663	0	1705	85	1
1	B	1673	0	1720	98	1
1	C	1673	0	1720	87	0
1	D	1673	0	1720	100	0
1	E	1673	0	1720	100	0
1	F	1673	0	1720	88	1
1	G	1673	0	1720	90	0
1	H	1673	0	1720	62	1
2	A	27	0	22	7	0
2	C	27	0	22	9	0
2	G	27	0	21	18	0
2	H	27	0	22	6	0
All	All	13482	0	13832	693	2

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 25.

The worst 5 of 693 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:96:ARG:HH11	1:A:96:ARG:CB	1.16	1.57
1:A:96:ARG:NH1	1:A:96:ARG:HB2	1.18	1.51
1:G:96:ARG:CB	1:G:96:ARG:HH11	1.28	1.45
1:H:96:ARG:NH1	1:H:96:ARG:HB2	1.31	1.43
1:C:96:ARG:NH1	1:C:96:ARG:HB2	1.22	1.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:B:96:ARG:CD[2_655]	1.87	0.33
1:F:132:ASP:OD1	1:H:58:ASN:OD1[1_554]	2.15	0.05

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	210/225 (93%)	174 (83%)	24 (11%)	12 (6%)	2	12
1	B	210/225 (93%)	176 (84%)	20 (10%)	14 (7%)	1	8
1	C	210/225 (93%)	185 (88%)	17 (8%)	8 (4%)	4	22
1	D	210/225 (93%)	174 (83%)	23 (11%)	13 (6%)	2	10
1	E	210/225 (93%)	168 (80%)	26 (12%)	16 (8%)	1	6
1	F	210/225 (93%)	171 (81%)	24 (11%)	15 (7%)	1	7
1	G	210/225 (93%)	175 (83%)	28 (13%)	7 (3%)	5	26
1	H	210/225 (93%)	179 (85%)	22 (10%)	9 (4%)	3	19
All	All	1680/1800 (93%)	1402 (84%)	184 (11%)	94 (6%)	2	13

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
1	B	17	ALA
1	B	50	GLY
1	B	78	ALA
1	B	109	LEU

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	176/188 (94%)	153 (87%)	23 (13%)	5	22
1	B	178/188 (95%)	147 (83%)	31 (17%)	2	12
1	C	178/188 (95%)	157 (88%)	21 (12%)	6	26
1	D	178/188 (95%)	142 (80%)	36 (20%)	1	8
1	E	178/188 (95%)	149 (84%)	29 (16%)	3	14
1	F	178/188 (95%)	144 (81%)	34 (19%)	2	10
1	G	178/188 (95%)	156 (88%)	22 (12%)	6	24
1	H	178/188 (95%)	152 (85%)	26 (15%)	4	18
All	All	1422/1504 (94%)	1200 (84%)	222 (16%)	3	16

5 of 222 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	168	ARG
1	E	100	ARG
1	H	74	ASN
1	D	186	GLN
1	E	36	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	133	HIS

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Mol	Chain	Res	Type
1	E	118	GLN
1	H	74	ASN
1	E	62	HIS
1	E	133	HIS

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 [i](#)

4 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	$\# Z > 2$
2	SAM	A	226	-	21,29,29	1.57	2 (9%)	17,42,42	2.84	8 (47%)
2	SAM	C	226	-	21,29,29	1.48	3 (14%)	17,42,42	2.83	7 (41%)
2	SAM	G	226	-	21,29,29	1.31	4 (19%)	17,42,42	3.23	4 (23%)
2	SAM	H	226	-	21,29,29	1.42	3 (14%)	17,42,42	3.14	7 (41%)

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
2	SAM	A	226	-	-	0/8/33/33	0/3/3/3
2	SAM	C	226	-	-	0/8/33/33	0/3/3/3
2	SAM	G	226	-	-	0/8/33/33	0/3/3/3
2	SAM	H	226	-	-	0/8/33/33	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	226	SAM	O4'-C4'	-2.31	1.39	1.45
2	H	226	SAM	C4-N3	-2.31	1.32	1.35
2	G	226	SAM	C4-N3	-2.26	1.32	1.35
2	G	226	SAM	C5-N7	-2.26	1.31	1.39
2	C	226	SAM	C5-N7	-2.11	1.32	1.39

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	226	SAM	N3-C2-N1	-9.60	121.54	128.89
2	H	226	SAM	C4'-O4'-C1'	-7.30	101.70	109.72
2	G	226	SAM	C4'-O4'-C1'	-7.01	102.01	109.72
2	C	226	SAM	N3-C2-N1	-6.37	124.01	128.89
2	H	226	SAM	N3-C2-N1	-6.31	124.06	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	226	SAM	7	0
2	C	226	SAM	9	0
2	G	226	SAM	18	0
2	H	226	SAM	6	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	214/225 (95%)	0.28	1 (0%) 91 76	60, 78, 107, 123	0
1	B	214/225 (95%)	0.29	2 (0%) 85 64	55, 79, 116, 131	0
1	C	214/225 (95%)	0.27	1 (0%) 91 76	60, 78, 109, 125	0
1	D	214/225 (95%)	0.36	5 (2%) 64 33	56, 81, 114, 131	0
1	E	214/225 (95%)	0.37	5 (2%) 64 33	55, 80, 120, 134	0
1	F	214/225 (95%)	0.41	6 (2%) 56 27	54, 80, 120, 134	0
1	G	214/225 (95%)	0.24	1 (0%) 91 76	59, 78, 107, 125	0
1	H	214/225 (95%)	0.24	1 (0%) 91 76	60, 78, 109, 125	0
All	All	1712/1800 (95%)	0.31	22 (1%) 79 53	54, 79, 113, 134	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	48	VAL	5.4
1	F	47	VAL	5.0
1	D	47	VAL	4.2
1	B	47	VAL	3.8
1	B	48	VAL	3.5

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(\AA^2)	Q<0.9
2	SAM	G	226	27/27	0.86	0.33	1.24	142,147,156,157	0
2	SAM	H	226	27/27	0.94	0.27	0.28	67,77,81,82	0
2	SAM	C	226	27/27	0.94	0.27	0.20	69,75,81,84	0
2	SAM	A	226	27/27	0.93	0.25	-0.04	64,73,81,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.