



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:07 PM GMT

PDB ID : 5C0O  
Title : m1A58 tRNA methyltransferase mutant - Y78A  
Authors : Degut, C.; Ponchon, L.; Folly-Klan, M.; Barraud, P.; Tisne, C.  
Deposited on : 2015-06-12  
Resolution : 2.62 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

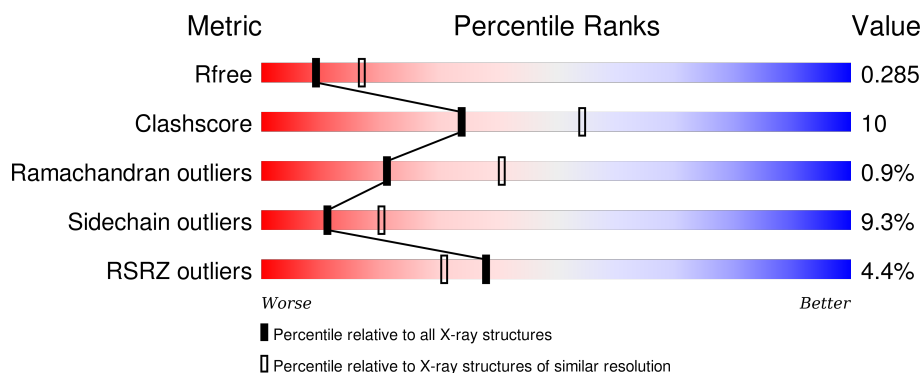
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.62 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	E	255	<div> <div>2%</div> <div>80% 13% 7%</div> </div>
1	F	255	<div> <div>8%</div> <div>63% 22% 6% 9%</div> </div>
1	G	255	<div> <div>4%</div> <div>71% 20% 7%</div> </div>
1	H	255	<div> <div>2%</div> <div>58% 18% 6% 17%</div> </div>

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	F	301	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7264 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.

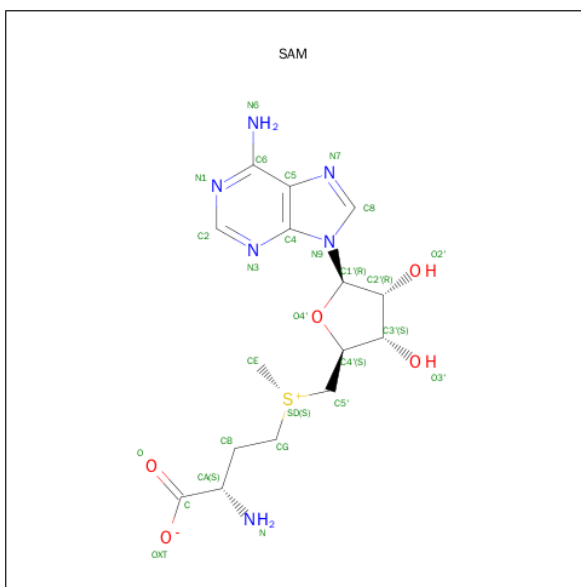
- Molecule 1 is a protein called tRNA (adenine(58)-N(1))-methyltransferase TrmI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	238	Total	C	N	O	S	0	0	0
			1823	1181	317	322	3			
1	F	232	Total	C	N	O	S	0	0	0
			1745	1134	302	306	3			
1	G	237	Total	C	N	O	S	0	0	0
			1819	1176	321	319	3			
1	H	211	Total	C	N	O	S	0	0	0
			1632	1051	293	285	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	78	ALA	TYR	engineered mutation	UNP Q8GBB2
F	78	ALA	TYR	engineered mutation	UNP Q8GBB2
G	78	ALA	TYR	engineered mutation	UNP Q8GBB2
H	78	ALA	TYR	engineered mutation	UNP Q8GBB2

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C<sub>15</sub>H<sub>22</sub>N<sub>6</sub>O<sub>5</sub>S).



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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	O	S	0	0
			5	4	1		

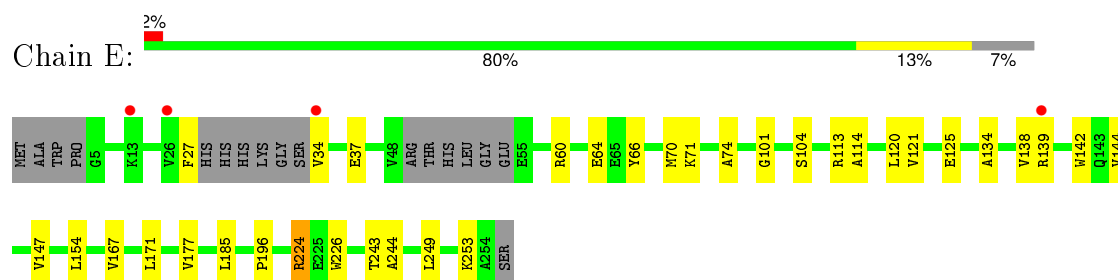
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	44	Total	O		0	0
			44	44			
4	F	27	Total	O		0	0
			27	27			
4	G	36	Total	O		0	0
			36	36			
4	H	25	Total	O		0	0
			25	25			

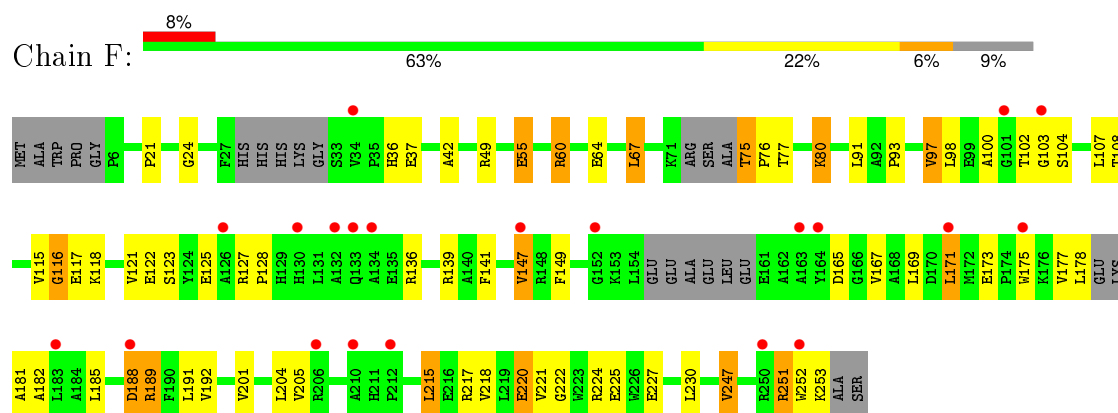
### 3 Residue-property plots [i](#)

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

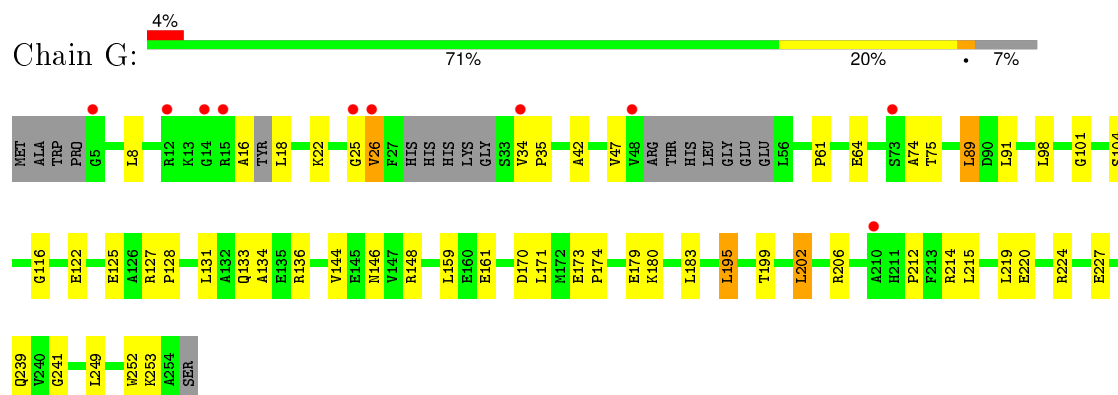
- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI



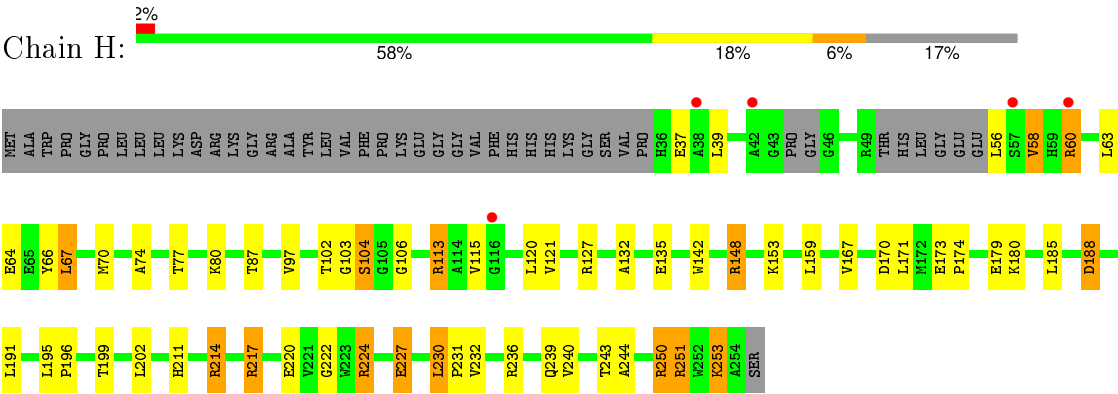
- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI



- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI



- Molecule 1: tRNA (adenine(58)-N(1))-methyltransferase TrmI





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.54Å 79.86Å 184.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.92 – 2.62 52.92 – 2.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) (52.92-2.62) 99.8 (52.92-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.05 (at 2.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.282 0.240 , 0.285	Depositor DCC
$R_{free}$ test set	1709 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 82.0	EDS
Estimated twinning fraction	0.058 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.35$ , $\langle L^2 \rangle = 0.18$	Xtriage
Outliers	1 of 40175 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	7264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 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	E	0.26	0/1867	0.48	0/2541
1	F	0.30	0/1789	0.54	0/2442
1	G	0.27	0/1862	0.50	0/2531
1	H	0.26	0/1670	0.50	0/2270
All	All	0.27	0/7188	0.51	0/9784

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	E	1823	0	1808	20	0
1	F	1745	0	1687	54	0
1	G	1819	0	1814	42	1
1	H	1632	0	1617	38	1
2	E	27	0	19	2	0
2	F	27	0	18	4	0
2	G	27	0	20	3	0
2	H	27	0	22	2	0
3	F	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	44	0	0	7	0
4	F	27	0	0	9	0
4	G	36	0	0	12	1
4	H	25	0	0	5	1
All	All	7264	0	7005	143	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 10.

All (143) 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:G:161:GLU:HG2	1:G:183:LEU:CD1	1.86	1.05
1:G:161:GLU:HG2	1:G:183:LEU:HD11	1.47	0.95
2:G:301:SAM:N	4:G:401:HOH:O	1.99	0.93
1:H:80:LYS:NZ	1:H:243:THR:OG1	2.06	0.89
1:F:42:ALA:O	1:H:253:LYS:NZ	2.05	0.89
1:G:161:GLU:CG	1:G:183:LEU:HD11	2.04	0.87
1:E:114:ALA:O	4:E:401:HOH:O	1.94	0.85
1:G:161:GLU:HG2	1:G:183:LEU:CG	2.08	0.83
1:G:25:GLY:N	4:G:404:HOH:O	2.10	0.82
1:F:218:VAL:HG22	1:F:247:VAL:HG13	1.62	0.80
1:H:148:ARG:NH1	4:H:401:HOH:O	2.05	0.79
1:H:103:GLY:HA3	2:H:301:SAM:HB1	1.66	0.76
1:G:239:GLN:O	4:G:402:HOH:O	2.03	0.76
1:G:144:VAL:O	4:G:403:HOH:O	2.05	0.75
1:F:188:ASP:OD2	1:H:60:ARG:N	2.18	0.75
1:G:18:LEU:N	4:G:405:HOH:O	2.19	0.74
1:H:87:THR:O	4:H:402:HOH:O	2.06	0.74
1:G:161:GLU:HG2	1:G:183:LEU:HG	1.68	0.73
1:G:22:LYS:O	4:G:404:HOH:O	2.05	0.72
1:F:75:THR:N	4:F:404:HOH:O	2.24	0.70
1:G:74:ALA:O	1:G:104:SER:OG	2.09	0.70
1:F:64:GLU:OE2	1:H:217:ARG:NH2	2.25	0.69
1:F:80:LYS:NZ	1:F:221:VAL:O	2.28	0.67
1:F:93:PRO:HG2	1:H:142:TRP:HH2	1.58	0.67
1:F:116:GLY:O	1:F:118:LYS:N	2.27	0.67
1:G:161:GLU:OE2	1:G:183:LEU:HD11	1.95	0.66
1:F:181:ALA:N	4:F:405:HOH:O	2.28	0.65
1:H:66:TYR:O	1:H:70:MET:N	2.28	0.65
1:F:182:ALA:O	4:F:401:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ARG:NH1	4:E:406:HOH:O	2.29	0.64
1:G:133:GLN:OE1	1:G:136:ARG:NH2	2.31	0.63
1:H:167:VAL:HG23	1:H:185:LEU:HD13	1.81	0.63
1:H:97:VAL:CG1	1:H:121:VAL:HG22	2.29	0.62
1:F:222:GLY:N	1:H:222:GLY:O	2.33	0.62
1:E:74:ALA:O	1:E:104:SER:OG	2.19	0.61
1:E:253:LYS:NZ	1:G:42:ALA:O	2.28	0.59
1:F:108:THR:CG2	1:F:147:VAL:HG11	2.33	0.59
1:F:97:VAL:HG13	1:F:121:VAL:HG22	1.84	0.59
1:F:189:ARG:N	4:F:402:HOH:O	2.35	0.59
1:F:169:LEU:CD1	1:F:191:LEU:HD11	2.32	0.59
1:G:161:GLU:CG	1:G:183:LEU:CD1	2.68	0.58
1:F:251:ARG:NH2	1:F:253:LYS:O	2.37	0.57
1:E:226:TRP:NE1	1:G:220:GLU:OE1	2.33	0.57
1:G:220:GLU:OE2	1:H:224:ARG:NH2	2.37	0.57
1:G:161:GLU:CD	1:G:183:LEU:HD11	2.25	0.57
1:G:18:LEU:N	4:G:412:HOH:O	2.37	0.57
1:F:169:LEU:HD12	1:F:191:LEU:HD11	1.87	0.56
1:G:116:GLY:O	1:G:146:ASN:ND2	2.36	0.56
1:F:167:VAL:HG23	1:F:185:LEU:HD12	1.87	0.56
1:H:37:GLU:N	4:H:405:HOH:O	2.37	0.56
1:F:115:VAL:HG21	1:F:121:VAL:HG23	1.88	0.56
1:F:169:LEU:HD23	1:F:171:LEU:HD23	1.88	0.56
1:F:165:ASP:HA	1:F:189:ARG:HG3	1.88	0.55
1:H:97:VAL:HG12	1:H:121:VAL:HG22	1.86	0.55
1:G:133:GLN:HB3	4:G:406:HOH:O	2.06	0.55
1:F:103:GLY:HA3	2:F:301:SAM:H4'	1.89	0.55
1:E:64:GLU:OE2	4:E:403:HOH:O	2.18	0.55
1:F:217:ARG:NH2	1:H:64:GLU:OE1	2.39	0.54
1:E:224:ARG:NH2	1:F:220:GLU:OE2	2.40	0.54
2:F:301:SAM:HE3	4:F:404:HOH:O	2.08	0.54
1:F:125:GLU:OE1	1:F:127:ARG:N	2.41	0.53
2:E:301:SAM:HA	4:E:402:HOH:O	2.08	0.53
1:F:121:VAL:HB	1:F:147:VAL:HG13	1.89	0.53
1:H:179:GLU:OE1	1:H:211:HIS:ND1	2.41	0.53
1:E:154:LEU:HD23	1:E:177:VAL:HG21	1.92	0.52
1:G:215:LEU:HA	1:G:249:LEU:HD23	1.91	0.52
1:G:101:GLY:O	4:G:401:HOH:O	2.18	0.52
1:E:134:ALA:O	1:E:138:VAL:HG23	2.10	0.52
1:E:101:GLY:O	4:E:402:HOH:O	2.17	0.51
1:F:230:LEU:HD21	1:H:202:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:GLY:CA	2:F:301:SAM:H4'	2.40	0.51
1:F:227:GLU:HA	3:F:302:SO4:O4	2.12	0.50
1:H:102:THR:O	2:H:301:SAM:HA	2.12	0.49
1:G:64:GLU:N	4:G:411:HOH:O	2.36	0.49
1:H:74:ALA:O	1:H:104:SER:OG	2.31	0.48
1:F:218:VAL:HG22	1:F:247:VAL:CG1	2.39	0.48
1:G:134:ALA:N	4:G:406:HOH:O	2.45	0.48
1:E:71:LYS:NZ	4:E:409:HOH:O	2.47	0.47
1:H:77:THR:OG1	1:H:170:ASP:OD2	2.32	0.47
1:G:241:GLY:HA3	1:H:239:GLN:HG3	1.96	0.47
1:G:8:LEU:HB2	1:G:61:PRO:HG3	1.97	0.47
1:H:188:ASP:HA	1:H:250:ARG:HD3	1.97	0.46
1:F:189:ARG:O	4:F:402:HOH:O	2.20	0.46
1:H:67:LEU:HD11	1:H:106:GLY:CA	2.46	0.46
1:G:173:GLU:N	1:G:174:PRO:HD3	2.32	0.45
1:G:212:PRO:HA	1:G:252:TRP:CE3	2.52	0.45
1:F:60:ARG:N	1:H:188:ASP:OD2	2.43	0.45
1:F:102:THR:H	1:F:125:GLU:CG	2.30	0.45
1:H:132:ALA:O	1:H:135:GLU:N	2.50	0.45
1:H:39:LEU:HD22	1:H:58:VAL:HG21	1.98	0.45
1:F:185:LEU:HD22	1:F:251:ARG:HG3	1.98	0.44
1:F:201:VAL:O	1:F:204:LEU:N	2.50	0.44
1:F:100:ALA:O	1:F:171:LEU:HD22	2.16	0.44
1:F:139:ARG:NE	4:F:408:HOH:O	2.49	0.44
1:E:27:PHE:O	1:E:34:VAL:N	2.50	0.44
1:F:21:PRO:HB3	1:F:36:HIS:HB3	2.00	0.44
1:G:214:ARG:HG2	1:G:252:TRP:CD1	2.52	0.44
1:G:125:GLU:HB3	1:G:131:LEU:HD13	2.00	0.44
1:F:102:THR:HG1	1:F:123:SER:HG	1.54	0.43
1:G:224:ARG:NH2	4:H:408:HOH:O	2.51	0.43
1:E:125:GLU:OE1	2:E:301:SAM:H1'	2.18	0.43
1:F:107:LEU:HB3	2:F:301:SAM:HN1	1.82	0.43
1:F:191:LEU:HD12	1:F:192:VAL:N	2.33	0.43
1:E:167:VAL:HG23	1:E:185:LEU:HD13	2.00	0.43
1:H:230:LEU:HA	1:H:232:VAL:N	2.33	0.43
1:F:67:LEU:CD2	1:F:76:PRO:HB3	2.47	0.43
1:H:191:LEU:HD23	1:H:191:LEU:C	2.39	0.43
1:H:214:ARG:NE	4:H:406:HOH:O	2.47	0.43
1:E:120:LEU:HG	1:E:121:VAL:N	2.34	0.43
1:F:173:GLU:HG3	1:F:175:TRP:CZ2	2.54	0.42
1:H:115:VAL:HG21	1:H:121:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:LEU:HD12	1:H:173:GLU:H	1.85	0.42
1:F:75:THR:N	4:F:409:HOH:O	2.52	0.42
1:F:49:ARG:HD2	1:F:55:GLU:HA	2.02	0.42
1:E:196:PRO:HA	1:E:244:ALA:HA	2.00	0.42
1:F:224:ARG:HB3	1:H:220:GLU:HB2	2.01	0.42
1:H:185:LEU:HD23	1:H:251:ARG:HB2	2.02	0.42
1:F:108:THR:HG23	1:F:147:VAL:HG11	2.00	0.42
1:F:98:LEU:HB3	1:F:167:VAL:HG13	2.02	0.42
1:F:91:LEU:HB3	4:F:406:HOH:O	2.18	0.42
1:E:142:TRP:CE2	1:E:144:VAL:HB	2.55	0.42
1:E:66:TYR:O	1:E:70:MET:N	2.49	0.42
1:G:26:VAL:HG13	1:G:35:PRO:HA	2.02	0.41
1:E:139:ARG:NE	4:E:411:HOH:O	2.50	0.41
1:G:202:LEU:O	1:G:206:ARG:N	2.51	0.41
1:G:173:GLU:N	1:G:174:PRO:CD	2.83	0.41
1:G:26:VAL:HA	1:G:35:PRO:HA	2.03	0.41
1:H:63:LEU:HD22	1:H:113:ARG:HD3	2.02	0.41
1:G:174:PRO:HG2	1:G:195:LEU:HD21	2.03	0.41
1:F:147:VAL:HB	1:F:149:PHE:CE1	2.56	0.41
1:E:121:VAL:HB	1:E:147:VAL:HG22	2.03	0.41
1:G:89:LEU:HB3	1:G:91:LEU:HG	2.03	0.41
1:H:227:GLU:HG2	1:H:236:ARG:HG2	2.01	0.41
1:H:196:PRO:HA	1:H:244:ALA:HA	2.03	0.41
1:G:170:ASP:OD2	2:G:301:SAM:N	2.54	0.40
1:G:16:ALA:O	4:G:405:HOH:O	2.22	0.40
1:F:252:TRP:O	1:F:253:LYS:CB	2.69	0.40
1:F:201:VAL:O	1:F:205:VAL:HG23	2.21	0.40
1:G:170:ASP:HB3	2:G:301:SAM:HN2	1.85	0.40
1:F:205:VAL:HG13	1:F:215:LEU:CD1	2.52	0.40
1:H:174:PRO:HG2	1:H:195:LEU:HD21	2.04	0.40
1:F:24:GLY:N	1:F:37:GLU:OE2	2.50	0.40
1:G:127:ARG:HA	1:G:128:PRO:HD3	1.96	0.40

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)
4:G:415:HOH:O	4:H:420:HOH:O[4_555]	2.07	0.13
1:G:180:LYS:NZ	1:H:179:GLU:OE2[1_565]	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	E	232/255 (91%)	218 (94%)	14 (6%)	0	100	100
1	F	222/255 (87%)	199 (90%)	16 (7%)	7 (3%)	5	7
1	G	229/255 (90%)	223 (97%)	6 (3%)	0	100	100
1	H	205/255 (80%)	195 (95%)	9 (4%)	1 (0%)	34	58
All	All	888/1020 (87%)	835 (94%)	45 (5%)	8 (1%)	21	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	117	GLU
1	F	128	PRO
1	F	116	GLY
1	F	141	PHE
1	F	188	ASP
1	F	177	VAL
1	F	55	GLU
1	H	231	PRO

### 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	E	179/204 (88%)	173 (97%)	6 (3%)	44	71
1	F	167/204 (82%)	149 (89%)	18 (11%)	8	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	180/204 (88%)	163 (91%)	17 (9%)	11	20
1	H	159/204 (78%)	136 (86%)	23 (14%)	4	6
All	All	685/816 (84%)	621 (91%)	64 (9%)	11	20

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	37	GLU
1	E	60	ARG
1	E	171	LEU
1	E	224	ARG
1	E	243	THR
1	E	249	LEU
1	F	60	ARG
1	F	67	LEU
1	F	75	THR
1	F	77	THR
1	F	80	LYS
1	F	97	VAL
1	F	104	SER
1	F	122	GLU
1	F	136	ARG
1	F	147	VAL
1	F	171	LEU
1	F	178	LEU
1	F	189	ARG
1	F	215	LEU
1	F	220	GLU
1	F	225	GLU
1	F	247	VAL
1	F	251	ARG
1	G	26	VAL
1	G	34	VAL
1	G	47	VAL
1	G	75	THR
1	G	89	LEU
1	G	98	LEU
1	G	122	GLU
1	G	148	ARG
1	G	159	LEU
1	G	171	LEU

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Mol	Chain	Res	Type
1	G	179	GLU
1	G	195	LEU
1	G	199	THR
1	G	202	LEU
1	G	219	LEU
1	G	227	GLU
1	G	253	LYS
1	H	56	LEU
1	H	58	VAL
1	H	60	ARG
1	H	67	LEU
1	H	104	SER
1	H	113	ARG
1	H	120	LEU
1	H	127	ARG
1	H	148	ARG
1	H	153	LYS
1	H	159	LEU
1	H	180	LYS
1	H	188	ASP
1	H	199	THR
1	H	214	ARG
1	H	217	ARG
1	H	224	ARG
1	H	227	GLU
1	H	230	LEU
1	H	240	VAL
1	H	250	ARG
1	H	251	ARG
1	H	253	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	130	HIS
1	G	36	HIS

### 5.3.3 RNA ⓘ

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](#)

5 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	E	301	-	23,29,29	1.06	2 (8%)	15,42,42	3.00	1 (6%)
2	SAM	F	301	-	23,29,29	1.05	2 (8%)	15,42,42	2.94	1 (6%)
3	SO4	F	302	-	4,4,4	1.48	0	6,6,6	1.72	1 (16%)
2	SAM	G	301	-	23,29,29	1.06	2 (8%)	15,42,42	2.98	1 (6%)
2	SAM	H	301	-	23,29,29	1.04	2 (8%)	15,42,42	3.22	2 (13%)

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	E	301	-	-	0/8/33/33	0/3/3/3
2	SAM	F	301	-	-	0/8/33/33	0/3/3/3
3	SO4	F	302	-	-	0/0/0/0	0/0/0/0
2	SAM	G	301	-	-	0/8/33/33	0/3/3/3
2	SAM	H	301	-	-	0/8/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	SAM	C2-N1	2.25	1.38	1.33
2	G	301	SAM	C2-N1	2.35	1.38	1.33
2	E	301	SAM	C2-N1	2.37	1.38	1.33
2	F	301	SAM	C2-N1	2.46	1.38	1.33
2	H	301	SAM	C2-N3	3.42	1.38	1.32
2	E	301	SAM	C2-N3	3.53	1.38	1.32
2	F	301	SAM	C2-N3	3.63	1.38	1.32
2	G	301	SAM	C2-N3	3.63	1.38	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	SAM	N3-C2-N1	-11.82	119.59	128.87
2	E	301	SAM	N3-C2-N1	-11.24	120.04	128.87
2	G	301	SAM	N3-C2-N1	-11.09	120.16	128.87
2	F	301	SAM	N3-C2-N1	-10.96	120.26	128.87
2	H	301	SAM	C1'-N9-C4	-2.99	123.47	126.81
3	F	302	SO4	O4-S-O3	4.04	125.39	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	SAM	2	0
2	F	301	SAM	4	0
3	F	302	SO4	1	0
2	G	301	SAM	3	0
2	H	301	SAM	2	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	E	238/255 (93%)	-0.17	4 (1%) 73 68	12, 29, 58, 82	0
1	F	232/255 (90%)	0.40	21 (9%) 11 7	18, 50, 71, 94	0
1	G	237/255 (92%)	0.04	10 (4%) 40 33	15, 37, 67, 88	0
1	H	211/255 (82%)	0.21	5 (2%) 62 56	21, 40, 65, 80	0
All	All	918/1020 (90%)	0.12	40 (4%) 38 31	12, 40, 67, 94	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	34	VAL	5.6
1	F	212	PRO	4.6
1	F	183	LEU	4.0
1	G	12	ARG	3.9
1	E	13	LYS	3.9
1	F	188	ASP	3.8
1	H	116	GLY	3.8
1	F	34	VAL	3.5
1	G	5	GLY	3.4
1	G	26	VAL	3.4
1	G	48	VAL	3.1
1	F	126	ALA	3.1
1	F	152	GLY	3.1
1	F	175	TRP	3.0
1	F	252	TRP	2.9
1	F	147	VAL	2.7
1	H	57	SER	2.7
1	F	103	GLY	2.6
1	F	206	ARG	2.6
1	H	42	ALA	2.5
1	F	101	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	14	GLY	2.5
1	F	250	ARG	2.5
1	G	210	ALA	2.5
1	F	210	ALA	2.5
1	G	25	GLY	2.4
1	E	34	VAL	2.4
1	F	164	TYR	2.3
1	E	139	ARG	2.3
1	F	163	ALA	2.3
1	G	73	SER	2.2
1	F	134	ALA	2.2
1	F	130	HIS	2.2
1	H	38	ALA	2.2
1	H	60	ARG	2.1
1	F	133	GLN	2.1
1	E	26	VAL	2.1
1	F	132	ALA	2.1
1	F	171	LEU	2.0
1	G	15	ARG	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SAM	F	301	27/27	0.71	0.42	2.62	64,91,107,108	0
2	SAM	G	301	27/27	0.88	0.19	0.60	26,37,57,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SAM	H	301	27/27	0.93	0.18	0.01	29,41,51,59	0
3	SO4	F	302	5/5	0.91	0.19	0.01	32,40,44,83	0
2	SAM	E	301	27/27	0.94	0.15	-0.16	15,26,40,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.