



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:52 AM UTC

PDB ID : 3ID5 / pdb_00003id5
Title : Crystal structure of Sulfolobus solfataricus C/D RNP assembled with Nop5, fibrillarin, L7Ae and a split half C/D RNA
Authors : Ye, K.
Deposited on : 2009-07-20
Resolution : 4.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

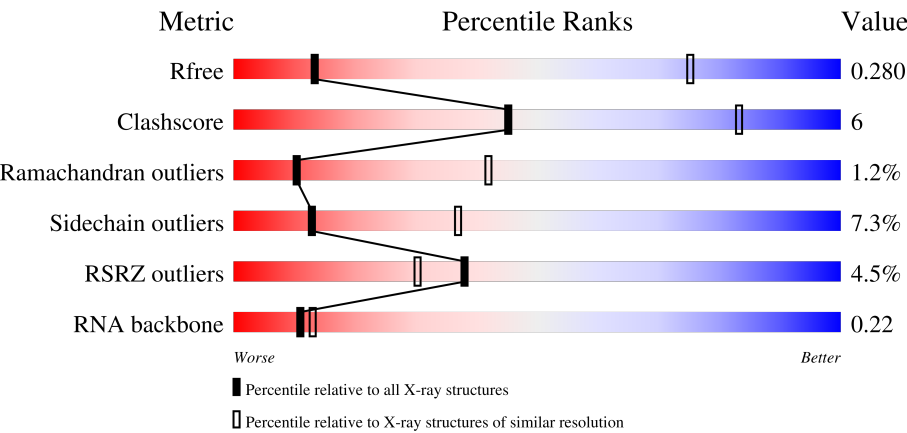
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1095 (4.24-3.80)
Clashscore	190562	1142 (4.24-3.80)
Ramachandran outliers	187476	1074 (4.24-3.80)
Sidechain outliers	187428	1065 (4.24-3.80)
RSRZ outliers	180081	1095 (4.24-3.80)
RNA backbone	3983	1017 (4.84-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	388	3% 79%14% . .
1	E	388	7% 78%15% . .
2	B	232	4% 70%23% . .
2	F	232	2% 68%25% . .

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Mol	Chain	Length	Quality of chain
3	C	130	2% 82% 10% • 8%
3	G	130	5% 82% 10% • 8%
4	D	35	6% 37% 37% 23% •
4	H	35	6% 31% 49% 14% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12730 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 Pre mRNA splicing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2931	1864	511	551	5			
1	E	371	Total	C	N	O	S	0	0	0
			2931	1864	511	551	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	MET	engineered mutation	UNP Q97ZH3
A	381	HIS	-	expression tag	UNP Q97ZH3
A	382	HIS	-	expression tag	UNP Q97ZH3
A	383	HIS	-	expression tag	UNP Q97ZH3
A	384	HIS	-	expression tag	UNP Q97ZH3
A	385	HIS	-	expression tag	UNP Q97ZH3
A	386	HIS	-	expression tag	UNP Q97ZH3
A	387	HIS	-	expression tag	UNP Q97ZH3
A	388	HIS	-	expression tag	UNP Q97ZH3
E	2	VAL	MET	engineered mutation	UNP Q97ZH3
E	381	HIS	-	expression tag	UNP Q97ZH3
E	382	HIS	-	expression tag	UNP Q97ZH3
E	383	HIS	-	expression tag	UNP Q97ZH3
E	384	HIS	-	expression tag	UNP Q97ZH3
E	385	HIS	-	expression tag	UNP Q97ZH3
E	386	HIS	-	expression tag	UNP Q97ZH3
E	387	HIS	-	expression tag	UNP Q97ZH3
E	388	HIS	-	expression tag	UNP Q97ZH3

- Molecule 2 is a protein called Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	223	Total	C	N	O	S	0	0	0
			1796	1156	302	334	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	223	Total	C	N	O	S	0	0	0
			1796	1156	302	334	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	SER	engineered mutation	UNP P58032
F	2	ALA	SER	engineered mutation	UNP P58032

- Molecule 3 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	120	Total	C	N	O	S	0	0	0
			911	578	153	178	2			
3	G	120	Total	C	N	O	S	0	0	0
			911	578	153	178	2			

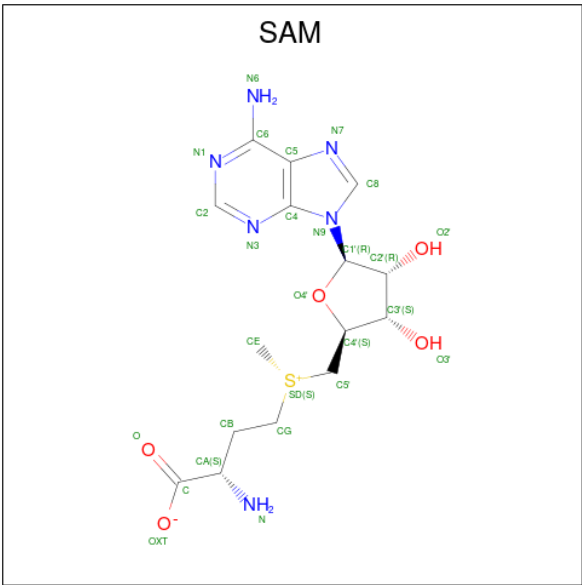
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	expression tag	UNP P55858
C	2	ASP	-	expression tag	UNP P55858
C	3	ALA	-	expression tag	UNP P55858
G	1	MET	-	expression tag	UNP P55858
G	2	ASP	-	expression tag	UNP P55858
G	3	ALA	-	expression tag	UNP P55858

- Molecule 4 is a RNA chain called half C/D RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	34	Total	C	N	O	P	0	0	0
			700	309	121	236	34			
4	H	34	Total	C	N	O	P	0	0	0
			700	309	121	236	34			

- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).

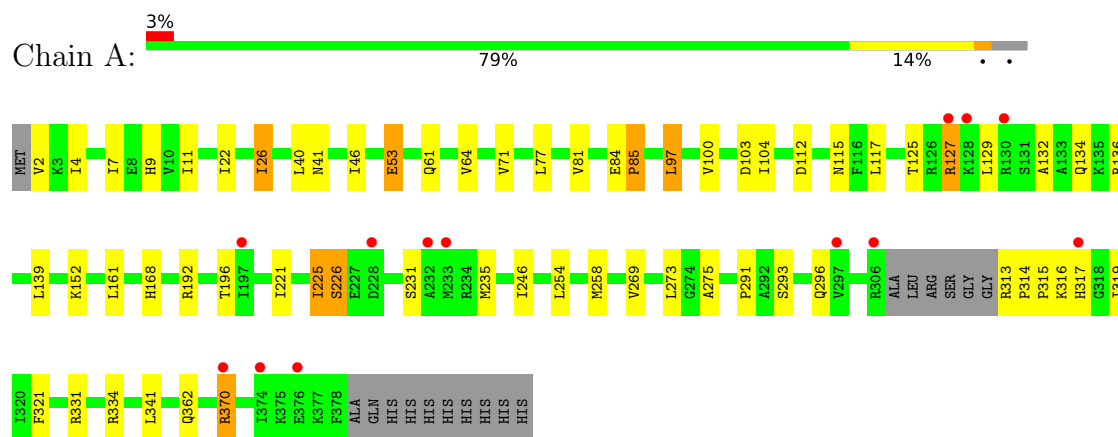


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
5	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

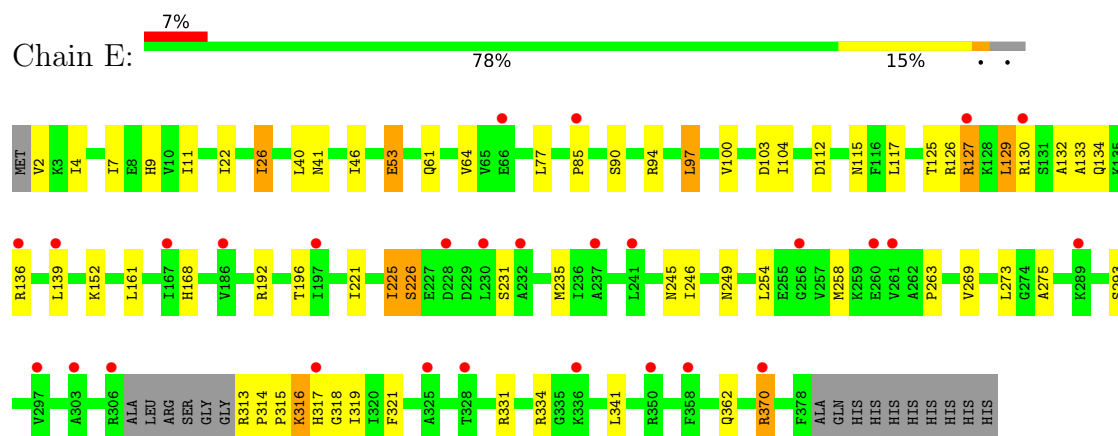
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

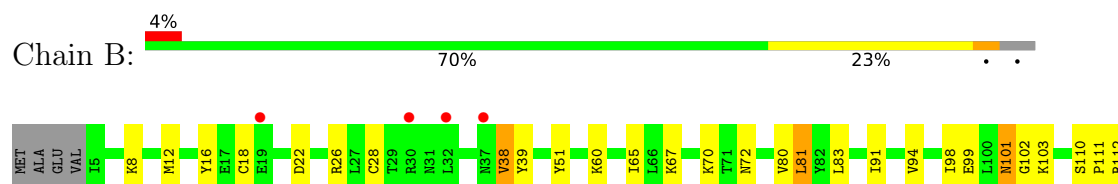
• Molecule 1: Pre mRNA splicing protein

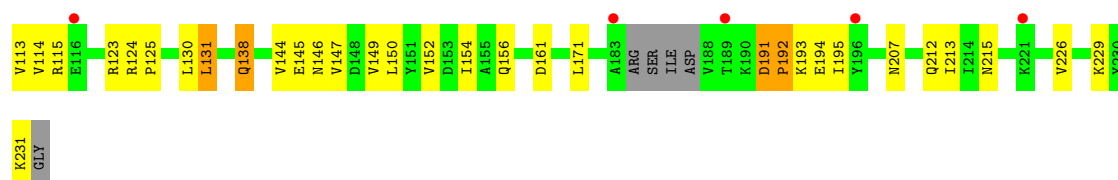


• Molecule 1: Pre mRNA splicing protein

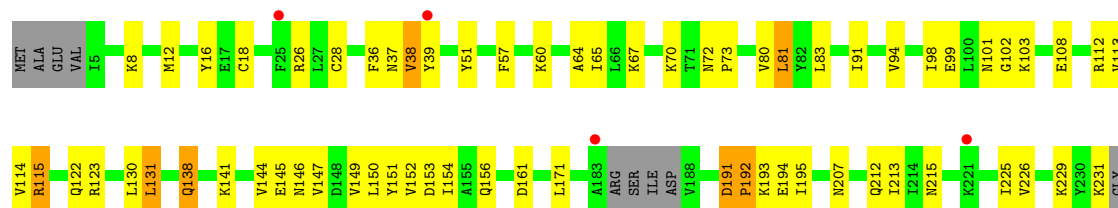


• Molecule 2: Fibrillarin-like rRNA/tRNA 2'-O-methyltransferase

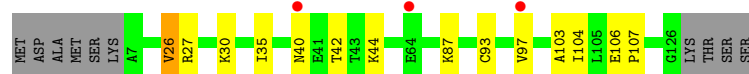
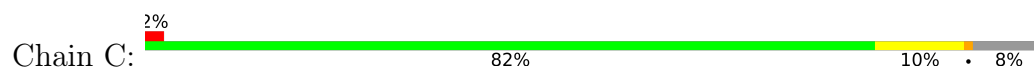




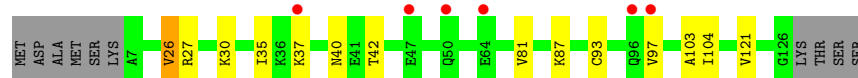
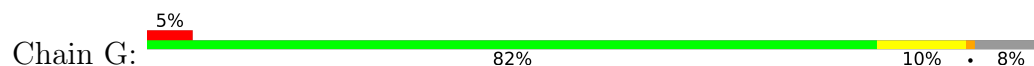
- Molecule 2: Fibrillar-like rRNA/tRNA 2'-O-methyltransferase



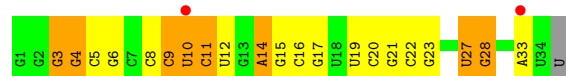
- Molecule 3: 50S ribosomal protein L7Ae



- Molecule 3: 50S ribosomal protein L7Ae



- Molecule 4: half C/D RNA



- Molecule 4: half C/D RNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	265.49Å 265.49Å 129.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.01 20.00 – 4.01	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-4.01) 95.7 (20.00-4.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 4.07Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.285 , 0.304 0.267 , 0.280	Depositor DCC
R_{free} test set	1888 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	135.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 196.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12730	wwPDB-VP
Average B, all atoms (Å ²)	166.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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

5.1 Standard geometry

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	0.39	0/2977	0.84	5/4021 (0.1%)
1	E	0.39	0/2977	0.84	5/4021 (0.1%)
2	B	0.41	0/1829	0.77	0/2474
2	F	0.41	0/1829	0.77	0/2474
3	C	0.45	0/920	0.76	0/1239
3	G	0.45	0/920	0.76	0/1239
4	D	0.60	0/780	1.18	10/1214 (0.8%)
4	H	0.58	0/780	1.08	8/1214 (0.7%)
All	All	0.43	0/13012	0.86	28/17896 (0.2%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	22	C	O3'-P-O5'	-13.63	83.56	104.00
4	D	22	C	O3'-P-O5'	-13.41	83.89	104.00
4	D	10	U	O3'-P-O5'	-13.01	84.48	104.00
4	H	8	C	O3'-P-O5'	9.14	117.72	104.00
4	D	8	C	O3'-P-O5'	8.99	117.49	104.00
4	H	12	U	OP1-P-OP2	-8.87	93.00	119.60
4	D	12	U	OP1-P-OP2	-8.69	93.52	119.60
1	E	314	PRO	CA-C-N	7.98	129.82	119.84
1	E	314	PRO	C-N-CA	7.98	129.82	119.84
4	H	9	C	O5'-P-OP2	-7.89	84.33	108.00
1	A	314	PRO	CA-C-N	7.89	129.70	119.84
1	A	314	PRO	C-N-CA	7.89	129.70	119.84
4	D	9	C	O5'-P-OP1	-7.33	86.02	108.00
4	D	22	C	OP2-P-O3'	-6.88	87.35	108.00
4	H	22	C	OP2-P-O3'	-6.66	88.03	108.00
1	E	313	ARG	CA-C-N	6.57	127.15	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	313	ARG	C-N-CA	6.57	127.15	120.38
4	H	22	C	OP1-P-O3'	-6.51	88.46	108.00
1	A	313	ARG	CA-C-N	6.50	127.07	120.38
1	A	313	ARG	C-N-CA	6.50	127.07	120.38
4	D	10	U	OP2-P-O3'	-6.23	89.31	108.00
4	D	14	A	P-O3'-C3'	5.84	128.96	120.20
4	H	14	A	P-O3'-C3'	5.79	128.88	120.20
1	E	136	ARG	N-CA-C	-5.55	108.29	114.62
4	D	10	U	OP1-P-O3'	-5.49	91.53	108.00
4	D	22	C	OP1-P-O3'	-5.36	91.92	108.00
1	A	136	ARG	N-CA-C	-5.31	108.56	114.62
4	H	27	U	P-O3'-C3'	5.18	127.97	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2931	0	2951	35	0
1	E	2931	0	2951	39	0
2	B	1796	0	1828	30	0
2	F	1796	0	1828	44	0
3	C	911	0	961	10	0
3	G	911	0	961	9	0
4	D	700	0	351	6	0
4	H	700	0	351	5	0
5	B	27	0	22	0	0
5	F	27	0	22	0	0
All	All	12730	0	12226	148	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 6.

All (148) 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:125:THR:HG21	2:B:130:LEU:HA	1.47	0.96
1:A:26:ILE:HD12	1:A:53:GLU:HB3	1.64	0.80
1:E:125:THR:HG21	2:F:130:LEU:HA	1.62	0.79
1:E:26:ILE:HD12	1:E:53:GLU:HB3	1.64	0.78
1:E:249:ASN:HB2	2:F:38:VAL:HG11	1.69	0.74
1:A:168:HIS:HB2	1:A:225:ILE:HD12	1.70	0.73
1:E:168:HIS:HB2	1:E:225:ILE:HD12	1.71	0.72
2:B:138:GLN:HE21	2:B:138:GLN:H	1.41	0.69
2:F:70:LYS:H	2:F:212:GLN:HE22	1.41	0.69
2:F:12:MET:HE1	2:F:65:ILE:HG12	1.75	0.68
2:F:138:GLN:HE21	2:F:138:GLN:H	1.39	0.68
2:B:70:LYS:H	2:B:212:GLN:HE22	1.42	0.68
1:A:293:SER:H	3:C:40:ASN:HD21	1.45	0.65
2:B:12:MET:HE1	2:B:65:ILE:HG12	1.78	0.63
2:B:80:VAL:HG12	2:B:149:VAL:HB	1.80	0.63
2:B:12:MET:HE3	2:B:72:ASN:HB2	1.79	0.63
1:E:331:ARG:HA	1:E:334:ARG:HE	1.64	0.63
2:F:80:VAL:HG12	2:F:149:VAL:HB	1.81	0.63
2:F:12:MET:HE3	2:F:72:ASN:HB2	1.80	0.63
4:H:3:G:H2'	4:H:4:G:H8	1.65	0.62
1:E:90:SER:HB2	2:F:141:LYS:NZ	2.14	0.62
1:E:370:ARG:NH2	4:H:29:A:OP1	2.34	0.61
1:A:40:LEU:HD11	1:A:127:ARG:HG2	1.83	0.61
1:A:125:THR:CG2	2:B:130:LEU:HA	2.26	0.61
1:A:331:ARG:HA	1:A:334:ARG:HE	1.66	0.61
4:D:3:G:H2'	4:D:4:G:H8	1.65	0.61
1:E:90:SER:HB2	2:F:141:LYS:HZ3	1.67	0.60
2:B:114:VAL:HG21	2:B:131:LEU:HD12	1.84	0.60
3:G:30:LYS:HE2	3:G:93:CYS:HA	1.84	0.60
3:C:30:LYS:HE2	3:C:93:CYS:HA	1.83	0.59
1:A:226:SER:HB3	2:F:112:ARG:HG3	1.85	0.59
2:B:28:CYS:SG	2:B:51:TYR:HB3	2.43	0.58
2:F:114:VAL:HG21	2:F:131:LEU:HD12	1.85	0.58
2:F:28:CYS:SG	2:F:51:TYR:HB3	2.44	0.58
1:E:40:LEU:HD11	1:E:127:ARG:HG2	1.84	0.58
2:B:22:ASP:HA	2:F:57:PHE:CZ	2.38	0.57
2:B:154:ILE:HG22	2:B:156:GLN:HG2	1.86	0.57
2:F:83:LEU:HD12	2:F:152:VAL:HG22	1.87	0.57
2:F:154:ILE:HG22	2:F:156:GLN:HG2	1.87	0.57
1:A:291:PRO:HG3	3:C:44:LYS:HG2	1.87	0.56
1:A:100:VAL:HA	1:A:103:ASP:HB2	1.87	0.56
3:C:42:THR:HG23	3:C:103:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:THR:CG2	2:F:130:LEU:HA	2.35	0.55
1:E:132:ALA:C	1:E:134:GLN:H	2.13	0.55
1:E:130:ARG:CZ	1:E:263:PRO:HG3	2.37	0.55
1:A:235:MET:HE2	1:E:246:ILE:HG12	1.89	0.55
2:F:38:VAL:HG12	2:F:39:TYR:N	2.21	0.55
1:A:246:ILE:HG12	1:E:235:MET:HE2	1.89	0.55
2:B:16:TYR:HB2	2:B:28:CYS:HB3	1.89	0.54
1:A:139:LEU:HD21	1:E:225:ILE:HD11	1.89	0.54
1:A:225:ILE:HD11	1:E:139:LEU:HD21	1.88	0.54
1:E:100:VAL:HA	1:E:103:ASP:HB2	1.88	0.54
2:B:83:LEU:HD12	2:B:152:VAL:HG22	1.89	0.54
2:F:16:TYR:HB2	2:F:28:CYS:HB3	1.89	0.53
3:G:42:THR:HG23	3:G:103:ALA:HB2	1.89	0.53
1:A:258:MET:HE3	1:A:275:ALA:HB2	1.91	0.53
2:F:12:MET:HE3	2:F:72:ASN:CB	2.40	0.52
1:A:11:ILE:HB	1:A:104:ILE:HD11	1.92	0.52
2:B:12:MET:HE3	2:B:72:ASN:CB	2.39	0.52
1:E:11:ILE:HB	1:E:104:ILE:HD11	1.93	0.51
3:G:30:LYS:CE	3:G:93:CYS:HA	2.41	0.51
1:E:9:HIS:HD2	1:E:11:ILE:HG12	1.75	0.51
2:B:192:PRO:HB3	2:B:195:ILE:HD12	1.93	0.51
1:E:126:ARG:NH2	2:F:122:GLN:HE21	2.09	0.51
1:E:293:SER:H	3:G:40:ASN:HD21	1.59	0.51
1:E:258:MET:HE3	1:E:275:ALA:HB2	1.93	0.50
1:E:112:ASP:HA	1:E:115:ASN:HB2	1.94	0.50
1:E:41:ASN:HB3	1:E:46:ILE:HB	1.94	0.50
1:A:41:ASN:HB3	1:A:46:ILE:HB	1.94	0.50
3:C:30:LYS:CE	3:C:93:CYS:HA	2.41	0.50
1:A:9:HIS:HD2	1:A:11:ILE:HG12	1.77	0.49
1:E:129:LEU:HD11	2:F:115:ARG:HD2	1.94	0.49
2:F:145:GLU:HG2	2:F:146:ASN:N	2.27	0.49
1:A:112:ASP:HA	1:A:115:ASN:HB2	1.93	0.49
2:B:145:GLU:HG2	2:B:146:ASN:N	2.27	0.49
2:F:81:LEU:HB2	2:F:147:VAL:HG21	1.94	0.49
1:A:293:SER:H	3:C:40:ASN:ND2	2.11	0.48
1:A:296:GLN:NE2	4:D:11:C:H41	2.12	0.48
2:F:192:PRO:HB3	2:F:195:ILE:HD12	1.94	0.48
1:E:94:ARG:HH22	2:F:141:LYS:NZ	2.11	0.48
4:D:27:U:H4'	4:D:28:G:OP2	2.12	0.48
1:E:132:ALA:C	1:E:134:GLN:N	2.70	0.48
1:A:2:VAL:HB	1:A:61:GLN:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:HIS:CE1	1:E:97:LEU:HD11	2.48	0.48
2:B:213:ILE:HG12	2:B:226:VAL:HG22	1.96	0.48
1:A:254:LEU:HD11	1:A:275:ALA:HB2	1.96	0.47
3:G:27:ARG:HA	3:G:30:LYS:HD2	1.96	0.47
2:B:81:LEU:HB2	2:B:147:VAL:HG21	1.97	0.47
4:H:27:U:H4'	4:H:28:G:OP2	2.15	0.47
1:E:254:LEU:HD11	1:E:275:ALA:HB2	1.96	0.47
1:A:226:SER:HB3	2:F:112:ARG:HA	1.96	0.47
1:A:132:ALA:C	1:A:134:GLN:H	2.23	0.47
2:B:38:VAL:HG12	2:B:39:TYR:N	2.30	0.47
3:C:27:ARG:HA	3:C:30:LYS:HD2	1.96	0.47
2:B:193:LYS:HD3	2:B:194:GLU:HG2	1.98	0.46
1:E:269:VAL:HB	1:E:273:LEU:HD23	1.98	0.46
2:F:193:LYS:HD3	2:F:194:GLU:HG2	1.98	0.46
1:E:245:ASN:HB3	2:F:38:VAL:HG13	1.96	0.46
2:F:213:ILE:HG12	2:F:226:VAL:HG22	1.96	0.46
1:E:2:VAL:HB	1:E:61:GLN:HG2	1.98	0.45
1:A:9:HIS:CE1	1:A:97:LEU:HD11	2.51	0.45
3:G:37:LYS:HG3	4:H:26:G:C8	2.52	0.45
1:A:168:HIS:NE2	1:A:192:ARG:HG3	2.32	0.45
2:B:18:CYS:SG	2:B:28:CYS:SG	3.15	0.45
2:F:36:PHE:HB3	2:F:37:ASN:H	1.56	0.45
2:B:112:ARG:HG3	1:E:226:SER:HB3	2.00	0.44
1:E:245:ASN:CB	2:F:38:VAL:HG13	2.47	0.44
1:A:235:MET:HE3	2:F:39:TYR:HB3	2.00	0.44
1:A:269:VAL:HB	1:A:273:LEU:HD23	1.99	0.44
2:B:191:ASP:N	2:B:192:PRO:CD	2.80	0.44
2:F:98:ILE:HG23	2:F:102:GLY:HA3	1.99	0.44
2:F:191:ASP:N	2:F:192:PRO:CD	2.81	0.44
2:F:207:ASN:OD1	2:F:207:ASN:N	2.50	0.44
3:G:35:ILE:HG22	3:G:104:ILE:HA	2.00	0.43
4:D:16:C:H2'	4:D:17:G:H8	1.84	0.43
1:E:9:HIS:CD2	1:E:11:ILE:HG12	2.54	0.43
1:E:168:HIS:NE2	1:E:192:ARG:HG3	2.33	0.43
2:B:207:ASN:OD1	2:B:207:ASN:N	2.51	0.42
4:D:3:G:H2'	4:D:4:G:C8	2.51	0.42
1:A:370:ARG:HH22	4:D:28:G:H5''	1.84	0.42
3:C:106:GLU:HA	3:C:107:PRO:HD3	1.91	0.42
2:F:70:LYS:N	2:F:212:GLN:HE22	2.13	0.42
1:A:226:SER:HB3	2:F:112:ARG:CG	2.48	0.42
4:H:16:C:H2'	4:H:17:G:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:26:VAL:HG12	3:C:30:LYS:HE3	2.01	0.42
2:B:110:SER:HA	2:B:111:PRO:HD3	1.90	0.42
2:F:108:GLU:HG3	2:F:114:VAL:HG23	2.01	0.42
3:C:35:ILE:HG22	3:C:104:ILE:HA	2.01	0.42
3:G:26:VAL:HG12	3:G:30:LYS:HE3	2.00	0.42
2:F:73:PRO:HB2	2:F:149:VAL:CG2	2.49	0.41
2:B:98:ILE:HG23	2:B:102:GLY:HA3	2.01	0.41
2:F:18:CYS:SG	2:F:28:CYS:SG	3.17	0.41
1:A:231:SER:O	1:A:235:MET:HG3	2.20	0.41
2:B:101:ASN:HD22	2:B:101:ASN:HA	1.69	0.41
1:E:316:LYS:O	1:E:318:GLY:N	2.53	0.41
1:A:71:VAL:HA	1:A:81:VAL:HG11	2.02	0.41
1:A:84:GLU:HA	1:A:85:PRO:HD3	1.91	0.41
1:E:231:SER:O	1:E:235:MET:HG3	2.20	0.41
2:F:98:ILE:HG22	2:F:99:GLU:O	2.20	0.41
2:B:98:ILE:HG22	2:B:99:GLU:O	2.21	0.41
2:B:207:ASN:O	2:B:231:LYS:HG2	2.20	0.41
1:E:127:ARG:HE	1:E:127:ARG:HB2	1.70	0.41
2:F:64:ALA:HB2	2:F:225:ILE:HD12	2.03	0.41
2:F:151:TYR:CE2	2:F:153:ASP:HB2	2.55	0.41
1:A:9:HIS:CD2	1:A:11:ILE:HG12	2.56	0.40
2:F:207:ASN:O	2:F:231:LYS:HG2	2.19	0.40
2:B:124:ARG:HA	2:B:125:PRO:HD3	1.85	0.40
3:G:81:VAL:HG22	3:G:121:VAL:HG11	2.03	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	367/388 (95%)	341 (93%)	22 (6%)	4 (1%)	11 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	367/388 (95%)	342 (93%)	20 (5%)	5 (1%)	9	39
2	B	219/232 (94%)	196 (90%)	19 (9%)	4 (2%)	6	34
2	F	219/232 (94%)	197 (90%)	18 (8%)	4 (2%)	6	34
3	C	118/130 (91%)	117 (99%)	1 (1%)	0	100	100
3	G	118/130 (91%)	117 (99%)	1 (1%)	0	100	100
All	All	1408/1500 (94%)	1310 (93%)	81 (6%)	17 (1%)	10	42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	PRO
1	A	316	LYS
1	A	317	HIS
1	E	315	PRO
1	E	316	LYS
1	E	317	HIS
1	A	85	PRO
1	E	85	PRO
2	B	38	VAL
1	E	133	ALA
2	F	38	VAL
2	B	192	PRO
2	F	192	PRO
2	B	191	ASP
2	F	191	ASP
2	B	144	VAL
2	F	144	VAL

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	307/330 (93%)	285 (93%)	22 (7%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	307/330 (93%)	285 (93%)	22 (7%)	13	37
2	B	198/205 (97%)	179 (90%)	19 (10%)	8	28
2	F	198/205 (97%)	179 (90%)	19 (10%)	8	28
3	C	98/107 (92%)	95 (97%)	3 (3%)	35	57
3	G	98/107 (92%)	95 (97%)	3 (3%)	35	57
All	All	1206/1284 (94%)	1118 (93%)	88 (7%)	13	37

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	7	ILE
1	A	22	ILE
1	A	26	ILE
1	A	53	GLU
1	A	64	VAL
1	A	77	LEU
1	A	97	LEU
1	A	117	LEU
1	A	127	ARG
1	A	129	LEU
1	A	152	LYS
1	A	161	LEU
1	A	196	THR
1	A	221	ILE
1	A	225	ILE
1	A	226	SER
1	A	319	ILE
1	A	321	PHE
1	A	341	LEU
1	A	362	GLN
1	A	370	ARG
2	B	8	LYS
2	B	26	ARG
2	B	60	LYS
2	B	67	LYS
2	B	81	LEU
2	B	91	ILE
2	B	94	VAL
2	B	101	ASN

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Mol	Chain	Res	Type
2	B	103	LYS
2	B	113	VAL
2	B	115	ARG
2	B	123	ARG
2	B	131	LEU
2	B	138	GLN
2	B	150	LEU
2	B	161	ASP
2	B	171	LEU
2	B	215	ASN
2	B	229	LYS
3	C	26	VAL
3	C	87	LYS
3	C	97	VAL
1	E	4	ILE
1	E	7	ILE
1	E	22	ILE
1	E	26	ILE
1	E	53	GLU
1	E	64	VAL
1	E	77	LEU
1	E	97	LEU
1	E	117	LEU
1	E	127	ARG
1	E	129	LEU
1	E	152	LYS
1	E	161	LEU
1	E	196	THR
1	E	221	ILE
1	E	225	ILE
1	E	226	SER
1	E	319	ILE
1	E	321	PHE
1	E	341	LEU
1	E	362	GLN
1	E	370	ARG
2	F	8	LYS
2	F	26	ARG
2	F	60	LYS
2	F	67	LYS
2	F	81	LEU
2	F	91	ILE

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Mol	Chain	Res	Type
2	F	94	VAL
2	F	101	ASN
2	F	103	LYS
2	F	113	VAL
2	F	115	ARG
2	F	123	ARG
2	F	131	LEU
2	F	138	GLN
2	F	150	LEU
2	F	161	ASP
2	F	171	LEU
2	F	215	ASN
2	F	229	LYS
3	G	26	VAL
3	G	87	LYS
3	G	97	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	59	ASN
1	A	251	ASN
1	A	296	GLN
2	B	31	ASN
2	B	101	ASN
2	B	138	GLN
2	B	156	GLN
2	B	174	ASN
2	B	212	GLN
2	B	215	ASN
3	C	40	ASN
1	E	9	HIS
1	E	59	ASN
1	E	109	ASN
1	E	251	ASN
1	E	296	GLN
2	F	31	ASN
2	F	101	ASN
2	F	122	GLN
2	F	138	GLN
2	F	156	GLN

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Mol	Chain	Res	Type
2	F	174	ASN
2	F	212	GLN
2	F	215	ASN
3	G	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	32/35 (91%)	16 (50%)	5 (15%)
4	H	32/35 (91%)	16 (50%)	4 (12%)
All	All	64/70 (91%)	32 (50%)	9 (14%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	3	G
4	D	4	G
4	D	5	C
4	D	6	G
4	D	9	C
4	D	10	U
4	D	11	C
4	D	14	A
4	D	15	G
4	D	19	U
4	D	20	C
4	D	21	G
4	D	23	G
4	D	27	U
4	D	28	G
4	D	33	A
4	H	3	G
4	H	4	G
4	H	5	C
4	H	6	G
4	H	9	C
4	H	10	U
4	H	11	C
4	H	14	A
4	H	15	G
4	H	19	U

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Mol	Chain	Res	Type
4	H	20	C
4	H	21	G
4	H	23	G
4	H	27	U
4	H	28	G
4	H	33	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	9	C
4	D	10	U
4	D	14	A
4	D	20	C
4	D	27	U
4	H	9	C
4	H	14	A
4	H	20	C
4	H	27	U

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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
5	SAM	B	301	-	27,29,29	1.17	4 (14%)	34,42,42	2.07	10 (29%)
5	SAM	F	301	-	27,29,29	1.16	4 (14%)	34,42,42	2.08	10 (29%)

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
5	SAM	B	301	-	-	4/17/33/33	0/3/3/3
5	SAM	F	301	-	-	4/17/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	SAM	C2-N3	2.87	1.39	1.33
5	F	301	SAM	C2-N3	2.85	1.39	1.33
5	B	301	SAM	C2-N1	2.79	1.38	1.33
5	F	301	SAM	C2-N1	2.69	1.38	1.33
5	B	301	SAM	OXT-C	-2.27	1.23	1.30
5	F	301	SAM	OXT-C	-2.27	1.23	1.30
5	B	301	SAM	C8-N7	2.09	1.35	1.31
5	F	301	SAM	C8-N7	2.08	1.35	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	SAM	N3-C2-N1	-5.61	120.09	128.58
5	F	301	SAM	N3-C2-N1	-5.59	120.12	128.58
5	F	301	SAM	C5-C4-N3	-5.07	119.73	126.72
5	B	301	SAM	C5-C4-N3	-5.02	119.80	126.72
5	F	301	SAM	C2-N3-C4	3.66	120.76	111.83
5	B	301	SAM	C2-N3-C4	3.62	120.67	111.83
5	F	301	SAM	N9-C8-N7	-3.39	109.12	113.94
5	B	301	SAM	N9-C8-N7	-3.39	109.13	113.94
5	F	301	SAM	C5-N7-C8	3.37	108.74	103.45
5	B	301	SAM	C5-N7-C8	3.32	108.67	103.45
5	F	301	SAM	N3-C4-N9	3.31	132.80	127.17
5	B	301	SAM	N3-C4-N9	3.27	132.72	127.17
5	B	301	SAM	OXT-C-O	-3.26	116.69	124.08
5	F	301	SAM	OXT-C-O	-3.02	117.22	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	301	SAM	O4'-C1'-N9	2.92	113.70	108.09
5	B	301	SAM	O4'-C1'-N9	2.82	113.51	108.09
5	F	301	SAM	C4-C5-N7	-2.44	107.79	110.58
5	B	301	SAM	C4-C5-N7	-2.38	107.86	110.58
5	B	301	SAM	C6-C5-C4	2.03	119.95	117.18
5	F	301	SAM	C6-C5-C4	2.01	119.92	117.18

There are no chirality outliers.

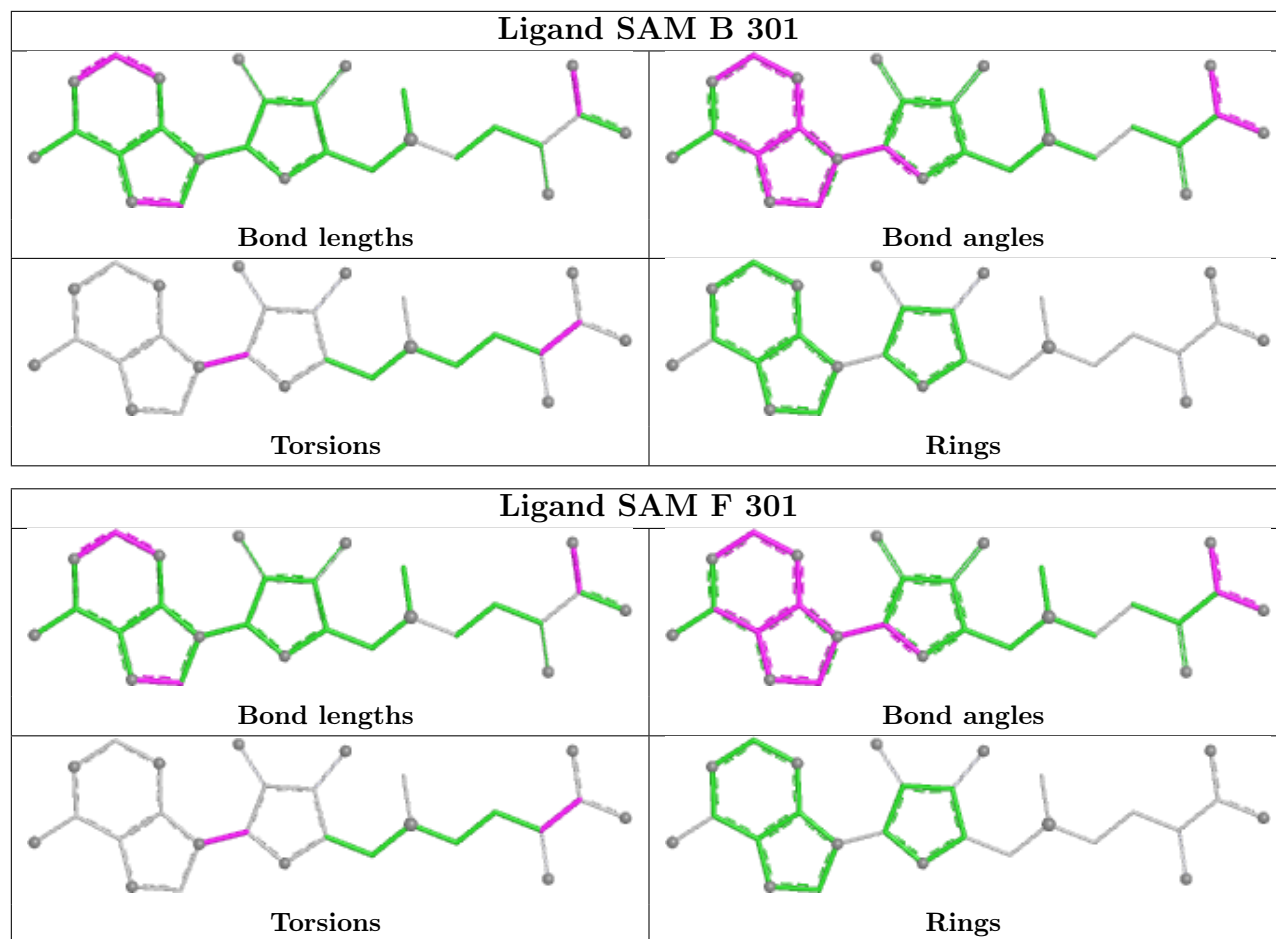
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	SAM	O-C-CA-N
5	F	301	SAM	O-C-CA-N
5	B	301	SAM	OXT-C-CA-N
5	F	301	SAM	OXT-C-CA-N
5	B	301	SAM	C2'-C1'-N9-C8
5	F	301	SAM	C2'-C1'-N9-C8
5	B	301	SAM	O4'-C1'-N9-C8
5	F	301	SAM	O4'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	371/388 (95%)	0.44	13 (3%) 47 35	63, 206, 210, 251	0
1	E	371/388 (95%)	0.70	28 (7%) 20 20	63, 206, 210, 251	0
2	B	223/232 (96%)	0.18	9 (4%) 42 33	58, 103, 180, 211	1 (0%)
2	F	223/232 (96%)	0.14	4 (1%) 67 50	58, 103, 180, 211	1 (0%)
3	C	120/130 (92%)	0.53	3 (2%) 58 43	207, 209, 210, 210	0
3	G	120/130 (92%)	0.46	6 (5%) 34 28	207, 209, 210, 210	0
4	D	34/35 (97%)	0.85	2 (5%) 28 25	207, 211, 281, 283	0
4	H	34/35 (97%)	0.86	2 (5%) 28 25	207, 211, 281, 283	0
All	All	1496/1570 (95%)	0.45	67 (4%) 38 30	58, 205, 210, 283	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	HIS	6.2
1	E	228	ASP	5.1
3	C	64	GLU	4.9
1	A	306	ARG	4.9
2	F	183	ALA	4.0
1	E	306	ARG	4.0
2	B	183	ALA	3.8
1	A	127	ARG	3.7
1	E	303	ALA	3.7
4	D	10	U	3.6
1	E	317	HIS	3.5
2	B	37	ASN	3.4
4	H	33	A	3.2
4	D	33	A	3.1
3	G	37	LYS	3.1
1	A	370	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	228	ASP	3.0
2	B	221	LYS	3.0
1	A	297	VAL	3.0
1	E	297	VAL	3.0
2	B	196	TYR	2.9
3	G	96	GLN	2.9
2	B	32	LEU	2.9
1	E	370	ARG	2.8
3	G	97	VAL	2.8
1	E	237	ALA	2.7
1	E	139	LEU	2.7
2	F	221	LYS	2.6
1	E	358	PHE	2.6
3	G	64	GLU	2.6
1	E	197	ILE	2.6
1	E	66	GLU	2.6
3	G	50	GLN	2.6
2	F	39	TYR	2.6
1	E	241	LEU	2.5
3	C	40	ASN	2.5
1	E	350	ARG	2.4
1	A	128	LYS	2.4
1	E	230	LEU	2.4
1	A	233	MET	2.3
1	A	197	ILE	2.3
2	B	189	THR	2.3
2	B	116	GLU	2.3
1	E	336	LYS	2.3
1	A	232	ALA	2.3
3	C	97	VAL	2.3
1	E	127	ARG	2.3
1	E	325	ALA	2.2
3	G	47	GLU	2.2
1	A	376	GLU	2.2
1	E	260	GLU	2.2
1	A	130	ARG	2.2
1	E	130	ARG	2.2
1	E	232	ALA	2.2
1	E	261	VAL	2.2
1	E	289	LYS	2.2
1	E	136	ARG	2.2
2	B	19	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	328	THR	2.1
2	F	25	PHE	2.1
1	E	256	GLY	2.1
1	A	374	ILE	2.1
1	E	85	PRO	2.1
1	E	167	ILE	2.1
2	B	30	ARG	2.1
4	H	11	C	2.1
1	E	186	VAL	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

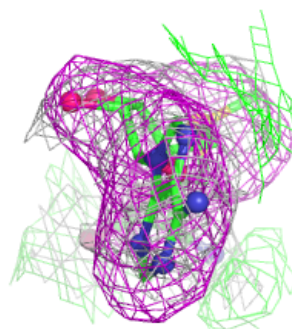
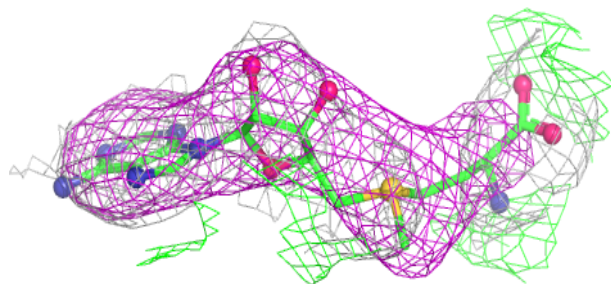
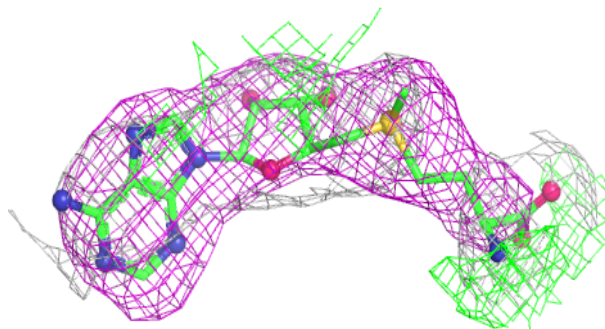
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SAM	B	301	27/27	0.55	0.27	145,145,146,147	0
5	SAM	F	301	27/27	0.60	0.28	145,145,146,147	0

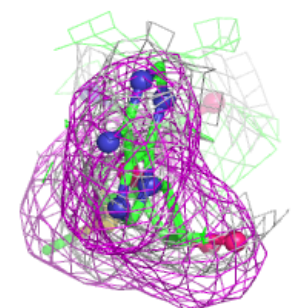
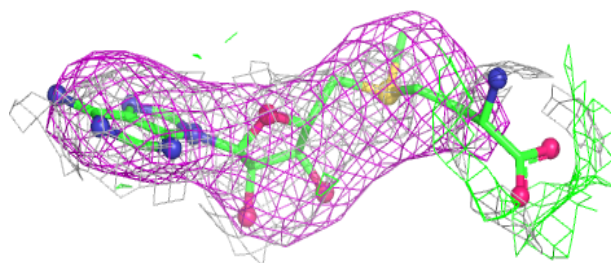
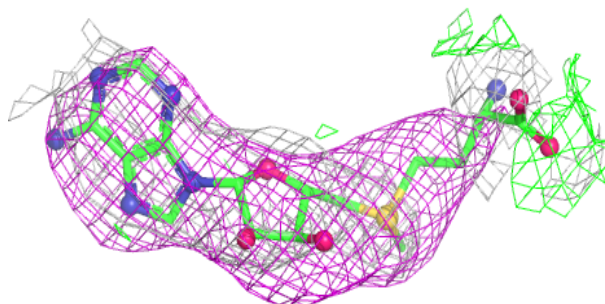
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAM B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SAM F 301:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.