



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:08 am GMT

PDB ID : 3ID5
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

<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

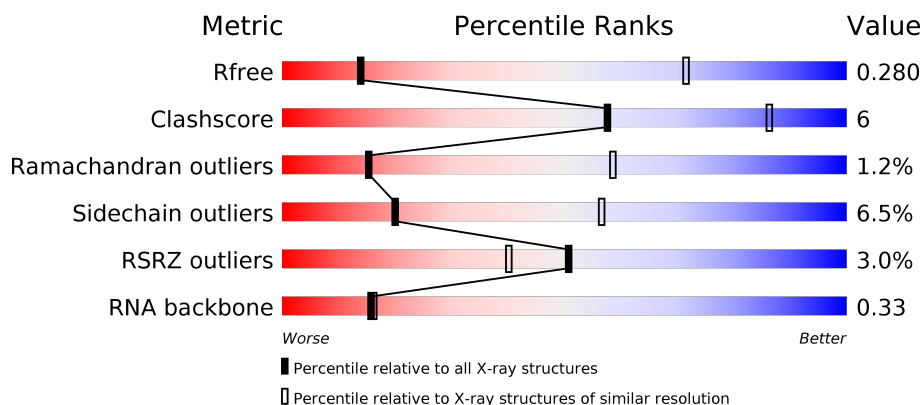
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1089 (4.42-3.60)
Clashscore	112137	1189 (4.44-3.60)
Ramachandran outliers	110173	1140 (4.42-3.60)
Sidechain outliers	110143	1127 (4.42-3.60)
RSRZ outliers	101464	1100 (4.42-3.60)
RNA backbone	2435	1026 (5.04-2.90)

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	388	<div> <div></div> <div>81% 13% . .</div> </div>
1	E	388	<div> <div></div> <div>80% 14% . .</div> </div>
2	B	232	<div> <div></div> <div>71% 22% . .</div> </div>
2	F	232	<div> <div></div> <div>69% 24% . .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	130	
3	G	130	
4	D	35	
4	H	35	

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
5	SAM	B	301	-	-	-	X
5	SAM	F	301	-	-	-	X

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	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	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			

Continued on next page...

Continued from previous page...

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	UNP P58032
F	2	ALA	SER	ENGINEERED	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			

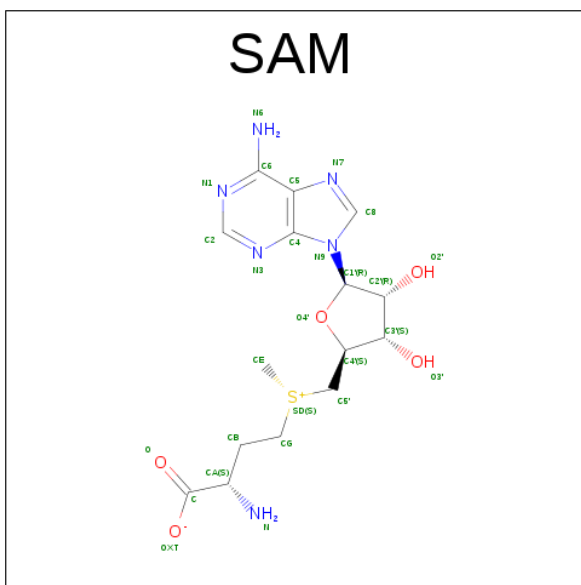
There are 6 discrepancies between the modelled and reference sequences:

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 (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).

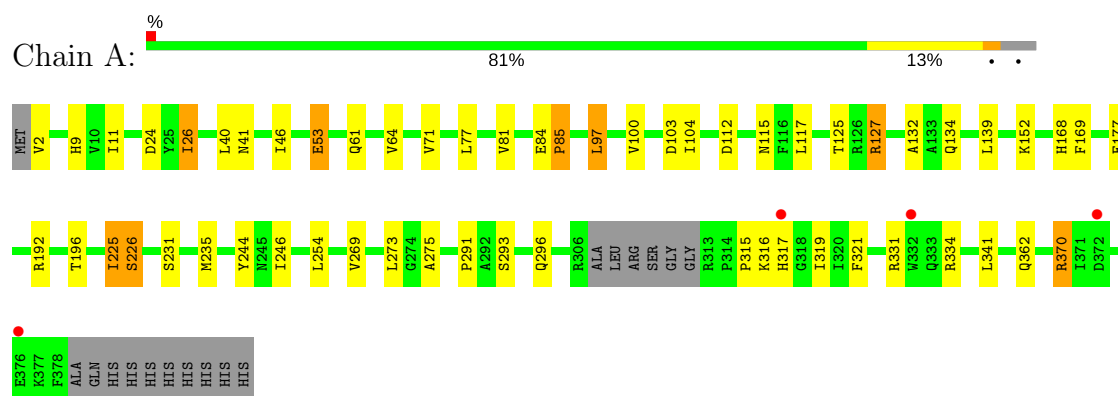


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total 27	C 15	N 6	O 5	S 1	0	0
5	F	1	Total 27	C 15	N 6	O 5	S 1	0	0

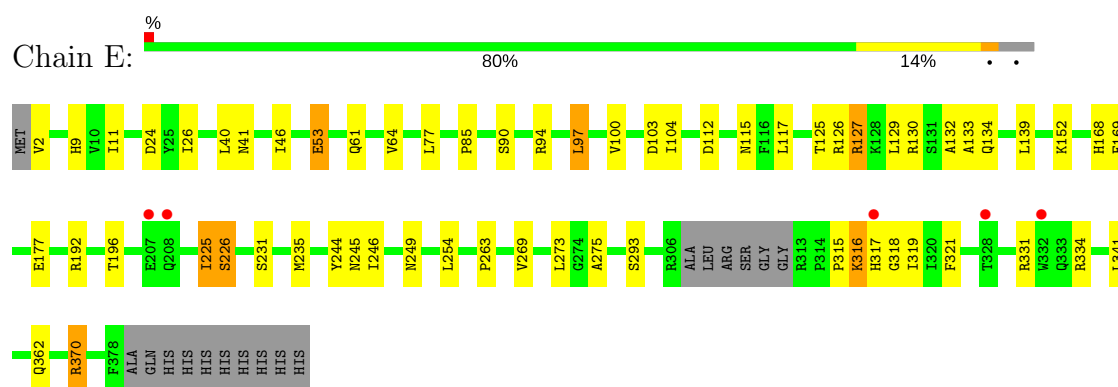
3 Residue-property plots [i](#)

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.

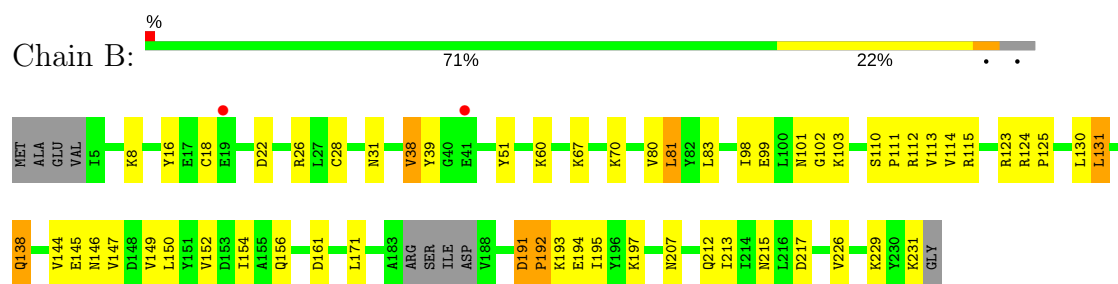
• Molecule 1: Pre mRNA splicing protein



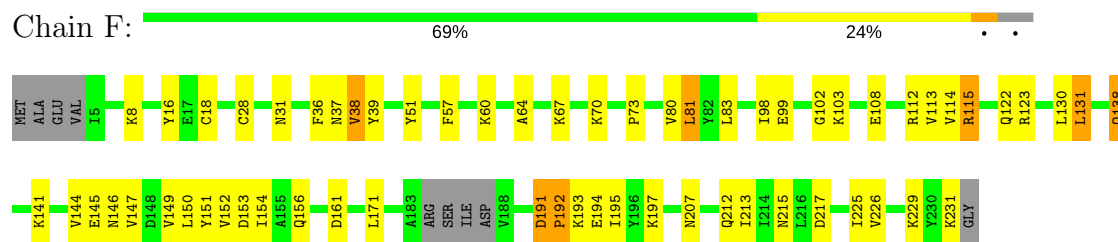
• Molecule 1: Pre mRNA splicing protein



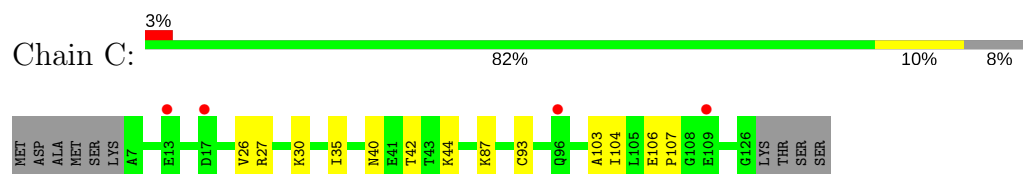
• Molecule 2: Fibrillar-like rRNA/tRNA 2'-O-methyltransferase



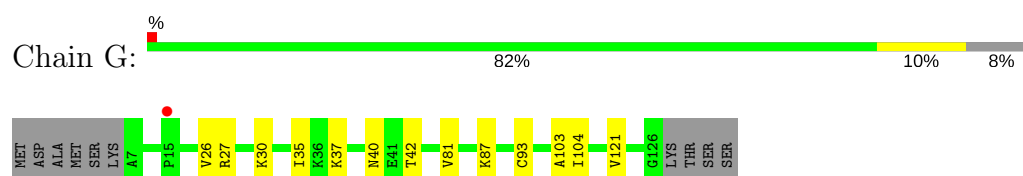
• Molecule 2: Fibrillar-like rRNA/tRNA 2'-O-methyltransferase



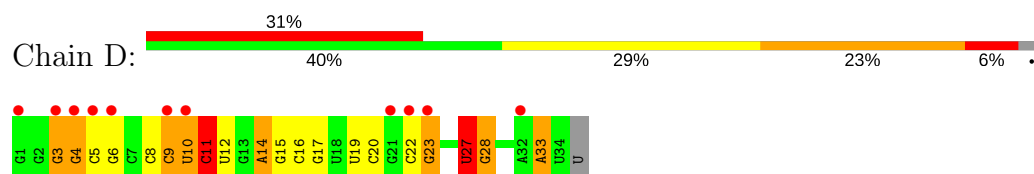
- Molecule 3: 50S ribosomal protein L7Ae



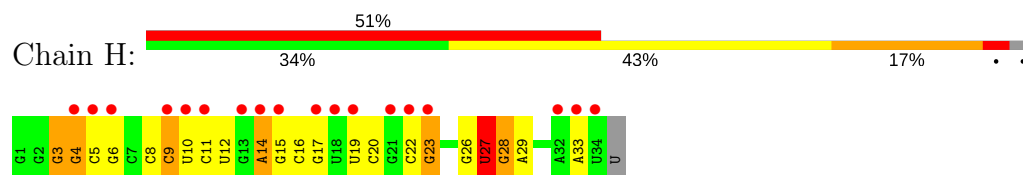
- Molecule 3: 50S ribosomal protein L7Ae



- 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 19.99 – 4.01	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-4.01) 96.5 (19.99-4.01)	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 (5.28%)	DCC
Wilson B-factor (Å ²)	135.9	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 181.9	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	0.90	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	0.31	0/2977	0.47	0/4021
1	E	0.31	0/2977	0.47	0/4021
2	B	0.34	0/1829	0.50	0/2474
2	F	0.34	0/1829	0.50	0/2474
3	C	0.30	0/920	0.44	0/1239
3	G	0.30	0/920	0.44	0/1239
4	D	0.73	0/780	1.57	16/1214 (1.3%)
4	H	0.71	0/780	1.52	9/1214 (0.7%)
All	All	0.39	0/13012	0.72	25/17896 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	9	C	O5'-P-OP2	-21.97	84.33	110.70
4	D	9	C	O5'-P-OP1	-20.57	86.02	110.70
4	H	12	U	OP1-P-OP2	-17.74	93.00	119.60
4	D	12	U	OP1-P-OP2	-17.38	93.52	119.60
4	H	22	C	O3'-P-O5'	-10.76	83.56	104.00
4	D	22	C	O3'-P-O5'	-10.58	83.89	104.00
4	D	10	U	O3'-P-O5'	-10.27	84.48	104.00
4	D	22	C	OP2-P-O3'	-8.11	87.35	105.20
4	H	22	C	OP2-P-O3'	-7.80	88.03	105.20
4	D	14	A	P-O3'-C3'	7.72	128.96	119.70
4	H	14	A	P-O3'-C3'	7.65	128.88	119.70
4	H	22	C	OP1-P-O3'	-7.61	88.46	105.20
4	D	23	G	O5'-P-OP2	7.31	119.48	110.70
4	D	10	U	OP2-P-O3'	-7.22	89.31	105.20
4	H	8	C	O3'-P-O5'	7.22	117.72	104.00
4	D	8	C	O3'-P-O5'	7.10	117.49	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	27	U	P-O3'-C3'	6.89	127.97	119.70
4	D	11	C	OP1-P-OP2	6.74	129.71	119.60
4	D	9	C	P-O3'-C3'	6.66	127.69	119.70
4	D	27	U	P-O3'-C3'	6.44	127.43	119.70
4	D	10	U	OP1-P-O3'	-6.22	91.53	105.20
4	H	23	G	O5'-P-OP2	6.20	118.14	110.70
4	D	22	C	OP1-P-O3'	-6.04	91.92	105.20
4	D	11	C	O5'-P-OP2	5.89	117.77	110.70
4	D	33	A	P-O3'-C3'	5.07	125.79	119.70

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	34	0
1	E	2931	0	2951	38	0
2	B	1796	0	1828	27	0
2	F	1796	0	1828	41	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	140	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 (140) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:138:GLN:H	2:F:138:GLN:HE21	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:80:VAL:HG12	2:B:149:VAL:HB	1.80	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
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:331:ARG:HA	1:A:334:ARG:HE	1.66	0.61
1:A:125:THR:CG2	2:B:130:LEU:HA	2.26	0.61
4:D:3:G:H2'	4:D:4:G:H8	1.65	0.61
2:B:114:VAL:HG21	2:B:131:LEU:HD12	1.84	0.60
1:E:90:SER:HB2	2:F:141:LYS:HZ3	1.67	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
1:E:125:THR:CG2	2:F:130:LEU:HA	2.35	0.55
1:E:130:ARG:CZ	1:E:263:PRO:HG3	2.37	0.55
2:F:38:VAL:HG12	2:F:39:TYR:N	2.21	0.55
2:B:16:TYR:HB2	2:B:28:CYS:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD21	1:E:225:ILE:HD11	1.89	0.54
1:E:100:VAL:HA	1:E:103:ASP:HB2	1.88	0.54
1:A:225:ILE:HD11	1:E:139:LEU:HD21	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
1:A:235:MET:HE3	2:F:39:TYR:HB3	1.90	0.53
3:G:42:THR:HG23	3:G:103:ALA:HB2	1.89	0.53
1:A:235:MET:HE1	1:E:246:ILE:HA	1.90	0.52
1:A:11:ILE:HB	1:A:104:ILE:HD11	1.92	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:132:ALA:C	1:E:134:GLN:H	2.13	0.51
1:E:293:SER:H	3:G:40:ASN:HD21	1.59	0.51
1:E:112:ASP:HA	1:E:115:ASN:HB2	1.94	0.50
1:A:246:ILE:HA	1:E:235:MET:HE1	1.94	0.50
2:B:145:GLU:HG2	2:B:146:ASN:N	2.27	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: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:A:2:VAL:HB	1:A:61:GLN:HG2	1.95	0.48
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:N	2:F:207:ASN:OD1	2.50	0.44
3:G:35:ILE:HG22	3:G:104:ILE:HA	2.00	0.43
1:E:132:ALA:C	1:E:134:GLN:N	2.70	0.43
4:D:16:C:H2'	4:D:17:G:H8	1.84	0.43
1:E:168:HIS:NE2	1:E:192:ARG:HG3	2.33	0.43
1:E:9:HIS:CD2	1:E:11:ILE:HG12	2.54	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
1:A:132:ALA:C	1:A:134:GLN:H	2.23	0.42
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:SER:O	1:A:235:MET:HG3	2.20	0.41
2:B:101:ASN:HA	2:B:101:ASN:HD22	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:207:ASN:O	2:B:231:LYS:HG2	2.20	0.41
2:B:98:ILE:HG22	2:B:99:GLU:O	2.21	0.41
1:E:127:ARG:HB2	1:E:127:ARG:HE	1.70	0.41
2:F:151:TYR:CE2	2:F:153:ASP:HB2	2.55	0.41
2:F:64:ALA:HB2	2:F:225:ILE:HD12	2.03	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 ⓘ

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	367/388 (95%)	341 (93%)	22 (6%)	4 (1%)	17	60
1	E	367/388 (95%)	342 (93%)	20 (5%)	5 (1%)	13	55
2	B	219/232 (94%)	196 (90%)	19 (9%)	4 (2%)	10	51
2	F	219/232 (94%)	197 (90%)	18 (8%)	4 (2%)	10	51
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%)	15	58

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%)	287 (94%)	20 (6%)	20	56
1	E	307/330 (93%)	288 (94%)	19 (6%)	21	58
2	B	198/205 (97%)	179 (90%)	19 (10%)	10	40
2	F	198/205 (97%)	180 (91%)	18 (9%)	11	43
3	C	98/107 (92%)	97 (99%)	1 (1%)	80	90
3	G	98/107 (92%)	97 (99%)	1 (1%)	80	90
All	All	1206/1284 (94%)	1128 (94%)	78 (6%)	20	56

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
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	152	LYS
1	A	169	PHE
1	A	177	GLU
1	A	196	THR
1	A	225	ILE
1	A	226	SER
1	A	244	TYR
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	31	ASN
2	B	60	LYS
2	B	67	LYS
2	B	81	LEU
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	197	LYS
2	B	215	ASN
2	B	217	ASP
2	B	229	LYS
3	C	87	LYS
1	E	24	ASP
1	E	53	GLU
1	E	64	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	77	LEU
1	E	97	LEU
1	E	117	LEU
1	E	127	ARG
1	E	152	LYS
1	E	169	PHE
1	E	177	GLU
1	E	196	THR
1	E	225	ILE
1	E	226	SER
1	E	244	TYR
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	31	ASN
2	F	60	LYS
2	F	67	LYS
2	F	81	LEU
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	197	LYS
2	F	215	ASN
2	F	217	ASP
2	F	229	LYS
3	G	87	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	59	ASN
1	A	251	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	296	GLN
2	B	31	ASN
2	B	101	ASN
2	B	138	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	249	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	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%)	15 (46%)	0
4	H	32/35 (91%)	15 (46%)	0
All	All	64/70 (91%)	30 (46%)	0

All (30) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	19	U
4	D	20	C
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
4	H	20	C
4	H	23	G
4	H	27	U
4	H	28	G
4	H	33	A

There are no RNA pucker outliers to report.

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](#)

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	-	21,29,29	1.22	2 (9%)	17,42,42	2.54	1 (5%)
5	SAM	F	301	-	21,29,29	1.21	2 (9%)	17,42,42	2.54	1 (5%)

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	-	-	0/8/33/33	0/3/3/3
5	SAM	F	301	-	-	0/8/33/33	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	301	SAM	C2-N1	2.56	1.38	1.33
5	B	301	SAM	C2-N1	2.66	1.38	1.33
5	F	301	SAM	C2-N3	4.10	1.39	1.32
5	B	301	SAM	C2-N3	4.12	1.39	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	SAM	N3-C2-N1	-10.07	120.09	128.86
5	F	301	SAM	N3-C2-N1	-10.03	120.12	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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%)	-0.30	4 (1%) 80 72	63, 206, 210, 251	0
1	E	371/388 (95%)	-0.26	5 (1%) 77 68	63, 206, 210, 251	0
2	B	223/232 (96%)	-0.26	2 (0%) 84 77	90, 104, 180, 211	1 (0%)
2	F	223/232 (96%)	-0.27	0 100 100	90, 104, 180, 211	1 (0%)
3	C	120/130 (92%)	0.11	4 (3%) 47 37	207, 209, 210, 210	0
3	G	120/130 (92%)	0.04	1 (0%) 86 79	207, 209, 210, 210	0
4	D	34/35 (97%)	1.77	11 (32%) 0 1	207, 211, 281, 283	0
4	H	34/35 (97%)	2.24	18 (52%) 0 1	207, 211, 281, 283	0
All	All	1496/1570 (95%)	-0.11	45 (3%) 51 40	63, 205, 210, 283	2 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	23	G	4.8
4	H	9	C	4.7
4	D	5	C	4.0
4	H	22	C	4.0
1	E	208	GLN	3.9
4	H	33	A	3.9
4	H	23	G	3.7
3	C	17	ASP	3.7
4	H	5	C	3.7
4	H	4	G	3.6
4	H	34	U	3.6
4	D	21	G	3.6
3	C	13	GLU	3.5
4	H	18	U	3.4
4	H	6	G	3.3
4	H	21	G	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	4	G	3.2
4	H	10	U	2.9
1	A	317	HIS	2.9
4	H	11	C	2.8
4	D	1	G	2.8
1	A	332	TRP	2.8
4	D	10	U	2.7
4	D	9	C	2.7
4	H	32	A	2.5
1	A	376	GLU	2.5
4	D	22	C	2.5
4	H	19	U	2.4
4	D	3	G	2.4
4	H	14	A	2.4
2	B	19	GLU	2.3
1	E	317	HIS	2.3
3	C	109	GLU	2.3
3	C	96	GLN	2.2
4	D	32	A	2.2
4	D	6	G	2.2
4	H	15	G	2.2
2	B	41	GLU	2.2
4	H	17	G	2.1
1	E	328	THR	2.1
1	E	332	TRP	2.1
1	A	372	ASP	2.1
1	E	207	GLU	2.1
3	G	15	PRO	2.0
4	H	13	G	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
5	SAM	F	301	27/27	0.67	0.52	3.27	145,145,146,147	0
5	SAM	B	301	27/27	0.77	0.48	2.32	145,145,146,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.