



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 20, 2016 – 12:30 PM EDT

PDB ID : 5HR6  
Title : X-ray crystal structure of C118A RlmN with cross-linked tRNA purified from Escherichia coli  
Authors : Schwalm, E.L.; Grove, T.L.; Booker, S.J.; Boal, A.K.  
Deposited on : 2016-01-22  
Resolution : 2.88 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-20027257  
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-20027257

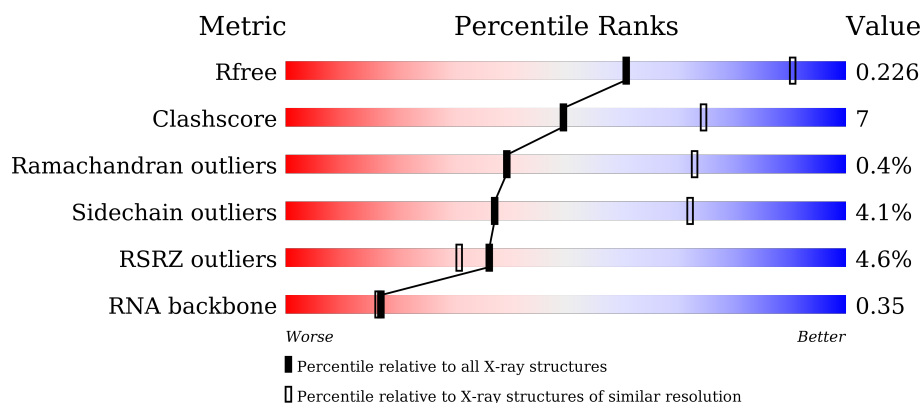
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.88 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)
RNA backbone	2183	1033 (3.26-2.50)

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	A	404	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>12%</div> </div> </div>
1	B	404	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>12%</div> </div> </div>
2	C	68	<div> <div></div> <div> <div>57%</div> <div>29%</div> <div>12%</div> </div> </div>
2	D	68	<div> <div></div> <div> <div>46%</div> <div>44%</div> <div>7%</div> </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
5	5AD	A	503	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8539 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 RlmN methylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2786	1747	498	522	19			
1	B	354	Total	C	N	O	S	0	0	0
			2786	1747	498	522	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	ALA	CYS	engineered mutation	UNP A7ZPW0
A	385	GLY	-	expression tag	UNP A7ZPW0
A	386	ASN	-	expression tag	UNP A7ZPW0
A	387	SER	-	expression tag	UNP A7ZPW0
A	388	SER	-	expression tag	UNP A7ZPW0
A	389	SER	-	expression tag	UNP A7ZPW0
A	390	VAL	-	expression tag	UNP A7ZPW0
A	391	ASP	-	expression tag	UNP A7ZPW0
A	392	LYS	-	expression tag	UNP A7ZPW0
A	393	LEU	-	expression tag	UNP A7ZPW0
A	394	ALA	-	expression tag	UNP A7ZPW0
A	395	ALA	-	expression tag	UNP A7ZPW0
A	396	ALA	-	expression tag	UNP A7ZPW0
A	397	LEU	-	expression tag	UNP A7ZPW0
A	398	GLU	-	expression tag	UNP A7ZPW0
A	399	HIS	-	expression tag	UNP A7ZPW0
A	400	HIS	-	expression tag	UNP A7ZPW0
A	401	HIS	-	expression tag	UNP A7ZPW0
A	402	HIS	-	expression tag	UNP A7ZPW0
A	403	HIS	-	expression tag	UNP A7ZPW0
A	404	HIS	-	expression tag	UNP A7ZPW0
B	118	ALA	CYS	engineered mutation	UNP A7ZPW0
B	385	GLY	-	expression tag	UNP A7ZPW0
B	386	ASN	-	expression tag	UNP A7ZPW0
B	387	SER	-	expression tag	UNP A7ZPW0

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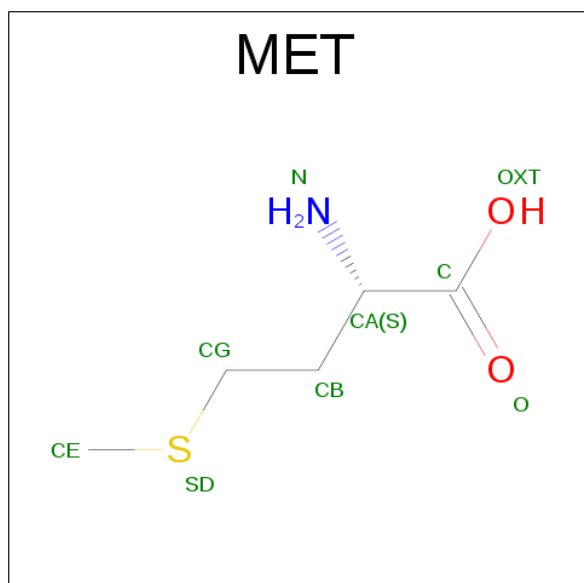
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Chain	Residue	Modelled	Actual	Comment	Reference
B	388	SER	-	expression tag	UNP A7ZPW0
B	389	SER	-	expression tag	UNP A7ZPW0
B	390	VAL	-	expression tag	UNP A7ZPW0
B	391	ASP	-	expression tag	UNP A7ZPW0
B	392	LYS	-	expression tag	UNP A7ZPW0
B	393	LEU	-	expression tag	UNP A7ZPW0
B	394	ALA	-	expression tag	UNP A7ZPW0
B	395	ALA	-	expression tag	UNP A7ZPW0
B	396	ALA	-	expression tag	UNP A7ZPW0
B	397	LEU	-	expression tag	UNP A7ZPW0
B	398	GLU	-	expression tag	UNP A7ZPW0
B	399	HIS	-	expression tag	UNP A7ZPW0
B	400	HIS	-	expression tag	UNP A7ZPW0
B	401	HIS	-	expression tag	UNP A7ZPW0
B	402	HIS	-	expression tag	UNP A7ZPW0
B	403	HIS	-	expression tag	UNP A7ZPW0
B	404	HIS	-	expression tag	UNP A7ZPW0

- Molecule 2 is a RNA chain called tRNA Glu.

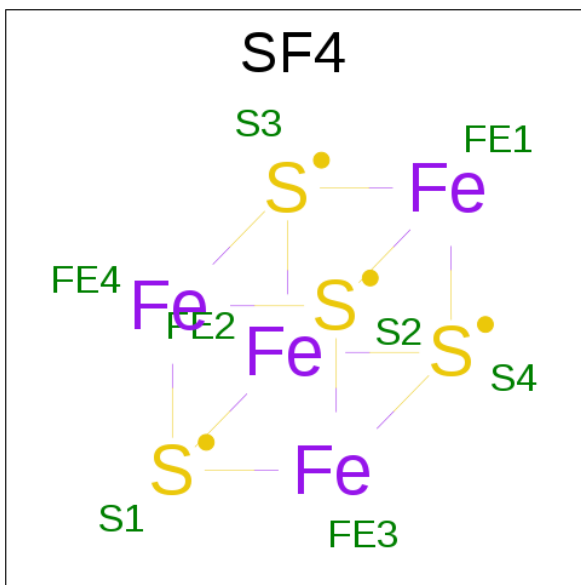
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	68	Total	C	N	O	P	0	0	0
			1444	644	256	476	68			
2	D	66	Total	C	N	O	P	0	0	0
			1401	625	248	462	66			

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>S).



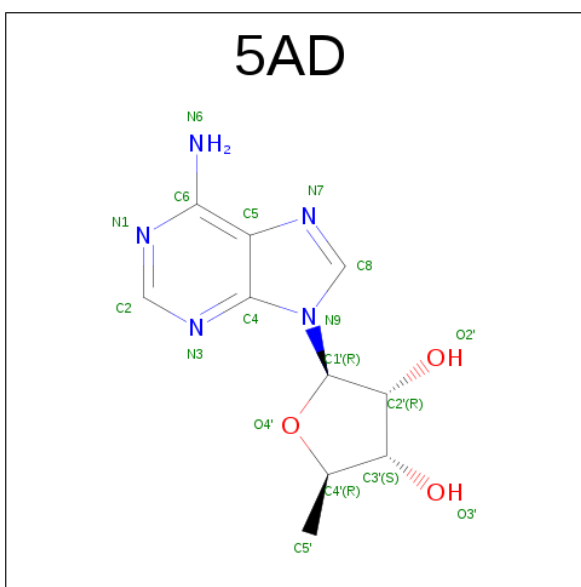
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $\text{C}_{10}\text{H}_{13}\text{N}_5\text{O}_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	3	Total	Mg	0	0
			3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total	O	0	0
			17	17		
7	C	4	Total	O	0	0
			4	4		
7	B	20	Total	O	0	0
			20	20		

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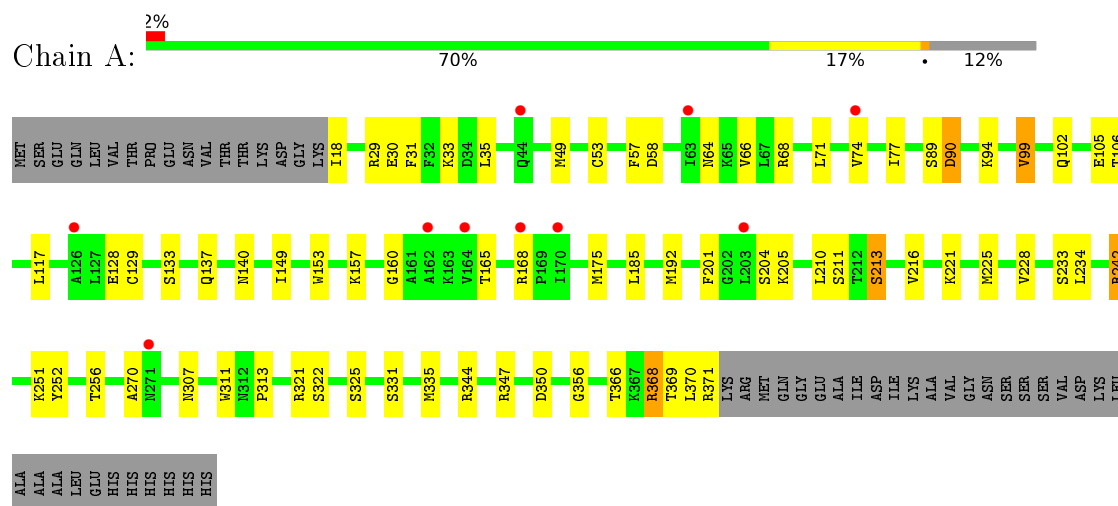
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	5	Total	O	0	0
			5	5		



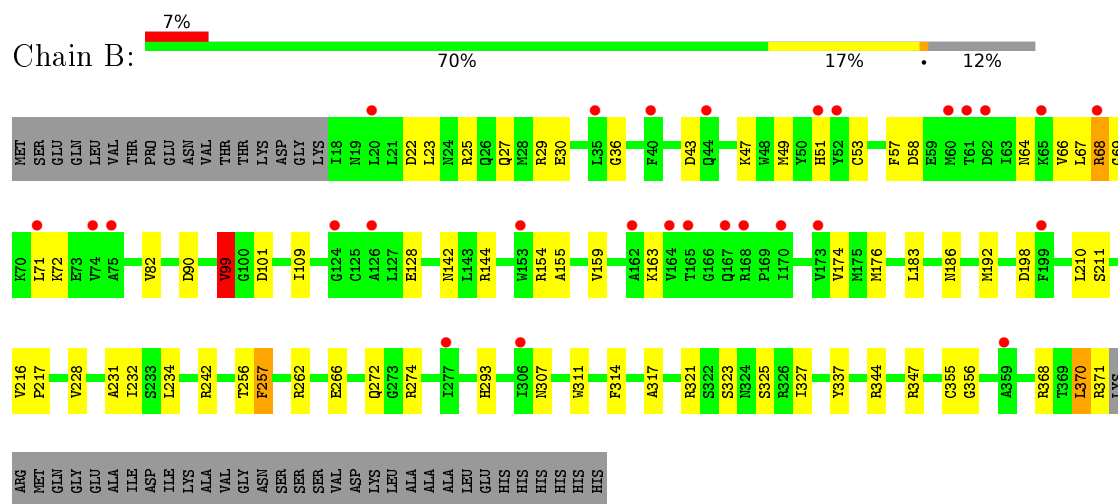
### 3 Residue-property plots [i](#)

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.

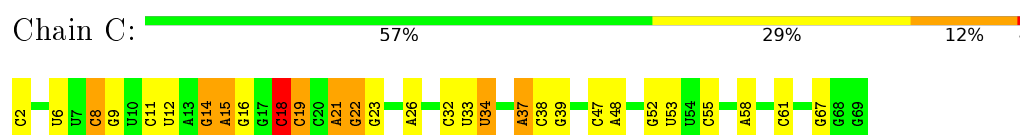
#### • Molecule 1: RlmN methylase



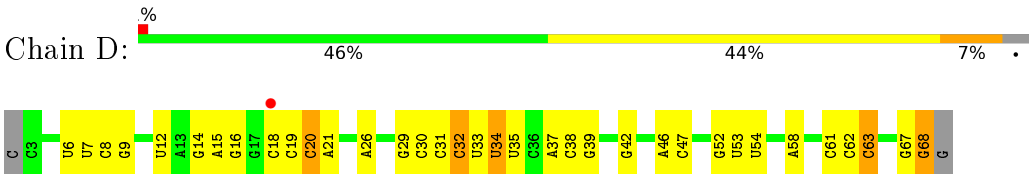
#### • Molecule 1: RlmN methylase



#### • Molecule 2: tRNA Glu



● Molecule 2: tRNA Glu



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.66 Å 69.82 Å 149.30 Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	88.66 – 2.88 49.77 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.9 (88.66-2.88) 98.2 (49.77-2.88)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.182 , 0.228 0.186 , 0.226	Depositor DCC
$R_{free}$ test set	1700 reflections (4.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.357 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, SMC, MG, 5AD

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	0.68	0/2824	0.88	4/3815 (0.1%)
1	B	0.68	0/2824	0.86	0/3815
2	C	0.49	0/1611	0.87	5/2508 (0.2%)
2	D	0.50	0/1563	0.85	3/2433 (0.1%)
All	All	0.62	0/8822	0.87	12/12571 (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
2	C	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	368	ARG	NE-CZ-NH1	9.23	124.92	120.30
2	C	11	C	O5'-P-OP2	-7.97	98.53	105.70
2	C	32	C	C2'-C3'-O3'	6.45	124.02	113.70
2	C	53	U	O5'-P-OP2	6.14	118.06	110.70
1	A	368	ARG	NE-CZ-NH2	-5.85	117.38	120.30
2	C	18	C	N1-C1'-C2'	5.53	121.18	114.00
2	D	34	U	C2'-C3'-O3'	5.37	122.30	113.70
2	C	14	G	O4'-C1'-N9	5.35	112.48	108.20
1	A	90	ASP	CB-CG-OD1	5.28	123.05	118.30
2	D	53	U	O5'-P-OP1	-5.17	101.05	105.70
2	D	53	U	O5'-P-OP2	5.11	116.83	110.70
1	A	90	ASP	CB-CA-C	-5.11	100.19	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	14	G	Sidechain

## 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	2786	0	2801	45	0
1	B	2786	0	2801	45	0
2	C	1444	0	736	17	0
2	D	1401	0	715	14	0
3	A	9	0	8	0	0
3	B	9	0	8	1	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	18	0	13	1	0
5	B	18	0	13	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	3	0	0	0	0
6	D	1	0	0	0	0
7	A	17	0	0	0	0
7	B	20	0	0	0	0
7	C	4	0	0	0	0
7	D	5	0	0	0	0
All	All	8539	0	7095	111	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 7.

All (111) 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:175:MET:HG3	1:A:192:MET:CE	2.17	0.75
1:A:192:MET:HE1	1:A:210:LEU:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LEU:O	1:A:242:ARG:HD2	1.92	0.68
1:A:18:ILE:HG22	1:A:74:VAL:O	1.94	0.68
1:A:94:LYS:HD2	1:A:105:GLU:OE1	1.97	0.65
2:C:18:C:H1'	1:B:142:ASN:ND2	2.13	0.64
1:B:234:LEU:O	1:B:242:ARG:HD2	1.99	0.63
1:A:18:ILE:CG2	1:A:74:VAL:O	2.47	0.62
1:B:370:LEU:O	1:B:371:ARG:O	2.18	0.62
1:A:369:THR:O	1:A:370:LEU:C	2.39	0.61
1:B:210:LEU:C	1:B:210:LEU:HD23	2.22	0.59
1:B:64:ASN:ND2	2:D:68:G:OP1	2.35	0.59
1:B:192:MET:HE2	1:B:228:VAL:HG11	1.83	0.59
1:B:82:VAL:HG13	1:B:154:ARG:HD2	1.85	0.59
1:B:49:MET:O	1:B:53:CYS:HA	2.03	0.58
1:B:99:VAL:HG12	1:B:99:VAL:O	2.03	0.57
2:D:7:U:C2	2:D:14:G:O6	2.58	0.57
1:A:90:ASP:HB3	1:A:347:ARG:HH21	1.70	0.57
1:B:192:MET:CE	1:B:228:VAL:HG11	2.35	0.57
1:B:90:ASP:HB3	1:B:347:ARG:HH21	1.70	0.57
1:B:58:ASP:OD1	1:B:72:LYS:CE	2.55	0.55
1:B:23:LEU:HD22	1:B:27:GLN:HB3	1.89	0.54
1:A:210:LEU:HD23	1:A:210:LEU:C	2.26	0.54
1:A:366:THR:O	1:A:371:ARG:NH1	2.40	0.54
2:C:34:U:C6	2:C:34:U:H5'	2.44	0.52
1:B:216:VAL:HB	1:B:217:PRO:HD3	1.89	0.52
1:B:128:GLU:HG2	1:B:368:ARG:HH12	1.73	0.52
1:B:109:ILE:HD13	2:D:37:A:C5	2.45	0.52
1:A:216:VAL:HG21	1:A:256:THR:HG22	1.91	0.52
1:A:106:THR:CG2	1:A:117:LEU:HD11	2.40	0.51
2:D:62:C:H2'	2:D:63:C:C6	2.45	0.51
2:C:15:A:H5'	2:C:15:A:H8	1.75	0.51
2:C:33:U:C4'	2:C:34:U:H5''	2.41	0.51
1:B:307:ASN:ND2	1:B:344:ARG:HE	2.08	0.51
1:A:185:LEU:HD13	1:A:225:MET:HE1	1.93	0.50
1:A:49:MET:O	1:A:53:CYS:HA	2.11	0.50
2:C:21:A:H5''	2:C:22:G:OP1	2.12	0.50
1:A:106:THR:HG22	1:A:117:LEU:HD11	1.92	0.50
1:B:293:HIS:ND1	1:B:337:TYR:OH	2.37	0.49
1:A:175:MET:HG3	1:A:192:MET:HE2	1.93	0.49
3:B:501:MET:C	3:B:501:MET:SD	2.91	0.48
2:C:33:U:H4'	2:C:34:U:H5''	1.93	0.48
1:A:133:SER:HB3	1:A:356:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:CZ	1:B:317:ALA:HB2	2.48	0.48
2:D:19:C:H4'	2:D:20:C:OP1	2.14	0.48
1:A:58:ASP:HA	1:A:68:ARG:HD3	1.95	0.47
2:D:21:A:H61	2:D:46:A:H2'	1.79	0.47
1:B:370:LEU:O	1:B:371:ARG:C	2.53	0.47
2:C:33:U:H4'	2:C:34:U:C5'	2.44	0.47
1:B:29:ARG:O	1:B:30:GLU:C	2.53	0.47
1:A:350:ASP:OD1	1:A:350:ASP:N	2.48	0.47
1:B:174:VAL:HG23	1:B:176:MET:HB2	1.97	0.47
1:B:274:ARG:HH12	2:D:32:C:H3'	1.79	0.46
1:B:311:TRP:O	1:B:321:ARG:HD2	2.15	0.46
1:A:307:ASN:ND2	1:A:344:ARG:HE	2.13	0.46
1:B:356:GLY:HA3	5:B:503:5AD:C5	2.46	0.46
1:A:149:ILE:HD11	1:A:201:PHE:HE2	1.81	0.46
1:B:57:PHE:O	1:B:68:ARG:HD2	2.16	0.46
2:C:15:A:H5'	2:C:15:A:C8	2.51	0.46
1:B:211:SER:HA	1:B:231:ALA:O	2.16	0.46
2:D:67:G:H2'	2:D:68:G:C8	2.51	0.46
1:B:216:VAL:HG21	1:B:256:THR:HG22	1.97	0.45
1:A:321:ARG:O	1:A:322:SER:C	2.52	0.45
2:C:18:C:O2	2:C:18:C:H2'	2.15	0.45
2:C:19:C:O2	2:C:21:A:H1'	2.17	0.45
1:B:22:ASP:OD2	1:B:144:ARG:NH2	2.50	0.44
1:A:213:SER:HA	1:A:233:SER:HB2	1.99	0.44
2:C:18:C:H1'	1:B:142:ASN:HD22	1.78	0.44
2:C:8:C:H5	2:C:23:G:O6	2.00	0.44
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.86	0.44
1:B:57:PHE:CE1	1:B:71:LEU:HD13	2.53	0.44
1:A:311:TRP:CH2	1:A:313:PRO:HA	2.53	0.44
1:A:31:PHE:O	1:A:35:LEU:HD13	2.18	0.44
1:B:67:LEU:O	1:B:69:GLY:N	2.50	0.44
1:B:370:LEU:H	1:B:370:LEU:HD23	1.83	0.43
1:A:102:GLN:HE22	1:A:140:ASN:CG	2.22	0.43
1:B:370:LEU:N	1:B:370:LEU:HD23	2.33	0.43
1:A:99:VAL:HG12	1:A:99:VAL:O	2.19	0.43
1:B:323:SER:O	1:B:327:ILE:HG13	2.18	0.43
1:A:185:LEU:HD13	1:A:225:MET:CE	2.48	0.43
2:C:55:C:C6	1:B:371:ARG:HD2	2.54	0.43
1:A:99:VAL:O	1:A:99:VAL:CG1	2.66	0.43
1:A:356:GLY:HA3	5:A:503:5AD:C5	2.48	0.43
2:C:2:C:H6	2:C:2:C:P	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:C:O2	1:B:186:ASN:HB2	2.19	0.43
1:A:160:GLY:HA3	1:A:165:THR:HG21	2.01	0.43
2:D:62:C:H2'	2:D:63:C:H6	1.83	0.42
1:B:64:ASN:HB2	1:B:67:LEU:H	1.84	0.42
2:D:29:G:H2'	2:D:30:C:C6	2.54	0.42
1:A:175:MET:HG3	1:A:192:MET:HE3	1.98	0.42
1:A:205:LYS:HB3	1:A:270:ALA:HB2	2.01	0.42
1:A:64:ASN:OD1	1:A:66:VAL:HG12	2.19	0.42
1:A:307:ASN:HD21	2:C:37:A:H5'	1.84	0.42
1:B:47:LYS:O	1:B:51:HIS:HB2	2.18	0.42
1:B:67:LEU:C	1:B:69:GLY:N	2.73	0.42
1:A:204:SER:HB2	2:C:26:A:H5''	2.01	0.41
1:A:251:LYS:HD2	1:A:252:TYR:CE2	2.55	0.41
1:A:331:SER:O	1:A:335:MET:HG3	2.20	0.41
1:A:153:TRP:CH2	1:A:157:LYS:HE3	2.55	0.41
1:A:29:ARG:O	1:A:30:GLU:C	2.58	0.41
1:A:149:ILE:HD11	1:A:201:PHE:CE2	2.56	0.41
1:A:33:LYS:HE2	1:A:33:LYS:HA	2.02	0.41
1:B:155:ALA:O	1:B:159:VAL:HG23	2.21	0.41
1:B:232:ILE:HB	1:B:257:PHE:CZ	2.55	0.41
2:D:31:C:C2'	2:D:32:C:H5'	2.51	0.41
2:D:31:C:H2'	2:D:32:C:H5'	2.03	0.41
1:A:57:PHE:CE1	1:A:71:LEU:HD13	2.55	0.40
1:B:272:GLN:OE1	2:D:30:C:N4	2.53	0.40
1:A:49:MET:HG2	1:A:77:ILE:HD13	2.03	0.40
1:B:355:SMC:SG	2:D:37:A:C6	3.15	0.40
1:A:128:GLU:O	1:A:129:CYS:C	2.59	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	351/404 (87%)	323 (92%)	28 (8%)	0	100	100
1	B	351/404 (87%)	321 (92%)	27 (8%)	3 (1%)	21	55
All	All	702/808 (87%)	644 (92%)	55 (8%)	3 (0%)	39	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ARG
1	B	99	VAL
1	B	36	GLY

### 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	303/345 (88%)	292 (96%)	11 (4%)	42	76
1	B	303/345 (88%)	291 (96%)	12 (4%)	38	73
All	All	606/690 (88%)	583 (96%)	23 (4%)	37	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	SER
1	A	99	VAL
1	A	137	GLN
1	A	168	ARG
1	A	211	SER
1	A	213	SER
1	A	221	LYS
1	A	228	VAL
1	A	242	ARG
1	A	325	SER
1	A	368	ARG
1	B	25	ARG
1	B	43	ASP

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Mol	Chain	Res	Type
1	B	66	VAL
1	B	99	VAL
1	B	101	ASP
1	B	163	LYS
1	B	198	ASP
1	B	257	PHE
1	B	262	ARG
1	B	266	GLU
1	B	325	SER
1	B	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	B	64	ASN
1	B	307	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	67/68 (98%)	20 (29%)	4 (5%)
2	D	65/68 (95%)	23 (35%)	4 (6%)
All	All	132/136 (97%)	43 (32%)	8 (6%)

All (43) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	6	U
2	C	8	C
2	C	9	G
2	C	12	U
2	C	15	A
2	C	16	G
2	C	18	C
2	C	19	C
2	C	21	A
2	C	22	G
2	C	34	U
2	C	37	A

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Mol	Chain	Res	Type
2	C	38	C
2	C	39	G
2	C	47	C
2	C	48	A
2	C	52	G
2	C	58	A
2	C	61	C
2	C	67	G
2	D	6	U
2	D	8	C
2	D	9	G
2	D	12	U
2	D	15	A
2	D	16	G
2	D	18	C
2	D	20	C
2	D	26	A
2	D	32	C
2	D	33	U
2	D	34	U
2	D	35	U
2	D	38	C
2	D	39	G
2	D	42	G
2	D	47	C
2	D	52	G
2	D	54	U
2	D	58	A
2	D	61	C
2	D	63	C
2	D	68	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	8	C
2	C	15	A
2	C	16	G
2	C	38	C
2	D	8	C
2	D	33	U
2	D	34	U

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Mol	Chain	Res	Type
2	D	38	C

## 5.4 Non-standard residues in protein, DNA, RNA chains

2 non-standard protein/DNA/RNA residues 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
1	SMC	A	355	1,2	4,6,7	1.69	1 (25%)	2,6,8	4.04	2 (100%)
1	SMC	B	355	1,2	4,6,7	1.56	1 (25%)	2,6,8	2.73	1 (50%)

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
1	SMC	A	355	1,2	-	0/3/5/7	0/0/0/0
1	SMC	B	355	1,2	-	0/3/5/7	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	SMC	CB-SG	-3.24	1.77	1.80
1	B	355	SMC	CB-SG	-2.85	1.77	1.80

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	SMC	O-C-CA	-2.18	119.87	125.72
1	B	355	SMC	CS-SG-CB	3.60	106.82	101.24
1	A	355	SMC	CS-SG-CB	5.28	109.41	101.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	355	SMC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MET	A	501	4	5,8,8	0.46	0	3,9,9	1.17	0
4	SF4	A	502	1,3	0,12,12	0.00	-	0,24,24	0.00	-
5	5AD	A	503	-	17,20,20	1.01	1 (5%)	15,30,30	3.01	3 (20%)
3	MET	B	501	4	5,8,8	0.35	0	3,9,9	0.65	0
4	SF4	B	502	1,3	0,12,12	0.00	-	0,24,24	0.00	-
5	5AD	B	503	-	17,20,20	1.04	2 (11%)	15,30,30	2.86	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MET	A	501	4	-	0/4/8/8	0/0/0/0
4	SF4	A	502	1,3	-	0/0/48/48	0/6/5/5
5	5AD	A	503	-	-	0/0/20/20	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MET	B	501	4	-	0/4/8/8	0/0/0/0
4	SF4	B	502	1,3	-	0/0/48/48	0/6/5/5
5	5AD	B	503	-	-	0/0/20/20	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	5AD	C4-N3	-2.03	1.32	1.35
5	B	503	5AD	C5-C4	2.10	1.45	1.40
5	A	503	5AD	C5-C4	2.16	1.45	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	503	5AD	C5'-C4'-C3'	-7.46	107.45	115.81
5	A	503	5AD	N3-C2-N1	-7.46	123.01	128.87
5	A	503	5AD	C5'-C4'-C3'	-6.61	108.40	115.81
5	B	503	5AD	N3-C2-N1	-5.16	124.82	128.87
5	A	503	5AD	C1'-N9-C4	-4.84	121.40	126.81
5	B	503	5AD	C4'-O4'-C1'	-4.12	105.28	109.64
5	B	503	5AD	C1'-N9-C4	-3.46	122.95	126.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	5AD	1	0
3	B	501	MET	1	0
5	B	503	5AD	1	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 ⓘ

### 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	A	353/404 (87%)	0.65	10 (2%) 56 51	46, 61, 97, 112	0
1	B	353/404 (87%)	0.75	28 (7%) 15 10	51, 65, 110, 133	0
2	C	68/68 (100%)	0.17	0 100 100	55, 73, 109, 128	0
2	D	66/68 (97%)	-0.06	1 (1%) 76 74	61, 87, 126, 135	0
All	All	840/944 (88%)	0.59	39 (4%) 36 31	46, 65, 110, 135	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	162	ALA	5.7
1	B	71	LEU	5.5
1	B	167	GLN	4.4
1	B	61	THR	4.0
1	A	162	ALA	3.6
1	B	306	ILE	3.5
1	B	44	GLN	3.4
1	B	62	ASP	3.3
1	B	40	PHE	3.3
1	B	359	ALA	3.1
1	B	164	VAL	3.1
1	B	52	TYR	3.0
1	A	63	ILE	3.0
1	B	277	ILE	2.8
1	B	74	VAL	2.8
1	B	199	PHE	2.8
1	B	168	ARG	2.7
1	B	35	LEU	2.7
1	A	168	ARG	2.7
1	A	170	ILE	2.6
1	B	173	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	68	ARG	2.5
1	B	170	ILE	2.4
1	B	124	GLY	2.4
1	B	153	TRP	2.4
1	A	74	VAL	2.4
1	A	44	GLN	2.4
1	B	165	THR	2.3
1	A	126	ALA	2.3
1	B	65	LYS	2.3
1	B	51	HIS	2.3
1	A	164	VAL	2.2
1	B	75	ALA	2.1
1	B	126	ALA	2.1
1	A	271	ASN	2.1
1	A	203	LEU	2.1
2	D	18	C	2.0
1	B	60	MET	2.0
1	B	20	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SMC	A	355	7/8	0.99	0.18	-	43,49,54,55	0
1	SMC	B	355	7/8	0.97	0.15	-	52,56,57,57	0

## 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
5	5AD	A	503	18/18	0.98	0.31	2.82	53,59,69,73	0
5	5AD	B	503	18/18	0.98	0.28	1.11	54,60,68,68	0
3	MET	A	501	9/9	0.98	0.23	-0.17	60,66,69,72	0
6	MG	A	504	1/1	0.81	0.22	-0.18	56,56,56,56	0
3	MET	B	501	9/9	0.99	0.22	-0.39	56,62,68,69	0
4	SF4	B	502	8/8	0.99	0.22	-0.58	42,43,57,59	0
4	SF4	A	502	8/8	0.99	0.22	-0.84	40,44,55,55	0
6	MG	B	504	1/1	0.99	0.14	-1.17	67,67,67,67	0
6	MG	D	101	1/1	0.98	0.14	-1.55	41,41,41,41	0
6	MG	C	102	1/1	0.93	0.29	-	70,70,70,70	0
6	MG	C	103	1/1	0.45	0.31	-	88,88,88,88	0
6	MG	C	101	1/1	0.98	0.31	-	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.