



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2016 – 10:59 PM EST

PDB ID : 5D8H  
Title : CRYSTAL STRUCTURE OF THE BASE OF THE RIBOSOMAL P  
STALK FROM METHANOCOCCUS JANNASCHII WITH ANTIBIOTIC  
THIOSTREPTON  
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Deposited on : 2015-08-17  
Resolution : 2.80 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-20028442  
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-20028442

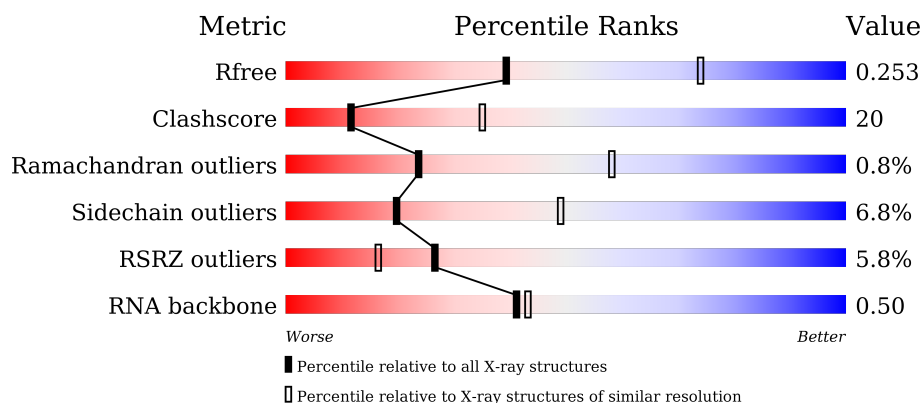
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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	74	<div> <div>8%</div> <div>55% 31% 14%</div> </div>
2	B	213	<div> <div>8%</div> <div>62% 29% 5%</div> </div>
3	C	161	<div> <div>4%</div> <div>53% 39%</div> </div>
4	D	19	<div> <div>74% 26%</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	MG	A	1303	-	-	-	X
6	NA	A	1313	-	-	-	X
7	TRS	A	1315	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4592 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	P	0	0	0
			1588	708	293	513	74			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	C	-	expression tag	REF 470491724

- Molecule 2 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	Se	0	0	0
			1589	1024	268	290	1	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MSE	VAL	engineered mutation	UNP P54049

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	158	Total	C	N	O	S	Se	0	0	0
			1197	762	197	232	1	5			

- Molecule 4 is a protein called THIOSTREPTON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	19	Total	C	N	O	S	1	0	1
			114	72	19	18	5			

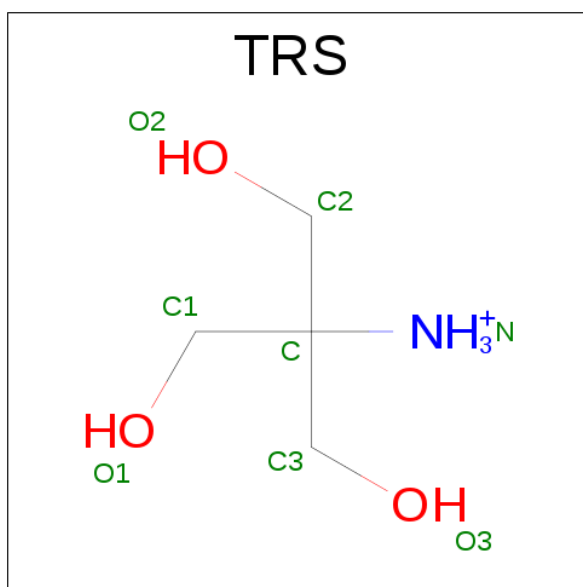
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	Mg	0	0
			10	10		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		
6	A	3	Total	Na	0	0
			3	3		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	58	Total 58	O 58	0	0
8	B	4	Total 4	O 4	0	0
8	C	3	Total 3	O 3	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 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.

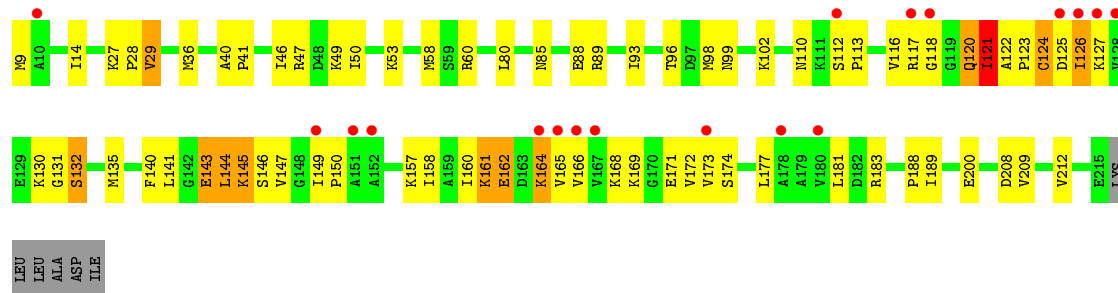
#### • Molecule 1: 23S ribosomal RNA

Chain A: 



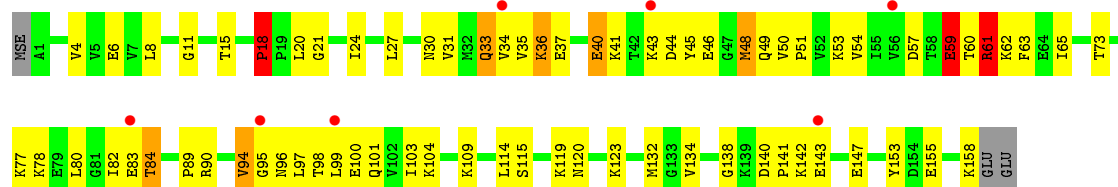
#### • Molecule 2: 50S ribosomal protein L10

Chain B: 



#### • Molecule 3: 50S ribosomal protein L11

Chain C: 



#### • Molecule 4: THIOSTREPTON

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	125.07Å 127.16Å 132.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.55 – 2.80 45.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.55-2.80) 99.9 (45.54-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.208 , 0.245 0.218 , 0.253	Depositor DCC
$R_{free}$ test set	1319 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.0	Xtriage
Anisotropy	0.799	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 69.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4592	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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, 0.333 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: MG, NA, DCY, DHA, QUA, BB9, NH2, MH6, TRS, DBU, TS9

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	0.89	1/1777 (0.1%)	1.50	21/2768 (0.8%)
2	B	0.63	0/1607	0.92	5/2161 (0.2%)
3	C	0.82	2/1208 (0.2%)	1.03	12/1624 (0.7%)
4	D	0.89	0/31	0.83	0/38
All	All	0.79	3/4623 (0.1%)	1.22	38/6591 (0.6%)

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	B	0	3
3	C	0	2
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	44	ASP	C-N	-18.32	0.92	1.34
1	A	1151	G	OP3-P	-9.67	1.49	1.61
3	C	41	LYS	C-N	7.84	1.52	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	44	ASP	C-N-CA	13.55	155.57	121.70
1	A	1179	A	O4'-C1'-N9	8.34	114.87	108.20
3	C	44	ASP	O-C-N	-8.33	109.37	122.70
3	C	59	GLU	C-N-CA	7.58	140.66	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	59	GLU	N-CA-CB	-7.30	97.47	110.60
1	A	1163	G	N1-C6-O6	-7.20	115.58	119.90
1	A	1163	G	C5-C6-O6	6.67	132.60	128.60
3	C	59	GLU	OE1-CD-OE2	-6.59	115.39	123.30
3	C	30	ASN	CB-CA-C	6.54	123.48	110.40
1	A	1205	A	C8-N9-C4	6.32	108.33	105.80
3	C	61	ARG	CB-CA-C	-6.18	98.04	110.40
1	A	1224	C	C5-C4-N4	-6.10	115.93	120.20
1	A	1216	C	C5-C4-N4	-6.06	115.96	120.20
2	B	80	LEU	CA-CB-CG	5.91	128.88	115.30
1	A	1197	G	N9-C4-C5	5.89	107.75	105.40
3	C	41	LYS	C-N-CA	-5.87	107.02	121.70
3	C	8	LEU	CA-CB-CG	5.84	128.74	115.30
3	C	44	ASP	CA-C-N	5.75	129.86	117.20
1	A	1199	G	C5-C6-O6	-5.65	125.21	128.60
1	A	1165	G	OP1-P-OP2	5.62	128.03	119.60
1	A	1224	C	N3-C4-N4	5.61	121.93	118.00
3	C	61	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	1202	C	N1-C2-O2	-5.53	115.58	118.90
1	A	1216	C	N1-C2-O2	-5.52	115.59	118.90
2	B	121	ILE	CG1-CB-CG2	-5.46	99.40	111.40
1	A	1197	G	N3-C4-N9	-5.35	122.79	126.00
1	A	1179	A	OP1-P-O3'	5.30	116.85	105.20
1	A	1196	A	O4'-C1'-N9	5.29	112.43	108.20
2	B	162	GLU	CA-CB-CG	5.25	124.96	113.40
2	B	118	GLY	N-CA-C	5.20	126.09	113.10
1	A	1197	G	C8-N9-C1'	5.15	133.70	127.00
1	A	1182	C	C5-C4-N4	-5.15	116.60	120.20
1	A	1174	C	N3-C4-C5	5.09	123.94	121.90
1	A	1211	U	C6-N1-C2	5.07	124.04	121.00
3	C	61	ARG	CA-CB-CG	5.05	124.50	113.40
1	A	1163	G	N1-C2-N2	-5.03	111.67	116.20
2	B	144	LEU	CB-CG-CD2	5.02	119.53	111.00
1	A	1165	G	O5'-P-OP2	-5.00	101.20	105.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	121	ILE	Peptide
2	B	126	ILE	Peptide
2	B	164	LYS	Peptide

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Mol	Chain	Res	Type	Group
3	C	18	PRO	Peptide
3	C	94	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1588	0	802	20	0
2	B	1589	0	1720	89	0
3	C	1197	0	1255	63	0
4	D	114	0	79	9	0
5	A	10	0	0	0	0
5	C	1	0	0	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
7	A	16	0	24	0	0
7	B	8	0	12	2	0
8	A	58	0	0	3	0
8	B	4	0	0	0	0
8	C	3	0	0	0	0
All	All	4592	0	3892	167	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 20.

All (167) 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)
4:D:0:QUA:C7	4:D:1:ILE:N	1.68	1.51
2:B:120:GLN:O	2:B:121:ILE:HG13	1.33	1.26
3:C:59:GLU:CD	3:C:60:THR:H	1.65	0.99
3:C:98:THR:HG22	3:C:101:GLN:HG3	1.43	0.98
2:B:127:LYS:HD2	2:B:165:VAL:HA	1.43	0.98
2:B:126:ILE:HD12	2:B:127:LYS:HA	1.47	0.95
2:B:120:GLN:C	2:B:121:ILE:HG13	1.82	0.94
1:A:1183:A:OP1	8:A:1401:HOH:O	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:0:QUA:C8	4:D:1:ILE:N	2.38	0.87
2:B:121:ILE:HG12	2:B:172:VAL:HA	1.57	0.84
2:B:120:GLN:O	2:B:121:ILE:CG1	2.24	0.83
2:B:145:LYS:HG3	2:B:146:SER:H	1.44	0.82
2:B:127:LYS:HE3	2:B:166:VAL:H	1.46	0.81
3:C:18:PRO:O	3:C:21:GLY:N	2.13	0.80
3:C:59:GLU:HG2	3:C:60:THR:HG23	1.64	0.79
2:B:161:LYS:HD2	2:B:161:LYS:O	1.82	0.78
3:C:34:VAL:HG13	3:C:65:ILE:HD11	1.66	0.78
2:B:121:ILE:HG22	2:B:122:ALA:H	1.48	0.77
2:B:147:VAL:HG23	2:B:149:ILE:H	1.52	0.74
3:C:98:THR:HG23	3:C:100:GLU:HG2	1.70	0.73
2:B:162:GLU:HG3	2:B:164:LYS:HB2	1.71	0.73
2:B:121:ILE:HG21	2:B:171:GLU:O	1.88	0.73
3:C:59:GLU:CG	3:C:60:THR:H	2.01	0.73
3:C:60:THR:O	3:C:61:ARG:NH2	2.23	0.71
3:C:94:VAL:H	3:C:95:GLY:HA3	1.55	0.70
1:A:1163:G:H21	2:B:36:MSE:CE	2.05	0.70
2:B:130:LYS:HG3	2:B:131:GLY:H	1.57	0.69
2:B:125:ASP:OD1	2:B:168:LYS:HG3	1.93	0.68
2:B:147:VAL:HG21	2:B:149:ILE:HD12	1.76	0.67
2:B:99:ASN:HD21	2:B:102:LYS:HG2	1.60	0.65
1:A:1196:A:O2'	1:A:1213:A:N1	2.27	0.65
3:C:59:GLU:CD	3:C:60:THR:N	2.46	0.65
2:B:123:PRO:O	2:B:169:LYS:NZ	2.30	0.64
2:B:145:LYS:HG3	2:B:146:SER:N	2.12	0.62
3:C:33:GLN:NE2	3:C:36:LYS:HE2	2.14	0.62
2:B:9:MSE:HB3	2:B:14:ILE:HD11	1.82	0.62
2:B:161:LYS:HE3	2:B:162:GLU:HB2	1.82	0.62
3:C:34:VAL:O	3:C:34:VAL:HG12	2.00	0.62
2:B:141:LEU:C	2:B:143:GLU:H	2.01	0.61
3:C:140:ASP:OD1	3:C:141:PRO:HD2	2.00	0.61
2:B:85:ASN:ND2	7:B:302:TRS:O2	2.32	0.61
2:B:122:ALA:HB1	2:B:124:CYS:O	1.99	0.61
1:A:1223:G:O6	8:A:1402:HOH:O	2.12	0.60
2:B:121:ILE:HG22	2:B:122:ALA:N	2.14	0.60
3:C:95:GLY:HA2	3:C:134:VAL:HG22	1.84	0.59
3:C:48:MSE:SE	3:C:78:LYS:HE2	2.53	0.59
2:B:116:VAL:HG23	2:B:188:PRO:HG2	1.85	0.58
2:B:127:LYS:CD	2:B:165:VAL:HA	2.27	0.58
3:C:6:GLU:HB2	3:C:53:LYS:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:VAL:HG23	2:B:149:ILE:N	2.19	0.57
2:B:140:PHE:CZ	2:B:183:ARG:HG2	2.39	0.57
1:A:1168:G:H1'	3:C:114:LEU:HG	1.87	0.57
2:B:143:GLU:O	2:B:143:GLU:HG3	2.05	0.57
2:B:125:ASP:OD1	2:B:168:LYS:HA	2.05	0.56
3:C:59:GLU:OE1	3:C:60:THR:N	2.38	0.56
2:B:140:PHE:CE1	2:B:183:ARG:HG2	2.39	0.56
1:A:1182:C:N3	1:A:1202:C:N4	2.52	0.56
2:B:145:LYS:HE2	2:B:146:SER:OG	2.05	0.56
3:C:31:VAL:O	3:C:35:VAL:HG23	2.05	0.56
3:C:59:GLU:N	3:C:59:GLU:OE1	2.39	0.55
2:B:130:LYS:HB2	2:B:160:ILE:HG13	1.87	0.55
3:C:34:VAL:CG1	3:C:65:ILE:HD11	2.36	0.55
2:B:29:VAL:HG12	2:B:200:GLU:HG3	1.89	0.54
3:C:73:THR:O	3:C:77:LYS:HG3	2.07	0.54
2:B:140:PHE:O	2:B:143:GLU:HB3	2.07	0.54
1:A:1173:G:H4'	3:C:132:MSE:HG2	1.89	0.54
1:A:1216:C:H4'	2:B:58:MSE:HE3	1.89	0.54
3:C:140:ASP:OD1	3:C:141:PRO:CD	2.56	0.54
3:C:34:VAL:HG11	3:C:54:VAL:HG11	1.90	0.54
1:A:1163:G:H21	2:B:36:MSE:HE3	1.71	0.54
2:B:130:LYS:CG	2:B:131:GLY:N	2.71	0.54
2:B:132:SER:HB3	2:B:157:LYS:CE	2.38	0.53
2:B:121:ILE:HG23	2:B:173:VAL:H	1.74	0.53
1:A:1156:A:C5	2:B:9:MSE:SE	3.11	0.53
2:B:130:LYS:HG3	2:B:131:GLY:N	2.22	0.53
4:D:0:QUA:HC8	4:D:1:ILE:N	2.23	0.53
1:A:1164:G:O6	8:A:1403:HOH:O	2.19	0.53
3:C:57:ASP:OD1	3:C:62:LYS:N	2.42	0.53
3:C:4:VAL:HG11	3:C:53:LYS:HE3	1.91	0.52
3:C:96:ASN:HD21	3:C:138:GLY:HA2	1.73	0.52
2:B:130:LYS:HD3	2:B:161:LYS:C	2.30	0.52
1:A:1170:U:OP2	3:C:109:LYS:NZ	2.43	0.52
3:C:80:LEU:HD21	3:C:97:LEU:HG	1.91	0.51
4:D:0:QUA:O16	4:D:10:TS9:HD13	2.11	0.51
3:C:94:VAL:N	3:C:95:GLY:HA3	2.20	0.51
1:A:1194:A:OP1	2:B:47:ARG:NH2	2.43	0.51
2:B:53:LYS:O	2:B:96:THR:OG1	2.28	0.50
3:C:57:ASP:OD2	3:C:62:LYS:HB2	2.11	0.50
2:B:135:MSE:HE3	2:B:140:PHE:CE2	2.45	0.50
3:C:99:LEU:HD22	3:C:153:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:TYR:O	3:C:155:GLU:N	2.40	0.50
1:A:1157:G:OP1	2:B:60:ARG:NH1	2.44	0.49
3:C:57:ASP:HB2	3:C:59:GLU:CD	2.33	0.49
3:C:119:LYS:O	3:C:123:LYS:HG3	2.13	0.49
2:B:177:LEU:O	2:B:181:LEU:HG	2.12	0.49
3:C:24:ILE:O	3:C:27:LEU:N	2.25	0.48
4:D:0:QUA:HC8	4:D:1:ILE:CA	2.42	0.48
2:B:147:VAL:CG2	2:B:149:ILE:H	2.23	0.48
4:D:0:QUA:C7	4:D:1:ILE:CA	2.81	0.48
3:C:60:THR:C	3:C:61:ARG:HG3	2.34	0.48
1:A:1166:G:H5''	1:A:1167:A:H5'	1.95	0.47
2:B:49:LYS:NZ	2:B:110:ASN:OD1	2.28	0.47
3:C:147:GLU:OE1	3:C:153:TYR:HE1	1.96	0.47
2:B:150:PRO:HB2	2:B:161:LYS:HB3	1.96	0.47
3:C:33:GLN:HE22	3:C:36:LYS:HE2	1.78	0.47
1:A:1164:G:H1'	2:B:36:MSE:HE2	1.96	0.46
1:A:1156:A:C4	2:B:9:MSE:SE	3.19	0.46
2:B:49:LYS:HE3	2:B:49:LYS:HB3	1.53	0.46
2:B:144:LEU:HD13	2:B:160:ILE:HG22	1.97	0.46
2:B:162:GLU:CG	2:B:164:LYS:HB2	2.44	0.46
2:B:93:ILE:HA	2:B:93:ILE:HD13	1.77	0.46
2:B:121:ILE:CG2	2:B:122:ALA:H	2.17	0.45
2:B:140:PHE:HB3	2:B:158:ILE:CD1	2.46	0.45
3:C:11:GLY:O	3:C:46:GLU:HA	2.16	0.45
3:C:98:THR:O	3:C:101:GLN:HB2	2.16	0.45
3:C:99:LEU:O	3:C:103:ILE:HG13	2.17	0.45
1:A:1180:A:C8	1:A:1207:C:O5'	2.70	0.45
4:D:0:QUA:O15	4:D:6:BB9:HB	2.16	0.44
3:C:49:GLN:OE1	3:C:49:GLN:N	2.50	0.44
3:C:115:SER:HB3	3:C:120:ASN:HB3	2.00	0.44
3:C:100:GLU:O	3:C:104:LYS:HG2	2.18	0.44
2:B:46:ILE:O	2:B:50:ILE:HG12	2.17	0.44
1:A:1186:C:H1'	3:C:89:PRO:HD2	1.98	0.44
2:B:120:GLN:C	2:B:121:ILE:CG1	2.69	0.44
3:C:45:TYR:CD2	3:C:50:VAL:HG21	2.53	0.44
3:C:37:GLU:OE1	3:C:65:ILE:HG13	2.17	0.44
2:B:144:LEU:HB3	2:B:149:ILE:O	2.18	0.43
2:B:96:THR:HG23	2:B:98:MSE:H	1.83	0.43
3:C:18:PRO:HD2	4:D:9:DCY:HB2	1.99	0.43
2:B:145:LYS:CG	2:B:146:SER:N	2.81	0.43
2:B:174:SER:HB3	2:B:177:LEU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:90:ARG:NH2	3:C:142:LYS:HG3	2.34	0.43
2:B:132:SER:HB3	2:B:157:LYS:HE2	2.01	0.43
3:C:45:TYR:HA	3:C:48:MSE:HE2	1.99	0.43
2:B:85:ASN:HD21	7:B:302:TRS:C2	2.31	0.43
3:C:37:GLU:HA	3:C:40:GLU:HB3	2.00	0.43
3:C:141:PRO:C	3:C:143:GLU:N	2.72	0.42
2:B:98:MSE:HE2	2:B:102:LYS:HB3	2.02	0.42
2:B:143:GLU:HA	2:B:145:LYS:HZ2	1.84	0.42
1:A:1174:C:H5"	3:C:84:THR:HG23	2.01	0.42
2:B:88:GLU:HG2	2:B:89:ARG:N	2.34	0.42
3:C:98:THR:CG2	3:C:100:GLU:HG2	2.47	0.42
3:C:20:LEU:O	3:C:24:ILE:HG12	2.20	0.42
2:B:141:LEU:C	2:B:143:GLU:N	2.72	0.42
2:B:127:LYS:HE2	2:B:127:LYS:HA	2.02	0.41
2:B:162:GLU:HG3	2:B:164:LYS:CB	2.47	0.41
3:C:50:VAL:HA	3:C:51:PRO:HD3	1.91	0.41
3:C:82:ILE:HG22	3:C:83:GLU:H	1.85	0.41
2:B:143:GLU:HA	2:B:145:LYS:NZ	2.35	0.41
3:C:82:ILE:HG22	3:C:83:GLU:N	2.35	0.41
2:B:127:LYS:NZ	2:B:166:VAL:HG23	2.35	0.41
2:B:140:PHE:O	2:B:141:LEU:C	2.59	0.41
2:B:122:ALA:HA	2:B:123:PRO:HD2	1.65	0.41
2:B:144:LEU:HB3	2:B:149:ILE:HB	2.03	0.41
2:B:27:LYS:HB3	2:B:28:PRO:HD2	2.02	0.41
2:B:150:PRO:HG2	2:B:161:LYS:HG3	2.02	0.41
4:D:0:QUA:H15	4:D:6:BB9:HB	1.85	0.41
2:B:121:ILE:CG1	2:B:172:VAL:HA	2.39	0.41
2:B:113:PRO:HA	2:B:189:ILE:O	2.21	0.41
2:B:40:ALA:HB3	2:B:41:PRO:HD3	2.03	0.41
3:C:97:LEU:HD12	3:C:134:VAL:HG11	2.01	0.41
2:B:9:MSE:HE2	2:B:9:MSE:N	2.36	0.41
3:C:59:GLU:CG	3:C:60:THR:N	2.79	0.40
2:B:140:PHE:HB3	2:B:158:ILE:HD13	2.04	0.40
2:B:209:VAL:O	2:B:212:VAL:HG22	2.22	0.40
2:B:29:VAL:HG22	2:B:96:THR:O	2.21	0.40
3:C:34:VAL:HG22	3:C:63:PHE:CG	2.56	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	
2	B	205/213 (96%)	193 (94%)	11 (5%)	1 (0%)	34	69
3	C	156/161 (97%)	146 (94%)	8 (5%)	2 (1%)	15	44
4	D	5/19 (26%)	4 (80%)	1 (20%)	0	100	100
All	All	366/393 (93%)	343 (94%)	20 (6%)	3 (1%)	24	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	ILE
3	C	59	GLU
3	C	18	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	175/174 (101%)	164 (94%)	11 (6%)	22	53
3	C	132/129 (102%)	122 (92%)	10 (8%)	16	42
4	D	3/4 (75%)	3 (100%)	0	100	100
All	All	310/307 (101%)	289 (93%)	21 (7%)	20	49

All (21) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
2	B	29	VAL
2	B	112	SER
2	B	117	ARG
2	B	120	GLN
2	B	121	ILE
2	B	124	CYS
2	B	132	SER
2	B	143	GLU
2	B	145	LYS
2	B	161	LYS
2	B	208	ASP
3	C	15	THR
3	C	33	GLN
3	C	36	LYS
3	C	40	GLU
3	C	43	LYS
3	C	48	MSE
3	C	59	GLU
3	C	61	ARG
3	C	84	THR
3	C	158	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	85	ASN
2	B	120	GLN
3	C	30	ASN
3	C	33	GLN
3	C	96	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	73/74 (98%)	8 (10%)	1 (1%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1170	U
1	A	1179	A

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Mol	Chain	Res	Type
1	A	1180	A
1	A	1193	U
1	A	1198	A
1	A	1207	C
1	A	1221	A
1	A	1222	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	A

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

11 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$
4	TS9	D	10	4	7,8,10	0.46	0	7,12,15	1.30	0
4	BB9	D	11	4	3,5,6	1.03	0	1,5,7	3.63	1 (100%)
4	BB9	D	13	4	2,4,6	0.88	0	3,4,7	4.61	3 (100%)
4	MH6	D	14	4	3,3,6	1.80	1 (33%)	1,3,7	1.78	0
4	BB9	D	15	4	3,5,6	1.40	0	1,5,7	4.10	1 (100%)
4	DHA	D	16	4	4,4,5	1.34	0	3,4,6	2.00	2 (66%)
4	DHA	D	17	4	4,4,5	0.89	0	3,4,6	2.46	2 (66%)
4	DHA	D	3	4	4,4,5	0.92	0	3,4,6	2.15	1 (33%)
4	BB9	D	6	4	3,5,6	1.45	0	1,5,7	4.41	1 (100%)
4	DBU	D	8	4	4,4,6	1.22	0	1,4,7	2.78	1 (100%)
4	DCY	D	9	4	3,5,6	2.02	1 (33%)	3,5,7	1.62	0

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
4	TS9	D	10	4	-	0/9/12/16	0/0/0/0
4	BB9	D	11	4	-	0/0/4/6	0/0/0/0
4	BB9	D	13	4	-	0/0/2/6	0/0/0/0
4	MH6	D	14	4	-	0/0/0/6	0/0/0/0
4	BB9	D	15	4	-	0/0/4/6	0/0/0/0
4	DHA	D	16	4	-	0/0/2/4	0/0/0/0
4	DHA	D	17	4	-	0/0/2/4	0/0/0/0
4	DHA	D	3	4	-	0/0/2/4	0/0/0/0
4	BB9	D	6	4	-	0/0/4/6	0/0/0/0
4	DBU	D	8	4	-	0/1/2/6	0/0/0/0
4	DCY	D	9	4	-	0/1/4/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	14	MH6	C-CA	-2.94	1.45	1.49
4	D	9	DCY	CB-SG	3.05	1.88	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	6	BB9	O-C-CA	-4.41	119.43	125.59
4	D	15	BB9	O-C-CA	-4.10	119.87	125.59
4	D	11	BB9	O-C-CA	-3.63	120.53	125.59
4	D	3	DHA	O-C-CA	-3.61	118.16	125.33
4	D	17	DHA	O-C-CA	-3.25	118.89	125.33
4	D	13	BB9	CB-CA-N	-3.12	111.36	122.39
4	D	17	DHA	CB-CA-N	-2.72	119.54	126.11
4	D	16	DHA	O-C-CA	-2.55	120.26	125.33
4	D	16	DHA	CB-CA-N	-2.23	120.71	126.11
4	D	13	BB9	C-CA-CB	2.36	124.03	120.96
4	D	8	DBU	C-CA-N	2.78	119.73	116.52
4	D	13	BB9	C-CA-N	6.97	124.56	116.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	10	TS9	1	0
4	D	6	BB9	2	0
4	D	9	DCY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	$\# Z  > 2$
7	TRS	A	1314	-	7,7,7	0.86	0	9,9,9	0.52	0
7	TRS	A	1315	-	7,7,7	1.03	0	9,9,9	1.62	3 (33%)
7	TRS	B	302	-	7,7,7	0.88	1 (14%)	9,9,9	1.02	0

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
7	TRS	A	1314	-	-	0/9/9/9	0/0/0/0
7	TRS	A	1315	-	-	0/9/9/9	0/0/0/0
7	TRS	B	302	-	-	0/9/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	302	TRS	C-N	-2.03	1.48	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	A	1315	TRS	C3-C-N	-2.55	103.55	107.88
7	A	1315	TRS	C2-C-N	2.30	111.78	107.88
7	A	1315	TRS	C1-C-N	2.34	111.85	107.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	302	TRS	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	1
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	11:BB9	C	12:THR	N	1.17
1	C	44:ASP	C	45:TYR	N	0.91

## 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	74/74 (100%)	-0.07	0 100 100	63, 72, 84, 93	0
2	B	201/213 (94%)	0.34	18 (8%) 12 6	63, 95, 170, 178	0
3	C	153/161 (95%)	0.28	7 (4%) 36 25	24, 112, 164, 177	0
4	D	6/19 (31%)	0.13	0 100 100	76, 77, 84, 87	0
All	All	434/467 (92%)	0.25	25 (5%) 26 16	24, 98, 168, 178	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	167	VAL	6.4
2	B	165	VAL	6.1
2	B	126	ILE	4.8
2	B	178	ALA	4.1
3	C	34	VAL	3.8
2	B	173	VAL	3.7
2	B	180	VAL	3.3
3	C	43	LYS	3.2
2	B	10	ALA	3.0
3	C	95	GLY	3.0
2	B	118	GLY	2.7
3	C	83	GLU	2.6
3	C	143	GLU	2.6
2	B	128	VAL	2.6
2	B	125	ASP	2.5
2	B	149	ILE	2.4
3	C	99	LEU	2.3
2	B	152	ALA	2.3
2	B	117	ARG	2.3
3	C	56	VAL	2.2
2	B	164	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	127	LYS	2.1
2	B	151	ALA	2.1
2	B	112	SER	2.0
2	B	166	VAL	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
4	DBU	D	8	5/7	0.98	0.21	-	79,81,83,83	0
4	BB9	D	11	6/7	0.96	0.15	-	85,86,89,97	0
4	BB9	D	6	6/7	0.91	0.17	-	63,68,71,77	0
4	BB9	D	13	5/7	0.95	0.14	-	76,76,83,83	0
4	MH6	D	14	4/7	0.93	0.10	-	80,80,80,87	0
4	DHA	D	17	5/6	0.82	1.02	-	122,127,128,129	1
4	DCY	D	9	6/7	0.93	0.14	-	85,88,95,101	0
4	TS9	D	10	9/11	0.92	0.20	-	74,85,90,92	0
4	BB9	D	15	6/7	0.90	0.13	-	97,107,112,114	0
4	DHA	D	16	5/6	0.69	0.57	-	121,122,130,130	0
4	DHA	D	3	5/6	0.96	0.19	-	77,79,81,83	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( $\text{\AA}^2$ )	Q<0.9
7	TRS	A	1315	8/8	0.82	0.37	6.58	75,82,90,91	0
6	NA	A	1313	1/1	0.91	0.24	5.63	84,84,84,84	0
5	MG	A	1303	1/1	0.81	0.26	5.00	68,68,68,68	0
5	MG	A	1308	1/1	0.54	0.14	-1.13	109,109,109,109	0
5	MG	A	1302	1/1	0.93	0.10	-2.71	71,71,71,71	0
6	NA	A	1312	1/1	0.28	1.24	-	114,114,114,114	0
5	MG	A	1306	1/1	0.93	0.03	-	95,95,95,95	0
5	MG	A	1310	1/1	0.84	0.52	-	125,125,125,125	0
5	MG	A	1309	1/1	0.68	0.15	-	82,82,82,82	0
7	TRS	A	1314	8/8	0.88	0.61	-	87,91,95,95	0
5	MG	A	1305	1/1	0.94	0.13	-	64,64,64,64	0
6	NA	B	301	1/1	0.89	0.42	-	86,86,86,86	0
5	MG	A	1304	1/1	0.95	0.11	-	65,65,65,65	0
5	MG	A	1301	1/1	0.97	0.11	-	60,60,60,60	0
5	MG	C	201	1/1	0.91	0.14	-	92,92,92,92	0
6	NA	A	1311	1/1	0.81	0.21	-	87,87,87,87	0
5	MG	A	1307	1/1	0.82	0.20	-	77,77,77,77	0
7	TRS	B	302	8/8	0.90	0.24	-	83,86,93,100	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.