



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:43 AM GMT

PDB ID : 1VQL  
Title : The structure of the transition state analogue "DCSN" bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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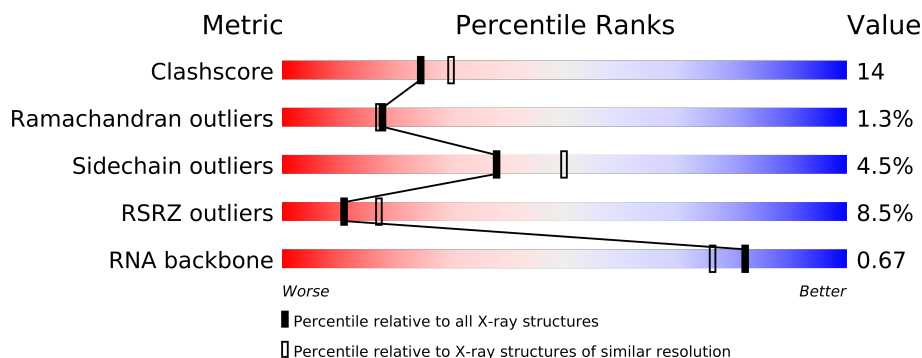
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.30 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.














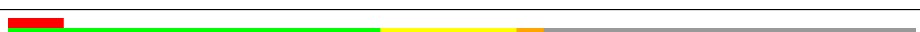
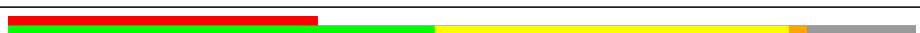

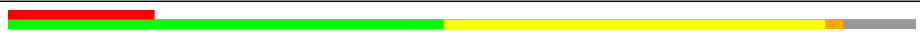



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)
RNA backbone	1838	1081 (3.00-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	4	7	
4	A	240	
5	B	338	
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	

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Mol	Chain	Length	Quality of chain
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	
32	I	162	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
34	MG	0	8001	-	X
34	MG	0	8008	-	X
34	MG	0	8012	-	X
34	MG	0	8013	-	X
34	MG	0	8014	-	X
34	MG	0	8021	-	X
34	MG	0	8022	-	X
34	MG	0	8024	-	X
34	MG	0	8025	-	X
34	MG	0	8026	-	X
34	MG	0	8027	-	X
34	MG	0	8029	-	X
34	MG	0	8038	-	X
34	MG	0	8040	-	X
34	MG	0	8047	-	X
34	MG	0	8050	-	X
34	MG	0	8051	-	X
34	MG	0	8052	-	X
34	MG	0	8055	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	MG	0	8057	-	X
34	MG	0	8058	-	X
34	MG	0	8059	-	X
34	MG	0	8065	-	X
34	MG	0	8070	-	X
34	MG	0	8082	-	X
34	MG	0	8084	-	X
34	MG	0	8089	-	X
34	MG	0	8090	-	X
34	MG	0	8092	-	X
34	MG	0	8094	-	X
34	MG	0	8101	-	X
34	MG	0	8103	-	X
34	MG	0	8108	-	X
34	MG	0	8114	-	X
34	MG	0	8118	-	X
34	MG	9	8095	-	X
34	MG	K	8069	-	X
35	K	0	9001	-	X
36	NA	0	9102	-	X
36	NA	0	9106	-	X
36	NA	0	9107	-	X
36	NA	0	9111	-	X
36	NA	0	9116	-	X
36	NA	0	9118	-	X
36	NA	0	9120	-	X
36	NA	0	9122	-	X
36	NA	0	9125	-	X
36	NA	0	9129	-	X
36	NA	0	9132	-	X
36	NA	0	9135	-	X
36	NA	0	9140	-	X
36	NA	0	9150	-	X
36	NA	0	9152	-	X
36	NA	0	9156	-	X
36	NA	0	9157	-	X
36	NA	0	9158	-	X
36	NA	0	9160	-	X
36	NA	0	9161	-	X
36	NA	0	9162	-	X
36	NA	0	9163	-	X
36	NA	0	9164	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	NA	0	9165	-	X
36	NA	0	9167	-	X
36	NA	0	9168	-	X
36	NA	0	9169	-	X
36	NA	0	9170	-	X
36	NA	0	9171	-	X
36	NA	0	9172	-	X
36	NA	0	9173	-	X
36	NA	0	9174	-	X
36	NA	0	9175	-	X
36	NA	0	9177	-	X
36	NA	0	9178	-	X
36	NA	0	9179	-	X
36	NA	0	9184	-	X
36	NA	0	9185	-	X
36	NA	9	9183	-	X
36	NA	R	9186	-	X
36	NA	S	9112	-	X
37	CL	0	9316	-	X
37	CL	0	9322	-	X
38	SR	0	9405	-	X
38	SR	0	9406	-	X
38	SR	0	9408	-	X
38	SR	0	9432	-	X
38	SR	0	9434	-	X
38	SR	0	9467	-	X
38	SR	0	9482	-	X
38	SR	0	9521	-	X
38	SR	0	9534	-	X
38	SR	0	9539	-	X
38	SR	0	9547	-	X
38	SR	0	9626	-	X
38	SR	C	9500	-	X

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99053 atoms, of which 0 are hydrogen and 0 are deuterium.

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	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 3377779
0	2587	OMU	U	MODIFIED RESIDUE	GB 3377779
0	2588	OMG	G	MODIFIED RESIDUE	GB 3377779
0	2619	UR3	U	MODIFIED RESIDUE	GB 3377779
0	2621	PSU	U	MODIFIED RESIDUE	GB 3377779

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(\*CP\*CP\*(PPU)\*(TSE)\*(DA)\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	S	0	0	0
			1118	670	222	226				

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

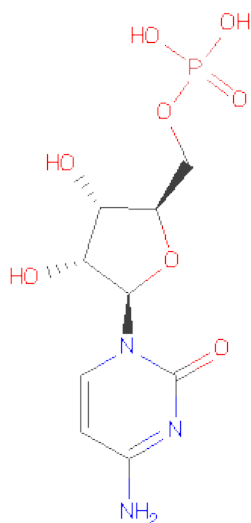
- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is THIOPHOSPHONOACETIC ACID (three-letter code: C, TSE, DA) (formula:  $C_9H_{14}N_3O_8P$ ,  $C_2H_5O_4PS$ ,  $C_{10}H_{14}N_5O_6P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	4	4	Total	C	N	O	P S	0	0
			64	30	11	19	3 1		

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	89	Total	Mg	0	0
			89	89		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	Y	1	Total 1	Mg 1	0	0
34	K	1	Total 1	Mg 1	0	0
34	A	1	Total 1	Mg 1	0	0
34	T	1	Total 1	Mg 1	0	0
34	9	1	Total 1	Mg 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total 2	K 2	0	0

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	64	Total 64	Na 64	0	0
36	J	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	T	1	Total 1	Na 1	0	0
36	R	3	Total 3	Na 3	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total	Cl	0	0
			10	10		
37	J	3	Total	Cl	0	0
			3	3		
37	B	1	Total	Cl	0	0
			1	1		
37	A	1	Total	Cl	0	0
			1	1		
37	N	1	Total	Cl	0	0
			1	1		
37	O	1	Total	Cl	0	0
			1	1		
37	R	1	Total	Cl	0	0
			1	1		
37	Y	1	Total	Cl	0	0
			1	1		
37	L	1	Total	Cl	0	0
			1	1		
37	3	1	Total	Cl	0	0
			1	1		
37	M	1	Total	Cl	0	0
			1	1		

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total	Sr	0	0
			98	98		
38	1	2	Total	Sr	0	0
			2	2		
38	H	1	Total	Sr	0	0
			1	1		
38	B	1	Total	Sr	0	0
			1	1		
38	C	1	Total	Sr	0	0
			1	1		
38	3	1	Total	Sr	0	0
			1	1		
38	A	3	Total	Sr	0	0
			3	3		
38	R	1	Total	Sr	0	0
			1	1		
38	9	3	Total	Sr	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5735	Total 5735	O 5735	0	0
40	9	136	Total 136	O 136	0	0
40	4	6	Total 6	O 6	0	0
40	A	128	Total 128	O 128	0	0
40	B	139	Total 139	O 139	0	0
40	C	174	Total 174	O 174	0	0
40	D	50	Total 50	O 50	0	0
40	E	43	Total 43	O 43	0	0
40	F	28	Total 28	O 28	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	G	16	Total 16	O 16	0	0
40	H	71	Total 71	O 71	0	0
40	J	52	Total 52	O 52	0	0
40	K	59	Total 59	O 59	0	0
40	L	80	Total 80	O 80	0	0
40	M	127	Total 127	O 127	0	0
40	N	60	Total 60	O 60	0	0
40	O	37	Total 37	O 37	0	0
40	P	58	Total 58	O 58	0	0
40	Q	48	Total 48	O 48	0	0
40	R	87	Total 87	O 87	0	0
40	S	29	Total 29	O 29	0	0
40	T	36	Total 36	O 36	0	0
40	U	27	Total 27	O 27	0	0
40	V	11	Total 11	O 11	0	0
40	W	69	Total 69	O 69	0	0
40	X	24	Total 24	O 24	0	0
40	Y	87	Total 87	O 87	0	0
40	Z	31	Total 31	O 31	0	0
40	1	55	Total 55	O 55	0	0
40	2	42	Total 42	O 42	0	0

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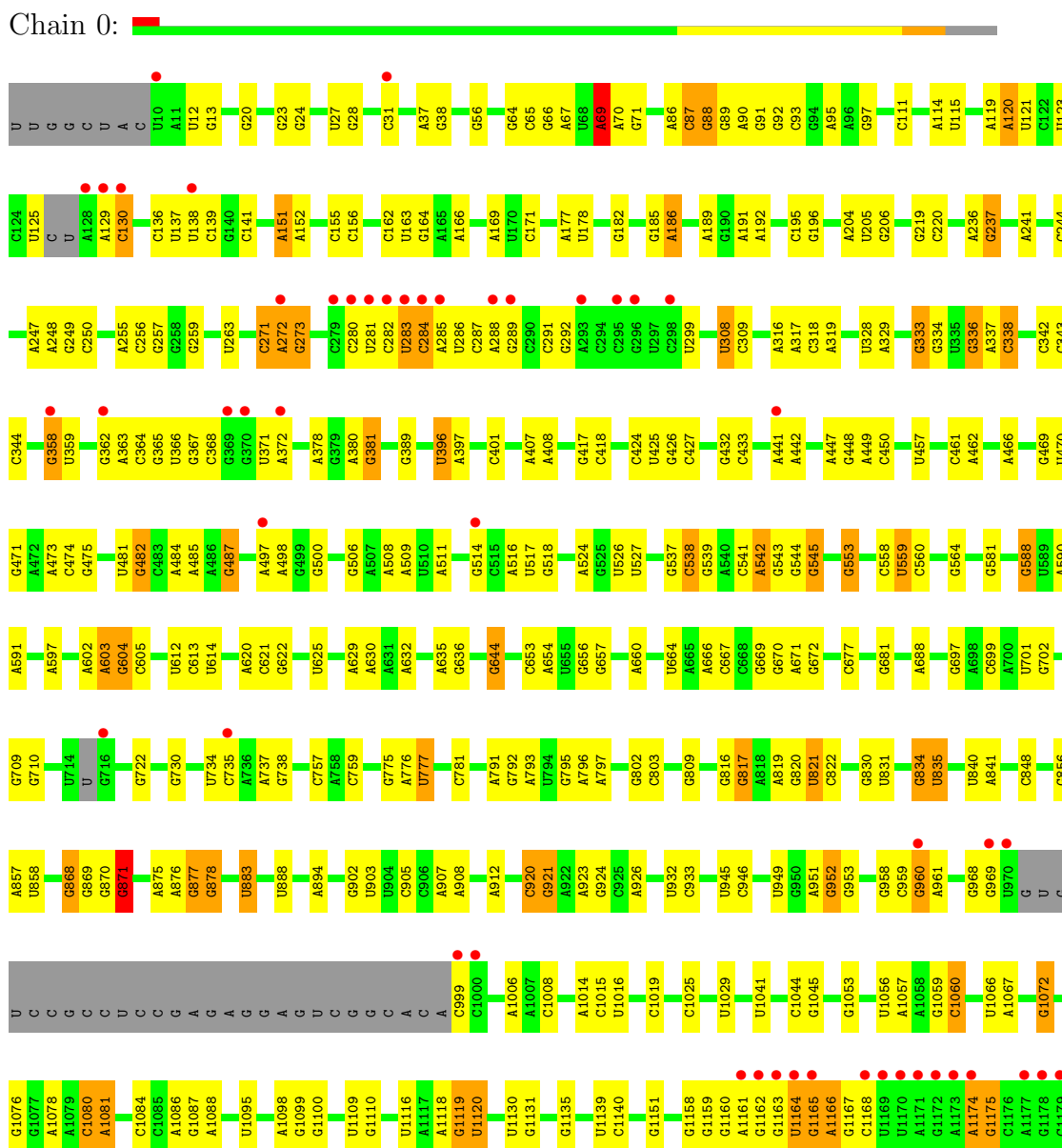
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	3	65	Total 65	O 65	0	0
40	I	9	Total 9	O 9	0	0



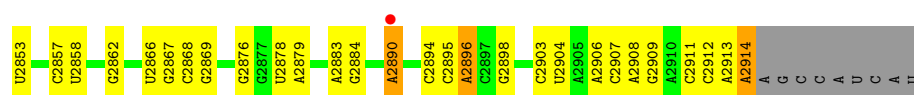
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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







• Molecule 2: 5S ribosomal RNA

Chain 9:



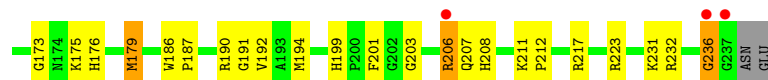
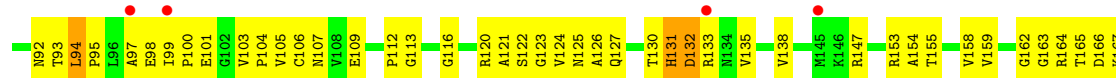
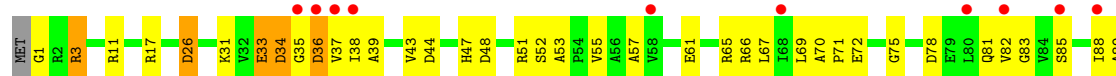
• Molecule 3: 5'-R(\*CP\*CP\*(PPU)\*(TSE)\*(DA)\*CP\*C)-3'

Chain 4:



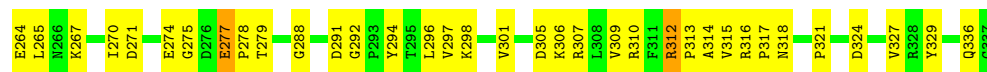
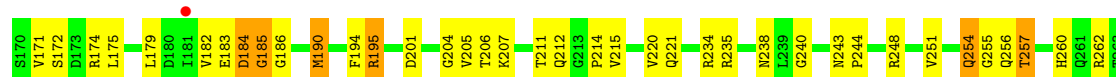
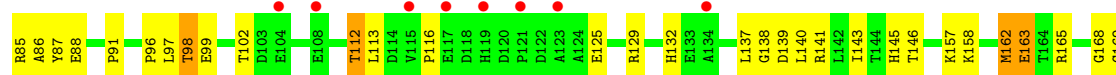
• Molecule 4: 50S ribosomal protein L2P

Chain A:



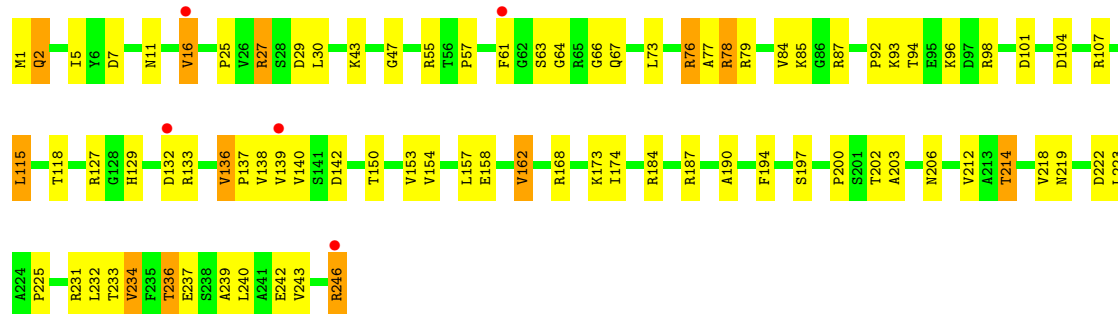
• Molecule 5: 50S ribosomal protein L3P

Chain B:



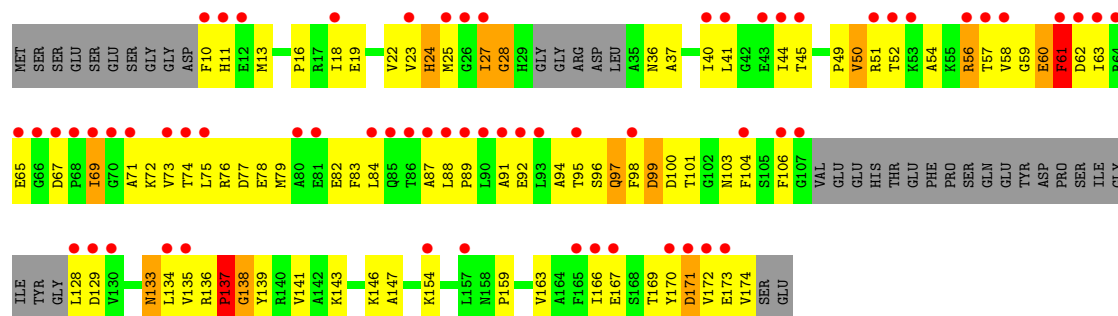
• Molecule 6: 50S ribosomal protein L4E

## Chain C:



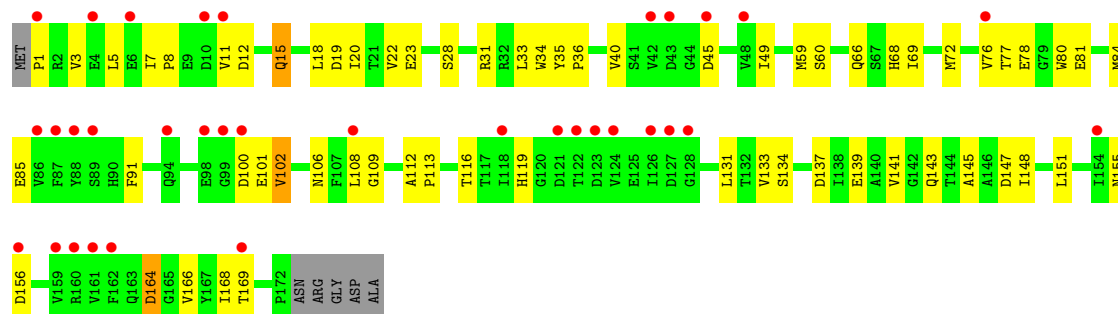
- Molecule 7: 50S ribosomal protein L5P

## Chain D:



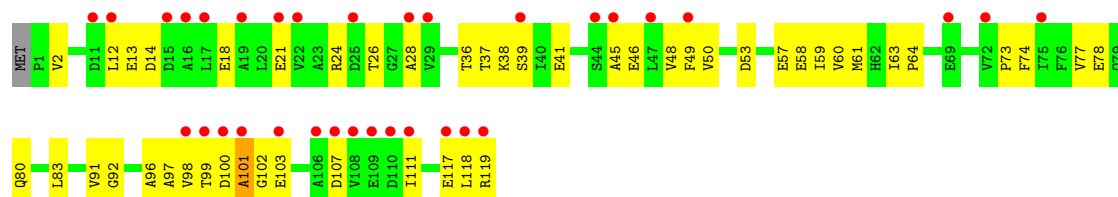
- Molecule 8: 50S ribosomal protein L6P

## Chain E:



- Molecule 9: 50S ribosomal protein L7AE

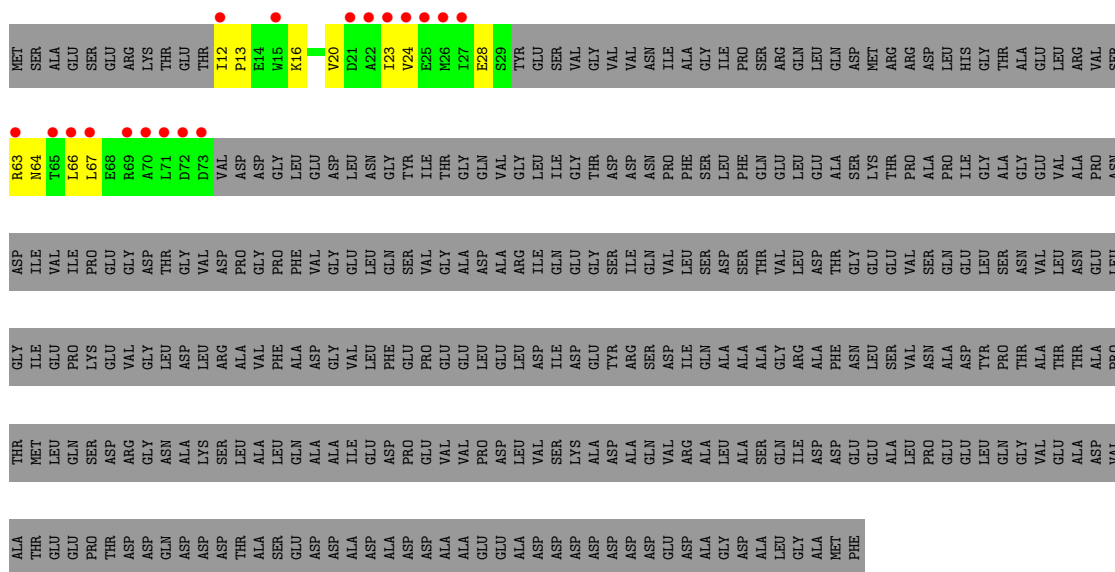
## Chain F:



- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

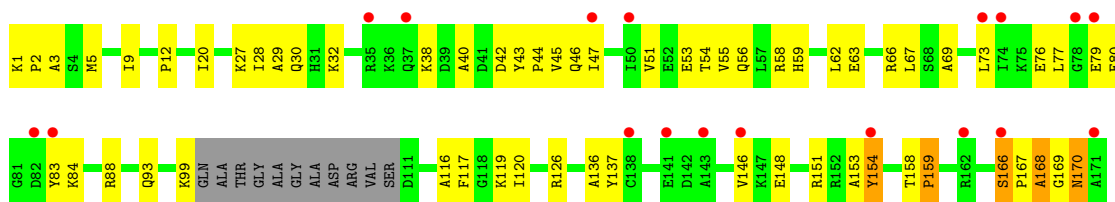
## Chain G:





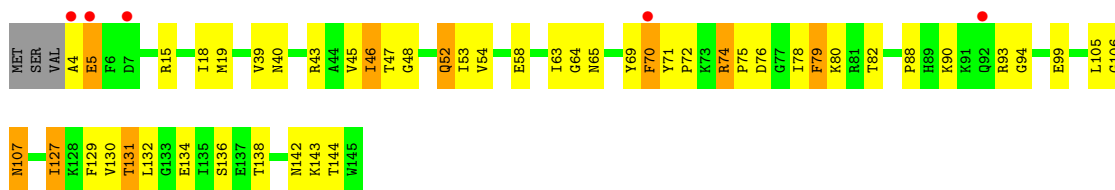
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



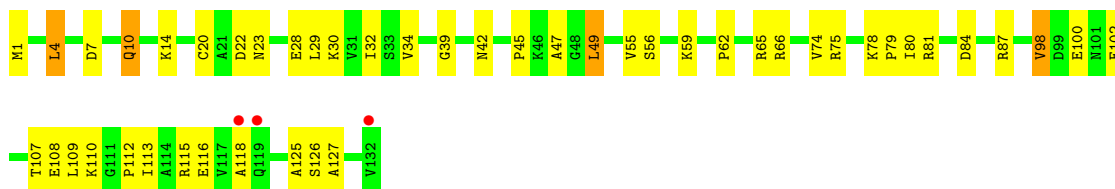
- Molecule 12: 50S ribosomal protein L13P

Chain J: 



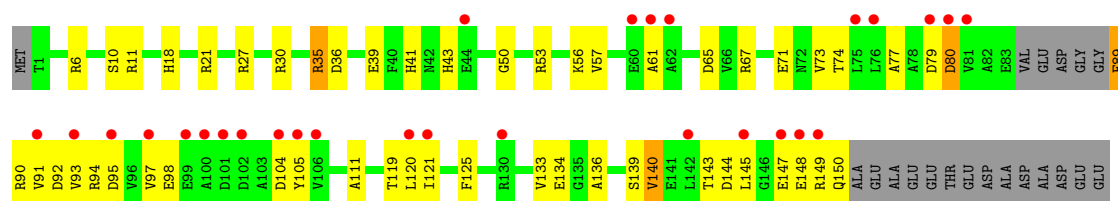
- Molecule 13: 50S ribosomal protein L14P

Chain K: 



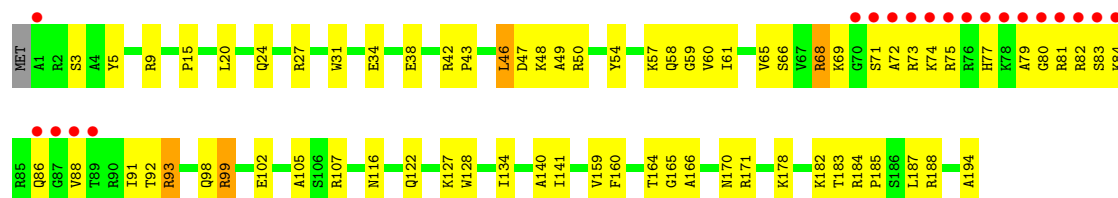
- Molecule 14: 50S ribosomal protein L15P

Chain L:



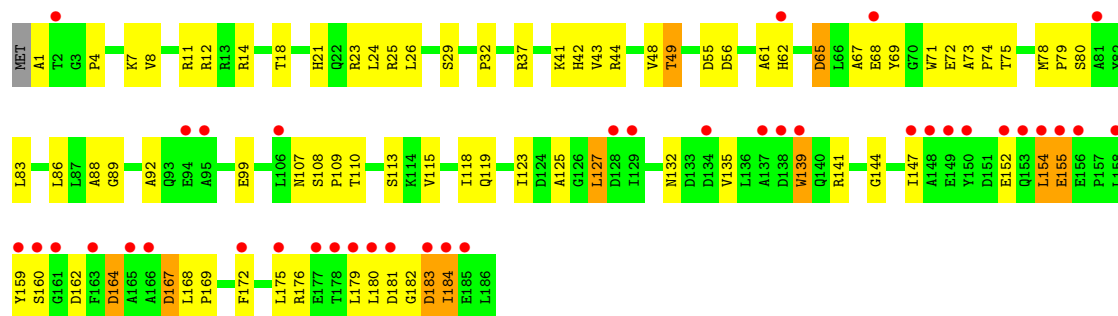
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



• Molecule 16: 50S ribosomal protein L18P

Chain N:



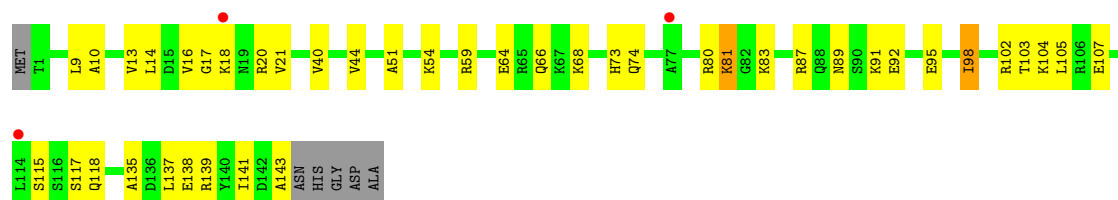
• Molecule 17: 50S ribosomal protein L18e

Chain O:



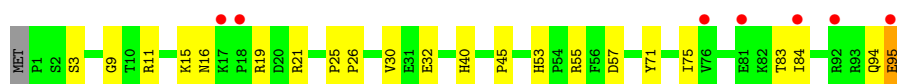
• Molecule 18: 50S ribosomal protein L19E

Chain P:



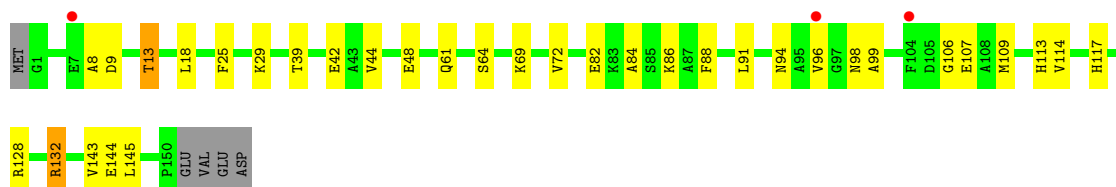
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



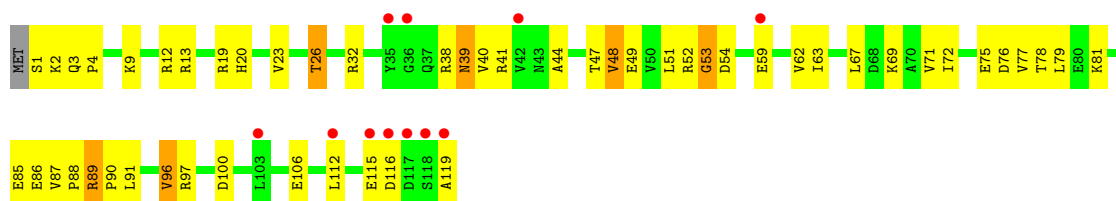
- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



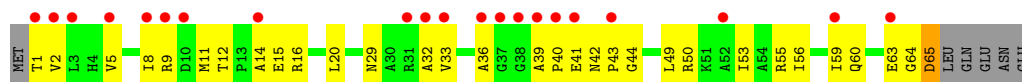
- Molecule 23: 50S ribosomal protein L24E

Chain U:



- Molecule 24: 50S ribosomal protein L29P

Chain V:



- Molecule 25: 50S ribosomal protein L30P

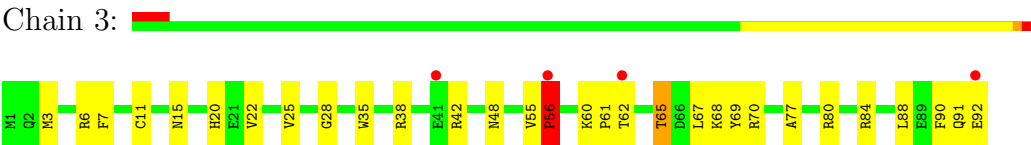
Chain W:



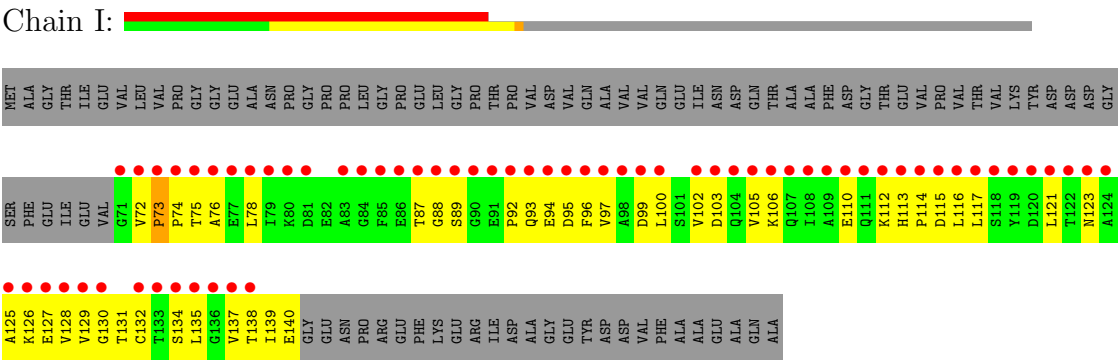




● Molecule 31: 50S ribosomal protein L44E



● Molecule 32: 50S RIBOSOMAL PROTEIN L11P



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.44Å 298.56Å 574.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.30) 89.4 (49.76-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.251 0.213 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 787866 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99053	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, PPU, CL, SR, NA, K, TSE, CD, OMU, UR3, 1MA, PSU

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	0	0.37	0/65959	0.69	27/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.52	0/40	0.54	0/60
4	A	0.33	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.56	0/1880
9	F	0.31	0/901	0.55	0/1224
10	G	0.27	0/241	0.46	0/324
11	H	0.33	0/1287	0.65	0/1725
12	J	0.34	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.61	0/2119
16	N	0.28	0/1474	0.61	0/1999
17	O	0.32	0/874	0.58	0/1181
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.36	0/749	0.69	0/1005
20	R	0.34	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.29	0/958	0.62	0/1289
23	U	0.35	0/417	0.57	0/562
24	V	0.27	0/502	0.51	0/675
25	W	0.33	0/1219	0.60	0/1655
26	X	0.33	0/664	0.57	0/895
27	Y	0.35	0/1146	0.64	0/1536
28	Z	0.33	0/589	0.58	0/787
29	1	0.44	0/438	0.67	0/578
30	2	0.34	0/401	0.60	0/529
31	3	0.37	0/771	0.57	0/1024
32	I	0.29	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98732	0.67	29/147637 (0.0%)

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
1	0	1	46
2	9	0	2
All	All	1	48

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.71	130.86	109.50
1	0	871	G	C5'-C4'-O4'	-7.68	99.89	109.10
2	9	3039	U	N1-C1'-C2'	7.28	123.46	114.00
1	0	1942	A	C5'-C4'-C3'	7.25	127.60	116.00
1	0	1592	G	N9-C1'-C2'	6.96	123.05	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	469	G	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	756	0
2	9	2600	0	1326	59	0
3	4	74	0	49	1	0
4	A	1753	0	1765	117	0
5	B	2625	0	2531	135	0
6	C	1859	0	1816	96	0
7	D	1094	0	1085	91	0
8	E	1357	0	1266	59	0
9	F	890	0	843	49	0
10	G	240	0	231	13	0
11	H	1266	0	1268	63	0
12	J	1120	0	1098	72	0
13	K	992	0	1031	51	0
14	L	1118	0	1076	51	0
15	M	1560	0	1568	71	0
16	N	1445	0	1401	83	0
17	O	865	0	873	35	0
18	P	1136	0	1123	39	0
19	Q	735	0	728	22	0
20	R	1149	0	1122	39	0
21	S	641	0	605	16	0
22	T	950	0	924	54	0
23	U	410	0	364	17	0
24	V	499	0	511	33	0
25	W	1196	0	1137	91	0
26	X	654	0	653	34	0
27	Y	1130	0	1133	47	0
28	Z	578	0	539	34	0
29	1	431	0	426	25	0
30	2	396	0	413	34	0
31	3	755	0	728	29	0
32	I	519	0	500	47	0
33	4	64	0	36	5	0
34	0	89	0	0	0	0
34	9	1	0	0	0	0
34	A	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	0	64	0	0	0	0
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	3	0	0	0	0
36	S	1	0	0	0	0
36	T	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	1	0	0	0	0
38	C	1	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5735	0	0	103	0
40	1	55	0	0	1	0
40	2	42	0	0	2	0
40	3	65	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	4	6	0	0	0	0
40	9	136	0	0	5	0
40	A	128	0	0	10	0
40	B	139	0	0	18	0
40	C	174	0	0	19	0
40	D	50	0	0	8	0
40	E	43	0	0	3	0
40	F	28	0	0	2	0
40	G	16	0	0	2	0
40	H	71	0	0	6	0
40	I	9	0	0	1	0
40	J	52	0	0	3	0
40	K	59	0	0	4	0
40	L	80	0	0	9	0
40	M	127	0	0	5	0
40	N	60	0	0	10	0
40	O	37	0	0	0	0
40	P	58	0	0	1	0
40	Q	48	0	0	4	0
40	R	87	0	0	5	0
40	S	29	0	0	2	0
40	T	36	0	0	6	0
40	U	27	0	0	2	0
40	V	11	0	0	1	0
40	W	69	0	0	4	0
40	X	24	0	0	5	0
40	Y	87	0	0	8	0
40	Z	31	0	0	5	0
All	All	99053	0	59982	2116	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 2116 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.11
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.32	1.06
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.22	1.04
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.73	1.03
2:9:3076:G:H3'	2:9:3077:A:H5''	1.40	1.00

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	
4	A	235/240 (98%)	214 (91%)	16 (7%)	5 (2%)	11	8
5	B	335/338 (99%)	313 (93%)	17 (5%)	5 (2%)	15	13
6	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
7	D	134/177 (76%)	106 (79%)	16 (12%)	12 (9%)	1	0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
9	F	117/120 (98%)	104 (89%)	12 (10%)	1 (1%)	25	26
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	18	17
12	J	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	11	8
13	K	130/132 (98%)	119 (92%)	10 (8%)	1 (1%)	27	30
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	30	34
15	M	192/195 (98%)	181 (94%)	10 (5%)	1 (0%)	38	45
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	5	2
17	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
18	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	14	11
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	14	12
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	3	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	21	21
32	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	7	4
All	All	3705/4431 (84%)	3420 (92%)	237 (6%)	48 (1%)	18	17

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
7	D	27	ILE
7	D	60	GLU
7	D	137	PRO
11	H	166	SER

### 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	
4	A	179/182 (98%)	168 (94%)	11 (6%)	26	34
5	B	282/283 (100%)	265 (94%)	17 (6%)	27	35
6	C	193/193 (100%)	174 (90%)	19 (10%)	12	13
7	D	117/148 (79%)	110 (94%)	7 (6%)	27	35
8	E	152/156 (97%)	146 (96%)	6 (4%)	43	57
9	F	93/94 (99%)	92 (99%)	1 (1%)	84	93
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	128 (97%)	4 (3%)	53	70
12	J	118/121 (98%)	110 (93%)	8 (7%)	22	28
13	K	106/106 (100%)	100 (94%)	6 (6%)	29	37
14	L	113/127 (89%)	109 (96%)	4 (4%)	48	63
15	M	158/159 (99%)	153 (97%)	5 (3%)	51	67
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	64
17	O	93/94 (99%)	90 (97%)	3 (3%)	51	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	113/117 (97%)	111 (98%)	2 (2%)	71	86
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	59
20	R	117/122 (96%)	115 (98%)	2 (2%)	73	87
21	S	71/74 (96%)	70 (99%)	1 (1%)	78	90
22	T	105/106 (99%)	100 (95%)	5 (5%)	35	46
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	68	84
25	W	130/130 (100%)	125 (96%)	5 (4%)	44	59
26	X	66/74 (89%)	59 (89%)	7 (11%)	10	10
27	Y	120/196 (61%)	111 (92%)	9 (8%)	19	23
28	Z	60/68 (88%)	57 (95%)	3 (5%)	34	45
29	1	46/47 (98%)	45 (98%)	1 (2%)	64	81
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	79
31	3	79/79 (100%)	77 (98%)	2 (2%)	60	77
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2955 (96%)	138 (4%)	38	50

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	154	TYR
13	K	98	VAL
27	Y	189	ASN
11	H	170	ASN
12	J	107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	143	ASN
18	P	73	HIS
30	2	16	ASN
15	M	170	ASN
17	O	53	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	237 (8%)	36 (1%)
2	9	121/122 (99%)	14 (11%)	2 (1%)
3	4	1/7 (14%)	0	0
All	All	2867/3051 (93%)	251 (8%)	38 (1%)

5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1563	G
1	0	1730	G
1	0	2852	A
1	0	1685	A
1	0	1856	C

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

6 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	OMU	0	2587	1	20,22,23	0.81	1 (5%)	24,31,34	0.74	0
1	OMG	0	2588	1,3	24,26,27	0.85	1 (4%)	32,38,41	5.07	3 (9%)
1	UR3	0	2619	1	20,22,23	0.82	0	23,32,35	0.80	0
1	PSU	0	2621	1	19,21,22	1.19	2 (10%)	23,30,33	1.05	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	1MA	0	628	1,36	23,25,26	0.80	0	32,37,40	0.98	1 (3%)
3	PPU	4	76	33,1,3	38,40,41	1.11	2 (5%)	54,57,60	1.01	4 (7%)

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	OMU	0	2587	1	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1,36	-	1/8/25/26	0/1/3/3
3	PPU	4	76	33,1,3	-	0/26/43/44	0/2/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.27	1.25	1.42
1	0	2621	PSU	C2-N1	3.21	1.43	1.37
1	0	2587	OMU	P-OP1	2.69	1.49	1.46
1	0	2621	PSU	C6-N1	2.37	1.34	1.32
1	0	2588	OMG	C2-N2	2.03	1.35	1.32

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-28.04	130.36	134.14
3	4	76	PPU	C2-N1-C6	3.39	118.89	111.53
1	0	2588	OMG	C6-N1-C2	3.25	125.20	119.51
1	0	628	1MA	C2-N3-C4	-3.14	110.86	116.23
3	4	76	PPU	C4'-C3'-N3'	-2.99	107.18	113.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 316 ligands modelled in this entry, 312 are monoatomic - leaving 4 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	$\# Z  > 2$
33	TSE	4	178	33,3	3,5,7	1.06	0	3,5,10	1.55	0
33	DA	4	179	33,1,34	21,23,24	0.66	0	30,33,36	0.76	0
33	C	4	180	33,34	19,21,22	0.97	2 (10%)	24,30,33	0.86	1 (4%)
33	C	4	181	33	18,18,22	0.79	1 (5%)	23,26,33	0.89	1 (4%)

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
33	TSE	4	178	33,3	-	0/0/3/5	0/0/0/0
33	DA	4	179	33,1,34	-	0/6/21/22	0/1/3/3
33	C	4	180	33,34	-	0/6/25/26	0/2/2/2
33	C	4	181	33	-	0/4/22/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	4	180	C	C2-N1	2.46	1.40	1.38
33	4	180	C	P-OP1	2.38	1.49	1.46
33	4	181	C	C2-N1	2.10	1.40	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
33	4	181	C	C2-N3-C4	3.13	120.10	115.57
33	4	180	C	C2-N3-C4	3.01	119.93	115.57

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	0	2754/2922 (94%)	-0.06	91 (3%) 44 54	24, 46, 90, 150	0
2	9	122/122 (100%)	0.22	5 (4%) 35 46	42, 65, 90, 149	0
3	4	3/7 (42%)	-0.49	0 100 100	40, 40, 45, 48	0
4	A	237/240 (98%)	0.48	17 (7%) 15 22	28, 50, 83, 105	0
5	B	337/338 (99%)	0.34	14 (4%) 35 45	29, 52, 78, 90	0
6	C	246/246 (100%)	0.13	5 (2%) 62 72	26, 47, 69, 81	0
7	D	140/177 (79%)	2.39	64 (45%) 1 1	59, 93, 123, 132	0
8	E	172/178 (96%)	1.03	34 (19%) 2 3	44, 66, 84, 89	0
9	F	119/120 (99%)	1.30	33 (27%) 1 1	46, 72, 98, 109	0
10	G	29/348 (8%)	2.55	18 (62%) 0 0	71, 91, 100, 102	0
11	H	160/171 (93%)	0.67	18 (11%) 6 9	41, 59, 92, 99	0
12	J	142/145 (97%)	0.30	5 (3%) 42 52	37, 50, 70, 89	0
13	K	132/132 (100%)	-0.05	3 (2%) 57 67	34, 46, 68, 78	0
14	L	145/165 (87%)	0.98	28 (19%) 2 3	26, 64, 108, 121	0
15	M	194/195 (99%)	0.61	20 (10%) 7 11	31, 45, 76, 85	0
16	N	186/187 (99%)	1.14	39 (20%) 1 3	44, 62, 110, 116	0
17	O	115/116 (99%)	0.34	3 (2%) 53 63	39, 55, 69, 77	0
18	P	143/149 (95%)	0.25	3 (2%) 60 70	37, 51, 65, 74	0
19	Q	95/96 (98%)	0.29	7 (7%) 14 21	38, 47, 64, 73	0
20	R	150/155 (96%)	0.04	3 (2%) 62 72	31, 44, 64, 74	0
21	S	81/85 (95%)	0.39	6 (7%) 14 21	41, 56, 77, 93	0
22	T	119/120 (99%)	0.69	11 (9%) 9 15	42, 55, 81, 110	0
23	U	53/66 (80%)	0.31	2 (3%) 38 49	41, 51, 72, 79	0
24	V	65/71 (91%)	2.32	21 (32%) 1 1	54, 75, 113, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.23	4 (2%) 53 63	40, 52, 71, 81	0
26	X	82/92 (89%)	0.76	9 (10%) 6 10	43, 55, 83, 100	0
27	Y	142/241 (58%)	0.36	14 (9%) 8 13	30, 45, 65, 87	0
28	Z	73/83 (87%)	2.08	28 (38%) 1 1	48, 78, 93, 101	0
29	1	56/57 (98%)	-0.34	0 100 100	27, 33, 41, 47	0
30	2	46/50 (92%)	1.05	8 (17%) 2 4	35, 59, 82, 94	0
31	3	92/92 (100%)	0.33	4 (4%) 34 44	35, 55, 69, 83	0
32	I	70/162 (43%)	6.41	65 (92%) 0 0	111, 123, 141, 141	0
All	All	6654/7482 (88%)	0.40	582 (8%) 11 16	24, 51, 97, 150	0

The worst 5 of 582 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	25.0
24	V	39	ALA	16.8
24	V	1	THR	16.2
32	I	79	ILE	14.1
32	I	133	THR	14.1

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	UR3	0	2619	21/22	0.13	0.75	33,36,40,41	0
1	1MA	0	628	23/24	0.13	-0.17	32,34,36,38	0
3	PPU	4	76	37/38	0.12	-0.22	36,42,57,61	0
1	OMG	0	2588	24/25	0.11	-0.48	30,33,37,38	0
1	OMU	0	2587	21/22	0.10	-0.83	30,36,38,38	0
1	PSU	0	2621	20/21	0.11	-1.36	31,34,41,42	0



## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	MG	0	8108	1/1	0.30	105.51	96,96,96,96	0
36	NA	0	9179	1/1	0.74	89.42	103,103,103,103	0
34	MG	0	8082	1/1	0.24	83.67	85,85,85,85	0
34	MG	0	8094	1/1	0.45	72.20	85,85,85,85	0
38	SR	0	9432	1/1	0.12	62.23	64,64,64,64	0
36	NA	0	9125	1/1	0.67	47.58	88,88,88,88	0
34	MG	0	8059	1/1	0.47	38.80	85,85,85,85	0
36	NA	0	9118	1/1	0.22	35.82	58,58,58,58	0
34	MG	0	8024	1/1	0.52	34.85	64,64,64,64	0
36	NA	0	9157	1/1	0.20	33.54	46,46,46,46	0
38	SR	0	9539	1/1	0.50	32.74	156,156,156,156	0
37	CL	0	9322	1/1	0.27	31.07	59,59,59,59	0
34	MG	0	8022	1/1	0.55	30.97	107,107,107,107	0
36	NA	0	9164	1/1	0.40	26.44	65,65,65,65	0
34	MG	0	8025	1/1	0.33	26.40	26,26,26,26	0
38	SR	0	9547	1/1	0.34	22.81	191,191,191,191	0
36	NA	0	9107	1/1	0.31	21.09	63,63,63,63	0
34	MG	0	8013	1/1	0.39	20.86	21,21,21,21	0
36	NA	0	9152	1/1	0.18	20.00	65,65,65,65	0
38	SR	C	9500	1/1	0.52	19.11	187,187,187,187	0
34	MG	0	8089	1/1	0.28	18.81	53,53,53,53	0
36	NA	0	9106	1/1	0.27	18.17	41,41,41,41	0
36	NA	0	9161	1/1	0.31	18.00	52,52,52,52	0
34	MG	0	8047	1/1	0.29	14.53	86,86,86,86	0
36	NA	0	9116	1/1	0.31	14.36	46,46,46,46	0
36	NA	0	9120	1/1	0.25	14.21	67,67,67,67	0
36	NA	0	9122	1/1	0.42	14.19	79,79,79,79	0
36	NA	0	9185	1/1	0.48	14.09	61,61,61,61	0
36	NA	0	9177	1/1	0.32	13.97	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8092	1/1	0.33	13.80	68,68,68,68	0
36	NA	0	9169	1/1	0.60	13.65	115,115,115,115	0
38	SR	0	9626	1/1	0.32	13.61	142,142,142,142	0
36	NA	0	9111	1/1	0.18	13.54	68,68,68,68	0
36	NA	0	9173	1/1	0.29	13.51	70,70,70,70	0
34	MG	0	8051	1/1	0.23	13.11	31,31,31,31	0
34	MG	0	8084	1/1	0.35	12.99	69,69,69,69	0
35	K	0	9001	1/1	0.25	12.78	81,81,81,81	0
36	NA	0	9178	1/1	0.35	12.78	52,52,52,52	0
34	MG	0	8050	1/1	0.27	12.62	87,87,87,87	0
36	NA	0	9174	1/1	0.25	12.41	70,70,70,70	0
34	MG	0	8052	1/1	0.29	12.00	82,82,82,82	0
34	MG	0	8038	1/1	0.24	11.45	25,25,25,25	0
34	MG	0	8055	1/1	0.20	10.42	103,103,103,103	0
36	NA	0	9170	1/1	0.31	10.26	84,84,84,84	0
36	NA	0	9129	1/1	0.20	9.94	81,81,81,81	0
36	NA	0	9140	1/1	0.35	9.85	63,63,63,63	0
34	MG	0	8114	1/1	0.27	9.11	63,63,63,63	0
36	NA	0	9102	1/1	0.19	9.08	58,58,58,58	0
36	NA	0	9184	1/1	0.27	9.08	74,74,74,74	0
38	SR	0	9482	1/1	0.23	9.01	117,117,117,117	0
36	NA	0	9175	1/1	0.19	8.81	53,53,53,53	0
36	NA	0	9158	1/1	0.18	8.77	56,56,56,56	0
36	NA	0	9168	1/1	0.18	8.74	67,67,67,67	0
34	MG	0	8029	1/1	0.28	8.57	33,33,33,33	0
36	NA	0	9171	1/1	0.20	8.48	63,63,63,63	0
36	NA	S	9112	1/1	0.36	7.42	74,74,74,74	0
36	NA	0	9156	1/1	0.20	7.33	61,61,61,61	0
34	MG	0	8070	1/1	0.15	7.15	26,26,26,26	0
34	MG	0	8008	1/1	0.16	7.04	19,19,19,19	0
36	NA	0	9172	1/1	0.30	7.01	76,76,76,76	0
34	MG	0	8057	1/1	0.39	6.98	68,68,68,68	0
34	MG	0	8027	1/1	0.22	6.77	37,37,37,37	0
36	NA	0	9167	1/1	0.16	6.76	54,54,54,54	0
34	MG	0	8001	1/1	0.20	6.60	20,20,20,20	0
34	MG	0	8090	1/1	0.31	6.36	79,79,79,79	0
34	MG	0	8014	1/1	0.31	6.24	84,84,84,84	0
36	NA	0	9162	1/1	0.19	5.94	47,47,47,47	0
34	MG	0	8103	1/1	0.17	5.82	64,64,64,64	0
34	MG	0	8012	1/1	0.20	5.38	39,39,39,39	0
36	NA	0	9165	1/1	0.30	5.21	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
38	SR	0	9405	1/1	0.13	5.03	58,58,58,58	0
34	MG	0	8026	1/1	0.14	4.94	32,32,32,32	0
34	MG	0	8101	1/1	0.16	4.92	70,70,70,70	0
34	MG	K	8069	1/1	0.17	4.41	24,24,24,24	0
36	NA	0	9132	1/1	0.21	4.37	59,59,59,59	0
36	NA	0	9135	1/1	0.17	4.21	47,47,47,47	0
36	NA	R	9186	1/1	0.20	4.19	66,66,66,66	0
38	SR	0	9521	1/1	0.25	3.82	175,175,175,175	0
36	NA	0	9160	1/1	0.15	3.72	43,43,43,43	0
34	MG	0	8021	1/1	0.14	3.62	56,56,56,56	0
38	SR	0	9406	1/1	0.14	3.55	33,33,33,33	0
34	MG	0	8040	1/1	0.35	3.35	103,103,103,103	0
38	SR	0	9408	1/1	0.15	3.30	39,39,39,39	0
36	NA	0	9163	1/1	0.16	3.19	68,68,68,68	0
34	MG	0	8065	1/1	0.27	3.10	86,86,86,86	0
38	SR	0	9467	1/1	0.12	3.08	84,84,84,84	0
37	CL	0	9316	1/1	0.20	3.03	73,73,73,73	0
34	MG	0	8058	1/1	0.22	3.01	43,43,43,43	0
36	NA	9	9183	1/1	0.18	2.77	76,76,76,76	0
38	SR	0	9534	1/1	0.17	2.68	102,102,102,102	0
34	MG	9	8095	1/1	0.18	2.43	51,51,51,51	0
36	NA	0	9150	1/1	0.14	2.22	47,47,47,47	0
34	MG	0	8118	1/1	0.16	2.17	29,29,29,29	0
38	SR	0	9434	1/1	0.13	2.12	62,62,62,62	0
34	MG	0	8020	1/1	0.18	1.86	33,33,33,33	0
34	MG	0	8009	1/1	0.13	1.76	21,21,21,21	0
33	TSE	4	178	6/8	0.16	1.66	45,50,55,58	0
34	MG	0	8056	1/1	0.19	1.63	45,45,45,45	0
34	MG	0	8045	1/1	0.20	1.54	76,76,76,76	0
36	NA	0	9159	1/1	0.16	1.48	48,48,48,48	0
38	SR	0	9433	1/1	0.11	1.48	71,71,71,71	0
36	NA	0	9155	1/1	0.22	1.33	57,57,57,57	0
34	MG	0	8107	1/1	0.18	1.33	62,62,62,62	0
36	NA	0	9182	1/1	0.14	1.30	87,87,87,87	0
38	SR	0	9411	1/1	0.14	1.26	42,42,42,42	0
38	SR	9	9588	1/1	0.12	1.18	131,131,131,131	0
34	MG	0	8074	1/1	0.18	1.16	31,31,31,31	0
34	MG	0	8054	1/1	0.12	1.16	47,47,47,47	0
36	NA	0	9131	1/1	0.14	1.13	44,44,44,44	0
36	NA	0	9181	1/1	0.12	1.10	53,53,53,53	0
33	DA	4	179	21/22	0.13	0.96	43,46,51,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	NA	0	9149	1/1	0.14	0.82	43,43,43,43	0
34	MG	0	8085	1/1	0.14	0.74	55,55,55,55	0
36	NA	0	9115	1/1	0.12	0.73	38,38,38,38	0
38	SR	H	9486	1/1	0.19	0.71	106,106,106,106	0
34	MG	0	8080	1/1	0.15	0.70	53,53,53,53	0
36	NA	0	9127	1/1	0.13	0.68	60,60,60,60	0
34	MG	0	8079	1/1	0.12	0.66	31,31,31,31	0
36	NA	0	9110	1/1	0.12	0.56	45,45,45,45	0
34	MG	0	8106	1/1	0.13	0.32	43,43,43,43	0
35	K	0	9002	1/1	0.18	0.31	80,80,80,80	0
33	C	4	181	17/21	0.11	0.29	51,53,55,56	0
38	SR	0	9407	1/1	0.11	0.27	43,43,43,43	0
36	NA	M	9147	1/1	0.15	0.26	41,41,41,41	0
38	SR	0	9515	1/1	0.12	0.26	95,95,95,95	0
38	SR	0	9420	1/1	0.12	0.26	66,66,66,66	0
34	MG	0	8036	1/1	0.11	0.15	54,54,54,54	0
38	SR	F	9595	1/1	0.14	0.08	103,103,103,103	0
34	MG	0	8017	1/1	0.09	-0.04	28,28,28,28	0
33	C	4	180	20/21	0.12	-0.07	47,49,51,51	0
37	CL	B	9319	1/1	0.13	-0.10	55,55,55,55	0
38	SR	0	9410	1/1	0.12	-0.14	39,39,39,39	0
38	SR	0	9537	1/1	0.12	-0.25	135,135,135,135	0
39	CD	Z	9203	1/1	0.18	-0.29	92,92,92,92	0
34	MG	0	8099	1/1	0.12	-0.31	68,68,68,68	0
34	MG	0	8041	1/1	0.11	-0.32	49,49,49,49	0
38	SR	0	9474	1/1	0.10	-0.35	60,60,60,60	0
36	NA	0	9139	1/1	0.13	-0.37	48,48,48,48	0
34	MG	0	8068	1/1	0.14	-0.51	45,45,45,45	0
34	MG	0	8076	1/1	0.10	-0.60	57,57,57,57	0
36	NA	0	9124	1/1	0.09	-0.62	49,49,49,49	0
36	NA	C	9104	1/1	0.12	-0.63	28,28,28,28	0
38	SR	0	9417	1/1	0.10	-0.65	59,59,59,59	0
34	MG	0	8031	1/1	0.11	-0.67	48,48,48,48	0
34	MG	0	8116	1/1	0.10	-0.70	57,57,57,57	0
36	NA	J	9146	1/1	0.11	-0.74	55,55,55,55	0
34	MG	0	8015	1/1	0.10	-0.79	31,31,31,31	0
38	SR	0	9509	1/1	0.12	-0.81	88,88,88,88	0
38	SR	0	9452	1/1	0.13	-0.83	105,105,105,105	0
34	MG	0	8088	1/1	0.08	-0.84	44,44,44,44	0
37	CL	R	9306	1/1	0.11	-0.84	45,45,45,45	0
36	NA	0	9130	1/1	0.11	-0.86	48,48,48,48	0
36	NA	0	9141	1/1	0.09	-0.91	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
38	SR	A	9437	1/1	0.10	-0.92	63,63,63,63	0
38	SR	O	9413	1/1	0.10	-0.92	44,44,44,44	0
38	SR	A	9497	1/1	0.09	-0.93	85,85,85,85	0
36	NA	D	9151	1/1	0.22	-0.93	66,66,66,66	0
36	NA	O	9126	1/1	0.10	-0.94	53,53,53,53	0
36	NA	R	9138	1/1	0.08	-0.96	66,66,66,66	0
37	CL	O	9314	1/1	0.10	-0.99	48,48,48,48	0
34	MG	O	8102	1/1	0.09	-1.08	67,67,67,67	0
38	SR	1	9419	1/1	0.09	-1.10	41,41,41,41	0
37	CL	J	9321	1/1	0.08	-1.11	63,63,63,63	0
38	SR	O	9475	1/1	0.09	-1.11	82,82,82,82	0
34	MG	O	8061	1/1	0.12	-1.15	71,71,71,71	0
36	NA	R	9137	1/1	0.09	-1.16	39,39,39,39	0
38	SR	S	9470	1/1	0.10	-1.20	96,96,96,96	0
38	SR	O	9451	1/1	0.10	-1.21	57,57,57,57	0
38	SR	R	9418	1/1	0.12	-1.21	54,54,54,54	0
38	SR	O	9504	1/1	0.10	-1.26	100,100,100,100	0
34	MG	O	8093	1/1	0.13	-1.26	40,40,40,40	0
38	SR	O	9545	1/1	0.03	-1.26	76,76,76,76	0
36	NA	O	9114	1/1	0.10	-1.27	46,46,46,46	0
37	CL	J	9301	1/1	0.09	-1.36	55,55,55,55	0
34	MG	T	8073	1/1	0.12	-1.36	47,47,47,47	0
36	NA	O	9134	1/1	0.07	-1.39	49,49,49,49	0
38	SR	O	9425	1/1	0.10	-1.39	52,52,52,52	0
37	CL	O	9312	1/1	0.08	-1.41	51,51,51,51	0
39	CD	U	9201	1/1	0.09	-1.41	52,52,52,52	0
34	MG	O	8060	1/1	0.11	-1.41	82,82,82,82	0
36	NA	O	9101	1/1	0.13	-1.42	45,45,45,45	0
34	MG	O	8096	1/1	0.10	-1.44	44,44,44,44	0
34	MG	O	8042	1/1	0.09	-1.45	56,56,56,56	0
38	SR	O	9415	1/1	0.09	-1.48	54,54,54,54	0
38	SR	O	9412	1/1	0.10	-1.48	41,41,41,41	0
36	NA	O	9108	1/1	0.09	-1.52	32,32,32,32	0
38	SR	O	9421	1/1	0.08	-1.52	68,68,68,68	0
39	CD	3	9204	1/1	0.04	-1.56	58,58,58,58	0
34	MG	A	8066	1/1	0.09	-1.56	57,57,57,57	0
36	NA	O	9136	1/1	0.10	-1.63	31,31,31,31	0
36	NA	O	9166	1/1	0.08	-1.64	61,61,61,61	0
34	MG	O	8104	1/1	0.09	-1.65	53,53,53,53	0
38	SR	O	9435	1/1	0.09	-1.66	73,73,73,73	0
38	SR	O	9581	1/1	0.10	-1.68	123,123,123,123	0
36	NA	O	9117	1/1	0.09	-1.68	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	CL	J	9302	1/1	0.05	-1.69	54,54,54,54	0
37	CL	0	9311	1/1	0.08	-1.74	61,61,61,61	0
34	MG	0	8039	1/1	0.10	-1.80	74,74,74,74	0
34	MG	0	8067	1/1	0.11	-1.82	40,40,40,40	0
38	SR	0	9508	1/1	0.10	-1.83	100,100,100,100	0
38	SR	0	9488	1/1	0.09	-1.86	77,77,77,77	0
36	NA	Q	9148	1/1	0.09	-1.86	45,45,45,45	0
34	MG	0	8046	1/1	0.08	-1.87	44,44,44,44	0
38	SR	0	9450	1/1	0.05	-1.94	74,74,74,74	0
37	CL	L	9310	1/1	0.10	-1.96	50,50,50,50	0
38	SR	0	9424	1/1	0.13	-2.09	46,46,46,46	0
34	MG	0	8005	1/1	0.11	-2.15	33,33,33,33	0
38	SR	1	9460	1/1	0.09	-2.16	48,48,48,48	0
38	SR	0	9422	1/1	0.10	-2.17	57,57,57,57	0
38	SR	3	9439	1/1	0.04	-2.17	67,67,67,67	0
38	SR	0	9517	1/1	0.04	-2.18	109,109,109,109	0
38	SR	0	9566	1/1	0.05	-2.18	79,79,79,79	0
37	CL	A	9309	1/1	0.10	-2.20	57,57,57,57	0
37	CL	0	9315	1/1	0.10	-2.26	48,48,48,48	0
38	SR	L	9409	1/1	0.09	-2.29	37,37,37,37	0
37	CL	M	9318	1/1	0.10	-2.35	38,38,38,38	0
37	CL	N	9307	1/1	0.11	-2.40	57,57,57,57	0
38	SR	0	9568	1/1	0.07	-2.42	71,71,71,71	0
37	CL	O	9308	1/1	0.07	-2.45	66,66,66,66	0
34	MG	0	8002	1/1	0.09	-2.47	33,33,33,33	0
38	SR	0	9530	1/1	0.12	-2.49	65,65,65,65	0
34	MG	0	8004	1/1	0.08	-2.58	31,31,31,31	0
34	MG	0	8110	1/1	0.11	-2.60	41,41,41,41	0
38	SR	0	9462	1/1	0.11	-2.64	67,67,67,67	0
38	SR	0	9414	1/1	0.08	-2.68	56,56,56,56	0
38	SR	0	9532	1/1	0.04	-2.71	118,118,118,118	0
38	SR	0	9430	1/1	0.09	-2.72	48,48,48,48	0
38	SR	0	9428	1/1	0.04	-2.75	52,52,52,52	0
34	MG	0	8115	1/1	0.07	-2.76	48,48,48,48	0
38	SR	0	9490	1/1	0.06	-2.77	99,99,99,99	0
37	CL	3	9304	1/1	0.05	-2.78	56,56,56,56	0
36	NA	T	9143	1/1	0.07	-2.82	38,38,38,38	0
38	SR	0	9448	1/1	0.05	-2.88	60,60,60,60	0
38	SR	0	9590	1/1	0.06	-2.90	102,102,102,102	0
38	SR	0	9455	1/1	0.05	-2.91	74,74,74,74	0
38	SR	0	9431	1/1	0.10	-3.06	60,60,60,60	0
34	MG	0	8072	1/1	0.11	-3.06	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8028	1/1	0.10	-3.15	37,37,37,37	0
38	SR	0	9438	1/1	0.07	-3.16	64,64,64,64	0
38	SR	0	9447	1/1	0.08	-3.16	68,68,68,68	0
38	SR	0	9461	1/1	0.04	-3.23	77,77,77,77	0
38	SR	0	9423	1/1	0.07	-3.35	54,54,54,54	0
39	CD	1	9202	1/1	0.02	-3.38	51,51,51,51	0
34	MG	0	8097	1/1	0.08	-3.38	58,58,58,58	0
38	SR	0	9426	1/1	0.07	-3.41	67,67,67,67	0
38	SR	0	9501	1/1	0.07	-3.52	96,96,96,96	0
38	SR	0	9442	1/1	0.08	-3.53	59,59,59,59	0
37	CL	Y	9320	1/1	0.07	-3.53	45,45,45,45	0
38	SR	0	9478	1/1	0.06	-3.56	75,75,75,75	0
37	CL	0	9303	1/1	0.09	-3.65	48,48,48,48	0
39	CD	O	9205	1/1	0.06	-3.67	124,124,124,124	0
34	MG	0	8098	1/1	0.05	-3.70	46,46,46,46	0
36	NA	0	9105	1/1	0.07	-3.77	38,38,38,38	0
38	SR	0	9473	1/1	0.03	-3.78	77,77,77,77	0
38	SR	0	9489	1/1	0.06	-3.78	86,86,86,86	0
38	SR	A	9436	1/1	0.04	-3.83	55,55,55,55	0
38	SR	0	9446	1/1	0.06	-3.86	86,86,86,86	0
38	SR	0	9505	1/1	0.10	-3.92	89,89,89,89	0
34	MG	0	8113	1/1	0.10	-3.93	42,42,42,42	0
34	MG	0	8044	1/1	0.06	-3.98	43,43,43,43	0
38	SR	0	9416	1/1	0.07	-4.06	45,45,45,45	0
34	MG	0	8003	1/1	0.11	-4.07	33,33,33,33	0
34	MG	0	8032	1/1	0.07	-4.23	39,39,39,39	0
38	SR	0	9444	1/1	0.04	-4.24	53,53,53,53	0
38	SR	0	9427	1/1	0.10	-4.27	53,53,53,53	0
38	SR	0	9469	1/1	0.03	-4.27	85,85,85,85	0
38	SR	9	9481	1/1	0.04	-4.35	83,83,83,83	0
38	SR	0	9468	1/1	0.04	-4.44	115,115,115,115	0
34	MG	0	8112	1/1	0.04	-4.48	41,41,41,41	0
38	SR	0	9629	1/1	0.08	-4.50	72,72,72,72	0
38	SR	0	9459	1/1	0.08	-4.52	104,104,104,104	0
38	SR	0	9445	1/1	0.07	-4.80	57,57,57,57	0
34	MG	0	8063	1/1	0.08	-4.83	57,57,57,57	0
34	MG	0	8117	1/1	0.06	-4.84	38,38,38,38	0
34	MG	0	8091	1/1	0.07	-4.93	54,54,54,54	0
37	CL	0	9305	1/1	0.04	-4.99	51,51,51,51	0
38	SR	0	9585	1/1	0.05	-5.00	85,85,85,85	0
37	CL	0	9313	1/1	0.07	-5.05	54,54,54,54	0
36	NA	0	9113	1/1	0.08	-5.18	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8030	1/1	0.05	-5.28	35,35,35,35	0
38	SR	0	9483	1/1	0.06	-5.34	77,77,77,77	0
36	NA	0	9123	1/1	0.08	-5.41	40,40,40,40	0
34	MG	0	8043	1/1	0.09	-5.49	50,50,50,50	0
38	SR	0	9529	1/1	0.07	-5.64	103,103,103,103	0
38	SR	0	9498	1/1	0.04	-5.64	59,59,59,59	0
38	SR	0	9466	1/1	0.05	-5.65	98,98,98,98	0
38	SR	0	9443	1/1	0.06	-5.66	57,57,57,57	0
38	SR	0	9441	1/1	0.06	-5.70	64,64,64,64	0
38	SR	0	9465	1/1	0.07	-5.76	98,98,98,98	0
34	MG	Y	8109	1/1	0.05	-5.85	41,41,41,41	0
38	SR	0	9506	1/1	0.04	-5.94	65,65,65,65	0
38	SR	0	9457	1/1	0.07	-5.99	53,53,53,53	0
38	SR	0	9477	1/1	0.07	-6.12	82,82,82,82	0
38	SR	0	9495	1/1	0.06	-6.25	97,97,97,97	0
38	SR	9	9503	1/1	0.04	-6.28	105,105,105,105	0
38	SR	0	9456	1/1	0.06	-6.30	60,60,60,60	0
38	SR	B	9458	1/1	0.05	-6.62	74,74,74,74	0
36	NA	0	9128	1/1	0.05	-6.62	42,42,42,42	0
38	SR	0	9453	1/1	0.06	-6.75	69,69,69,69	0
34	MG	0	8075	1/1	0.05	-6.83	40,40,40,40	0
38	SR	0	9464	1/1	0.04	-7.16	77,77,77,77	0
34	MG	0	8019	1/1	0.04	-7.23	45,45,45,45	0
38	SR	0	9522	1/1	0.06	-7.70	109,109,109,109	0
38	SR	0	9429	1/1	0.08	-7.83	62,62,62,62	0
36	NA	0	9154	1/1	0.09	-8.03	47,47,47,47	0
38	SR	0	9480	1/1	0.03	-8.08	90,90,90,90	0
38	SR	0	9449	1/1	0.04	-8.35	61,61,61,61	0
38	SR	0	9560	1/1	0.04	-8.60	94,94,94,94	0
34	MG	0	8083	1/1	0.07	-8.92	51,51,51,51	0
38	SR	0	9570	1/1	0.04	-9.17	100,100,100,100	0
37	CL	0	9317	1/1	0.05	-9.77	54,54,54,54	0
38	SR	0	9440	1/1	0.03	-11.33	70,70,70,70	0
34	MG	0	8037	1/1	0.03	-11.61	39,39,39,39	0
38	SR	0	9454	1/1	0.04	-17.22	75,75,75,75	0
38	SR	0	9484	1/1	0.07	-25.67	136,136,136,136	0
38	SR	0	9601	1/1	0.03	-	94,94,94,94	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.