



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:19 PM GMT

PDB ID : 3CCR  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488C. Density for anisomycin is visible but not included in the model.  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 3.00 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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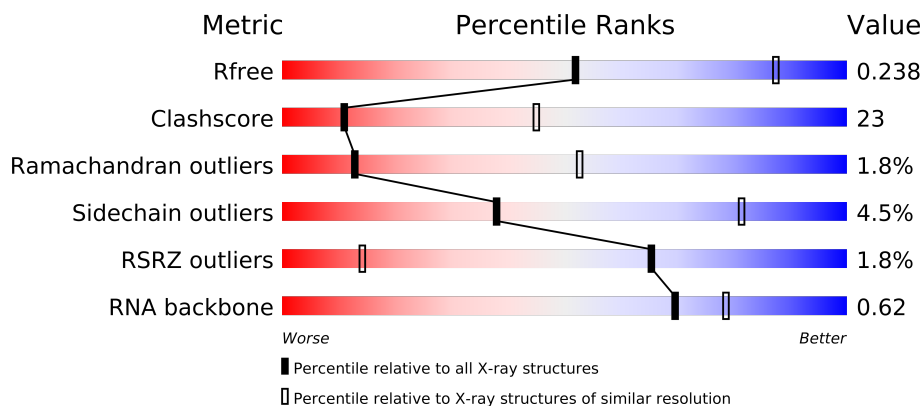
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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. 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	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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Mol	Chain	Length	Quality of chain
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8004	-	X
32	MG	0	8005	-	X
32	MG	0	8009	-	X
32	MG	0	8011	-	X
32	MG	0	8014	-	X
32	MG	0	8015	-	X
32	MG	0	8016	-	X
32	MG	0	8020	-	X
32	MG	0	8022	-	X
32	MG	0	8023	-	X
32	MG	0	8030	-	X
32	MG	0	8031	-	X
32	MG	0	8033	-	X
32	MG	0	8037	-	X
32	MG	0	8040	-	X
32	MG	0	8041	-	X
32	MG	0	8044	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8048	-	X
32	MG	0	8063	-	X
32	MG	0	8066	-	X
32	MG	0	8071	-	X
32	MG	0	8078	-	X
32	MG	0	8081	-	X
32	MG	0	8085	-	X
32	MG	A	8051	-	X
32	MG	K	8054	-	X
33	K	0	8401	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X
34	NA	0	8513	-	X
34	NA	0	8518	-	X
34	NA	0	8519	-	X
34	NA	0	8520	-	X
34	NA	0	8521	-	X
34	NA	0	8522	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8526	-	X
34	NA	0	8528	-	X
34	NA	0	8529	-	X
34	NA	0	8530	-	X
34	NA	0	8534	-	X
34	NA	0	8535	-	X
34	NA	0	8537	-	X
34	NA	0	8541	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8550	-	X
34	NA	0	8552	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X
34	NA	0	8558	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8569	-	X
34	NA	0	8571	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	9	8572	-	X
34	NA	R	8532	-	X
34	NA	R	8575	-	X
35	CL	0	8814	-	X
35	CL	0	8816	-	X
35	CL	0	8817	-	X
35	CL	0	8822	-	X
35	CL	A	8809	-	X
36	SR	0	8901	-	X
36	SR	0	8904	-	X
36	SR	0	8905	-	X
36	SR	0	8909	-	X
36	SR	0	8914	-	X
36	SR	0	8919	-	X
36	SR	0	8922	-	X
36	SR	0	8924	-	X
36	SR	0	8925	-	X
36	SR	0	8927	-	X
36	SR	0	8947	-	X
36	SR	0	8955	-	X
36	SR	0	8957	-	X
36	SR	0	8959	-	X
36	SR	0	8969	-	X
36	SR	0	8971	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8986	-	X
36	SR	0	8989	-	X
36	SR	0	8991	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	8998	-	X
36	SR	0	9000	-	X
36	SR	0	9004	-	X
36	SR	0	9007	-	X
36	SR	9	8980	-	X
36	SR	B	8987	-	X
37	CD	3	8704	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99120 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.



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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59018	26348	10871	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	84	Total	Mg	0	0
			84	84		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	1	Total K 1 1	0	0
33	M	1	Total K 1 1	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	93	Total 93	Sr 93	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5897	Total 5897	O 5897	0	0
38	9	154	Total 154	O 154	0	0
38	A	121	Total 121	O 121	0	0
38	B	145	Total 145	O 145	0	0
38	C	166	Total 166	O 166	0	0
38	D	46	Total 46	O 46	0	0
38	E	43	Total 43	O 43	0	0
38	F	31	Total 31	O 31	0	0
38	G	17	Total 17	O 17	0	0
38	H	72	Total 72	O 72	0	0
38	I	5	Total 5	O 5	0	0
38	J	52	Total 52	O 52	0	0
38	K	52	Total 52	O 52	0	0
38	L	81	Total 81	O 81	0	0
38	M	133	Total 133	O 133	0	0
38	N	56	Total 56	O 56	0	0
38	O	41	Total 41	O 41	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	P	63	Total 63	O 63	0	0
38	Q	52	Total 52	O 52	0	0
38	R	75	Total 75	O 75	0	0
38	S	37	Total 37	O 37	0	0
38	T	40	Total 40	O 40	0	0
38	U	28	Total 28	O 28	0	0
38	V	15	Total 15	O 15	0	0
38	W	69	Total 69	O 69	0	0
38	X	22	Total 22	O 22	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	28	Total 28	O 28	0	0
38	1	61	Total 61	O 61	0	0
38	2	45	Total 45	O 45	0	0
38	3	76	Total 76	O 76	0	0





- Chain D: 

T153	T70	MET
K154	A71	SER
H155	T74	SER
R156	R75	GLU
	R76	GLU
P159		SER
	M79	GLY
V163		ASP
V172	L84	F10
E173	Q85	H11
V174	T86	E12
SER	A87	M13
GLU	L88	R14
	P89	E15
		P16
	E92	R17
		I18
	M103	E19
	F104	K20
	S105	V21
	F106	V22
	G107	V23
	VAL	H24
	GLU	M25
	GLU	
	HIS	G28
	THR	H29
	GLU	GLY
	PHE	GLY
	PRO	ARG
	SER	ASP
	GLN	LEU
	GLU	
	TYR	A35
	ASP	N36
	PRO	A37
	SER	
	ILE	I40
	GLY	
	ILE	V50
	TYR	R51
	GLY	T52
		K53
	L128	A54
	D129	
	V130	K55
	T131	R56
	V132	T57
	N133	
	L134	V58
	V135	G59
	R136	E90
	P137	F61
	G138	D62
	Y139	I63
	R140	R64
		E85
		G86
	K146	D67
		P68
		T69

- Chain E: 

V103	N106	F107	L108	G109	E110	R115	T116	L117	H118	H119	G120	D121	E125	L126	D127	G128	E129	E130	L131	T132	V133	S134	D137	L138	E139	A140	Q143	T144	A145	I148	L151	T152	R153	L154	M155	D156	D164	G165	V166	L168	P172	ASN	ARC	GLY	ASP	ALA	D100	F101	H102							
Met	P1	I7		V11	D12		Q15	D16		T20	T21	V22		S28	V29	T30		L33	Q34	Y35	P36	V40		D45		I49		E53	D54	N55		S60		I69		M72		V76	T77	E78	G79	W80	E81		M84	E85		H90	F91	P92		V95		D100	F101	H102

- Chain F: 

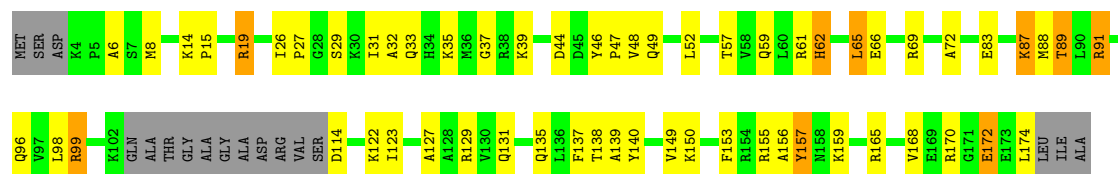
ME1	P1	L12	E13	E21	R24	D25	T26	K30	N34	E35	T36	I37	K38	V48	F49	V50	D63	E57	E58	I59	V60	M61	H62	I63	P64	F74	E78	Q79	Q80	L89	E90	V91	G92	A96	A97	D100	A101	G102	D107	D110	I111	V114
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- Chain G: 

[illegible]

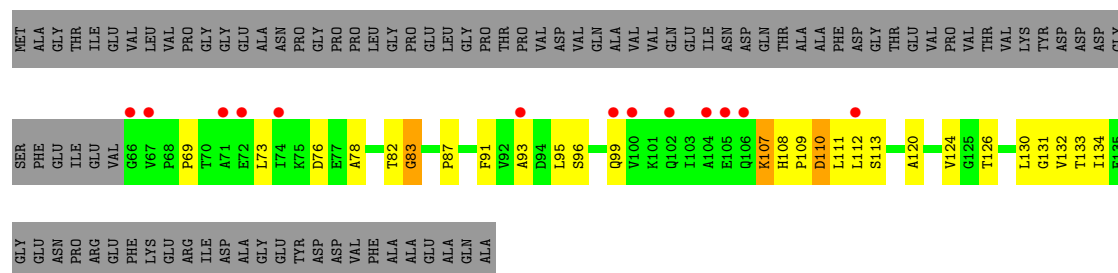
- Molecule 8: 50S ribosomal protein L10e

Chain H:



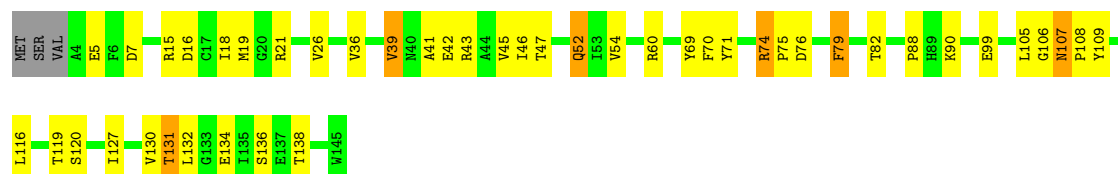
- Molecule 9: 50S ribosomal protein L11P

Chain I:



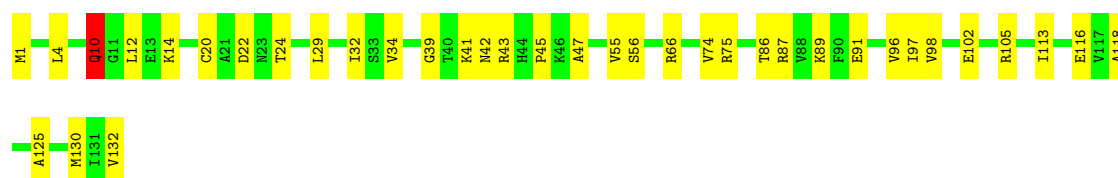
- Molecule 10: 50S ribosomal protein L13P

Chain J:



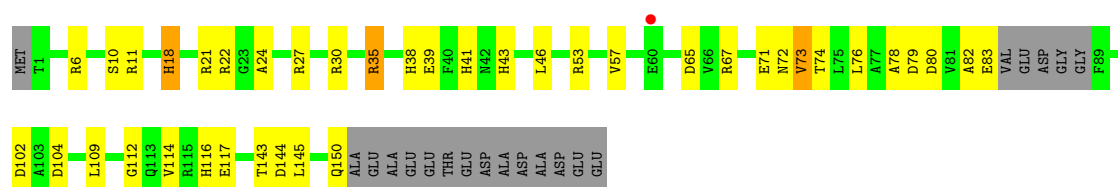
- Molecule 11: 50S ribosomal protein L14P

Chain K:



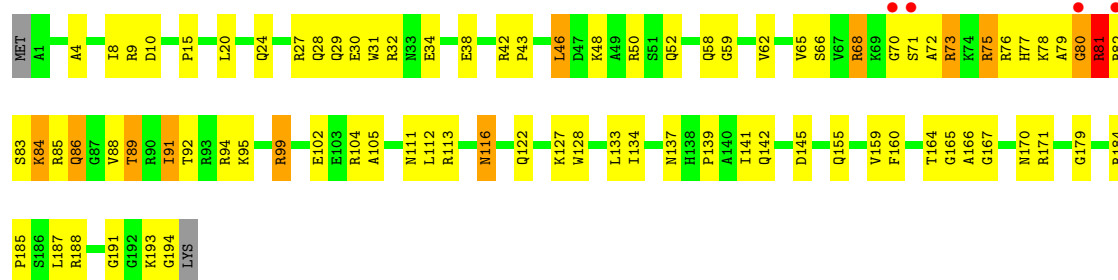
- Molecule 12: 50S ribosomal protein L15P

Chain L:



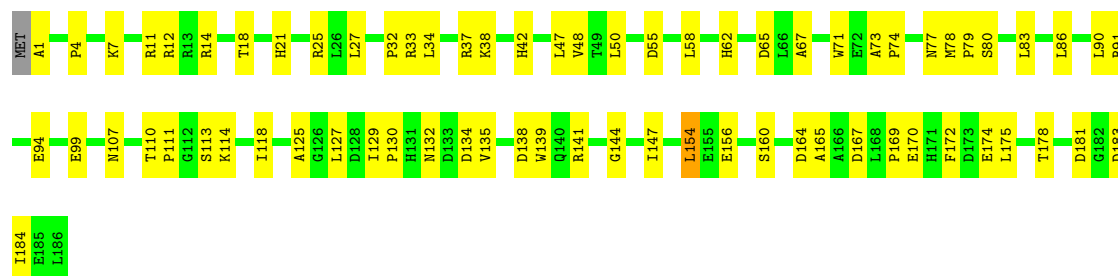
- Molecule 13: 50S ribosomal protein L15e

Chain M: 



- Molecule 14: 50S ribosomal protein L18P

Chain N: 



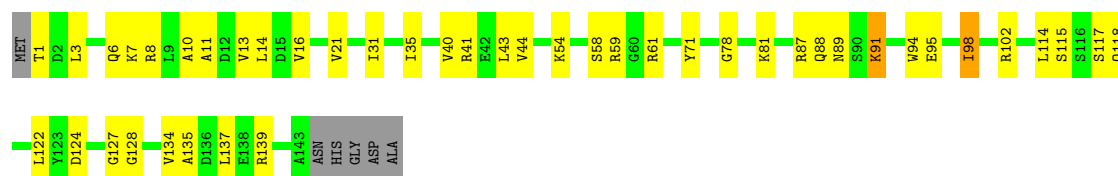
- Molecule 15: 50S ribosomal protein L18e

Chain O: 



- Molecule 16: 50S ribosomal protein L19e

Chain P: 



- Molecule 17: 50S ribosomal protein L21e

Chain Q: 



- Molecule 18: 50S ribosomal protein L22P

Chain R: 





- Molecule 19: 50S ribosomal protein L23P

Chain S:



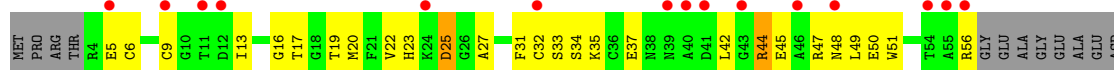
- Molecule 20: 50S ribosomal protein L24P

Chain T:



- Molecule 21: 50S ribosomal protein L24e

Chain U:



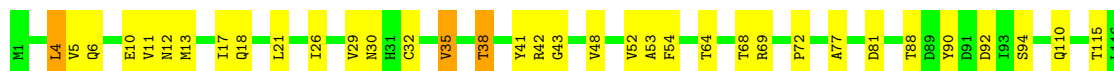
- Molecule 22: 50S ribosomal protein L29P

Chain V:



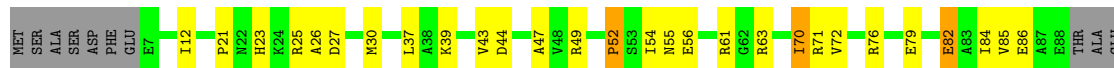
- Molecule 23: 50S ribosomal protein L30P

Chain W:



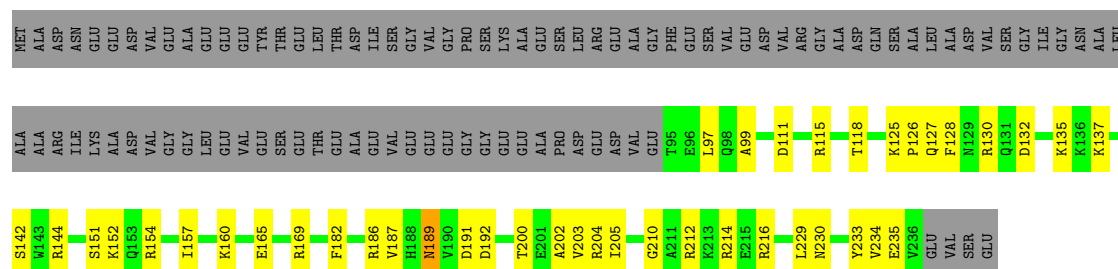
- Molecule 24: 50S ribosomal protein L31e

Chain X:



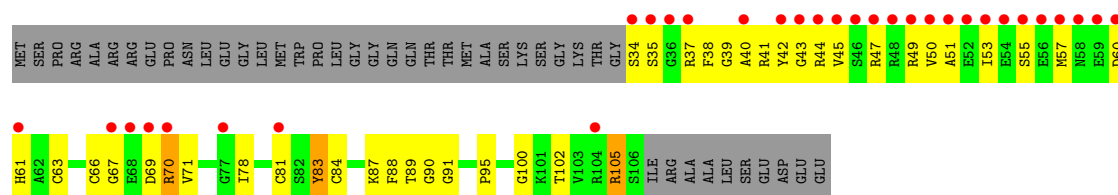
- Molecule 25: 50S ribosomal protein L32e

Chain Y:



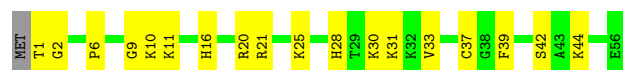
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 27: 50S ribosomal protein L37e

Chain 1:



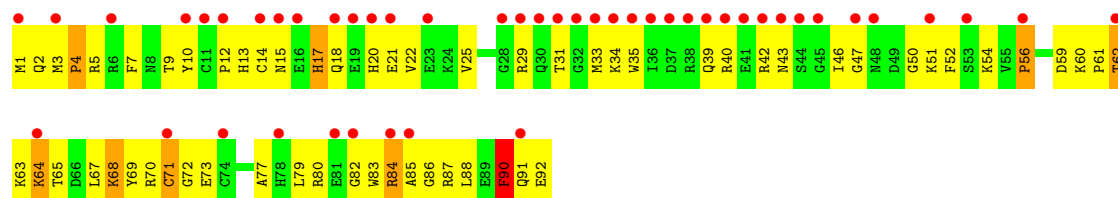
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



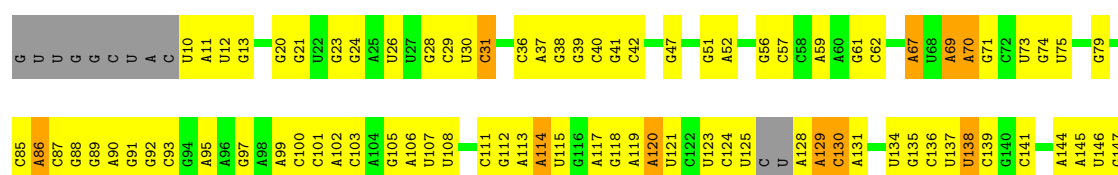
- Molecule 29: 50S ribosomal protein L44E

Chain 3:



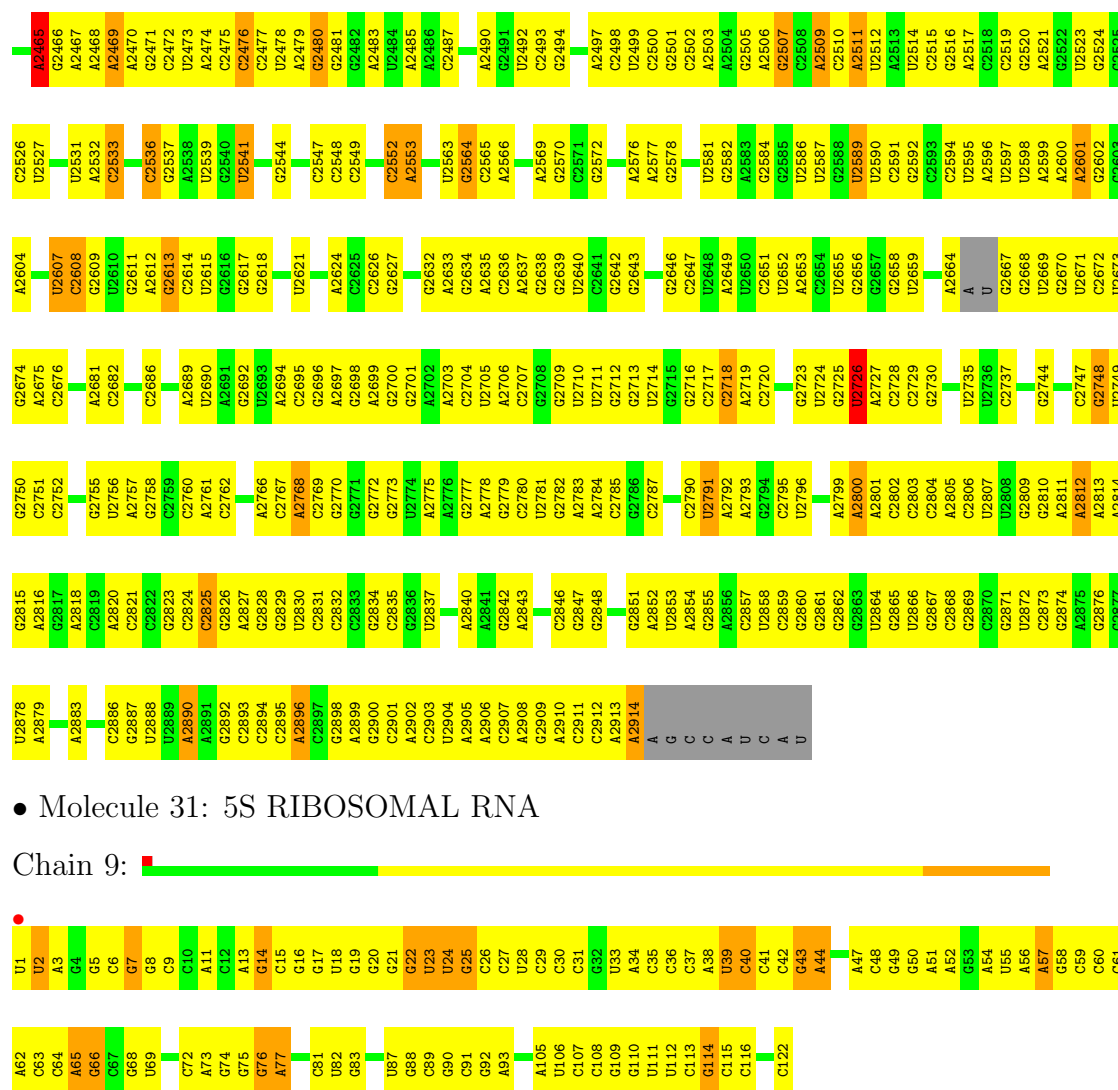
- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:



WORLDWIDE  
 PDB  
PROTEIN DATA BANK







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.41 Å   299.52 Å   574.90 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.81 – 3.00 85.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	77.8 (49.81-3.00) 77.4 (85.66-2.40)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.180   ,   0.247 0.179   ,   0.238	Depositor DCC
$R_{free}$ test set	2791 reflections (1.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.9	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 667115 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, CL, SR, NA, K, 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	A	0.34	0/1786	0.65	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.38	0/1885	0.65	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.34	0/1382	0.59	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.33	0/241	0.48	0/324
8	H	0.34	0/1302	0.65	0/1743
9	I	0.31	0/526	0.51	0/716
10	J	0.38	0/1136	0.62	0/1530
11	K	0.36	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.62	0/1509
13	M	0.38	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.63	0/1999
15	O	0.37	0/874	0.60	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.69	0/1005
18	R	0.37	0/1172	0.63	0/1578
19	S	0.38	0/648	0.60	0/875
20	T	0.34	0/958	0.66	1/1289 (0.1%)
21	U	0.45	0/417	0.67	0/562
22	V	0.32	0/502	0.55	0/675
23	W	0.36	0/1219	0.64	0/1655
24	X	0.35	0/664	0.61	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.45	0/584	0.63	0/781
27	1	0.43	0/438	0.57	0/578
28	2	0.35	0/401	0.60	0/529
29	3	0.48	0/771	0.66	0/1024
30	0	0.41	0/65954	0.68	4/102862 (0.0%)
31	9	0.35	0/2904	0.68	0/4526
All	All	0.39	0/98698	0.67	5/147581 (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
23	W	0	1
30	0	0	18
31	9	0	1
All	All	0	20

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C5'-C4'-C3'	5.99	125.59	116.00
30	0	871	G	C5'-C4'-O4'	-5.85	102.08	109.10
30	0	1504	A	C1'-O4'-C4'	-5.36	105.62	109.90
20	T	52	ARG	N-CA-C	5.08	124.73	111.00
30	0	2726	U	N1-C1'-C2'	5.01	120.52	114.00

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	214	U	Sidechain
30	0	324	G	Sidechain
30	0	393	G	Sidechain
30	0	435	A	Sidechain
23	W	90	TYR	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	A	1753	0	1766	97	0
2	B	2625	0	2532	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1860	0	1813	70	0
4	D	1094	0	1085	50	0
5	E	1357	0	1266	55	0
6	F	890	0	843	27	0
7	G	240	0	231	11	0
8	H	1282	0	1292	55	0
9	I	519	0	500	26	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	98	0
14	N	1445	0	1401	59	0
15	O	865	0	873	32	0
16	P	1136	0	1123	44	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	16	0
20	T	950	0	924	33	0
21	U	410	0	368	38	0
22	V	499	0	511	19	0
23	W	1196	0	1137	52	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	44	0
26	Z	573	0	535	64	0
27	1	431	0	426	20	0
28	2	396	0	413	21	0
29	3	755	0	732	90	0
30	0	59018	0	29810	2239	0
31	9	2599	0	1325	161	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
33	M	1	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	9	0	0	2	0
35	3	1	0	0	3	0
35	A	1	0	0	1	0
35	B	1	0	0	2	0
35	J	3	0	0	2	0
35	K	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	2	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	93	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5897	0	0	323	0
38	1	61	0	0	3	0
38	2	45	0	0	1	0
38	3	76	0	0	7	0
38	9	154	0	0	11	0
38	A	121	0	0	3	0
38	B	145	0	0	20	0
38	C	166	0	0	13	0
38	D	46	0	0	7	0
38	E	43	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	31	0	0	1	0
38	G	17	0	0	0	0
38	H	72	0	0	10	0
38	I	5	0	0	2	0
38	J	52	0	0	4	0
38	K	52	0	0	3	0
38	L	81	0	0	4	0
38	M	133	0	0	12	0
38	N	56	0	0	6	0
38	O	41	0	0	2	0
38	P	63	0	0	5	0
38	Q	52	0	0	1	0
38	R	75	0	0	2	0
38	S	37	0	0	0	0
38	T	40	0	0	3	0
38	U	28	0	0	5	0
38	V	15	0	0	1	0
38	W	69	0	0	7	0
38	X	22	0	0	4	0
38	Y	100	0	0	5	0
38	Z	28	0	0	5	0
All	All	99120	0	59922	3377	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 23.

The worst 5 of 3377 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:0:871:G:C8	30:0:871:G:H5'	1.74	1.22
30:0:1160:G:H5'	30:0:1161:A:C5'	1.70	1.20
30:0:1160:G:C5'	30:0:1161:A:H5'	1.73	1.18
30:0:1278:A:H4'	30:0:1279:U:C4	1.81	1.16
13:M:171:ARG:HD3	30:0:156:C:H5''	1.15	1.13

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	235/240 (98%)	200 (85%)	30 (13%)	5 (2%)	11	47
2	B	335/338 (99%)	305 (91%)	23 (7%)	7 (2%)	11	47
3	C	244/246 (99%)	216 (88%)	26 (11%)	2 (1%)	27	76
4	D	134/177 (76%)	105 (78%)	23 (17%)	6 (4%)	4	22
5	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	33	81
6	F	117/120 (98%)	97 (83%)	16 (14%)	4 (3%)	6	31
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	156/177 (88%)	139 (89%)	16 (10%)	1 (1%)	33	81
9	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	4	22
10	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	16	60
11	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	27	76
12	L	141/165 (86%)	116 (82%)	22 (16%)	3 (2%)	11	47
13	M	192/196 (98%)	171 (89%)	17 (9%)	4 (2%)	11	47
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	10	45
15	O	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	10	45
18	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	30	78
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
21	U	51/67 (76%)	44 (86%)	6 (12%)	1 (2%)	11	48
22	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	14	56
23	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	30	78
24	X	80/92 (87%)	72 (90%)	6 (8%)	2 (2%)	9	40
25	Y	140/241 (58%)	132 (94%)	7 (5%)	1 (1%)	30	78
26	Z	71/116 (61%)	55 (78%)	12 (17%)	4 (6%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	64 (71%)	17 (19%)	9 (10%)	1	4
All	All	3705/4472 (83%)	3292 (89%)	348 (9%)	65 (2%)	13	53

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	206	THR
2	B	306	LYS
4	D	137	PRO
6	F	61	MET
6	F	101	ALA

### 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	179/182 (98%)	170 (95%)	9 (5%)	34	77
2	B	282/283 (100%)	263 (93%)	19 (7%)	23	64
3	C	193/193 (100%)	180 (93%)	13 (7%)	23	64
4	D	117/148 (79%)	110 (94%)	7 (6%)	27	69
5	E	152/156 (97%)	146 (96%)	6 (4%)	43	85
6	F	93/94 (99%)	92 (99%)	1 (1%)	84	97
7	G	27/282 (10%)	25 (93%)	2 (7%)	20	58
8	H	134/145 (92%)	124 (92%)	10 (8%)	19	57
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	95
10	J	118/121 (98%)	109 (92%)	9 (8%)	19	57
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	91
12	L	113/127 (89%)	106 (94%)	7 (6%)	26	67
13	M	158/160 (99%)	147 (93%)	11 (7%)	21	62
14	N	149/150 (99%)	146 (98%)	3 (2%)	68	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	95
17	Q	79/80 (99%)	74 (94%)	5 (6%)	25	66
18	R	117/122 (96%)	113 (97%)	4 (3%)	49	88
19	S	71/74 (96%)	70 (99%)	1 (1%)	78	96
20	T	105/106 (99%)	98 (93%)	7 (7%)	23	64
21	U	44/53 (83%)	43 (98%)	1 (2%)	63	93
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	130/130 (100%)	126 (97%)	4 (3%)	52	89
24	X	66/74 (89%)	61 (92%)	5 (8%)	19	57
25	Y	120/196 (61%)	117 (98%)	3 (2%)	60	92
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	92
29	3	79/79 (100%)	73 (92%)	6 (8%)	19	57
All	All	3095/3646 (85%)	2955 (96%)	140 (4%)	38	81

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	99	ARG
11	K	24	THR
24	X	82	GLU
8	H	157	TYR
10	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	116	HIS
16	P	50	GLN
28	2	45	ASN
13	M	24	GLN
13	M	137	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	243 (8%)	22 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	262 (9%)	24 (0%)

5 of 262 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	871	G
30	0	1237	U
31	9	43	G
30	0	877	G
30	0	1080	C

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

5 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	$\# Z  > 2$
30	OMU	0	2587	30	20,22,23	0.64	0	24,31,34	0.83	0
30	OMG	0	2588	30	24,26,27	0.74	0	32,38,41	5.18	3 (9%)
30	UR3	0	2619	30	20,22,23	0.77	0	23,32,35	0.84	0
30	PSU	0	2621	30	19,21,22	1.12	2 (10%)	23,30,33	1.00	1 (4%)
30	1MA	0	628	30	23,25,26	0.86	0	32,37,40	0.90	1 (3%)

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
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30	-	0/8/25/26	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	3.08	1.43	1.37
30	0	2621	PSU	C6-N1	2.15	1.34	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.74	130.27	134.14
30	0	628	1MA	C2-N3-C4	-3.23	110.71	116.23
30	0	2588	OMG	C6-N1-C2	3.19	125.08	119.51
30	0	2588	OMG	C2-N3-C4	-2.37	111.76	115.09
30	0	2621	PSU	C5-C4-N3	-2.15	114.94	118.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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	A	237/240 (98%)	-0.38	1 (0%) 90 41	29, 65, 98, 115	0
2	B	337/338 (99%)	-0.47	0 100 100	31, 59, 87, 97	0
3	C	246/246 (100%)	-0.52	0 100 100	23, 47, 69, 80	0
4	D	140/177 (79%)	0.26	1 (0%) 84 28	74, 109, 132, 140	0
5	E	172/178 (96%)	-0.42	0 100 100	50, 74, 97, 103	0
6	F	119/120 (99%)	-0.18	0 100 100	50, 73, 106, 113	0
7	G	29/348 (8%)	0.12	0 100 100	75, 96, 105, 109	0
8	H	160/177 (90%)	-0.30	0 100 100	48, 67, 99, 109	0
9	I	70/162 (43%)	1.11	13 (18%) 2 1	134, 152, 167, 169	0
10	J	142/145 (97%)	-0.49	0 100 100	40, 58, 75, 97	0
11	K	132/132 (100%)	-0.56	0 100 100	39, 55, 81, 86	0
12	L	145/165 (87%)	-0.16	1 (0%) 84 28	35, 72, 113, 129	0
13	M	194/196 (98%)	-0.35	4 (2%) 60 12	31, 46, 99, 106	0
14	N	186/187 (99%)	-0.17	0 100 100	60, 80, 126, 132	0
15	O	115/116 (99%)	-0.49	0 100 100	43, 56, 74, 80	0
16	P	143/149 (95%)	-0.48	0 100 100	40, 59, 79, 85	0
17	Q	95/96 (98%)	-0.42	0 100 100	44, 56, 72, 88	0
18	R	150/155 (96%)	-0.53	0 100 100	33, 49, 70, 83	0
19	S	81/85 (95%)	-0.37	0 100 100	40, 62, 82, 92	0
20	T	119/120 (99%)	-0.36	0 100 100	40, 59, 87, 116	0
21	U	53/67 (79%)	1.56	15 (28%) 1 0	107, 117, 125, 126	0
22	V	65/71 (91%)	-0.03	3 (4%) 31 7	47, 74, 118, 123	0
23	W	154/154 (100%)	-0.42	0 100 100	39, 54, 73, 87	0
24	X	82/92 (89%)	-0.28	0 100 100	46, 65, 94, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.57	0 100 100	30, 49, 71, 92	0
26	Z	73/116 (62%)	2.06	32 (43%) 1 0	98, 116, 126, 130	0
27	1	56/57 (98%)	-0.52	0 100 100	28, 36, 43, 48	0
28	2	46/50 (92%)	-0.31	0 100 100	31, 66, 97, 104	0
29	3	92/92 (100%)	2.55	47 (51%) 0 0	104, 119, 130, 134	0
30	0	2754/2923 (94%)	-0.88	2 (0%) 93 63	23, 51, 96, 175	0
31	9	122/122 (100%)	-0.99	1 (0%) 83 26	45, 75, 103, 154	0
All	All	6651/7517 (88%)	-0.49	120 (1%) 65 14	23, 57, 116, 175	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	41	GLU	8.2
29	3	38	ARG	8.1
29	3	34	LYS	7.8
29	3	39	GLN	7.8
26	Z	46	SER	7.6

## 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
30	UR3	0	2619	21/22	0.13	0.47	39,43,45,48	0
30	PSU	0	2621	20/21	0.16	0.16	40,43,44,44	0
30	OMU	0	2587	21/22	0.11	0.10	41,44,50,50	0
30	OMG	0	2588	24/25	0.12	-0.82	39,41,42,45	0
30	1MA	0	628	23/24	0.14	-1.13	31,36,38,38	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
36	SR	0	8997	1/1	0.56	187.79	194,194,194,194	0
36	SR	0	8982	1/1	1.74	127.39	200,200,200,200	0
34	NA	0	8565	1/1	0.72	70.85	70,70,70,70	0
34	NA	0	8559	1/1	0.64	59.86	122,122,122,122	0
35	CL	A	8809	1/1	0.43	50.92	100,100,100,100	0
34	NA	0	8505	1/1	1.07	50.76	53,53,53,53	0
34	NA	0	8547	1/1	0.42	44.26	47,47,47,47	0
34	NA	0	8508	1/1	0.31	41.08	61,61,61,61	0
35	CL	0	8822	1/1	0.56	37.17	97,97,97,97	0
34	NA	0	8566	1/1	0.34	36.52	62,62,62,62	0
34	NA	0	8562	1/1	0.54	33.30	89,89,89,89	0
34	NA	0	8506	1/1	0.45	27.31	58,58,58,58	0
34	NA	0	8528	1/1	0.79	25.17	83,83,83,83	0
36	SR	0	8919	1/1	0.33	24.08	200,200,200,200	0
36	SR	0	8983	1/1	0.27	23.63	191,191,191,191	0
32	MG	0	8081	1/1	0.30	21.97	80,80,80,80	0
34	NA	0	8574	1/1	0.35	21.70	54,54,54,54	0
36	SR	0	8925	1/1	0.14	21.40	94,94,94,94	0
32	MG	0	8037	1/1	0.15	20.00	76,76,76,76	0
32	MG	0	8066	1/1	0.37	19.56	75,75,75,75	0
34	NA	0	8573	1/1	0.41	19.27	55,55,55,55	0
36	SR	0	8922	1/1	0.35	19.25	169,169,169,169	0
36	SR	0	8957	1/1	0.64	18.80	200,200,200,200	0
36	SR	0	9004	1/1	0.95	18.19	200,200,200,200	0
36	SR	0	9007	1/1	0.23	18.14	179,179,179,179	0
36	SR	0	9000	1/1	0.27	18.12	200,200,200,200	0
34	NA	0	8558	1/1	0.33	17.83	44,44,44,44	0
34	NA	0	8545	1/1	0.24	16.89	33,33,33,33	0
34	NA	0	8554	1/1	0.53	16.83	65,65,65,65	0
34	NA	0	8563	1/1	0.50	15.82	65,65,65,65	0
32	MG	0	8031	1/1	0.22	14.99	52,52,52,52	0
34	NA	0	8561	1/1	0.40	14.73	57,57,57,57	0
34	NA	R	8575	1/1	0.40	13.67	89,89,89,89	0
34	NA	0	8530	1/1	0.45	13.50	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8033	1/1	0.15	13.15	40,40,40,40	0
32	MG	0	8016	1/1	0.26	12.78	48,48,48,48	0
34	NA	0	8519	1/1	0.29	12.69	51,51,51,51	0
36	SR	0	8959	1/1	0.27	12.67	200,200,200,200	0
36	SR	0	8927	1/1	0.17	12.28	196,196,196,196	0
34	NA	0	8524	1/1	0.29	12.00	54,54,54,54	0
32	MG	0	8041	1/1	0.30	11.50	36,36,36,36	0
36	SR	0	8994	1/1	0.27	11.03	200,200,200,200	0
34	NA	0	8525	1/1	0.15	10.69	85,85,85,85	0
34	NA	0	8553	1/1	0.34	10.33	70,70,70,70	0
34	NA	0	8564	1/1	0.27	10.03	57,57,57,57	0
36	SR	0	8955	1/1	0.18	9.95	200,200,200,200	0
34	NA	0	8509	1/1	0.14	9.76	54,54,54,54	0
36	SR	0	8991	1/1	0.29	9.75	193,193,193,193	0
34	NA	0	8535	1/1	0.20	9.62	64,64,64,64	0
34	NA	0	8518	1/1	0.22	9.50	75,75,75,75	0
36	SR	0	8947	1/1	0.31	8.92	194,194,194,194	0
34	NA	0	8526	1/1	0.13	8.80	33,33,33,33	0
36	SR	0	8986	1/1	0.43	8.67	200,200,200,200	0
34	NA	0	8556	1/1	0.58	8.38	63,63,63,63	0
34	NA	0	8555	1/1	0.40	7.65	50,50,50,50	0
34	NA	0	8567	1/1	0.27	7.28	68,68,68,68	0
36	SR	B	8987	1/1	0.41	7.19	200,200,200,200	0
36	SR	0	8976	1/1	0.23	6.91	197,197,197,197	0
36	SR	0	8998	1/1	0.33	6.86	184,184,184,184	0
34	NA	0	8521	1/1	0.23	6.40	53,53,53,53	0
34	NA	0	8550	1/1	0.28	6.29	47,47,47,47	0
35	CL	0	8816	1/1	0.23	6.11	94,94,94,94	0
34	NA	0	8513	1/1	0.33	5.99	66,66,66,66	0
32	MG	0	8085	1/1	0.18	5.96	67,67,67,67	0
32	MG	0	8078	1/1	0.27	5.58	51,51,51,51	0
36	SR	0	8905	1/1	0.22	5.39	62,62,62,62	0
36	SR	0	8914	1/1	0.20	5.30	105,105,105,105	0
35	CL	0	8814	1/1	0.19	5.15	72,72,72,72	0
32	MG	0	8063	1/1	0.23	4.91	86,86,86,86	0
34	NA	9	8572	1/1	0.17	4.82	71,71,71,71	0
33	K	0	8401	1/1	0.17	4.78	156,156,156,156	0
34	NA	0	8546	1/1	0.36	4.74	80,80,80,80	0
32	MG	0	8005	1/1	0.24	4.65	34,34,34,34	0
36	SR	0	8971	1/1	0.11	4.47	170,170,170,170	0
36	SR	0	8989	1/1	0.21	4.46	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8569	1/1	0.23	4.30	67,67,67,67	0
36	SR	0	8969	1/1	0.22	4.28	192,192,192,192	0
36	SR	0	8901	1/1	0.14	4.22	63,63,63,63	0
32	MG	0	8040	1/1	0.20	4.16	54,54,54,54	0
34	NA	0	8541	1/1	0.25	4.09	54,54,54,54	0
34	NA	0	8529	1/1	0.15	3.89	41,41,41,41	0
34	NA	0	8552	1/1	0.26	3.82	58,58,58,58	0
32	MG	0	8014	1/1	0.20	3.78	21,21,21,21	0
36	SR	0	8924	1/1	0.16	3.67	133,133,133,133	0
34	NA	0	8522	1/1	0.20	3.66	45,45,45,45	0
36	SR	0	8979	1/1	0.13	3.51	198,198,198,198	0
34	NA	0	8520	1/1	0.14	3.25	39,39,39,39	0
32	MG	0	8011	1/1	0.22	2.89	24,24,24,24	0
34	NA	0	8534	1/1	0.21	2.84	37,37,37,37	0
35	CL	0	8817	1/1	0.19	2.83	69,69,69,69	0
32	MG	0	8004	1/1	0.19	2.79	21,21,21,21	0
36	SR	0	8904	1/1	0.17	2.76	58,58,58,58	0
32	MG	0	8023	1/1	0.15	2.60	24,24,24,24	0
32	MG	K	8054	1/1	0.14	2.59	40,40,40,40	0
36	SR	9	8980	1/1	0.13	2.48	182,182,182,182	0
32	MG	A	8051	1/1	0.31	2.44	101,101,101,101	0
32	MG	0	8009	1/1	0.19	2.43	24,24,24,24	0
34	NA	0	8537	1/1	0.21	2.43	29,29,29,29	0
36	SR	0	8909	1/1	0.14	2.35	89,89,89,89	0
32	MG	0	8048	1/1	0.21	2.33	20,20,20,20	0
32	MG	0	8044	1/1	0.15	2.26	52,52,52,52	0
32	MG	0	8015	1/1	0.13	2.24	25,25,25,25	0
32	MG	0	8022	1/1	0.13	2.20	17,17,17,17	0
34	NA	0	8571	1/1	0.14	2.07	46,46,46,46	0
32	MG	0	8030	1/1	0.35	2.07	86,86,86,86	0
32	MG	0	8071	1/1	0.15	2.04	31,31,31,31	0
34	NA	R	8532	1/1	0.15	2.01	37,37,37,37	0
32	MG	0	8020	1/1	0.12	2.01	29,29,29,29	0
36	SR	0	8996	1/1	0.17	2.01	199,199,199,199	0
32	MG	0	8007	1/1	0.19	1.97	18,18,18,18	0
35	CL	N	8807	1/1	0.34	1.94	99,99,99,99	0
32	MG	0	8075	1/1	0.13	1.93	83,83,83,83	0
32	MG	0	8047	1/1	0.20	1.84	67,67,67,67	0
36	SR	0	9008	1/1	0.16	1.71	97,97,97,97	0
32	MG	0	8018	1/1	0.13	1.70	34,34,34,34	0
32	MG	0	8059	1/1	0.12	1.63	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8010	1/1	0.18	1.61	24,24,24,24	0
36	SR	0	8906	1/1	0.20	1.51	64,64,64,64	0
32	MG	0	8003	1/1	0.17	1.46	22,22,22,22	0
34	NA	0	8502	1/1	0.14	1.38	56,56,56,56	0
34	NA	0	8507	1/1	0.15	1.35	32,32,32,32	0
35	CL	0	8811	1/1	0.28	1.34	79,79,79,79	0
32	MG	0	8008	1/1	0.13	1.27	26,26,26,26	0
34	NA	0	8560	1/1	0.94	1.27	74,74,74,74	0
34	NA	0	8548	1/1	0.12	1.16	68,68,68,68	0
32	MG	0	8088	1/1	0.15	1.14	35,35,35,35	0
36	SR	0	8903	1/1	0.13	1.13	46,46,46,46	0
32	MG	0	8062	1/1	0.19	1.08	57,57,57,57	0
36	SR	0	8902	1/1	0.16	0.92	67,67,67,67	0
36	SR	0	8968	1/1	0.13	0.86	177,177,177,177	0
32	MG	0	8019	1/1	0.16	0.72	23,23,23,23	0
36	SR	0	8941	1/1	0.17	0.56	122,122,122,122	0
36	SR	0	8985	1/1	0.12	0.54	182,182,182,182	0
32	MG	0	8084	1/1	0.13	0.49	24,24,24,24	0
32	MG	0	8061	1/1	0.19	0.42	19,19,19,19	0
36	SR	0	8937	1/1	0.15	0.42	100,100,100,100	0
32	MG	0	8029	1/1	0.12	0.35	68,68,68,68	0
37	CD	3	8704	1/1	0.70	0.25	200,200,200,200	0
32	MG	2	8060	1/1	0.11	0.18	35,35,35,35	0
32	MG	0	8083	1/1	0.12	0.17	71,71,71,71	0
35	CL	0	8803	1/1	0.14	0.14	69,69,69,69	0
32	MG	0	8027	1/1	0.11	0.11	26,26,26,26	0
34	NA	0	8515	1/1	0.14	0.06	44,44,44,44	0
36	SR	0	8943	1/1	0.10	0.04	72,72,72,72	0
34	NA	0	8551	1/1	0.13	0.03	55,55,55,55	0
34	NA	0	8544	1/1	0.10	-0.00	41,41,41,41	0
34	NA	0	8557	1/1	0.08	-0.05	59,59,59,59	0
32	MG	0	8006	1/1	0.13	-0.06	20,20,20,20	0
32	MG	0	8068	1/1	0.11	-0.18	49,49,49,49	0
34	NA	C	8503	1/1	0.15	-0.20	45,45,45,45	0
32	MG	0	8077	1/1	0.10	-0.21	43,43,43,43	0
36	SR	0	8908	1/1	0.12	-0.21	77,77,77,77	0
35	CL	R	8806	1/1	0.12	-0.22	47,47,47,47	0
32	MG	0	8080	1/1	0.22	-0.24	68,68,68,68	0
36	SR	0	8951	1/1	0.10	-0.25	139,139,139,139	0
34	NA	Q	8540	1/1	0.14	-0.27	67,67,67,67	0
32	MG	0	8021	1/1	0.11	-0.29	25,25,25,25	0
32	MG	0	8028	1/1	0.13	-0.30	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8514	1/1	0.17	-0.33	17,17,17,17	0
32	MG	0	8039	1/1	0.14	-0.33	71,71,71,71	0
34	NA	0	8527	1/1	0.19	-0.35	54,54,54,54	0
36	SR	0	8926	1/1	0.09	-0.36	109,109,109,109	0
35	CL	0	8805	1/1	0.10	-0.36	70,70,70,70	0
36	SR	0	8988	1/1	0.11	-0.38	170,170,170,170	0
32	MG	0	8034	1/1	0.14	-0.39	53,53,53,53	0
32	MG	3	8090	1/1	0.14	-0.41	80,80,80,80	0
35	CL	O	8808	1/1	0.14	-0.43	87,87,87,87	0
32	MG	B	8043	1/1	0.11	-0.47	53,53,53,53	0
35	CL	J	8801	1/1	0.15	-0.50	71,71,71,71	0
34	NA	0	8517	1/1	0.13	-0.55	21,21,21,21	0
37	CD	1	8702	1/1	0.11	-0.57	61,61,61,61	0
33	K	M	8402	1/1	0.14	-0.59	60,60,60,60	0
36	SR	0	8940	1/1	0.10	-0.61	77,77,77,77	0
32	MG	0	8070	1/1	0.10	-0.68	40,40,40,40	0
36	SR	F	9005	1/1	0.10	-0.68	131,131,131,131	0
32	MG	0	8069	1/1	0.14	-0.69	55,55,55,55	0
35	CL	J	8821	1/1	0.11	-0.72	66,66,66,66	0
35	CL	Y	8820	1/1	0.10	-0.73	47,47,47,47	0
36	SR	B	8950	1/1	0.15	-0.75	113,113,113,113	0
36	SR	0	8923	1/1	0.11	-0.76	85,85,85,85	0
34	NA	0	8501	1/1	0.11	-0.84	43,43,43,43	0
36	SR	A	8993	1/1	0.08	-0.85	159,159,159,159	0
32	MG	0	8056	1/1	0.11	-0.86	75,75,75,75	0
32	MG	0	8024	1/1	0.11	-0.91	96,96,96,96	0
36	SR	0	8990	1/1	0.13	-0.92	125,125,125,125	0
36	SR	0	8953	1/1	0.07	-0.93	200,200,200,200	0
36	SR	R	8912	1/1	0.12	-0.95	86,86,86,86	0
36	SR	0	8954	1/1	0.11	-0.95	103,103,103,103	0
36	SR	0	8918	1/1	0.10	-0.96	71,71,71,71	0
36	SR	0	8916	1/1	0.10	-0.98	114,114,114,114	0
32	MG	B	8042	1/1	0.08	-1.03	56,56,56,56	0
36	SR	0	8964	1/1	0.08	-1.04	129,129,129,129	0
36	SR	0	8977	1/1	0.09	-1.04	181,181,181,181	0
36	SR	1	8913	1/1	0.12	-1.07	100,100,100,100	0
36	SR	0	8915	1/1	0.10	-1.09	118,118,118,118	0
36	SR	0	8972	1/1	0.09	-1.09	150,150,150,150	0
36	SR	0	8907	1/1	0.10	-1.12	40,40,40,40	0
36	SR	0	8946	1/1	0.13	-1.15	123,123,123,123	0
34	NA	0	8549	1/1	0.15	-1.22	77,77,77,77	0
32	MG	0	8012	1/1	0.14	-1.25	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8046	1/1	0.12	-1.26	26,26,26,26	0
37	CD	U	8701	1/1	0.36	-1.30	200,200,200,200	0
35	CL	J	8802	1/1	0.07	-1.32	76,76,76,76	0
32	MG	0	8058	1/1	0.07	-1.35	22,22,22,22	0
36	SR	A	8930	1/1	0.11	-1.35	125,125,125,125	0
36	SR	3	8932	1/1	0.11	-1.36	158,158,158,158	0
36	SR	0	8939	1/1	0.08	-1.39	152,152,152,152	0
36	SR	9	9003	1/1	0.11	-1.40	177,177,177,177	0
35	CL	0	8815	1/1	0.09	-1.42	87,87,87,87	0
34	NA	9	8543	1/1	0.09	-1.43	38,38,38,38	0
34	NA	0	8523	1/1	0.10	-1.47	51,51,51,51	0
36	SR	0	8956	1/1	0.04	-1.49	151,151,151,151	0
36	SR	0	8958	1/1	0.07	-1.50	114,114,114,114	0
32	MG	0	8082	1/1	0.11	-1.50	66,66,66,66	0
34	NA	J	8538	1/1	0.07	-1.50	49,49,49,49	0
36	SR	0	8995	1/1	0.15	-1.54	140,140,140,140	0
32	MG	0	8067	1/1	0.14	-1.57	32,32,32,32	0
35	CL	L	8810	1/1	0.11	-1.68	64,64,64,64	0
36	SR	0	8936	1/1	0.08	-1.71	87,87,87,87	0
36	SR	0	8975	1/1	0.08	-1.74	171,171,171,171	0
35	CL	K	8812	1/1	0.08	-1.76	48,48,48,48	0
36	SR	1	8952	1/1	0.11	-1.77	72,72,72,72	0
36	SR	0	8984	1/1	0.08	-1.80	105,105,105,105	0
36	SR	0	9002	1/1	0.07	-1.81	157,157,157,157	0
36	SR	0	8981	1/1	0.09	-1.83	157,157,157,157	0
36	SR	0	8935	1/1	0.08	-1.87	87,87,87,87	0
34	NA	0	8531	1/1	0.09	-1.89	15,15,15,15	0
36	SR	9	8978	1/1	0.07	-1.91	125,125,125,125	0
32	MG	0	8001	1/1	0.12	-1.92	26,26,26,26	0
36	SR	A	8929	1/1	0.05	-1.98	117,117,117,117	0
35	CL	B	8819	1/1	0.11	-1.99	59,59,59,59	0
36	SR	0	8928	1/1	0.07	-2.04	146,146,146,146	0
32	MG	0	8036	1/1	0.07	-2.13	37,37,37,37	0
34	NA	0	8504	1/1	0.09	-2.19	27,27,27,27	0
36	SR	0	8944	1/1	0.06	-2.21	165,165,165,165	0
34	NA	0	8570	1/1	0.07	-2.26	25,25,25,25	0
32	MG	0	8076	1/1	0.10	-2.37	27,27,27,27	0
36	SR	0	8933	1/1	0.07	-2.40	126,126,126,126	0
32	MG	0	8017	1/1	0.09	-2.43	20,20,20,20	0
37	CD	Z	8703	1/1	0.30	-2.49	200,200,200,200	0
36	SR	0	8921	1/1	0.09	-2.59	75,75,75,75	0
36	SR	0	8938	1/1	0.07	-2.59	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8052	1/1	0.06	-2.60	51,51,51,51	0
36	SR	0	8911	1/1	0.06	-2.66	79,79,79,79	0
32	MG	0	8053	1/1	0.05	-2.69	45,45,45,45	0
36	SR	0	8931	1/1	0.07	-2.72	110,110,110,110	0
32	MG	0	8073	1/1	0.07	-2.80	51,51,51,51	0
34	NA	M	8539	1/1	0.07	-2.81	32,32,32,32	0
35	CL	3	8804	1/1	0.13	-2.98	120,120,120,120	0
32	MG	0	8038	1/1	0.07	-3.04	61,61,61,61	0
32	MG	0	8065	1/1	0.09	-3.06	50,50,50,50	0
34	NA	0	8568	1/1	0.10	-3.08	38,38,38,38	0
35	CL	M	8818	1/1	0.05	-3.12	39,39,39,39	0
32	MG	T	8057	1/1	0.04	-3.17	63,63,63,63	0
34	NA	0	8533	1/1	0.08	-3.20	53,53,53,53	0
36	SR	0	8910	1/1	0.07	-3.22	99,99,99,99	0
36	SR	0	8960	1/1	0.06	-3.22	152,152,152,152	0
32	MG	0	8055	1/1	0.09	-3.23	45,45,45,45	0
36	SR	0	8967	1/1	0.05	-3.27	133,133,133,133	0
34	NA	0	8511	1/1	0.07	-3.27	48,48,48,48	0
32	MG	0	8079	1/1	0.09	-3.44	36,36,36,36	0
32	MG	0	8087	1/1	0.08	-3.59	26,26,26,26	0
36	SR	0	8934	1/1	0.08	-3.65	99,99,99,99	0
36	SR	0	8917	1/1	0.09	-3.67	109,109,109,109	0
36	SR	0	8948	1/1	0.08	-3.73	103,103,103,103	0
34	NA	0	8536	1/1	0.07	-3.98	40,40,40,40	0
36	SR	0	9001	1/1	0.07	-4.11	166,166,166,166	0
34	NA	0	8542	1/1	0.14	-4.13	51,51,51,51	0
36	SR	S	8961	1/1	0.05	-4.14	126,126,126,126	0
36	SR	0	8974	1/1	0.13	-4.53	164,164,164,164	0
36	SR	0	8992	1/1	0.06	-4.66	130,130,130,130	0
32	MG	Y	8086	1/1	0.04	-4.84	37,37,37,37	0
34	NA	0	8512	1/1	0.08	-4.88	36,36,36,36	0
32	MG	0	8045	1/1	0.07	-4.94	24,24,24,24	0
32	MG	0	8089	1/1	0.16	-5.00	59,59,59,59	0
34	NA	0	8516	1/1	0.09	-5.40	20,20,20,20	0
34	NA	S	8510	1/1	0.03	-5.50	26,26,26,26	0
36	SR	0	8970	1/1	0.03	-5.52	131,131,131,131	0
36	SR	0	8965	1/1	0.07	-5.53	127,127,127,127	0
32	MG	0	8013	1/1	0.04	-5.59	24,24,24,24	0
32	MG	0	8091	1/1	0.08	-5.67	58,58,58,58	0
32	MG	0	8025	1/1	0.09	-5.74	30,30,30,30	0
32	MG	0	8093	1/1	0.05	-5.83	28,28,28,28	0
36	SR	0	8942	1/1	0.06	-5.85	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8962	1/1	0.08	-5.96	179,179,179,179	0
32	MG	0	8064	1/1	0.06	-6.20	33,33,33,33	0
36	SR	0	8949	1/1	0.07	-6.43	102,102,102,102	0
36	SR	0	8945	1/1	0.06	-6.66	107,107,107,107	0
32	MG	9	8074	1/1	0.03	-6.67	63,63,63,63	0
36	SR	0	8920	1/1	0.04	-6.95	106,106,106,106	0
32	MG	0	8072	1/1	0.08	-6.97	47,47,47,47	0
32	MG	0	8050	1/1	0.07	-7.45	52,52,52,52	0
32	MG	0	8002	1/1	0.09	-7.47	29,29,29,29	0
35	CL	0	8813	1/1	0.04	-7.55	46,46,46,46	0
36	SR	3	8999	1/1	0.25	-7.85	172,172,172,172	0
36	SR	0	8966	1/1	0.07	-8.83	97,97,97,97	0
32	MG	0	8032	1/1	0.07	-11.31	27,27,27,27	0
32	MG	0	8026	1/1	0.04	-11.48	27,27,27,27	0
32	MG	0	8035	1/1	0.06	-17.00	61,61,61,61	0
36	SR	0	8963	1/1	0.06	-18.00	123,123,123,123	0
37	CD	O	8705	1/1	0.06	-20.20	93,93,93,93	0
32	MG	0	8092	1/1	0.05	-48.00	44,44,44,44	0
36	SR	0	8973	1/1	0.12	-	112,112,112,112	0
32	MG	0	8049	1/1	0.56	-	74,74,74,74	0
36	SR	0	9006	1/1	0.53	-	180,180,180,180	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.