



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:17 PM GMT

PDB ID : 3CCQ
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.90 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

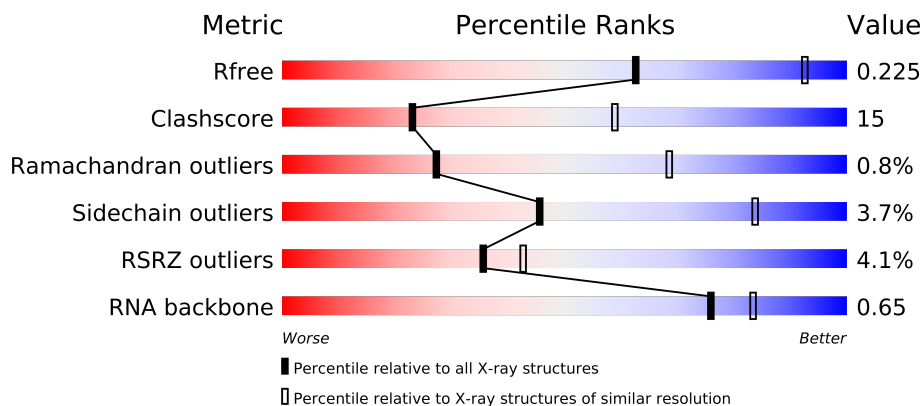
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	8003	-	X
32	MG	0	8009	-	X
32	MG	0	8014	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8022	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8033	-	X
32	MG	0	8039	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8061	-	X
32	MG	0	8063	-	X
32	MG	0	8066	-	X
32	MG	0	8069	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8071	-	X
32	MG	0	8072	-	X
32	MG	0	8073	-	X
32	MG	0	8078	-	X
32	MG	0	8081	-	X
32	MG	0	8082	-	X
32	MG	0	8085	-	X
32	MG	0	8089	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
33	K	0	8402	-	X
34	NA	0	8505	-	X
34	NA	0	8509	-	X
34	NA	0	8511	-	X
34	NA	0	8513	-	X
34	NA	0	8516	-	X
34	NA	0	8518	-	X
34	NA	0	8519	-	X
34	NA	0	8521	-	X
34	NA	0	8522	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8527	-	X
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8534	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8548	-	X
34	NA	0	8549	-	X
34	NA	0	8550	-	X
34	NA	0	8551	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8559	-	X
34	NA	0	8560	-	X
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	8568	-	X
34	NA	0	8571	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	9	8572	-	X
34	NA	B	8552	-	X
34	NA	R	8575	-	X
34	NA	S	8510	-	X
35	CL	0	8822	-	X
35	CL	B	8819	-	X
36	SR	0	8903	-	X
36	SR	0	8905	-	X
36	SR	0	8906	-	X
36	SR	0	8909	-	X
36	SR	0	8914	-	X
36	SR	0	8921	-	X
36	SR	0	8922	-	X
36	SR	0	8926	-	X
36	SR	0	8934	-	X
36	SR	0	8937	-	X
36	SR	0	8947	-	X
36	SR	0	8949	-	X
36	SR	0	8959	-	X
36	SR	0	8962	-	X
36	SR	0	8963	-	X
36	SR	0	8976	-	X
36	SR	0	8981	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8986	-	X
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8997	-	X
36	SR	0	9002	-	X
36	SR	0	9004	-	X
36	SR	0	9006	-	X
36	SR	0	9007	-	X
36	SR	9	8980	-	X
36	SR	B	8987	-	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	10870	19055	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	87	Total	Mg	0	0
			87	87		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	9	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	2	Total K 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	65	Total Na 65 65	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	B	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	Q	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
35	R	1	Total Cl 1 1	0	0

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5950	Total	O	0	0
			5950	5950		
38	9	148	Total	O	0	0
			148	148		
38	A	112	Total	O	0	0
			112	112		
38	B	142	Total	O	0	0
			142	142		
38	C	168	Total	O	0	0
			168	168		
38	D	45	Total	O	0	0
			45	45		
38	E	42	Total	O	0	0
			42	42		
38	F	26	Total	O	0	0
			26	26		
38	G	17	Total	O	0	0
			17	17		
38	H	65	Total	O	0	0
			65	65		
38	I	5	Total	O	0	0
			5	5		
38	J	56	Total	O	0	0
			56	56		
38	K	60	Total	O	0	0
			60	60		
38	L	82	Total	O	0	0
			82	82		
38	M	123	Total	O	0	0
			123	123		
38	N	59	Total	O	0	0
			59	59		
38	O	47	Total	O	0	0
			47	47		
38	P	59	Total	O	0	0
			59	59		

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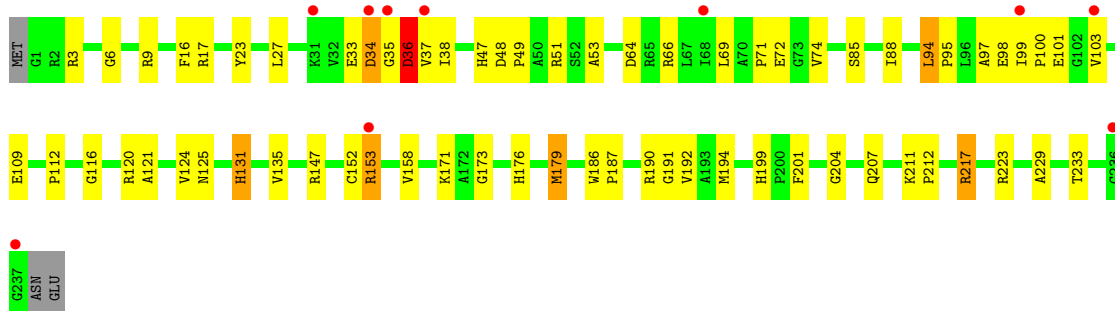
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Q	47	Total 47	O 47	0	0
38	R	76	Total 76	O 76	0	0
38	S	33	Total 33	O 33	0	0
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	12	Total 12	O 12	0	0
38	W	66	Total 66	O 66	0	0
38	X	28	Total 28	O 28	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	31	Total 31	O 31	0	0
38	1	54	Total 54	O 54	0	0
38	2	43	Total 43	O 43	0	0
38	3	68	Total 68	O 68	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 ($RSRZ > 2$). 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.

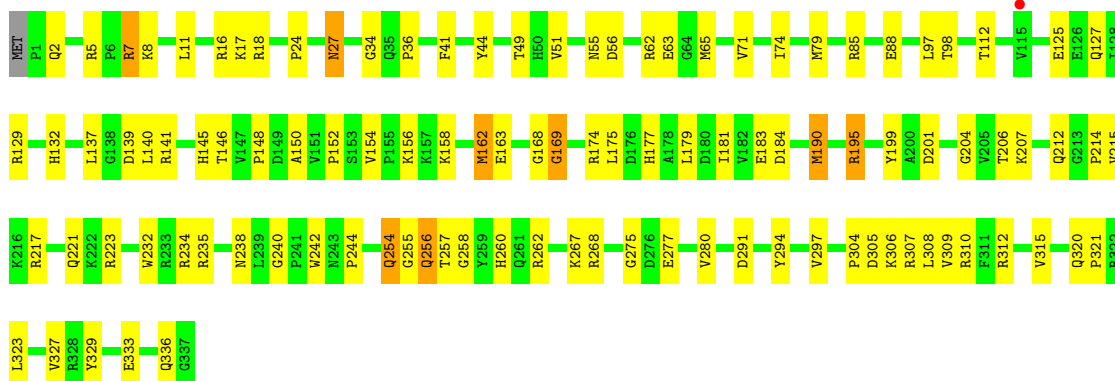
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



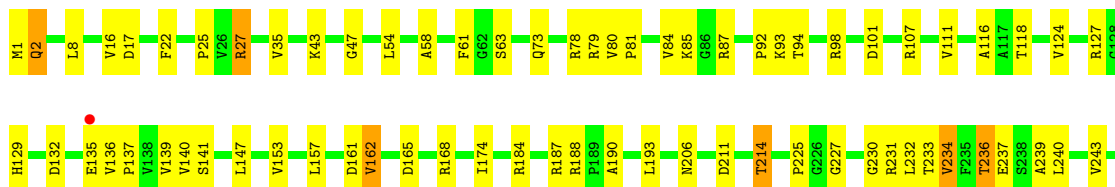
- Molecule 2: 50S ribosomal protein L3P

Chain B: 



- Molecule 3: 50S ribosomal protein L4P

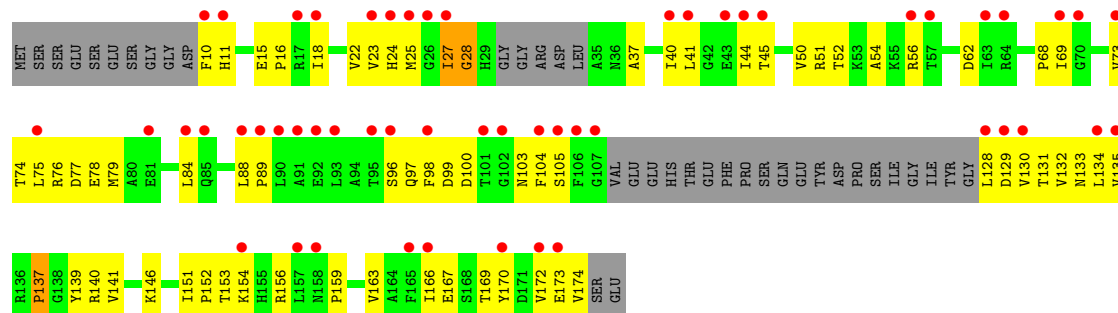
Chain C: 



R246

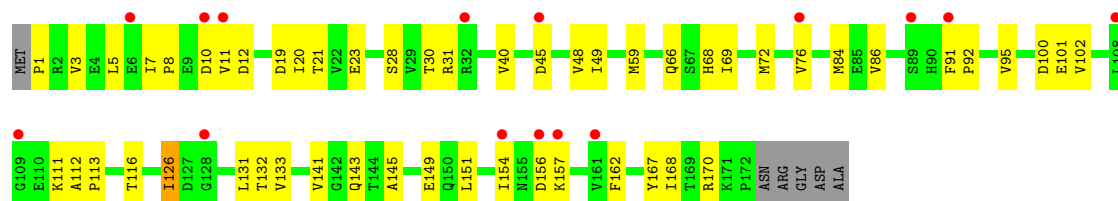
- Molecule 4: 50S ribosomal protein L5P

Chain D:



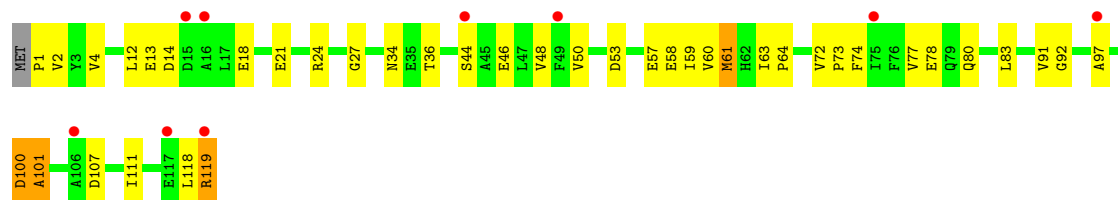
- Molecule 5: 50S ribosomal protein L6P

Chain E:



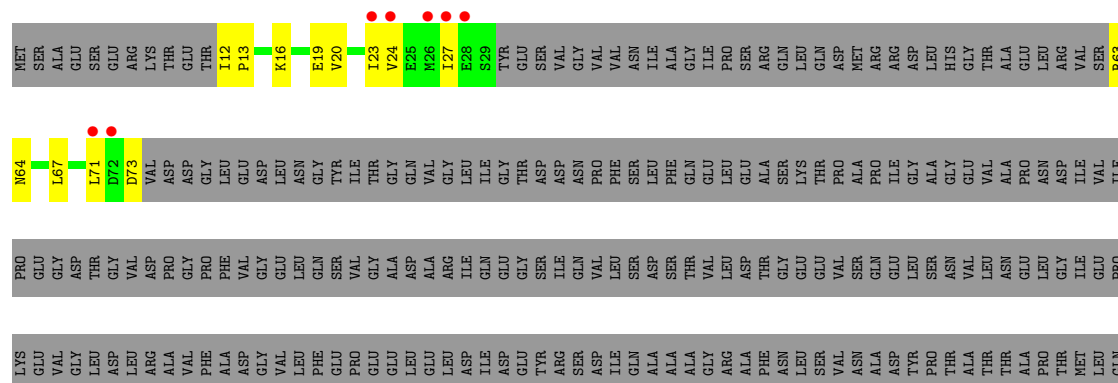
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



- Molecule 7: 50S ribosomal protein L10E

Chain G:



SER
ALA
ARG
GLY
ASN
ALA
LYS
SER
LEU
ALA
LEU
GLN
ALA
ALA
ILE
GLU
ASP
PRO
GLU
VAL
VAL
VAL
PRO
ASP
LEU
VAL
SER
LYS
ALA
ASP
ALA
GLN
VAL
ARG
ALA
LEU
ALA
SER
GLN
ILE
ASP
GLU
GLU
ALA
LEU
PRO
GLU
GLU
LEU
GLN
GLY
VAL
GLU
ALA
ASP
VAL
ALA
THR
GLU

PRO
THR
ASP
GLN
ASP
ASP
THR
ALA
SER
GLU
ASP
ASP
ASP
ALA
ASP
ALA
ALA
ALA
GLU
GLU
ALA
ALA
ASP
ASP
ASP
ASP
GLU
ASP
ALA
GLY
ALA
ASP
LEU
GLY
MET
PHE

• Molecule 8: 50S ribosomal protein L10e

Chain H:

MET
SER
ASP
K4
P5
A6
P15
R19
R20
E21
Y22
I26
P27
G28
S29
K30
I31
A32
K39
Q40
K41
D42
Y46
P47
V48
L52
Q59
L60
R61
H62
G63
S64
L65
E66
R69
A72
N73
R74
Y86
K87
R91
R99
E100
N101
K102
GLN
ALA
THR

GLY
ALA
GLY
ALA
ASP
ARG
VAL
D114
I123
V124
R129
F137
T138
A139
V149
R155
A156
Y157
M158
V168
E169
R170
E173
L174
LEU
ILE
ALA

• Molecule 9: 50S ribosomal protein L11P

Chain I:

MET
ALA
GLY
THR
ILE
GLU
VAL
VAL
LEU
PRO
GLY
GLY
ALA
ASN
PRO
GLY
PRO
PRO
LEU
PRO
PRO
LEU
GLY
LEU
PRO
THR
PRO
VAL
ASP
VAL
GLN
ALA
VAL
VAL
GLN
ILE
ASN
ASP
GLN
THR
ALA
ALA
PHE
ASP
GLY
THR
VAL
VAL
VAL
LYS
TYR
ASP
ASP
GLY

SER
PHE
GLU
ILE
GLU
VAL
G66
V67
P68
P69
T70
A71
E72
L73
I74
K75
D76
E77
A78
G79
F80
E81
T82
G83
S84
G85
E86
P87
Q88
F91
V92
A93
D94
V97
D98
Q99
V100
K101
Q102
I103
E104
A105
Q106
K107
H108
P109
D110
L111
L112
S113
Y114
A120
K121
V124
G125
T126

G127
T128
S129
L130
G131
V132
T133
T134
I135
GLY
ASN
PRO
ARG
GLU
PHE
LYS
GLU
ARG
ILE
ASP
ALA
GLY
TVR
ASP
VAL
PHE
ALA
ALA
GLU
GLN
ALA

• Molecule 10: 50S ribosomal protein L13P

Chain J:

MET
SER
VAL
A4
E5
T18
M19
V39
N40
A41
E42
V45
I46
T47
Q52
I53
V54
R60
Y69
F70
R74
P75
D76
G77
I78
F79
T82
P88
H89
K90
L106
G106
N107
P108
Y109
L121
I127
V130
T131
L132
S136
E137
T138
W145

• Molecule 11: 50S ribosomal protein L14P

Chain K:

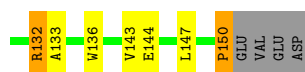
M1
L4
D7
Q10
K14
C20
L29
I32
S33
V34
G39
T40
K41
N42
P45
K46
A47
V55
S56
E63
M64
R65
R66
Q67
V74
R75
K78
P79
I80
R81
R87
V88
K89
V98
E102
E108
I113
E116
V117
A118
A125
S126
A127
A128
T129
M130
T131
V132

• Molecule 12: 50S ribosomal protein L15P

Chain L:

MET
T1
R6
R11
H18
R22
R30
G31
D32
R35
D36
E39
F40
H41
N42
H43
R53
K56
V57
Q58
E59
F60
M61
A62
V66
R67
E71
D80
V81
A82
E83
VAL
GLU
ASP
GLY
GLY
F89
E99
A100
D101
D104
Y105
V106
G112
Q113





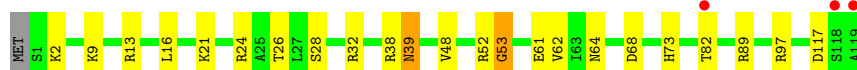
- Molecule 19: 50S ribosomal protein L23P

Chain S:



- Molecule 20: 50S ribosomal protein L24P

Chain T:



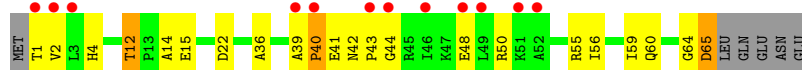
- Molecule 21: 50S ribosomal protein L24e

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:

MET ALA ASP ASN GLU GLU ASP VAL GLU ALA GLU TYR THR LEU THR ASP ILE SER GLY VAL GLY PRO SER LYS ALA GLU SER LEU ARG GLU ALA GLY PHE SER VAL ASP ARG GLY ALA ASP GLN SER ALA LEU ALA ASP VAL SER GLY ILE GLY ASN LEU

ALA ARG ILE LYS ALA ASP VAL GLY ASN LEU VAL GLU SER THR LEU GLU ALA GLY THR ASP VAL T995 A99 P107 R115 K125 P126 Q127 F128 N129 R130 Q131 D132 H133 H134 T141 S142 W143 R144 S151

R154 T163 R169 S170 V174 R175 G176 K177 G181 F182 R186 V187 H188 H189 D192 T200 E201 A202 V203 R204 R212 R216 I217 E218 E219 E220 Y233 Y234 Y236 VAL SER GLU

- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:

MET SER PRO ARG ALA ARG GLU PRO ASN LEU GLY LEU LEU TRP PRO LEU GLY GLN THR MET ALA SER LYS SER GLY THR GLY S34 S35 F38 G39 A40 G43 R44 V45 S46 R47 R48 R49 V50 E54 S55 E56 M57 N58 E59 D60 H61 C66 G67

E68 D69 R70 V71 D72 R73 D74 G75 G76 G77 I78 C81 S82 Y83 C84 D85 G90 S106 ILE ARG ALA LEU SER GLU ASP GLU

- Molecule 27: 50S ribosomal protein L37e

Chain 1:

MET T1 Q8 G9 K10 K11 N12 H16 R20 R21 C22 K25 H28 K31 K32 C37 G38 F39 S42 E56

- Molecule 28: 50S ribosomal protein L39e

Chain 2:

MET G1 K2 K5 K8 K9 L11 M18 P22 V25 K28 K31 K32 VAL GLN K35 K38 R39 R40 H41 R42 R43 R44 R45 T47 D48 E49

- Molecule 29: 50S ribosomal protein L44E

Chain 3:

M1 Q2 M3 P4 N8 C11 N15 H20 V25 G28 R29 Q30 N43 K60 P61 K68 Y69 R70 C71 G72 E73 A77 W83 F90 Q91 E92

- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

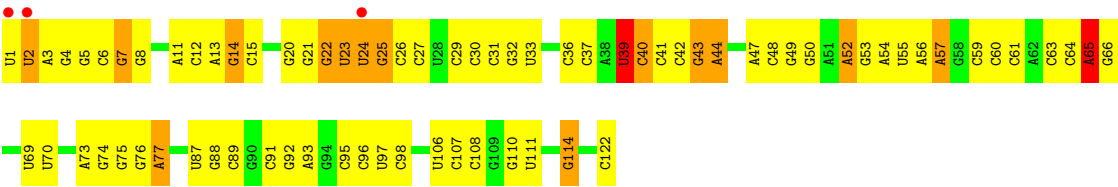
G U G G C C A U10 A11 U12 G13 G17 C18 G23 G24 A25 U26 U27 C31 A37 G38 G39 G47 A48 G51 A52 G56 A60 G61 G62 U63 G64 G65 G66 A67 U68 A69 A70 G71 G74 U75 G81 G85 A86 C87 G88 G89

A90 G91 G92 C93 A98 A99 C100 G105 A111 U107 U108 G111 G112 A113 A114 U115 A119 A120 U121 C122 U123 C124 U125 C U128 A129 C130 A131 C136 U137 G138 C139 G140 C141 A151 A152 C153 C154 C155 A156 A157 A158 G159 C162 U163 G164 A165 A166 A167 C168 A169

U172 A177 U178 G182 G185 A186 A189 G190 A191 A192 G196 A198 U202 G203 A204 U205 A212 G213 U214 G219 G220 G221 A222 G223 U224 G225 C228 G229 A232 G237 C238 C239 C240 A241 G249 C250 U253 C254 A255 C256 G257 A258 G259 C260 U263







4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 85.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.90) 98.2 (85.65-2.41)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.186 , 0.233 0.184 , 0.225	Depositor DCC
R_{free} test set	3844 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 667142 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.33	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.32	0/1111	0.56	1/1498 (0.1%)
5	E	0.33	0/1382	0.57	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.33	0/241	0.51	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.61	0/1530
11	K	0.34	0/1004	0.66	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.36	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.61	0/1999
15	O	0.35	0/874	0.59	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.09	6/1578 (0.4%)
19	S	0.33	0/648	0.54	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.32	0/417	0.57	0/562
22	V	0.32	0/502	0.54	0/675
23	W	0.36	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.37	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.63	0/781
27	1	0.39	0/438	0.62	0/578
28	2	0.34	0/401	0.58	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.39	0/65954	0.68	9/102862 (0.0%)
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.40	7/98698 (0.0%)	0.67	17/147581 (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
18	R	1	0
23	W	0	1
30	0	0	32
31	9	0	3
All	All	1	36

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.45	2.87	1.50
18	R	150	PRO	CA-C	-18.11	1.16	1.52
18	R	150	PRO	CG-CD	13.90	1.96	1.50
18	R	150	PRO	C-O	11.92	1.47	1.23
18	R	150	PRO	N-CA	11.35	1.66	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.81	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.28	128.89	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.52	99.75	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	202	U	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	48	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	66	0
2	B	2625	0	2533	94	0
3	C	1860	0	1813	53	0
4	D	1094	0	1085	52	0
5	E	1357	0	1266	36	0
6	F	890	0	843	30	0
7	G	240	0	231	11	0
8	H	1282	0	1292	41	0
9	I	519	0	500	21	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	33	0
13	M	1558	0	1573	59	0
14	N	1445	0	1401	54	0
15	O	865	0	873	18	0
16	P	1136	0	1123	30	0
17	Q	735	0	729	26	0
18	R	1149	0	1122	32	0
19	S	641	0	605	10	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	17	0
23	W	1196	0	1137	66	0
24	X	654	0	653	22	0
25	Y	1130	0	1133	33	0
26	Z	573	0	531	21	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	728	17	0
30	0	59018	0	29809	1329	0
31	9	2599	0	1325	97	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	65	0	0	0	0
34	9	2	0	0	0	0
34	B	1	0	0	0	0
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	3	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	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	5950	0	0	203	0
38	1	54	0	0	3	0
38	2	43	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	3	68	0	0	6	0
38	9	148	0	0	9	0
38	A	112	0	0	5	0
38	B	142	0	0	14	0
38	C	168	0	0	13	0
38	D	45	0	0	4	0
38	E	42	0	0	4	0
38	F	26	0	0	1	0
38	G	17	0	0	1	0
38	H	65	0	0	5	0
38	I	5	0	0	0	0
38	J	56	0	0	2	0
38	K	60	0	0	5	0
38	L	82	0	0	8	0
38	M	123	0	0	2	0
38	N	59	0	0	3	0
38	O	47	0	0	4	0
38	P	59	0	0	2	0
38	Q	47	0	0	2	0
38	R	76	0	0	1	0
38	S	33	0	0	0	0
38	T	36	0	0	4	0
38	U	26	0	0	2	0
38	V	12	0	0	1	0
38	W	66	0	0	6	0
38	X	28	0	0	3	0
38	Y	97	0	0	7	0
38	Z	31	0	0	4	0
All	All	99120	0	59910	2191	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 15.

The worst 5 of 2191 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:871:G:C8	30:0:871:G:H5'	1.75	1.21
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.12
31:9:56:A:H2'	31:9:57:A:H5''	1.21	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.79	1.11

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%)	213 (91%)	18 (8%)	4 (2%)	14	45
2	B	335/338 (99%)	309 (92%)	22 (7%)	4 (1%)	19	57
3	C	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
4	D	134/177 (76%)	107 (80%)	22 (16%)	5 (4%)	5	20
5	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
6	F	117/120 (98%)	104 (89%)	9 (8%)	4 (3%)	6	23
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	145 (93%)	11 (7%)	0	100	100
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	15	50
10	J	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	11	39
13	M	192/196 (98%)	182 (95%)	10 (5%)	0	100	100
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	10	37
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
19	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
20	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	25	66
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	6	25
23	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	30	72
24	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	18	54
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	62 (87%)	8 (11%)	1 (1%)	16	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	37 (88%)	5 (12%)	0	100	100
29	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4472 (83%)	3416 (92%)	258 (7%)	31 (1%)	27	68

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ASP
1	A	37	VAL
6	F	101	ALA
14	N	154	LEU

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%)	171 (96%)	8 (4%)	38	77
2	B	282/283 (100%)	268 (95%)	14 (5%)	34	73
3	C	193/193 (100%)	180 (93%)	13 (7%)	23	56
4	D	117/148 (79%)	113 (97%)	4 (3%)	49	86
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	90
6	F	93/94 (99%)	91 (98%)	2 (2%)	64	92
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	84
8	H	134/145 (92%)	128 (96%)	6 (4%)	38	77
9	I	58/130 (45%)	56 (97%)	2 (3%)	49	86
10	J	118/121 (98%)	110 (93%)	8 (7%)	22	55
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	90
12	L	113/127 (89%)	108 (96%)	5 (4%)	39	77
13	M	158/160 (99%)	151 (96%)	7 (4%)	39	77
14	N	149/150 (99%)	147 (99%)	2 (1%)	80	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	93/94 (99%)	92 (99%)	1 (1%)	84	97
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	94
17	Q	79/80 (99%)	75 (95%)	4 (5%)	33	72
18	R	117/122 (96%)	112 (96%)	5 (4%)	40	78
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	101 (96%)	4 (4%)	44	83
21	U	44/53 (83%)	42 (96%)	2 (4%)	38	77
22	V	51/57 (90%)	48 (94%)	3 (6%)	28	64
23	W	130/130 (100%)	127 (98%)	3 (2%)	63	92
24	X	66/74 (89%)	63 (96%)	3 (4%)	38	77
25	Y	120/196 (61%)	116 (97%)	4 (3%)	50	87
26	Z	60/94 (64%)	59 (98%)	1 (2%)	73	94
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	91
29	3	79/79 (100%)	78 (99%)	1 (1%)	80	96
All	All	3095/3646 (85%)	2982 (96%)	113 (4%)	45	84

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	173	GLU
11	K	10	GLN
24	X	46	ASP
9	I	110	ASP
10	J	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	88	GLN
27	1	28	HIS
13	M	137	ASN
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	22 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	23 (0%)

5 of 260 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 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1246	A
30	0	1377	C
30	0	2718	C
30	0	1352	A
30	0	1474	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	0.72	1 (5%)	24,31,34	0.73	0
30	OMG	0	2588	30	24,26,27	0.84	1 (4%)	32,38,41	5.05	3 (9%)
30	UR3	0	2619	30	20,22,23	0.73	0	23,32,35	0.87	0
30	PSU	0	2621	30	19,21,22	1.11	3 (15%)	23,30,33	1.10	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	1MA	0	628	30	23,25,26	0.85	0	32,37,40	0.94	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	-	1/8/25/26	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	2.73	1.42	1.37
30	0	2588	OMG	P-OP1	2.32	1.49	1.46
30	0	2621	PSU	C6-N1	2.24	1.34	1.32
30	0	2587	OMU	P-OP1	2.11	1.49	1.46
30	0	2621	PSU	P-OP1	2.04	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.00	130.37	134.14
30	0	628	1MA	C2-N3-C4	-3.29	110.61	116.23
30	0	2588	OMG	C6-N1-C2	3.26	125.21	119.51
30	0	2621	PSU	C5-C4-N3	-2.26	114.74	118.86
30	0	2588	OMG	C2-N3-C4	-2.24	111.94	115.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	-0.18	10 (4%) 35 41	34, 56, 94, 116	0
2	B	337/338 (99%)	-0.50	1 (0%) 91 95	34, 58, 89, 99	0
3	C	246/246 (100%)	-0.38	1 (0%) 90 94	32, 51, 75, 87	0
4	D	140/177 (79%)	1.64	53 (37%) 1 0	69, 106, 134, 144	0
5	E	172/178 (96%)	0.24	15 (8%) 10 13	49, 73, 97, 102	0
6	F	119/120 (99%)	0.14	9 (7%) 14 17	52, 76, 109, 124	0
7	G	29/348 (8%)	0.98	7 (24%) 1 2	79, 103, 110, 113	0
8	H	160/177 (90%)	-0.16	5 (3%) 47 55	53, 73, 107, 111	0
9	I	70/162 (43%)	3.42	44 (62%) 0 0	137, 155, 173, 175	0
10	J	142/145 (97%)	-0.56	0 100 100	43, 57, 77, 99	0
11	K	132/132 (100%)	-0.33	5 (3%) 38 45	39, 54, 79, 83	0
12	L	145/165 (87%)	0.48	11 (7%) 14 17	32, 71, 123, 134	0
13	M	194/196 (98%)	-0.53	1 (0%) 88 93	35, 49, 64, 71	0
14	N	186/187 (99%)	0.02	15 (8%) 12 15	51, 74, 121, 131	0
15	O	115/116 (99%)	-0.49	0 100 100	44, 61, 78, 85	0
16	P	143/149 (95%)	-0.32	1 (0%) 84 90	47, 61, 74, 83	0
17	Q	95/96 (98%)	-0.54	0 100 100	44, 55, 72, 85	0
18	R	150/155 (96%)	-0.47	0 100 100	37, 51, 73, 84	0
19	S	81/85 (95%)	-0.06	2 (2%) 54 64	49, 64, 87, 97	0
20	T	119/120 (99%)	-0.24	3 (2%) 54 64	42, 62, 92, 121	0
21	U	53/67 (79%)	0.10	1 (1%) 64 72	51, 64, 83, 91	0
22	V	65/71 (91%)	0.97	12 (18%) 2 3	53, 76, 130, 134	0
23	W	154/154 (100%)	-0.75	0 100 100	41, 56, 74, 88	0
24	X	82/92 (89%)	-0.14	3 (3%) 39 47	49, 66, 91, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.66	1 (0%) 84 90	34, 48, 72, 94	0
26	Z	73/116 (62%)	0.50	10 (13%) 4 5	59, 77, 92, 101	0
27	1	56/57 (98%)	-0.50	0 100 100	33, 39, 48, 56	0
28	2	46/50 (92%)	-0.20	1 (2%) 59 67	41, 69, 102, 114	0
29	3	92/92 (100%)	-0.17	2 (2%) 59 67	43, 65, 78, 91	0
30	0	2754/2923 (94%)	-0.23	54 (1%) 62 71	28, 51, 95, 171	0
31	9	122/122 (100%)	-0.18	3 (2%) 54 64	45, 72, 95, 154	0
All	All	6651/7517 (88%)	-0.15	270 (4%) 35 43	28, 57, 106, 175	0

The worst 5 of 270 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	9	1	U	13.5
9	I	71	ALA	13.1
9	I	74	ILE	12.4
22	V	1	THR	12.2
9	I	80	PHE	9.8

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	UR3	0	2619	21/22	0.14	1.23	42,44,47,47	0
30	OMG	0	2588	24/25	0.13	0.72	36,39,42,43	0
30	1MA	0	628	23/24	0.17	0.49	33,37,38,39	0
30	OMU	0	2587	21/22	0.12	-0.21	38,40,44,45	0
30	PSU	0	2621	20/21	0.15	-0.75	34,35,47,48	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
36	SR	0	9006	1/1	1.82	3413.00	200,200,200,200	0
34	NA	0	8509	1/1	1.24	164.24	85,85,85,85	0
36	SR	0	8982	1/1	1.94	154.42	200,200,200,200	0
36	SR	0	8996	1/1	0.74	126.61	200,200,200,200	0
36	SR	0	8994	1/1	0.82	125.75	200,200,200,200	0
36	SR	0	9007	1/1	0.94	102.57	200,200,200,200	0
34	NA	0	8505	1/1	1.08	78.69	48,48,48,48	0
34	NA	0	8562	1/1	1.15	69.64	78,78,78,78	0
34	NA	0	8565	1/1	0.55	61.89	79,79,79,79	0
34	NA	0	8549	1/1	0.87	59.99	52,52,52,52	0
34	NA	0	8547	1/1	0.72	59.47	80,80,80,80	0
36	SR	0	8997	1/1	0.71	57.66	200,200,200,200	0
33	K	0	8401	1/1	0.96	55.00	128,128,128,128	0
34	NA	0	8550	1/1	1.28	54.87	57,57,57,57	0
34	NA	0	8553	1/1	0.87	53.50	65,65,65,65	0
34	NA	0	8560	1/1	0.81	44.25	101,101,101,101	0
34	NA	0	8545	1/1	0.61	43.53	47,47,47,47	0
34	NA	B	8552	1/1	0.50	33.19	83,83,83,83	0
34	NA	0	8535	1/1	0.52	31.52	61,61,61,61	0
32	MG	0	8039	1/1	0.37	28.48	76,76,76,76	0
34	NA	0	8536	1/1	0.23	28.39	61,61,61,61	0
34	NA	0	8551	1/1	0.81	26.07	52,52,52,52	0
34	NA	0	8522	1/1	0.75	24.98	79,79,79,79	0
34	NA	0	8564	1/1	0.31	23.69	68,68,68,68	0
36	SR	0	8963	1/1	0.14	23.00	112,112,112,112	0
32	MG	0	8073	1/1	0.31	22.14	73,73,73,73	0
34	NA	0	8513	1/1	0.46	21.11	54,54,54,54	0
34	NA	0	8573	1/1	0.43	20.48	73,73,73,73	0
34	NA	0	8559	1/1	0.30	20.37	91,91,91,91	0
34	NA	0	8567	1/1	0.56	19.99	76,76,76,76	0
34	NA	0	8521	1/1	0.50	19.51	61,61,61,61	0
32	MG	0	8085	1/1	0.44	18.50	97,97,97,97	0
34	NA	9	8572	1/1	0.81	17.53	81,81,81,81	0
34	NA	0	8544	1/1	0.18	17.25	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8548	1/1	0.22	16.54	58,58,58,58	0
34	NA	0	8555	1/1	0.52	16.48	75,75,75,75	0
35	CL	0	8822	1/1	0.31	15.46	81,81,81,81	0
36	SR	0	8962	1/1	0.30	15.36	169,169,169,169	0
34	NA	0	8554	1/1	0.83	15.32	65,65,65,65	0
33	K	0	8402	1/1	0.46	15.17	76,76,76,76	0
34	NA	0	8525	1/1	0.23	14.87	92,92,92,92	0
34	NA	0	8528	1/1	0.60	14.82	66,66,66,66	0
32	MG	0	8081	1/1	0.24	14.41	73,73,73,73	0
36	SR	0	8947	1/1	0.43	13.74	200,200,200,200	0
34	NA	0	8524	1/1	0.26	13.50	58,58,58,58	0
36	SR	0	8959	1/1	0.26	13.20	163,163,163,163	0
36	SR	0	8986	1/1	0.39	13.16	200,200,200,200	0
34	NA	0	8527	1/1	0.31	11.05	71,71,71,71	0
36	SR	0	8914	1/1	0.27	10.32	120,120,120,120	0
36	SR	0	8922	1/1	0.39	10.30	161,161,161,161	0
36	SR	B	8987	1/1	0.49	9.93	200,200,200,200	0
32	MG	0	8089	1/1	0.22	9.90	72,72,72,72	0
34	NA	0	8518	1/1	0.43	9.75	88,88,88,88	0
34	NA	0	8519	1/1	0.25	9.63	43,43,43,43	0
32	MG	0	8030	1/1	0.27	9.57	68,68,68,68	0
34	NA	0	8563	1/1	0.40	9.42	88,88,88,88	0
32	MG	0	8082	1/1	0.59	9.36	89,89,89,89	0
34	NA	S	8510	1/1	0.46	9.28	64,64,64,64	0
34	NA	0	8534	1/1	0.27	9.21	44,44,44,44	0
34	NA	0	8556	1/1	0.85	9.15	64,64,64,64	0
32	MG	0	8049	1/1	0.31	9.13	69,69,69,69	0
34	NA	0	8566	1/1	0.35	9.03	64,64,64,64	0
32	MG	0	8022	1/1	0.22	8.44	44,44,44,44	0
36	SR	0	8903	1/1	0.18	7.72	59,59,59,59	0
34	NA	0	8516	1/1	0.17	7.65	45,45,45,45	0
32	MG	0	8047	1/1	0.27	7.41	51,51,51,51	0
32	MG	A	8051	1/1	0.71	7.37	70,70,70,70	0
34	NA	0	8571	1/1	0.18	7.37	76,76,76,76	0
34	NA	0	8561	1/1	0.24	7.28	68,68,68,68	0
32	MG	0	8029	1/1	0.17	6.96	49,49,49,49	0
36	SR	0	8934	1/1	0.27	6.92	134,134,134,134	0
36	SR	0	8976	1/1	0.30	6.75	194,194,194,194	0
32	MG	0	8018	1/1	0.21	6.60	40,40,40,40	0
36	SR	0	8905	1/1	0.25	6.49	61,61,61,61	0
34	NA	0	8568	1/1	0.39	6.49	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8992	1/1	0.20	6.47	136,136,136,136	0
36	SR	0	8949	1/1	0.16	6.37	122,122,122,122	0
32	MG	0	8009	1/1	0.24	6.33	36,36,36,36	0
34	NA	R	8575	1/1	0.27	6.26	99,99,99,99	0
34	NA	0	8541	1/1	0.21	6.22	75,75,75,75	0
32	MG	0	8033	1/1	0.16	5.84	55,55,55,55	0
36	SR	9	8980	1/1	0.21	5.82	175,175,175,175	0
34	NA	0	8511	1/1	0.30	5.68	69,69,69,69	0
34	NA	0	8542	1/1	0.36	5.64	49,49,49,49	0
34	NA	0	8530	1/1	0.37	5.63	59,59,59,59	0
32	MG	0	8014	1/1	0.22	5.61	33,33,33,33	0
36	SR	0	8926	1/1	0.16	5.57	108,108,108,108	0
36	SR	0	9002	1/1	0.15	5.28	177,177,177,177	0
34	NA	0	8546	1/1	0.28	5.14	65,65,65,65	0
34	NA	0	8574	1/1	0.20	5.12	59,59,59,59	0
32	MG	0	8078	1/1	0.25	5.09	69,69,69,69	0
36	SR	0	8981	1/1	0.21	4.80	178,178,178,178	0
32	MG	0	8072	1/1	0.19	4.58	63,63,63,63	0
32	MG	0	8071	1/1	0.17	4.55	72,72,72,72	0
36	SR	0	8983	1/1	0.19	4.32	170,170,170,170	0
32	MG	0	8017	1/1	0.18	3.78	52,52,52,52	0
36	SR	0	8937	1/1	0.21	3.67	112,112,112,112	0
32	MG	0	8069	1/1	0.32	3.42	73,73,73,73	0
32	MG	0	8066	1/1	0.17	3.29	70,70,70,70	0
36	SR	0	9004	1/1	0.32	2.89	200,200,200,200	0
36	SR	0	8909	1/1	0.14	2.41	88,88,88,88	0
32	MG	0	8063	1/1	0.14	2.41	80,80,80,80	0
32	MG	0	8048	1/1	0.18	2.30	33,33,33,33	0
36	SR	0	8921	1/1	0.14	2.25	96,96,96,96	0
32	MG	0	8003	1/1	0.20	2.21	45,45,45,45	0
35	CL	B	8819	1/1	0.17	2.20	58,58,58,58	0
32	MG	0	8061	1/1	0.17	2.17	37,37,37,37	0
36	SR	0	8906	1/1	0.21	2.05	64,64,64,64	0
32	MG	0	8084	1/1	0.15	1.94	33,33,33,33	0
32	MG	0	8036	1/1	0.11	1.88	56,56,56,56	0
35	CL	R	8806	1/1	0.16	1.85	57,57,57,57	0
32	MG	0	8019	1/1	0.17	1.82	28,28,28,28	0
32	MG	0	8028	1/1	0.14	1.81	26,26,26,26	0
36	SR	0	8904	1/1	0.15	1.65	65,65,65,65	0
36	SR	0	8998	1/1	0.18	1.44	173,173,173,173	0
32	MG	K	8054	1/1	0.17	1.40	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8045	1/1	0.14	1.30	44,44,44,44	0
32	MG	0	8037	1/1	0.14	1.26	88,88,88,88	0
36	SR	0	8918	1/1	0.15	1.25	80,80,80,80	0
32	MG	0	8064	1/1	0.18	1.15	44,44,44,44	0
32	MG	0	8088	1/1	0.19	1.09	52,52,52,52	0
35	CL	J	8802	1/1	0.19	1.04	75,75,75,75	0
36	SR	0	8955	1/1	0.11	1.04	199,199,199,199	0
36	SR	A	8929	1/1	0.17	0.97	144,144,144,144	0
32	MG	0	8011	1/1	0.20	0.97	25,25,25,25	0
32	MG	0	8041	1/1	0.15	0.79	29,29,29,29	0
36	SR	0	8907	1/1	0.14	0.75	56,56,56,56	0
32	MG	0	8015	1/1	0.13	0.74	30,30,30,30	0
34	NA	0	8502	1/1	0.12	0.68	66,66,66,66	0
36	SR	0	9001	1/1	0.11	0.68	173,173,173,173	0
34	NA	0	8533	1/1	0.14	0.68	55,55,55,55	0
36	SR	0	8989	1/1	0.15	0.67	168,168,168,168	0
35	CL	0	8814	1/1	0.16	0.61	72,72,72,72	0
32	MG	0	8027	1/1	0.12	0.54	51,51,51,51	0
36	SR	0	8933	1/1	0.11	0.54	139,139,139,139	0
36	SR	R	8912	1/1	0.15	0.48	92,92,92,92	0
36	SR	0	8946	1/1	0.16	0.47	123,123,123,123	0
32	MG	0	8005	1/1	0.20	0.45	35,35,35,35	0
34	NA	M	8539	1/1	0.14	0.42	34,34,34,34	0
36	SR	0	8924	1/1	0.12	0.42	154,154,154,154	0
34	NA	0	8515	1/1	0.19	0.39	41,41,41,41	0
36	SR	0	8985	1/1	0.12	0.33	134,134,134,134	0
34	NA	J	8538	1/1	0.18	0.17	56,56,56,56	0
36	SR	0	8965	1/1	0.11	0.17	132,132,132,132	0
32	MG	0	8010	1/1	0.21	0.02	45,45,45,45	0
36	SR	0	8966	1/1	0.10	0.00	107,107,107,107	0
32	MG	0	8040	1/1	0.12	-0.02	96,96,96,96	0
32	MG	0	8038	1/1	0.20	-0.04	70,70,70,70	0
36	SR	0	9008	1/1	0.15	-0.06	95,95,95,95	0
35	CL	0	8817	1/1	0.12	-0.13	67,67,67,67	0
34	NA	0	8569	1/1	0.15	-0.16	48,48,48,48	0
34	NA	0	8514	1/1	0.17	-0.17	56,56,56,56	0
34	NA	0	8504	1/1	0.15	-0.17	44,44,44,44	0
37	CD	Z	8703	1/1	0.12	-0.27	75,75,75,75	0
32	MG	0	8053	1/1	0.14	-0.28	47,47,47,47	0
35	CL	J	8801	1/1	0.10	-0.34	79,79,79,79	0
35	CL	0	8816	1/1	0.12	-0.41	79,79,79,79	0
32	MG	0	8046	1/1	0.13	-0.41	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8957	1/1	0.11	-0.45	195,195,195,195	0
32	MG	0	8004	1/1	0.13	-0.46	32,32,32,32	0
36	SR	0	8972	1/1	0.14	-0.52	146,146,146,146	0
36	SR	0	8967	1/1	0.10	-0.53	133,133,133,133	0
36	SR	0	8964	1/1	0.09	-0.53	131,131,131,131	0
34	NA	C	8503	1/1	0.15	-0.60	36,36,36,36	0
32	MG	0	8090	1/1	0.14	-0.62	65,65,65,65	0
36	SR	0	8936	1/1	0.11	-0.63	94,94,94,94	0
34	NA	0	8506	1/1	0.11	-0.71	64,64,64,64	0
36	SR	0	8927	1/1	0.11	-0.74	153,153,153,153	0
34	NA	0	8526	1/1	0.11	-0.83	47,47,47,47	0
36	SR	3	8932	1/1	0.11	-0.85	76,76,76,76	0
37	CD	1	8702	1/1	0.11	-0.88	67,67,67,67	0
36	SR	3	8999	1/1	0.10	-0.89	110,110,110,110	0
35	CL	J	8821	1/1	0.11	-0.89	67,67,67,67	0
32	MG	0	8002	1/1	0.14	-0.94	36,36,36,36	0
35	CL	0	8813	1/1	0.10	-0.94	66,66,66,66	0
34	NA	0	8520	1/1	0.07	-1.00	49,49,49,49	0
34	NA	0	8558	1/1	0.13	-1.01	49,49,49,49	0
32	MG	0	8067	1/1	0.12	-1.04	40,40,40,40	0
37	CD	3	8704	1/1	0.09	-1.04	74,74,74,74	0
36	SR	0	8993	1/1	0.07	-1.05	176,176,176,176	0
36	SR	0	8939	1/1	0.09	-1.07	149,149,149,149	0
34	NA	Q	8540	1/1	0.12	-1.07	64,64,64,64	0
36	SR	0	8979	1/1	0.10	-1.08	200,200,200,200	0
36	SR	0	8935	1/1	0.09	-1.10	79,79,79,79	0
32	MG	0	8083	1/1	0.08	-1.15	60,60,60,60	0
35	CL	N	8807	1/1	0.09	-1.23	69,69,69,69	0
35	CL	A	8809	1/1	0.12	-1.24	80,80,80,80	0
32	MG	0	8058	1/1	0.08	-1.28	22,22,22,22	0
36	SR	0	8956	1/1	0.05	-1.31	155,155,155,155	0
36	SR	0	8944	1/1	0.10	-1.32	169,169,169,169	0
34	NA	0	8523	1/1	0.10	-1.35	50,50,50,50	0
36	SR	0	8968	1/1	0.07	-1.35	160,160,160,160	0
35	CL	L	8810	1/1	0.10	-1.41	68,68,68,68	0
36	SR	0	8990	1/1	0.10	-1.42	139,139,139,139	0
32	MG	0	8043	1/1	0.06	-1.42	52,52,52,52	0
32	MG	0	8060	1/1	0.07	-1.45	53,53,53,53	0
32	MG	T	8057	1/1	0.11	-1.50	60,60,60,60	0
32	MG	0	8065	1/1	0.10	-1.54	57,57,57,57	0
36	SR	0	8975	1/1	0.10	-1.59	130,130,130,130	0
36	SR	1	8952	1/1	0.13	-1.62	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8902	1/1	0.14	-1.66	66,66,66,66	0
35	CL	O	8808	1/1	0.09	-1.66	70,70,70,70	0
32	MG	B	8042	1/1	0.06	-1.66	44,44,44,44	0
36	SR	1	8913	1/1	0.12	-1.68	95,95,95,95	0
36	SR	0	8911	1/1	0.08	-1.70	85,85,85,85	0
34	NA	0	8537	1/1	0.08	-1.70	38,38,38,38	0
36	SR	F	9005	1/1	0.06	-1.71	133,133,133,133	0
37	CD	U	8701	1/1	0.09	-1.72	63,63,63,63	0
32	MG	0	8056	1/1	0.12	-1.79	47,47,47,47	0
32	MG	0	8008	1/1	0.10	-1.87	28,28,28,28	0
36	SR	0	8954	1/1	0.09	-1.90	109,109,109,109	0
35	CL	0	8815	1/1	0.09	-1.91	77,77,77,77	0
35	CL	Q	8811	1/1	0.12	-1.93	82,82,82,82	0
32	MG	0	8023	1/1	0.09	-1.97	37,37,37,37	0
32	MG	0	8050	1/1	0.07	-1.97	32,32,32,32	0
36	SR	0	8953	1/1	0.12	-2.01	144,144,144,144	0
34	NA	9	8543	1/1	0.08	-2.06	74,74,74,74	0
34	NA	R	8532	1/1	0.09	-2.11	58,58,58,58	0
32	MG	0	8034	1/1	0.14	-2.17	46,46,46,46	0
36	SR	0	8969	1/1	0.08	-2.19	159,159,159,159	0
35	CL	M	8818	1/1	0.08	-2.25	40,40,40,40	0
32	MG	0	8025	1/1	0.11	-2.32	37,37,37,37	0
36	SR	0	8908	1/1	0.07	-2.35	116,116,116,116	0
32	MG	0	8044	1/1	0.09	-2.37	50,50,50,50	0
36	SR	A	8977	1/1	0.05	-2.39	160,160,160,160	0
32	MG	0	8007	1/1	0.11	-2.45	32,32,32,32	0
36	SR	0	8974	1/1	0.17	-2.45	165,165,165,165	0
32	MG	0	8021	1/1	0.05	-2.48	40,40,40,40	0
35	CL	0	8803	1/1	0.09	-2.51	58,58,58,58	0
36	SR	A	8930	1/1	0.05	-2.57	97,97,97,97	0
36	SR	9	8978	1/1	0.07	-2.61	135,135,135,135	0
36	SR	0	8917	1/1	0.06	-2.61	107,107,107,107	0
32	MG	0	8001	1/1	0.11	-2.68	33,33,33,33	0
35	CL	3	8804	1/1	0.06	-2.69	63,63,63,63	0
32	MG	0	8070	1/1	0.10	-2.73	46,46,46,46	0
36	SR	0	8958	1/1	0.05	-2.74	122,122,122,122	0
34	NA	0	8557	1/1	0.05	-2.77	53,53,53,53	0
36	SR	0	8943	1/1	0.05	-2.81	124,124,124,124	0
32	MG	0	8062	1/1	0.11	-2.86	59,59,59,59	0
36	SR	0	8960	1/1	0.07	-2.86	141,141,141,141	0
34	NA	0	8570	1/1	0.07	-2.88	52,52,52,52	0
32	MG	0	8052	1/1	0.08	-2.92	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CL	0	8812	1/1	0.06	-2.94	58,58,58,58	0
36	SR	0	8951	1/1	0.04	-2.96	148,148,148,148	0
32	MG	0	8068	1/1	0.09	-2.96	51,51,51,51	0
32	MG	0	8016	1/1	0.11	-2.99	48,48,48,48	0
32	MG	Y	8086	1/1	0.07	-3.01	44,44,44,44	0
35	CL	0	8805	1/1	0.05	-3.05	67,67,67,67	0
32	MG	0	8087	1/1	0.10	-3.15	51,51,51,51	0
34	NA	0	8529	1/1	0.06	-3.17	39,39,39,39	0
36	SR	0	8940	1/1	0.06	-3.18	97,97,97,97	0
32	MG	0	8079	1/1	0.08	-3.18	51,51,51,51	0
36	SR	0	8991	1/1	0.07	-3.23	199,199,199,199	0
34	NA	0	8512	1/1	0.13	-3.24	52,52,52,52	0
37	CD	O	8705	1/1	0.05	-3.28	118,118,118,118	0
36	SR	0	8942	1/1	0.09	-3.29	122,122,122,122	0
36	SR	0	8920	1/1	0.07	-3.36	135,135,135,135	0
32	MG	0	8020	1/1	0.07	-3.41	40,40,40,40	0
36	SR	0	8919	1/1	0.11	-3.47	170,170,170,170	0
32	MG	0	8075	1/1	0.07	-3.75	42,42,42,42	0
36	SR	0	8915	1/1	0.08	-3.79	121,121,121,121	0
36	SR	0	8928	1/1	0.06	-3.83	135,135,135,135	0
36	SR	0	8923	1/1	0.07	-3.89	101,101,101,101	0
32	MG	9	8074	1/1	0.08	-3.95	86,86,86,86	0
36	SR	0	8948	1/1	0.09	-3.95	92,92,92,92	0
35	CL	Y	8820	1/1	0.06	-3.96	48,48,48,48	0
36	SR	0	8931	1/1	0.07	-3.98	113,113,113,113	0
32	MG	0	8031	1/1	0.07	-3.98	62,62,62,62	0
36	SR	0	8984	1/1	0.06	-4.08	121,121,121,121	0
32	MG	0	8013	1/1	0.04	-4.26	25,25,25,25	0
32	MG	0	8026	1/1	0.08	-4.40	35,35,35,35	0
36	SR	S	8961	1/1	0.06	-4.45	121,121,121,121	0
32	MG	0	8035	1/1	0.07	-4.47	54,54,54,54	0
36	SR	0	8973	1/1	0.06	-4.68	130,130,130,130	0
32	MG	0	8055	1/1	0.09	-4.71	53,53,53,53	0
32	MG	0	8077	1/1	0.03	-4.86	45,45,45,45	0
36	SR	9	9003	1/1	0.05	-5.02	171,171,171,171	0
34	NA	0	8507	1/1	0.07	-5.20	37,37,37,37	0
36	SR	0	8941	1/1	0.11	-5.34	108,108,108,108	0
32	MG	0	8093	1/1	0.08	-5.39	42,42,42,42	0
36	SR	0	8938	1/1	0.02	-5.53	147,147,147,147	0
36	SR	0	8995	1/1	0.10	-5.56	136,136,136,136	0
36	SR	0	8910	1/1	0.05	-5.56	100,100,100,100	0
36	SR	0	8945	1/1	0.06	-5.62	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8508	1/1	0.05	-5.64	35,35,35,35	0
32	MG	0	8076	1/1	0.07	-5.93	40,40,40,40	0
36	SR	B	8950	1/1	0.08	-6.22	116,116,116,116	0
32	MG	0	8059	1/1	0.07	-6.25	57,57,57,57	0
32	MG	0	8006	1/1	0.07	-6.35	32,32,32,32	0
36	SR	0	8970	1/1	0.01	-6.55	123,123,123,123	0
34	NA	0	8517	1/1	0.06	-6.70	31,31,31,31	0
32	MG	0	8012	1/1	0.09	-6.80	18,18,18,18	0
32	MG	0	8091	1/1	0.03	-7.50	57,57,57,57	0
36	SR	0	8925	1/1	0.06	-8.55	86,86,86,86	0
32	MG	0	8080	1/1	0.03	-8.87	75,75,75,75	0
34	NA	0	8501	1/1	0.07	-9.09	40,40,40,40	0
34	NA	0	8531	1/1	0.05	-9.36	40,40,40,40	0
36	SR	0	8988	1/1	0.06	-10.67	158,158,158,158	0
36	SR	0	9000	1/1	0.04	-10.78	176,176,176,176	0
36	SR	0	8916	1/1	0.03	-11.34	120,120,120,120	0
32	MG	0	8032	1/1	0.05	-12.45	44,44,44,44	0
32	MG	0	8092	1/1	0.10	-13.00	53,53,53,53	0
36	SR	0	8901	1/1	0.07	-13.72	91,91,91,91	0
32	MG	0	8024	1/1	0.09	-15.60	49,49,49,49	0
36	SR	0	8971	1/1	0.07	-39.00	171,171,171,171	0

6.5 Other polymers ⓘ

There are no such residues in this entry.