



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:56 AM 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

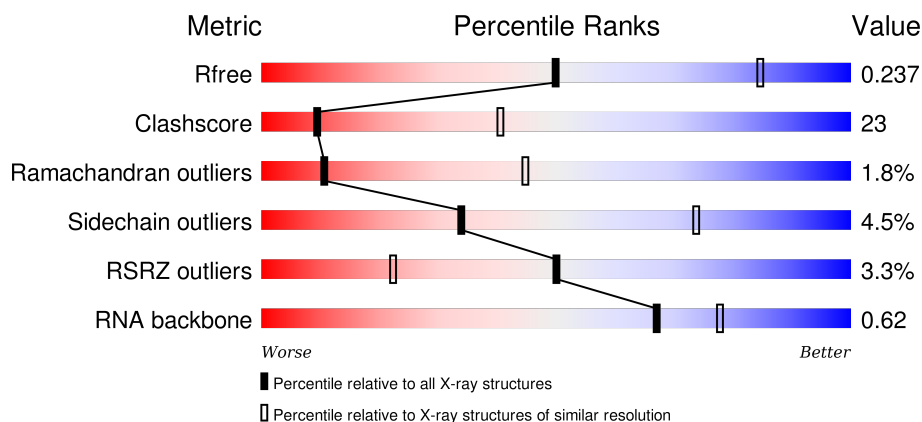
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div style="width: 62%;"></div> <div style="width: 33%;"></div> <div style="width: 5%;"></div> <div style="width: 5%;"></div> <div style="width: 5%;"></div> </div> <div> <div style="width: 62%;"></div> <div style="width: 33%;"></div> <div style="width: 5%;"></div> <div style="width: 5%;"></div> <div style="width: 5%;"></div> </div>
2	B	338	<div> <div style="width: 58%;"></div> <div style="width: 37%;"></div> <div style="width: 5%;"></div> </div> <div> <div style="width: 58%;"></div> <div style="width: 37%;"></div> <div style="width: 5%;"></div> </div>
3	C	246	<div> <div style="width: 68%;"></div> <div style="width: 27%;"></div> <div style="width: 5%;"></div> </div> <div> <div style="width: 68%;"></div> <div style="width: 27%;"></div> <div style="width: 5%;"></div> </div>
4	D	177	<div> <div style="width: 9%;"></div> <div style="width: 42%;"></div> <div style="width: 35%;"></div> <div style="width: 21%;"></div> </div> <div> <div style="width: 9%;"></div> <div style="width: 42%;"></div> <div style="width: 35%;"></div> <div style="width: 21%;"></div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8009	-	-	-	X
32	MG	0	8011	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8016	-	-	-	X
32	MG	0	8044	-	-	-	X
32	MG	A	8051	-	-	-	X
34	NA	0	8513	-	-	-	X
34	NA	0	8519	-	-	-	X
34	NA	0	8521	-	-	-	X
34	NA	0	8522	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8545	-	-	-	X
34	NA	0	8546	-	-	-	X
34	NA	0	8550	-	-	-	X
34	NA	0	8552	-	-	-	X
34	NA	0	8553	-	-	-	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
34	NA	0	8562	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8567	-	-	-	X
34	NA	0	8569	-	-	-	X
34	NA	0	8571	-	-	-	X
34	NA	R	8575	-	-	-	X
35	CL	0	8805	-	-	-	X
35	CL	0	8811	-	-	-	X
35	CL	0	8816	-	-	-	X
35	CL	3	8804	-	-	X	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	B	8819	-	-	X	-
35	CL	M	8818	-	-	X	-
36	SR	0	8904	-	-	-	X
36	SR	0	8947	-	-	-	X
36	SR	0	8957	-	-	-	X
36	SR	0	8969	-	-	-	X
36	SR	B	8987	-	-	-	X
37	CD	3	8704	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99120 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 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

Continued on next page...

Continued from previous page...

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 38 is water.

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

Continued on next page...

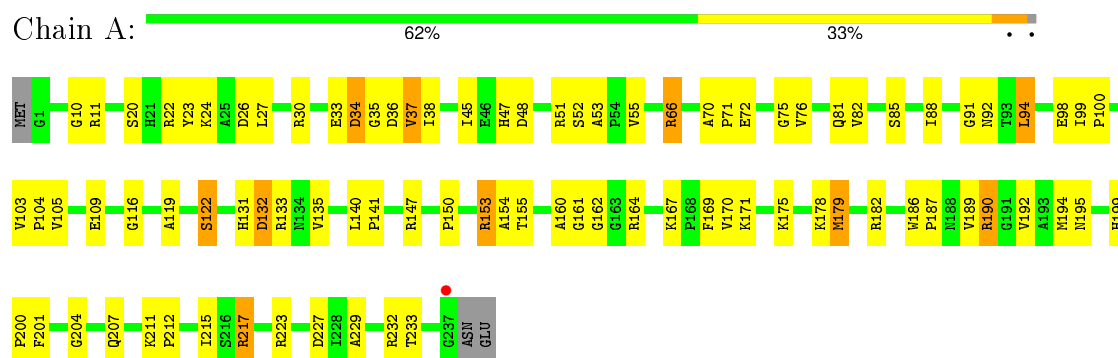
Continued from previous page...

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

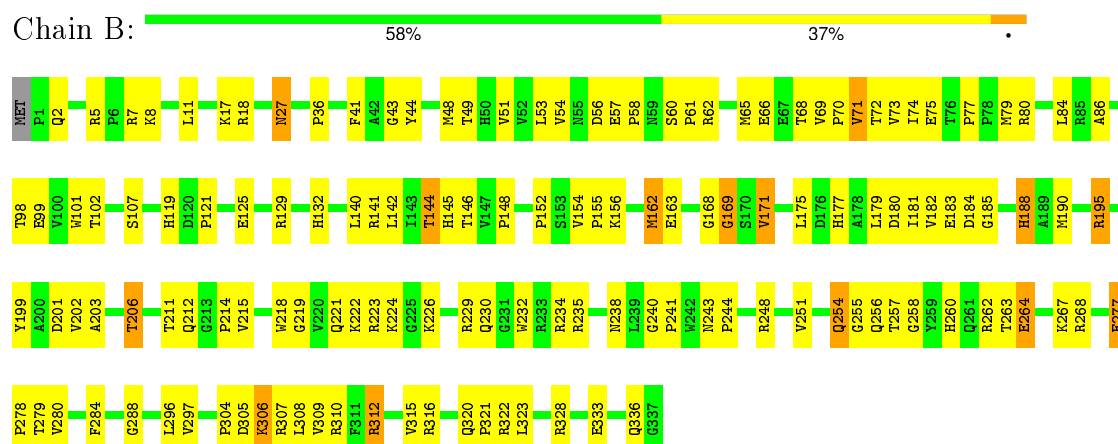
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

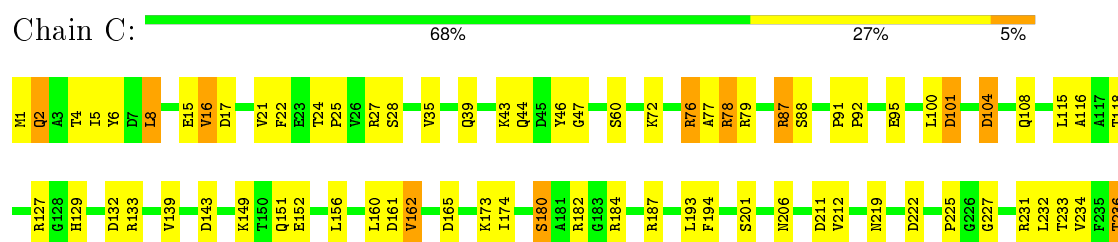
• Molecule 1: 50S ribosomal protein L2P

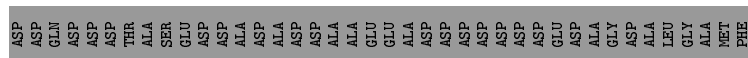


• Molecule 2: 50S ribosomal protein L3P

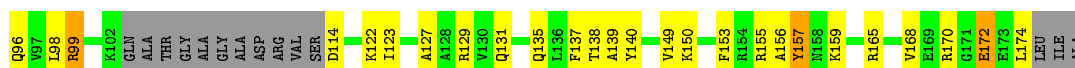


• Molecule 3: 50S ribosomal protein L4P

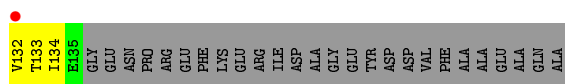




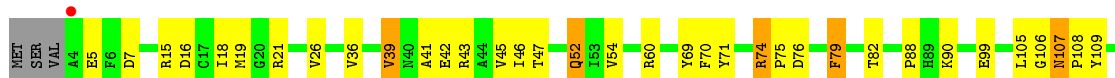
- Chain H:  57% 28% 5% 10%



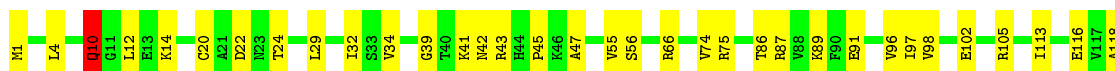
- Chain I: 19% 27% 15% 57%



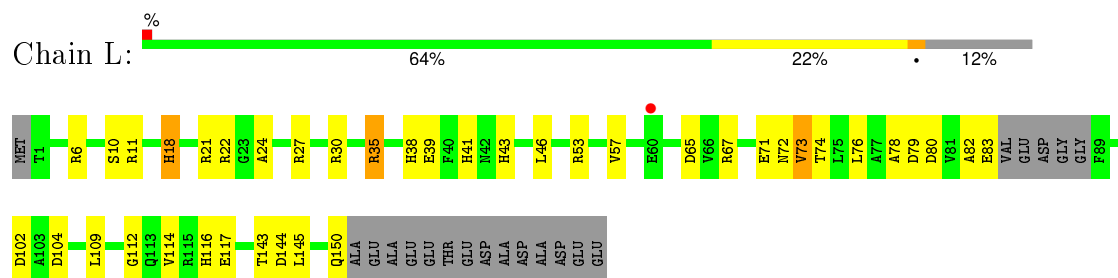
- Chain J:  67% 27% . .



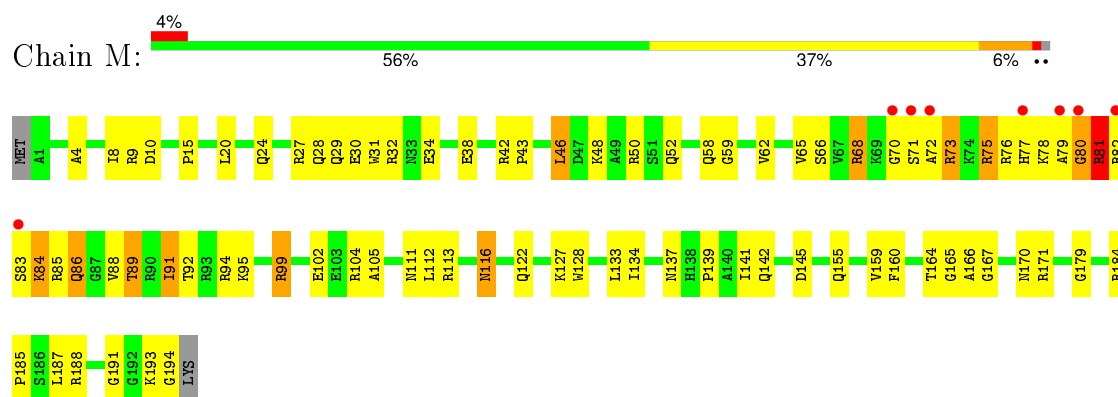
- Chain K:  72% 27%



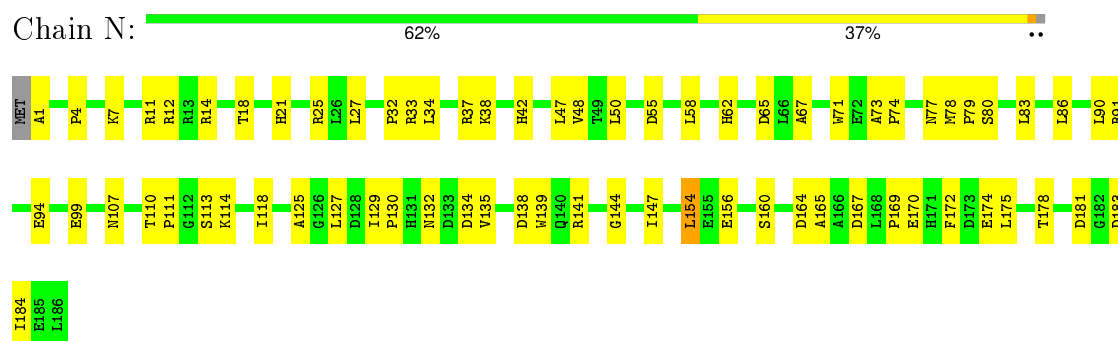
- 
- WORLDWIDE
PDB
PROTEIN DATA BANK



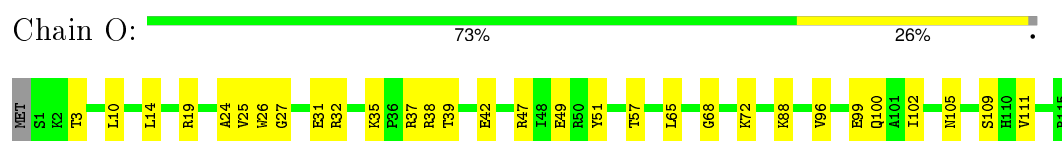
- Molecule 13: 50S ribosomal protein L15e



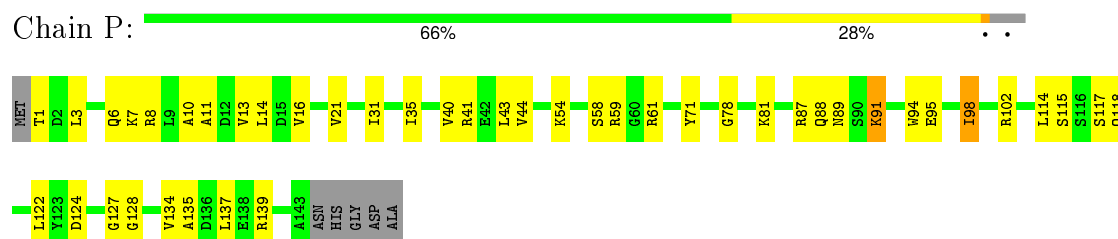
- Molecule 14: 50S ribosomal protein L18P



- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e



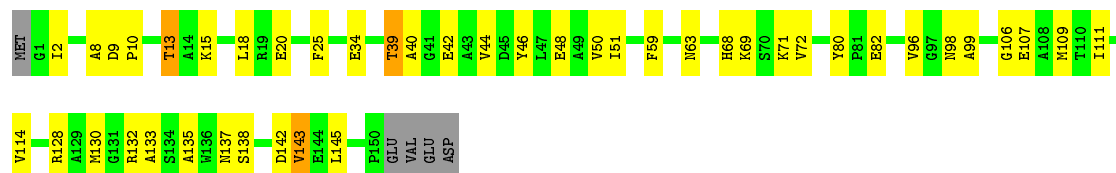
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  69% 27% ..



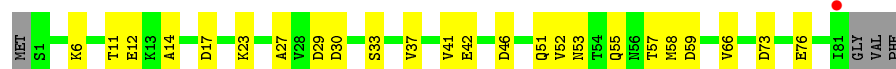
- Molecule 18: 50S ribosomal protein L22P

Chain R:  68% 26% . .



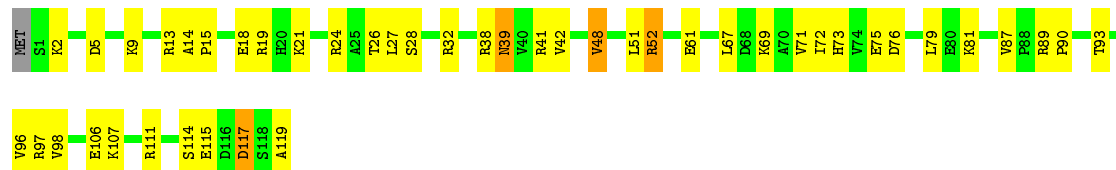
- Molecule 19: 50S ribosomal protein L23P

Chain S:  67% 28% 5%




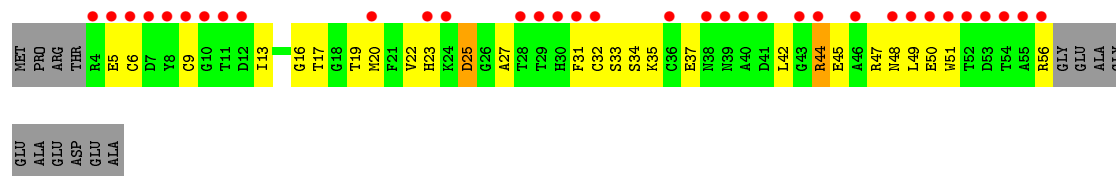
- Molecule 20: 50S ribosomal protein L24P

Chain T:  62% 34% ..



- Molecule 21: 50S ribosomal protein L24e

Chain U:  39% 51% 37% 21%

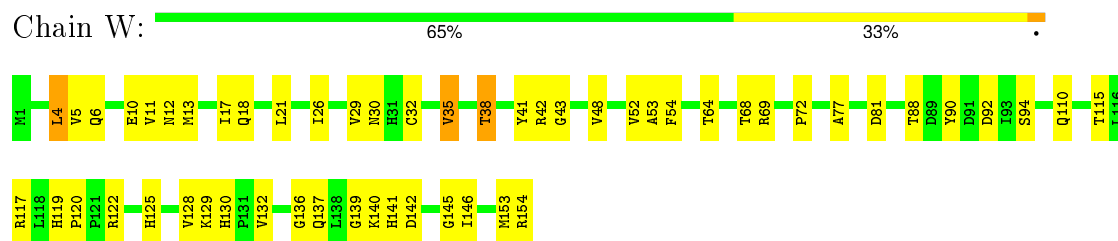


- Molecule 22: 50S ribosomal protein L29P

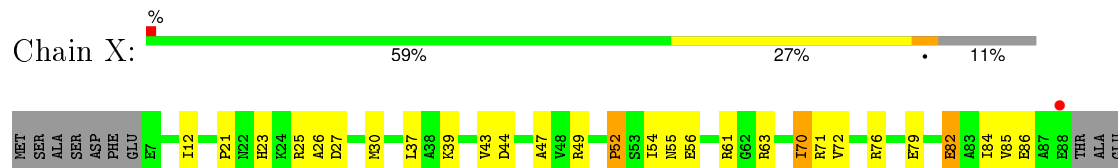
Chain V:  6% 62% 28% 8%



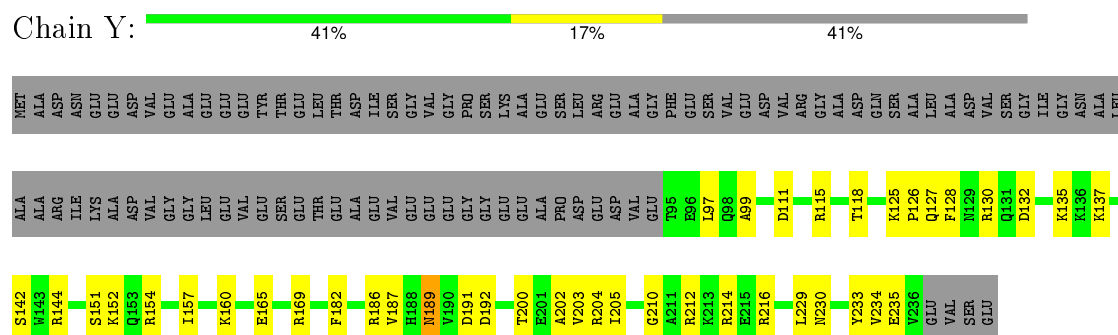
- Molecule 23: 50S ribosomal protein L30P



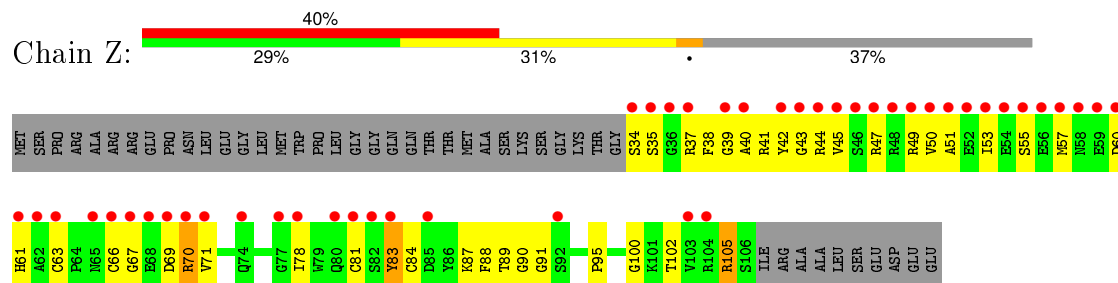
- Molecule 24: 50S ribosomal protein L31e



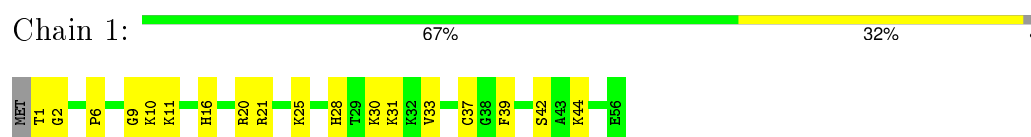
- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae



- Molecule 27: 50S ribosomal protein L37e

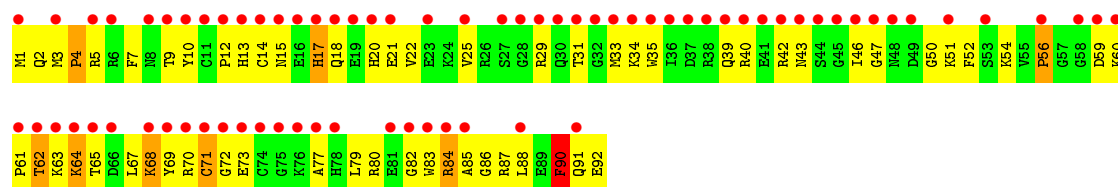
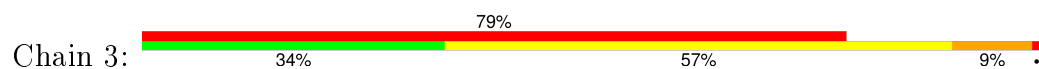


- Molecule 28: 50S ribosomal protein L39e

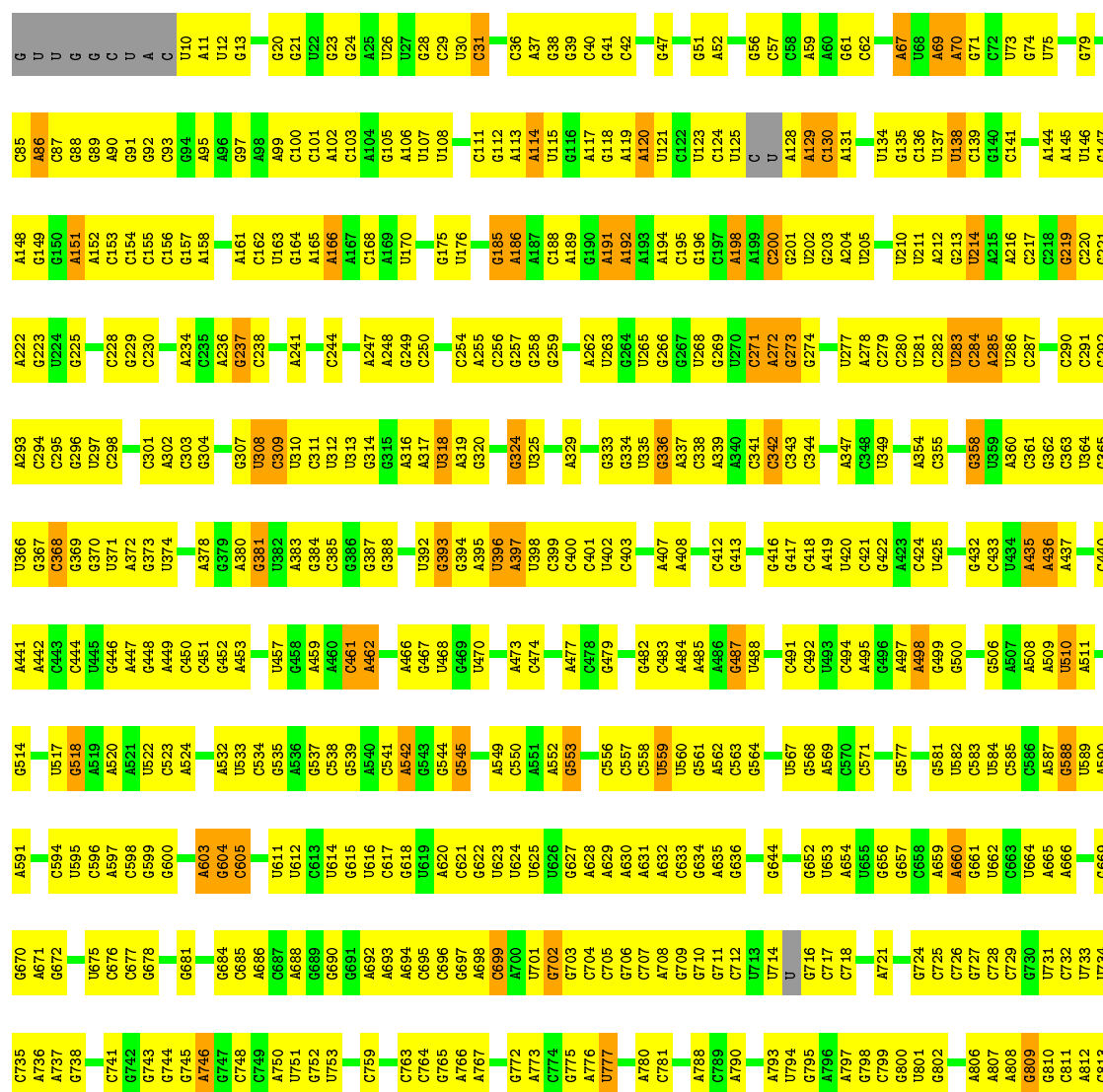




- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S RIBOSOMAL RNA



A1924	C1856	A1778	C1705	G1823	G1555	G1475	U1405	U1251	C1186	G1112	C1025	G964	G887	G814
G1925	A1857	A1778	G1706	A1624	G1556	A1476	A1406	C1255	U1187	U1115	U1026	A965	U888	U815
G1926	A1858	C1787	G1707	U1625	G1557	A1477	A1407	C1256	A1188	U1116	U1028	U966	C889	G816
A1927	A1859	C1787	G1708	A1626	C1558	U1478	U1408	C1267	A1189	A1117	U1029	G967	C890	G817
G1928	U1860	G1788	G1709	G1627	U1559	G1484	G1410	G1260	G1190	A1118	U1030	G968	A818	A819
G1929	C1861	G1789	A1710	U1630	U1561	A1485	G1411	U1264	A1192	G1119	G1031	U970	A819	A820
A1930	C1862	C1790	A1711	A1631	C1562	A1490	A1413	U1265	A1193	U1120	A1032	G	A821	U821
A1931	G1863	U1791	G1712	A1632	C1563	G1490	A1414	G1266	A1194	U1121	U1041	U	C822	U822
G1932	C1864	A1796	A1716	C1633	C1566	C1495	G1415	C1267	G1195	C1127	U1042	U	C898	U823
G1933	A1865	C1798	G1717	G1634	G1567	A1496	G1416	C1268	C1196	U1128	C1043	U	C899	U824
A1934	A1866	G1798	G1718	U1635	G1568	G1497	G1417	G1269	G1197	C1129	C1044	C	G802	U825
G1935	G1867	G1799	G1718	U1635	G1568	G1497	U1418	U1270	U1198	U1130	G1045	G	U903	U826
G1936	G1868	G1800	G1719	A1641	U1569	U1500	U1419	U1271	A1199	U1131	U1046	C	U904	U827
U1937	A1871	G1801	U1722	A1642	A1572	C1500	C1420	C1271	A1200	A1132	U1047	C	C905	G828
G1938	C1872	G1802	U1723	C1643	A1573	U1503	C1421	C1272	G1131	A1133	U1047	C	U905	A829
U1939	G1873	C1803	G1724	U1644	C1574	A1504	U1422	C1273	A1201	A1133	U1047	U	C906	G830
G1940	A1874	A1804	U1724	C1645	C1574	U1505	C1423	A1274	A1202	G1134	G1052	C	C910	G911
A1941	C1875	G1805	C1725	G1649	G1575	U1506	G1425	C1275	G1203	U1137	G1053	C	G911	G912
A1942	C1876	G1806	G1725	G1649	G1576	C1507	G1426	U1276	U1205	G1138	G1054	G	A912	A913
C1943	G1877	U1807	G1730	A1653	U1577	C1507	C1426	U1277	U1206	G1139	U1055	A	A916	C838
G1947	U1878	C1808	C1731	A1653	C1578	U1511	U1427	U1278	A1207	U1139	U1056	G	U917	C839
G1948	U1879	G1809	A1732	C1654	C1578	G1512	C1428	U1279	C1208	C1140	A1057	A	C920	U840
G1949	C1880	C1810	A1733	G1655	U1583	G1513	U1429	G1284	G1209	U1149	A1058	G	C921	U841
G1950	A1881	A1811	C1734	A1656	C1585	G1514	G1430	U1285	G1211	A1150	C1060	A	G922	C842
G1951	C1882	G1812	C1735	C1662	C1586	A1515	A1434	U1286	C1212	G1151	U1062	U	G923	A844
U	U1883	U1813	A1736	G1663	U1587	U1516	U1435	A1287	C1213	A1154	U1063	C	G924	C848
A	A1884	G1814	A1737	C1664	C1588	G1517	C1436	U1288	G1214	G1155	G1066	G	C925	C853
C	A1885	A1815	U1741	G1665	G1589	A1518	A1437	U1289	A1215	G1156	U1067	C	C926	C854
U	A1886	G1816	A1742	G1666	G1590	G1519	C1438	G1290	G1216	C1157	C1068	A	U927	U855
A	C1889	U1817	G1743	C1667	A1591	G1520	C1439	U1291	G1217	G1158	A1070	C	A928	C857
U	U1890	G1819	G1744	U1668	C1592	C1521	U1440	G1292	U1218	G1159	A1071	C	A929	C858
G	C1891	C1820	G1745	G1669	C1593	G1523	G1441	U1293	U1219	G1160	G1072	A	C999	C859
A	C1894	U1748	U1748	A1670	C1594	G1524	A1442	A1294	U1220	A1161	G1071	C1000	G938	U860
C	U1825	U1749	U1749	U1671	G1595	U1824	G1443	C1305	C1229	G1162	G1072	C999	G939	U861
C	G1898	C1826	G1752	C1675	U1596	G1525	G1444	U1309	U1234	G1163	A1073	U1009	G940	U862
C	C1899	G1827	C1753	G1676	A1597	A1526	G1445	G1300	G1235	G1164	A1074	U1009	U941	U863
U1964	G1902	G1828	C1754	U1677	U1598	A1527	U1446	U1300	C1226	G1165	U1079	U1004	U942	C863
C1965	U1903	A1829	A1755	A1678	U1599	G1528	U1447	C1303	G1227	G1166	A1080	U1005	U943	C864
U1966	C1904	C1830	A1756	C1679	G1600	G1529	A1448	U1304	C1228	G1167	C1081	A1006	U944	C865
U1967	U1905	U1831	G1756	C1679	G1601	G1530	G1449	U1305	C1229	G1168	A1081	A1007	U945	C866
A1968	U1906	G1832	U1757	C1680	C1602	A1533	G1450	C1305	C1229	G1169	A1082	U1008	U946	C867
A1969	U1907	U1833	U1758	G1681	A1603	A1533	G1451	U1309	U1234	U1170	G1087	U1009	U947	C868
G1970	U1907	C1834	A1759	A1682	G1604	C1537	G1452	U1309	G1235	A1171	A1088	U1009	U948	C869
G1971	U1908	U1835	G1760	G1683	G1605	C1538	U1453	U1310	A1236	G1172	A1089	C1010	U949	C870
U1972	A1909	U1761	U1761	A1684	A1606	U1539	U1454	G1311	U1237	G1173	C1089	C1011	U950	C871
A1973	A1910	C1762	C1762	A1685	A1607	G1540	G1461	G1312	C1238	A1173	A1098	A1012	G951	U872
G1974	C1913	C1763	C1763	C1686	G1608	G1541	G1462	G1313	G1239	A1174	U1095	A1013	A951	C873
U1977	C1914	G1765	G1765	C1687	G1608	G1542	U1463	U1314	G1240	G1175	U1096	A1014	G952	A874
C1978	U1915	U1766	U1766	A1691	C1613	G1543	C1462	G1315	G1241	C1176	A1097	C1015	G953	A875
G1979	C1916	C1692	C1692	A1615	G1614	U1544	U1463	G1316	A1242	G1177	A1098	U1016	G956	A876
U1980	G1917	G1697	G1697	A1616	U1616	C1545	C1464	G1324	U1244	G1178	C1102	U1017	G957	C877
A1981	U1918	U1770	U1770	C1617	A1617	G1546	U1471	G1325	C1243	C1179	G1102	U1018	G958	C878
U1982	C1919	U1771	U1771	G1618	U1548	U1548	C1469	C1326	A1246	U1180	C1103	C1019	A1020	C879
C1983	U1919	U1771	U1771	G1618	U1548	U1548	C1469	G1327	A1247	C1182	G1104	G1021	C959	A882
U1985	C1920	G1772	G1772	A1701	G1619	U1552	A1471	G1328	A1248	C1183	U1109	A1022	G960	U883
G1986	A1921	G1773	G1773	U1702	C1620	G1552	C1472	A1328	U1248	C1184	U1110	C1023	A961	C884
C1987	A1922	G1774	G1774	G1703	C1621	C1553	U1473	G1329	U1249	C1185	G1111	C1024	C962	C885
G1988	G1923	A1775	A1775	G1704	G1622	C1554	C1474	A1330	C1250	U1185	U1111	G1024	C963	A886



A62	C63	C64	A65	G66	C67	G68	U69		C72	A73	G74	G75	G76	A77		C81	U82	G83		U87	G88	C89	G90	C91	G92	A93		A105	U106	C107	C108	G109	G110	U111	U112	C113	G114	C115	C116		C122
-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	--	------	------	------	------	------	------	------	------	------	------	------	------	--	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.41Å 299.52Å 574.90Å 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
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.180 , 0.247 0.178 , 0.237	Depositor DCC
R_{free} test set	3540 reflections (1.27%)	DCC
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	97	0
2	B	2625	0	2532	127	0
3	C	1860	0	1813	70	0
4	D	1094	0	1085	50	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
34	C	1	0	0	0	0
34	J	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
38	F	31	0	0	1	0
38	G	17	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 3377 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	9	40
2	B	335/338 (99%)	305 (91%)	23 (7%)	7 (2%)	9	40
3	C	244/246 (99%)	216 (88%)	26 (11%)	2 (1%)	24	66
4	D	134/177 (76%)	105 (78%)	23 (17%)	6 (4%)	3	18
5	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	30	72
6	F	117/120 (98%)	97 (83%)	16 (14%)	4 (3%)	5	25
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	156/177 (88%)	139 (89%)	16 (10%)	1 (1%)	30	72
9	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	3	18
10	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	14	51
11	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	24	66
12	L	141/165 (86%)	116 (82%)	22 (16%)	3 (2%)	9	40
13	M	192/196 (98%)	171 (89%)	17 (9%)	4 (2%)	9	40
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	8	38
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%)	8	38
18	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	26	70
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%)	9	41
22	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	12	48
23	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	26	70
24	X	80/92 (87%)	72 (90%)	6 (8%)	2 (2%)	7	34
25	Y	140/241 (58%)	132 (94%)	7 (5%)	1 (1%)	26	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	55 (78%)	12 (17%)	4 (6%)	2	13
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	3
All	All	3705/4472 (83%)	3292 (89%)	348 (9%)	65 (2%)	11	45

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%)	30	70
2	B	282/283 (100%)	263 (93%)	19 (7%)	20	57
3	C	193/193 (100%)	180 (93%)	13 (7%)	20	57
4	D	117/148 (79%)	110 (94%)	7 (6%)	24	62
5	E	152/156 (97%)	146 (96%)	6 (4%)	39	77
6	F	93/94 (99%)	92 (99%)	1 (1%)	80	94
7	G	27/282 (10%)	25 (93%)	2 (7%)	17	52
8	H	134/145 (92%)	124 (92%)	10 (8%)	17	51
9	I	58/130 (45%)	57 (98%)	1 (2%)	68	91
10	J	118/121 (98%)	109 (92%)	9 (8%)	16	51
11	K	106/106 (100%)	103 (97%)	3 (3%)	51	84
12	L	113/127 (89%)	106 (94%)	7 (6%)	23	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	147 (93%)	11 (7%)	19	55
14	N	149/150 (99%)	146 (98%)	3 (2%)	63	89
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	66	91
17	Q	79/80 (99%)	74 (94%)	5 (6%)	22	60
18	R	117/122 (96%)	113 (97%)	4 (3%)	44	81
19	S	71/74 (96%)	70 (99%)	1 (1%)	74	93
20	T	105/106 (99%)	98 (93%)	7 (7%)	20	57
21	U	44/53 (83%)	43 (98%)	1 (2%)	58	87
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	130/130 (100%)	126 (97%)	4 (3%)	47	83
24	X	66/74 (89%)	61 (92%)	5 (8%)	16	51
25	Y	120/196 (61%)	117 (98%)	3 (2%)	55	86
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%)	57	87
29	3	79/79 (100%)	73 (92%)	6 (8%)	16	51
All	All	3095/3646 (85%)	2955 (96%)	140 (4%)	34	74

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	30,34	12,22,23	0.99	1 (8%)	19,31,34	3.14	2 (10%)
30	OMG	0	2588	30	17,26,27	1.07	1 (5%)	21,38,41	2.52	3 (14%)
30	UR3	0	2619	30	12,22,23	0.73	0	16,32,35	0.72	0
30	PSU	0	2621	30	13,21,22	1.66	2 (15%)	18,30,33	6.08	4 (22%)
30	1MA	0	628	30,34	14,25,26	1.00	1 (7%)	15,37,40	1.10	1 (6%)

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	30,34	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,34	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.07	1.47	1.52
30	0	2621	PSU	C4-N3	2.47	1.37	1.33
30	0	2587	OMU	C4-N3	2.51	1.37	1.33
30	0	628	1MA	C6-N6	2.71	1.34	1.29
30	0	2588	OMG	C6-N1	3.45	1.39	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-21.32	114.73	128.33
30	0	2588	OMG	C5-C6-N1	-8.70	111.69	123.59
30	0	628	1MA	C2-N3-C4	-3.68	110.71	116.40
30	0	2587	OMU	C5-C4-N3	-3.35	114.53	123.12
30	0	2588	OMG	N3-C2-N1	-2.33	123.89	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0
30	0	2621	PSU	2	0
30	0	628	1MA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.59	1 (0%) 93 80	29, 65, 98, 115	0
2	B	337/338 (99%)	-0.72	0 100 100	31, 59, 87, 97	0
3	C	246/246 (100%)	-0.82	0 100 100	23, 47, 69, 80	0
4	D	140/177 (79%)	0.49	16 (11%) 7 2	74, 109, 132, 140	0
5	E	172/178 (96%)	-0.63	0 100 100	50, 74, 97, 103	0
6	F	119/120 (99%)	-0.29	1 (0%) 87 67	50, 73, 106, 113	0
7	G	29/348 (8%)	0.08	0 100 100	75, 96, 105, 109	0
8	H	160/177 (90%)	-0.48	0 100 100	48, 67, 99, 109	0
9	I	70/162 (43%)	1.87	30 (42%) 0 0	134, 152, 167, 169	0
10	J	142/145 (97%)	-0.79	1 (0%) 89 70	40, 58, 75, 97	0
11	K	132/132 (100%)	-0.87	0 100 100	39, 55, 81, 86	0
12	L	145/165 (87%)	-0.23	1 (0%) 89 70	35, 72, 113, 129	0
13	M	194/196 (98%)	-0.50	8 (4%) 41 16	31, 46, 99, 106	0
14	N	186/187 (99%)	-0.31	0 100 100	60, 80, 126, 132	0
15	O	115/116 (99%)	-0.86	0 100 100	43, 56, 74, 80	0
16	P	143/149 (95%)	-0.74	0 100 100	40, 59, 79, 85	0
17	Q	95/96 (98%)	-0.70	0 100 100	44, 56, 72, 88	0
18	R	150/155 (96%)	-0.83	0 100 100	33, 49, 70, 83	0
19	S	81/85 (95%)	-0.67	1 (1%) 81 55	40, 62, 82, 92	0
20	T	119/120 (99%)	-0.54	0 100 100	40, 59, 87, 116	0
21	U	53/67 (79%)	2.76	34 (64%) 0 0	107, 117, 125, 126	0
22	V	65/71 (91%)	-0.01	4 (6%) 24 9	47, 74, 118, 123	0
23	W	154/154 (100%)	-0.67	0 100 100	39, 54, 73, 87	0
24	X	82/92 (89%)	-0.44	1 (1%) 81 55	46, 65, 94, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.88	0 100 100	30, 49, 71, 92	0
26	Z	73/116 (62%)	3.71	46 (63%) 0 0	98, 116, 126, 130	0
27	1	56/57 (98%)	-0.77	0 100 100	28, 36, 43, 48	0
28	2	46/50 (92%)	-0.57	1 (2%) 65 35	31, 66, 97, 104	0
29	3	92/92 (100%)	4.35	73 (79%) 0 0	104, 119, 130, 134	0
30	0	2749/2923 (94%)	-0.82	2 (0%) 95 90	23, 51, 96, 175	0
31	9	122/122 (100%)	-0.97	1 (0%) 87 67	45, 75, 103, 154	0
All	All	6646/7517 (88%)	-0.52	221 (3%) 50 22	23, 57, 116, 175	0

The worst 5 of 221 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	46	SER	17.6
26	Z	58	ASN	13.0
29	3	39	GLN	12.5
26	Z	36	GLY	11.7
29	3	34	LYS	11.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	OMG	0	2588	24/25	0.98	0.13	-	39,41,42,45	0
30	UR3	0	2619	21/22	0.98	0.14	-	39,43,45,48	0
30	1MA	0	628	23/24	0.98	0.15	-	31,36,38,38	0
30	PSU	0	2621	20/21	0.98	0.18	-	40,43,44,44	0
30	OMU	0	2587	21/22	0.98	0.12	-	41,44,50,50	0

6.3 Carbohydrates [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	NA	0	8559	1/1	0.79	0.45	33.62	122,122,122,122	0
34	NA	0	8528	1/1	0.64	0.91	31.75	83,83,83,83	0
34	NA	0	8562	1/1	0.88	0.53	29.60	89,89,89,89	0
36	SR	0	8957	1/1	0.56	0.75	22.57	200,200,200,200	0
34	NA	0	8545	1/1	0.88	0.24	19.26	33,33,33,33	0
34	NA	0	8564	1/1	0.86	0.35	13.61	57,57,57,57	0
35	CL	0	8816	1/1	0.96	0.39	12.34	94,94,94,94	0
36	SR	0	8947	1/1	0.83	0.30	10.53	194,194,194,194	0
34	NA	R	8575	1/1	0.98	0.34	10.32	89,89,89,89	0
34	NA	0	8530	1/1	0.88	0.36	8.58	49,49,49,49	0
34	NA	0	8546	1/1	0.86	0.48	8.53	80,80,80,80	0
36	SR	0	8969	1/1	0.78	0.30	8.16	192,192,192,192	0
34	NA	0	8553	1/1	0.63	0.32	8.15	70,70,70,70	0
34	NA	0	8535	1/1	0.83	0.20	7.84	64,64,64,64	0
36	SR	B	8987	1/1	0.87	0.39	7.69	200,200,200,200	0
34	NA	0	8513	1/1	0.96	0.34	7.62	66,66,66,66	0
34	NA	0	8567	1/1	0.51	0.30	7.25	68,68,68,68	0
32	MG	0	8016	1/1	0.93	0.21	6.97	48,48,48,48	0
34	NA	0	8519	1/1	0.92	0.26	6.82	51,51,51,51	0
34	NA	0	8550	1/1	0.96	0.28	6.15	47,47,47,47	0
34	NA	0	8556	1/1	0.81	0.45	5.38	63,63,63,63	0
34	NA	0	8555	1/1	0.98	0.34	5.04	50,50,50,50	0
32	MG	0	8014	1/1	0.98	0.19	4.75	21,21,21,21	0
34	NA	0	8552	1/1	0.90	0.26	4.61	58,58,58,58	0
34	NA	0	8521	1/1	0.93	0.21	4.17	53,53,53,53	0
34	NA	0	8558	1/1	0.98	0.21	3.42	44,44,44,44	0
34	NA	0	8571	1/1	0.82	0.17	3.27	46,46,46,46	0
32	MG	0	8011	1/1	1.00	0.21	3.02	24,24,24,24	0
34	NA	0	8522	1/1	0.90	0.21	2.97	45,45,45,45	0
35	CL	0	8811	1/1	0.99	0.37	2.88	79,79,79,79	0
32	MG	0	8009	1/1	0.98	0.21	2.69	24,24,24,24	0
36	SR	0	8904	1/1	1.00	0.17	2.50	58,58,58,58	0
35	CL	0	8805	1/1	0.99	0.14	2.38	70,70,70,70	0
32	MG	0	8044	1/1	0.99	0.14	2.28	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	8051	1/1	0.84	0.22	2.09	101,101,101,101	0
34	NA	0	8569	1/1	0.99	0.21	2.06	67,67,67,67	0
32	MG	0	8008	1/1	0.99	0.14	1.74	26,26,26,26	0
32	MG	0	8004	1/1	0.96	0.18	1.74	21,21,21,21	0
32	MG	0	8003	1/1	0.99	0.17	1.61	22,22,22,22	0
34	NA	0	8517	1/1	0.99	0.15	1.54	21,21,21,21	0
32	MG	0	8015	1/1	0.99	0.13	1.28	25,25,25,25	0
32	MG	0	8088	1/1	0.94	0.16	1.25	35,35,35,35	0
36	SR	0	8903	1/1	1.00	0.13	1.24	46,46,46,46	0
34	NA	0	8507	1/1	0.86	0.16	1.23	32,32,32,32	0
32	MG	0	8085	1/1	0.99	0.12	1.22	67,67,67,67	0
32	MG	0	8062	1/1	0.95	0.20	1.22	57,57,57,57	0
36	SR	0	8902	1/1	0.99	0.16	1.03	67,67,67,67	0
34	NA	0	8534	1/1	0.97	0.18	0.99	37,37,37,37	0
34	NA	0	8537	1/1	1.00	0.17	0.91	29,29,29,29	0
32	MG	0	8010	1/1	0.93	0.17	0.91	24,24,24,24	0
34	NA	0	8560	1/1	0.94	0.79	0.89	74,74,74,74	0
32	MG	0	8084	1/1	0.99	0.14	0.72	24,24,24,24	0
32	MG	0	8065	1/1	0.95	0.12	0.57	50,50,50,50	0
36	SR	0	8975	1/1	0.64	0.11	0.52	171,171,171,171	0
36	SR	0	8985	1/1	0.44	0.12	0.50	182,182,182,182	0
34	NA	0	8515	1/1	0.87	0.15	0.06	44,44,44,44	0
37	CD	3	8704	1/1	0.90	0.71	-0.04	200,200,200,200	0
32	MG	0	8080	1/1	0.95	0.30	-0.13	68,68,68,68	0
35	CL	B	8819	1/1	0.99	0.15	-0.16	59,59,59,59	0
36	SR	0	8923	1/1	0.98	0.12	-0.25	85,85,85,85	0
32	MG	0	8006	1/1	0.98	0.13	-0.34	20,20,20,20	0
37	CD	1	8702	1/1	1.00	0.13	-0.35	61,61,61,61	0
32	MG	0	8021	1/1	0.98	0.11	-0.43	25,25,25,25	0
32	MG	0	8028	1/1	1.00	0.13	-0.47	19,19,19,19	0
34	NA	0	8557	1/1	0.40	0.08	-0.52	59,59,59,59	0
32	MG	0	8047	1/1	0.90	0.15	-0.57	67,67,67,67	0
32	MG	0	8045	1/1	0.99	0.10	-0.63	24,24,24,24	0
34	NA	0	8523	1/1	0.99	0.11	-0.66	51,51,51,51	0
34	NA	0	8542	1/1	0.98	0.17	-0.70	51,51,51,51	0
34	NA	Q	8540	1/1	0.96	0.11	-0.70	67,67,67,67	0
35	CL	J	8821	1/1	0.94	0.12	-0.72	66,66,66,66	0
33	K	M	8402	1/1	0.98	0.11	-0.79	60,60,60,60	0
32	MG	0	8034	1/1	0.98	0.13	-0.90	53,53,53,53	0
36	SR	0	8943	1/1	0.96	0.09	-0.94	72,72,72,72	0
36	SR	0	8972	1/1	0.96	0.10	-1.00	150,150,150,150	0
32	MG	B	8043	1/1	0.96	0.11	-1.21	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8001	1/1	0.99	0.13	-1.26	26,26,26,26	0
36	SR	0	8964	1/1	0.88	0.08	-1.32	129,129,129,129	0
36	SR	0	8944	1/1	0.80	0.08	-1.42	165,165,165,165	0
34	NA	J	8538	1/1	0.94	0.08	-1.42	49,49,49,49	0
32	MG	0	8012	1/1	0.99	0.15	-1.50	15,15,15,15	0
36	SR	3	8932	1/1	0.82	0.08	-1.51	158,158,158,158	0
35	CL	O	8808	1/1	0.99	0.10	-1.53	87,87,87,87	0
37	CD	U	8701	1/1	0.74	0.35	-1.61	200,200,200,200	0
32	MG	0	8058	1/1	0.99	0.06	-1.74	22,22,22,22	0
34	NA	M	8539	1/1	0.96	0.09	-1.85	32,32,32,32	0
36	SR	A	8930	1/1	0.99	0.07	-2.06	125,125,125,125	0
37	CD	Z	8703	1/1	0.86	0.28	-2.09	200,200,200,200	0
36	SR	0	8936	1/1	0.98	0.08	-2.17	87,87,87,87	0
34	NA	0	8533	1/1	0.96	0.08	-2.19	53,53,53,53	0
34	NA	0	8504	1/1	0.95	0.10	-2.27	27,27,27,27	0
36	SR	0	8984	1/1	0.91	0.07	-2.34	105,105,105,105	0
36	SR	A	8929	1/1	0.96	0.04	-2.47	117,117,117,117	0
36	SR	0	9001	1/1	0.55	0.08	-2.53	166,166,166,166	0
32	MG	T	8057	1/1	0.97	0.04	-2.71	63,63,63,63	0
34	NA	0	8568	1/1	0.99	0.10	-2.75	38,38,38,38	0
35	CL	K	8812	1/1	0.95	0.07	-2.82	48,48,48,48	0
35	CL	3	8804	1/1	0.90	0.19	-2.98	120,120,120,120	0
32	MG	0	8025	1/1	0.97	0.10	-3.14	30,30,30,30	0
36	SR	0	8910	1/1	0.94	0.08	-3.23	99,99,99,99	0
36	SR	0	8992	1/1	0.98	0.08	-3.40	130,130,130,130	0
32	MG	0	8052	1/1	0.91	0.04	-3.67	51,51,51,51	0
36	SR	0	8948	1/1	0.97	0.08	-3.90	103,103,103,103	0
32	MG	Y	8086	1/1	0.97	0.06	-4.07	37,37,37,37	0
35	CL	M	8818	1/1	0.99	0.05	-4.17	39,39,39,39	0
32	MG	0	8087	1/1	0.98	0.09	-4.79	26,26,26,26	0
32	MG	0	8050	1/1	0.91	0.08	-4.90	52,52,52,52	0
32	MG	0	8072	1/1	0.99	0.08	-5.76	47,47,47,47	0
32	MG	0	8002	1/1	0.98	0.08	-6.07	29,29,29,29	0
32	MG	0	8013	1/1	0.99	0.04	-7.18	24,24,24,24	0
36	SR	0	8945	1/1	0.95	0.06	-8.05	107,107,107,107	0
36	SR	0	8949	1/1	0.99	0.05	-11.90	102,102,102,102	0
36	SR	0	8982	1/1	0.78	1.84	-	200,200,200,200	0
32	MG	0	8026	1/1	1.00	0.04	-	27,27,27,27	0
36	SR	0	8908	1/1	0.98	0.13	-	77,77,77,77	0
36	SR	0	8914	1/1	0.95	0.20	-	105,105,105,105	0
36	SR	0	8990	1/1	0.96	0.15	-	125,125,125,125	0
36	SR	0	8968	1/1	0.82	0.15	-	177,177,177,177	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	S	8510	1/1	0.96	0.04	-	26,26,26,26	0
34	NA	0	8544	1/1	0.94	0.11	-	41,41,41,41	0
32	MG	0	8033	1/1	0.94	0.13	-	40,40,40,40	0
36	SR	0	8973	1/1	0.80	0.14	-	112,112,112,112	0
36	SR	0	8965	1/1	0.91	0.07	-	127,127,127,127	0
34	NA	0	8514	1/1	0.99	0.19	-	17,17,17,17	0
36	SR	0	8931	1/1	0.83	0.07	-	110,110,110,110	0
36	SR	1	8952	1/1	1.00	0.12	-	72,72,72,72	0
34	NA	0	8563	1/1	0.52	0.67	-	65,65,65,65	0
36	SR	0	8988	1/1	0.81	0.14	-	170,170,170,170	0
32	MG	0	8019	1/1	0.99	0.15	-	23,23,23,23	0
36	SR	0	8924	1/1	0.97	0.17	-	133,133,133,133	0
34	NA	0	8529	1/1	0.98	0.18	-	41,41,41,41	0
36	SR	0	8907	1/1	1.00	0.12	-	40,40,40,40	0
32	MG	0	8056	1/1	0.99	0.09	-	75,75,75,75	0
36	SR	0	8905	1/1	0.99	0.23	-	62,62,62,62	0
34	NA	0	8524	1/1	0.99	0.39	-	54,54,54,54	0
34	NA	0	8518	1/1	0.79	0.26	-	75,75,75,75	0
36	SR	1	8913	1/1	0.99	0.11	-	100,100,100,100	0
34	NA	0	8520	1/1	0.98	0.10	-	39,39,39,39	0
32	MG	0	8023	1/1	0.98	0.18	-	24,24,24,24	0
34	NA	0	8548	1/1	0.85	0.13	-	68,68,68,68	0
35	CL	0	8817	1/1	0.96	0.19	-	69,69,69,69	0
32	MG	0	8066	1/1	0.98	0.31	-	75,75,75,75	0
32	MG	0	8031	1/1	0.99	0.23	-	52,52,52,52	0
36	SR	0	8909	1/1	0.98	0.13	-	89,89,89,89	0
32	MG	0	8079	1/1	1.00	0.11	-	36,36,36,36	0
36	SR	0	8911	1/1	0.98	0.06	-	79,79,79,79	0
36	SR	0	8953	1/1	0.89	0.07	-	200,200,200,200	0
34	NA	0	8566	1/1	0.81	0.33	-	62,62,62,62	0
36	SR	0	9000	1/1	0.93	0.32	-	200,200,200,200	0
36	SR	0	8974	1/1	0.57	0.14	-	164,164,164,164	0
34	NA	C	8503	1/1	0.98	0.17	-	45,45,45,45	0
34	NA	0	8551	1/1	0.98	0.15	-	55,55,55,55	0
34	NA	0	8554	1/1	0.96	0.55	-	65,65,65,65	0
34	NA	0	8526	1/1	0.95	0.13	-	33,33,33,33	0
36	SR	0	8983	1/1	0.95	0.28	-	191,191,191,191	0
36	SR	0	8921	1/1	0.98	0.09	-	75,75,75,75	0
34	NA	0	8516	1/1	0.96	0.08	-	20,20,20,20	0
32	MG	0	8036	1/1	0.90	0.05	-	37,37,37,37	0
36	SR	0	8956	1/1	0.91	0.05	-	151,151,151,151	0
36	SR	9	9003	1/1	0.90	0.09	-	177,177,177,177	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8954	1/1	1.00	0.12	-	103,103,103,103	0
34	NA	0	8549	1/1	0.90	0.17	-	77,77,77,77	0
32	MG	0	8038	1/1	0.99	0.05	-	61,61,61,61	0
34	NA	0	8509	1/1	0.92	0.14	-	54,54,54,54	0
37	CD	O	8705	1/1	0.98	0.08	-	93,93,93,93	0
32	MG	0	8070	1/1	0.99	0.10	-	40,40,40,40	0
36	SR	0	8996	1/1	0.96	0.21	-	199,199,199,199	0
36	SR	0	8920	1/1	0.97	0.05	-	106,106,106,106	0
34	NA	0	8541	1/1	0.83	0.24	-	54,54,54,54	0
35	CL	Y	8820	1/1	0.94	0.11	-	47,47,47,47	0
36	SR	0	8997	1/1	0.54	0.85	-	194,194,194,194	0
32	MG	K	8054	1/1	0.92	0.15	-	40,40,40,40	0
36	SR	0	8979	1/1	0.61	0.18	-	198,198,198,198	0
32	MG	2	8060	1/1	0.86	0.10	-	35,35,35,35	0
32	MG	0	8082	1/1	0.95	0.12	-	66,66,66,66	0
32	MG	0	8089	1/1	0.97	0.17	-	59,59,59,59	0
36	SR	0	8998	1/1	0.76	0.31	-	184,184,184,184	0
34	NA	9	8572	1/1	0.82	0.17	-	71,71,71,71	0
36	SR	9	8978	1/1	1.00	0.07	-	125,125,125,125	0
35	CL	0	8813	1/1	0.99	0.03	-	46,46,46,46	0
32	MG	0	8024	1/1	0.98	0.12	-	96,96,96,96	0
36	SR	0	8933	1/1	0.99	0.07	-	126,126,126,126	0
36	SR	0	8939	1/1	0.88	0.08	-	152,152,152,152	0
36	SR	B	8950	1/1	0.98	0.15	-	113,113,113,113	0
36	SR	0	8916	1/1	0.94	0.10	-	114,114,114,114	0
34	NA	0	8502	1/1	0.99	0.05	-	56,56,56,56	0
36	SR	0	8934	1/1	0.99	0.09	-	99,99,99,99	0
36	SR	0	8922	1/1	0.75	0.29	-	169,169,169,169	0
32	MG	0	8017	1/1	0.98	0.11	-	20,20,20,20	0
36	SR	0	8901	1/1	0.98	0.14	-	63,63,63,63	0
36	SR	0	8958	1/1	0.98	0.07	-	114,114,114,114	0
36	SR	S	8961	1/1	0.98	0.05	-	126,126,126,126	0
32	MG	0	8029	1/1	0.97	0.07	-	68,68,68,68	0
36	SR	0	8989	1/1	0.86	0.19	-	200,200,200,200	0
32	MG	0	8078	1/1	0.98	0.23	-	51,51,51,51	0
32	MG	0	8068	1/1	0.92	0.11	-	49,49,49,49	0
32	MG	9	8074	1/1	0.99	0.05	-	63,63,63,63	0
32	MG	0	8037	1/1	0.94	0.16	-	76,76,76,76	0
32	MG	0	8076	1/1	0.99	0.10	-	27,27,27,27	0
35	CL	A	8809	1/1	0.97	0.34	-	100,100,100,100	0
36	SR	0	8942	1/1	0.88	0.07	-	130,130,130,130	0
32	MG	3	8090	1/1	0.96	0.12	-	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8059	1/1	0.99	0.12	-	53,53,53,53	0
32	MG	0	8020	1/1	0.97	0.14	-	29,29,29,29	0
32	MG	0	8063	1/1	0.79	0.23	-	86,86,86,86	0
32	MG	0	8067	1/1	0.98	0.14	-	32,32,32,32	0
36	SR	0	8960	1/1	0.76	0.05	-	152,152,152,152	0
36	SR	3	8999	1/1	0.91	0.28	-	172,172,172,172	0
35	CL	0	8815	1/1	0.84	0.09	-	87,87,87,87	0
32	MG	0	8030	1/1	0.99	0.34	-	86,86,86,86	0
36	SR	0	8940	1/1	0.98	0.11	-	77,77,77,77	0
32	MG	0	8077	1/1	0.99	0.10	-	43,43,43,43	0
36	SR	0	8963	1/1	0.98	0.06	-	123,123,123,123	0
34	NA	0	8547	1/1	0.94	0.68	-	47,47,47,47	0
36	SR	0	8962	1/1	0.67	0.08	-	179,179,179,179	0
36	SR	F	9005	1/1	0.92	0.09	-	131,131,131,131	0
32	MG	0	8005	1/1	0.98	0.22	-	34,34,34,34	0
36	SR	R	8912	1/1	1.00	0.12	-	86,86,86,86	0
34	NA	0	8511	1/1	0.93	0.10	-	48,48,48,48	0
36	SR	0	9008	1/1	0.99	0.17	-	97,97,97,97	0
32	MG	0	8048	1/1	0.99	0.21	-	20,20,20,20	0
32	MG	0	8075	1/1	0.91	0.09	-	83,83,83,83	0
36	SR	0	8971	1/1	0.55	0.10	-	170,170,170,170	0
33	K	0	8401	1/1	0.75	0.14	-	156,156,156,156	0
36	SR	0	9006	1/1	0.31	0.83	-	180,180,180,180	0
32	MG	0	8053	1/1	0.98	0.05	-	45,45,45,45	0
36	SR	0	8976	1/1	0.91	0.24	-	197,197,197,197	0
36	SR	0	9004	1/1	0.45	1.04	-	200,200,200,200	0
32	MG	0	8081	1/1	0.86	0.32	-	80,80,80,80	0
34	NA	0	8561	1/1	0.96	0.36	-	57,57,57,57	0
36	SR	0	8986	1/1	0.62	0.47	-	200,200,200,200	0
36	SR	0	8955	1/1	0.85	0.18	-	200,200,200,200	0
36	SR	0	8928	1/1	0.89	0.09	-	146,146,146,146	0
34	NA	0	8505	1/1	0.90	1.17	-	53,53,53,53	0
32	MG	0	8073	1/1	0.98	0.06	-	51,51,51,51	0
32	MG	0	8055	1/1	0.97	0.10	-	45,45,45,45	0
36	SR	0	8938	1/1	0.98	0.07	-	164,164,164,164	0
32	MG	0	8039	1/1	0.94	0.18	-	71,71,71,71	0
36	SR	0	8981	1/1	0.91	0.14	-	157,157,157,157	0
36	SR	0	8951	1/1	0.98	0.08	-	139,139,139,139	0
32	MG	0	8092	1/1	0.98	0.02	-	44,44,44,44	0
35	CL	N	8807	1/1	0.94	0.35	-	99,99,99,99	0
32	MG	B	8042	1/1	0.90	0.08	-	56,56,56,56	0
34	NA	0	8570	1/1	0.88	0.07	-	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8022	1/1	0.99	0.12	-	17,17,17,17	0
34	NA	0	8531	1/1	0.99	0.10	-	15,15,15,15	0
36	SR	0	8994	1/1	0.93	0.24	-	200,200,200,200	0
34	NA	0	8527	1/1	0.96	0.15	-	54,54,54,54	0
36	SR	0	8937	1/1	0.93	0.17	-	100,100,100,100	0
36	SR	0	8970	1/1	0.94	0.04	-	131,131,131,131	0
32	MG	0	8041	1/1	0.96	0.31	-	36,36,36,36	0
34	NA	9	8543	1/1	0.99	0.12	-	38,38,38,38	0
32	MG	0	8027	1/1	0.97	0.12	-	26,26,26,26	0
34	NA	0	8508	1/1	0.95	0.56	-	61,61,61,61	0
35	CL	0	8803	1/1	0.95	0.14	-	69,69,69,69	0
35	CL	J	8801	1/1	0.96	0.13	-	71,71,71,71	0
36	SR	0	8918	1/1	0.98	0.10	-	71,71,71,71	0
34	NA	0	8506	1/1	0.95	0.53	-	58,58,58,58	0
36	SR	0	8926	1/1	0.98	0.09	-	109,109,109,109	0
34	NA	0	8525	1/1	0.86	0.26	-	85,85,85,85	0
32	MG	0	8064	1/1	0.97	0.06	-	33,33,33,33	0
34	NA	0	8512	1/1	0.99	0.08	-	36,36,36,36	0
36	SR	0	8959	1/1	0.56	0.29	-	200,200,200,200	0
35	CL	R	8806	1/1	0.95	0.11	-	47,47,47,47	0
32	MG	0	8018	1/1	0.98	0.14	-	34,34,34,34	0
34	NA	0	8573	1/1	0.82	0.27	-	55,55,55,55	0
36	SR	0	8967	1/1	0.81	0.05	-	133,133,133,133	0
36	SR	0	9007	1/1	0.82	0.23	-	179,179,179,179	0
35	CL	0	8822	1/1	0.95	0.60	-	97,97,97,97	0
36	SR	0	8966	1/1	0.99	0.07	-	97,97,97,97	0
32	MG	0	8061	1/1	0.99	0.18	-	19,19,19,19	0
35	CL	0	8814	1/1	0.78	0.18	-	72,72,72,72	0
36	SR	0	8919	1/1	0.75	0.32	-	200,200,200,200	0
35	CL	J	8802	1/1	0.54	0.08	-	76,76,76,76	0
32	MG	0	8046	1/1	0.92	0.13	-	26,26,26,26	0
36	SR	A	8993	1/1	0.86	0.08	-	159,159,159,159	0
32	MG	0	8083	1/1	0.97	0.12	-	71,71,71,71	0
36	SR	0	8917	1/1	0.96	0.10	-	109,109,109,109	0
32	MG	0	8093	1/1	0.87	0.06	-	28,28,28,28	0
32	MG	0	8032	1/1	0.91	0.05	-	27,27,27,27	0
36	SR	0	8977	1/1	0.72	0.12	-	181,181,181,181	0
36	SR	9	8980	1/1	0.75	0.14	-	182,182,182,182	0
32	MG	0	8049	1/1	0.92	0.38	-	74,74,74,74	0
35	CL	L	8810	1/1	0.93	0.09	-	64,64,64,64	0
34	NA	0	8565	1/1	0.92	0.95	-	70,70,70,70	0
36	SR	0	8915	1/1	0.87	0.07	-	118,118,118,118	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8946	1/1	0.85	0.12	-	123,123,123,123	0
36	SR	0	8906	1/1	1.00	0.20	-	64,64,64,64	0
32	MG	0	8071	1/1	0.89	0.13	-	31,31,31,31	0
34	NA	0	8536	1/1	0.97	0.07	-	40,40,40,40	0
36	SR	0	8995	1/1	0.97	0.14	-	140,140,140,140	0
32	MG	0	8040	1/1	0.96	0.21	-	54,54,54,54	0
32	MG	0	8091	1/1	0.73	0.07	-	58,58,58,58	0
36	SR	0	8941	1/1	0.98	0.18	-	122,122,122,122	0
36	SR	0	9002	1/1	0.84	0.06	-	157,157,157,157	0
32	MG	0	8069	1/1	0.90	0.19	-	55,55,55,55	0
32	MG	0	8007	1/1	1.00	0.19	-	18,18,18,18	0
36	SR	0	8935	1/1	0.98	0.09	-	87,87,87,87	0
34	NA	0	8501	1/1	0.96	0.14	-	43,43,43,43	0
34	NA	0	8574	1/1	0.96	0.35	-	54,54,54,54	0
34	NA	R	8532	1/1	0.94	0.13	-	37,37,37,37	0
32	MG	0	8035	1/1	0.96	0.10	-	61,61,61,61	0
36	SR	0	8991	1/1	0.88	0.34	-	193,193,193,193	0
36	SR	0	8927	1/1	0.94	0.20	-	196,196,196,196	0
36	SR	0	8925	1/1	0.99	0.15	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.