



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 07:36 PM EDT

PDB ID : 3CCL
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535C. Density for Anisomycin is visible but not included in model.
Authors : Blaha, G.; Gurel, G.
Deposited on : unknown
Resolution : 2.90 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

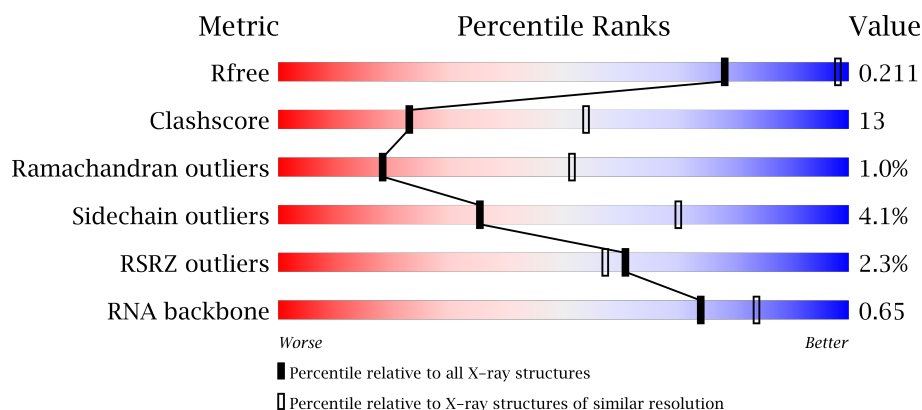
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



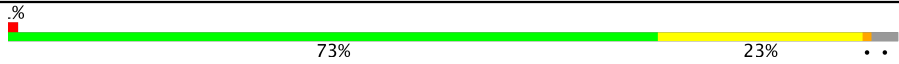

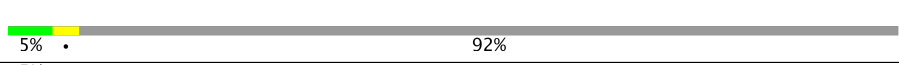

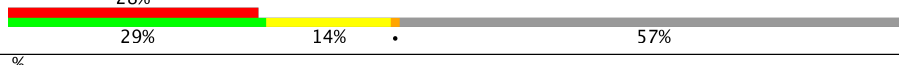
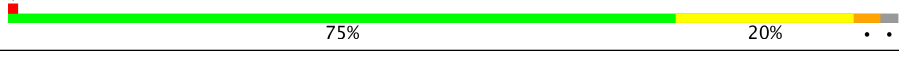
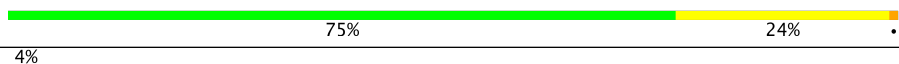

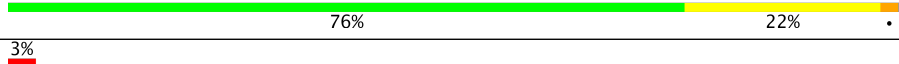


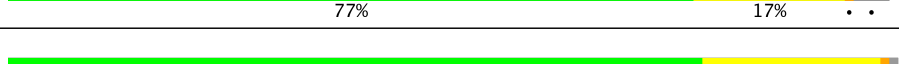
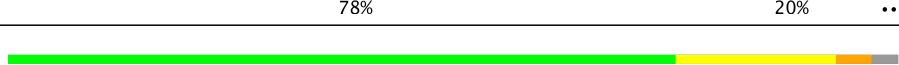
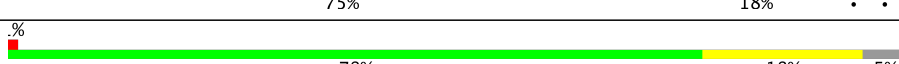

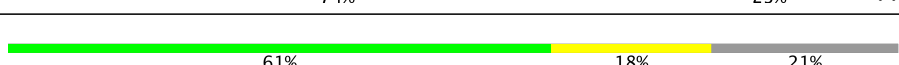
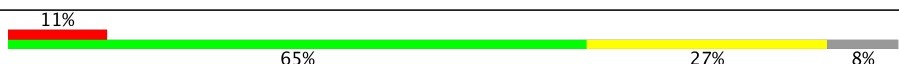
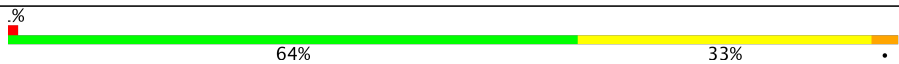
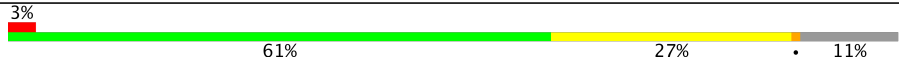
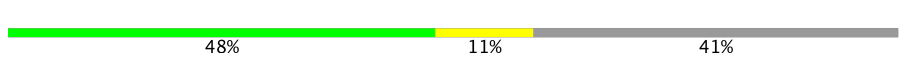
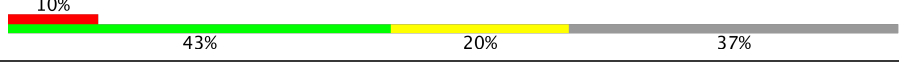
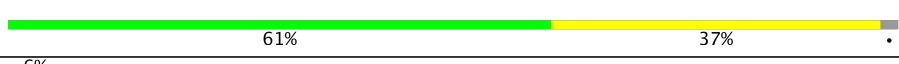
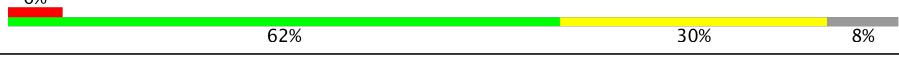


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
2	B	338	<div> <div>66%</div> <div>31%</div> <div>•</div> </div>
3	C	246	<div> <div>72%</div> <div>24%</div> <div>•</div> </div>
4	D	177	<div> <div>16%</div> <div>45%</div> <div>32%</div> <div>21%</div> <div>•</div> </div>

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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	

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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	8008	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8084	-	-	-	X
32	MG	A	8051	-	-	-	X
34	SR	0	8903	-	-	-	X
34	SR	0	8904	-	-	-	X
34	SR	0	8947	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8508	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8517	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8534	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8552	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	9	8572	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	K	0	8402	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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
			59020	26349	10874	19052	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	9	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	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	10	Total Cl 10 10	0	0
33	J	3	Total Cl 3 3	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	93	Total Sr 93 93	0	0
34	1	2	Total Sr 2 2	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	3	Total Sr 3 3	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	S	1	Total Sr 1 1	0	0
34	F	1	Total Sr 1 1	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	67	Total 67	Na 67	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	2	Total 2	K 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	116	Total 116	O 116	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	B	141	Total 141	O 141	0	0
38	C	170	Total 170	O 170	0	0
38	D	44	Total 44	O 44	0	0
38	E	45	Total 45	O 45	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	63	Total 63	O 63	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	85	Total 85	O 85	0	0
38	M	123	Total 123	O 123	0	0
38	N	55	Total 55	O 55	0	0
38	O	43	Total 43	O 43	0	0
38	P	67	Total 67	O 67	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	33	Total 33	O 33	0	0
38	T	34	Total 34	O 34	0	0
38	U	27	Total 27	O 27	0	0
38	V	13	Total 13	O 13	0	0

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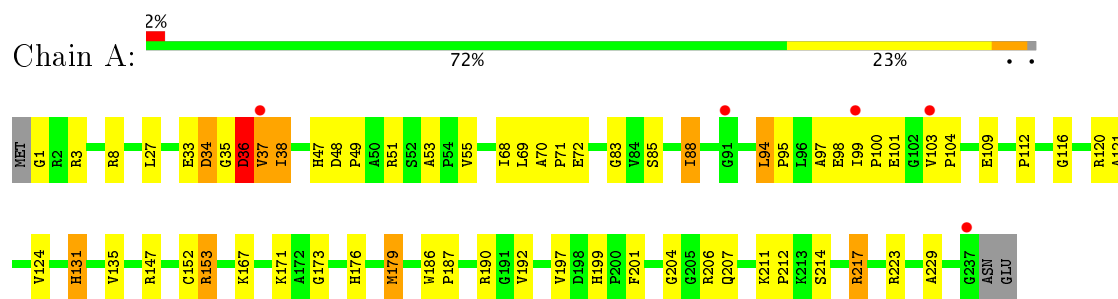
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	69	Total 69	O 69	0	0
38	X	25	Total 25	O 25	0	0
38	Y	95	Total 95	O 95	0	0
38	Z	26	Total 26	O 26	0	0
38	1	63	Total 63	O 63	0	0
38	2	50	Total 50	O 50	0	0
38	3	62	Total 62	O 62	0	0
38	0	5929	Total 5929	O 5929	0	0
38	9	147	Total 147	O 147	0	0

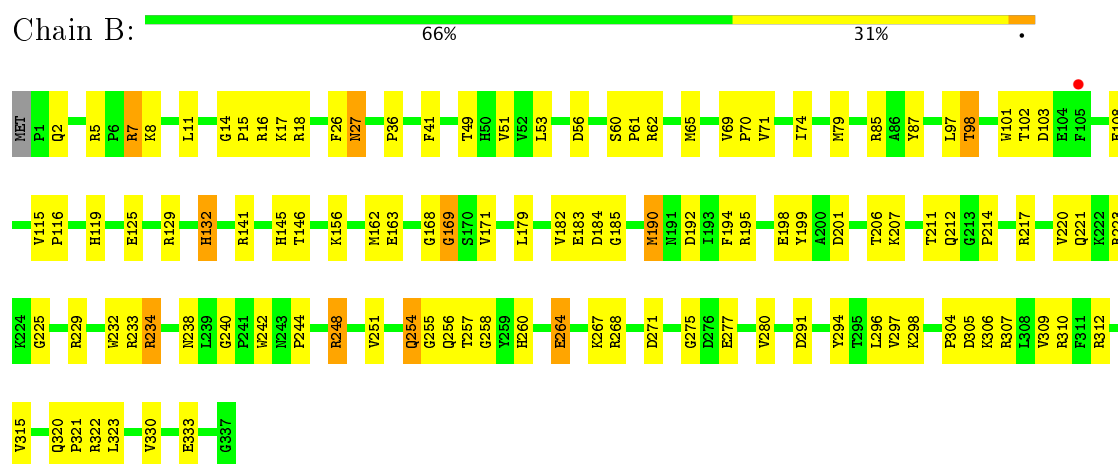
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

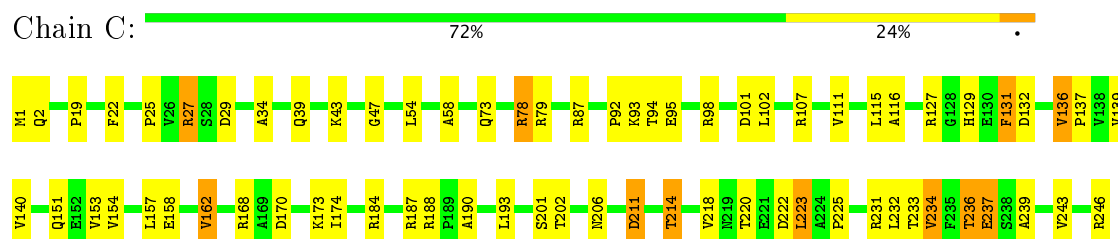
- Molecule 1: 50S ribosomal protein L2P



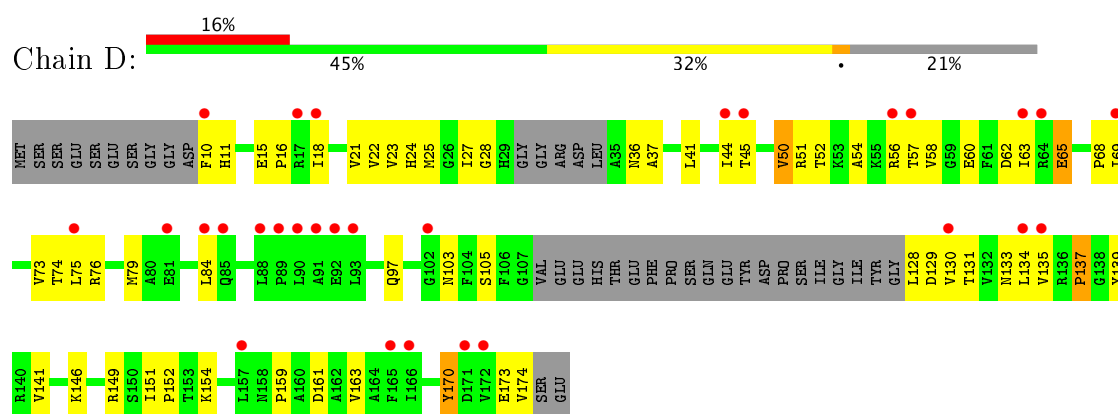
- Molecule 2: 50S ribosomal protein L3P



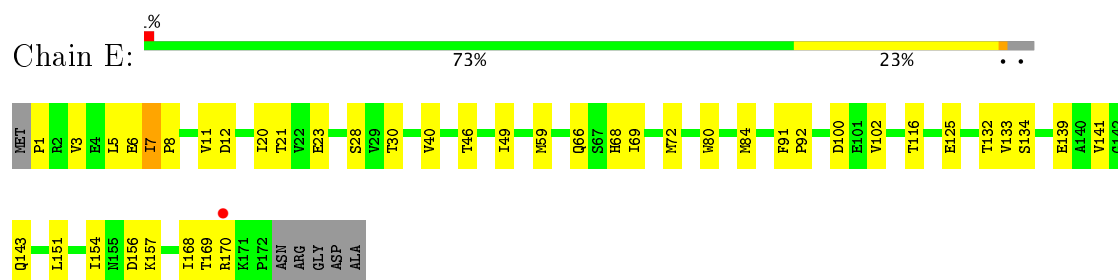
- Molecule 3: 50S ribosomal protein L4P



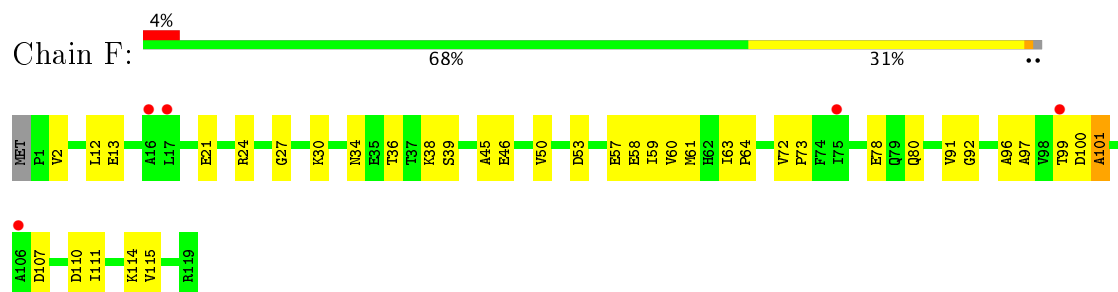
- Molecule 4: 50S ribosomal protein L5P



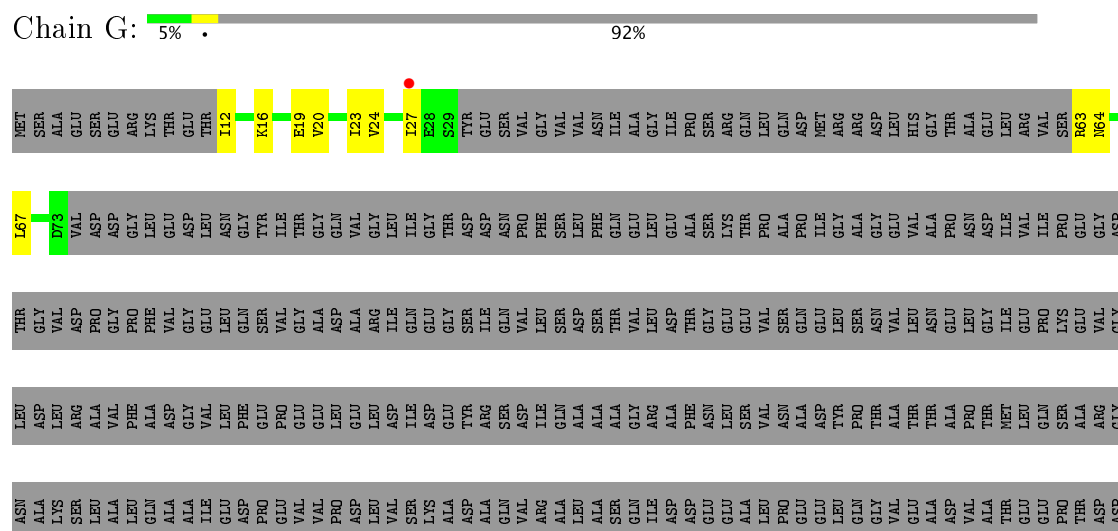
- Molecule 5: 50S ribosomal protein L6P



- Molecule 6: 50S ribosomal protein L7Ae

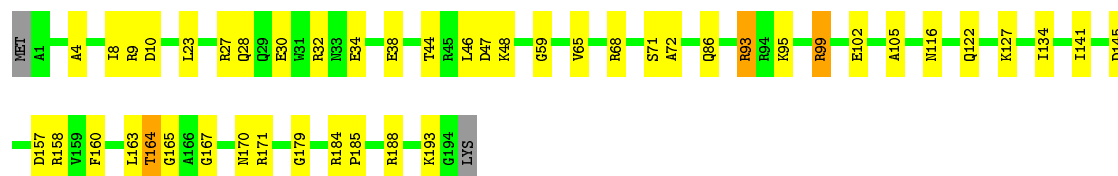


- Molecule 7: 50S ribosomal protein L10E



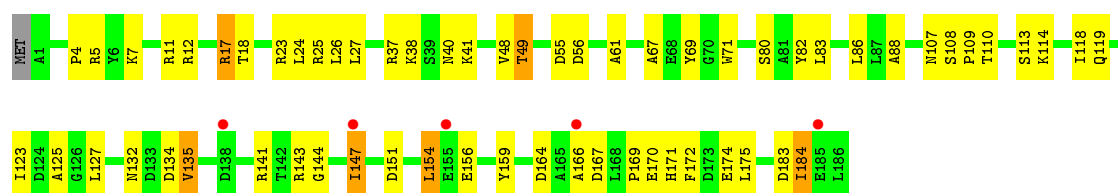
- Molecule 13: 50S ribosomal protein L15e

Chain M:  76% 22% ..

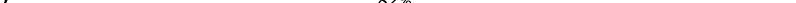


- Molecule 14: 50S ribosomal protein L18P

Chain N:  3% 66% 30% ..



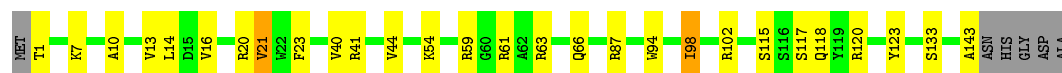
- Molecule 15: 50S ribosomal protein L18e

Chain 0:  82% 16% ..

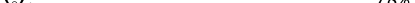


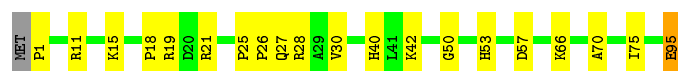
- Molecule 16: 50S ribosomal protein L19e

Chain P: 77% 17% ..



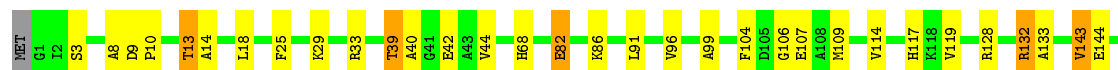
- Molecule 17: 50S ribosomal protein L21e

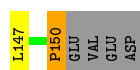
Chain Q:  78% 20% ..



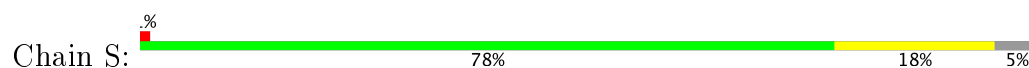
- Molecule 18: 50S ribosomal protein L22P

Chain R:  75% 18% . .

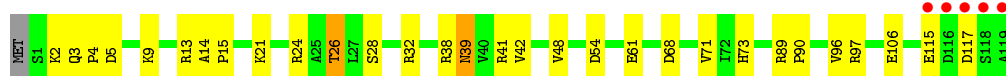
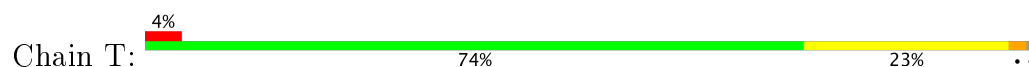




- Molecule 19: 50S ribosomal protein L23P



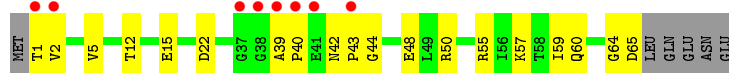
- Molecule 20: 50S ribosomal protein L24P



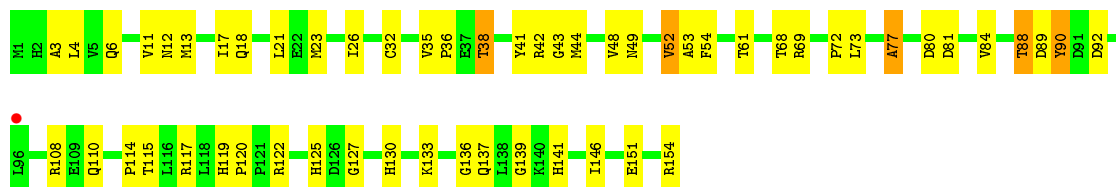
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

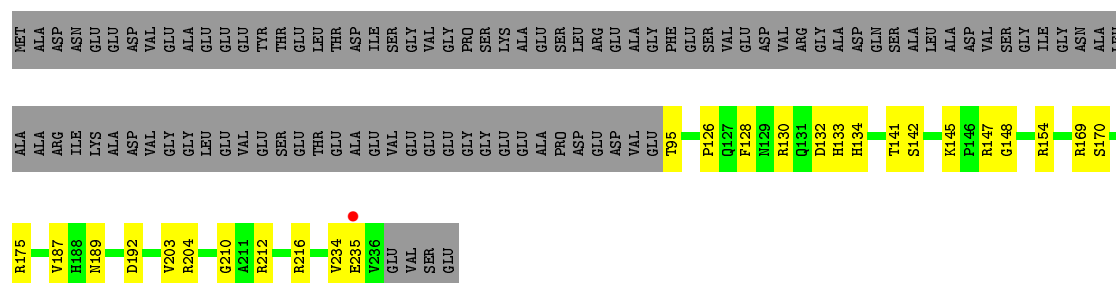


- Molecule 24: 50S ribosomal protein L31e




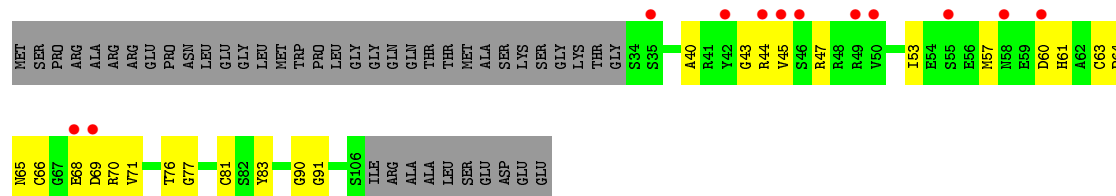
- Molecule 25: 50S ribosomal protein L32e

Chain Y:  48% 11% 41%



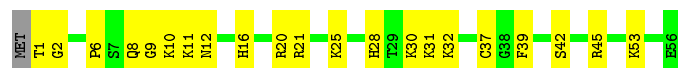
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:  10% 43% 20% 37%



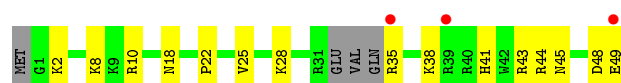
- Molecule 27: 50S ribosomal protein L37e

Chain 1:  61% 37% 2%



- Molecule 28: 50S ribosomal protein L39e

Chain 2:  6% 62% 30% 8%



- Molecule 29: 50S ribosomal protein L44E

Chain 3:  77% 22% 1%

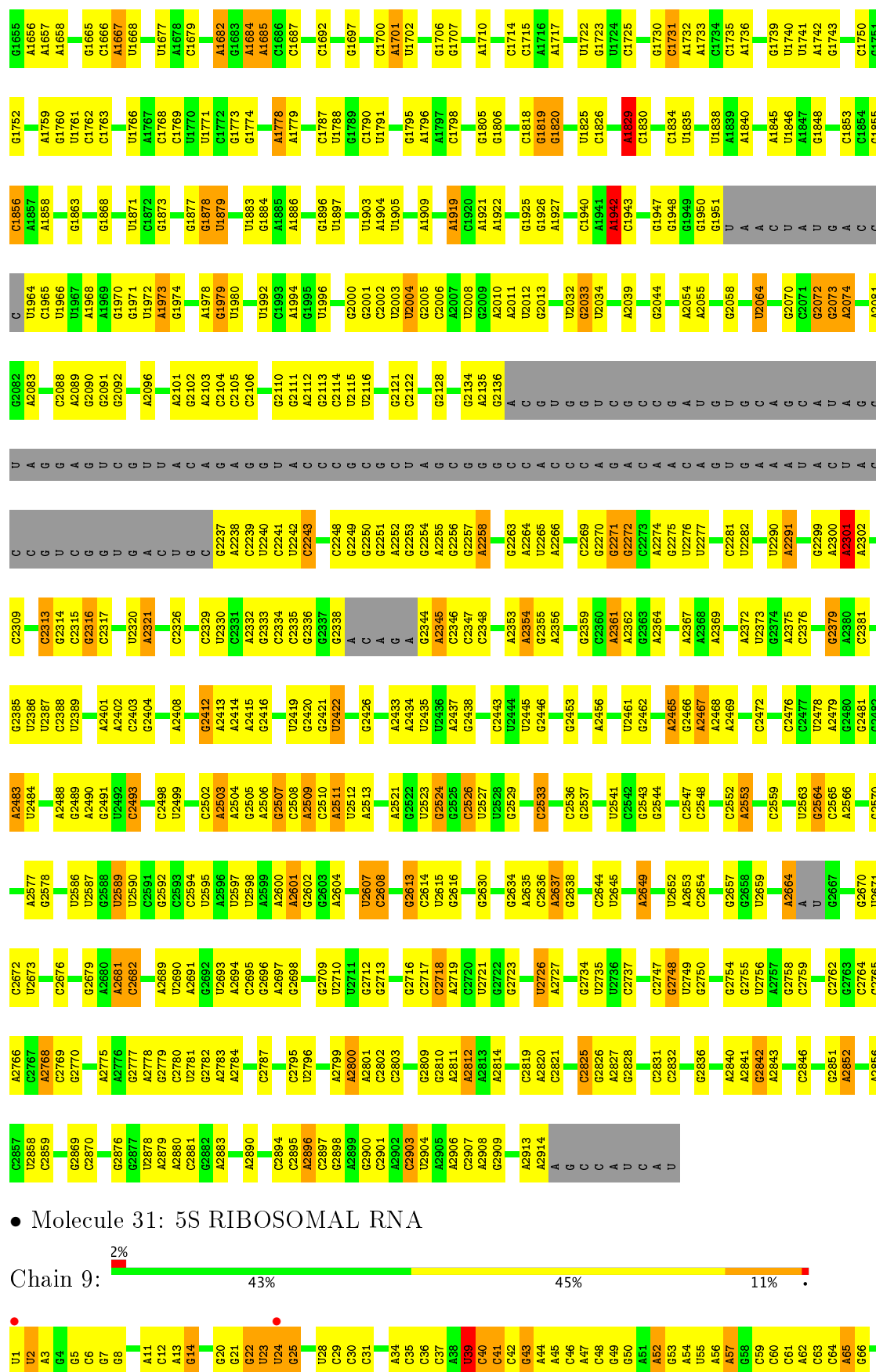


- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:  54% 35% 5% 6%



C1554	G1555	A1559	U	U1561	C1562	A1573	G1586	U1587	G1588	G1589	C1592	C1593	C1594	G1595	U1596	A1597	A1598	A1603	G1604	G1605	A1606	A1607	C1613	G1614	A1615	A1616	C1617	G1622	C1623	A1624	G1625	A1626	G1627	A1630	A1631	A1632	C1633	G1634	U1635	G1636	A1637	A1641	A1642	C1643	U1644	C1645	C1652	A1653																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
G1441	A1442	U1446	U1447	C1450	C1451	U1461	C1462	C1463	C1474	C1477	U1478	A1482	C1483	C1484	A1485	A1486	A1487	U1488	G1493	G1494	G1495	G1496	U1503	A1504	U1505	U1506	C1513	C1514	A1515	U1516	G1520	C1521	A1522	G1523	U1524	A1525	A1526	C1527	A1528	G1529	U1635	G1636	A1637	A1641	A1642	C1643	U1644	C1645	C1652	A1653																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
C1245	A1246	U1249	C1250	C1268	G1269	C1273	A1278	U1279	A1280	A1287	U1288	C1289	U1290	A1291	A1294	G1295	A1296	U1297	U1298	G1299	G1300	U1304	C1305	U1306	A1307	A1308	G1311	G1312	A1313	U1314	A1321	G1322	G1325	A1328	G1331	C1332	U1333	C1334	G1339	G1340	A1341	G1342	G1343	G1344	U1350																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C1168	U1169	A1171	G1172	A1173	A1174	U1180	C1181	C1182	C1183	A1184	U1185	U1186	A1188	U1189	G1190	A1191	A1192	A1193	A1194	U1198	A1199	G1200	G1203	U1205	U1206	A1207	C1208	G1209	A1210	G1211	C1212	G1216	G1221	C1229	A1230	A1231	U1232	U1233	A1236	U1237	C1238	G1239	A1242	C1243	U1244																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C1068	C1069	G1071	G1072	A1078	A1079	C1080	A1081	A1088	A1097	A1098	G1099	C1104	U1109	G1110	U1115	U1116	A1117	A1118	G1119	U1120	G1121	C1127	U1128	C1129	U1130	G1131	A1132	G1135	U1136	G1137	G1138	U1139	C1140	U1149	A1150	G1151	A1154	U1155	G1159	G1160	A1161	G1162	G1163	U1164	G1165	A1166	C1167																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
C980	G985	A986	G987	U988	G989	G998	C999	U903	U904	C905	A912	C920	G921	A922	A923	A926	U932	A939	G940	G941	U942	A943	G944	U945	C946	U947	G948	U949	G950	A951	G952	G953	G958	C959	G960	A961	C962	C963	G968	G969	U970	G	U	G	U	C	C	G	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
A790	A791	G792	G800	U801	A807	A808	G809	A812	C813	G814	U815	G816	G817	G820	U821	C822	U823	G824	U825	U826	A827	G834	U835	G836	U840	A841	C842	A843	A846	G847	C848	C853	G854	A857	U858	A861	A867	G868	G869	U870	G	U	G	U	C	C	G	C																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
C583	U584	G588	G589	G590	G604	G605	C613	U614	G615	U616	U619	A620	C621	G622	U623	U624	U625	U626	G627	C628	A629	A632	C633	G634	A635	G636	C637	G638	A639	G644	U645	G652	U653	A654	U655	G656	G657	G658	A659	A660	G661	G669	G670	A671	G672	G677	G678	G681	A682	C683																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G378	G379	A380	G381	U382	A383	G384	U392	U396	A397	U398	A507	A508	A509	U510	A511	G512	A513	U514	U515	G518	U522	C523	A524	A532	G535	A536	G537	C538	A449	C450	A451	G452	U457	A458	A459	G461	U468	U470	G482	U487	A488	A489	C492	A493	A494	A495	A496	A497	A498	A499	A500	A501	A502	A503	A504	A505	A506	A507	A508	A509	A510	A511	A512	A513	A514	A515	A516	A517	A518	A519	A520	A521	A522	A523	A524	A525	A526	A527	A528	A529	A530	A531	A532	A533	A534	A535	A536	A537	A538	A539	A540	A541	A542	A543	A544	A545	A546	A547	A548	A549	A550	A551	A552	A553	A554	A555	A556	A557	A558	A559	A560	A561	A562	A563	A564	A565	A566	A567	A568	A569	A570	A571	A572	A573	A574	A575	A576	A577	A578	A579	A580	A581	A582	A583	A584	A585	A586	A587	A588	A589	A590	A591	A592	A593	A594	A595	A596	A597	A598	A599	A600	A601	A602	A603	A604	A605	A606	A607	A608	A609	A610	A611	A612	A613	A614	A615	A616	A617	A618	A619	A620	A621	A622	A623	A624	A625	A626	A627	A628	A629	A630	A631	A632	A633	A634	A635	A636	A637	A638	A639	A640	A641	A642	A643	A644	A645	A646	A647	A648	A649	A650	A651	A652	A653	A654	A655	A656	A657	A658	A659	A660	A661	A662	A663	A664	A665	A666	A667	A668	A669	A670	A671	A672	A673	A674	A675	A676	A677	A678	A679	A680	A681	A682	A683	A684	A685	A686	A687	A688	A689	A690	A691	A692	A693	A694	A695	A696	A697	A698	A699	A700	A701	A702	A703	A704	A705	A706	A707	A708	A709	A710	A711	A712	A713	A714	A715	A716	A717	A718	A719	A720	A721	A722	A723	A724	A725	A726	A727	A728	A729	A730	A731	A732	A733	A734	A735	A736	A737	A738	A739	A740	A741	A742	A743	A744	A745	A746	A747	A748	A749	A750	A751	A752	A753	A754	A755	A756	A757	A758	A759	A760	A761	A762	A763	A764	A765	A766	A767	A768	A769	A770	A771	A772	A773	A774	A775	A776	A777	A778	A779	A780	A781	A782	A783	A784	A785	A786	A787	A788	A789	A790	A791	A792	A793	A794	A795	A796	A797	A798	A799	A800	A801	A802	A803	A804	A805	A806	A807	A808	A809	A810	A811	A812	A813	A814	A815	A816	A817	A818	A819	A820	A821	A822	A823	A824	A825	A826	A827	A828	A829	A830	A831	A832	A833	A834	A835	A836	A837	A838	A839	A840	A841	A842	A843	A844	A845	A846	A847	A848	A849	A850	A851	A852	A853	A854	A855	A856	A857	A858	A859	A860	A861	A862	A863	A864	A865	A866	A867	A868	A869	A870	A871	A872	A873	A874	A875	A876	A877	A878	A879	A880	A881	A882	A883	A884	A885	A886	A887	A888	A889	A890	A891	A892	A893	A894	A895	A896	A897	A898	A899	A900	A901	A902	A903	A904	A905	A906	A907	A908	A909	A910	A911	A912	A913	A914	A915	A916	A917	A918	A919	A920	A921	A922	A923	A924	A925	A926	A927	A928	A929	A930	A931	A932	A933	A934	A935	A936	A937	A938	A939	A940	A941	A942	A943	A944	A945	A946	A947	A948	A949	A950	A951	A952	A953	A954	A955	A956	A957	A958	A959	A960	A961	A962	A963	A964	A965	A966	A967	A968	A969	A970	A971	A972	A973	A974	A975	A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050	A1051	A1052	A1053	A1054	A1055	A1056	A1057	A1058	A1059	A1060	A1061	A1062	A1063	A1064	A1065	A1066	A1067	A1068	A1069	A1070	A1071	A1072	A1073	A1074	A1075	A1076	A1077	A1078	A1079	A1080	A1081	A1082	A1083	A1084	A1085	A1086	A1087	A1088	A1089	A1090	A1091	A1092	A1093	A1094	A1095	A1096	A1097	A1098	A1099	A1100	A1101	A1102	A1103	A1104	A1105	A1106	A1107	A1108	A1109	A1110	A1111	A1112	A1113	A1114	A1115	A1116	A1117	A1118	A1119	A1120	A1121	A1122	A1123	A1124	A1125	A1126	A1127	A1128	A1129	A1130	A1131	A1132	A1133	A1134	A1135	A1136	A1137	A1138	A1139	A1140	A1141	A1142	A1143	A1144	A1145	A1146	A1147	A1148	A1149	A1150	A1151	A1152	A1153	A1154	A1155	A1156	A1157	A1158	A1159	A1160	A1161	A1162	A1163	A1164	A1165	A1166	A1167	A1168	A1169	A1170	A1171	A1172	A1173	A1174	A1175	A1176	A1177	A1178	A1179	A1180	A1181	A1182	A1183	A1184	A1185	A1186	A1187	A1188	A1189	A1190	A1191	A1192	A1193	A1194	A1195	A1196	A1197	A1198	A1199	A1200	A1201	A1202	A1203	A1204	A1205	A1206	A1207	A1208	A1209	A1210	A1211	A1212	A1213	A1214	A1215	A1216	A1217	A1218	A1219	A1220	A1221	A1222	A1223	A1224	A1225	A1226	A1227	A1228	A1229	A1230	A1231	A1232	A1233	A1234	A1235	A1236	A1237	A1238	A1239	A1240	A1241	A1242	A1243	A1244	A1245	A1246	A1247	A1248	A1249	A1250	A1251	A1252	A1253	A1254	A1255	A1256	A1257	A1258	A1259	A1260	A1261	A1262	A1263	A1264	A1265	A1266	A1267	A1268	A1269	A1270	A1271	A1272	A1273	A1274	A1275	A1276	A1277	A1278	A1279	A1280	A1281	A1282	A1283	A1284	A1285	A1286	A1287	A1288	A1289	A1290	A1291	A1292	A1293	A1294	A1295	A1296	A1297	A1298	A1299	A1300	A1301	A1302	A1303	A1304	A1305	A1306	A1307	A1308	A1309	A1310	A1311	A1312	A1313	A1314	A1315	A1316	A1317	A1318	A1319	A1320	A1321	A1322	A1323	A1324	A1325	A1326	A1327	A1328	A1329	A1330	A1331	A1332	A1333	A1334	A1335	A1336	A1337	A1338	A1339	A1340	A1341	A1342	A1343	A1344	A1345	A1346	A1347	A1348	A1349	A1350	A1351	A1352	A1353	A1354	A1355	A1356	A1357	A1358	A1359	A1360	A1361	A1362	A1363	A1364	A1365	A1366	A1367	A1368	A1369	A1370	A1371	A1372	A1373	A1374	A1375	A1376	A1377	A1378	A1379	A1380	A1381	A1382	A1383	A1384	A1385	A1386	A1387	A1388	A1389	A1390	A1391	A1392	A1393	A1394	A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	A1416	A1417	A1418	A1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	A1440	A1441	A1442	A1443	A1444	A1445	A1446	A1447	A1448	A1449	A1450	A1451	A1452	A1453	A1454	A1455	A1456	A1457	A1458	A1459	A1460	A1461	A1462	A1463	A1464	A1465	A1466	A1467	A1468	A1469	A1470	A1471	A1472	A1473	A1474	A1475	A1476	A1477	A1478	A1479	A1480	A1481	A1482	A1483	A1484	A1485	A1486	A1487	A1488	A1489	A1490	A1491	A1492	A1493	A1494	A1495	A1496	A1497	A1498	A1499	A1500	A1501	A1502	A1503</



U69	U70	G75	G76	A77	G88	C91	C92	A93	G94	C95	C96	G101	U106	C107	C108	U112	C113	G114	C115	C122
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.16Å 300.03Å 576.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.90 85.91 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.98-2.90) 92.3 (85.91-2.41)	Depositor EDS
R_{merge}	0.13	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}	0.171 , 0.220 0.167 , 0.211	Depositor DCC
R_{free} test set	3626 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.31	0/241	0.49	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.36	0/1136	0.60	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.59	0/1181
16	P	0.32	0/1147	0.51	0/1528
17	Q	0.33	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.32	0/648	0.55	0/875
20	T	0.33	0/958	0.64	0/1289
21	U	0.33	0/417	0.59	0/562
22	V	0.33	0/502	0.52	0/675
23	W	0.34	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.37	0/584	0.60	0/781
27	1	0.39	0/438	0.59	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.55	0/1024
30	0	0.37	0/65957	0.68	13/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	20/147586 (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	28
31	9	0	1
All	All	1	30

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	27.29	2.86	1.50
18	R	150	PRO	CA-C	-18.25	1.16	1.52
18	R	150	PRO	CG-CD	13.93	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.37	1.66	1.47

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.40	61.65	112.10
18	R	150	PRO	CA-N-CD	12.30	128.92	111.70
18	R	150	PRO	N-CA-CB	10.97	116.46	103.30
18	R	150	PRO	CA-C-O	-8.51	99.79	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 30 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	131	A	Sidechain
30	0	220	C	Sidechain
30	0	333	G	Sidechain
30	0	48	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	63	0
2	B	2625	0	2533	89	0
3	C	1860	0	1813	59	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	29	0
6	F	890	0	843	26	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	32	0
11	K	994	0	1027	32	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	51	0
15	O	865	0	873	18	0
16	P	1136	0	1123	24	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	10	0
20	T	950	0	924	21	0
21	U	410	0	364	8	0
22	V	499	0	511	17	0
23	W	1196	0	1137	56	0
24	X	654	0	653	18	0
25	Y	1130	0	1133	23	0
26	Z	573	0	532	15	0
27	1	431	0	426	23	0
28	2	396	0	413	15	0
29	3	755	0	728	18	0
30	0	59020	0	29811	1159	0
31	9	2599	0	1325	100	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
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	4	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	67	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5929	0	0	185	0
38	1	63	0	0	4	0
38	2	50	0	0	1	0
38	3	62	0	0	3	0
38	9	147	0	0	7	0
38	A	116	0	0	5	0
38	B	141	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	170	0	0	13	0
38	D	44	0	0	3	0
38	E	45	0	0	2	0
38	F	27	0	0	2	0
38	G	19	0	0	1	0
38	H	63	0	0	7	0
38	I	8	0	0	3	0
38	J	53	0	0	1	0
38	K	56	0	0	5	0
38	L	85	0	0	6	0
38	M	123	0	0	2	0
38	N	55	0	0	5	0
38	O	43	0	0	3	0
38	P	67	0	0	2	0
38	Q	50	0	0	3	0
38	R	85	0	0	1	0
38	S	33	0	0	2	0
38	T	34	0	0	2	0
38	U	27	0	0	2	0
38	V	13	0	0	2	0
38	W	69	0	0	4	0
38	X	25	0	0	2	0
38	Y	95	0	0	5	0
38	Z	26	0	0	3	0
All	All	99122	0	59913	1941	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 13.

The worst 5 of 1941 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.77	1.12
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11
30:0:871:G:H8	30:0:871:G:H5'	1.09	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.31	1.10

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%)	211 (90%)	18 (8%)	6 (3%)	6	24
2	B	335/338 (99%)	306 (91%)	25 (8%)	4 (1%)	15	46
3	C	244/246 (99%)	224 (92%)	19 (8%)	1 (0%)	38	72
4	D	134/177 (76%)	113 (84%)	16 (12%)	5 (4%)	4	16
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	6	24
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	147 (94%)	8 (5%)	1 (1%)	28	64
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	12	39
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	25	60
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	22	57
12	L	141/165 (86%)	125 (89%)	14 (10%)	2 (1%)	13	41
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	32	68
14	N	184/187 (98%)	169 (92%)	12 (6%)	3 (2%)	11	37
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	110 (94%)	7 (6%)	0	100	100
21	U	51/67 (76%)	45 (88%)	5 (10%)	1 (2%)	9	31
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	11	37
23	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	14	43
24	X	80/92 (87%)	75 (94%)	4 (5%)	1 (1%)	14	43
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	62 (87%)	7 (10%)	2 (3%)	6	22
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3447 (93%)	222 (6%)	36 (1%)	18	51

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP

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%)	28	62
2	B	282/283 (100%)	263 (93%)	19 (7%)	19	48
3	C	193/193 (100%)	176 (91%)	17 (9%)	12	34
4	D	117/148 (79%)	110 (94%)	7 (6%)	22	54
5	E	152/156 (97%)	149 (98%)	3 (2%)	60	87
6	F	93/94 (99%)	91 (98%)	2 (2%)	57	86
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	39	74
9	I	58/130 (45%)	57 (98%)	1 (2%)	66	89
10	J	118/121 (98%)	110 (93%)	8 (7%)	18	47
11	K	106/106 (100%)	104 (98%)	2 (2%)	62	88
12	L	113/127 (89%)	110 (97%)	3 (3%)	50	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	151 (96%)	7 (4%)	33	67
14	N	149/150 (99%)	142 (95%)	7 (5%)	30	65
15	O	93/94 (99%)	92 (99%)	1 (1%)	78	94
16	P	113/117 (97%)	111 (98%)	2 (2%)	64	89
17	Q	79/80 (99%)	76 (96%)	3 (4%)	38	73
18	R	117/122 (96%)	111 (95%)	6 (5%)	28	62
19	S	71/74 (96%)	70 (99%)	1 (1%)	71	91
20	T	105/106 (99%)	97 (92%)	8 (8%)	15	41
21	U	44/53 (83%)	43 (98%)	1 (2%)	56	85
22	V	51/57 (90%)	50 (98%)	1 (2%)	60	87
23	W	130/130 (100%)	126 (97%)	4 (3%)	45	79
24	X	66/74 (89%)	62 (94%)	4 (6%)	22	53
25	Y	120/196 (61%)	116 (97%)	4 (3%)	43	77
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%)	54	84
29	3	79/79 (100%)	78 (99%)	1 (1%)	73	93
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	35	70

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	62	HIS
11	K	10	GLN
24	X	27	ASP
8	H	87	LYS
10	J	46	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	66	GLN
27	1	28	HIS
13	M	77	HIS

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Mol	Chain	Res	Type
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	27 (0%)
31	9	121/122 (99%)	15 (12%)	1 (0%)
All	All	2866/3045 (94%)	257 (8%)	28 (0%)

5 of 257 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 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1237	U
30	0	1377	C
30	0	2718	C
30	0	1246	A
30	0	1352	A

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	14,22,23	0.96	1 (7%)	18,31,34	3.67	2 (11%)
30	OMG	0	2588	30	18,26,27	1.03	2 (11%)	22,38,41	2.45	5 (22%)
30	UR3	0	2619	30	14,22,23	0.72	0	16,32,35	0.73	0
30	PSU	0	2621	30	16,21,22	1.75	3 (18%)	20,30,33	6.10	5 (25%)
30	1MA	0	628	30	16,25,26	1.09	1 (6%)	13,37,40	1.18	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	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	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.58	1.47	1.52
30	0	2588	OMG	C8-N7	-2.01	1.30	1.34
30	0	2621	PSU	C2-N1	2.44	1.43	1.38
30	0	2587	OMU	C4-N3	2.52	1.37	1.33
30	0	2621	PSU	C4-N3	2.69	1.37	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.17	114.61	128.40
30	0	2621	PSU	C5-C4-N3	-12.85	114.89	125.43
30	0	2588	OMG	C5-C6-N1	-8.23	111.77	123.48
30	0	628	1MA	C2-N3-C4	-3.68	110.76	116.41
30	0	2587	OMU	C5-C4-N3	-3.53	114.70	123.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	3	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 ⓘ

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%)	-0.39	5 (2%) 64 60	35, 59, 97, 117	0
2	B	337/338 (99%)	-0.60	1 (0%) 93 93	36, 60, 90, 100	0
3	C	246/246 (100%)	-0.58	0 100 100	30, 51, 75, 89	0
4	D	140/177 (79%)	1.08	29 (20%) 1 1	73, 108, 135, 146	0
5	E	172/178 (96%)	-0.51	1 (0%) 89 88	51, 74, 96, 104	0
6	F	119/120 (99%)	0.12	5 (4%) 37 32	55, 78, 111, 125	0
7	G	29/348 (8%)	0.48	1 (3%) 46 39	83, 103, 109, 112	0
8	H	160/177 (90%)	0.03	9 (5%) 25 20	50, 73, 106, 113	0
9	I	70/162 (43%)	3.12	46 (65%) 0 0	137, 156, 173, 174	0
10	J	142/145 (97%)	-0.57	1 (0%) 87 86	41, 58, 78, 97	0
11	K	132/132 (100%)	-0.71	0 100 100	40, 55, 79, 82	0
12	L	145/165 (87%)	0.07	7 (4%) 31 27	34, 73, 123, 136	0
13	M	194/196 (98%)	-0.71	0 100 100	35, 50, 66, 73	0
14	N	186/187 (99%)	-0.08	5 (2%) 55 50	52, 75, 123, 135	0
15	O	115/116 (99%)	-0.60	0 100 100	45, 61, 78, 84	0
16	P	143/149 (95%)	-0.64	0 100 100	46, 61, 77, 84	0
17	Q	95/96 (98%)	-0.60	0 100 100	44, 55, 71, 86	0
18	R	150/155 (96%)	-0.73	0 100 100	39, 52, 71, 86	0
19	S	81/85 (95%)	-0.51	1 (1%) 79 77	49, 65, 86, 98	0
20	T	119/120 (99%)	-0.35	5 (4%) 37 32	47, 62, 89, 123	0
21	U	53/67 (79%)	-0.63	0 100 100	48, 62, 79, 88	0
22	V	65/71 (91%)	0.69	8 (12%) 5 3	55, 80, 129, 134	0
23	W	154/154 (100%)	-0.52	1 (0%) 89 88	41, 57, 74, 88	0
24	X	82/92 (89%)	-0.19	3 (3%) 42 37	49, 67, 90, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.76	1 (0%) 87 86	31, 50, 73, 94	0
26	Z	73/116 (62%)	0.73	12 (16%) 2 1	63, 87, 101, 106	0
27	1	56/57 (98%)	-0.66	0 100 100	32, 39, 45, 53	0
28	2	46/50 (92%)	-0.12	3 (6%) 20 15	41, 69, 104, 115	0
29	3	92/92 (100%)	-0.38	0 100 100	44, 68, 81, 91	0
30	0	2749/2923 (94%)	-0.67	8 (0%) 93 93	28, 53, 96, 172	0
31	9	122/122 (100%)	-0.83	2 (1%) 72 70	45, 74, 96, 153	0
All	All	6646/7517 (88%)	-0.45	154 (2%) 61 57	28, 58, 108, 174	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	10.0
22	V	39	ALA	8.0
22	V	1	THR	7.6
26	Z	46	SER	7.5
4	D	63	ILE	7.5

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	OMU	0	2587	21/22	0.99	0.13	-	40,43,46,49	0
30	1MA	0	628	23/24	0.99	0.15	-	35,38,38,39	0
30	OMG	0	2588	24/25	0.98	0.12	-	38,42,43,43	0
30	PSU	0	2621	20/21	0.99	0.14	-	35,38,47,48	0
30	UR3	0	2619	21/22	0.98	0.14	-	43,45,48,49	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
35	NA	0	8565	1/1	0.94	0.93	67.70	68,68,68,68	0
35	NA	0	8562	1/1	0.55	0.80	63.04	74,74,74,74	0
35	NA	0	8564	1/1	0.96	0.42	34.64	81,81,81,81	0
35	NA	0	8547	1/1	0.93	0.60	26.69	54,54,54,54	0
35	NA	0	8522	1/1	0.54	0.39	21.22	83,83,83,83	0
35	NA	0	8568	1/1	0.97	0.50	18.72	50,50,50,50	0
35	NA	0	8512	1/1	0.99	0.42	15.04	56,56,56,56	0
35	NA	0	8542	1/1	0.96	0.39	14.61	66,66,66,66	0
35	NA	0	8555	1/1	0.64	0.49	14.54	51,51,51,51	0
35	NA	0	8553	1/1	0.99	0.36	13.94	68,68,68,68	0
35	NA	9	8572	1/1	0.72	0.34	13.34	111,111,111,111	0
34	SR	B	8987	1/1	0.67	0.49	13.33	200,200,200,200	0
35	NA	0	8563	1/1	0.71	0.36	11.31	94,94,94,94	0
35	NA	0	8528	1/1	0.85	0.29	10.62	58,58,58,58	0
34	SR	0	8903	1/1	0.99	0.18	8.43	58,58,58,58	0
35	NA	0	8530	1/1	0.91	0.28	6.97	55,55,55,55	0
35	NA	0	8556	1/1	0.96	0.40	6.75	49,49,49,49	0
35	NA	0	8517	1/1	0.99	0.20	6.69	36,36,36,36	0
35	NA	0	8552	1/1	1.00	0.29	6.17	72,72,72,72	0
32	MG	0	8047	1/1	0.99	0.28	5.86	65,65,65,65	0
35	NA	0	8527	1/1	0.87	0.23	5.38	71,71,71,71	0
34	SR	0	8947	1/1	0.82	0.27	5.32	200,200,200,200	0
35	NA	0	8508	1/1	0.98	0.18	5.08	39,39,39,39	0
35	NA	0	8559	1/1	0.90	0.14	4.95	76,76,76,76	0
32	MG	A	8051	1/1	0.88	0.41	4.92	72,72,72,72	0
32	MG	0	8041	1/1	0.98	0.20	4.74	31,31,31,31	0
37	K	0	8402	1/1	0.97	0.27	4.36	87,87,87,87	0
32	MG	0	8008	1/1	0.99	0.15	3.89	27,27,27,27	0
35	NA	0	8534	1/1	0.96	0.23	3.66	42,42,42,42	0
32	MG	0	8084	1/1	0.99	0.15	3.05	37,37,37,37	0
34	SR	0	8904	1/1	0.99	0.19	2.90	66,66,66,66	0
32	MG	0	8009	1/1	0.99	0.20	2.80	29,29,29,29	0
35	NA	0	8569	1/1	0.96	0.20	2.10	54,54,54,54	0
35	NA	0	8507	1/1	0.95	0.16	2.09	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8014	1/1	0.99	0.15	1.96	35,35,35,35	0
34	SR	0	8918	1/1	0.98	0.14	1.90	85,85,85,85	0
32	MG	0	8003	1/1	1.00	0.18	1.86	34,34,34,34	0
32	MG	0	8067	1/1	0.97	0.20	1.76	34,34,34,34	0
32	MG	0	8028	1/1	0.99	0.16	1.58	27,27,27,27	0
32	MG	0	8016	1/1	0.98	0.18	1.35	60,60,60,60	0
35	NA	0	8575	1/1	0.97	0.18	1.31	86,86,86,86	0
32	MG	0	8006	1/1	0.94	0.14	1.30	30,30,30,30	0
34	SR	A	8929	1/1	0.95	0.16	1.26	137,137,137,137	0
34	SR	0	8992	1/1	0.95	0.15	1.21	137,137,137,137	0
32	MG	0	8045	1/1	0.99	0.11	1.08	35,35,35,35	0
34	SR	R	8912	1/1	0.99	0.16	1.03	86,86,86,86	0
32	MG	0	8004	1/1	1.00	0.17	0.89	30,30,30,30	0
35	NA	0	8557	1/1	0.87	0.10	0.82	52,52,52,52	0
35	NA	0	8558	1/1	0.94	0.18	0.68	50,50,50,50	0
32	MG	0	8062	1/1	0.88	0.17	0.61	50,50,50,50	0
35	NA	0	8533	1/1	0.90	0.13	0.60	67,67,67,67	0
33	CL	0	8815	1/1	0.96	0.10	0.53	78,78,78,78	0
34	SR	0	8948	1/1	0.97	0.12	0.48	102,102,102,102	0
35	NA	0	8504	1/1	0.99	0.16	0.31	37,37,37,37	0
35	NA	0	8537	1/1	0.96	0.11	0.13	41,41,41,41	0
35	NA	0	8502	1/1	0.89	0.12	0.11	65,65,65,65	0
32	MG	0	8070	1/1	0.98	0.13	0.00	45,45,45,45	0
35	NA	C	8503	1/1	0.91	0.16	-0.06	44,44,44,44	0
35	NA	J	8538	1/1	0.85	0.16	-0.27	60,60,60,60	0
35	NA	0	8523	1/1	0.98	0.12	-0.28	45,45,45,45	0
32	MG	0	8088	1/1	0.98	0.13	-0.28	42,42,42,42	0
36	CD	U	8701	1/1	0.99	0.11	-0.30	72,72,72,72	0
37	K	0	8401	1/1	0.93	0.13	-0.31	74,74,74,74	0
34	SR	0	8972	1/1	0.96	0.14	-0.32	141,141,141,141	0
32	MG	0	8011	1/1	1.00	0.16	-0.36	33,33,33,33	0
33	CL	J	8821	1/1	0.99	0.13	-0.48	71,71,71,71	0
32	MG	0	8012	1/1	0.98	0.16	-0.56	25,25,25,25	0
32	MG	0	8043	1/1	0.96	0.10	-0.62	49,49,49,49	0
34	SR	3	8932	1/1	1.00	0.12	-0.62	79,79,79,79	0
35	NA	0	8515	1/1	0.96	0.14	-0.63	37,37,37,37	0
32	MG	K	8054	1/1	0.95	0.13	-0.80	50,50,50,50	0
32	MG	0	8050	1/1	0.98	0.12	-0.83	37,37,37,37	0
32	MG	B	8042	1/1	0.98	0.09	-0.84	50,50,50,50	0
33	CL	M	8818	1/1	0.98	0.10	-0.88	47,47,47,47	0
34	SR	0	8935	1/1	0.99	0.10	-0.89	80,80,80,80	0
32	MG	0	8021	1/1	0.96	0.10	-0.92	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	M	8539	1/1	0.99	0.10	-0.97	34,34,34,34	0
34	SR	0	8936	1/1	0.98	0.10	-1.14	94,94,94,94	0
35	NA	0	8520	1/1	0.97	0.08	-1.21	53,53,53,53	0
32	MG	0	8010	1/1	0.96	0.12	-1.31	35,35,35,35	0
34	SR	F	9005	1/1	0.98	0.07	-1.32	134,134,134,134	0
36	CD	Z	8703	1/1	0.99	0.09	-1.34	91,91,91,91	0
36	CD	1	8702	1/1	0.99	0.10	-1.40	65,65,65,65	0
35	NA	R	8532	1/1	0.97	0.08	-1.44	46,46,46,46	0
35	NA	Q	8540	1/1	0.92	0.08	-1.49	60,60,60,60	0
33	CL	L	8810	1/1	0.96	0.08	-1.54	61,61,61,61	0
34	SR	0	8943	1/1	0.99	0.07	-1.64	117,117,117,117	0
36	CD	3	8704	1/1	1.00	0.07	-1.69	81,81,81,81	0
32	MG	0	8025	1/1	0.99	0.11	-1.85	35,35,35,35	0
34	SR	0	8969	1/1	0.97	0.10	-1.88	160,160,160,160	0
32	MG	T	8057	1/1	0.93	0.07	-1.89	65,65,65,65	0
32	MG	0	8058	1/1	0.99	0.08	-1.90	23,23,23,23	0
33	CL	O	8808	1/1	0.93	0.07	-1.99	81,81,81,81	0
34	SR	0	8975	1/1	0.97	0.07	-1.99	135,135,135,135	0
34	SR	A	8930	1/1	0.99	0.05	-2.05	104,104,104,104	0
34	SR	9	8978	1/1	0.99	0.07	-2.27	133,133,133,133	0
32	MG	0	8085	1/1	0.96	0.08	-2.52	73,73,73,73	0
32	MG	0	8052	1/1	0.93	0.07	-2.53	52,52,52,52	0
34	SR	0	8985	1/1	0.89	0.06	-2.78	143,143,143,143	0
33	CL	0	8813	1/1	0.99	0.06	-2.78	61,61,61,61	0
33	CL	0	8805	1/1	0.97	0.06	-2.83	67,67,67,67	0
34	SR	0	8949	1/1	0.97	0.09	-3.09	119,119,119,119	0
34	SR	0	8945	1/1	0.95	0.07	-3.28	112,112,112,112	0
32	MG	0	8001	1/1	0.97	0.09	-3.61	33,33,33,33	0
34	SR	0	8902	1/1	1.00	0.11	-3.64	66,66,66,66	0
33	CL	0	8812	1/1	0.97	0.06	-3.82	54,54,54,54	0
33	CL	3	8804	1/1	0.99	0.06	-3.88	67,67,67,67	0
35	NA	0	8519	1/1	0.92	0.12	-3.89	50,50,50,50	0
32	MG	0	8060	1/1	0.95	0.06	-3.96	61,61,61,61	0
32	MG	0	8002	1/1	0.99	0.07	-4.04	32,32,32,32	0
32	MG	Y	8086	1/1	0.98	0.05	-4.19	46,46,46,46	0
33	CL	B	8819	1/1	0.98	0.09	-4.22	54,54,54,54	0
34	SR	1	8913	1/1	1.00	0.09	-4.26	96,96,96,96	0
34	SR	0	8910	1/1	0.99	0.05	-4.51	101,101,101,101	0
32	MG	0	8065	1/1	0.99	0.06	-4.57	49,49,49,49	0
35	NA	0	8521	1/1	0.97	0.07	-4.60	65,65,65,65	0
32	MG	0	8034	1/1	0.99	0.07	-4.64	45,45,45,45	0
34	SR	0	8984	1/1	0.92	0.04	-5.67	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8075	1/1	0.90	0.03	-5.85	46,46,46,46	0
34	SR	0	8970	1/1	0.95	0.03	-6.52	128,128,128,128	0
32	MG	0	8044	1/1	0.98	0.05	-6.72	53,53,53,53	0
32	MG	0	8013	1/1	0.99	0.03	-8.68	30,30,30,30	0
32	MG	0	8005	1/1	0.99	0.17	-	33,33,33,33	0
34	SR	0	8990	1/1	0.99	0.10	-	137,137,137,137	0
34	SR	0	8996	1/1	0.84	1.02	-	200,200,200,200	0
34	SR	9	8980	1/1	0.76	0.15	-	200,200,200,200	0
35	NA	0	8571	1/1	0.85	0.09	-	77,77,77,77	0
35	NA	0	8509	1/1	0.92	0.15	-	69,69,69,69	0
32	MG	0	8055	1/1	0.98	0.20	-	46,46,46,46	0
32	MG	0	8063	1/1	0.96	0.17	-	71,71,71,71	0
34	SR	0	8924	1/1	0.94	0.16	-	135,135,135,135	0
34	SR	0	8939	1/1	0.94	0.04	-	160,160,160,160	0
34	SR	0	8988	1/1	0.78	0.13	-	173,173,173,173	0
34	SR	0	8920	1/1	0.98	0.05	-	134,134,134,134	0
33	CL	0	8822	1/1	0.98	0.55	-	106,106,106,106	0
32	MG	0	8090	1/1	0.93	0.33	-	62,62,62,62	0
34	SR	0	8994	1/1	0.40	0.98	-	200,200,200,200	0
34	SR	0	8907	1/1	1.00	0.14	-	56,56,56,56	0
32	MG	0	8015	1/1	0.99	0.17	-	36,36,36,36	0
34	SR	0	8953	1/1	0.98	0.08	-	157,157,157,157	0
35	NA	0	8573	1/1	0.95	0.26	-	77,77,77,77	0
32	MG	0	8048	1/1	0.95	0.20	-	26,26,26,26	0
34	SR	0	8906	1/1	1.00	0.21	-	60,60,60,60	0
34	SR	0	8928	1/1	0.88	0.06	-	135,135,135,135	0
34	SR	0	8993	1/1	0.78	0.09	-	182,182,182,182	0
32	MG	9	8074	1/1	0.96	0.11	-	77,77,77,77	0
32	MG	0	8089	1/1	0.58	0.12	-	57,57,57,57	0
34	SR	0	8997	1/1	0.72	0.47	-	200,200,200,200	0
35	NA	0	8567	1/1	0.94	0.21	-	80,80,80,80	0
34	SR	0	8941	1/1	0.95	0.13	-	116,116,116,116	0
32	MG	0	8061	1/1	0.96	0.21	-	30,30,30,30	0
32	MG	0	8017	1/1	0.99	0.22	-	25,25,25,25	0
35	NA	0	8506	1/1	0.81	0.25	-	68,68,68,68	0
35	NA	S	8510	1/1	0.91	0.06	-	49,49,49,49	0
32	MG	0	8072	1/1	0.91	0.10	-	53,53,53,53	0
34	SR	3	8999	1/1	0.99	0.04	-	106,106,106,106	0
32	MG	0	8053	1/1	0.98	0.04	-	59,59,59,59	0
34	SR	0	9006	1/1	0.11	1.24	-	200,200,200,200	0
33	CL	R	8806	1/1	0.97	0.13	-	52,52,52,52	0
33	CL	0	8811	1/1	0.92	0.11	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	9002	1/1	0.97	0.08	-	184,184,184,184	0
35	NA	9	8543	1/1	0.96	0.18	-	49,49,49,49	0
34	SR	0	8926	1/1	0.98	0.10	-	127,127,127,127	0
34	SR	0	8979	1/1	0.90	0.20	-	198,198,198,198	0
35	NA	0	8549	1/1	0.97	0.28	-	58,58,58,58	0
32	MG	0	8046	1/1	0.97	0.13	-	41,41,41,41	0
34	SR	0	8964	1/1	0.98	0.10	-	139,139,139,139	0
35	NA	0	8554	1/1	0.97	0.89	-	78,78,78,78	0
34	SR	0	8911	1/1	0.97	0.08	-	85,85,85,85	0
35	NA	0	8505	1/1	0.80	1.03	-	49,49,49,49	0
33	CL	J	8802	1/1	0.97	0.09	-	76,76,76,76	0
34	SR	0	8960	1/1	0.92	0.05	-	150,150,150,150	0
35	NA	0	8536	1/1	0.94	0.08	-	65,65,65,65	0
32	MG	0	8081	1/1	0.85	0.19	-	74,74,74,74	0
32	MG	0	8091	1/1	0.77	0.06	-	62,62,62,62	0
34	SR	0	8956	1/1	0.94	0.09	-	155,155,155,155	0
34	SR	0	8983	1/1	0.91	0.45	-	195,195,195,195	0
35	NA	0	8570	1/1	0.71	0.13	-	60,60,60,60	0
34	SR	0	8914	1/1	1.00	0.27	-	110,110,110,110	0
34	SR	1	8952	1/1	0.99	0.13	-	91,91,91,91	0
34	SR	0	8973	1/1	0.98	0.07	-	137,137,137,137	0
34	SR	0	8931	1/1	0.98	0.09	-	117,117,117,117	0
33	CL	0	8817	1/1	0.99	0.10	-	65,65,65,65	0
32	MG	0	8037	1/1	0.74	0.33	-	90,90,90,90	0
35	NA	0	8560	1/1	0.78	0.37	-	83,83,83,83	0
35	NA	0	8566	1/1	0.93	0.25	-	60,60,60,60	0
34	SR	0	9008	1/1	0.99	0.14	-	89,89,89,89	0
34	SR	0	8989	1/1	0.92	0.13	-	185,185,185,185	0
32	MG	0	8069	1/1	0.99	0.17	-	72,72,72,72	0
35	NA	0	8526	1/1	0.96	0.05	-	57,57,57,57	0
32	MG	0	8026	1/1	0.98	0.07	-	37,37,37,37	0
34	SR	0	8995	1/1	0.96	0.17	-	140,140,140,140	0
32	MG	0	8022	1/1	0.99	0.11	-	32,32,32,32	0
34	SR	0	8963	1/1	0.97	0.04	-	134,134,134,134	0
34	SR	0	8966	1/1	0.94	0.08	-	111,111,111,111	0
32	MG	0	8035	1/1	0.94	0.14	-	68,68,68,68	0
35	NA	0	8516	1/1	0.96	0.12	-	42,42,42,42	0
32	MG	0	8082	1/1	0.90	0.28	-	69,69,69,69	0
32	MG	0	8030	1/1	0.98	0.48	-	69,69,69,69	0
35	NA	0	8501	1/1	0.98	0.22	-	44,44,44,44	0
34	SR	0	8922	1/1	0.42	0.22	-	170,170,170,170	0
34	SR	0	8927	1/1	0.87	0.06	-	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8059	1/1	0.91	0.06	-	59,59,59,59	0
32	MG	0	8064	1/1	0.96	0.15	-	37,37,37,37	0
34	SR	0	8958	1/1	0.92	0.11	-	123,123,123,123	0
35	NA	0	8518	1/1	0.71	0.47	-	94,94,94,94	0
35	NA	0	8548	1/1	0.90	0.16	-	55,55,55,55	0
34	SR	9	9003	1/1	0.97	0.01	-	170,170,170,170	0
34	SR	0	8965	1/1	0.98	0.05	-	124,124,124,124	0
34	SR	0	8991	1/1	0.58	0.09	-	197,197,197,197	0
35	NA	0	8561	1/1	0.91	0.50	-	78,78,78,78	0
35	NA	0	8531	1/1	0.94	0.11	-	44,44,44,44	0
32	MG	0	8049	1/1	0.98	0.38	-	68,68,68,68	0
34	SR	0	8998	1/1	0.89	0.13	-	175,175,175,175	0
33	CL	0	8814	1/1	0.98	0.10	-	60,60,60,60	0
32	MG	0	8038	1/1	0.93	0.10	-	75,75,75,75	0
32	MG	0	8020	1/1	0.98	0.13	-	43,43,43,43	0
34	SR	0	8954	1/1	0.97	0.12	-	112,112,112,112	0
33	CL	J	8801	1/1	0.96	0.17	-	79,79,79,79	0
33	CL	Y	8820	1/1	0.99	0.23	-	51,51,51,51	0
32	MG	0	8073	1/1	0.99	0.07	-	83,83,83,83	0
32	MG	0	8092	1/1	0.96	0.26	-	67,67,67,67	0
32	MG	0	8066	1/1	0.92	0.15	-	76,76,76,76	0
35	NA	0	8551	1/1	0.97	0.24	-	59,59,59,59	0
32	MG	0	8039	1/1	0.96	0.25	-	77,77,77,77	0
32	MG	0	8077	1/1	0.88	0.07	-	49,49,49,49	0
34	SR	0	8917	1/1	0.95	0.13	-	111,111,111,111	0
34	SR	0	9004	1/1	0.98	0.64	-	200,200,200,200	0
34	SR	0	8944	1/1	0.80	0.12	-	182,182,182,182	0
35	NA	0	8524	1/1	0.95	0.18	-	58,58,58,58	0
34	SR	0	9000	1/1	0.99	0.12	-	177,177,177,177	0
35	NA	0	8525	1/1	0.78	0.19	-	78,78,78,78	0
35	NA	0	8541	1/1	0.92	0.22	-	69,69,69,69	0
34	SR	0	8962	1/1	0.93	0.05	-	175,175,175,175	0
34	SR	0	8959	1/1	0.81	0.20	-	174,174,174,174	0
34	SR	0	8905	1/1	0.99	0.28	-	68,68,68,68	0
32	MG	0	8079	1/1	0.96	0.10	-	55,55,55,55	0
34	SR	0	8955	1/1	0.97	0.16	-	200,200,200,200	0
32	MG	0	8080	1/1	0.99	0.36	-	69,69,69,69	0
34	SR	0	8908	1/1	0.96	0.10	-	110,110,110,110	0
36	CD	O	8705	1/1	1.00	0.07	-	94,94,94,94	0
32	MG	0	8083	1/1	0.92	0.11	-	73,73,73,73	0
32	MG	0	8023	1/1	0.99	0.14	-	32,32,32,32	0
34	SR	0	8901	1/1	0.98	0.10	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8546	1/1	0.60	1.30	-	112,112,112,112	0
32	MG	0	8007	1/1	0.95	0.20	-	38,38,38,38	0
32	MG	0	8068	1/1	0.99	0.09	-	54,54,54,54	0
35	NA	0	8574	1/1	0.90	0.38	-	55,55,55,55	0
34	SR	0	8937	1/1	0.97	0.21	-	115,115,115,115	0
34	SR	0	8957	1/1	0.86	0.10	-	196,196,196,196	0
32	MG	0	8087	1/1	0.91	0.08	-	47,47,47,47	0
34	SR	0	8933	1/1	0.97	0.17	-	150,150,150,150	0
34	SR	0	8974	1/1	0.93	0.13	-	149,149,149,149	0
35	NA	0	8544	1/1	0.84	0.20	-	75,75,75,75	0
34	SR	0	8925	1/1	1.00	0.12	-	91,91,91,91	0
32	MG	0	8019	1/1	0.99	0.18	-	27,27,27,27	0
32	MG	0	8027	1/1	0.99	0.09	-	49,49,49,49	0
35	NA	0	8535	1/1	0.94	0.25	-	53,53,53,53	0
32	MG	0	8024	1/1	0.96	0.13	-	55,55,55,55	0
32	MG	0	8076	1/1	0.98	0.07	-	42,42,42,42	0
34	SR	0	8981	1/1	0.98	0.16	-	153,153,153,153	0
35	NA	0	8514	1/1	0.96	0.59	-	48,48,48,48	0
34	SR	0	8946	1/1	0.94	0.23	-	122,122,122,122	0
34	SR	0	8986	1/1	0.61	0.17	-	200,200,200,200	0
34	SR	0	8916	1/1	0.99	0.06	-	113,113,113,113	0
32	MG	0	8078	1/1	0.97	0.32	-	61,61,61,61	0
34	SR	0	8982	1/1	0.75	1.20	-	200,200,200,200	0
34	SR	0	8938	1/1	0.77	0.13	-	192,192,192,192	0
32	MG	0	8032	1/1	0.98	0.05	-	46,46,46,46	0
34	SR	A	8977	1/1	0.87	0.06	-	161,161,161,161	0
32	MG	0	8031	1/1	0.97	0.39	-	72,72,72,72	0
32	MG	0	8071	1/1	0.89	0.19	-	71,71,71,71	0
34	SR	0	8915	1/1	0.91	0.09	-	131,131,131,131	0
32	MG	0	8093	1/1	0.98	0.08	-	35,35,35,35	0
34	SR	0	8951	1/1	0.88	0.07	-	142,142,142,142	0
32	MG	0	8056	1/1	0.98	0.11	-	51,51,51,51	0
32	MG	0	8018	1/1	0.99	0.19	-	46,46,46,46	0
34	SR	0	8919	1/1	0.61	0.13	-	192,192,192,192	0
34	SR	S	8961	1/1	0.93	0.10	-	122,122,122,122	0
32	MG	0	8033	1/1	0.98	0.09	-	49,49,49,49	0
34	SR	0	9007	1/1	0.89	1.35	-	200,200,200,200	0
33	CL	A	8809	1/1	0.94	0.09	-	74,74,74,74	0
34	SR	0	8968	1/1	0.90	0.08	-	165,165,165,165	0
34	SR	0	8976	1/1	0.81	0.25	-	200,200,200,200	0
34	SR	0	8940	1/1	0.99	0.08	-	93,93,93,93	0
34	SR	0	8971	1/1	0.95	0.07	-	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	CL	0	8816	1/1	0.97	0.18	-	85,85,85,85	0
33	CL	N	8807	1/1	0.97	0.10	-	71,71,71,71	0
35	NA	0	8529	1/1	0.93	0.05	-	45,45,45,45	0
34	SR	0	8967	1/1	0.97	0.08	-	132,132,132,132	0
33	CL	0	8803	1/1	0.97	0.08	-	62,62,62,62	0
32	MG	0	8036	1/1	0.83	0.09	-	50,50,50,50	0
34	SR	0	9001	1/1	0.71	0.10	-	173,173,173,173	0
35	NA	0	8513	1/1	0.97	0.13	-	58,58,58,58	0
34	SR	B	8950	1/1	0.98	0.17	-	132,132,132,132	0
35	NA	0	8545	1/1	0.95	0.14	-	41,41,41,41	0
34	SR	0	8909	1/1	0.98	0.14	-	85,85,85,85	0
35	NA	0	8511	1/1	0.96	0.13	-	59,59,59,59	0
34	SR	0	8934	1/1	0.99	0.11	-	130,130,130,130	0
32	MG	0	8029	1/1	0.97	0.17	-	48,48,48,48	0
32	MG	0	8040	1/1	0.98	0.16	-	96,96,96,96	0
34	SR	0	8921	1/1	0.97	0.12	-	92,92,92,92	0
35	NA	0	8550	1/1	0.82	0.52	-	61,61,61,61	0
34	SR	0	8942	1/1	0.92	0.08	-	133,133,133,133	0
34	SR	0	8923	1/1	0.98	0.10	-	116,116,116,116	0

6.5 Other polymers

There are no such residues in this entry.