



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 08:24 PM GMT

PDB ID : 4WFA  
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with linezolid  
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.E.  
Deposited on : 2014-09-14  
Resolution : 3.39 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

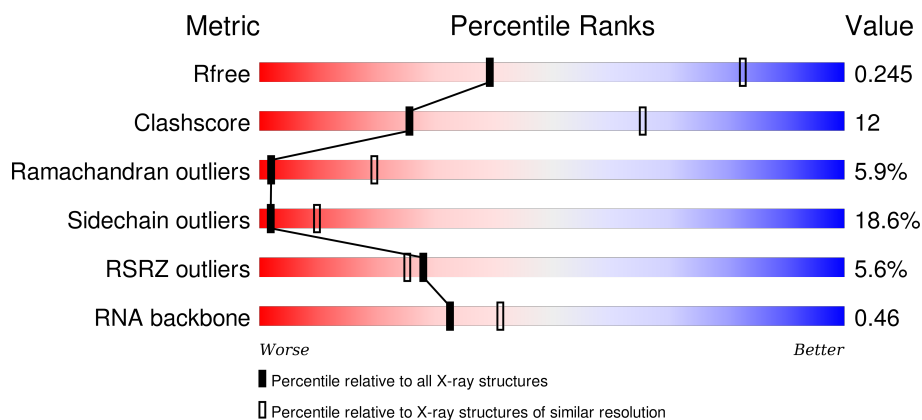
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.39 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)
RNA backbone	2183	1041 (4.00-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	X	2923	<div> <div>45%</div> <div>37%</div> <div>10%</div> <div>7%</div> </div>
2	Y	114	<div> <div>52%</div> <div>41%</div> <div>7%</div> </div>
3	A	277	<div> <div>21%</div> <div>61%</div> <div>30%</div> <div>6%</div> </div>
4	B	220	<div> <div>2%</div> <div>54%</div> <div>35%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	ZLD	X	3001	-	-	-	X
30	MPD	X	3003	-	-	-	X
30	MPD	X	3004	-	-	-	X
30	MPD	X	3006	-	-	-	X
30	MPD	X	3007	-	-	-	X
30	MPD	X	3008	-	-	-	X
30	MPD	X	3009	-	-	-	X
30	MPD	X	3010	-	-	-	X
31	MG	A	302	-	-	-	X
31	MG	X	3021	-	-	-	X
31	MG	X	3024	-	-	-	X
31	MG	X	3032	-	-	-	X
31	MG	X	3035	-	-	-	X
31	MG	X	3037	-	-	-	X
31	MG	X	3062	-	-	-	X
31	MG	X	3063	-	-	-	X
31	MG	X	3249	-	-	-	X
31	MG	X	3287	-	-	-	X
31	MG	X	3294	-	-	-	X
31	MG	X	3308	-	-	-	X
31	MG	X	3310	-	-	-	X
31	MG	X	3314	-	-	-	X
31	MG	X	3319	-	-	-	X
31	MG	X	3323	-	-	-	X
31	MG	X	3335	-	-	-	X
31	MG	X	3344	-	-	-	X
31	MG	X	3345	-	-	-	X
31	MG	X	3384	-	-	-	X
31	MG	X	3415	-	-	-	X
31	MG	X	3418	-	-	-	X
31	MG	X	3420	-	-	-	X
31	MG	X	3441	-	-	-	X
31	MG	Y	206	-	-	-	X
32	MN	X	3079	-	-	-	X
32	MN	X	3084	-	-	-	X
32	MN	X	3119	-	-	-	X
32	MN	X	3124	-	-	-	X
32	MN	X	3130	-	-	-	X
32	MN	X	3131	-	-	-	X
32	MN	X	3132	-	-	-	X
32	MN	X	3133	-	-	-	X
32	MN	X	3142	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MN	X	3143	-	-	-	X
32	MN	X	3146	-	-	-	X
32	MN	X	3147	-	-	-	X
32	MN	X	3148	-	-	-	X
32	MN	X	3150	-	-	-	X
32	MN	X	3151	-	-	-	X
32	MN	X	3152	-	-	-	X
32	MN	X	3153	-	-	-	X
32	MN	X	3154	-	-	-	X
32	MN	X	3157	-	-	-	X
32	MN	X	3159	-	-	-	X
32	MN	X	3161	-	-	-	X
32	MN	X	3162	-	-	-	X
32	MN	X	3168	-	-	-	X
32	MN	X	3172	-	-	-	X
32	MN	X	3176	-	-	-	X
32	MN	X	3184	-	-	-	X
32	MN	X	3187	-	-	-	X
32	MN	X	3195	-	-	-	X
32	MN	X	3199	-	-	-	X
32	MN	X	3215	-	-	-	X
32	MN	X	3220	-	-	-	X
32	MN	X	3221	-	-	-	X
32	MN	X	3223	-	-	-	X
32	MN	X	3224	-	-	-	X
32	MN	X	3227	-	-	-	X
32	MN	X	3231	-	-	-	X
32	MN	X	3239	-	-	-	X
32	MN	X	3240	-	-	-	X
32	MN	X	3442	-	-	-	X
34	EPE	X	3423	-	-	-	X
34	EPE	X	3424	-	-	-	X
34	EPE	X	3425	-	-	-	X
34	EPE	X	3426	-	-	X	X
35	SPD	J	201	-	-	-	X
35	SPD	X	3427	-	-	-	X
35	SPD	X	3428	-	-	-	X
35	SPD	X	3429	-	-	-	X
35	SPD	X	3431	-	-	-	X
35	SPD	X	3432	-	-	-	X
35	SPD	X	3433	-	-	-	X
35	SPD	X	3434	-	-	-	X

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 81465 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2711	Total	C	N	O	P	0	0	0
			58151	25961	10662	18817	2711			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	268	Total	C	N	O	S	0	0	0
			1620	985	315	316	4			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1531	957	283	286	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1321	818	253	248	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	155	Total	C	N	O	S	0	0	0
			794	478	155	160	1			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			926	567	172	186	1			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1087	679	202	203	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			840	517	163	157	3			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			817	500	164	152	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1003	642	185	173	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			896	551	176	168	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	108	Total	C	N	O	0	0	0
			659	399	134	126			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O			
			809	513	158	138	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	188	153	4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	101	Total	C	N	O	S			
			751	477	137	136	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	88	Total	C	N	O	S			
			586	363	108	113	2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			680	425	121	133	1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1048	656	187	203	2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			530	328	100	102			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	44	Total	C	N	O	0	0	0
			254	154	52	48			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			414	261	74	79			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O	0	0	0
			441	274	83	84			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	44	Total	C	N	O	S	0	0	0
			336	208	70	55	3			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			368	225	89	53	1			

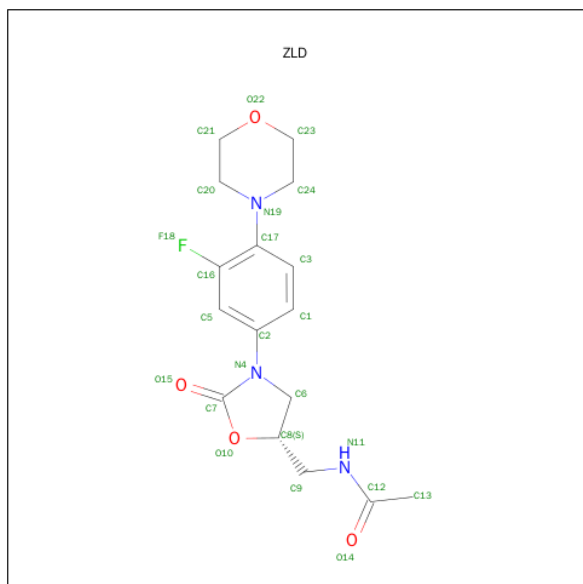
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			414	256	83	73	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

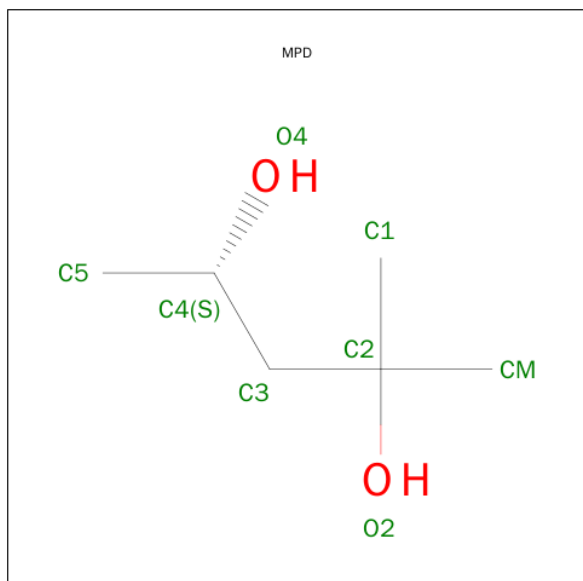
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			262	164	52	41	5			

- Molecule 29 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (three-letter code: ZLD) (formula:  $C_{16}H_{20}FN_3O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	X	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

- Molecule 30 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0
30	X	1	Total C O 8 6 2	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	G	2	Total Mg 2 2	0	0
31	K	1	Total Mg 1 1	0	0
31	B	1	Total Mg 1 1	0	0
31	I	1	Total Mg 1 1	0	0
31	C	1	Total Mg 1 1	0	0
31	W	1	Total Mg 1 1	0	0
31	Z	2	Total Mg 2 2	0	0
31	A	2	Total Mg 2 2	0	0
31	N	1	Total Mg 1 1	0	0
31	X	226	Total Mg 226 226	0	0
31	O	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	Y	6	Total 6	Mg 6	0	0

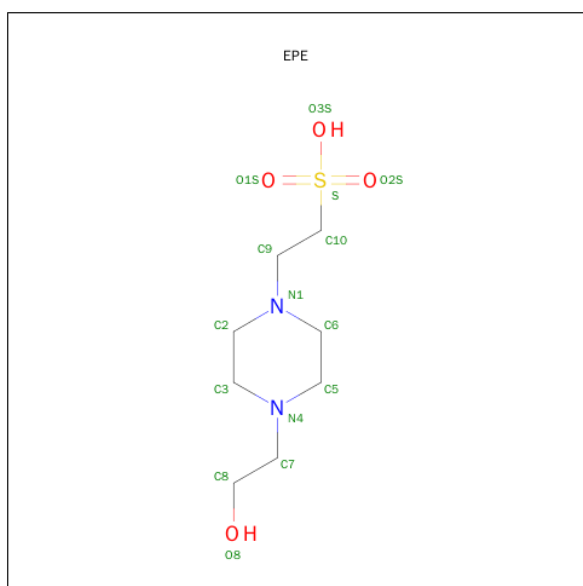
- Molecule 32 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	191	Total 191	Mn 191	0	0
32	Z	1	Total 1	Mn 1	0	0
32	Y	2	Total 2	Mn 2	0	0
32	M	1	Total 1	Mn 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

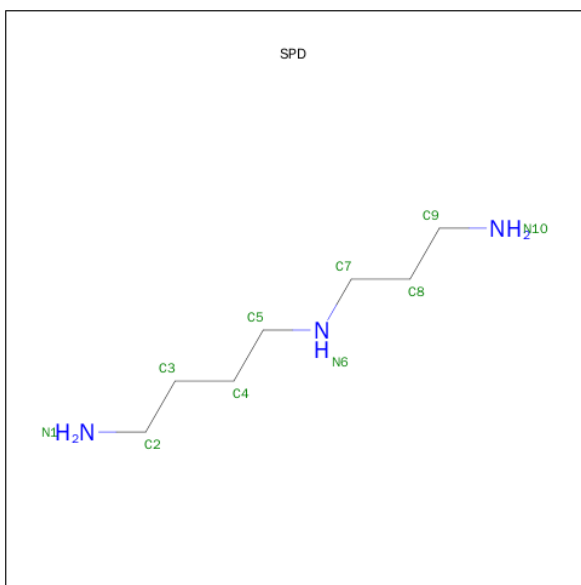
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total 1	Na 1	0	0

- Molecule 34 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
34	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 35 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



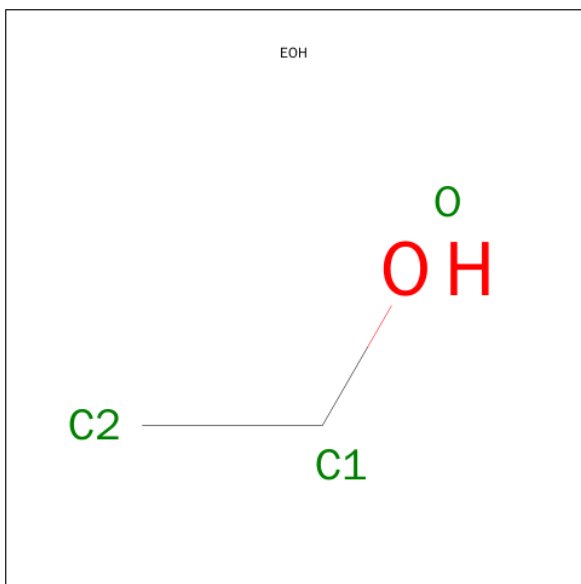
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		
35	X	1	Total	C	N	0	0
			10	7	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	J	1	Total	C	N	0	0
			10	7	3		

- Molecule 36 is ETHANOL (three-letter code: EOH) (formula: C<sub>2</sub>H<sub>6</sub>O).

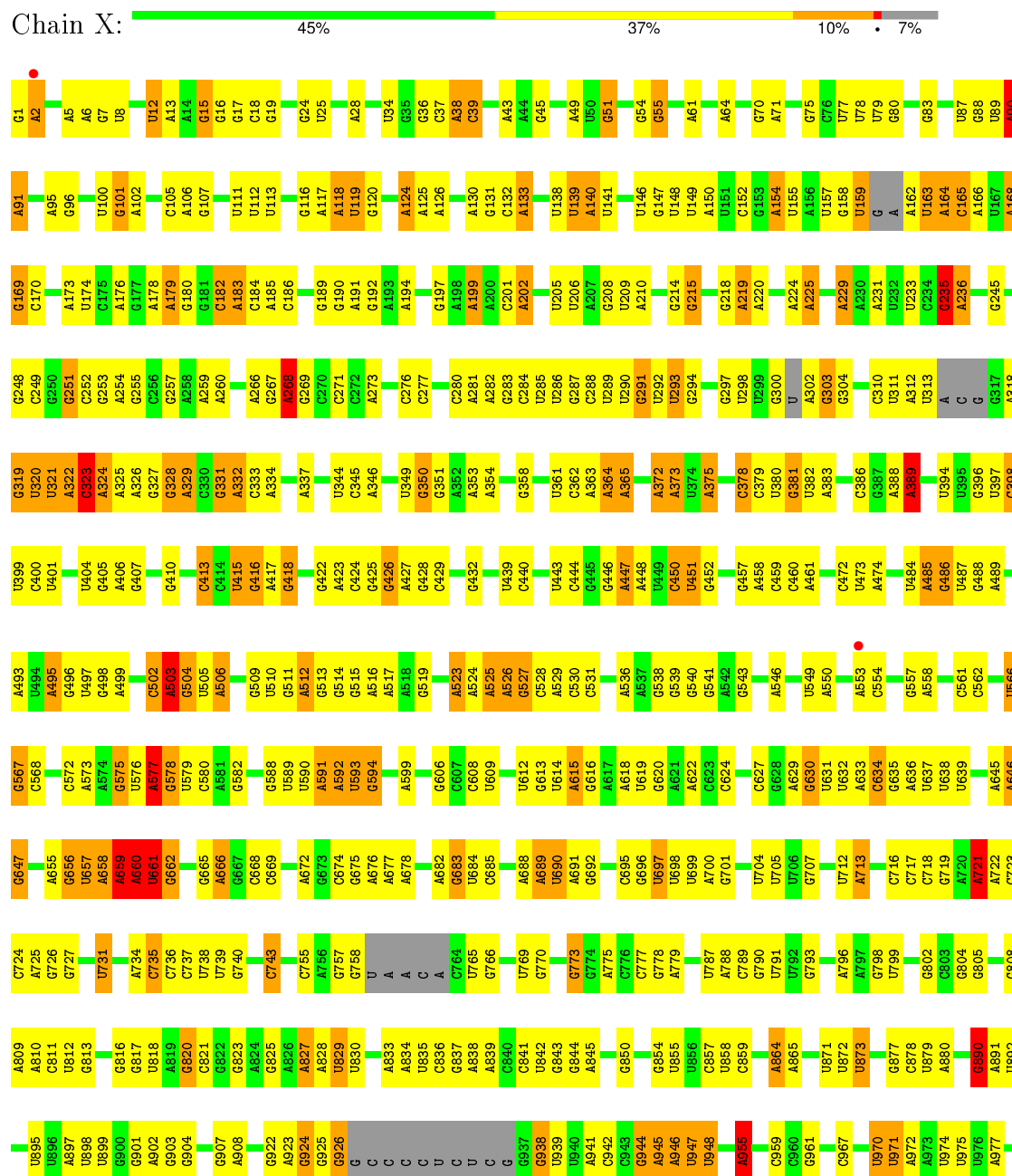


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	X	1	Total	C	O	0	0
			3	2	1		
36	Y	1	Total	C	O	0	0
			3	2	1		

### 3 Residue-property plots

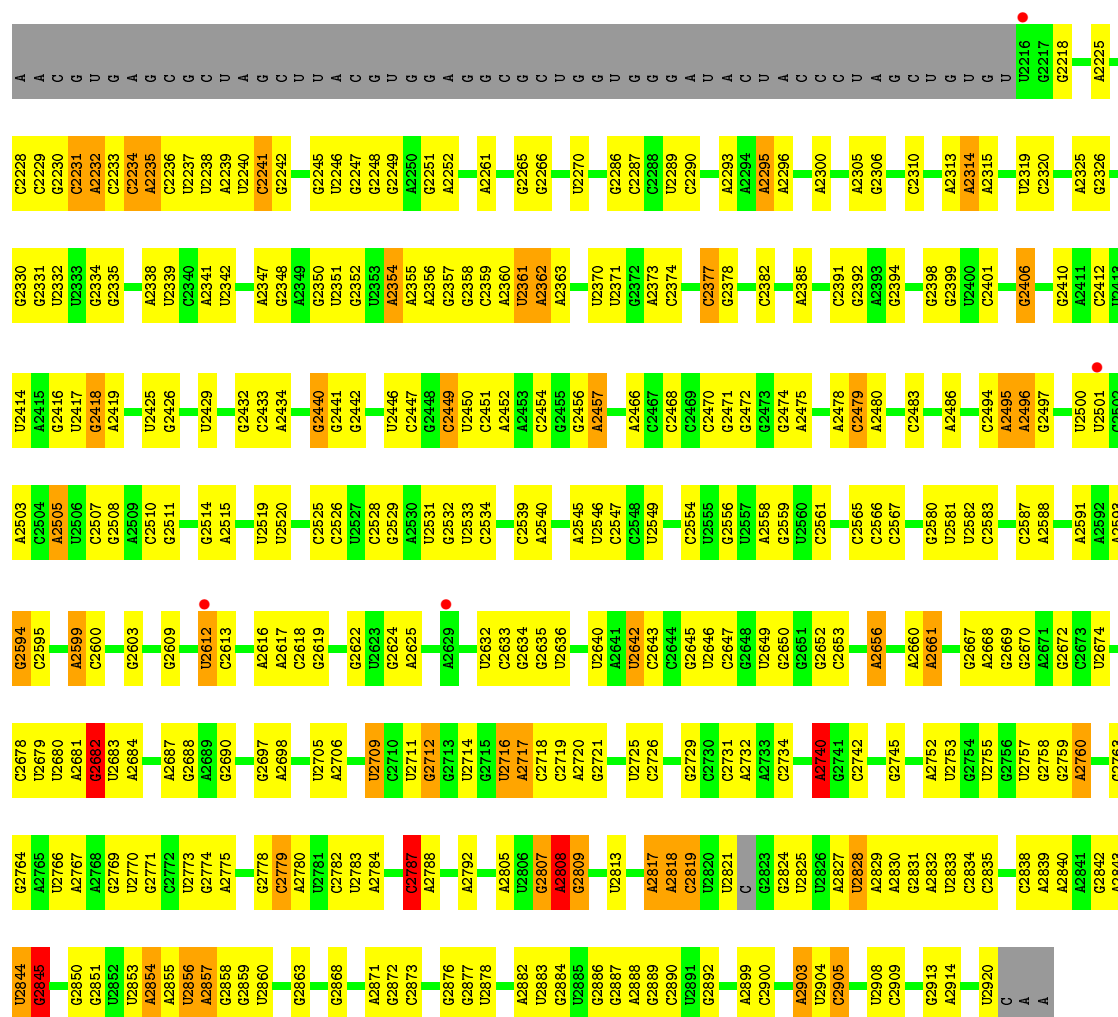
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: 23S rRNA



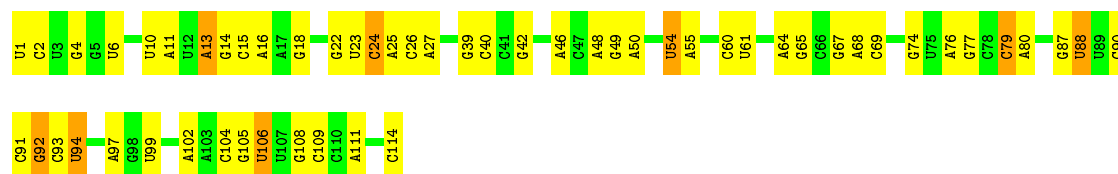
A2089	C2001	A1912	G1838	G1761	U1683	U1594	A	G1469	C1399	G1314	G1226	A	A1072	G982
G2094	A2005	C1922	G1839	U1762	A1684	C1595	G	G1470	C1400	C1315	G1227	U	U1077	G983
U2095	C2006	A1923	U1840	U1763	U1764	G1596	G	A1471	G1316	G1316	U1227	A	U1078	G984
G2096	G2007	U1923	G1841	A1764	A1690	U1597	C	C1472	A1402	G1317	G1228	G	U1079	A985
G2097	A2008	U1925	U1943	A1765	G1691	U1598	A1537	G1473	G1405	G1322	G1229	U1145	U987	G986
A2098	U2009	A1926	U1944	G1766	C1692	G1599	A1538	C1474	G1405	G1322	G1230	U1146	C1082	G988
G2099			G1844	G1767		A1600	A1539	A1475	G1411	C1328	C1235			A989
	G2013		U1845	C1768		U1601	U1540	G1476	G1412	G1329	U1238	A1150	U1085	G990
U2102			A1846	C1769		U1602	C1541	A1477		G1330	C1239	G1151	G1086	
C2105	C2017	G1930	U1847	C1770	A1696	U1603	G1542		A1415	C1331	U1240	U1152	C1087	G1000
U2106	U2018	G1931	A1948	A1771	C1694	U1604	G1543	A1481	A1415	C1331	U1241	G1153	C1088	A1001
	G2019	G1932	G1949	A1699	A1605	A1605	G1544	U1482	U1416	C1332	A1241	G1154	C1089	
	U2020	G1933	G1850	C1700	U1609	U1609	U1545	A1483	G1417	C1335	G1242	A1155	A1090	G1005
C2112		G1934	G1851	U1701	U1610	G1610	A1546	G1487	G1418	C1336	G1247	U1156	G1091	
	C2023	C1935		U1776	G1702	G1611	C1547	A1488	A1421	G1337	U1248	U1157	A1092	C1008
U2116	A2024	G	U1854	G1780	U1703	G1613	C1549	A	A1422	A1337	U1249	G1158	C1093	U1013
A2117	A2025	U	G1855	C1781	G1710	A1614	G	G1490	A1423	U1338	G1250	A1161	U1098	U1014
U2118	C2026	A	A1856	A1782	G1711	G1615	U	C1491	A1424				G1099	G1016
U2119		A	G1862	G1783	A1712	A1616	U	A1492	G1425	G1346			A	A1017
	G2037	C			A1713	A1617	A	U1493					U	A1018
A2123	U2038	U	C1865	A1787	G1718	A1618	A	G1494	G1429	U1349	A1267	C1168	U	G1022
U2124	G2039	A	G	U1788	C1719	A1619	G1555	C1495	A1430	U1350	A1268	U1176	G	A1023
U2125	A2040	U	G1867	A1789	A1720	G1620	G1556	G1496	U1431	C1352	U1272	G1175	U	
C2126		A	U1868	G1790	A1721	G1621	C1557	A1497	A1432	A1353	G1273	U1174	U	
G	U2043	A	G1869	G1791	A1722	G1622	U1558	U1498	U1433	G1354	G1274	G1176	G	C1026
G	C2044	C		C1792	A1723	C1624	G1559	U1499	U1434	A1355	A1275	A1177	U	A1027
C	A2047	G	A1874	U1724	G1725	U1625	G1560	G1500	C1435	G1356	G1276	C1178	C	G1028
A	G2048	U	G	U1726	G1726	A1626	G1562	A1502	U1437	A1358	G1277	G1179	U	C1029
C	U2049	C	G1876	U1806	A1726	G1627	U1563	U	G1438	A1359	G1278	G1180	U	C1030
G	A2050	C	G1877	U1807		A1828	U1564	U1504	U1439		G1279		A	C1031
C	C2051	U	G1882	U1808	U1732	A1829	G1565	G1505	A1440	C1362	U1280	G1183	G	A1032
U	U2052	A	A1883	C1809	A1733	G1630	G1566	C1506	C1441	U1366	U1281	U1184	A	
U	G2053	A	G1884	A1810	A1734	G1631	A1567	A1507			A1282	U1185	A	
G	A2054	U	G1885	A1811	C1735	A1632	U1568	C1508	C1444	G1370	A1285	A1186	G	A1037
U		C	A1886	A1812	U1736	A	G1569	G1509	G1445	U1371	G1286	A1187	C	C1038
A	A2057	A	G1887	A1813	U1737	A	G1570	U1510	U1446	U1372	U1287		A	C1039
C	A2058	C	U1888	C1738	C1738	A1635	G1571	U1511	A1447	G1373	G1288	A1192	C	A1040
A	G2059	A	G1889	A1814	A1739	U1636		U1512	U1448	U1374	A1289	A1195	C	A1044
G	A2060	G	G1890	C1815	G1740	A1637	A1575	A1513	A1450	G1375	G1290	C1196	A	A1045
U	U2061	U	U1891	A1818	G1741	G1638	A1576	A1515	U1451	G1376	A1291	C1197	U	G1046
A	G2062	U	U1892				G1577	C1516	C1452	U1377	A1292	G1198	C	G1047
U		C	U1893	U1821	A1744	C1642	A1578	A1517	G1453	U1378	U1293	A1199	A	
A	C2070	U	U1896	C1822	A1745	G1643	C	U1518	U1454	A1379	G1294	A1200	U	A1053
G	C2071	G	U	U1823	G1746	C1644	A	U1519	U				U	A1054
G	C2072	C	U	C1824	G1747	C1644	C	U1519	U				U	A1055
U		U	U	U1825	G1748	C1651	U	A	U	G1382	G1300	G1211	U	A1056
A	G2075	A	U	G1826	U1749	A1652	U	A1521	U	G1383	U1301	U1212	U	A1057
G	A2076	C	G1900	C1827	U1750	A1653	G	G1522	A		G1302	C1213	A	
G	C2077	G	C1901	U1828	G1751	A1654		G1523	A1459	U1389	A1303	C1214	A	
A		A	A1902	A1829	C1752		G	G1524	U1460	A1390	U1304	U	G	U1063
G	A2078	C	A1903	U1753	C1754	G1657	C	U1525	C1461	A1391	G1305	C1215	A	A1064
U	G2079	U	U1893	A1831	C1754	A1658	U	G1526	G1462	G1392	A1306	U1217	G	A1065
C	G2080	C	C1906	C1832	U1755	C1659	U	A1527	U1463	G1393	G1309	G1218	U	G1066
U	A2081	U	U1907	C1833	U1756	A1660	U	G1528	A1464	C1394	G1309	G1219	G	U1067
U	C2082	U	U1907	C1833	U1756	A1660	U	G1528	U1464	C1394	G1309	G1219	G	G1068
U	G2083	U	A1908	G1834	U1757	C1661	C	U1529	G1465	A1395	A1310	A1220	C	G1069
U		U	C1909	U1835	A1758	A1662		U1530	G1466	A1396	A1311	C1221	G	
G	A2087	G	G1910	A1836	G1759	A1663	G1591	U	G1467	G1397	A1312	A1222	U	A1070
A	G2088	A	A1911	A1837	G1760	G1663	G1593	U	G1468	G1398	G1313	A1223	A	A1071





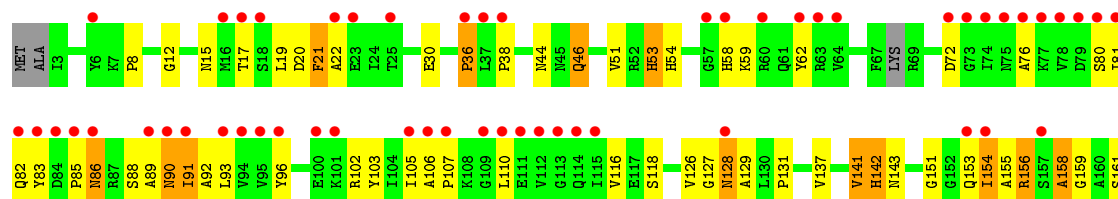
## • Molecule 2: 5S rRNA

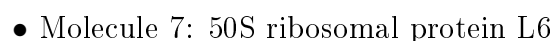
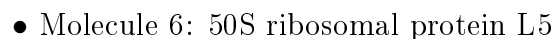
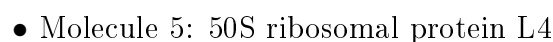
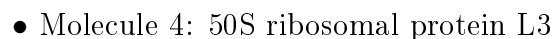
Chain Y: 52% 41% 7%



## • Molecule 3: 50S ribosomal protein L2

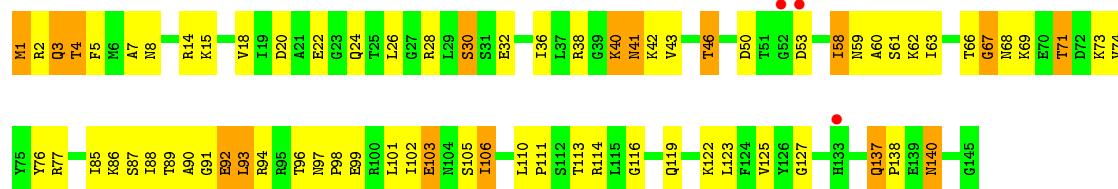
Chain A: 21% 61% 30% 6%



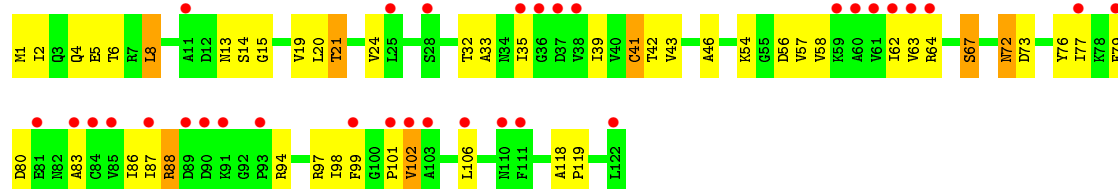




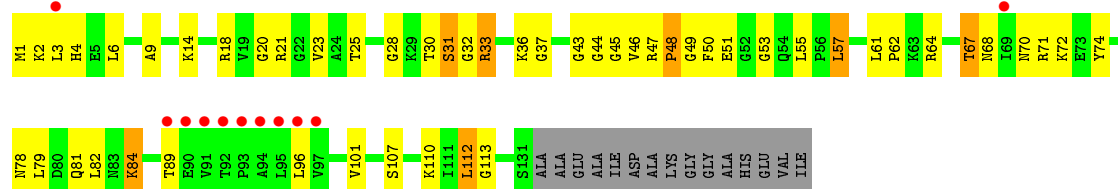
• Molecule 8: 50S ribosomal protein L13



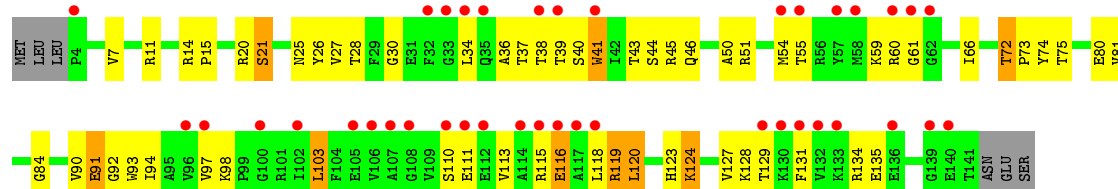
• Molecule 9: 50S ribosomal protein L14



• Molecule 10: 50S ribosomal protein L15

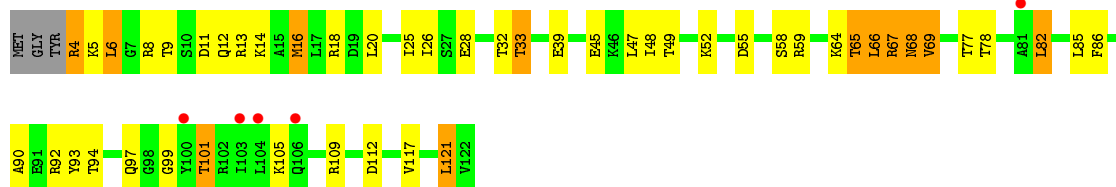


• Molecule 11: 50S ribosomal protein L16

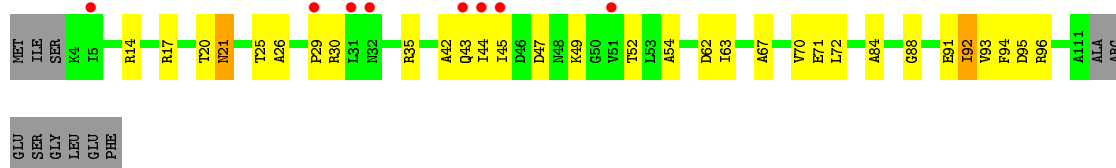


• Molecule 12: 50S ribosomal protein L17

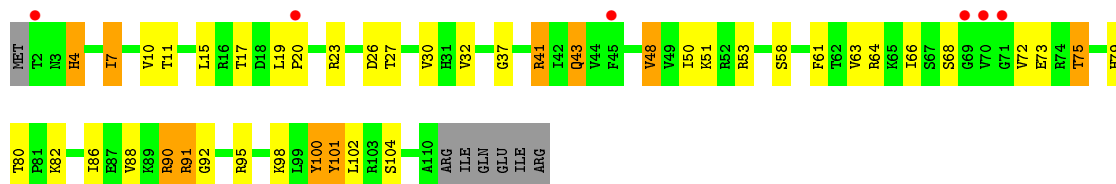




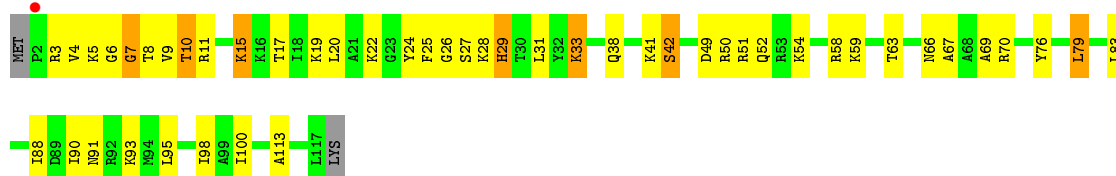
• Molecule 13: 50S ribosomal protein L18



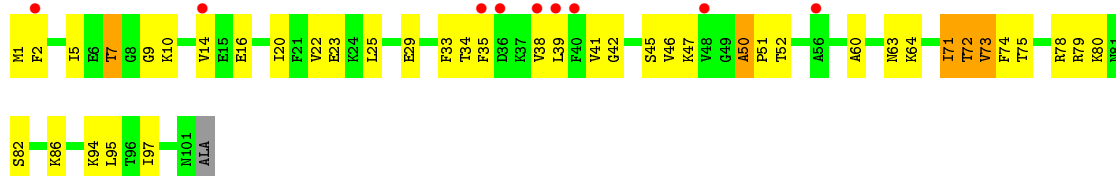
• Molecule 14: 50S ribosomal protein L19



• Molecule 15: 50S ribosomal protein L20

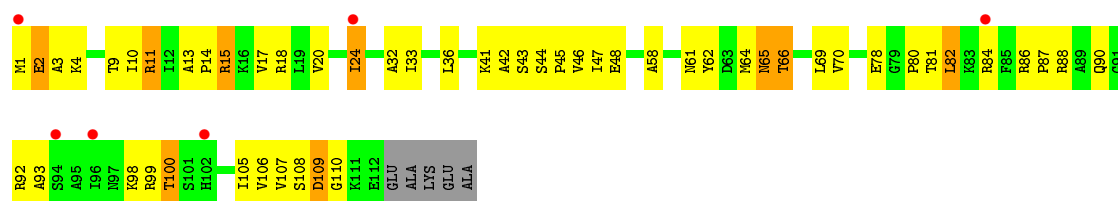


• Molecule 16: 50S ribosomal protein L21

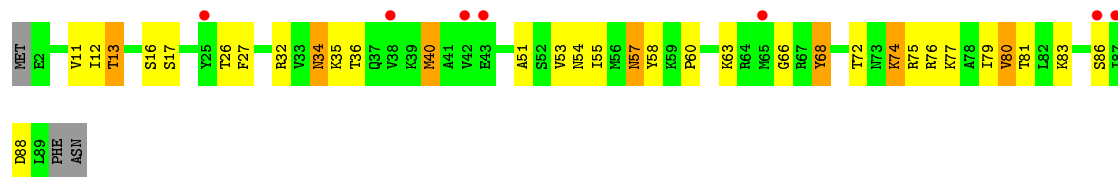


• Molecule 17: 50S ribosomal protein L22

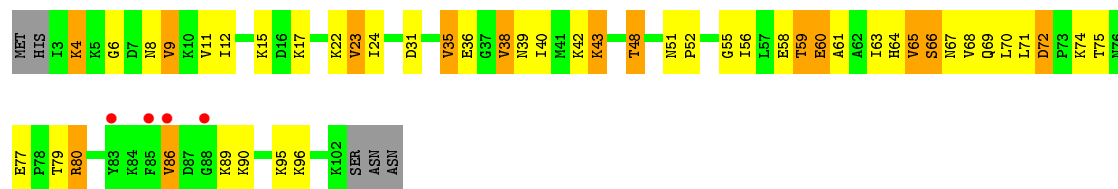




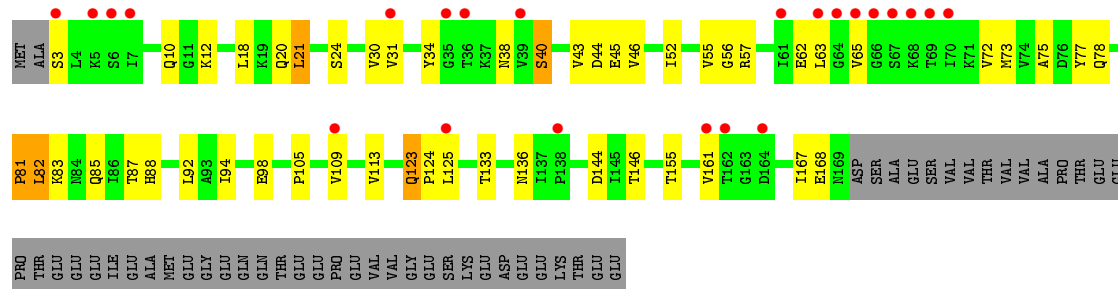
• Molecule 18: 50S ribosomal protein L23



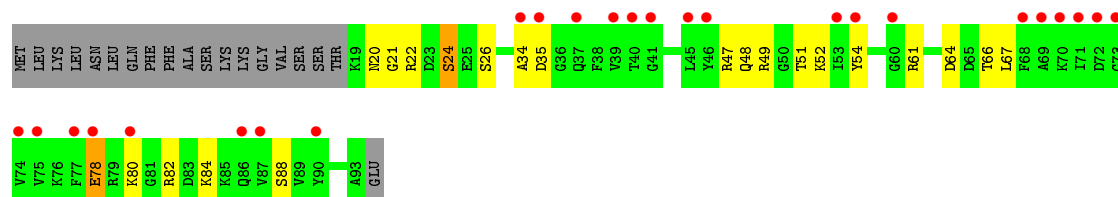
• Molecule 19: 50S ribosomal protein L24



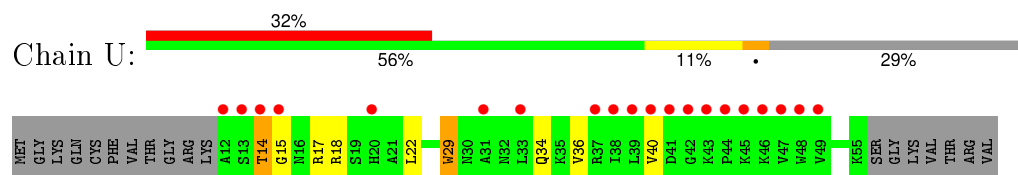
• Molecule 20: 50S ribosomal protein L25



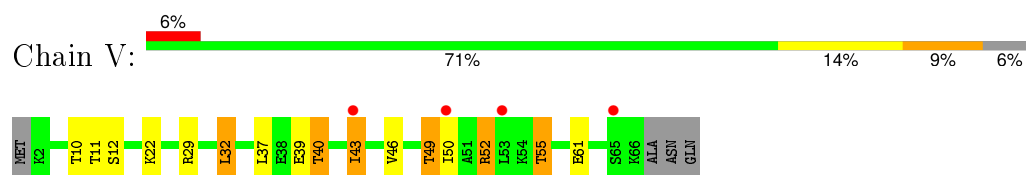
• Molecule 21: 50S ribosomal protein L27



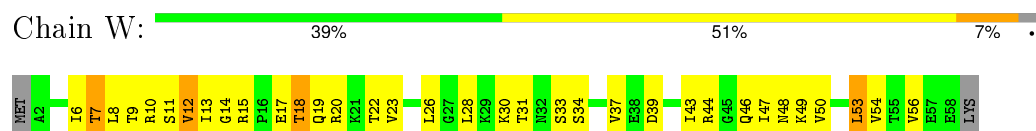
- Molecule 22: 50S ribosomal protein L28



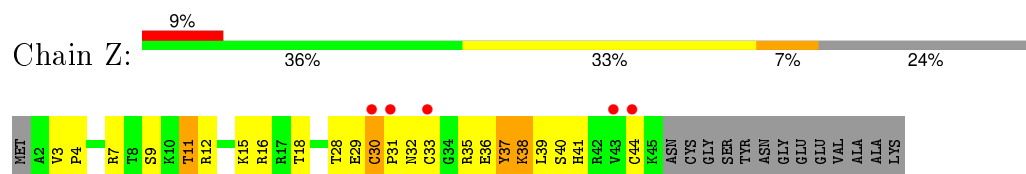
- Molecule 23: 50S ribosomal protein L29



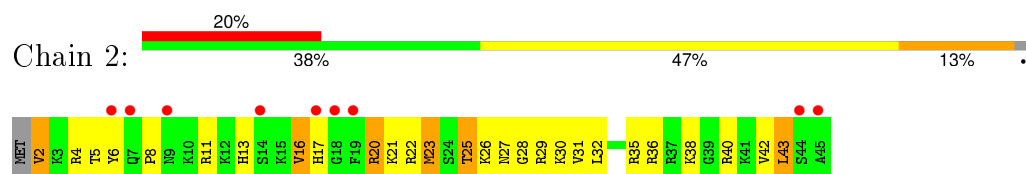
- Molecule 24: 50S ribosomal protein L30



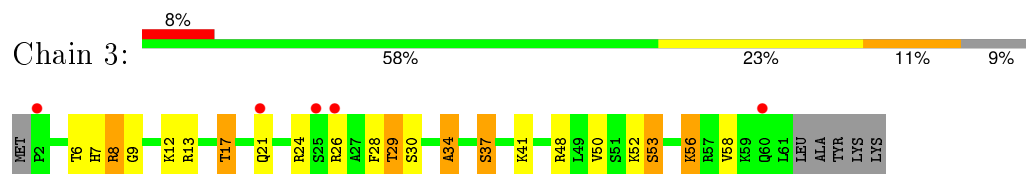
- Molecule 25: 50S ribosomal protein L32



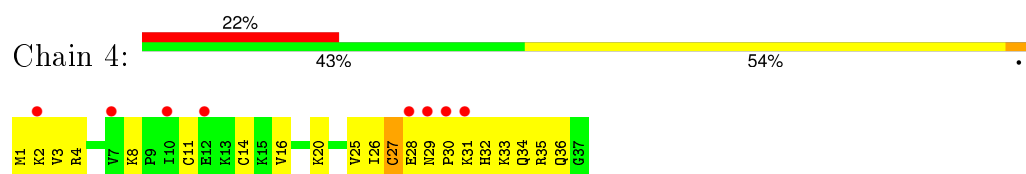
- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.92Å 279.92Å 870.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.88 – 3.39 100.73 – 3.39	Depositor EDS
% Data completeness (in resolution range)	88.9 (64.88-3.39) 88.9 (100.73-3.39)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.202 , 0.243 0.205 , 0.245	Depositor DCC
$R_{free}$ test set	12433 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	109.3	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 88.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 245649 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	81465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

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

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

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZLD, MG, MN, NA, EOH, MPD, EPE, SPD

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	X	0.53	7/65113 (0.0%)	1.03	150/101510 (0.1%)
2	Y	0.50	0/2717	1.03	10/4232 (0.2%)
3	A	0.36	0/1652	0.67	0/2280
4	B	0.49	0/1554	0.76	0/2101
5	C	0.49	0/1339	0.76	0/1832
6	D	0.27	0/796	0.54	0/1104
7	E	0.36	0/937	0.64	0/1296
8	G	0.45	0/1109	0.69	0/1504
9	H	0.47	0/847	0.68	0/1150
10	I	0.56	0/825	0.90	1/1119 (0.1%)
11	J	0.47	0/1026	0.70	0/1390
12	K	0.44	0/899	0.71	0/1204
13	L	0.36	0/664	0.67	0/907
14	M	0.43	0/821	0.71	0/1110
15	N	0.53	0/944	0.73	0/1252
16	O	0.47	0/761	0.73	0/1022
17	P	0.48	0/870	0.69	0/1171
18	Q	0.35	0/591	0.60	0/809
19	R	0.36	0/686	0.63	0/934
20	S	0.45	0/1060	0.71	2/1461 (0.1%)
21	T	0.42	0/536	0.64	0/720
22	U	0.30	0/257	0.59	0/356
23	V	0.35	0/415	0.55	0/569
24	W	0.44	0/443	0.66	0/597
25	Z	0.57	0/342	0.89	0/457
26	2	0.41	0/372	0.63	0/487
27	3	0.50	0/418	0.80	0/558
28	4	0.37	0/265	0.58	0/356
All	All	0.51	7/88259 (0.0%)	0.97	163/133488 (0.1%)

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
3	A	0	1
4	B	0	1
9	H	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	577	A	N9-C4	-8.16	1.32	1.37
1	X	1065	A	N9-C4	-7.99	1.33	1.37
1	X	577	A	C5-C6	-6.29	1.35	1.41
1	X	350	G	N9-C4	5.82	1.42	1.38
1	X	2845	G	N9-C4	-5.62	1.33	1.38

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	577	A	N1-C6-N6	13.04	126.42	118.60
1	X	577	A	C2-N3-C4	-11.54	104.83	110.60
1	X	2845	G	N3-C4-N9	-11.21	119.27	126.00
1	X	2845	G	N3-C4-C5	11.11	134.15	128.60
1	X	2048	G	C4-C5-N7	10.77	115.11	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	128	ASN	Peptide
4	B	166	GLY	Peptide
9	H	83	ALA	Peptide

## 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	X	58151	0	29248	918	0
2	Y	2430	0	1229	37	0
3	A	1620	0	1213	57	0
4	B	1531	0	1483	66	0
5	C	1321	0	1184	54	0
6	D	794	0	415	4	0
7	E	926	0	656	18	0
8	G	1087	0	1022	47	0
9	H	840	0	802	35	0
10	I	817	0	688	27	0
11	J	1003	0	970	44	0
12	K	896	0	921	35	0
13	L	659	0	505	17	0
14	M	809	0	811	23	0
15	N	932	0	997	45	0
16	O	751	0	744	24	0
17	P	862	0	920	45	0
18	Q	586	0	493	24	0
19	R	680	0	650	32	0
20	S	1048	0	847	15	0
21	T	530	0	494	19	0
22	U	254	0	165	4	0
23	V	414	0	354	9	0
24	W	441	0	478	20	0
25	Z	336	0	340	22	0
26	2	368	0	409	20	0
27	3	414	0	392	12	0
28	4	262	0	266	19	0
29	X	24	0	20	5	0
30	X	72	0	126	5	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	G	2	0	0	0	0
31	I	1	0	0	0	0
31	K	1	0	0	0	0
31	N	1	0	0	0	0
31	O	2	0	0	0	0
31	W	1	0	0	0	0
31	X	226	0	0	0	0
31	Y	6	0	0	0	0
31	Z	2	0	0	0	0
32	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	191	0	0	0	0
32	Y	2	0	0	0	0
32	Z	1	0	0	0	0
33	X	1	0	0	0	0
34	X	60	0	68	20	0
35	J	10	0	19	0	0
35	X	80	0	152	11	0
36	X	12	0	24	0	0
36	Y	3	0	6	0	0
All	All	81465	0	49111	1518	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 12.

The worst 5 of 1518 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)
3:A:116:VAL:HG11	3:A:127:GLY:HA3	1.41	0.97
34:X:3426:EPE:H52	15:N:7:GLY:HA2	1.50	0.94
1:X:1521:A:N6	1:X:1560:A:N3	2.17	0.93
1:X:1247:G:O2'	1:X:1275:A:N6	2.02	0.92
5:C:17:ILE:HD11	5:C:124:THR:HG21	1.56	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	
3	A	266/277 (96%)	208 (78%)	35 (13%)	23 (9%)	1	10
4	B	213/220 (97%)	183 (86%)	17 (8%)	13 (6%)	2	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	197/207 (95%)	162 (82%)	18 (9%)	17 (9%)	1	10
6	D	151/179 (84%)	118 (78%)	20 (13%)	13 (9%)	1	10
7	E	155/178 (87%)	109 (70%)	30 (19%)	16 (10%)	1	7
8	G	143/145 (99%)	122 (85%)	12 (8%)	9 (6%)	2	18
9	H	120/122 (98%)	109 (91%)	10 (8%)	1 (1%)	24	67
10	I	129/146 (88%)	91 (70%)	23 (18%)	15 (12%)	0	5
11	J	136/144 (94%)	119 (88%)	11 (8%)	6 (4%)	3	28
12	K	117/122 (96%)	106 (91%)	5 (4%)	6 (5%)	2	24
13	L	106/119 (89%)	82 (77%)	15 (14%)	9 (8%)	1	11
14	M	107/116 (92%)	95 (89%)	9 (8%)	3 (3%)	6	41
15	N	114/118 (97%)	110 (96%)	3 (3%)	1 (1%)	21	65
16	O	99/102 (97%)	86 (87%)	8 (8%)	5 (5%)	2	24
17	P	110/117 (94%)	106 (96%)	4 (4%)	0	100	100
18	Q	86/91 (94%)	75 (87%)	9 (10%)	2 (2%)	8	45
19	R	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	2	18
20	S	165/217 (76%)	130 (79%)	25 (15%)	10 (6%)	2	18
21	T	73/94 (78%)	67 (92%)	5 (7%)	1 (1%)	14	55
22	U	42/62 (68%)	32 (76%)	6 (14%)	4 (10%)	1	8
23	V	63/69 (91%)	52 (82%)	10 (16%)	1 (2%)	12	53
24	W	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
25	Z	42/58 (72%)	36 (86%)	2 (5%)	4 (10%)	1	8
26	2	42/45 (93%)	36 (86%)	5 (12%)	1 (2%)	7	44
27	3	58/66 (88%)	47 (81%)	7 (12%)	4 (7%)	1	15
28	4	35/37 (95%)	30 (86%)	3 (9%)	2 (6%)	2	20
All	All	2922/3215 (91%)	2440 (84%)	310 (11%)	172 (6%)	2	19

5 of 172 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	141	VAL
3	A	154	ILE
3	A	192	ILE
4	B	60	LYS
4	B	61	LYS

### 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	
3	A	102/224 (46%)	84 (82%)	18 (18%)	2	12
4	B	148/177 (84%)	115 (78%)	33 (22%)	1	5
5	C	107/169 (63%)	84 (78%)	23 (22%)	1	6
6	D	13/158 (8%)	11 (85%)	2 (15%)	3	18
7	E	53/155 (34%)	47 (89%)	6 (11%)	7	32
8	G	105/123 (85%)	87 (83%)	18 (17%)	2	14
9	H	77/100 (77%)	66 (86%)	11 (14%)	4	22
10	I	54/112 (48%)	40 (74%)	14 (26%)	0	3
11	J	91/119 (76%)	75 (82%)	16 (18%)	2	12
12	K	88/102 (86%)	73 (83%)	15 (17%)	2	14
13	L	35/95 (37%)	33 (94%)	2 (6%)	25	65
14	M	78/102 (76%)	58 (74%)	20 (26%)	0	3
15	N	93/98 (95%)	80 (86%)	13 (14%)	4	23
16	O	72/86 (84%)	64 (89%)	8 (11%)	8	33
17	P	91/94 (97%)	78 (86%)	13 (14%)	4	22
18	Q	44/82 (54%)	35 (80%)	9 (20%)	1	7
19	R	64/90 (71%)	45 (70%)	19 (30%)	0	2
20	S	75/190 (40%)	56 (75%)	19 (25%)	1	3
21	T	47/75 (63%)	42 (89%)	5 (11%)	8	36
22	U	10/52 (19%)	8 (80%)	2 (20%)	1	8
23	V	30/62 (48%)	22 (73%)	8 (27%)	0	3
24	W	51/53 (96%)	41 (80%)	10 (20%)	1	8
25	Z	35/51 (69%)	30 (86%)	5 (14%)	4	22
26	2	38/40 (95%)	29 (76%)	9 (24%)	1	4
27	3	35/57 (61%)	25 (71%)	10 (29%)	0	2
28	4	27/35 (77%)	26 (96%)	1 (4%)	41	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1663/2701 (62%)	1354 (81%)	309 (19%)	<b>2</b> <b>10</b>

5 of 309 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	120	LEU
14	M	73	GLU
25	Z	11	THR
12	K	8	ARG
13	L	21	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
24	W	40	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	33 (1%)
2	Y	113/114 (99%)	14 (12%)	0
All	All	2804/3037 (92%)	641 (22%)	33 (1%)

5 of 641 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	15	G
1	X	34	U
1	X	36	G
1	X	39	C

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1311	A
1	X	1510	U
1	X	2778	G
1	X	1432	A
1	X	1466	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 470 ligands modelled in this entry, 442 are monoatomic - leaving 28 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
35	SPD	J	201	-	9,9,9	0.18	0	8,8,8	0.20	0
29	ZLD	X	3001	-	26,26,26	1.05	1 (3%)	36,36,36	1.42	7 (19%)
30	MPD	X	3002	-	6,7,7	0.28	0	6,10,10	0.13	0
30	MPD	X	3003	-	6,7,7	0.45	0	6,10,10	0.23	0
30	MPD	X	3004	-	6,7,7	0.33	0	6,10,10	0.11	0
30	MPD	X	3005	-	6,7,7	0.30	0	6,10,10	0.33	0
30	MPD	X	3006	-	6,7,7	0.40	0	6,10,10	0.21	0
30	MPD	X	3007	-	6,7,7	0.48	0	6,10,10	0.24	0
30	MPD	X	3008	-	6,7,7	0.29	0	6,10,10	0.09	0
30	MPD	X	3009	-	6,7,7	0.33	0	6,10,10	0.10	0
30	MPD	X	3010	-	6,7,7	0.32	0	6,10,10	0.14	0
34	EPE	X	3423	-	15,15,15	1.21	1 (6%)	19,20,20	0.75	1 (5%)
34	EPE	X	3424	-	15,15,15	1.38	1 (6%)	19,20,20	0.95	1 (5%)
34	EPE	X	3425	-	15,15,15	1.01	1 (6%)	19,20,20	0.71	1 (5%)
34	EPE	X	3426	-	15,15,15	2.86	1 (6%)	19,20,20	0.87	0
35	SPD	X	3427	-	9,9,9	0.22	0	8,8,8	0.38	0
35	SPD	X	3428	-	9,9,9	0.20	0	8,8,8	0.18	0
35	SPD	X	3429	-	9,9,9	0.23	0	8,8,8	0.16	0
35	SPD	X	3430	-	9,9,9	0.15	0	8,8,8	0.20	0
35	SPD	X	3431	-	9,9,9	0.19	0	8,8,8	0.18	0
35	SPD	X	3432	-	9,9,9	0.24	0	8,8,8	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	SPD	X	3433	-	9,9,9	0.19	0	8,8,8	0.23	0
35	SPD	X	3434	-	9,9,9	0.19	0	8,8,8	0.22	0
36	EOH	X	3435	-	2,2,2	0.63	0	1,1,1	0.38	0
36	EOH	X	3436	-	2,2,2	0.52	0	1,1,1	0.67	0
36	EOH	X	3437	-	2,2,2	0.51	0	1,1,1	0.72	0
36	EOH	X	3438	-	2,2,2	0.60	0	1,1,1	0.54	0
36	EOH	Y	209	-	2,2,2	0.52	0	1,1,1	0.67	0

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
35	SPD	J	201	-	-	0/7/7/7	0/0/0/0
29	ZLD	X	3001	-	-	0/13/33/33	0/3/3/3
30	MPD	X	3002	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3003	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
30	MPD	X	3010	-	-	0/5/5/5	0/0/0/0
34	EPE	X	3423	-	-	0/9/19/19	0/1/1/1
34	EPE	X	3424	-	-	0/9/19/19	0/1/1/1
34	EPE	X	3425	-	-	0/9/19/19	0/1/1/1
34	EPE	X	3426	-	-	0/9/19/19	0/1/1/1
35	SPD	X	3427	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3428	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3429	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3430	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3431	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3432	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3433	-	-	0/7/7/7	0/0/0/0
35	SPD	X	3434	-	-	0/7/7/7	0/0/0/0
36	EOH	X	3435	-	-	0/0/0/0	0/0/0/0
36	EOH	X	3436	-	-	0/0/0/0	0/0/0/0
36	EOH	X	3437	-	-	0/0/0/0	0/0/0/0
36	EOH	X	3438	-	-	0/0/0/0	0/0/0/0
36	EOH	Y	209	-	-	0/0/0/0	0/0/0/0



All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	X	3426	EPE	C10-S	-10.95	1.61	1.77
34	X	3424	EPE	C10-S	-5.24	1.69	1.77
34	X	3423	EPE	C10-S	-4.54	1.70	1.77
34	X	3425	EPE	C10-S	-3.77	1.71	1.77
29	X	3001	ZLD	C7-N4	4.23	1.41	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	X	3424	EPE	O2S-S-C10	-3.66	104.28	106.87
29	X	3001	ZLD	O10-C7-N4	-2.98	107.98	109.97
29	X	3001	ZLD	O15-C7-N4	-2.67	126.68	128.84
29	X	3001	ZLD	C6-C8-C9	-2.63	109.24	114.64
34	X	3423	EPE	O2S-S-C10	-2.55	105.07	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3001	ZLD	5	0
30	X	3005	MPD	3	0
30	X	3009	MPD	1	0
30	X	3010	MPD	1	0
34	X	3423	EPE	1	0
34	X	3424	EPE	1	0
34	X	3425	EPE	4	0
34	X	3426	EPE	14	0
35	X	3428	SPD	3	0
35	X	3430	SPD	3	0
35	X	3432	SPD	2	0
35	X	3433	SPD	2	0
35	X	3434	SPD	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	X	2711/2923 (92%)	-0.50	9 (0%) <span>94</span> <span>92</span>	39, 91, 192, 340	0
2	Y	114/114 (100%)	-0.79	0 <span>100</span> <span>100</span>	61, 106, 172, 208	0
3	A	268/277 (96%)	0.74	57 (21%) <span>1</span> <span>1</span>	64, 121, 176, 224	0
4	B	215/220 (97%)	-0.04	5 (2%) <span>64</span> <span>58</span>	50, 66, 114, 194	0
5	C	199/207 (96%)	0.02	7 (3%) <span>48</span> <span>42</span>	56, 82, 132, 163	0
6	D	155/179 (86%)	-0.26	6 (3%) <span>43</span> <span>38</span>	96, 156, 222, 311	0
7	E	157/178 (88%)	-0.36	8 (5%) <span>32</span> <span>28</span>	88, 136, 197, 264	0
8	G	145/145 (100%)	0.01	3 (2%) <span>67</span> <span>61</span>	47, 63, 98, 129	0
9	H	122/122 (100%)	0.95	32 (26%) <span>1</span> <span>1</span>	66, 89, 129, 146	0
10	I	131/146 (89%)	0.24	11 (8%) <span>14</span> <span>13</span>	34, 94, 152, 175	0
11	J	138/144 (95%)	1.10	39 (28%) <span>1</span> <span>1</span>	54, 83, 183, 312	0
12	K	119/122 (97%)	-0.03	5 (4%) <span>40</span> <span>35</span>	37, 74, 127, 175	0
13	L	108/119 (90%)	-0.31	8 (7%) <span>17</span> <span>17</span>	68, 109, 149, 173	0
14	M	109/116 (93%)	0.10	6 (5%) <span>29</span> <span>26</span>	54, 86, 155, 201	0
15	N	116/118 (98%)	-0.14	1 (0%) <span>85</span> <span>81</span>	35, 60, 98, 125	0
16	O	101/102 (99%)	0.10	9 (8%) <span>12</span> <span>11</span>	38, 73, 127, 149	0
17	P	112/117 (95%)	0.45	6 (5%) <span>29</span> <span>27</span>	43, 63, 114, 179	0
18	Q	88/91 (96%)	0.11	7 (7%) <span>15</span> <span>14</span>	84, 110, 167, 193	0
19	R	100/105 (95%)	-0.31	4 (4%) <span>42</span> <span>37</span>	60, 110, 228, 298	0
20	S	167/217 (76%)	0.22	23 (13%) <span>4</span> <span>4</span>	55, 104, 213, 309	0
21	T	75/94 (79%)	1.29	25 (33%) <span>0</span> <span>1</span>	66, 78, 132, 178	0
22	U	44/62 (70%)	2.31	20 (45%) <span>0</span> <span>0</span>	89, 163, 227, 254	0
23	V	65/69 (94%)	-0.12	4 (6%) <span>24</span> <span>22</span>	75, 114, 166, 228	0
24	W	57/59 (96%)	-0.29	0 <span>100</span> <span>100</span>	37, 62, 114, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	44/58 (75%)	0.44	5 (11%) 7 7	34, 74, 140, 227	0
26	2	44/45 (97%)	0.84	9 (20%) 1 1	57, 83, 118, 145	0
27	3	60/66 (90%)	0.14	5 (8%) 14 13	41, 77, 118, 148	0
28	4	37/37 (100%)	0.86	8 (21%) 1 1	96, 104, 144, 162	0
All	All	5801/6252 (92%)	-0.13	322 (5%) 28 25	34, 92, 181, 340	0

The worst 5 of 322 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	42	GLY	12.5
3	A	82	GLN	12.3
22	U	41	ASP	10.0
20	S	164	ASP	8.6
22	U	39	LEU	8.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
31	MG	X	3418	1/1	0.65	0.76	62.14	81,81,81,81	0
31	MG	X	3420	1/1	0.47	0.64	36.08	79,79,79,79	0
31	MG	X	3287	1/1	0.91	0.93	28.89	67,67,67,67	0
30	MPD	X	3008	8/8	0.80	0.51	27.69	144,144,144,144	0
32	MN	X	3151	1/1	0.85	0.62	23.92	106,106,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MN	X	3231	1/1	0.97	0.75	23.57	135,135,135,135	0
32	MN	X	3119	1/1	0.83	0.70	23.18	155,155,155,155	0
31	MG	X	3384	1/1	0.94	0.54	21.93	81,81,81,81	0
32	MN	X	3161	1/1	0.85	0.58	20.51	98,98,98,98	0
32	MN	X	3146	1/1	0.95	0.34	18.58	100,100,100,100	0
35	SPD	X	3431	10/10	0.75	0.39	17.60	98,98,98,98	0
35	SPD	X	3429	10/10	0.61	0.64	17.39	106,106,106,106	0
31	MG	X	3344	1/1	0.69	0.68	16.44	92,92,92,92	0
32	MN	X	3079	1/1	0.98	0.47	14.54	71,71,71,71	0
32	MN	X	3172	1/1	0.89	0.57	14.26	82,82,82,82	0
31	MG	X	3294	1/1	0.97	0.36	14.02	51,51,51,51	0
31	MG	X	3032	1/1	0.78	0.48	13.90	64,64,64,64	0
32	MN	X	3221	1/1	0.79	0.35	13.31	130,130,130,130	0
32	MN	X	3224	1/1	0.96	0.35	13.12	99,99,99,99	0
32	MN	X	3150	1/1	0.99	0.40	12.86	39,39,39,39	0
30	MPD	X	3006	8/8	0.65	0.42	12.63	133,133,133,133	0
32	MN	X	3159	1/1	0.99	0.43	11.41	61,61,61,61	0
31	MG	Y	206	1/1	0.82	0.42	10.89	65,65,65,65	0
35	SPD	X	3434	10/10	0.84	0.26	10.53	98,98,98,98	0
32	MN	X	3133	1/1	0.99	0.35	10.22	58,58,58,58	0
32	MN	X	3148	1/1	0.87	0.39	9.99	102,102,102,102	0
32	MN	X	3124	1/1	0.98	0.36	9.52	80,80,80,80	0
31	MG	X	3314	1/1	0.97	0.34	9.40	45,45,45,45	0
31	MG	X	3037	1/1	0.85	0.23	9.26	69,69,69,69	0
32	MN	X	3152	1/1	0.98	0.38	9.21	60,60,60,60	0
32	MN	X	3168	1/1	0.93	0.42	9.19	85,85,85,85	0
32	MN	X	3239	1/1	0.96	0.44	8.90	60,60,60,60	0
32	MN	X	3157	1/1	0.94	0.42	8.39	85,85,85,85	0
31	MG	X	3345	1/1	0.98	0.34	8.32	78,78,78,78	0
32	MN	X	3153	1/1	0.97	0.32	8.22	75,75,75,75	0
32	MN	X	3154	1/1	0.95	0.39	7.84	46,46,46,46	0
31	MG	X	3063	1/1	0.83	0.32	7.23	49,49,49,49	0
35	SPD	X	3427	10/10	0.85	0.33	6.77	56,56,56,56	0
32	MN	X	3184	1/1	0.95	0.34	6.73	86,86,86,86	0
32	MN	X	3220	1/1	0.97	0.21	6.48	111,111,111,111	0
35	SPD	X	3428	10/10	0.91	0.22	6.45	82,82,82,82	0
31	MG	X	3021	1/1	0.92	0.31	6.44	76,76,76,76	0
30	MPD	X	3009	8/8	0.84	0.42	6.39	107,107,107,107	0
31	MG	X	3308	1/1	0.94	0.24	6.09	39,39,39,39	0
32	MN	X	3195	1/1	0.97	0.27	6.08	90,90,90,90	0
32	MN	X	3187	1/1	0.97	0.33	5.98	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MPD	X	3007	8/8	0.89	0.19	5.78	114,114,114,114	0
31	MG	X	3310	1/1	0.95	0.23	5.74	66,66,66,66	0
32	MN	X	3132	1/1	0.99	0.30	5.70	66,66,66,66	0
32	MN	X	3143	1/1	0.99	0.32	5.64	76,76,76,76	0
30	MPD	X	3004	8/8	0.87	0.24	5.29	109,109,109,109	0
35	SPD	X	3433	10/10	0.94	0.22	5.10	93,93,93,93	0
32	MN	X	3084	1/1	0.98	0.28	4.96	81,81,81,81	0
32	MN	X	3215	1/1	0.95	0.37	4.91	154,154,154,154	0
31	MG	X	3323	1/1	0.93	0.27	4.82	76,76,76,76	0
31	MG	X	3062	1/1	0.86	0.32	4.63	56,56,56,56	0
32	MN	X	3162	1/1	0.92	0.28	4.53	74,74,74,74	0
31	MG	X	3335	1/1	0.97	0.67	4.47	260,260,260,260	0
32	MN	X	3130	1/1	0.98	0.26	3.82	70,70,70,70	0
31	MG	X	3024	1/1	0.92	0.32	3.78	67,67,67,67	0
32	MN	X	3442	1/1	0.96	0.32	3.71	51,51,51,51	0
32	MN	X	3147	1/1	0.98	0.33	3.67	82,82,82,82	0
32	MN	X	3227	1/1	0.88	0.23	3.61	107,107,107,107	0
30	MPD	X	3003	8/8	0.95	0.20	3.39	92,92,92,92	0
30	MPD	X	3010	8/8	0.90	0.31	3.33	122,122,122,122	0
31	MG	X	3415	1/1	0.98	0.29	3.06	45,45,45,45	0
32	MN	X	3199	1/1	0.99	0.30	2.94	93,93,93,93	0
31	MG	X	3249	1/1	0.98	0.38	2.78	16,16,16,16	0
31	MG	X	3319	1/1	0.98	0.26	2.75	26,26,26,26	0
35	SPD	X	3432	10/10	0.87	0.25	2.67	77,77,77,77	0
29	ZLD	X	3001	24/24	0.92	0.40	2.65	87,88,90,91	0
32	MN	X	3240	1/1	0.82	0.36	2.52	123,123,123,123	0
34	EPE	X	3424	15/15	0.77	0.39	2.51	194,194,194,194	0
32	MN	X	3131	1/1	0.97	0.23	2.46	66,66,66,66	0
31	MG	X	3035	1/1	0.94	0.27	2.43	39,39,39,39	0
35	SPD	J	201	10/10	0.75	0.27	2.43	82,82,82,82	0
34	EPE	X	3425	15/15	0.72	0.33	2.41	152,152,152,152	0
32	MN	X	3223	1/1	0.96	0.15	2.40	127,127,127,127	0
34	EPE	X	3423	15/15	0.86	0.32	2.26	152,152,152,152	0
32	MN	X	3142	1/1	0.98	0.18	2.18	108,108,108,108	0
31	MG	A	302	1/1	0.86	0.33	2.16	58,58,58,58	0
34	EPE	X	3426	15/15	0.94	0.27	2.11	101,101,101,101	3
32	MN	X	3176	1/1	0.96	0.31	2.09	80,80,80,80	0
31	MG	X	3039	1/1	0.88	0.19	2.00	53,53,53,53	0
31	MG	X	3441	1/1	0.89	0.76	1.88	72,72,72,72	0
32	MN	X	3439	1/1	0.94	0.29	1.77	97,97,97,97	0
31	MG	X	3352	1/1	0.94	0.16	1.60	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MN	X	3111	1/1	0.95	0.27	1.51	125,125,125,125	0
32	MN	X	3126	1/1	0.98	0.21	1.50	96,96,96,96	0
32	MN	X	3087	1/1	0.98	0.20	1.34	104,104,104,104	0
30	MPD	X	3005	8/8	0.90	0.14	1.32	64,64,64,64	0
31	MG	X	3406	1/1	0.93	0.21	1.19	55,55,55,55	0
32	MN	X	3268	1/1	0.94	0.19	1.13	94,94,94,94	0
32	MN	X	3201	1/1	0.98	0.19	0.96	49,49,49,49	0
32	MN	X	3189	1/1	0.98	0.28	0.89	53,53,53,53	0
32	MN	X	3066	1/1	0.96	0.26	0.83	64,64,64,64	0
31	MG	X	3440	1/1	0.85	0.21	0.51	37,37,37,37	0
32	MN	X	3123	1/1	0.91	0.25	0.47	97,97,97,97	0
31	MG	X	3349	1/1	0.91	0.12	0.37	45,45,45,45	0
31	MG	X	3211	1/1	0.84	0.23	0.34	32,32,32,32	0
35	SPD	X	3430	10/10	0.91	0.28	0.26	80,80,80,80	0
31	MG	N	201	1/1	0.95	0.27	0.22	25,25,25,25	0
31	MG	X	3209	1/1	0.91	0.29	0.21	34,34,34,34	0
31	MG	X	3444	1/1	0.85	0.24	0.10	44,44,44,44	0
32	MN	X	3099	1/1	0.98	0.14	0.09	128,128,128,128	0
32	MN	X	3103	1/1	0.99	0.16	0.08	81,81,81,81	0
32	MN	X	3262	1/1	0.77	0.10	-0.01	191,191,191,191	0
32	MN	X	3120	1/1	0.98	0.14	-0.02	75,75,75,75	0
32	MN	X	3136	1/1	0.99	0.21	-0.04	84,84,84,84	0
31	MG	X	3252	1/1	0.66	0.30	-0.15	50,50,50,50	0
32	MN	X	3416	1/1	0.91	0.13	-0.41	111,111,111,111	0
31	MG	X	3304	1/1	0.84	0.18	-0.48	70,70,70,70	0
31	MG	X	3332	1/1	1.00	0.17	-0.81	28,28,28,28	0
31	MG	X	3338	1/1	0.97	0.15	-1.03	43,43,43,43	0
32	MN	X	3205	1/1	0.87	0.14	-1.17	113,113,113,113	0
31	MG	Z	103	1/1	0.97	0.11	-1.42	39,39,39,39	0
32	MN	X	3228	1/1	0.94	0.13	-	110,110,110,110	0
31	MG	X	3419	1/1	0.70	1.75	-	100,100,100,100	0
31	MG	X	3034	1/1	0.76	0.39	-	75,75,75,75	0
31	MG	X	3011	1/1	0.84	0.38	-	85,85,85,85	0
31	MG	G	202	1/1	0.84	0.28	-	77,77,77,77	0
31	MG	X	3041	1/1	0.96	0.36	-	68,68,68,68	0
31	MG	X	3060	1/1	0.99	0.44	-	16,16,16,16	0
31	MG	X	3290	1/1	0.88	0.40	-	46,46,46,46	0
32	MN	X	3095	1/1	0.93	0.25	-	133,133,133,133	0
31	MG	X	3023	1/1	0.93	0.23	-	56,56,56,56	0
32	MN	X	3140	1/1	0.87	0.33	-	111,111,111,111	0
31	MG	X	3040	1/1	0.97	0.91	-	58,58,58,58	0
31	MG	X	3289	1/1	0.95	0.31	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3208	1/1	0.56	0.43	-	78,78,78,78	0
32	MN	X	3102	1/1	0.96	0.29	-	96,96,96,96	0
32	MN	X	3192	1/1	0.91	0.20	-	85,85,85,85	0
32	MN	X	3180	1/1	0.99	0.27	-	70,70,70,70	0
31	MG	X	3348	1/1	0.75	0.41	-	85,85,85,85	0
31	MG	X	3320	1/1	0.98	0.43	-	43,43,43,43	0
31	MG	X	3316	1/1	0.82	0.86	-	88,88,88,88	0
32	MN	X	3100	1/1	0.95	0.76	-	129,129,129,129	0
32	MN	X	3179	1/1	0.99	0.28	-	77,77,77,77	0
31	MG	X	3411	1/1	0.71	0.42	-	83,83,83,83	0
36	EOH	X	3437	3/3	0.89	0.21	-	92,92,92,92	0
31	MG	X	3256	1/1	0.87	1.16	-	82,82,82,82	0
31	MG	X	3347	1/1	0.86	0.19	-	77,77,77,77	0
31	MG	X	3372	1/1	0.81	0.18	-	49,49,49,49	0
31	MG	Y	204	1/1	0.91	0.46	-	63,63,63,63	0
32	MN	X	3074	1/1	0.97	0.24	-	98,98,98,98	0
31	MG	X	3363	1/1	0.75	0.46	-	81,81,81,81	0
32	MN	X	3443	1/1	0.95	0.35	-	91,91,91,91	0
36	EOH	X	3438	3/3	0.83	0.31	-	63,63,63,63	0
31	MG	X	3412	1/1	0.91	1.01	-	82,82,82,82	0
31	MG	X	3312	1/1	0.73	1.02	-	57,57,57,57	0
31	MG	X	3043	1/1	0.97	0.41	-	64,64,64,64	0
32	MN	X	3219	1/1	0.91	0.22	-	139,139,139,139	0
32	MN	X	3078	1/1	0.99	0.25	-	56,56,56,56	0
31	MG	X	3306	1/1	0.82	0.31	-	77,77,77,77	0
31	MG	X	3355	1/1	0.97	0.19	-	71,71,71,71	0
32	MN	X	3108	1/1	0.93	0.50	-	182,182,182,182	0
31	MG	X	3390	1/1	0.96	0.20	-	47,47,47,47	0
31	MG	X	3044	1/1	0.90	0.39	-	20,20,20,20	1
31	MG	X	3400	1/1	0.78	0.37	-	50,50,50,50	0
31	MG	X	3025	1/1	0.90	0.46	-	10,10,10,10	1
32	MN	X	3125	1/1	0.96	0.80	-	122,122,122,122	0
32	MN	X	3182	1/1	0.94	0.37	-	88,88,88,88	0
32	MN	X	3077	1/1	0.96	0.21	-	61,61,61,61	0
32	MN	X	3113	1/1	0.67	0.24	-	123,123,123,123	0
31	MG	X	3027	1/1	0.91	0.59	-	66,66,66,66	0
32	MN	X	3417	1/1	0.93	0.23	-	156,156,156,156	0
32	MN	X	3169	1/1	0.95	0.51	-	76,76,76,76	0
31	MG	X	3309	1/1	0.81	0.10	-	53,53,53,53	0
31	MG	Y	207	1/1	0.65	0.54	-	101,101,101,101	0
36	EOH	X	3436	3/3	0.83	0.36	-	92,92,92,92	0
32	MN	X	3139	1/1	0.98	0.42	-	143,143,143,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3018	1/1	0.86	0.87	-	76,76,76,76	0
32	MN	X	3232	1/1	0.90	0.25	-	105,105,105,105	0
31	MG	X	3038	1/1	0.79	0.22	-	75,75,75,75	0
31	MG	X	3413	1/1	0.92	0.38	-	57,57,57,57	0
32	MN	X	3267	1/1	0.83	0.43	-	140,140,140,140	0
31	MG	X	3272	1/1	0.88	1.14	-	69,69,69,69	0
31	MG	X	3377	1/1	0.90	0.21	-	73,73,73,73	0
31	MG	X	3058	1/1	0.93	0.69	-	45,45,45,45	0
32	MN	X	3217	1/1	0.76	0.54	-	113,113,113,113	0
32	MN	Y	202	1/1	0.96	0.18	-	92,92,92,92	0
31	MG	X	3245	1/1	0.46	0.39	-	93,93,93,93	0
31	MG	X	3045	1/1	0.75	0.34	-	87,87,87,87	0
32	MN	X	3264	1/1	0.76	0.29	-	128,128,128,128	0
31	MG	X	3284	1/1	0.49	0.77	-	94,94,94,94	0
31	MG	X	3206	1/1	0.87	0.52	-	74,74,74,74	0
31	MG	X	3303	1/1	0.94	0.44	-	63,63,63,63	0
31	MG	X	3343	1/1	0.61	0.67	-	108,108,108,108	0
32	MN	X	3144	1/1	0.91	0.48	-	143,143,143,143	0
31	MG	X	3210	1/1	0.97	0.32	-	57,57,57,57	0
31	MG	X	3399	1/1	0.53	1.35	-	101,101,101,101	0
31	MG	X	3033	1/1	0.84	0.56	-	12,12,12,12	1
32	MN	X	3097	1/1	0.88	0.51	-	118,118,118,118	0
31	MG	X	3251	1/1	0.96	0.39	-	47,47,47,47	0
31	MG	X	3396	1/1	0.87	0.81	-	85,85,85,85	0
31	MG	X	3351	1/1	0.41	0.56	-	41,41,41,41	0
31	MG	X	3405	1/1	0.86	0.97	-	79,79,79,79	0
31	MG	X	3339	1/1	0.93	0.23	-	59,59,59,59	0
31	MG	X	3361	1/1	0.65	1.08	-	76,76,76,76	0
31	MG	X	3054	1/1	0.99	0.24	-	20,20,20,20	0
30	MPD	X	3002	8/8	0.84	0.38	-	132,132,132,132	0
31	MG	X	3329	1/1	0.94	0.28	-	60,60,60,60	0
31	MG	X	3280	1/1	0.68	1.21	-	87,87,87,87	0
31	MG	X	3315	1/1	0.96	0.86	-	87,87,87,87	0
31	MG	X	3042	1/1	0.97	0.69	-	59,59,59,59	0
32	MN	X	3177	1/1	0.88	0.14	-	56,56,56,56	0
31	MG	X	3395	1/1	0.95	0.90	-	93,93,93,93	0
32	MN	X	3271	1/1	0.87	0.20	-	117,117,117,117	0
32	MN	X	3109	1/1	0.90	0.39	-	145,145,145,145	0
31	MG	X	3402	1/1	0.94	0.17	-	84,84,84,84	0
31	MG	Z	102	1/1	0.92	0.26	-	68,68,68,68	0
31	MG	A	301	1/1	0.90	0.16	-	81,81,81,81	0
31	MG	X	3274	1/1	0.94	0.27	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MN	X	3235	1/1	0.72	0.16	-	134,134,134,134	0
31	MG	X	3031	1/1	0.88	0.28	-	70,70,70,70	0
31	MG	X	3055	1/1	0.92	0.54	-	53,53,53,53	0
31	MG	X	3253	1/1	0.94	0.41	-	45,45,45,45	0
31	MG	X	3292	1/1	0.54	0.17	-	70,70,70,70	0
31	MG	X	3414	1/1	0.92	0.35	-	59,59,59,59	0
32	MN	X	3263	1/1	0.96	0.18	-	80,80,80,80	0
31	MG	X	3340	1/1	0.72	0.43	-	56,56,56,56	0
31	MG	X	3404	1/1	0.98	0.34	-	78,78,78,78	0
31	MG	G	201	1/1	0.50	0.98	-	68,68,68,68	0
31	MG	X	3026	1/1	0.83	0.24	-	64,64,64,64	0
31	MG	X	3276	1/1	0.88	0.55	-	85,85,85,85	0
31	MG	Y	205	1/1	0.92	0.16	-	77,77,77,77	0
31	MG	X	3048	1/1	0.91	0.41	-	31,31,31,31	1
32	MN	X	3122	1/1	0.97	0.18	-	123,123,123,123	0
31	MG	X	3030	1/1	0.75	0.23	-	38,38,38,38	1
31	MG	X	3305	1/1	0.93	0.47	-	68,68,68,68	0
31	MG	X	3394	1/1	0.80	0.30	-	80,80,80,80	0
32	MN	X	3194	1/1	0.96	0.36	-	93,93,93,93	0
31	MG	X	3358	1/1	0.96	0.35	-	46,46,46,46	0
32	MN	X	3265	1/1	0.15	0.89	-	158,158,158,158	0
31	MG	X	3255	1/1	0.84	0.63	-	69,69,69,69	0
32	MN	X	3203	1/1	0.96	0.33	-	69,69,69,69	0
32	MN	X	3089	1/1	0.94	0.13	-	92,92,92,92	0
31	MG	X	3371	1/1	0.88	1.00	-	91,91,91,91	0
32	MN	X	3261	1/1	0.95	0.35	-	132,132,132,132	0
31	MG	X	3017	1/1	0.92	0.31	-	75,75,75,75	0
32	MN	X	3233	1/1	0.99	0.34	-	66,66,66,66	0
32	MN	Y	203	1/1	0.75	0.18	-	99,99,99,99	0
31	MG	X	3353	1/1	0.98	0.16	-	81,81,81,81	0
32	MN	X	3067	1/1	0.82	0.36	-	166,166,166,166	0
31	MG	X	3354	1/1	0.92	0.33	-	64,64,64,64	0
32	MN	X	3118	1/1	0.98	0.36	-	123,123,123,123	0
32	MN	X	3080	1/1	0.94	0.39	-	130,130,130,130	0
32	MN	X	3164	1/1	0.95	0.32	-	92,92,92,92	0
31	MG	X	3250	1/1	0.92	0.57	-	70,70,70,70	0
31	MG	X	3356	1/1	0.94	0.22	-	70,70,70,70	0
32	MN	X	3128	1/1	0.98	0.23	-	77,77,77,77	0
32	MN	X	3197	1/1	0.90	0.20	-	102,102,102,102	0
31	MG	X	3056	1/1	0.72	0.80	-	55,55,55,55	1
32	MN	X	3075	1/1	0.95	0.31	-	116,116,116,116	0
32	MN	X	3137	1/1	0.99	0.26	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MN	X	3214	1/1	0.79	0.28	-	163,163,163,163	0
32	MN	X	3163	1/1	0.96	0.37	-	61,61,61,61	0
32	MN	X	3098	1/1	0.69	0.26	-	131,131,131,131	0
32	MN	X	3135	1/1	0.96	0.27	-	76,76,76,76	0
32	MN	X	3200	1/1	0.97	0.21	-	126,126,126,126	0
32	MN	X	3186	1/1	0.97	0.28	-	69,69,69,69	0
32	MN	X	3064	1/1	0.93	0.25	-	145,145,145,145	0
31	MG	X	3301	1/1	0.99	0.12	-	43,43,43,43	0
31	MG	X	3241	1/1	0.83	0.67	-	66,66,66,66	0
31	MG	X	3328	1/1	0.92	0.50	-	59,59,59,59	0
31	MG	O	201	1/1	0.92	0.33	-	41,41,41,41	0
32	MN	X	3085	1/1	0.71	0.59	-	128,128,128,128	0
32	MN	X	3106	1/1	0.95	0.24	-	96,96,96,96	0
32	MN	X	3259	1/1	0.84	0.12	-	140,140,140,140	0
31	MG	X	3248	1/1	0.33	0.26	-	65,65,65,65	0
31	MG	X	3047	1/1	0.62	0.35	-	71,71,71,71	0
31	MG	C	301	1/1	0.92	0.25	-	46,46,46,46	0
31	MG	X	3383	1/1	0.93	0.66	-	58,58,58,58	0
31	MG	X	3288	1/1	0.99	0.26	-	79,79,79,79	0
32	MN	X	3069	1/1	0.97	0.22	-	121,121,121,121	0
31	MG	X	3213	1/1	0.92	0.38	-	22,22,22,22	0
32	MN	X	3237	1/1	0.98	0.27	-	71,71,71,71	0
31	MG	X	3330	1/1	0.96	0.16	-	55,55,55,55	0
31	MG	I	201	1/1	0.86	0.63	-	47,47,47,47	0
32	MN	X	3173	1/1	0.98	0.14	-	87,87,87,87	0
31	MG	X	3409	1/1	0.90	1.05	-	67,67,67,67	0
31	MG	X	3388	1/1	0.88	0.22	-	65,65,65,65	0
31	MG	X	3293	1/1	0.94	0.16	-	91,91,91,91	0
32	MN	X	3191	1/1	0.86	0.18	-	107,107,107,107	0
31	MG	X	3365	1/1	0.99	0.09	-	63,63,63,63	0
31	MG	X	3019	1/1	0.79	0.63	-	69,69,69,69	0
31	MG	X	3050	1/1	0.88	0.80	-	2,2,2,2	1
32	MN	X	3091	1/1	0.92	0.41	-	100,100,100,100	0
31	MG	X	3334	1/1	0.91	0.21	-	57,57,57,57	0
32	MN	X	3065	1/1	0.99	0.19	-	78,78,78,78	0
31	MG	X	3013	1/1	0.98	0.75	-	61,61,61,61	0
32	MN	X	3141	1/1	0.82	0.48	-	100,100,100,100	0
31	MG	X	3242	1/1	0.62	0.72	-	90,90,90,90	0
32	MN	X	3117	1/1	0.75	0.52	-	166,166,166,166	0
31	MG	X	3401	1/1	0.58	0.54	-	63,63,63,63	0
31	MG	W	101	1/1	0.97	0.61	-	84,84,84,84	0
31	MG	X	3307	1/1	0.95	0.51	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MN	X	3138	1/1	0.92	0.25	-	120,120,120,120	0
32	MN	X	3202	1/1	0.85	0.27	-	117,117,117,117	0
32	MN	X	3145	1/1	0.99	0.19	-	47,47,47,47	0
31	MG	X	3333	1/1	0.98	0.95	-	71,71,71,71	0
31	MG	X	3380	1/1	0.57	0.43	-	83,83,83,83	0
31	MG	X	3300	1/1	0.93	0.76	-	80,80,80,80	0
31	MG	X	3061	1/1	0.92	0.28	-	41,41,41,41	0
31	MG	X	3368	1/1	0.85	0.37	-	70,70,70,70	0
32	MN	X	3238	1/1	0.93	0.17	-	174,174,174,174	0
31	MG	X	3366	1/1	0.12	0.38	-	69,69,69,69	0
31	MG	X	3350	1/1	0.92	0.12	-	28,28,28,28	0
31	MG	X	3318	1/1	0.75	0.36	-	65,65,65,65	0
31	MG	X	3364	1/1	0.85	0.33	-	80,80,80,80	0
32	MN	X	3178	1/1	0.97	0.39	-	92,92,92,92	0
31	MG	X	3286	1/1	0.80	0.57	-	82,82,82,82	0
32	MN	X	3134	1/1	0.96	0.41	-	57,57,57,57	0
31	MG	X	3311	1/1	0.67	0.12	-	86,86,86,86	0
31	MG	X	3020	1/1	0.96	0.23	-	53,53,53,53	0
32	MN	X	3226	1/1	0.77	0.22	-	112,112,112,112	0
36	EOH	Y	209	3/3	0.66	0.27	-	93,93,93,93	0
31	MG	X	3403	1/1	0.97	0.08	-	52,52,52,52	0
31	MG	X	3410	1/1	0.90	0.37	-	78,78,78,78	0
31	MG	X	3393	1/1	0.80	0.12	-	67,67,67,67	0
32	MN	X	3090	1/1	0.85	0.14	-	123,123,123,123	0
31	MG	X	3298	1/1	0.94	0.30	-	72,72,72,72	0
32	MN	X	3422	1/1	0.57	1.08	-	201,201,201,201	0
32	MN	X	3104	1/1	0.98	0.42	-	88,88,88,88	0
31	MG	X	3302	1/1	0.72	0.21	-	51,51,51,51	0
31	MG	Y	201	1/1	0.96	0.42	-	24,24,24,24	1
32	MN	X	3092	1/1	0.90	0.29	-	104,104,104,104	0
32	MN	Z	101	1/1	0.98	0.38	-	88,88,88,88	0
31	MG	X	3015	1/1	0.89	0.40	-	36,36,36,36	1
32	MN	X	3170	1/1	0.96	0.28	-	95,95,95,95	0
32	MN	X	3129	1/1	0.94	0.60	-	106,106,106,106	0
31	MG	X	3378	1/1	0.83	0.23	-	83,83,83,83	0
31	MG	X	3370	1/1	0.58	0.34	-	103,103,103,103	0
31	MG	X	3036	1/1	0.95	0.65	-	85,85,85,85	0
36	EOH	X	3435	3/3	0.90	0.23	-	36,36,36,36	0
32	MN	X	3185	1/1	0.92	0.84	-	132,132,132,132	0
32	MN	X	3072	1/1	0.80	0.20	-	91,91,91,91	0
31	MG	X	3283	1/1	0.93	0.13	-	62,62,62,62	0
32	MN	X	3258	1/1	0.95	0.20	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3317	1/1	0.95	0.24	-	39,39,39,39	0
32	MN	X	3110	1/1	0.95	0.21	-	103,103,103,103	0
31	MG	X	3376	1/1	0.95	0.27	-	93,93,93,93	0
31	MG	X	3046	1/1	0.92	0.23	-	43,43,43,43	1
31	MG	X	3243	1/1	0.77	0.36	-	82,82,82,82	0
32	MN	X	3160	1/1	0.99	0.28	-	39,39,39,39	0
31	MG	X	3049	1/1	0.95	0.54	-	14,14,14,14	1
31	MG	X	3254	1/1	0.76	0.86	-	47,47,47,47	1
32	MN	X	3269	1/1	0.96	0.33	-	131,131,131,131	0
31	MG	X	3022	1/1	0.91	0.30	-	83,83,83,83	0
32	MN	X	3193	1/1	0.96	0.17	-	87,87,87,87	0
32	MN	X	3174	1/1	0.98	0.34	-	81,81,81,81	0
32	MN	X	3114	1/1	0.56	0.85	-	150,150,150,150	0
31	MG	X	3052	1/1	0.98	0.28	-	27,27,27,27	0
32	MN	X	3225	1/1	0.96	0.86	-	133,133,133,133	0
31	MG	B	301	1/1	0.85	0.28	-	65,65,65,65	0
32	MN	X	3071	1/1	0.60	0.15	-	134,134,134,134	0
31	MG	X	3331	1/1	0.98	0.20	-	60,60,60,60	0
32	MN	X	3070	1/1	0.83	0.18	-	148,148,148,148	0
32	MN	X	3266	1/1	0.78	0.14	-	104,104,104,104	0
31	MG	X	3285	1/1	0.78	0.30	-	73,73,73,73	0
32	MN	X	3234	1/1	0.97	0.06	-	91,91,91,91	0
32	MN	X	3260	1/1	0.87	0.26	-	126,126,126,126	0
31	MG	X	3016	1/1	0.91	0.43	-	81,81,81,81	0
31	MG	X	3408	1/1	0.87	0.24	-	48,48,48,48	0
32	MN	X	3073	1/1	0.90	0.09	-	105,105,105,105	0
31	MG	X	3327	1/1	0.63	0.47	-	103,103,103,103	0
31	MG	X	3326	1/1	0.99	0.25	-	32,32,32,32	0
31	MG	X	3341	1/1	0.83	0.47	-	43,43,43,43	0
32	MN	X	3086	1/1	0.87	0.21	-	82,82,82,82	0
31	MG	X	3359	1/1	0.58	1.18	-	87,87,87,87	0
32	MN	X	3183	1/1	0.97	0.22	-	63,63,63,63	0
31	MG	X	3297	1/1	0.68	0.47	-	85,85,85,85	0
32	MN	X	3083	1/1	0.84	0.31	-	150,150,150,150	0
31	MG	X	3281	1/1	0.90	0.40	-	72,72,72,72	0
32	MN	X	3165	1/1	0.98	0.25	-	79,79,79,79	0
32	MN	X	3188	1/1	0.93	0.38	-	100,100,100,100	0
32	MN	X	3204	1/1	0.95	0.15	-	126,126,126,126	0
31	MG	X	3028	1/1	0.84	0.24	-	58,58,58,58	0
31	MG	X	3379	1/1	0.98	0.20	-	40,40,40,40	0
31	MG	X	3324	1/1	0.95	0.66	-	88,88,88,88	0
31	MG	X	3279	1/1	0.94	0.29	-	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3277	1/1	0.94	0.07	-	55,55,55,55	0
31	MG	X	3059	1/1	0.86	0.26	-	35,35,35,35	0
31	MG	X	3386	1/1	0.40	1.38	-	112,112,112,112	0
32	MN	X	3196	1/1	0.97	0.26	-	77,77,77,77	0
32	MN	X	3236	1/1	0.95	0.17	-	104,104,104,104	0
32	MN	X	3107	1/1	0.98	0.15	-	71,71,71,71	0
31	MG	X	3369	1/1	0.76	0.80	-	76,76,76,76	0
31	MG	X	3382	1/1	0.78	0.72	-	68,68,68,68	0
31	MG	X	3257	1/1	0.96	0.26	-	71,71,71,71	0
32	MN	X	3190	1/1	0.98	0.47	-	91,91,91,91	0
31	MG	X	3296	1/1	0.77	0.30	-	75,75,75,75	0
31	MG	X	3346	1/1	0.91	0.92	-	81,81,81,81	0
31	MG	X	3029	1/1	0.41	0.41	-	65,65,65,65	1
32	MN	X	3374	1/1	0.92	0.21	-	153,153,153,153	0
31	MG	X	3357	1/1	0.75	0.65	-	56,56,56,56	0
33	NA	X	3367	1/1	0.83	0.36	-	64,64,64,64	0
31	MG	X	3014	1/1	0.70	1.10	-	85,85,85,85	0
31	MG	X	3381	1/1	0.86	0.31	-	82,82,82,82	0
32	MN	X	3155	1/1	0.97	0.35	-	75,75,75,75	0
31	MG	X	3291	1/1	0.80	0.97	-	62,62,62,62	0
31	MG	X	3360	1/1	0.85	0.61	-	123,123,123,123	0
32	MN	X	3101	1/1	0.99	0.17	-	86,86,86,86	0
31	MG	K	201	1/1	0.65	0.34	-	72,72,72,72	0
32	MN	X	3158	1/1	0.98	0.36	-	58,58,58,58	0
31	MG	X	3421	1/1	0.94	0.26	-	60,60,60,60	0
32	MN	X	3121	1/1	0.83	0.38	-	126,126,126,126	0
31	MG	X	3278	1/1	0.90	0.24	-	67,67,67,67	0
31	MG	O	202	1/1	0.34	0.74	-	67,67,67,67	0
31	MG	X	3407	1/1	0.85	0.52	-	89,89,89,89	0
31	MG	X	3244	1/1	0.81	0.44	-	78,78,78,78	0
32	MN	X	3181	1/1	0.96	0.27	-	73,73,73,73	0
32	MN	X	3270	1/1	0.88	0.11	-	109,109,109,109	0
31	MG	X	3337	1/1	0.97	0.31	-	44,44,44,44	0
32	MN	X	3216	1/1	0.93	0.13	-	112,112,112,112	0
32	MN	X	3096	1/1	0.75	0.10	-	153,153,153,153	0
31	MG	X	3313	1/1	0.99	0.41	-	59,59,59,59	0
31	MG	X	3362	1/1	0.89	0.23	-	47,47,47,47	0
32	MN	X	3149	1/1	0.96	0.37	-	64,64,64,64	0
31	MG	X	3057	1/1	0.94	0.45	-	41,41,41,41	0
32	MN	X	3229	1/1	0.93	0.43	-	135,135,135,135	0
32	MN	X	3082	1/1	0.96	0.19	-	109,109,109,109	0
31	MG	Y	208	1/1	0.79	0.52	-	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3282	1/1	0.96	0.29	-	68,68,68,68	0
31	MG	X	3273	1/1	0.84	0.25	-	79,79,79,79	0
31	MG	X	3392	1/1	0.92	0.16	-	91,91,91,91	0
31	MG	X	3398	1/1	0.94	1.58	-	107,107,107,107	0
32	MN	X	3105	1/1	0.73	0.37	-	87,87,87,87	0
32	MN	X	3076	1/1	0.93	0.47	-	148,148,148,148	0
32	MN	X	3112	1/1	0.82	0.12	-	155,155,155,155	0
31	MG	X	3275	1/1	0.33	0.22	-	73,73,73,73	0
31	MG	X	3295	1/1	0.99	0.06	-	56,56,56,56	0
32	MN	X	3116	1/1	0.91	0.17	-	84,84,84,84	0
32	MN	X	3156	1/1	0.95	0.26	-	83,83,83,83	0
32	MN	X	3171	1/1	0.97	0.39	-	88,88,88,88	0
32	MN	X	3127	1/1	0.97	0.22	-	108,108,108,108	0
31	MG	X	3325	1/1	0.98	0.39	-	93,93,93,93	0
32	MN	X	3093	1/1	0.95	0.14	-	122,122,122,122	0
31	MG	X	3246	1/1	0.92	0.37	-	69,69,69,69	0
31	MG	X	3212	1/1	0.96	0.71	-	40,40,40,40	0
32	MN	X	3198	1/1	0.99	0.42	-	73,73,73,73	0
31	MG	X	3053	1/1	0.90	0.70	-	42,42,42,42	1
31	MG	X	3322	1/1	0.95	0.50	-	50,50,50,50	0
31	MG	X	3051	1/1	0.85	0.51	-	14,14,14,14	1
32	MN	X	3167	1/1	0.91	0.42	-	91,91,91,91	0
32	MN	M	201	1/1	0.65	0.16	-	122,122,122,122	0
32	MN	X	3094	1/1	0.90	0.18	-	139,139,139,139	0
31	MG	X	3336	1/1	0.97	0.09	-	69,69,69,69	0
31	MG	X	3385	1/1	0.94	0.18	-	63,63,63,63	0
31	MG	X	3012	1/1	0.74	1.29	-	13,13,13,13	1
31	MG	X	3342	1/1	0.96	0.18	-	67,67,67,67	0
32	MN	X	3373	1/1	0.91	0.29	-	94,94,94,94	0
32	MN	X	3218	1/1	0.93	0.53	-	151,151,151,151	0
31	MG	X	3247	1/1	0.94	0.20	-	49,49,49,49	0
32	MN	X	3230	1/1	0.95	0.30	-	100,100,100,100	0
31	MG	X	3207	1/1	0.97	0.12	-	56,56,56,56	0
32	MN	X	3166	1/1	0.99	0.30	-	90,90,90,90	0
31	MG	X	3321	1/1	0.89	0.52	-	80,80,80,80	0
32	MN	X	3175	1/1	0.98	0.20	-	86,86,86,86	0
31	MG	X	3397	1/1	0.79	0.40	-	95,95,95,95	0
31	MG	X	3387	1/1	0.86	0.29	-	60,60,60,60	0
31	MG	X	3391	1/1	0.83	0.35	-	73,73,73,73	0
31	MG	X	3375	1/1	0.87	0.18	-	69,69,69,69	0
32	MN	X	3222	1/1	0.79	1.24	-	171,171,171,171	0
31	MG	X	3299	1/1	0.90	0.07	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MN	X	3068	1/1	0.77	0.15	-	130,130,130,130	0
32	MN	X	3115	1/1	0.70	0.28	-	135,135,135,135	0
31	MG	X	3389	1/1	0.62	0.29	-	66,66,66,66	0
32	MN	X	3088	1/1	0.86	0.15	-	110,110,110,110	0
32	MN	X	3081	1/1	0.98	0.30	-	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.