



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 7, 2023 – 09:01 PM EST

PDB ID : 2ZJP  
Title : Thiopeptide antibiotic Nosiheptide bound to the large ribosomal subunit of *Deinococcus radiodurans*  
Authors : Harms, J.M.; Wilson, D.N.; Schluenzen, F.; Connell, S.R.; Stachelhaus, T.; Zaborowska, Z.; Spahn, C.M.T.; Fucini, P.  
Deposited on : 2008-03-07  
Resolution : 3.70 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

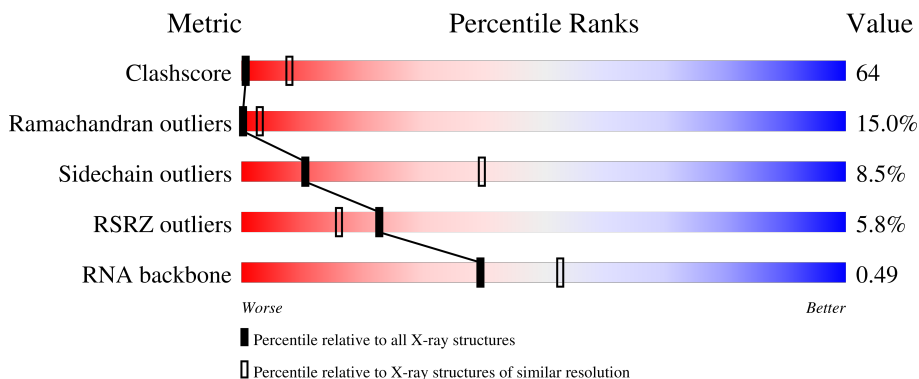
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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.



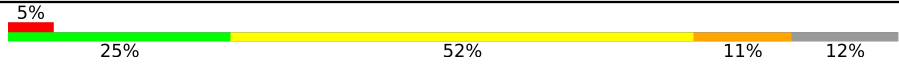
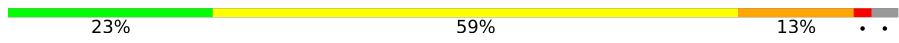

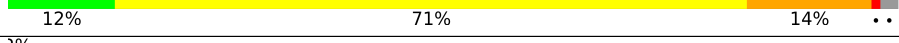
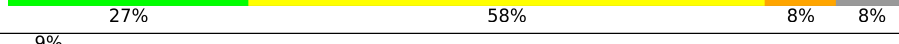
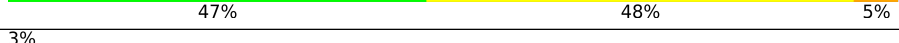
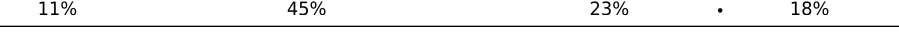
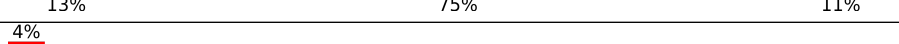
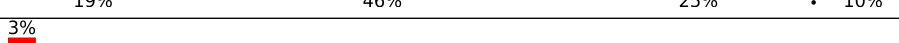
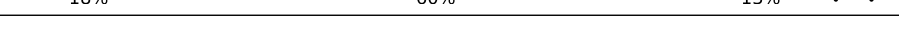
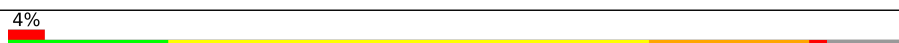

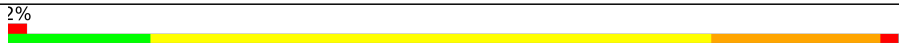

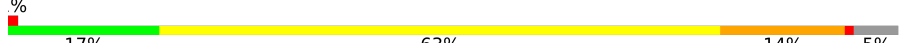
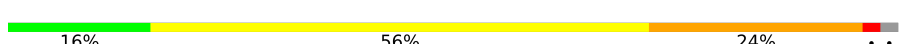
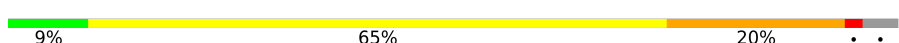

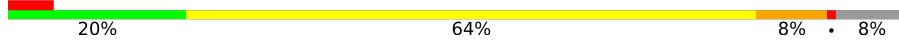
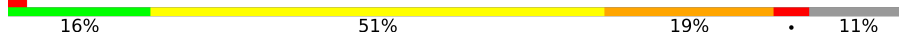
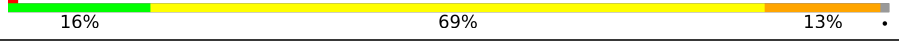
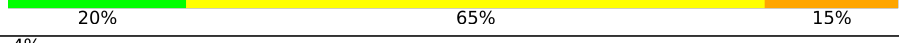

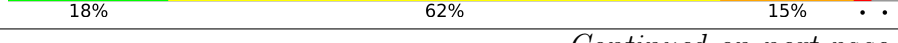

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	1	55	
2	2	47	
3	3	66	
4	4	37	
5	5	13	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	A	274	
7	B	211	
8	C	205	
9	D	180	
10	E	185	
11	F	144	
12	G	174	
13	H	134	
14	I	156	
15	J	142	
16	K	116	
17	L	114	
18	M	166	
19	N	118	
20	O	100	
21	P	134	
22	Q	95	
23	R	115	
24	S	237	
25	T	91	
26	U	81	
27	V	67	
28	W	55	
29	X	2880	
30	Y	60	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
31	Z	123	

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
34	MG	X	2883	-	-	-	X
34	MG	X	2889	-	-	-	X
34	MG	X	2891	-	-	-	X
34	MG	X	2903	-	-	-	X
34	MG	X	2908	-	-	-	X
34	MG	Z	127	-	-	-	X
5	MH6	5	10	-	X	-	-
5	DHA	5	12	-	X	-	-
5	DBU	5	4	-	X	-	-
5	BB9	5	7	-	-	-	X

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 84444 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 L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	1	53	Total C 53 53	0	0	53

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	2	46	Total C 46 46	0	0	46

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	3	63	Total C 63 63	0	0	63

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 5 is a protein called NOSIHEPTIDE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	5	13	Total C N O S 69 40 12 11 6	0	0	1

- Molecule 6 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	A	240	Total C N O S 1826 1137 366 321 2	0	0	0

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	B	205	1539	965	295	271	8	0	0	0

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	C	197	1506	935	287	282	2	0	0	0

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	D	177	1400	892	247	254	7	0	0	0

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	E	171	1286	812	237	236	1	0	0	0

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	F	144	1044	663	179	197	5	0	0	0

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	G	142	1114	704	209	198	3	0	0	0

- Molecule 13 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	H	134	997	614	198	180	5	0	0	0

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	I	141	1067	655	216	196	0	0	0

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	J	136	1090	696	202	185	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q9RXJ5

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	K	113	878	541	178	157	2	0	0	0

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	L	104	779	476	161	142	0	0	0

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	M	108	871	543	172	156	0	0	0

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	N	117	978	608	210	159	1	0	0	0

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	O	94	741	465	139	137	0	0	0

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	P	127	1014	639	199	174	2	0	0	0

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	Q	93	726	458	136	130	2	0	0	0

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	R	110	825	513	160	151	1	0	0	0

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	S	175	1345	849	236	254	6	0	0	0

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	T	84	625	393	122	109	1	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
26	U	72	552	341	116	95	0	0	0

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	V	66	533	327	107	96	3	0	0	0

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	W	55	424	264	82	76	2	0	0	0

- Molecule 29 is a RNA chain called RIBOSOMAL 23S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
29	X	2686	57651	25718	10642	18606	2685	0	0	0

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	Y	58	457	281	94	77	5	0	0	0

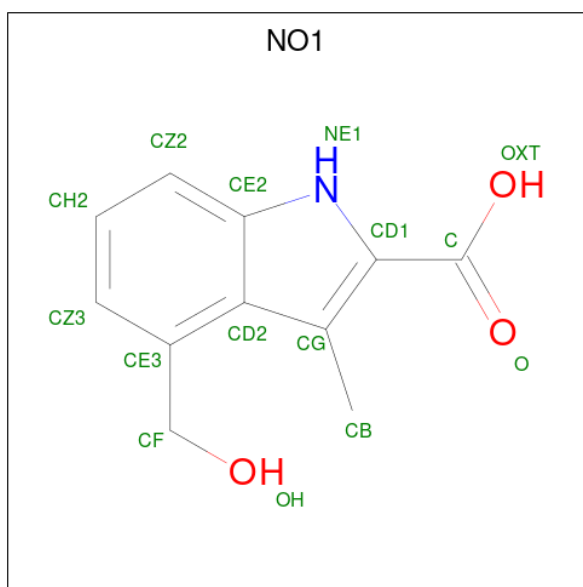
- Molecule 31 is a RNA chain called RIBOSOMAL 5S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
31	Z	122	2598	1161	476	840	121	0	0	0

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	4	1	Total	Zn	0	0
			1	1		
32	Y	1	Total	Zn	0	0
			1	1		

- Molecule 33 is 4-(hydroxymethyl)-3-methyl-1H-indole-2-carboxylic acid (three-letter code: NO1) (formula: C<sub>11</sub>H<sub>11</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
33	5	1	13	11	1	1	0	0

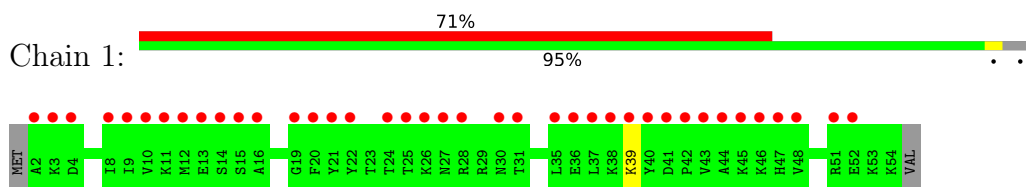
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
34	M	1	1	1	0	0
34	X	28	28	28	0	0
34	Z	6	6	6	0	0

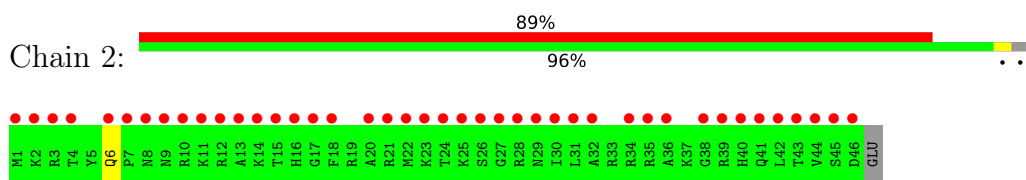
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

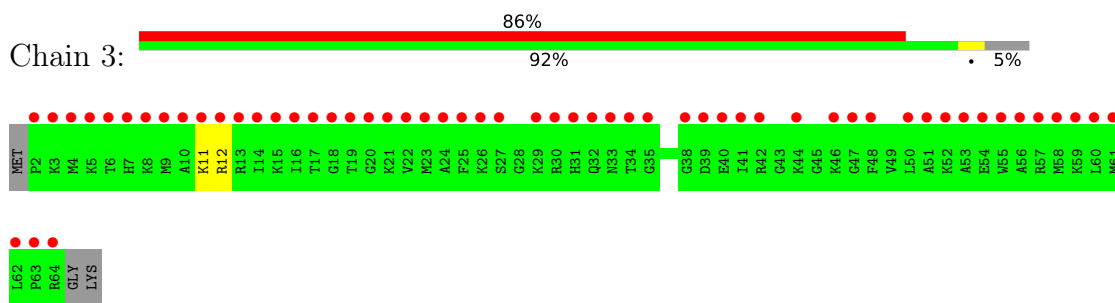
- Molecule 1: 50S RIBOSOMAL PROTEIN L33



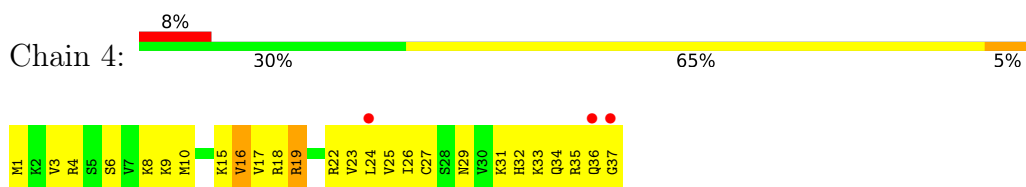
- Molecule 2: 50S RIBOSOMAL PROTEIN L34



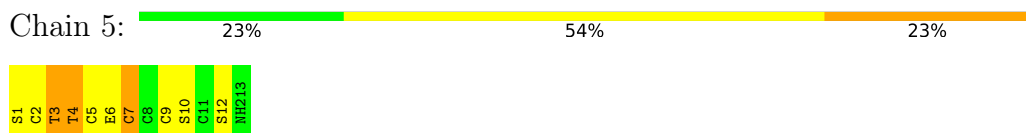
- Molecule 3: 50S RIBOSOMAL PROTEIN L35



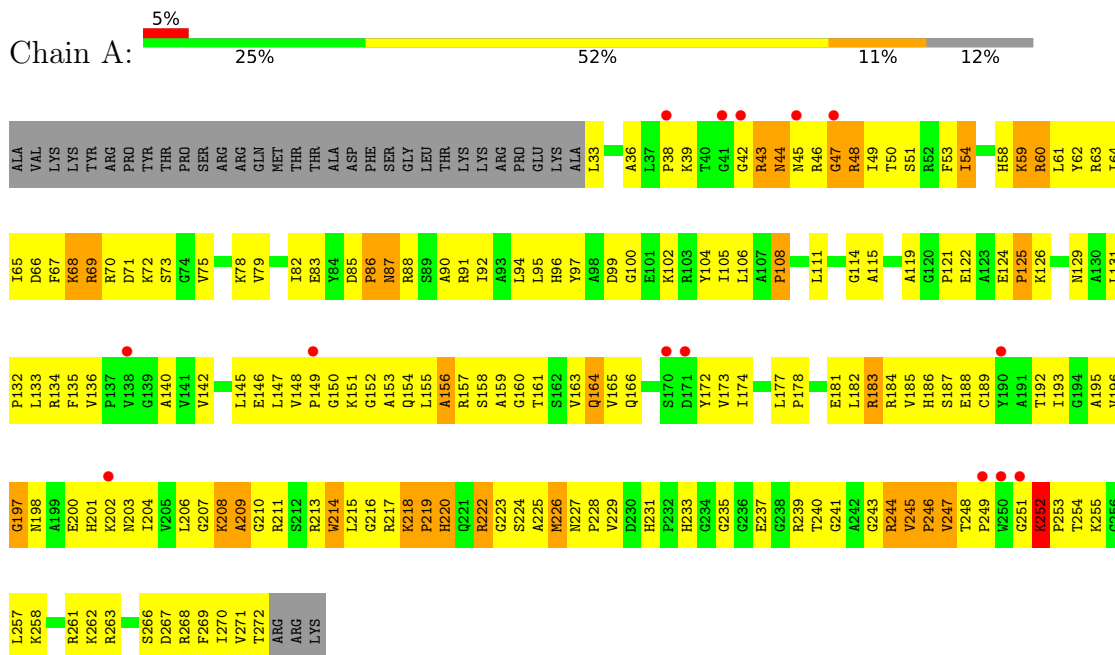
- Molecule 4: 50S RIBOSOMAL PROTEIN L36



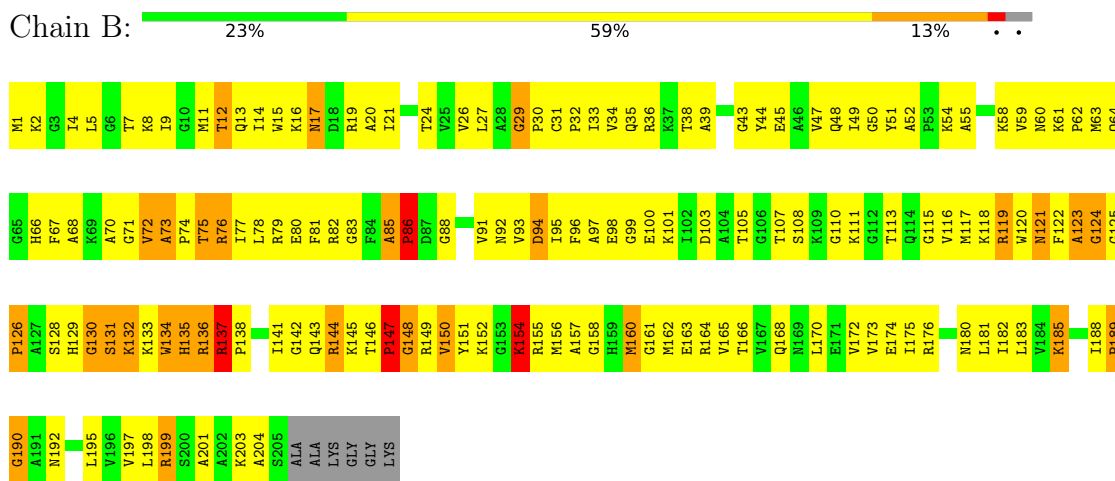
- Molecule 5: NOSIHEPTIDE



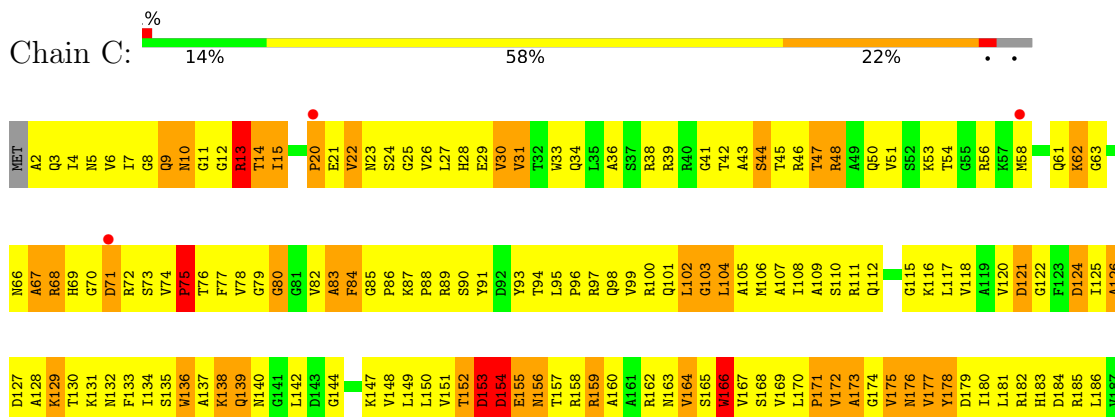
• Molecule 6: 50S RIBOSOMAL PROTEIN L2



• Molecule 7: 50S RIBOSOMAL PROTEIN L3

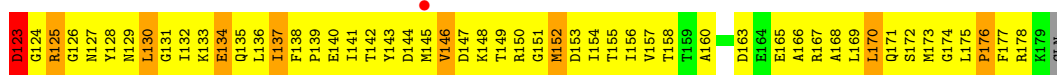


• Molecule 8: 50S RIBOSOMAL PROTEIN L4

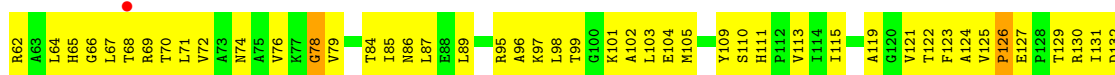
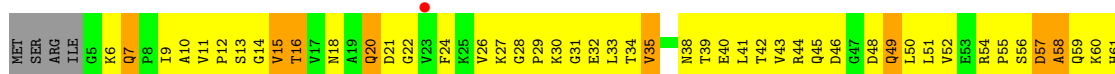




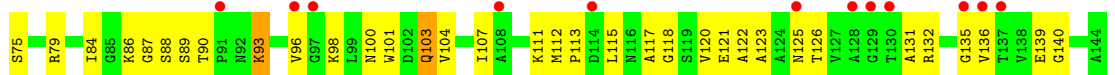
• Molecule 9: 50S RIBOSOMAL PROTEIN L5



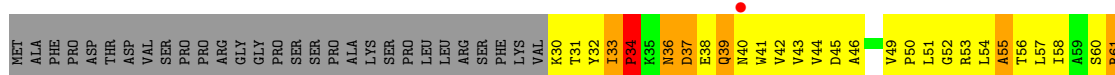
• Molecule 10: 50S RIBOSOMAL PROTEIN L6

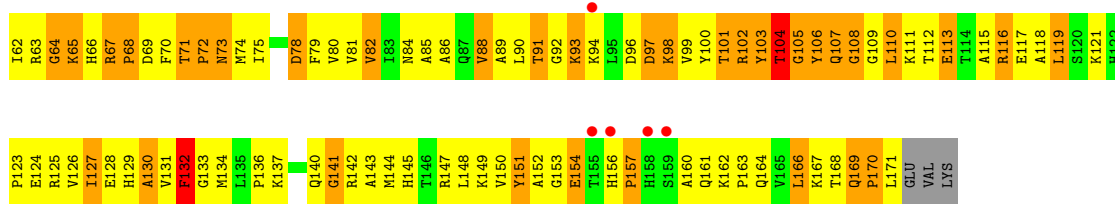


• Molecule 11: 50S RIBOSOMAL PROTEIN L11

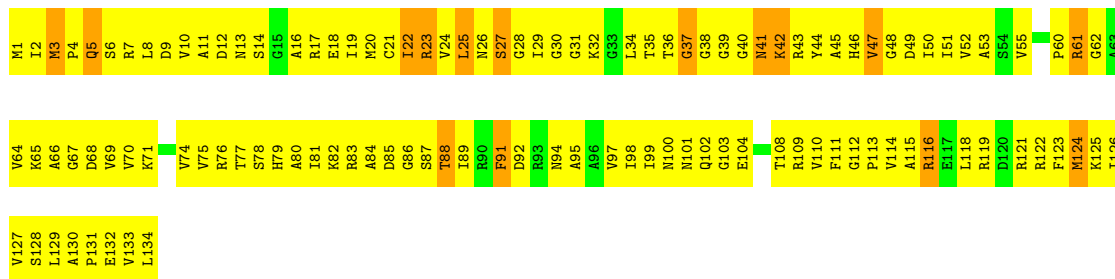


• Molecule 12: 50S RIBOSOMAL PROTEIN L13

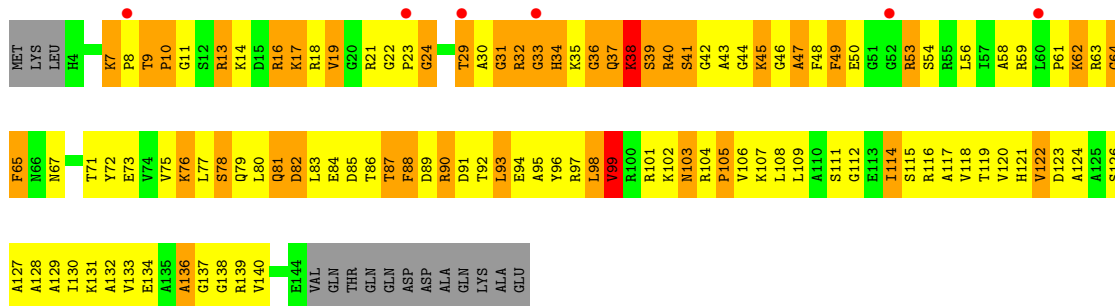
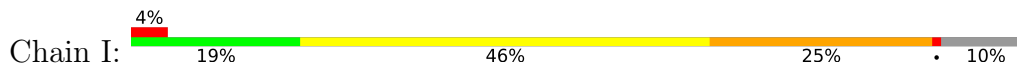




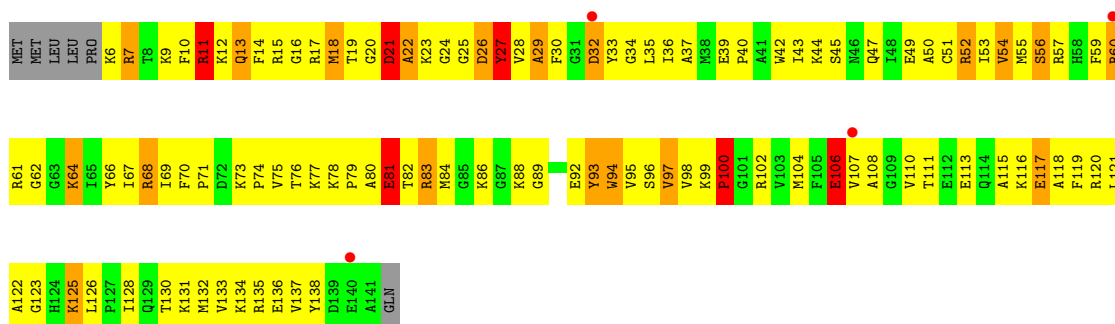
● Molecule 13: 50S RIBOSOMAL PROTEIN L14



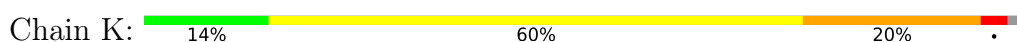
● Molecule 14: 50S RIBOSOMAL PROTEIN L15



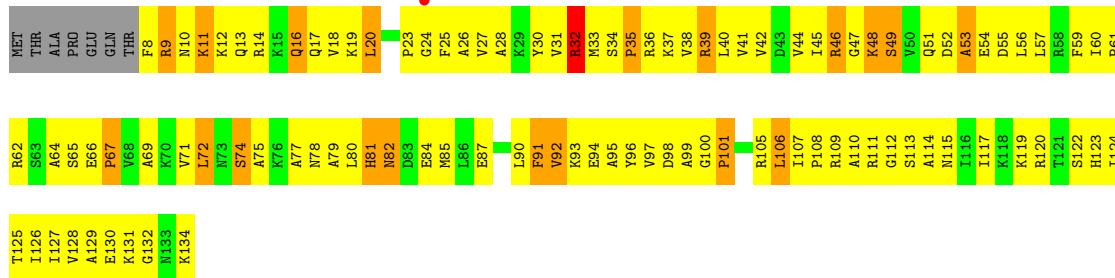
● Molecule 15: 50S RIBOSOMAL PROTEIN L16



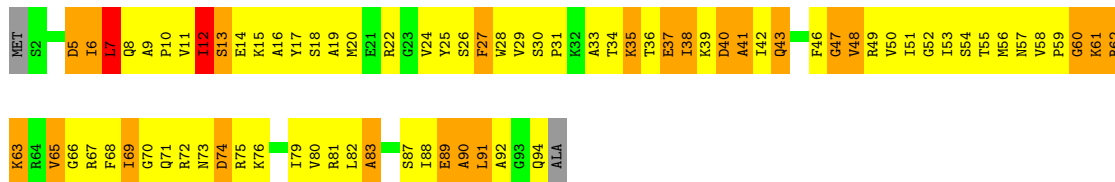
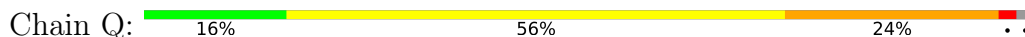
● Molecule 16: 50S RIBOSOMAL PROTEIN L17



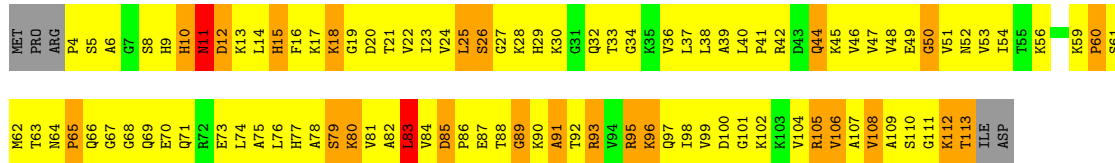
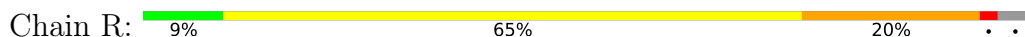




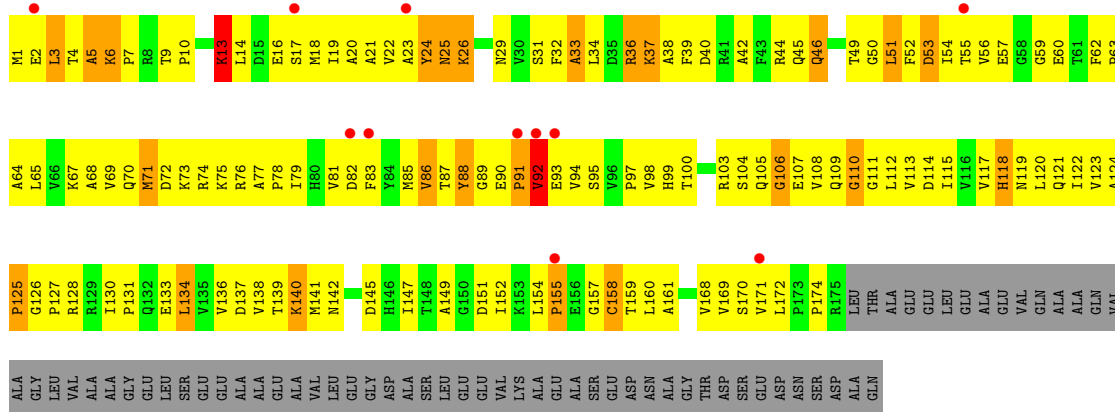
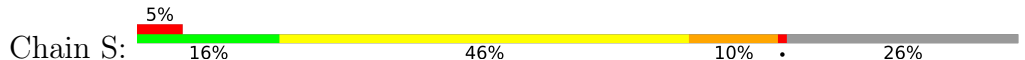
• Molecule 22: 50S RIBOSOMAL PROTEIN L23



• Molecule 23: 50S RIBOSOMAL PROTEIN L24

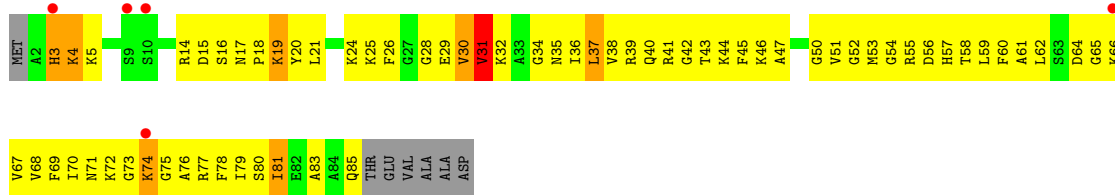


• Molecule 24: 50S RIBOSOMAL PROTEIN L25

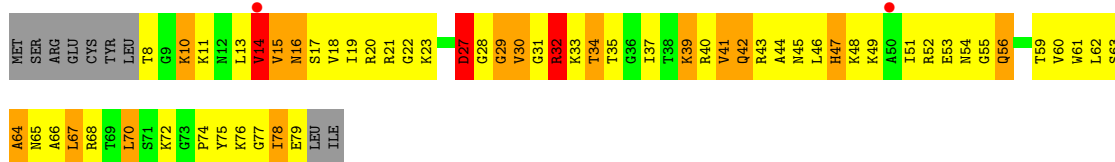
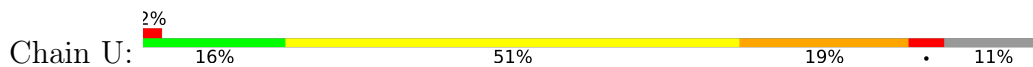


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

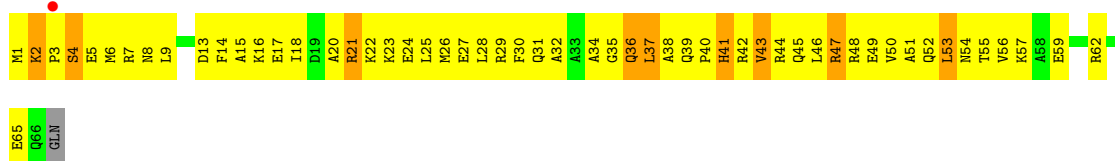




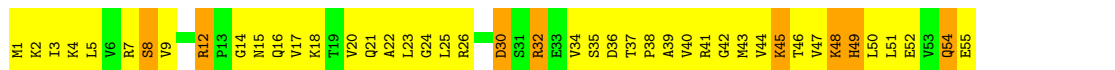
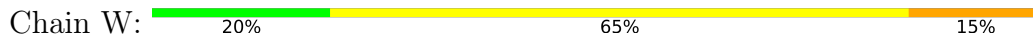
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



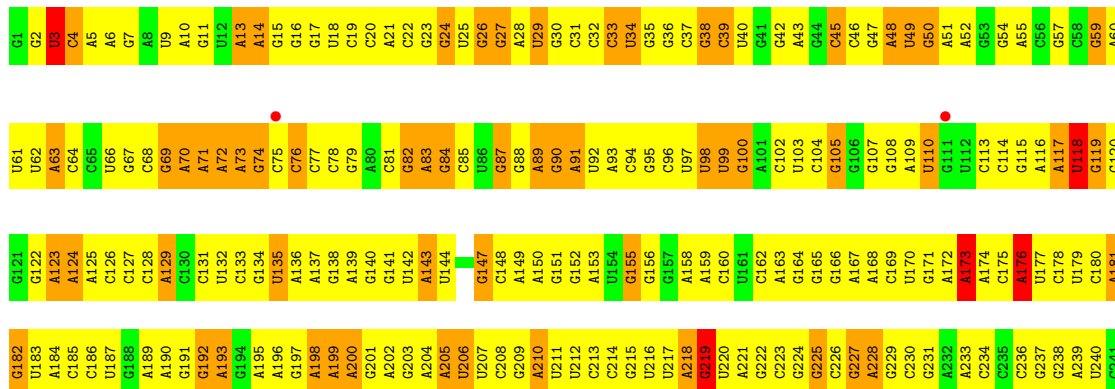
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30



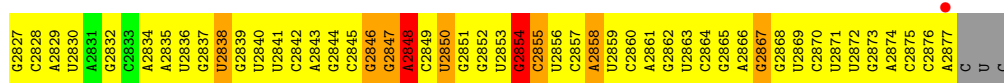
• Molecule 29: RIBOSOMAL 23S RNA



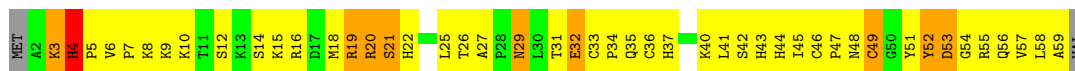
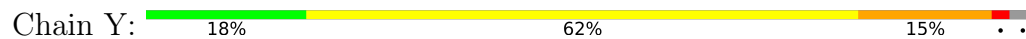
U1034	U1035	U1037	U1038	U1039	U1040	U1041	U1042	U1043	U1044	U1045	U1046	U1047	U1048	U1049	U1050	U1051	U1052	U1053	U1054	U1055	U1056	U1057	U1058	U1059	U1060	U1061	U1062	U1063	U1064	U1065	U1066	U1067	U1068	U1069	U1070	U1071	U1072	U1073	U1074	U1075	U1076	U1077	U1078	U1079	U1080	U1081	U1082	U1083	U1084	U1085	U1086	U1087	U1088	U1089	U1090	U1091	U1092	U1093																																																																																																																																																																																																																																																																																																																																																											
U973	U974	C975	C976	C977	U978	A979	G980	C981	C982	C983	A984	A985	A986	C987	C988	C989	A990	A991	A992	C993	A994	A995	A996	C997	C998	A999	G1000	A1001	C1002	C1003	A1004	U1005	C1006	A1007	C1008	C1009	U1010	A1011	A1012	G1013	G1014	U1015	U1016	C1017	U1018	U1019	C959	U960	G961	C962	C963	A964	C965	A966	C1027	C968	C969	U1030	C1031	A1032	G1033																																																																																																																																																																																																																																																																																																																																																								
A913	C914	C915	U916	U917	U918	U919	G920	A921	A922	A923	C924	U925	U926	C926	C927	G928	A929	A930	C931	C932	C933	C934	C935	A936	C937	C938	C939	A940	U941	U942	U943	A944	G945	U946	C947	C948	G949	C950	G951	A952	G953	U954	C955	A956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033																																																																																																																																																																																																																																																																																												
A851	U852	G853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033																																																																																																																																																																																																																															
A790	G791	U792	U793	U794	U795	U796	U797	U798	U799	U800	A801	A802	C803	C804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033																																																																																																																																																																		
A729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1011	U1012	U1013	U1014	U1015	U1016	U1017	U1018	U1019	U1020	U1021	U1022	U1023	U1024	U1025	U1026	U1027	U1028	U1029	U1030	U1031	U1032	U1033																																																																																																					
A606	U607	G608	U609	C610	C611	C612	A613	A614	C615	U616	U617	A618	A619	G620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	A632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	C651	C652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000	U1001	U1002	U1003	U1004	U1005	U1006	U1007	U1008	U1009	U1010	U1

G	C1094	G1155	G1219	G1279	U1339	G1402	A1463	U1526	G1589	C1653	A1718	U1778	G1842	G	C1945
G	A1095	U1159	G1220	U1280	C1940	U1403	A1464	G1527	U1527	A1654	G1716	C1779	U1843	G	C1946
U	A1096	C1160	C1221	A1281	G1941	U1404	A1465	C1528	U1592	C1655	A1717	C1779	C1844	C	C1947
C	A1097	C1166	G1222	A1282	U1942	A1405	C1466	C1593	C1594	C1656	G1722	C1781	A1845	U	C1948
C	G1098	U1161	A1223	C1283	C1943	A1406	U1467	U1530	A1596	A1658	U1723	A1782	A1846	C	C1949
A	A1099	A1162	G1224	G1284	C1944	G1407	A1468	A1597	A1598	C1659	C1724	G1783	U1943	U	C1950
U	G1100	C1163	G1225	A1285	G1945	A1408	U1469	A1599	C1599	C1660	C1725	A1785	G1849	U	C1951
U	U1101	C1164	G1226	U1286	C1946	U1409	G1470	U1534	C1598	C1661	C1726	A1786	G1850	U	C1952
C	U1102	G1165	A1227	U1287	C1947	U1410	A1471	C1535	C1598	C1662	C1727	C1786	G1851	U	C1953
C	U1103	G1166	G1228	U1288	C1948	C1411	U1472	C1536	C1599	C1663	A1728	U1787	A1851	U	C1954
C	A1106	A1167	C1229	A1289	A1949	A1412	C1473	U1537	U1600	G1663	A1729	C1788	G1852	U	C1955
U	U1107	A1168	G1230	U1290	C1950	U1413	A1474	A1538	A1538	C1664	G1729	U1789	G1853	U	C1956
U	U1108	C1169	A1231	G1291	G1951	G1414	U1475	U1539	G1601	C1665	C1730	G1790	G1854	U	C1957
U	U1109	C1170	U1232	U1292	C1952	C1415	G1476	C1540	A1603	G1666	C1731	C1791	G1855	U	C1958
U	U1110	A1171	A1233	A1293	A1953	U1416	U1477	G1541	A1604	G1667	U1732	C1792	G1856	U	C1959
U	G1110	U1172	C1234	U1294	A1954	C1417	U1478	G1542	U1607	G1668	U1733	C1793	G1857	U	C1960
U	C1111	A1173	G1235	U1295	A1955	A1418	G1479	G1543	A1608	A1669	C1734	A1794	G1858	U	C1961
U	U1112	G1174	G1236	U1296	A1956	G1419	U1480	U1551	U1612	G1670	G1735	C1795	A1859	U	C1962
U	C1113	A1175	G1237	A1297	U1957	A1420	U1481	G1552	G1614	U1671	C1736	A1796	A1860	U	C1963
U	U1114	U1176	A1238	G1298	U1958	U1421	U1482	U1547	C1615	C1672	G1737	C1797	A1861	U	C1964
U	U1115	U1177	A1239	U1299	G1959	U1422	U1483	U1548	U1611	C1673	U1738	C1798	G1862	U	C1965
U	U1116	C1178	G1240	U1300	C1363	A1423	U1484	U1549	U1612	U1674	G1739	A1800	C1863	U	C1966
U	G1117	A1179	G1241	U1301	C1364	A1424	U1485	C1550	U1613	C1675	G1740	C1801	G1864	U	C1967
U	U1118	A1180	G1242	U1302	C1365	U1425	U1486	U1551	G1614	U1676	G1741	A1802	G1865	U	C1968
U	U1119	C1181	G1243	U1303	U1365	G1426	C1487	G1552	C1615	C1677	G1742	G1803	G1866	U	C1969
U	C1120	U1182	U1244	U1304	U1366	G1427	G1488	G1554	U1615	C1678	C1743	U1804	A1867	U	C1970
U	G1121	C1183	G1245	U1305	A1367	U1428	U1489	A1555	U1618	U1679	G1744	G1805	A1868	U	C1971
U	U1122	G1184	G1246	C1306	A1368	A1429	U1490	A1556	U1619	U1680	G1745	G1806	A1869	U	C1972
U	U1123	C1185	U1247	U1307	C1369	G1430	C1491	U1557	U1620	U1681	A1746	A1807	U1870	U	C1973
U	U1124	G1186	G1248	U1308	U1370	U1431	U1492	U1558	C1621	A1682	G1747	C1808	G1871	U	C1974
U	G1125	A1187	G1249	U1309	C1371	G1432	U1493	G1559	G1622	G1683	U1748	G1809	A1872	U	C1975
U	A1126	U1188	A1250	U1310	A1372	U1433	G1494	U1560	G1623	C1684	G1749	U1810	A1873	U	C1976
U	U1127	G1189	G1251	C1311	G1373	U1434	U1495	A1561	A1624	A1685	A1750	A1811	G1874	U	C1977
U	G1128	C1190	C1252	U1312	G1374	G1435	G1496	U1562	U1625	C1686	A1751	A1812	U1875	U	C1978
U	U1129	G1191	C1253	U1313	C1375	G1436	C1497	G1563	A1626	C1687	U1752	A1813	C1876	U	C1979
U	U1130	A1192	G1254	U1314	C1376	A1437	G1498	U1564	C1627	U1688	A1753	G1814	G1877	U	C1980
U	G1131	G1193	A1255	A1315	C1377	G1438	A1499	G1565	G1628	U1689	G1754	G1815	G1878	U	C1981
U	C1132	U1194	C1256	G1316	C1378	G1439	U1500	G1566	G1629	U1690	G1755	G1816	G1879	U	C1982
U	U1133	U1195	U1257	G1317	A1379	G1440	C1501	A1567	A1630	C1691	G1756	U1817	G1880	U	C1983
U	C1134	G1196	G1258	U1318	C1380	A1441	U1502	A1568	C1631	C1692	C1757	G1818	G1881	U	C1984
U	G1135	U1197	A1259	C1319	G1381	C1442	G1503	A1569	A1632	A1693	C1758	U1819	A1882	U	C1985
U	U1136	C1198	U1260	U1320	G1382	G1443	U1504	C1570	C1633	A1694	A1759	G1820	C1883	U	C1986
U	A1137	U1199	G1261	A1321	C1383	C1444	U1505	G1571	A1634	U1695	G1760	A1821	G1884	U	C1987
U	U1138	G1200	U1262	G1322	G1384	A1445	C1506	C1572	A1635	C1696	C1761	C1822	G1885	U	C1988
U	A1139	G1201	G1263	U1323	C1385	U1446	A1507	G1573	G1636	C1697	C1762	G1825	C1886	U	C1989
U	U1140	U1202	C1264	G1324	A1386	U1447	G1508	A1574	A1637	A1699	G1763	C1826	G1887	U	C1990
U	U1141	A1203	G1265	U1325	G1387	A1448	A1509	C1575	G1638	C1700	A1764	U1826	G1888	U	C1991
U	G1142	G1204	G1266	U1326	C1388	C1449	A1510	G1576	U1639	C1701	C1765	G1827	A1952	U	C1992
U	U1143	U1205	A1267	G1327	C1389	G1450	A1511	G1577	C1640	U1706	U1766	C1830	A1953	U	C1993
U	U1144	G1206	U1268	C1328	G1390	C1451	A1512	U1578	C1641	G1704	G1767	C1831	G1955	U	C1994
U	C1145	C1210	G1269	U1329	A1391	U1452	U1513	G1579	G1644	U1705	U1768	G1832	G1956	U	C1995
U	G1146	C1211	C1270	G1330	U1392	U1453	U1514	C1580	G1644	A1706	U1769	G1833	C1957	U	C1996
U	G1147	C1212	C1271	U1331	U1393	U1454	U1515	U1454	U1645	A1707	U1770	C1834	C1958	U	C1997
U	G1148	U1212	G1272	G1332	G1394	C1455	A1516	A1455	G1646	C1708	A1771	C1835	U1959	U	C1998
U	C1149	C1213	G1273	G1333	G1395	C1456	C1517	A1456	A1647	U1709	C1772	C1836	U1960	U	C1999
U	U1150	U1214	C1274	A1395	A1395	C1456	C1517	G1584	C1648	U1710	C1773	G1837	A1961	U	C2000
U	U1151	A1215	A1275	A1334	A1334	C1456	C1517	G1585	A1649	C1711	A1774	G1838	A1962	U	C2001
U	C1152	G1216	A1276	A1335	A1335	U1459	U1522	A1585	A1649	C1712	A1775	G1839	G1963	U	C2002
U	U1217	G1277	A1277	A1336	A1336	G1460	A1523	A1586	A1650	G1713	A1776	A1839	U1964	U	C2003
U	A1153	G1218	G1278	U1337	A1400	G1462	C1524	A1587	A1651	G1714	A1777	A1840	G1965	U	C2004
U	U1154	C1218	A1278	G1338	G1401	C1462	A1525	A1588	G1652	A1714	A1777	G1841	U1966	U	C2005

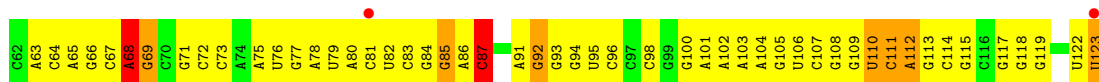
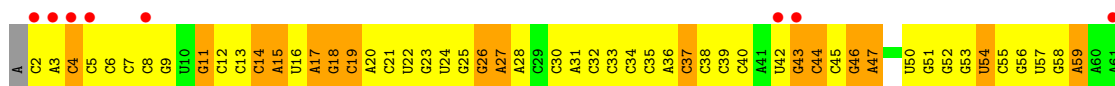
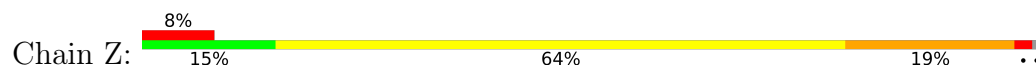




- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 31: RIBOSOMAL 5S RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.90Å 408.90Å 694.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.70 29.75 – 3.61	Depositor EDS
% Data completeness (in resolution range)	85.6 (30.00-3.70) 87.2 (29.75-3.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.65Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.300 , 0.340 0.323 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	109.2	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 129.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	84444	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	114.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DHA, BB9, MH6, NO1, ZN, 3GL, DBU, MG, NH2

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
4	4	0.48	0/298	0.63	0/390
5	5	3.86	2/12 (16.7%)	2.59	1/12 (8.3%)
6	A	0.46	0/1862	0.66	0/2510
7	B	0.73	0/1567	0.93	0/2105
8	C	0.54	0/1529	0.75	0/2070
9	D	0.40	0/1419	0.62	0/1903
10	E	0.42	0/1308	0.64	0/1771
11	F	0.42	0/1063	0.57	0/1440
12	G	0.57	0/1138	0.79	1/1539 (0.1%)
13	H	0.81	0/1007	1.03	1/1352 (0.1%)
14	I	0.51	0/1081	0.76	0/1448
15	J	0.60	0/1113	0.82	1/1486 (0.1%)
16	K	0.84	0/886	1.07	0/1188
17	L	0.48	0/785	0.72	0/1048
18	M	0.76	0/884	1.03	1/1186 (0.1%)
19	N	0.60	0/994	0.79	1/1323 (0.1%)
20	O	0.55	0/750	0.79	0/1000
21	P	0.72	0/1027	0.95	1/1373 (0.1%)
22	Q	0.52	0/737	0.70	0/988
23	R	0.47	0/835	0.76	0/1121
24	S	0.46	0/1370	0.66	0/1862
25	T	0.50	0/633	0.72	0/838
26	U	0.46	0/556	0.75	0/741
27	V	0.46	0/537	0.62	0/714
28	W	0.59	0/426	0.83	0/568
29	X	0.84	68/64561 (0.1%)	1.00	396/100708 (0.4%)
30	Y	0.69	0/469	0.95	1/629 (0.2%)
31	Z	0.58	1/2904 (0.0%)	0.76	0/4525
All	All	0.77	71/91751 (0.1%)	0.95	404/137838 (0.3%)

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
5	5	1	0
19	N	0	1
29	X	1	199
30	Y	0	1
31	Z	0	4
All	All	2	205

The worst 5 of 71 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	1	SER	CA-CB	-10.07	1.37	1.52
29	X	2533	U	N1-C2	9.78	1.47	1.38
29	X	2492	G	C5-C6	-9.33	1.33	1.42
29	X	2533	U	C4-C5	8.27	1.50	1.43
29	X	2424	G	C5-C6	-7.50	1.34	1.42

The worst 5 of 404 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1055	A	N9-C1'-C2'	-28.05	77.53	114.00
29	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
29	X	417	C	N1-C1'-C2'	17.87	137.23	114.00
29	X	558	G	C3'-C2'-C1'	-13.92	90.37	101.50
29	X	556	A	N9-C1'-C2'	12.66	130.46	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	5	1	SER	CA
29	X	2592	U	C1'

5 of 205 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
19	N	32	TYR	Sidechain
29	X	228	A	Sidechain
29	X	24	G	Sidechain
29	X	26	G	Sidechain
29	X	321	A	Sidechain



## 5.2 Too-close contacts [i](#)

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	1	53	0	0	2	0
2	2	46	0	0	1	0
3	3	63	0	0	2	0
4	4	297	0	328	63	0
5	5	69	0	34	3	0
6	A	1826	0	1885	312	0
7	B	1539	0	1600	305	0
8	C	1506	0	1525	334	0
9	D	1400	0	1481	313	0
10	E	1286	0	1336	201	0
11	F	1044	0	1088	101	0
12	G	1114	0	1144	278	0
13	H	997	0	1046	205	0
14	I	1067	0	1103	244	0
15	J	1090	0	1125	258	0
16	K	878	0	930	205	0
17	L	779	0	820	180	0
18	M	871	0	894	218	0
19	N	978	0	1020	200	0
20	O	741	0	756	191	0
21	P	1014	0	1096	200	0
22	Q	726	0	753	142	0
23	R	825	0	881	212	0
24	S	1345	0	1372	221	0
25	T	625	0	655	118	0
26	U	552	0	604	150	0
27	V	533	0	558	88	0
28	W	424	0	470	67	0
29	X	57651	0	29048	4666	0
30	Y	457	0	460	109	0
31	Z	2598	0	1328	176	0
32	4	1	0	0	0	0
32	Y	1	0	0	0	0
33	5	13	0	7	0	0
34	M	1	0	0	0	0
34	X	28	0	0	0	0
34	Z	6	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	84444	0	55347	8931	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 64.

The worst 5 of 8931 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:M:108:ARG:O	18:M:109:GLU:HG3	1.25	1.33
29:X:1854:G:O2'	29:X:1855:G:H5'	1.31	1.28
29:X:1053:G:H2'	29:X:1054:C:C6	1.71	1.25
29:X:1386:A:H5''	29:X:2191:A:N6	1.48	1.25
29:X:2196:U:H2'	29:X:2197:U:O4'	1.31	1.23

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
4	4	35/37 (95%)	20 (57%)	12 (34%)	3 (9%)	<a href="#">1</a> <a href="#">10</a>
5	5	2/13 (15%)	1 (50%)	1 (50%)	0	<a href="#">100</a> <a href="#">100</a>
6	A	238/274 (87%)	166 (70%)	51 (21%)	21 (9%)	<a href="#">1</a> <a href="#">10</a>
7	B	203/211 (96%)	143 (70%)	33 (16%)	27 (13%)	<a href="#">0</a> <a href="#">4</a>
8	C	195/205 (95%)	94 (48%)	55 (28%)	46 (24%)	<a href="#">0</a> <a href="#">0</a>
9	D	175/180 (97%)	99 (57%)	50 (29%)	26 (15%)	<a href="#">0</a> <a href="#">3</a>
10	E	169/185 (91%)	110 (65%)	40 (24%)	19 (11%)	<a href="#">0</a> <a href="#">5</a>
11	F	142/144 (99%)	101 (71%)	33 (23%)	8 (6%)	<a href="#">2</a> <a href="#">19</a>
12	G	140/174 (80%)	76 (54%)	34 (24%)	30 (21%)	<a href="#">0</a> <a href="#">1</a>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	H	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	1	18
14	I	139/156 (89%)	60 (43%)	41 (30%)	38 (27%)	0	0
15	J	134/142 (94%)	76 (57%)	41 (31%)	17 (13%)	0	4
16	K	111/116 (96%)	70 (63%)	23 (21%)	18 (16%)	0	3
17	L	102/114 (90%)	65 (64%)	23 (22%)	14 (14%)	0	3
18	M	106/166 (64%)	64 (60%)	22 (21%)	20 (19%)	0	1
19	N	115/118 (98%)	65 (56%)	30 (26%)	20 (17%)	0	2
20	O	92/100 (92%)	52 (56%)	23 (25%)	17 (18%)	0	1
21	P	125/134 (93%)	84 (67%)	26 (21%)	15 (12%)	0	5
22	Q	91/95 (96%)	45 (50%)	25 (28%)	21 (23%)	0	0
23	R	108/115 (94%)	61 (56%)	28 (26%)	19 (18%)	0	2
24	S	173/237 (73%)	96 (56%)	50 (29%)	27 (16%)	0	3
25	T	82/91 (90%)	56 (68%)	16 (20%)	10 (12%)	0	4
26	U	70/81 (86%)	34 (49%)	19 (27%)	17 (24%)	0	0
27	V	64/67 (96%)	44 (69%)	12 (19%)	8 (12%)	0	4
28	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	13
30	Y	56/60 (93%)	35 (62%)	15 (27%)	6 (11%)	0	6
All	All	3052/3404 (90%)	1859 (61%)	734 (24%)	459 (15%)	0	3

5 of 459 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	54	ILE
6	A	59	LYS
7	B	76	ARG
7	B	85	ALA
7	B	86	PRO

### 5.3.2 Protein sidechains [i](#)

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	
4	4	35/35 (100%)	35 (100%)	0	100	100
5	5	2/3 (67%)	2 (100%)	0	100	100
6	A	185/215 (86%)	170 (92%)	15 (8%)	11	41
7	B	155/157 (99%)	145 (94%)	10 (6%)	17	48
8	C	157/163 (96%)	146 (93%)	11 (7%)	15	45
9	D	153/156 (98%)	145 (95%)	8 (5%)	23	55
10	E	136/144 (94%)	133 (98%)	3 (2%)	52	72
11	F	107/107 (100%)	103 (96%)	4 (4%)	34	61
12	G	118/146 (81%)	100 (85%)	18 (15%)	2	17
13	H	103/103 (100%)	94 (91%)	9 (9%)	10	38
14	I	108/121 (89%)	99 (92%)	9 (8%)	11	40
15	J	110/116 (95%)	94 (86%)	16 (14%)	3	18
16	K	90/93 (97%)	74 (82%)	16 (18%)	2	12
17	L	74/82 (90%)	62 (84%)	12 (16%)	2	15
18	M	94/134 (70%)	79 (84%)	15 (16%)	2	15
19	N	96/97 (99%)	91 (95%)	5 (5%)	23	55
20	O	75/79 (95%)	70 (93%)	5 (7%)	16	47
21	P	109/115 (95%)	101 (93%)	8 (7%)	14	44
22	Q	75/76 (99%)	68 (91%)	7 (9%)	9	35
23	R	91/96 (95%)	79 (87%)	12 (13%)	4	22
24	S	149/192 (78%)	141 (95%)	8 (5%)	22	54
25	T	62/67 (92%)	59 (95%)	3 (5%)	25	56
26	U	57/66 (86%)	50 (88%)	7 (12%)	4	24
27	V	54/55 (98%)	52 (96%)	2 (4%)	34	61
28	W	48/48 (100%)	44 (92%)	4 (8%)	11	40
30	Y	51/53 (96%)	46 (90%)	5 (10%)	8	33
All	All	2494/2719 (92%)	2282 (92%)	212 (8%)	10	40

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	K	97	ILE
18	M	90	GLN
26	U	70	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
17	L	8	ARG
17	L	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
24	S	146	HIS
25	T	57	HIS
30	Y	29	ASN
14	I	34	HIS
13	H	79	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2680/2880 (93%)	653 (24%)	239 (8%)
31	Z	121/123 (98%)	24 (19%)	1 (0%)
All	All	2801/3003 (93%)	677 (24%)	240 (8%)

5 of 677 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	4	C
29	X	13	A
29	X	14	A
29	X	27	G
29	X	29	U

5 of 240 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1299	A
29	X	2660	C
29	X	1632	A
29	X	2593	A
29	X	2848	A

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

Of 10 non-standard protein/DNA/RNA residues modelled in this entry, 1 is modelled with single atom - leaving 9 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
5	DBU	5	4	5	4,4,6	4.92	4 (100%)	4,4,7	2.20	1 (25%)
5	BB9	5	9	5	2,4,6	1.52	1 (50%)	3,4,7	2.11	2 (66%)
5	MH6	5	10	5	3,4,6	3.22	1 (33%)	2,4,7	3.95	2 (100%)
5	BB9	5	5	5	3,5,6	4.14	1 (33%)	1,5,7	0.14	0
5	DHA	5	12	5	4,4,5	4.99	2 (50%)	2,4,6	2.86	2 (100%)
5	BB9	5	7	5	3,5,6	3.15	2 (66%)	1,5,7	4.72	1 (100%)
5	BB9	5	11	5	3,5,6	0.69	0	1,5,7	1.85	0
5	BB9	5	2	5	3,5,6	6.54	2 (66%)	1,5,7	5.98	1 (100%)
5	3GL	5	6	5,33	8,8,10	4.24	6 (75%)	10,10,13	1.36	1 (10%)

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
5	DBU	5	4	5	-	1/1/2/6	-
5	BB9	5	9	5	-	0/0/2/6	-
5	MH6	5	10	5	-	1/1/2/6	-
5	BB9	5	5	5	-	0/0/4/6	-
5	DHA	5	12	5	-	0/0/2/4	-
5	BB9	5	7	5	-	0/0/4/6	-
5	BB9	5	11	5	-	0/0/4/6	-
5	BB9	5	2	5	-	0/0/4/6	-
5	3GL	5	6	5,33	-	0/8/8/12	-

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	2	BB9	C-CA	10.97	1.62	1.45
5	5	12	DHA	C-CA	9.31	1.60	1.45
5	5	6	3GL	CG-CD	8.81	1.65	1.52
5	5	5	BB9	C-CA	7.11	1.56	1.45
5	5	4	DBU	CA-N	6.37	1.49	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	2	BB9	O-C-CA	-5.98	117.79	125.39
5	5	7	BB9	O-C-CA	-4.72	119.39	125.39
5	5	10	MH6	OG-CB-CA	4.21	120.27	112.19
5	5	10	MH6	C-CA-CB	3.67	126.14	118.30
5	5	4	DBU	C-CA-N	-3.67	112.42	116.53

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	5	10	MH6	C-CA-CB-OG
5	5	4	DBU	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	4	DBU	1	0
5	5	7	BB9	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 37 are monoatomic - leaving 1 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
33	NO1	5	14	5	11,14,16	4.69	6 (54%)	12,20,23	4.52	9 (75%)

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
33	NO1	5	14	5	-	0/0/2/6	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	14	NO1	CE3-CD2	10.42	1.61	1.44
33	5	14	NO1	CF-CE3	-7.89	1.36	1.51
33	5	14	NO1	CH2-CZ3	6.13	1.51	1.38
33	5	14	NO1	CZ3-CE3	-4.06	1.29	1.37
33	5	14	NO1	CD1-C	-2.31	1.46	1.48

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5	14	NO1	CE3-CD2-CE2	-9.91	106.80	122.70
33	5	14	NO1	CZ2-CE2-CD2	7.96	135.30	120.76
33	5	14	NO1	CF-CE3-CD2	-5.37	114.51	124.37
33	5	14	NO1	CH2-CZ2-CE2	-4.22	114.00	120.08
33	5	14	NO1	CZ2-CE2-NE1	-3.05	121.93	130.78

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

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1	53/55 (96%)	3.66	39 (73%) 0 0	91, 120, 138, 158	0
2	2	46/47 (97%)	5.49	42 (91%) 0 0	42, 90, 116, 151	0
3	3	63/66 (95%)	4.98	57 (90%) 0 0	52, 106, 135, 145	0
4	4	37/37 (100%)	0.53	3 (8%) 12 9	73, 124, 148, 152	0
5	5	3/13 (23%)	-0.10	0 100 100	84, 84, 84, 84	0
6	A	240/274 (87%)	0.28	14 (5%) 23 16	36, 129, 160, 198	0
7	B	205/211 (97%)	-0.53	0 100 100	13, 85, 130, 161	0
8	C	197/205 (96%)	-0.28	3 (1%) 73 63	24, 110, 147, 170	0
9	D	177/180 (98%)	-0.02	7 (3%) 38 28	101, 136, 160, 179	0
10	E	171/185 (92%)	-0.23	3 (1%) 68 57	79, 131, 158, 176	0
11	F	144/144 (100%)	0.62	13 (9%) 9 7	117, 148, 172, 188	0
12	G	142/174 (81%)	0.02	6 (4%) 36 27	30, 112, 143, 169	0
13	H	134/134 (100%)	-0.69	0 100 100	13, 67, 106, 127	0
14	I	141/156 (90%)	0.18	6 (4%) 35 26	13, 128, 156, 181	0
15	J	136/142 (95%)	-0.03	4 (2%) 51 39	25, 112, 155, 202	0
16	K	113/116 (97%)	-0.67	0 100 100	13, 57, 111, 148	0
17	L	104/114 (91%)	0.18	5 (4%) 30 22	73, 125, 149, 167	0
18	M	108/166 (65%)	-0.56	0 100 100	13, 76, 121, 150	0
19	N	117/118 (99%)	-0.30	2 (1%) 70 59	16, 104, 144, 182	0
20	O	94/100 (94%)	-0.15	1 (1%) 80 71	28, 117, 151, 160	0
21	P	127/134 (94%)	-0.61	1 (0%) 86 78	13, 76, 126, 155	0
22	Q	93/95 (97%)	-0.34	0 100 100	35, 114, 152, 159	0
23	R	110/115 (95%)	-0.41	0 100 100	53, 118, 145, 161	0
24	S	175/237 (73%)	0.25	11 (6%) 20 13	78, 136, 159, 184	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	T	84/91 (92%)	0.20	5 (5%) 21 15	75, 117, 145, 181	0
26	U	72/81 (88%)	0.27	2 (2%) 53 40	60, 130, 160, 180	0
27	V	66/67 (98%)	-0.42	1 (1%) 73 63	83, 126, 158, 168	0
28	W	55/55 (100%)	-0.20	0 100 100	35, 105, 140, 169	0
29	X	2686/2880 (93%)	0.25	116 (4%) 35 26	13, 114, 186, 250	0
30	Y	58/60 (96%)	-0.66	0 100 100	13, 70, 119, 132	0
31	Z	122/123 (99%)	0.67	10 (8%) 11 9	38, 143, 188, 205	0
All	All	6073/6575 (92%)	0.18	351 (5%) 23 16	13, 116, 174, 250	0

The worst 5 of 351 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	2	6	GLN	16.9
3	3	35	GLY	13.4
3	3	7	HIS	13.4
2	2	8	ASN	13.2
3	3	33	ASN	11.9

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	BB9	5	7	6/7	0.74	0.43	83,83,83,83	0
5	3GL	5	6	9/11	0.77	0.36	83,83,83,83	0
5	DHA	5	12	5/6	0.81	0.50	83,83,83,83	0
5	BB9	5	9	5/7	0.84	0.26	83,83,83,83	0
5	BB9	5	2	6/7	0.84	0.18	83,83,83,83	0
5	DBU	5	4	5/7	0.85	0.26	83,83,83,83	0
5	MH6	5	10	5/7	0.86	0.27	83,83,83,83	0
5	BB9	5	5	6/7	0.86	0.26	83,83,83,83	0
5	BB9	5	11	6/7	0.91	0.34	83,83,83,83	0
5	NH2	5	13	1/1	0.95	0.42	83,83,83,83	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
34	MG	X	2908	1/1	0.69	1.05	83,83,83,83	0
34	MG	X	2889	1/1	0.70	0.83	131,131,131,131	0
34	MG	X	2891	1/1	0.74	0.52	84,84,84,84	0
34	MG	X	2903	1/1	0.74	2.21	82,82,82,82	0
34	MG	X	2883	1/1	0.74	1.51	104,104,104,104	0
34	MG	Z	127	1/1	0.78	0.91	98,98,98,98	0
34	MG	X	2902	1/1	0.81	1.36	76,76,76,76	0
34	MG	X	2881	1/1	0.81	0.70	77,77,77,77	0
34	MG	Z	128	1/1	0.81	0.26	110,110,110,110	0
34	MG	X	2892	1/1	0.82	0.57	109,109,109,109	0
34	MG	Z	125	1/1	0.82	1.00	83,83,83,83	0
34	MG	X	2882	1/1	0.82	0.35	112,112,112,112	0
34	MG	X	2885	1/1	0.82	0.69	98,98,98,98	0
33	NO1	5	14	13/15	0.83	0.28	83,83,83,83	0
34	MG	X	2895	1/1	0.83	0.22	81,81,81,81	0
34	MG	Z	129	1/1	0.83	0.86	101,101,101,101	0
34	MG	Z	126	1/1	0.84	1.16	122,122,122,122	0
34	MG	X	2896	1/1	0.85	1.48	86,86,86,86	0
34	MG	X	2893	1/1	0.88	1.13	85,85,85,85	0
34	MG	X	2901	1/1	0.89	0.54	100,100,100,100	0
32	ZN	4	38	1/1	0.89	0.05	125,125,125,125	0
34	MG	X	2888	1/1	0.89	2.17	73,73,73,73	0
32	ZN	Y	61	1/1	0.91	0.08	118,118,118,118	0
34	MG	M	167	1/1	0.91	1.30	68,68,68,68	0
34	MG	Z	124	1/1	0.92	0.63	113,113,113,113	0
34	MG	X	2906	1/1	0.93	1.36	82,82,82,82	0
34	MG	X	2907	1/1	0.94	0.38	66,66,66,66	0
34	MG	X	2886	1/1	0.94	0.20	80,80,80,80	0
34	MG	X	2905	1/1	0.95	0.57	123,123,123,123	0
34	MG	X	2897	1/1	0.95	0.95	100,100,100,100	0
34	MG	X	2898	1/1	0.96	0.57	57,57,57,57	0
34	MG	X	2900	1/1	0.97	0.12	104,104,104,104	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	X	2904	1/1	0.97	0.79	81,81,81,81	0
34	MG	X	2890	1/1	0.97	0.22	58,58,58,58	0
34	MG	X	2899	1/1	0.97	0.65	57,57,57,57	0
34	MG	X	2894	1/1	0.98	0.60	57,57,57,57	0
34	MG	X	2884	1/1	0.98	0.28	98,98,98,98	0
34	MG	X	2887	1/1	0.98	0.75	98,98,98,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.