



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:14 AM GMT

PDB ID : 2ZJP
Title : Thiopeptide antibiotic Nosiheptide bound to the large ribosomal subunit of *Deinococcus radiodurans*
Authors : Harms, J.M.; Wilson, D.N.; Schlutzen, 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

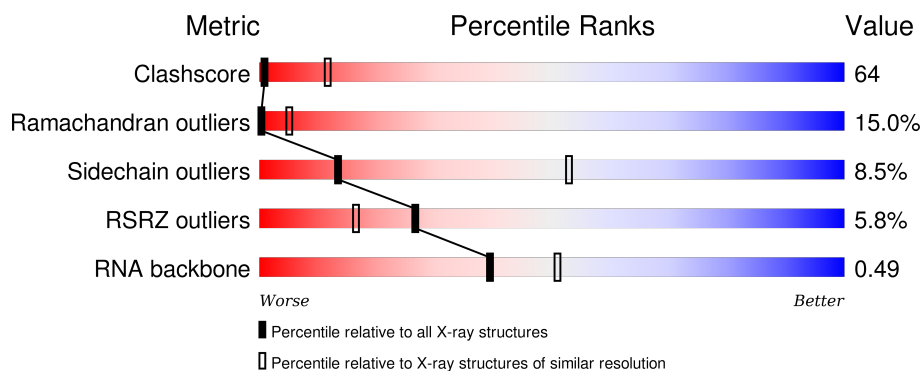
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)
RNA backbone	2183	1067 (4.60-2.80)

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 ≥ 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	1	55	<div> <div>73%</div> <div>95%</div> <div>..</div> </div>
2	2	47	<div> <div>89%</div> <div>96%</div> <div>..</div> </div>
3	3	66	<div> <div>86%</div> <div>92%</div> <div>• 5%</div> </div>
4	4	37	<div> <div>8%</div> <div>30%</div> <div>65%</div> <div>5%</div> </div>
5	5	13	<div> <div>69%</div> <div>23%</div> <div>8%</div> </div>

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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	

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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	2881	-	-	-	X
34	MG	X	2887	-	-	-	X
34	MG	X	2888	-	-	-	X
34	MG	X	2894	-	-	-	X
34	MG	X	2897	-	-	-	X
34	MG	X	2902	-	-	-	X
34	MG	X	2903	-	-	-	X
34	MG	X	2904	-	-	-	X
34	MG	X	2906	-	-	-	X
34	MG	X	2908	-	-	-	X
34	MG	Z	124	-	-	-	X
5	DHA	5	12	-	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
7	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
16	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

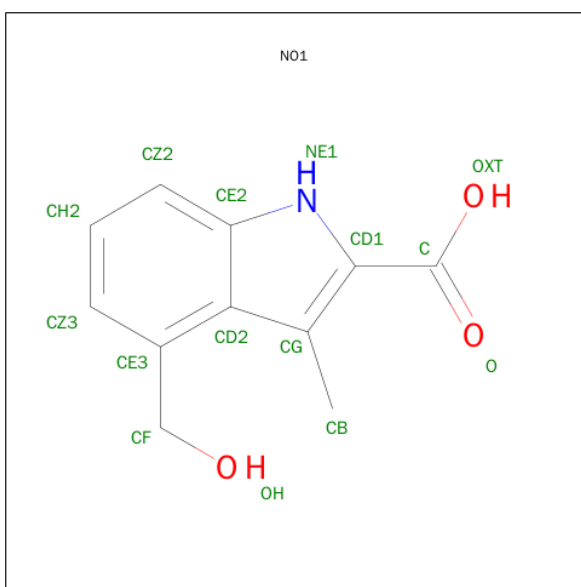
- Molecule 31 is a RNA chain called RIBOSOMAL 5S RNA.

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

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

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

- Molecule 33 is 4-(HYDROXYMETHYL)-3-METHYL-1H-INDOLE-2-CARBOXYLIC ACID (three-letter code: NO1) (formula: C₁₁H₁₁NO₃).



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

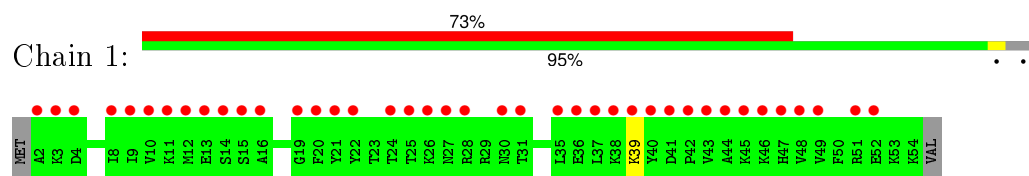
- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

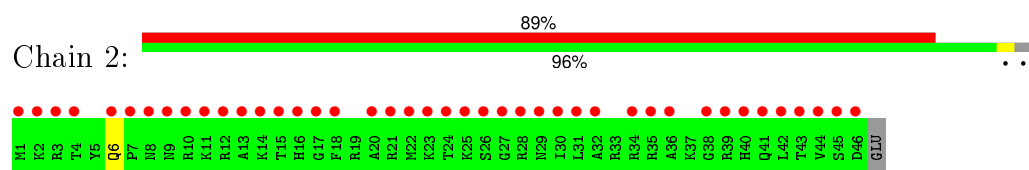
3 Residue-property plots

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 ($RSRZ > 2$). 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.

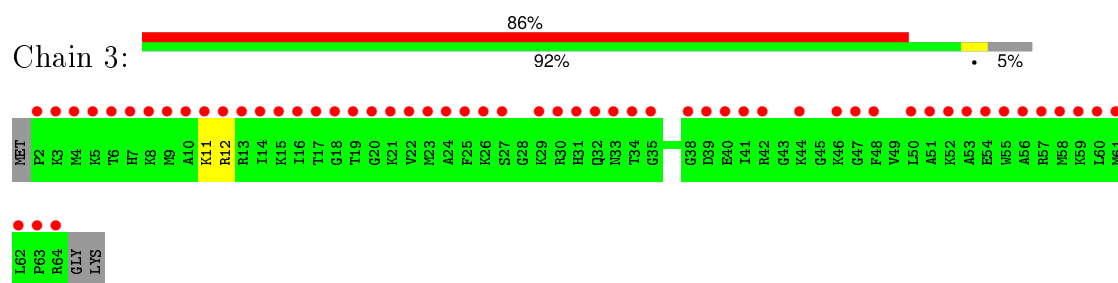
• Molecule 1: 50S RIBOSOMAL PROTEIN L33



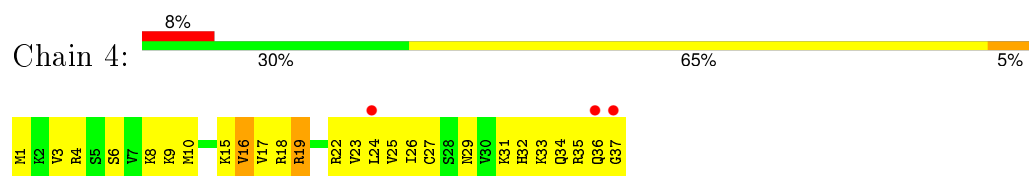
• Molecule 2: 50S RIBOSOMAL PROTEIN L34



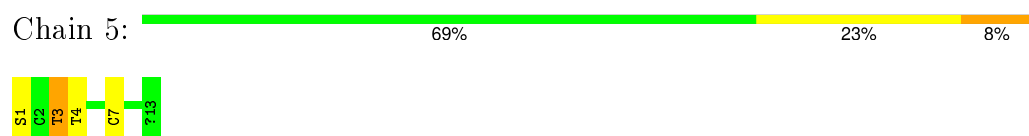
• Molecule 3: 50S RIBOSOMAL PROTEIN L35



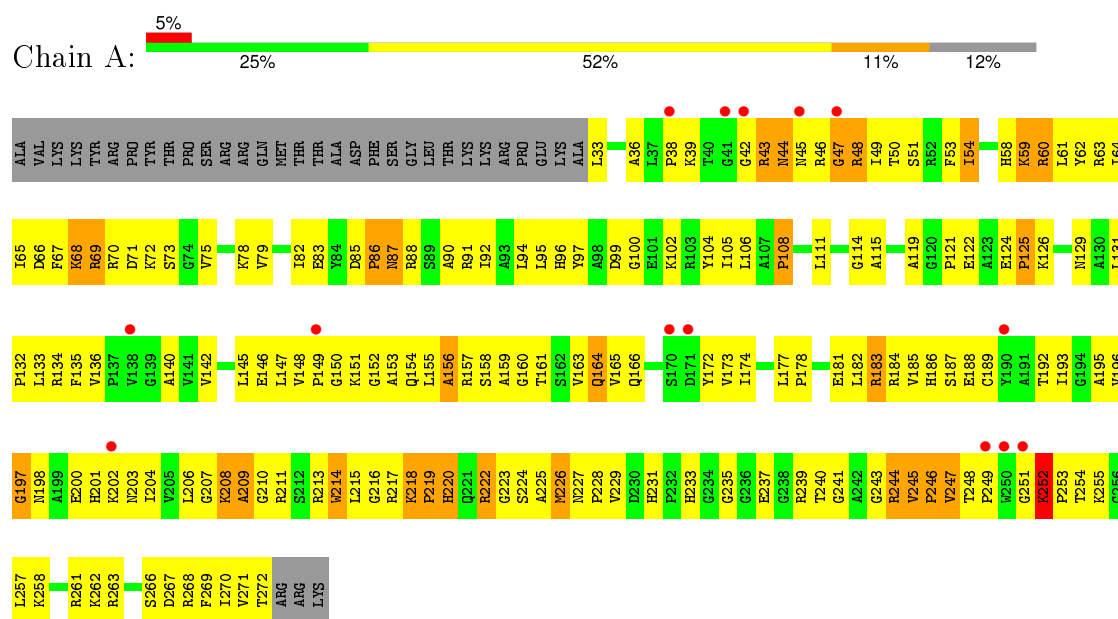
• Molecule 4: 50S RIBOSOMAL PROTEIN L36



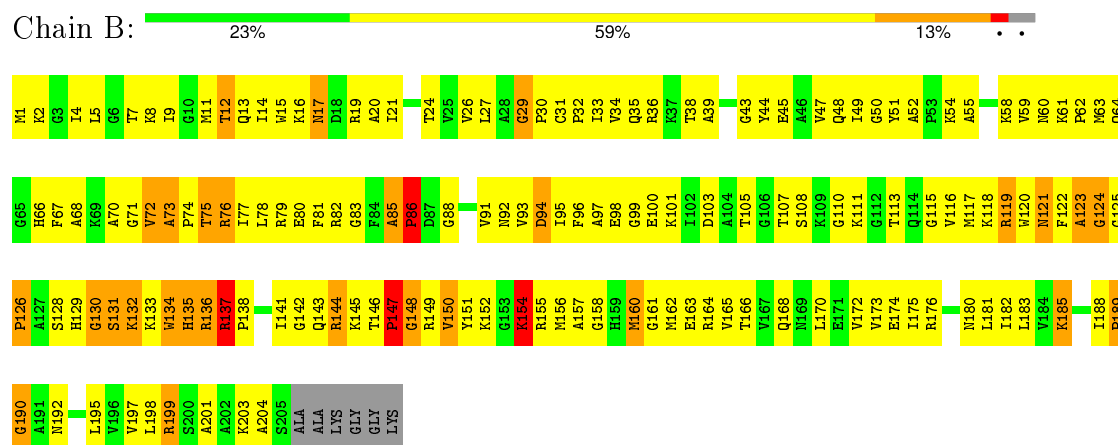
• Molecule 5: NOSIHEPTIDE



• Molecule 6: 50S RIBOSOMAL PROTEIN L2



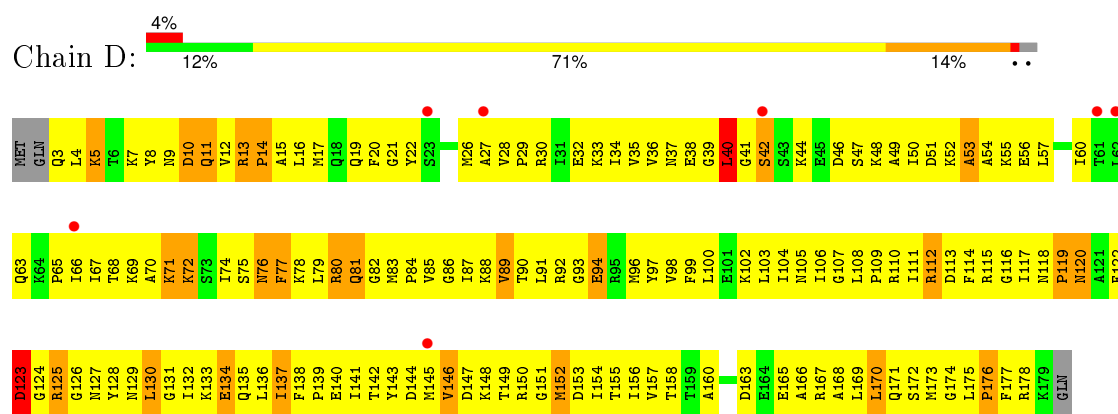
• Molecule 7: 50S RIBOSOMAL PROTEIN L3



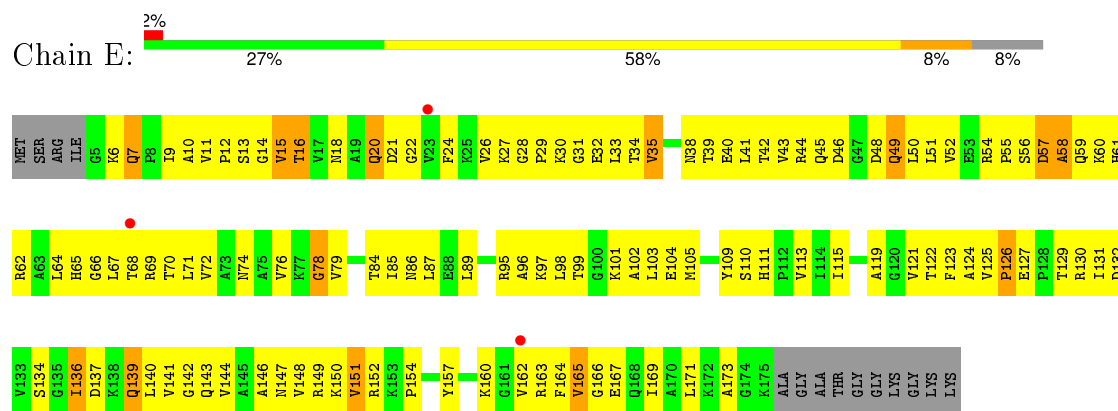
• Molecule 8: 50S RIBOSOMAL PROTEIN L4



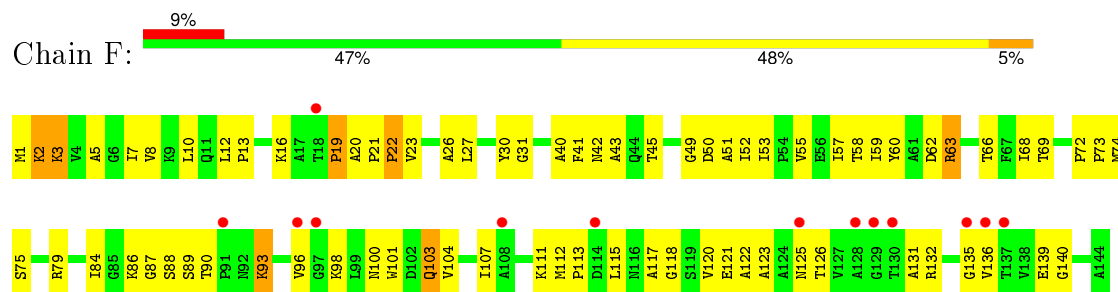
• Molecule 9: 50S RIBOSOMAL PROTEIN L5



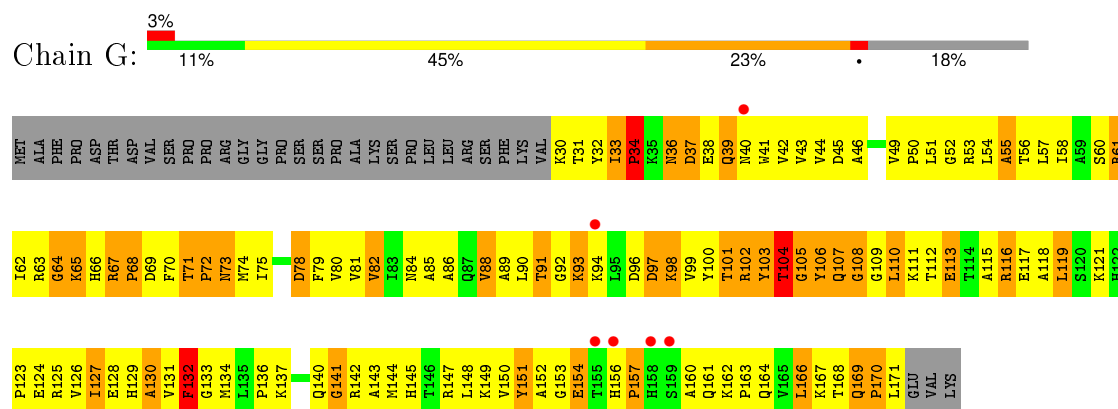
- Molecule 10: 50S RIBOSOMAL PROTEIN L6



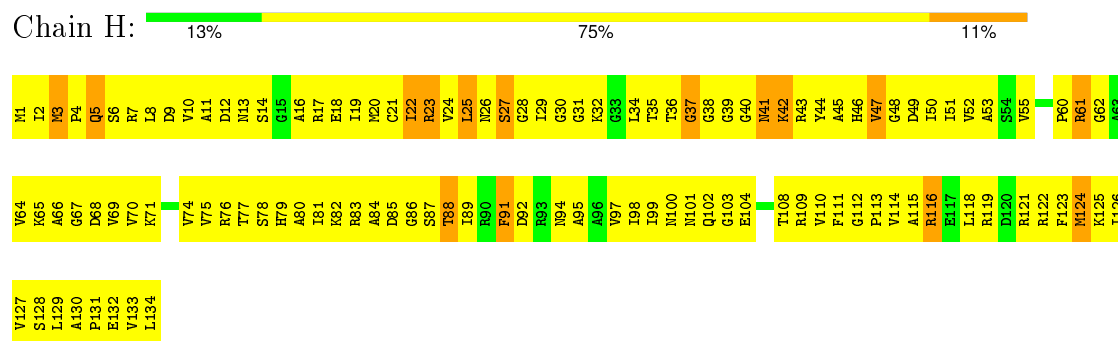
- Molecule 11: 50S RIBOSOMAL PROTEIN L11



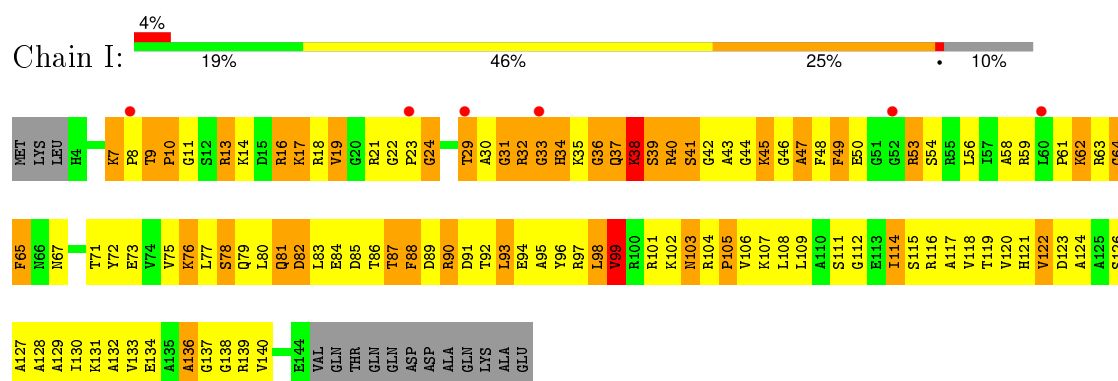
- Molecule 12: 50S RIBOSOMAL PROTEIN L13



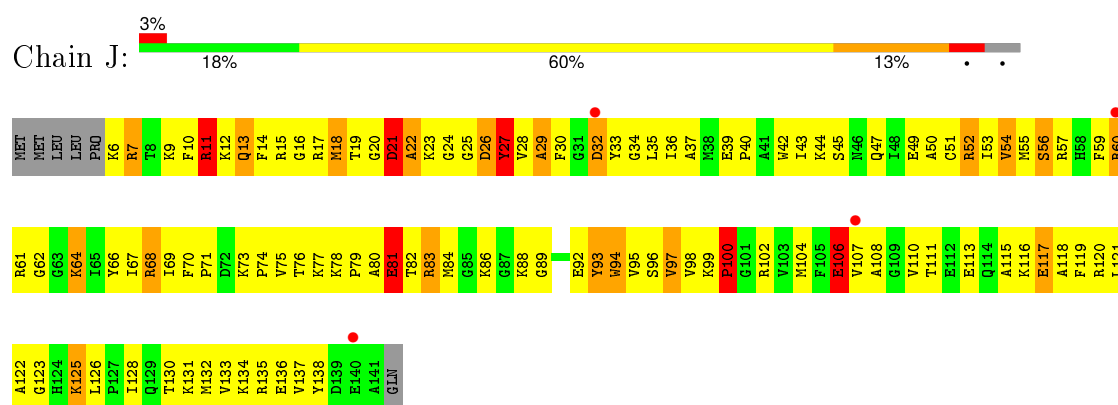
- Molecule 13: 50S RIBOSOMAL PROTEIN L14



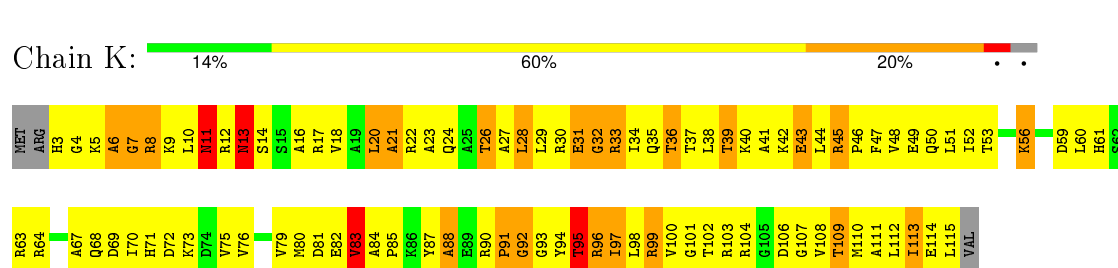
• Molecule 14: 50S RIBOSOMAL PROTEIN L15



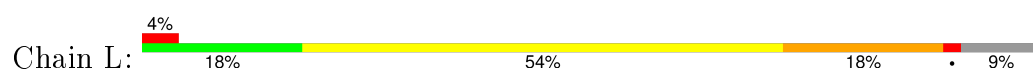
• Molecule 15: 50S RIBOSOMAL PROTEIN L16

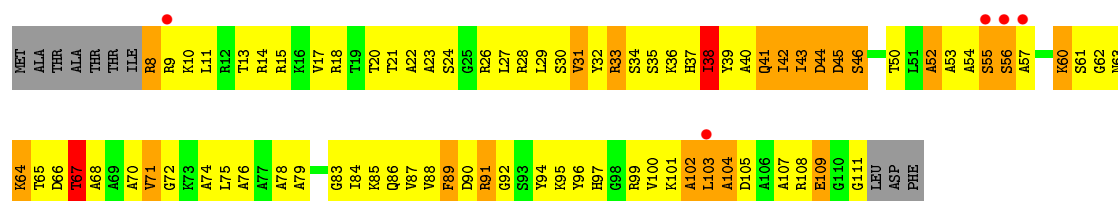


• Molecule 16: 50S RIBOSOMAL PROTEIN L17

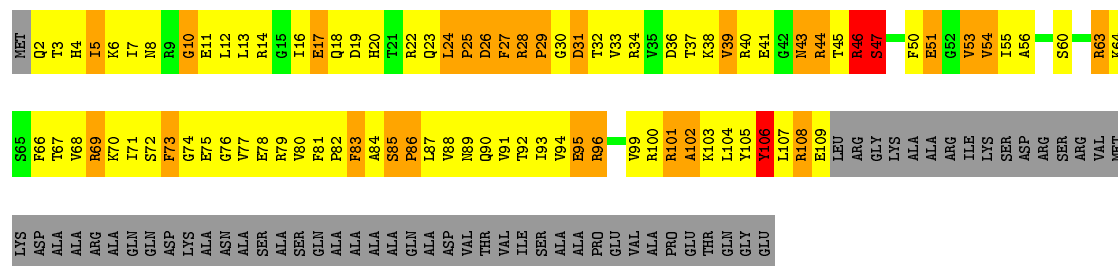
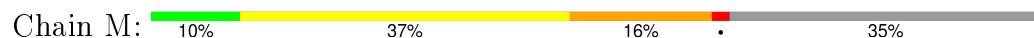


• Molecule 17: 50S RIBOSOMAL PROTEIN L18

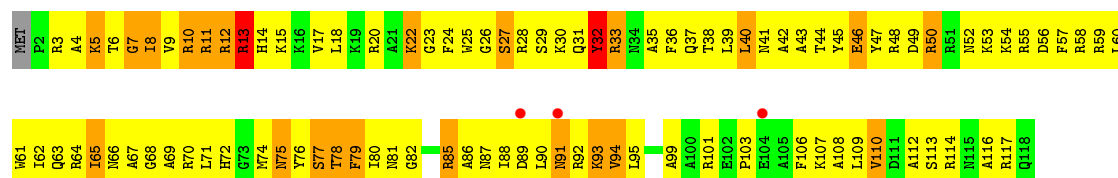




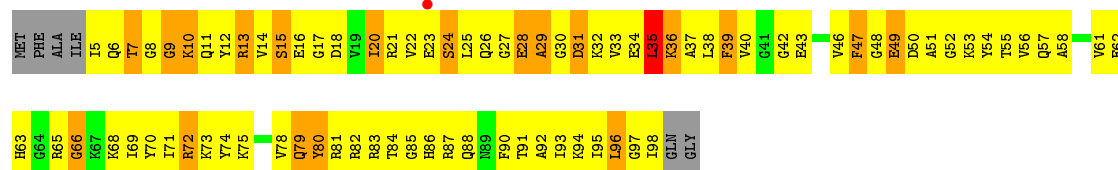
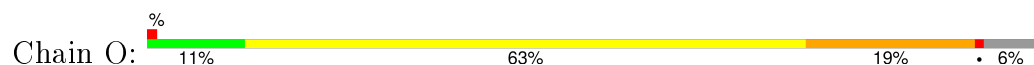
• Molecule 18: 50S RIBOSOMAL PROTEIN L19



• Molecule 19: 50S RIBOSOMAL PROTEIN L20



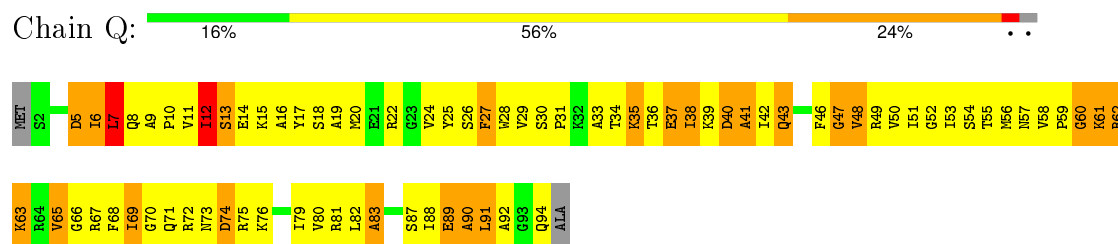
• Molecule 20: 50S RIBOSOMAL PROTEIN L21



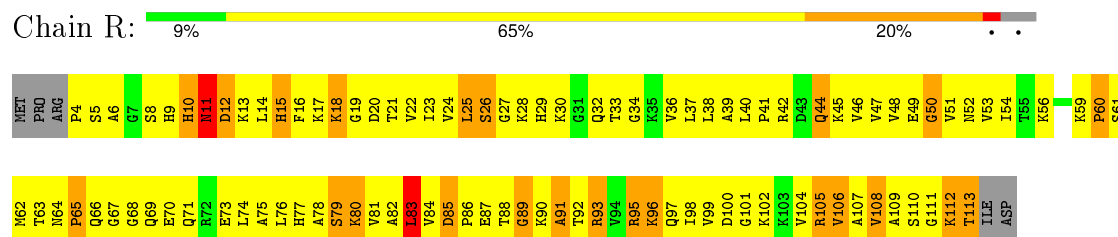
• Molecule 21: 50S RIBOSOMAL PROTEIN L22



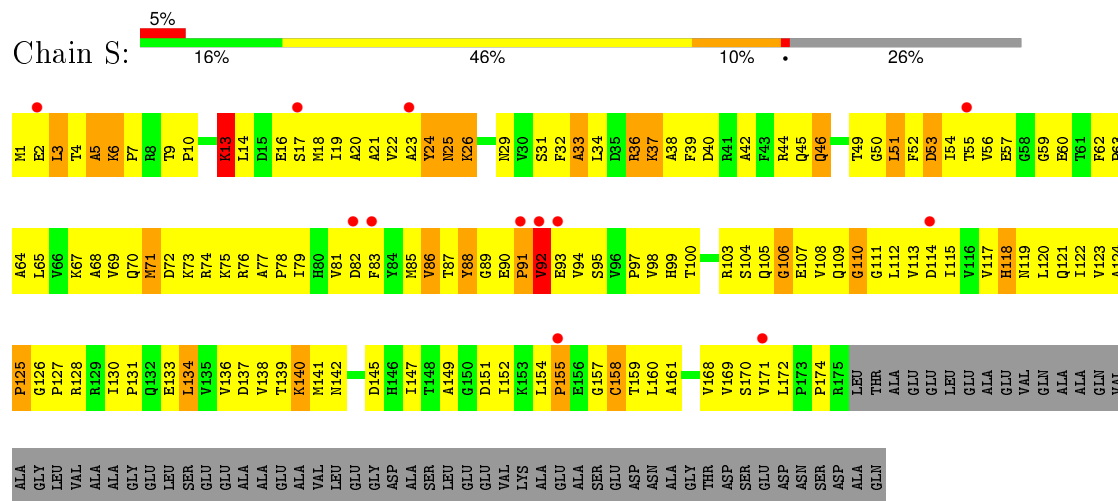
• Molecule 22: 50S RIBOSOMAL PROTEIN L23



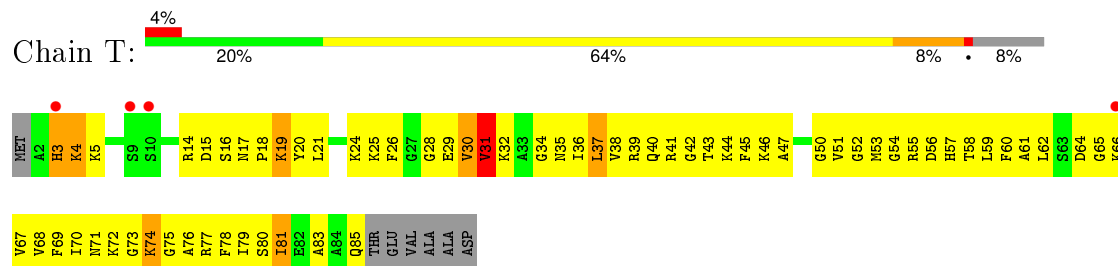
- Molecule 23: 50S RIBOSOMAL PROTEIN L24



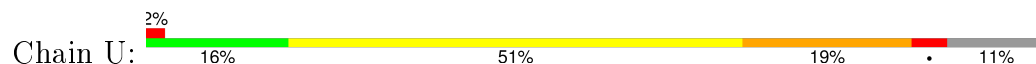
- Molecule 24: 50S RIBOSOMAL PROTEIN L25

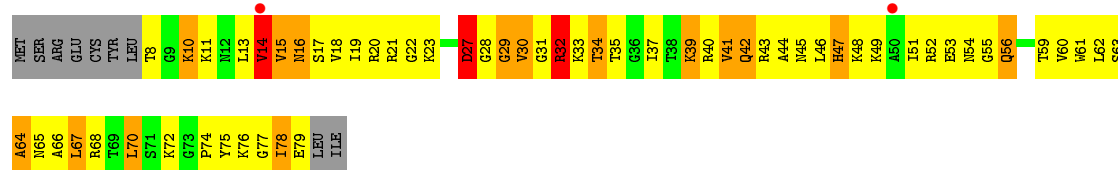


● Molecule 25: 50S RIBOSOMAL PROTEIN L27

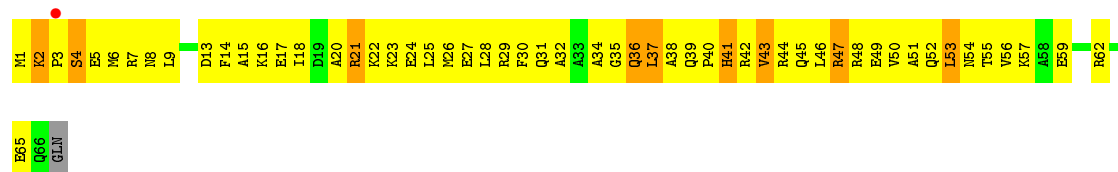


- Molecule 26: 50S RIBOSOMAL PROTEIN L28

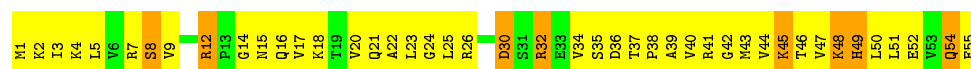




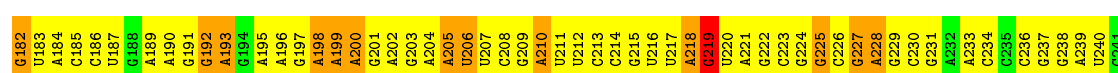
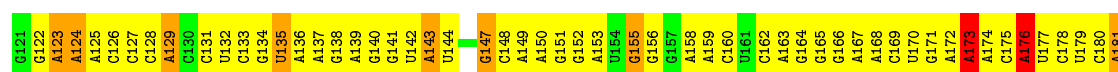
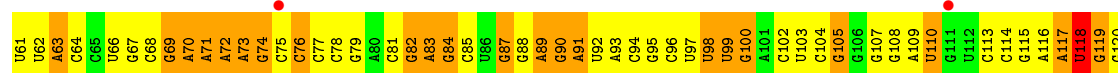
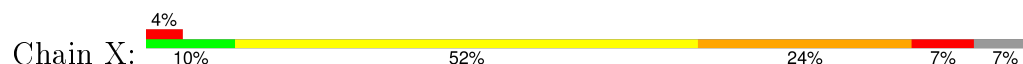
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



• Molecule 28: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: RIBOSOMAL 23S RNA



U1339	C1219	G1094	U1034	U973	A913	C851	A790	A729	U667	A806	A546	G485
C1340	G1220	A1095	G1035	U974	C914	U852	G791	C730	A668	C607	U547	U486
U1341	U1159	A1096	G1036	C975	C915	C853	U792	A731	G669	G507	G548	A487
A1282	G1222	A1097	U1037	C976	U916	G854	G793	G732	U670	U609	G549	A488
C1283	U1160	G1098	U1038	C977	U917	U857	A794	G733	A671	G610	C550	A489
G1284	A1162	A1099	U1039	U978	A918	U858	U795	G734	G734	C611	A551	A490
A1285	C1163	G1100	A1040	A979	U919	C859	U796	G735	U674	G612	C552	A491
U1286	U1101	G1101	G1041	G980	G920	U859	A797	G736	C675	A613	C553	A492
A1287	G1165	U1102	A1042	C981	A921	U860	G798	C737	G676	G614	U554	A493
A1288	A1166	C1103	U1043	C982	A922	G861	C799	G738	G677	C615	U555	C494
A1289	A1167	U1044	A1044	C983	A923	G862	U800	G739	G678	U616	A556	C495
G1290	G1168	U1045	A984	A984	C924	C863	A801	A740	C679	U617	U557	C496
A1291	A1107	G1045	G985	C985	U925	C864	A802	G741	U680	A618	G558	C497
U1292	U1108	G1047	A986	A986	C926	A865	C803	G742	A681	A619	C559	C498
A1293	U1109	U1048	G987	G987	C927	U866	C804	A743	G682	G820	G560	G499
A1294	G1110	U1049	G988	G988	G928	G867	G805	C744	A683	G821	U561	G500
U1295	C1111	G1050	A989	C989	A929	U868	A806	C745	C684	A628	G562	G501
G1296	G1174	U1051	A990	A990	A930	C869	A807	G746	U685	U563	U563	A502
A1297	C1113	C1052	A991	A991	G931	C870	C808	A747	C686	A625	U564	G503
U1298	U1175	U1053	A992	A992	G932	U871	C809	A748	G687	A626	A565	G504
G1299	U1177	C1054	C993	C993	G933	U872	U810	C749	A688	A627	U566	G507
A1300	C1178	U1055	A994	A994	G934	U873	G811	C750	A689	A628	G567	G508
U1301	U1116	U1056	A995	A995	G935	A874	G812	G751	A690	C629	G568	A512
A1302	G1117	A1057	A996	A996	A936	G875	A813	C752	C691	G630	G569	U509
U1303	U1118	G1058	C997	C997	A937	A876	G814	U753	C692	G631	G570	G510
U1304	C1181	A1059	C998	C998	G938	G877	A815	G754	A693	A632	U571	A511
C1305	U1120	G1121	C1060	A999	C939	C878	U816	C755	G694	G633	G572	A512
A1306	G1122	A1061	G940	G1000	G940	U879	G817	C756	G695	G634	C573	A513
U1307	U1123	C1062	A1001	A1001	U941	G882	C819	G757	U696	G635	C574	G514
G1308	G1124	G1063	C1002	C1002	U942	C883	G820	U758	G697	G636	U575	A515
U1309	U1125	C1064	C1003	C1003	U943	C884	A821	C759	A698	G637	A576	G516
A1310	A1126	A1065	A1004	A1004	A944	C885	G822	U760	G699	A638	U577	A517
U1311	C1127	G1066	U1005	U1005	G945	A886	G823	G761	C700	G639	U578	A518
G1312	G1128	G1067	C1006	C1006	U946	C887	U823	A762	U701	C640	G579	C519
A1313	A1129	A1068	A1007	A1007	C947	G887	U824	U763	A702	G641	A581	G520
U1314	U1130	G1069	G1008	G1008	C948	C888	C825	A764	A703	A642	G582	U521
A1315	G1131	G1070	U1071	U1071	G949	U890	C826	C765	G704	A643	G522	G522
G1316	C1132	U1072	U1072	U1072	C950	U891	C827	A766	C705	C583	A523	A523
U1317	U1133	G1073	A1073	A1011	G951	G	C828	G767	A706	G645	A584	A524
U1195	C1134	G1074	C1073	A1012	A952	G	C829	U768	U707	C646	U585	A525
G1136	U1135	C1075	G1075	G1013	G953	G	C830	C769	G708	A647	G586	C526
U1197	G1136	U1076	U1076	G1014	U954	G	G831	G769	A709	A648	A587	C527
A1321	A1137	U1077	C1016	U1015	G955	G	A832	G772	A712	G649	G588	G528
G1200	A1138	A1077	C1017	C1016	A956	C	A833	G773	A713	U650	C589	U529
G1201	A1139	A1078	C1018	C1017	G957	C	A834	A774	G713	C651	G590	G530
U1202	A1140	G1079	U1018	U1018	G958	C	U835	U775	G714	C652	G591	G531
A1203	U1141	A1080	U1019	U1019	C959	U	G836	G776	U715	G653	G592	A532
G1204	G1142	A1081	A1020	A1020	U960	A	A837	A777	U716	A654	C593	C533
G1205	A1143	C1082	A1021	A1021	G961	C	U838	G778	G717	G655	G594	U534
U1144	U1144	C1083	A1022	A1022	C962	C	U839	U779	A718	U656	A595	U535
G1145	U1145	A1084	U1023	U1023	G963	A	U840	U780	A719	A657	C586	A536
G1146	G1146	G1085	A1024	A1024	A964	G	U841	G781	A720	G658	U597	C537
U1147	C1086	C1086	A1025	A1025	G965	C	A842	U782	C721	G659	U598	A538
G1148	U1087	A1087	U1026	U1026	A966	U	G843	G783	G722	G660	A539	A539
A1149	A1088	A1088	C1027	C1027	G967	U	G844	U784	C723	G661	G600	G540
C1150	C1089	C1089	U1030	U1030	C968	A	U845	U785	C724	G662	A601	C541
U1151	U1090	C1090	C1031	U1031	U969	C	A848	U786	C725	G663	C602	A542
U1092	U1091	C1091	A1032	A1032	A970	C	G849	G787	G726	C664	G603	G543
A1153	U1092	U1092	G1033	G1033	A971	A911	C850	G788	U727	U665	U604	U544
A1154	U1093	U1093			C972	A912		G789	G728	U666	G605	C545

C2210	G	U2088	C2027	G	G1842	U1778	A1715	C1653	G1589	U1526	A1463	G1402
U2211	G	C2089	C2028	G	U1843	C1779	G1716	A1654	U1592	G1527	A1464	U1403
G2212	U	U2090	G2029	U	C1844	A1780	A1717	C1655	U1593	C1528	G1465	A1404
G2213	U	C	U2030	C	A1845	C1781		U1656	C1529	C1529	A1466	A1405
G2214	A	U	A2031	C	A1846	G1782	G1723	A1657	U1594	U1467	U1467	A1406
G2215	A	G	G2032	U	A1847	G1783	U1722	A1658	C1595	C1530	A1468	G1407
G2216	A	C	C2033	A	U1848	G1784	C1724	G1659	U1596	C1531	U1469	A1408
G2217	U	G	C2034	A	G1849	A1785	C1725	G1660	A1597		U1470	U1409
G2218	A	U	G2035	U	G1850	C1786	C1726	C1661	C1598	A1594	U1471	U1410
U2219	C	A	U1976	U	A1851	G1787	C1727	C1662	C1599	U1472	C1472	C1411
A2220	C	G	C1977	U	G1852	C1788	A1728	C1663	U1600	U1473	C1412	C1412
G2221	A	G	U1978	U	C1853	G1789	G1729	G1664	U1601	U1474	U1413	U1413
U2222	C	A	C1979	U	G1854	G1790	G1730	C1665	U1602	U1475	U1414	U1414
U2223	C	U	A1980	U	G1855	C1791	C1731	G1666	A1603	U1476	C1415	C1415
U2224	C	A	U1981	U	U1856	G1792	U1732	A1667	U1604	U1477	A1416	A1416
G2225	U	G	C1982	U	G1857	A1793	U1733	C1668		U1478	U1417	U1417
A2226	G	U	G1983	U	A1858	G1794	C1734	A1669	U1607	G1479	C1418	C1418
U2228	G	U	U1984	U	A1859	C1795	G1735	G1670	U1608	U1480	G1480	G1419
G2229	G	G	U1985	U	A1860	A1796	C1736	A1671	G1609	U1481	A1420	A1420
G2230	G	G	G1986	U	G1861	C1797	G1737	G1672	A1610	U1482	U1421	U1421
G2231	A	G	U1987	U	C1862		U1738	C1673	U1611	G1483	C1422	C1422
G2232	A	G	A1988	U	U1863	C1801	G1739	C1674	U1612	U1484	A1423	A1423
G2233	C	G	C1989	U	G1864	G1802	G1740	C1675	C1613	U1485	U1424	U1424
G2234	C	C	U1990	U	C1865	A1802	G1741	U1676	C1614	A1486	G1425	G1425
G2235	C	U	G1991	U	G1866	G1803	G1742	C1677	C1615	C1487	U1426	U1426
U2236	U	U	G1992	U	A1867	U1804	C1743	G1678		U1488	G1427	G1427
U2237	G	G	U1993	U	A1868	G1805	G1744	U1679	U1618	C1489	G1428	G1428
U2238	C	C	U1994	U	A1869	A1806	C1745	U1680	A1555	A1529	A1429	A1429
G2239	A	G	G1995	U	G1870	A1807	A1746	A1681	C1620	C1491	G1430	G1430
C2240	A	A	A1996	U	G1871	C1808	G1747	A1682	C1621	U1557	A1492	U1431
U2241	A	A	U1997	U	A1872	G1809	U1748	G1683	G1622	G1559	A1493	G1432
G2242	A	C	U1998	U	A1873	U1810	C1749	G1684	C1623	A1560	A1433	A1433
			U2059	U	G1874	A1811	A1750	A1685	A1624	U1561	A1434	A1434
A2245	U	U	A2060	U	C1875	U1812	G1751	A1686	A1625	U1562	G1495	G1435
A2246	U	G	C2061	U	G1878	A1813	U1752	C1687	A1626	G1563	G1496	G1436
A2247	C	C	U2062	U	G1879	G1814	A1753	U1688	C1627	U1564	C1497	A1437
A2248	C	C	A2063	U	G1880	G1815	G1754	U1689	C1628	A1499	G1438	G1438
U2249	C	U	U2064	U	U1881	G1816	G1755	U1690	G1629	U1500	G1439	G1439
G2250	U	U	A2065	U	G1882	U1817	C1756	G1691	U1630	C1501	G1440	G1440
U2251	U	U	G2006	U	A1883	G1818	C1757	C1692	C1631	A1567	A1441	A1441
A2252	U	U	C2007	U	A1884	U1819	C1758	A1693	C1632	C1570	G1502	G1502
A2253	U	G	U2008	U	G1885	G1820	G1759	A1694	C1633	C1571	G1503	G1503
G2254	G	G	G2009	U	A1886	A1821	G1760	U1695	A1634	C1572	U1505	C1444
C2193	G	G	G2010	U	G1887	C1822	G1761		G1635	C1571	C1506	C1445
A2194	G	G	U2011	U	C1888		C1762	C1688	G1636	G1572	U1507	U1446
C2195	G	G	A2012	U	G	C1825	G1763	A1699	U1637	G1573	G1508	U1447
U2196	U	U	A2013	U	C	U1826	A1764	C1700	C1574	C1575	A1509	C1448
U2197	C	U	A2014	U	C	G1827	C1765	C1701	U1638	G1576	A1510	C1449
G2258	G	C	G2015	U	C		U1766	G1704	C1640	G1577	A1511	G1450
C2199	G	G	A2016	U	G	G1830	G1767	U1705	C1641	U1578	C1451	C1451
G2260	U	U	U2017	U	U	G1831	U1768			G1579	U1512	U1452
G2261	G	G	G2018	U	A		U1769	U1706	G1644	C1580	U1513	U1453
G2262	G	G	C2019	U	A	G1834	U1770	A1707	U1645	C1581	C1514	A1454
C2263	A	A	U2080	U	C	C1835	A1771	C1708	U1646	A1582	U1515	U1454
C2264	C	C	U2081	U	U	G1836	C1772	U1709	U1647	A1583	C1516	C1455
A2265	G	G	C2082	U	A	A1960	G1773	U1710	C1648	G1584	C1517	C1456
A2266	C	C	G2083	U	U	G1837	A1774		A1649	A1585	C1522	U1459
A2267	C	C	G2084	U	U	G1838		C1711		A1586	A1523	G1460
G2268	A	A	U2024	U	A	A1839	A1775	G1712	U1650	C1524	C1461	C1461
A2086	A	A	A2025	U	A	A1840	A1776	G1713	A1587	A1588	A1525	C1462
U2087	C	C	C2026	U	C	G1841	A1777	A1714	G1652			





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.65Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.300 , 0.340 0.324 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	109.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 130.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	1 of 240234 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	84444	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 ⓘ

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

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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:1386:A:H5''	29:X:2191:A:N6	1.48	1.25
29:X:1053:G:H2'	29:X:1054:C:C6	1.71	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%)	1	16
5	5	2/13 (15%)	1 (50%)	1 (50%)	0	100	100
6	A	238/274 (87%)	166 (70%)	51 (21%)	21 (9%)	1	15
7	B	203/211 (96%)	143 (70%)	33 (16%)	27 (13%)	0	6
8	C	195/205 (95%)	94 (48%)	55 (28%)	46 (24%)	0	1
9	D	175/180 (97%)	99 (57%)	50 (29%)	26 (15%)	0	5
10	E	169/185 (91%)	110 (65%)	40 (24%)	19 (11%)	0	9
11	F	142/144 (99%)	101 (71%)	33 (23%)	8 (6%)	2	28
12	G	140/174 (80%)	76 (54%)	34 (24%)	30 (21%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	H	132/134 (98%)	106 (80%)	18 (14%)	8 (6%)	2	26
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	7
16	K	111/116 (96%)	70 (63%)	23 (21%)	18 (16%)	0	5
17	L	102/114 (90%)	65 (64%)	23 (22%)	14 (14%)	0	6
18	M	106/166 (64%)	64 (60%)	22 (21%)	20 (19%)	0	3
19	N	115/118 (98%)	65 (56%)	30 (26%)	20 (17%)	0	3
20	O	92/100 (92%)	52 (56%)	23 (25%)	17 (18%)	0	3
21	P	125/134 (93%)	84 (67%)	26 (21%)	15 (12%)	0	8
22	Q	91/95 (96%)	45 (50%)	25 (28%)	21 (23%)	0	1
23	R	108/115 (94%)	61 (56%)	28 (26%)	19 (18%)	0	3
24	S	173/237 (73%)	96 (56%)	50 (29%)	27 (16%)	0	5
25	T	82/91 (90%)	56 (68%)	16 (20%)	10 (12%)	0	8
26	U	70/81 (86%)	34 (49%)	19 (27%)	17 (24%)	0	1
27	V	64/67 (96%)	44 (69%)	12 (19%)	8 (12%)	0	8
28	W	53/55 (96%)	36 (68%)	13 (24%)	4 (8%)	1	20
30	Y	56/60 (93%)	35 (62%)	15 (27%)	6 (11%)	0	10
All	All	3052/3404 (90%)	1859 (61%)	734 (24%)	459 (15%)	0	5

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 ⓘ

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%)	15	54
7	B	155/157 (99%)	145 (94%)	10 (6%)	21	64
8	C	157/163 (96%)	146 (93%)	11 (7%)	19	61
9	D	153/156 (98%)	145 (95%)	8 (5%)	29	70
10	E	136/144 (94%)	133 (98%)	3 (2%)	60	86
11	F	107/107 (100%)	103 (96%)	4 (4%)	41	77
12	G	118/146 (81%)	100 (85%)	18 (15%)	3	25
13	H	103/103 (100%)	94 (91%)	9 (9%)	13	51
14	I	108/121 (89%)	99 (92%)	9 (8%)	14	53
15	J	110/116 (95%)	94 (86%)	16 (14%)	4	27
16	K	90/93 (97%)	74 (82%)	16 (18%)	2	16
17	L	74/82 (90%)	62 (84%)	12 (16%)	3	21
18	M	94/134 (70%)	79 (84%)	15 (16%)	3	22
19	N	96/97 (99%)	91 (95%)	5 (5%)	29	70
20	O	75/79 (95%)	70 (93%)	5 (7%)	20	63
21	P	109/115 (95%)	101 (93%)	8 (7%)	17	59
22	Q	75/76 (99%)	68 (91%)	7 (9%)	11	49
23	R	91/96 (95%)	79 (87%)	12 (13%)	5	31
24	S	149/192 (78%)	141 (95%)	8 (5%)	27	69
25	T	62/67 (92%)	59 (95%)	3 (5%)	31	72
26	U	57/66 (86%)	50 (88%)	7 (12%)	6	34
27	V	54/55 (98%)	52 (96%)	2 (4%)	41	77
28	W	48/48 (100%)	44 (92%)	4 (8%)	14	53
30	Y	51/53 (96%)	46 (90%)	5 (10%)	10	45
All	All	2494/2719 (92%)	2282 (92%)	212 (8%)	13	53

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

Mol	Chain	Res	Type
15	J	68	ARG
16	K	113	ILE
26	U	27	ASP

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Mol	Chain	Res	Type
15	J	93	TYR
16	K	33	ARG

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

Mol	Chain	Res	Type
16	K	11	ASN
17	L	86	GLN
28	W	49	HIS
16	K	13	ASN
17	L	41	GLN

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	1261	G
29	X	1496	G
29	X	2660	C
29	X	1265	G
29	X	1338	G

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

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	MH6	5	10	5	3,4,6	2.54	1 (33%)	0,4,7	0.00	-
5	BB9	5	11	5	3,5,6	0.71	0	1,5,7	1.61	0
5	DHA	5	12	5	4,4,5	5.30	2 (50%)	3,4,6	2.27	2 (66%)
5	BB9	5	2	5	3,5,6	6.98	2 (66%)	1,5,7	5.17	1 (100%)
5	DBU	5	4	5	2,4,6	4.51	2 (100%)	0,4,7	0.00	-
5	BB9	5	5	5	3,5,6	4.43	1 (33%)	1,5,7	0.11	0
5	3GL	5	6	33,5	5,8,10	2.43	3 (60%)	7,10,13	1.68	1 (14%)
5	BB9	5	7	5	3,5,6	3.17	2 (66%)	1,5,7	4.08	1 (100%)
5	BB9	5	9	5	0,4,6	0.00	-	0,4,7	0.00	-

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	4	DBU	CB-CA	-5.29	1.27	1.33
5	5	6	3GL	CA-N	-3.74	1.39	1.48
5	5	12	DHA	O-C	-3.24	1.14	1.22
5	5	6	3GL	OH-CG	-2.48	1.37	1.42
5	5	6	3GL	CB-CA	2.40	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	2	BB9	O-C-CA	-5.17	117.79	125.40
5	5	7	BB9	O-C-CA	-4.08	119.39	125.40
5	5	12	DHA	O-C-CA	-3.18	119.22	125.35
5	5	12	DHA	CB-CA-N	2.15	131.03	126.27
5	5	6	3GL	OH-CG-CB	3.76	116.39	108.94

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates 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	4.36	4 (36%)	13,20,23	3.43	9 (69%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	5	14	NO1	CF-CE3	-7.63	1.36	1.51
33	5	14	NO1	CZ3-CE3	-3.54	1.29	1.37
33	5	14	NO1	CH2-CZ3	6.29	1.51	1.38
33	5	14	NO1	CE3-CD2	9.26	1.61	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	5	14	NO1	CF-CE3-CD2	-4.44	114.51	124.25
33	5	14	NO1	CH2-CZ2-CE2	-3.78	114.00	120.06
33	5	14	NO1	CD2-CE2-NE1	-3.15	102.72	108.92
33	5	14	NO1	CZ2-CE2-NE1	-2.96	121.93	130.72
33	5	14	NO1	CZ2-CH2-CZ3	-2.11	117.45	120.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	53/55 (96%)	3.66	40 (75%) 0 1	91, 120, 138, 158	0
2	2	46/47 (97%)	5.48	42 (91%) 0 0	42, 90, 117, 151	0
3	3	63/66 (95%)	4.93	57 (90%) 0 0	52, 106, 135, 145	0
4	4	37/37 (100%)	0.55	3 (8%) 15 9	73, 124, 148, 152	0
5	5	3/13 (23%)	-0.04	0 100 100	84, 84, 84, 84	0
6	A	240/274 (87%)	0.31	14 (5%) 26 16	36, 129, 160, 198	0
7	B	205/211 (97%)	-0.50	0 100 100	13, 85, 130, 161	0
8	C	197/205 (96%)	-0.25	3 (1%) 76 62	24, 110, 147, 170	0
9	D	177/180 (98%)	0.01	7 (3%) 42 28	101, 136, 160, 179	0
10	E	171/185 (92%)	-0.20	3 (1%) 71 57	79, 131, 158, 176	0
11	F	144/144 (100%)	0.63	13 (9%) 12 7	117, 148, 172, 188	0
12	G	142/174 (81%)	0.05	6 (4%) 40 27	30, 112, 143, 169	0
13	H	134/134 (100%)	-0.66	0 100 100	13, 67, 106, 127	0
14	I	141/156 (90%)	0.21	6 (4%) 39 26	13, 128, 156, 181	0
15	J	136/142 (95%)	-0.00	4 (2%) 55 39	25, 112, 155, 202	0
16	K	113/116 (97%)	-0.64	0 100 100	13, 57, 111, 148	0
17	L	104/114 (91%)	0.20	5 (4%) 34 22	73, 125, 149, 167	0
18	M	108/166 (65%)	-0.54	0 100 100	13, 76, 121, 150	0
19	N	117/118 (99%)	-0.28	3 (2%) 59 43	16, 104, 144, 182	0
20	O	94/100 (94%)	-0.13	1 (1%) 82 70	28, 117, 151, 160	0
21	P	127/134 (94%)	-0.58	1 (0%) 87 77	13, 76, 126, 155	0
22	Q	93/95 (97%)	-0.31	0 100 100	35, 114, 152, 159	0
23	R	110/115 (95%)	-0.38	0 100 100	53, 118, 145, 161	0
24	S	175/237 (73%)	0.28	12 (6%) 20 12	78, 136, 159, 184	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	T	84/91 (92%)	0.22	4 (4%) 34 22	75, 117, 145, 181	0
26	U	72/81 (88%)	0.29	2 (2%) 56 41	60, 130, 160, 180	0
27	V	66/67 (98%)	-0.39	1 (1%) 76 62	83, 126, 158, 169	0
28	W	55/55 (100%)	-0.17	0 100 100	35, 105, 140, 169	0
29	X	2686/2880 (93%)	0.29	114 (4%) 40 27	13, 114, 186, 250	0
30	Y	58/60 (96%)	-0.62	0 100 100	13, 70, 119, 132	0
31	Z	122/123 (99%)	0.70	10 (8%) 14 9	38, 143, 188, 205	0
All	All	6073/6575 (92%)	0.21	351 (5%) 26 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	17.1
2	2	8	ASN	13.0
3	3	7	HIS	12.8
3	3	35	GLY	12.7
3	3	33	ASN	12.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NH2	5	13	1/1	0.95	0.41	-	83,83,83,83	0
5	BB9	5	5	6/7	0.86	0.26	-	83,83,83,83	0
5	BB9	5	7	6/7	0.75	0.43	-	83,83,83,83	0
5	BB9	5	11	6/7	0.91	0.34	-	83,83,83,83	0
5	DBU	5	4	5/7	0.85	0.26	-	83,83,83,83	0
5	DHA	5	12	5/6	0.81	0.49	-	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	3GL	5	6	9/11	0.77	0.37	-	83,83,83,83	0
5	MH6	5	10	5/7	0.86	0.27	-	83,83,83,83	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	MG	X	2903	1/1	0.74	2.20	53.88	82,82,82,82	0
34	MG	X	2888	1/1	0.89	2.19	39.33	73,73,73,73	0
34	MG	X	2897	1/1	0.95	0.95	32.28	100,100,100,100	0
34	MG	X	2902	1/1	0.81	1.35	26.97	76,76,76,76	0
34	MG	X	2906	1/1	0.93	1.36	26.86	82,82,82,82	0
34	MG	X	2908	1/1	0.70	1.07	25.72	83,83,83,83	0
34	MG	X	2881	1/1	0.82	0.70	20.90	77,77,77,77	0
34	MG	X	2887	1/1	0.98	0.75	9.72	98,98,98,98	0
34	MG	X	2904	1/1	0.97	0.79	7.73	81,81,81,81	0
34	MG	X	2894	1/1	0.98	0.61	5.96	57,57,57,57	0
34	MG	Z	124	1/1	0.92	0.63	4.48	113,113,113,113	0
34	MG	X	2890	1/1	0.97	0.22	-0.40	58,58,58,58	0
32	ZN	Y	61	1/1	0.91	0.08	-1.28	118,118,118,118	0
32	ZN	4	38	1/1	0.90	0.05	-2.02	125,125,125,125	0
33	NO1	5	14	13/15	0.83	0.28	-	83,83,83,83	0
34	MG	M	167	1/1	0.90	1.30	-	68,68,68,68	0
34	MG	X	2893	1/1	0.88	1.14	-	85,85,85,85	0
34	MG	Z	126	1/1	0.84	1.18	-	122,122,122,122	0
34	MG	X	2895	1/1	0.84	0.22	-	81,81,81,81	0
34	MG	X	2907	1/1	0.95	0.38	-	66,66,66,66	0
34	MG	X	2886	1/1	0.94	0.20	-	80,80,80,80	0
34	MG	Z	129	1/1	0.82	0.87	-	101,101,101,101	0
34	MG	X	2900	1/1	0.97	0.12	-	104,104,104,104	0
34	MG	X	2883	1/1	0.75	1.52	-	104,104,104,104	0
34	MG	X	2896	1/1	0.85	1.48	-	86,86,86,86	0
34	MG	X	2882	1/1	0.83	0.35	-	112,112,112,112	0
34	MG	Z	128	1/1	0.81	0.26	-	110,110,110,110	0
34	MG	X	2901	1/1	0.89	0.53	-	100,100,100,100	0
34	MG	X	2905	1/1	0.95	0.57	-	123,123,123,123	0
34	MG	X	2899	1/1	0.97	0.65	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	X	2889	1/1	0.70	0.83	-	131,131,131,131	0
34	MG	Z	125	1/1	0.81	1.00	-	83,83,83,83	0
34	MG	X	2885	1/1	0.83	0.67	-	98,98,98,98	0
34	MG	X	2884	1/1	0.98	0.28	-	98,98,98,98	0
34	MG	Z	127	1/1	0.79	0.92	-	98,98,98,98	0
34	MG	X	2891	1/1	0.75	0.51	-	84,84,84,84	0
34	MG	X	2898	1/1	0.96	0.58	-	57,57,57,57	0
34	MG	X	2892	1/1	0.82	0.57	-	109,109,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.