



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:34 am GMT

PDB ID : 3CF5
Title : Thiopeptide antibiotic Thiostrepton 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 : 2008-03-02
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

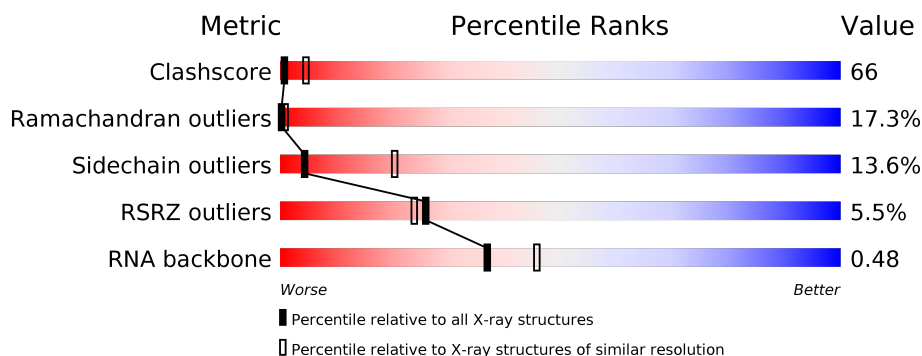
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	112137	1100 (3.36-3.24)
Ramachandran outliers	110173	1081 (3.36-3.24)
Sidechain outliers	110143	1080 (3.36-3.24)
RSRZ outliers	101464	1039 (3.36-3.24)
RNA backbone	2435	1111 (3.80-2.80)

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>71%</div> <div>96%</div> <div>.</div> </div>
2	2	47	<div> <div>98%</div> <div>98%</div> <div>.</div> </div>
3	3	66	<div> <div>89%</div> <div>94%</div> <div>5%</div> </div>
4	4	37	<div> <div>19%</div> <div>8%</div> <div>73%</div> <div>19%</div> </div>
5	5	19	<div> <div>5%</div> <div>68%</div> <div>32%</div> </div>
6	A	274	<div> <div>2%</div> <div>17%</div> <div>54%</div> <div>15%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
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
32	MG	X	2888	-	-	-	X
32	MG	X	2903	-	-	-	X
32	MG	X	2905	-	-	-	X
32	MG	X	2907	-	-	-	X
32	MG	X	2909	-	-	-	X
32	MG	Z	124	-	-	-	X
5	BB9	5	13	-	X	-	-

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 84475 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 THIOSTREPTON.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	5	19	Total C N O S 114 72 19 18 5	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			
			741	465	139	137	0	0	0

- 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		
			1014	639	199	174	2	0	0

- 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		
			726	458	136	130	2	0	0

- 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		
			825	513	160	151	1	0	0

- 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		
			1345	849	236	254	6	0	0

- 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		
			625	393	122	109	1	0	0

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

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

- 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 RRNA-23S RIBOSOMAL 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 RRNA-5S RIBOSOMAL RNA.

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

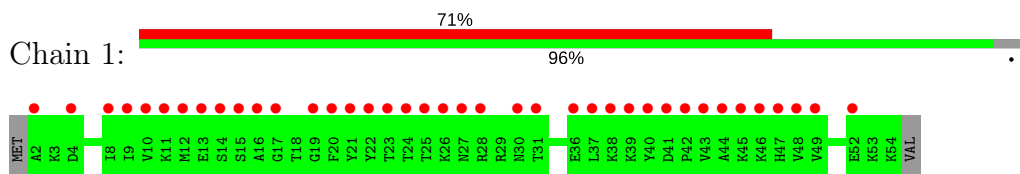
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	X	30	Total	Mg	0	0
			30	30		
32	Z	5	Total	Mg	0	0
			5	5		
32	M	1	Total	Mg	0	0
			1	1		

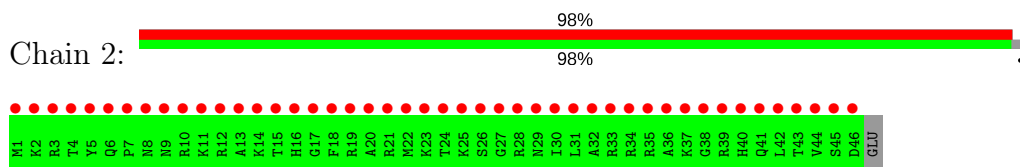
3 Residue-property plots [i](#)

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

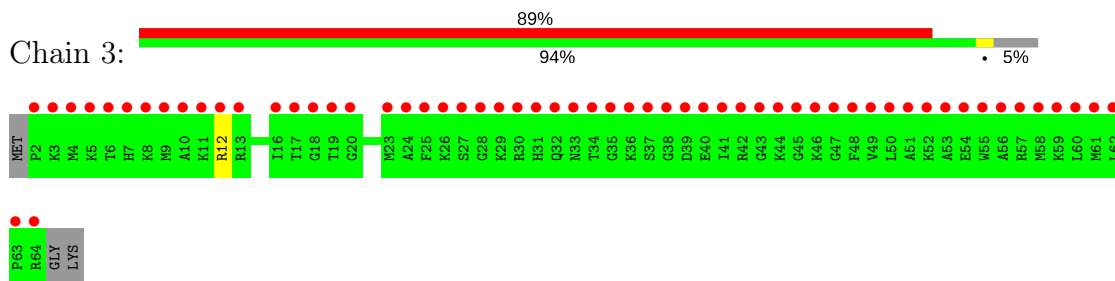
- Molecule 1: 50S RIBOSOMAL PROTEIN L33



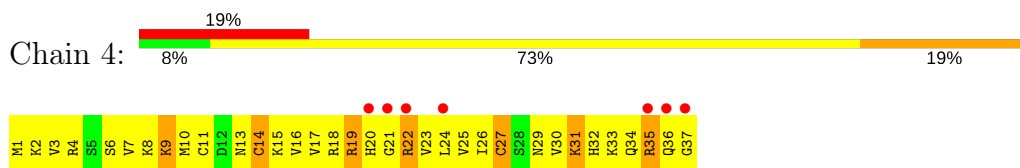
- Molecule 2: 50S RIBOSOMAL PROTEIN L34



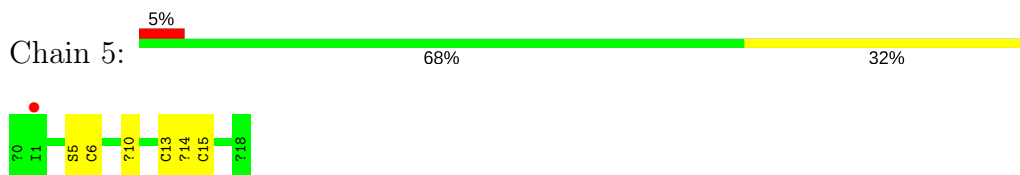
- Molecule 3: 50S RIBOSOMAL PROTEIN L35



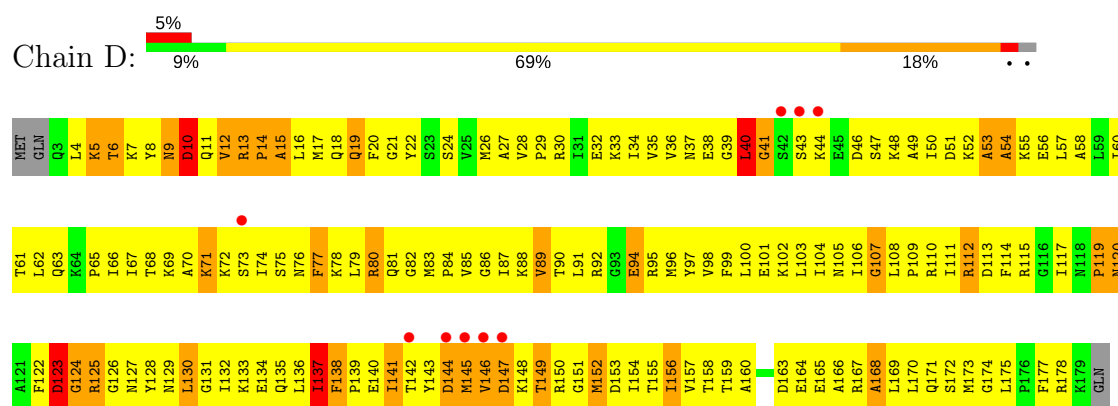
- Molecule 4: 50S RIBOSOMAL PROTEIN L36



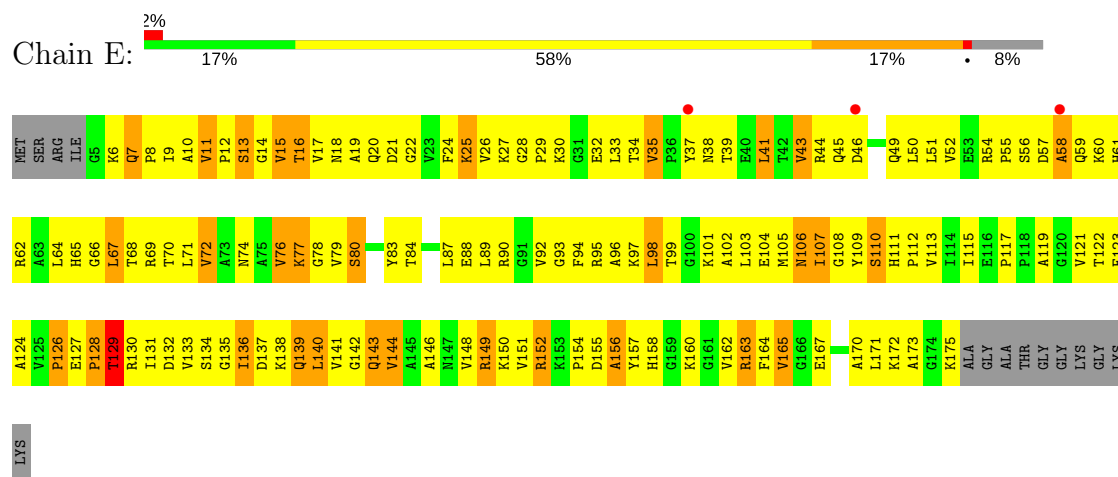
- Molecule 5: THIOSTREPTON



- Molecule 6: 50S RIBOSOMAL PROTEIN L2



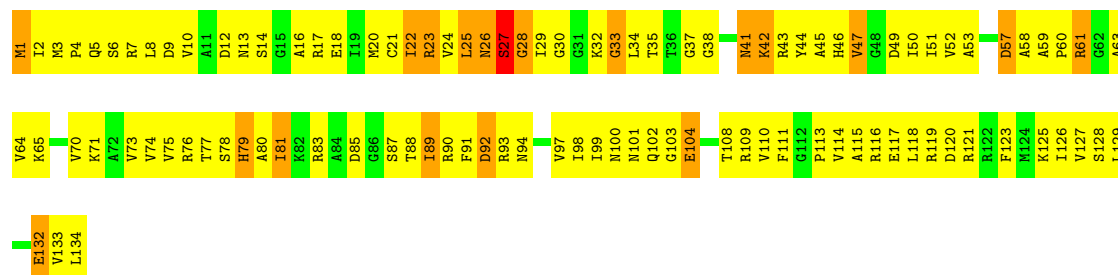
• Molecule 10: 50S RIBOSOMAL PROTEIN L6





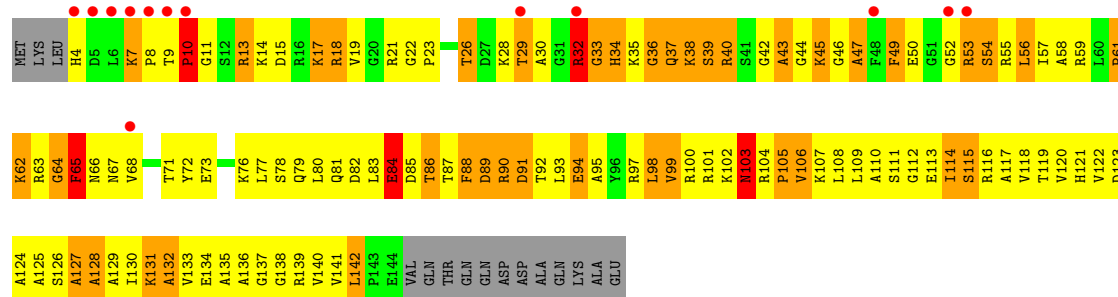
• Molecule 13: 50S RIBOSOMAL PROTEIN L14

Chain H: 22% 63% 13%



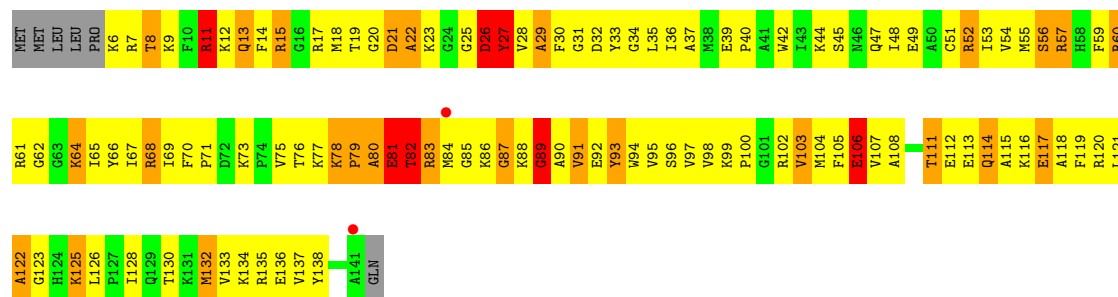
• Molecule 14: 50S RIBOSOMAL PROTEIN L15

Chain I: 8% 13% 49% 26% 10%



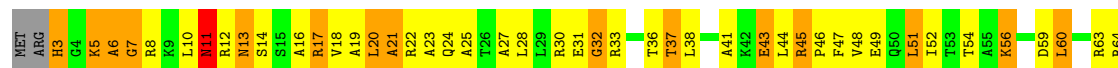
• Molecule 15: 50S RIBOSOMAL PROTEIN L16

Chain J: 15% 57% 18% 5%



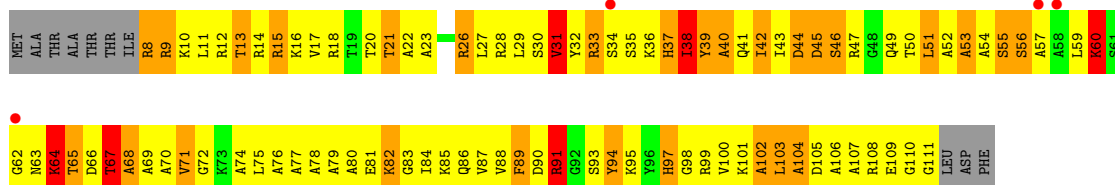
• Molecule 16: 50S RIBOSOMAL PROTEIN L17

Chain K: 24% 53% 19%

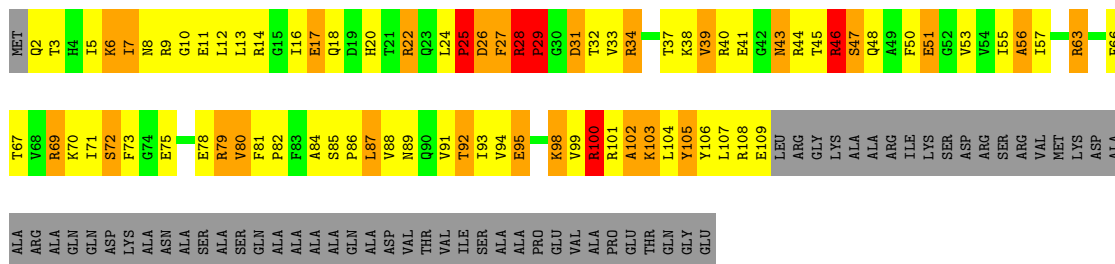




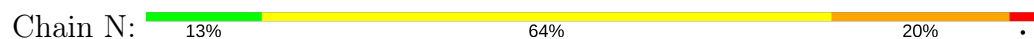
• Molecule 17: 50S RIBOSOMAL PROTEIN L18



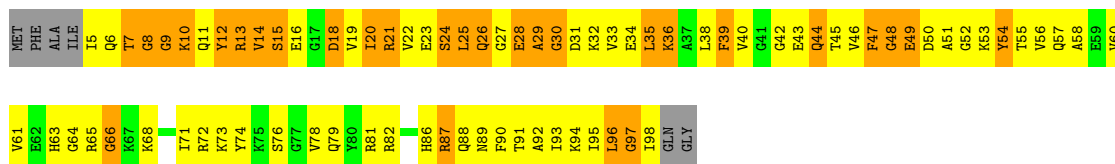
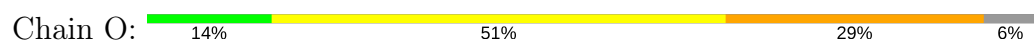
• Molecule 18: 50S RIBOSOMAL PROTEIN L19



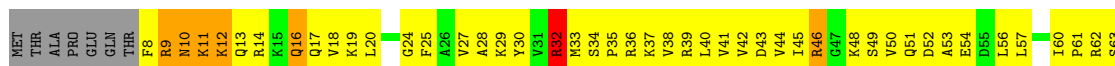
• Molecule 19: 50S RIBOSOMAL PROTEIN L20



• Molecule 20: 50S RIBOSOMAL PROTEIN L21

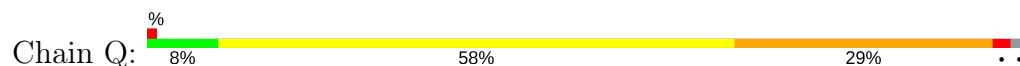


• Molecule 21: 50S RIBOSOMAL PROTEIN L22

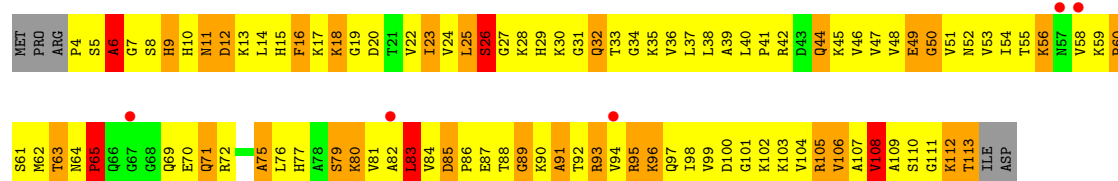
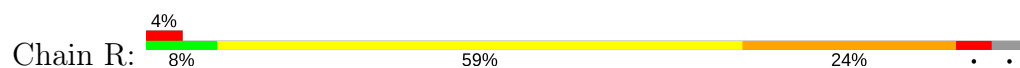




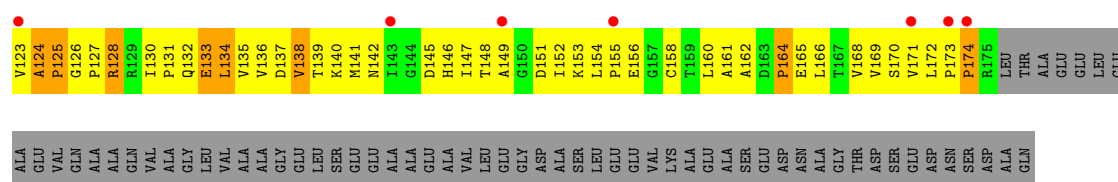
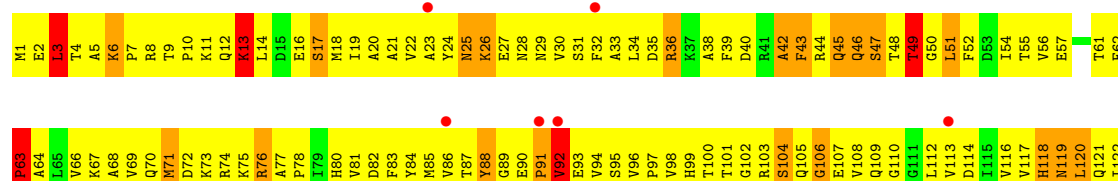
• Molecule 22: 50S RIBOSOMAL PROTEIN L23



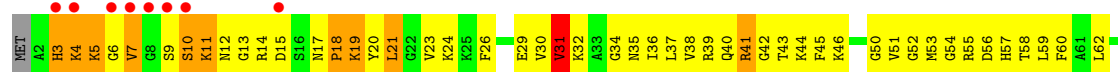
• Molecule 23: 50S RIBOSOMAL PROTEIN L24



• Molecule 24: 50S RIBOSOMAL PROTEIN L25

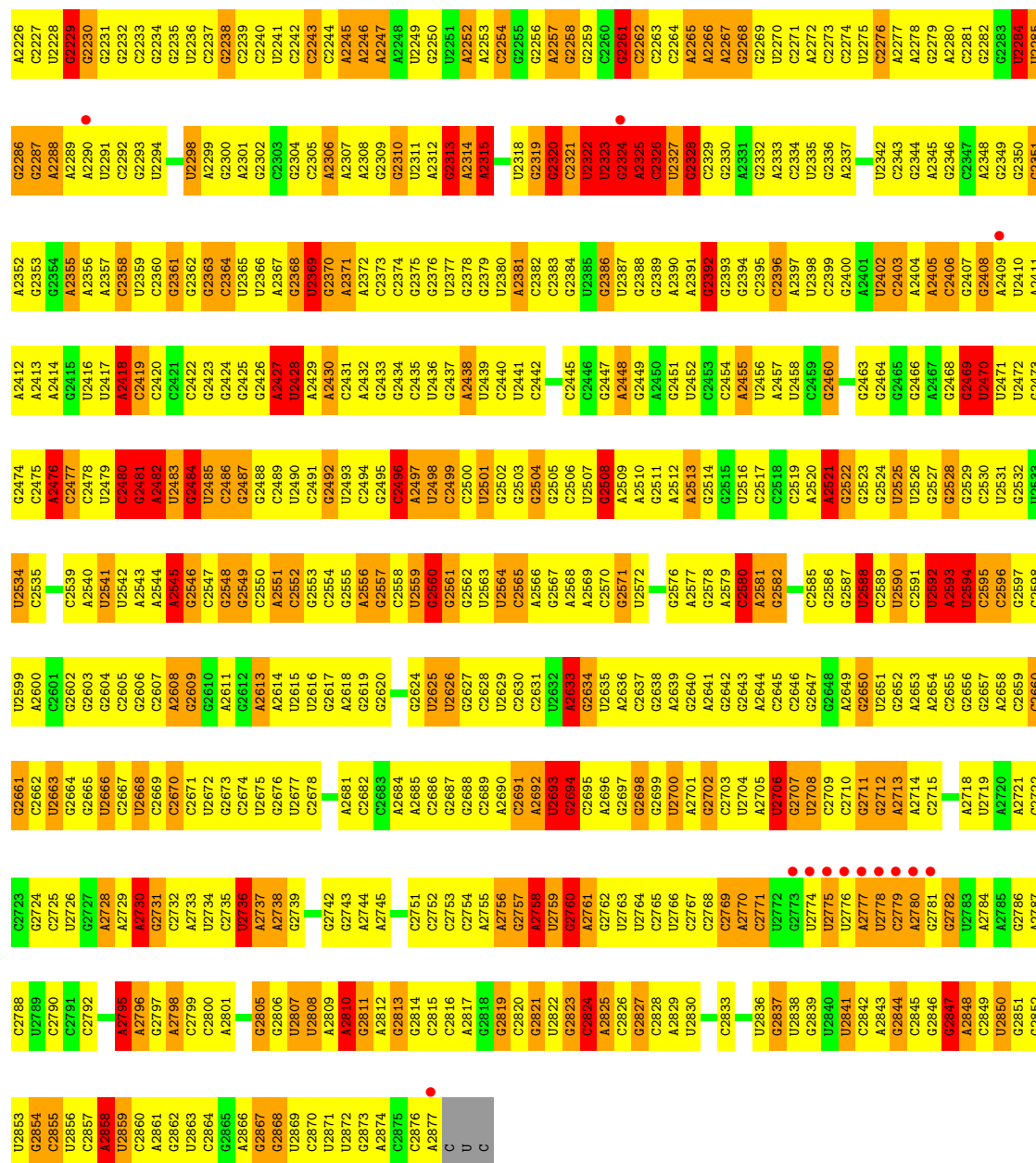


• Molecule 25: 50S RIBOSOMAL PROTEIN L27



A1239	A1240	G1241	A1242	G1243	U1244	G1245	A1246	U1247	A1248	G1249	A1250	G1251	C1252	C1253	G1254	A1255	C1256	U1257	G1258	A1259	A1260	G1261	U1262	C1263	G1264	C1265	G1266	U1267	U1268	G1269	C1270	G1271	G1272	C1273	C1274	A1275	U1276	G1277	A1278	U1279	U1280	A1281	A1282	C1283	G1284	A1285	U1286	A1287	A1288	A1289	A1290	G1291	A1292	A1293	A1294	U1295	G1296	A1297	A1298	A1299		
C1178	G1179	U1118	A1180	C1181	G1182	C1183	G1184	U1185	A1186	G1187	A1188	C1189	C1190	A1191	C1192	U1193	U1194	U1195	U1196	U1197	C1198	U1199	A1199	A1199	A1140	A1141	A1142	A1143	U1144	G1145	G1146	G1147	G1148	C1149	C1150	U1151	C1152	C1153	A1154	G1155	U1156	U1159	C1160	U1161	A1162	C1163	C1164	G1165	A1166	A1167	G1168	C1169	U1170	A1171	A1172	G1173	C1174	A1175	G1176	U1177		
U1056	A1057	G1058	A1059	C1060	A1061	G1062	C1063	U1064	A1065	G1066	U1067	C1068	A1069	G1070	U1071	G1072	U1073	G1074	C1075	U1076	U1077	A1078	G1079	A1080	A1081	C1082	C1083	A1084	G1085	C1086	C1087	A1088	C1089	C1090	C1091	U1092	U1093	A1094	U1095	A1096	A1097	G1098	A1099	U1100	U1101	G1102	C1103	G1104	U1105	A1106	U1107	A1108	A1109	U1110	U1112	C1113	A1114	C1115	U1116	U1117		
A994	A995	C996	C997	C998	A999	G1000	A1001	C1002	A1003	C1004	U1005	C1006	A1007	G1008	U1009	U1010	A1011	A1012	G1013	U1014	U1015	C1016	U1017	C1018	U1019	U1020	A1021	U1022	G1023	G1024	A1025	U1026	C1027	U1030	C1031	A1032	U1033	U1034	G1035	A1036	G1037	U1038	A1039	U1040	G1041	U1042	C1043	U1044	U1045	U1046	G1047	U1048	C1049	U1050	U1051	C1052	G1053	A1054	C1055	U1056		
U800	A801	C802	C803	G804	G805	A806	A807	C808	C809	U810	G811	G812	A813	G814	A815	U816	A817	G818	C819	U820	A821	G822	U823	U824	C825	U826	G827	C828	C829	C830	G831	A832	A833	A834	U835	G836	U837	A838	U839	U840	C841	A842	G843	U844	U845	C846	U847	A848	C849	C850	U851	U852	U853	U854	C855	C856	C857					
A740	G741	G742	A743	C744	C745	G746	A747	A748	C749	G750	G751	G752	U753	G754	C755	G756	U757	G758	C759	U760	G761	A762	A763	A764	C765	A766	G767	U768	C769	U770	C771	G772	G773	A774	U775	U776	A777	G778	U779	U780	G781	U782	G783	U784	U785	U786	A787	G788	G789	A790	G791	U792	G793	A794	U795	A796	A797	G798	C799			
A619	G620	U621	G622	C623	A624	G625	U626	A627	G628	A629	C630	G631	A632	G633	C634	G635	C636	G637	A638	G639	C640	G641	A642	A643	C644	G645	G646	G647	A648	G649	U650	C651	G652	C653	A654	A655	U656	A657	G658	U659	C660	C661	G662	G663	A664	U665	U666	U667	A668	G669	U670	C671	G672	C673	G674	U675	C676	G677	G678			
C679	U680	A681	G682	A683	C684	U685	C686	G687	A688	C689	G690	C691	C692	A693	G694	U695	G696	G697	A698	G699	U700	U701	A702	C703	A704	G705	A706	U707	G708	A709	C710	C711	A712	G713	G714	U715	U716	A717	A718	U719	A720	C721	C722	C723	C724	C725	G726	U727	U728	A729	C730	A731	C732	G733	G734	G735	C736	C737	G738	G739		
A556	U557	G558	C559	G560	C561	U562	G563	U564	A565	C566	G567	C568	C569	G570	U571	G572	C573	C574	U575	A576	U577	U578	C579	A580	A581	G582	C583	A584	U585	G586	A587	G588	C589	C590	G591	A592	C593	G594	U595	U596	U597	U598	A599	G600	A601	C602	C603	U604	U605	U606	U607	C608	U609	C610	C611	G612	A613	C614	C615	U616	U617	A618
C432	C433	C434	C435	C436	C437	C438	C439	U440	A441	A442	U443	U444	A445	C446	U447	C448	G449	A450	C451	A452	U453	C454	A455	C456	C457	G458	C459	U460	A461	A462	C463	A403	C404	C405	G406	U467	A407	A468	G469	U470	A471	C472	C473	U474	U475	C476	A477	G480	U481	A482	A483	G484	C485	U486	G487	C488	A489	A490	U491	C492		
U	A	C	U	G	G	C	A	C	C	U	G	A	G	U	U	A387	G388	G389	U390	C391	G392	U393	U394	A395	U396	U397	C398	G399	U400	A401	A402	A403	A404	C405	G406	U407	A408	G409	C410	C411	U412	G413	A414	A415	U416	C417	C418	G419	C420	G421	G422	A423	A424	C425	G426	C427	A428	C429	C430	A431		

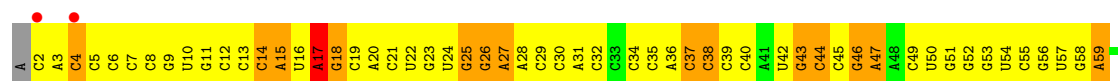
WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 30: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: RRNA-5S RIBOSOMAL RNA





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 – 3.30 29.76 – 3.31	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-3.30) 93.2 (29.76-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 3.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.318 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	67.5	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	84475	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DCY, DHA, QUA, BB9, NH2, MH6, DBU, TS9

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	0.46	0/298	0.67	0/390
5	5	1.46	0/31	1.18	0/38
6	A	0.55	0/1862	0.85	2/2510 (0.1%)
7	B	0.77	0/1567	1.04	4/2105 (0.2%)
8	C	0.63	0/1529	0.91	0/2070
9	D	0.48	0/1419	0.71	0/1903
10	E	0.48	0/1308	0.80	1/1771 (0.1%)
11	F	0.50	0/1063	0.71	0/1440
12	G	0.69	0/1138	1.00	3/1539 (0.2%)
13	H	0.79	0/1007	0.96	1/1352 (0.1%)
14	I	0.65	0/1081	0.94	3/1448 (0.2%)
15	J	0.67	0/1113	0.91	2/1486 (0.1%)
16	K	0.87	0/886	1.06	2/1188 (0.2%)
17	L	0.52	0/785	0.86	0/1048
18	M	0.73	0/884	1.20	6/1186 (0.5%)
19	N	0.63	0/994	0.89	0/1323
20	O	0.61	0/750	0.90	0/1000
21	P	0.77	0/1027	0.93	1/1373 (0.1%)
22	Q	0.67	0/737	0.98	4/988 (0.4%)
23	R	0.55	0/835	0.95	2/1121 (0.2%)
24	S	0.50	0/1370	0.75	0/1862
25	T	0.56	0/633	0.83	1/838 (0.1%)
26	U	0.58	0/556	0.95	1/741 (0.1%)
27	V	0.44	0/537	0.67	0/714
28	W	0.56	0/426	0.84	0/568
29	X	0.88	59/64561 (0.1%)	1.05	497/100708 (0.5%)
30	Y	0.70	0/469	1.11	2/629 (0.3%)
31	Z	0.55	0/2904	0.76	0/4525
All	All	0.81	59/91770 (0.1%)	1.01	532/137864 (0.4%)

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
6	A	0	1
19	N	0	2
22	Q	0	1
29	X	2	257
30	Y	0	1
31	Z	0	4
All	All	2	266

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	1856	U	C4'-C3'	-9.30	1.43	1.53
29	X	1856	U	O3'-P	-8.64	1.50	1.61
29	X	1056	U	P-O5'	8.52	1.68	1.59
29	X	1855	G	O3'-P	-8.11	1.51	1.61
29	X	551	A	O3'-P	-8.05	1.51	1.61

The worst 5 of 532 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	X	1055	A	N9-C1'-C2'	-29.46	75.70	114.00
29	X	2324	G	N9-C1'-C2'	22.22	142.88	114.00
29	X	557	U	N1-C1'-C2'	19.61	139.50	114.00
29	X	417	C	N1-C1'-C2'	18.73	138.35	114.00
18	M	28	ARG	C-N-CD	-18.52	79.85	120.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	X	1278	A	C1'
29	X	2592	U	C1'

5 of 266 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	104	TYR	Sidechain
19	N	32	TYR	Sidechain
19	N	76	TYR	Sidechain
22	Q	25	TYR	Sidechain

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Mol	Chain	Res	Type	Group
29	X	12	U	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	0	0
2	2	46	0	0	0	0
3	3	63	0	0	1	0
4	4	297	0	330	62	0
5	5	114	0	79	5	0
6	A	1826	0	1885	451	0
7	B	1539	0	1600	303	0
8	C	1506	0	1525	371	0
9	D	1400	0	1481	373	0
10	E	1286	0	1336	264	0
11	F	1044	0	1088	176	0
12	G	1114	0	1144	310	0
13	H	997	0	1046	194	0
14	I	1067	0	1103	301	0
15	J	1090	0	1125	273	0
16	K	878	0	930	135	0
17	L	779	0	820	231	0
18	M	871	0	894	208	0
19	N	978	0	1020	239	0
20	O	741	0	756	186	0
21	P	1014	0	1096	181	0
22	Q	726	0	753	150	0
23	R	825	0	881	266	0
24	S	1345	0	1372	303	0
25	T	625	0	655	111	0
26	U	552	0	604	207	0
27	V	533	0	558	109	0
28	W	424	0	470	83	0
29	X	57651	0	29049	4301	0
30	Y	457	0	462	86	0
31	Z	2598	0	1328	185	0
32	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	30	0	0	0	0
32	Z	5	0	0	0	0
All	All	84475	0	55390	9214	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 66.

The worst 5 of 9214 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)
7:B:116:VAL:N	7:B:136:ARG:HE	1.23	1.30
29:X:1053:G:H2'	29:X:1054:C:C6	1.70	1.26
29:X:2196:U:H2'	29:X:2197:U:O4'	1.31	1.23
29:X:2736:U:O2'	29:X:2737:A:H5''	1.36	1.21
29:X:2496:C:O2'	29:X:2497:A:H3'	1.40	1.19

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%)	10 (29%)	5 (14%)	0	1
5	5	5/19 (26%)	4 (80%)	1 (20%)	0	100	100
6	A	238/274 (87%)	154 (65%)	50 (21%)	34 (14%)	0	1
7	B	203/211 (96%)	148 (73%)	32 (16%)	23 (11%)	0	3
8	C	195/205 (95%)	97 (50%)	54 (28%)	44 (23%)	0	0
9	D	175/180 (97%)	95 (54%)	48 (27%)	32 (18%)	0	1
10	E	169/185 (91%)	100 (59%)	38 (22%)	31 (18%)	0	1
11	F	142/144 (99%)	94 (66%)	29 (20%)	19 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	G	140/174 (80%)	76 (54%)	34 (24%)	30 (21%)	0	0
13	H	132/134 (98%)	105 (80%)	18 (14%)	9 (7%)	1	10
14	I	139/156 (89%)	59 (42%)	45 (32%)	35 (25%)	0	0
15	J	134/142 (94%)	82 (61%)	31 (23%)	21 (16%)	0	1
16	K	111/116 (96%)	74 (67%)	25 (22%)	12 (11%)	0	3
17	L	102/114 (90%)	59 (58%)	19 (19%)	24 (24%)	0	0
18	M	106/166 (64%)	70 (66%)	23 (22%)	13 (12%)	0	2
19	N	115/118 (98%)	57 (50%)	40 (35%)	18 (16%)	0	1
20	O	92/100 (92%)	57 (62%)	10 (11%)	25 (27%)	0	0
21	P	125/134 (93%)	89 (71%)	21 (17%)	15 (12%)	0	2
22	Q	91/95 (96%)	39 (43%)	28 (31%)	24 (26%)	0	0
23	R	108/115 (94%)	62 (57%)	27 (25%)	19 (18%)	0	1
24	S	173/237 (73%)	93 (54%)	46 (27%)	34 (20%)	0	1
25	T	82/91 (90%)	47 (57%)	19 (23%)	16 (20%)	0	1
26	U	70/81 (86%)	35 (50%)	16 (23%)	19 (27%)	0	0
27	V	64/67 (96%)	35 (55%)	16 (25%)	13 (20%)	0	1
28	W	53/55 (96%)	38 (72%)	9 (17%)	6 (11%)	0	3
30	Y	56/60 (93%)	40 (71%)	9 (16%)	7 (12%)	0	2
All	All	3055/3410 (90%)	1829 (60%)	698 (23%)	528 (17%)	0	1

5 of 528 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	59	LYS
6	A	145	LEU
6	A	168	LYS
6	A	217	ARG
6	A	220	HIS

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%)	32 (91%)	3 (9%)	12	42
5	5	3/4 (75%)	3 (100%)	0	100	100
6	A	185/215 (86%)	161 (87%)	24 (13%)	5	22
7	B	155/157 (99%)	132 (85%)	23 (15%)	3	17
8	C	157/163 (96%)	131 (83%)	26 (17%)	2	12
9	D	153/156 (98%)	138 (90%)	15 (10%)	9	34
10	E	136/144 (94%)	128 (94%)	8 (6%)	23	58
11	F	107/107 (100%)	100 (94%)	7 (6%)	20	55
12	G	118/146 (81%)	96 (81%)	22 (19%)	2	8
13	H	103/103 (100%)	88 (85%)	15 (15%)	3	18
14	I	108/121 (89%)	91 (84%)	17 (16%)	3	15
15	J	110/116 (95%)	89 (81%)	21 (19%)	2	7
16	K	90/93 (97%)	76 (84%)	14 (16%)	3	15
17	L	74/82 (90%)	54 (73%)	20 (27%)	0	2
18	M	94/134 (70%)	72 (77%)	22 (23%)	1	3
19	N	96/97 (99%)	83 (86%)	13 (14%)	4	20
20	O	75/79 (95%)	70 (93%)	5 (7%)	19	53
21	P	109/115 (95%)	100 (92%)	9 (8%)	13	43
22	Q	75/76 (99%)	67 (89%)	8 (11%)	8	30
23	R	91/96 (95%)	72 (79%)	19 (21%)	1	5
24	S	149/192 (78%)	137 (92%)	12 (8%)	14	44
25	T	62/67 (92%)	57 (92%)	5 (8%)	14	44
26	U	57/66 (86%)	44 (77%)	13 (23%)	1	4
27	V	54/55 (98%)	48 (89%)	6 (11%)	7	29
28	W	48/48 (100%)	38 (79%)	10 (21%)	1	5
30	Y	51/53 (96%)	48 (94%)	3 (6%)	23	58
All	All	2495/2720 (92%)	2155 (86%)	340 (14%)	4	20

5 of 340 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	I	65	PHE

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Mol	Chain	Res	Type
16	K	83	VAL
26	U	47	HIS
14	I	103	ASN
15	J	82	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
13	H	41	ASN
16	K	13	ASN
27	V	45	GLN
13	H	79	HIS
14	I	66	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2680/2880 (93%)	688 (25%)	0
31	Z	121/123 (98%)	24 (19%)	0
All	All	2801/3003 (93%)	712 (25%)	0

5 of 712 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	2	G
29	X	4	C
29	X	13	A
29	X	14	A
29	X	27	G

There are no RNA pucker outliers to report.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	TS9	5	10	5	6,8,10	0.87	0	5,12,15	1.11	0
5	BB9	5	11	5	3,5,6	1.27	0	1,5,7	2.58	1 (100%)
5	BB9	5	13	5	2,4,6	1.64	1 (50%)	3,4,7	2.70	3 (100%)
5	MH6	5	14	5	3,3,6	1.53	1 (33%)	1,3,7	0.40	0
5	BB9	5	15	5	3,5,6	3.66	1 (33%)	1,5,7	3.90	1 (100%)
5	DHA	5	16	5	4,4,5	4.25	2 (50%)	3,4,6	4.43	1 (33%)
5	DHA	5	17	5	4,4,5	1.88	1 (25%)	3,4,6	2.13	1 (33%)
5	DHA	5	3	5	4,4,5	2.04	2 (50%)	3,4,6	1.81	1 (33%)
5	BB9	5	6	5	3,5,6	1.81	1 (33%)	1,5,7	2.60	1 (100%)
5	DBU	5	8	5	4,4,6	3.09	2 (50%)	4,4,7	1.52	1 (25%)
5	DCY	5	9	5	5,5,6	0.59	0	2,5,7	3.68	2 (100%)

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	TS9	5	10	5	-	0/9/12/16	0/0/0/0
5	BB9	5	11	5	-	0/0/4/6	0/0/0/0
5	BB9	5	13	5	-	0/0/2/6	0/0/0/0
5	MH6	5	14	5	-	0/0/0/6	0/0/0/0
5	BB9	5	15	5	-	0/0/4/6	0/0/0/0
5	DHA	5	16	5	-	0/0/2/4	0/0/0/0
5	DHA	5	17	5	-	0/0/2/4	0/0/0/0
5	DHA	5	3	5	-	0/0/2/4	0/0/0/0
5	BB9	5	6	5	-	0/0/4/6	0/0/0/0
5	DBU	5	8	5	-	0/1/2/6	0/0/0/0
5	DCY	5	9	5	-	0/1/4/6	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	15	BB9	O-C	-6.31	1.07	1.22
5	5	16	DHA	C-CA	-2.52	1.40	1.45
5	5	8	DBU	C-CA	-2.03	1.43	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	14	MH6	C-CA	2.03	1.53	1.49
5	5	3	DHA	C-CA	2.22	1.48	1.45

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	5	16	DHA	O-C-CA	-7.61	111.08	125.50
5	5	9	DCY	CA-CB-SG	-4.54	104.20	114.42
5	5	17	DHA	O-C-CA	-2.95	119.92	125.50
5	5	13	BB9	CB-CA-N	-2.67	113.96	122.50
5	5	6	BB9	O-C-CA	-2.60	122.15	125.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	10	TS9	1	0
5	5	13	BB9	1	0
5	5	14	MH6	1	0
5	5	15	BB9	1	0
5	5	6	BB9	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 36 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	53/55 (96%)	3.44	39 (73%) 0 0	48, 56, 77, 82	0
2	2	46/47 (97%)	5.52	46 (100%) 0 0	9, 29, 38, 40	0
3	3	63/66 (95%)	5.06	59 (93%) 0 0	23, 41, 51, 57	0
4	4	37/37 (100%)	1.16	7 (18%) 1 1	60, 69, 77, 81	0
5	5	6/19 (31%)	1.09	1 (16%) 2 2	79, 83, 86, 86	0
6	A	240/274 (87%)	-0.11	6 (2%) 58 54	25, 63, 77, 84	0
7	B	205/211 (97%)	-0.69	1 (0%) 90 90	3, 22, 49, 63	0
8	C	197/205 (96%)	-0.30	4 (2%) 65 63	8, 51, 73, 83	0
9	D	177/180 (98%)	0.03	9 (5%) 29 26	60, 75, 85, 91	0
10	E	171/185 (92%)	-0.35	3 (1%) 69 66	44, 66, 79, 88	0
11	F	144/144 (100%)	1.48	40 (27%) 1 1	74, 89, 98, 102	0
12	G	142/174 (81%)	-0.29	3 (2%) 64 61	22, 43, 67, 72	0
13	H	134/134 (100%)	-0.78	0 100 100	3, 16, 37, 45	0
14	I	141/156 (90%)	0.25	13 (9%) 10 9	22, 62, 77, 85	0
15	J	136/142 (95%)	-0.32	2 (1%) 74 70	27, 51, 73, 80	0
16	K	113/116 (97%)	-0.83	0 100 100	3, 9, 24, 34	0
17	L	104/114 (91%)	-0.06	4 (3%) 41 37	43, 62, 72, 75	0
18	M	108/166 (65%)	-0.74	0 100 100	4, 19, 43, 64	0
19	N	117/118 (99%)	-0.57	0 100 100	4, 40, 62, 73	0
20	O	94/100 (94%)	-0.43	0 100 100	18, 53, 71, 81	0
21	P	127/134 (94%)	-0.72	0 100 100	4, 18, 53, 76	0
22	Q	93/95 (97%)	-0.41	1 (1%) 80 79	32, 50, 69, 80	0
23	R	110/115 (95%)	-0.15	5 (4%) 34 32	36, 54, 80, 87	0
24	S	175/237 (73%)	0.23	13 (7%) 15 15	61, 71, 82, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	T	84/91 (92%)	0.02	8 (9%) 9 8	35, 51, 80, 90	0
26	U	72/81 (88%)	0.09	3 (4%) 37 34	45, 61, 72, 78	0
27	V	66/67 (98%)	-0.49	0 100 100	49, 61, 81, 88	0
28	W	55/55 (100%)	-0.42	0 100 100	23, 41, 61, 78	0
29	X	2686/2880 (93%)	-0.37	61 (2%) 61 58	4, 41, 116, 151	0
30	Y	58/60 (96%)	-0.52	1 (1%) 70 67	4, 17, 44, 52	0
31	Z	122/123 (99%)	-0.11	3 (2%) 58 54	30, 75, 102, 129	0
All	All	6076/6581 (92%)	-0.15	332 (5%) 26 24	3, 49, 95, 151	0

The worst 5 of 332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	3	39	ASP	15.9
2	2	26	SER	9.7
1	1	2	ALA	9.6
3	3	31	HIS	9.6
2	2	4	THR	9.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	BB9	5	15	6/7	0.78	0.48	-	88,88,88,88	0
5	TS9	5	10	9/11	0.87	0.38	-	87,88,89,89	0
5	BB9	5	6	6/7	0.89	0.18	-	82,84,85,86	0
5	BB9	5	11	6/7	0.86	0.23	-	85,87,87,88	0
5	DHA	5	3	5/6	0.77	0.47	-	82,83,84,85	0
5	DHA	5	16	5/6	0.51	0.55	-	83,83,85,86	0
5	BB9	5	13	5/7	0.83	0.22	-	85,86,86,87	0
5	DHA	5	17	5/6	0.55	0.39	-	76,77,78,80	2
5	MH6	5	14	4/7	0.85	0.30	-	86,86,87,87	0
5	DCY	5	9	6/7	0.81	0.18	-	87,87,87,87	0
5	DBU	5	8	5/7	0.93	0.16	-	85,86,87,87	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
32	MG	X	2907	1/1	0.96	0.73	64.14	17,17,17,17	0
32	MG	X	2905	1/1	0.97	0.50	9.49	13,13,13,13	0
32	MG	X	2888	1/1	0.95	0.30	8.48	3,3,3,3	0
32	MG	X	2903	1/1	0.95	0.30	6.42	3,3,3,3	0
32	MG	Z	124	1/1	0.95	0.31	6.28	26,26,26,26	0
32	MG	X	2909	1/1	0.96	0.21	5.34	3,3,3,3	0
32	MG	X	2895	1/1	0.98	0.25	1.39	3,3,3,3	0
32	MG	X	2910	1/1	0.90	0.38	-	19,19,19,19	0
32	MG	X	2885	1/1	0.93	0.41	-	56,56,56,56	0
32	MG	X	2901	1/1	0.98	0.08	-	60,60,60,60	0
32	MG	X	2887	1/1	0.98	0.18	-	3,3,3,3	0
32	MG	X	2881	1/1	0.95	0.25	-	59,59,59,59	0
32	MG	X	2899	1/1	0.99	0.54	-	3,3,3,3	0
32	MG	X	2882	1/1	0.97	0.36	-	12,12,12,12	0
32	MG	X	2906	1/1	0.98	0.19	-	58,58,58,58	0
32	MG	X	2883	1/1	0.99	0.10	-	49,49,49,49	0
32	MG	X	2897	1/1	0.98	0.47	-	3,3,3,3	0
32	MG	X	2884	1/1	0.83	0.79	-	55,55,55,55	0
32	MG	X	2904	1/1	0.97	0.32	-	6,6,6,6	0
32	MG	X	2900	1/1	0.96	0.26	-	3,3,3,3	0
32	MG	Z	126	1/1	0.95	0.34	-	25,25,25,25	0
32	MG	X	2893	1/1	0.96	0.15	-	13,13,13,13	0
32	MG	M	167	1/1	0.98	0.54	-	3,3,3,3	0
32	MG	X	2894	1/1	0.99	0.40	-	15,15,15,15	0
32	MG	X	2898	1/1	0.90	0.54	-	19,19,19,19	0
32	MG	X	2902	1/1	0.96	0.38	-	24,24,24,24	0
32	MG	Z	128	1/1	0.95	0.09	-	41,41,41,41	0
32	MG	X	2889	1/1	0.95	0.77	-	3,3,3,3	0
32	MG	X	2890	1/1	0.91	0.34	-	49,49,49,49	0
32	MG	X	2886	1/1	0.91	0.26	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	Z	127	1/1	0.95	0.17	-	12,12,12,12	0
32	MG	X	2892	1/1	0.95	0.16	-	22,22,22,22	0
32	MG	X	2896	1/1	0.95	0.27	-	3,3,3,3	0
32	MG	X	2908	1/1	0.97	0.11	-	3,3,3,3	0
32	MG	X	2891	1/1	0.99	0.41	-	12,12,12,12	0
32	MG	Z	125	1/1	0.98	0.29	-	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.