



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 06:08 PM BST

PDB ID : 4KD8
Title : 70S Ribosome translocation intermediate FA-3.6A CONTAINING ELONGATION FACTOR EFG/FUSIDIC ACID/GDP, MRNA, AND TRNA BOUND IN THE pe^*/E STATE. THIS ENTRY CONTAINS THE 30S RIBOSOMAL SUBUNIT A. THE 50S SUBUNIT A CAN BE FOUND IN 4KD9. MOLECULE B IN THE SAME ASYMMETRIC UNIT IS DEPOSITED AS 4KDA (30S) AND 4KDB (50S).
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
Resolution : 3.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

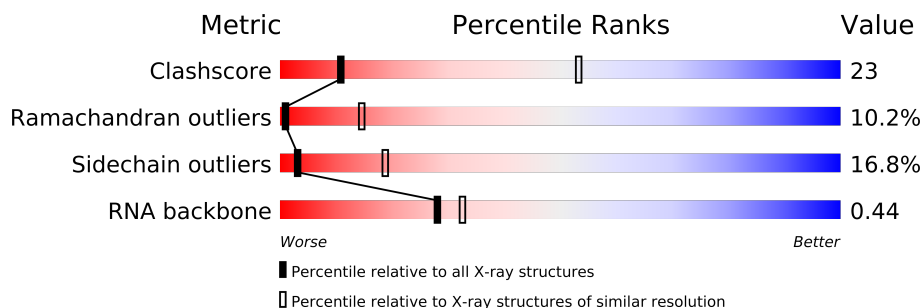
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	FAILED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.50 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	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RNA backbone	1838	1007 (4.22-2.76)


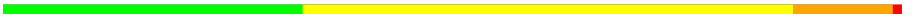
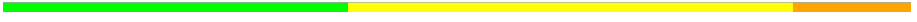

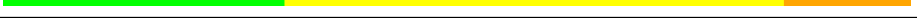

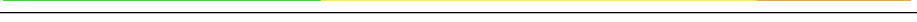

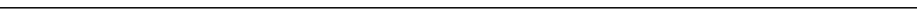
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	235	
2	C	207	
3	D	208	
4	E	151	
5	F	101	
6	G	155	
7	H	138	
8	I	127	
9	J	99	
10	K	119	
11	L	125	
12	M	125	
13	N	60	
14	O	88	
15	P	84	

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Mol	Chain	Length	Quality of chain
16	Q	100	
17	R	70	
18	S	79	
19	T	99	
20	A	1511	
21	W	77	
22	V	23	
23	Y	687	
24	U	6	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 58959 atoms, of which 0 are hydrogen and 0 are deuterium.

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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total	C	N	O	S	0	0	0
			1621	1022	315	283	1			

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	151	Total	C	N	O	S	0	0	0
			1156	729	218	205	4			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	58	HIS	ARG	CONFLICT	UNP P62669

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Q	100	Total	C	N	O	S	0	0	0
			835	534	155	144	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLU	GLN	CONFLICT	UNP P62658

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	S	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	ILE	VAL	CONFLICT	UNP P62661

- Molecule 20 is a RNA chain called ribosomal RNA 16S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	A	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	W	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	23	Total	C	N	O	P	0	0	0
			503	227	106	148	22			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Y	667	Total	C	N	O	S	0	0	0
			5219	3318	893	990	18			

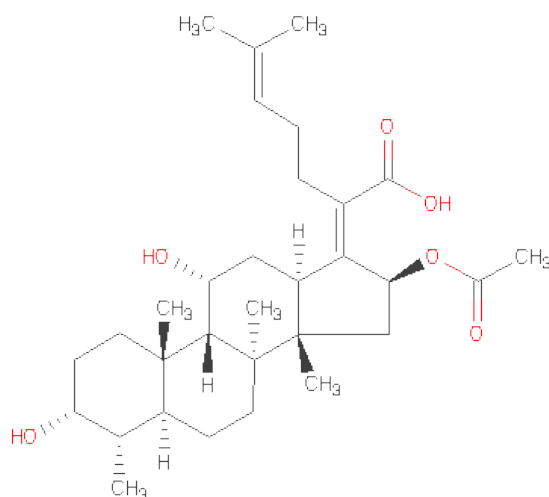
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	129	LYS	HIS	CONFLICT	UNP Q72I01
Y	226	ASN	HIS	CONFLICT	UNP Q72I01

- Molecule 24 is a protein called VIOMYCIN.

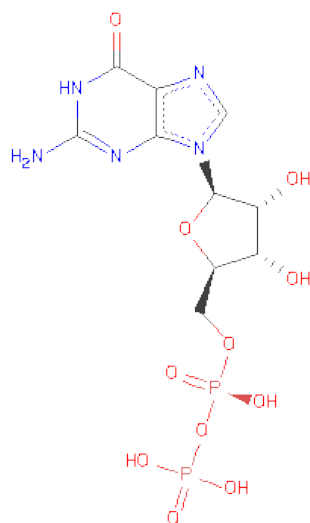
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	U	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	Y	1	Total	C	O	0	0
			37	31	6		

- Molecule 26 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	Y	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	Y	1	Total	Mg	0	0
			1	1		

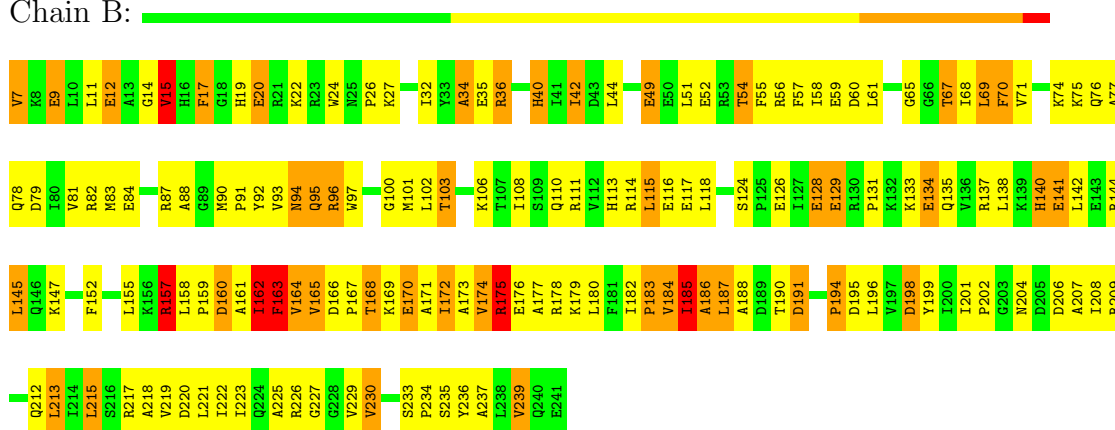
3 Residue-property plots

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.

Note EDS was not executed.

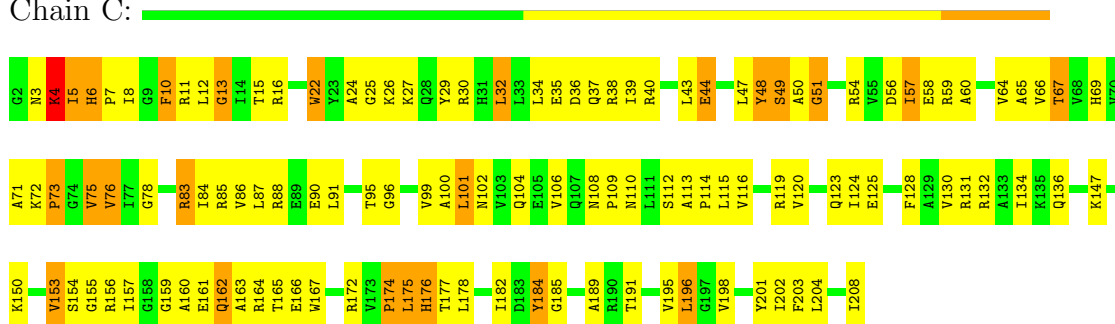
- Molecule 1: 30S ribosomal protein S2

Chain B:



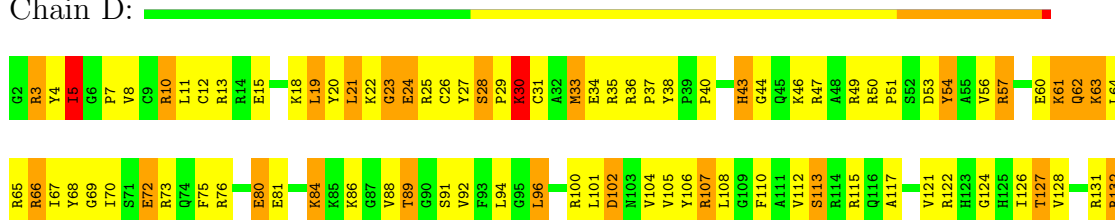
- Molecule 2: 30S ribosomal protein S3

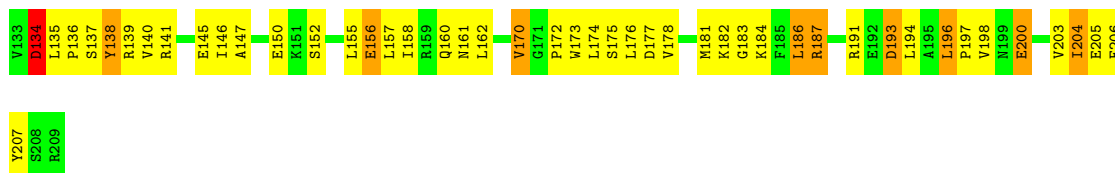
Chain C:



- Molecule 3: 30S ribosomal protein S4

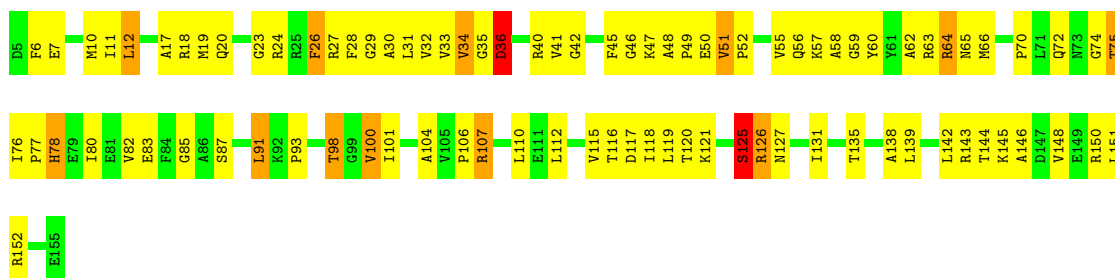
Chain D:





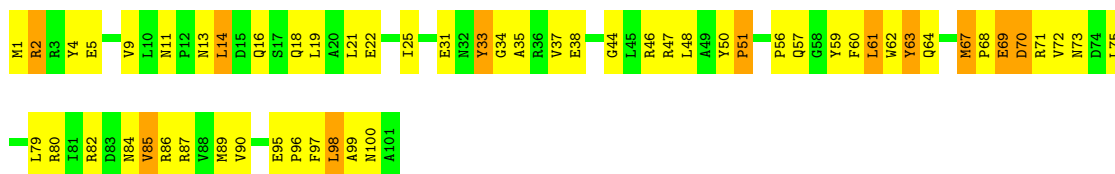
• Molecule 4: 30S ribosomal protein S5

Chain E:



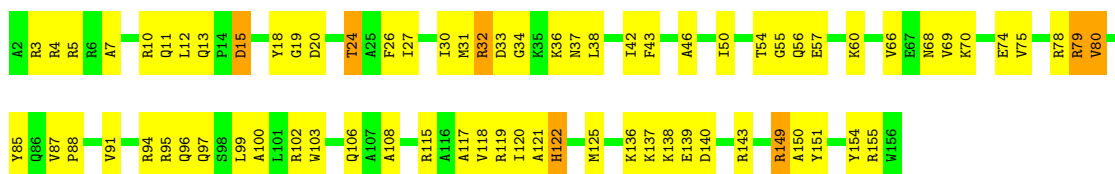
• Molecule 5: 30S ribosomal protein S6

Chain F:



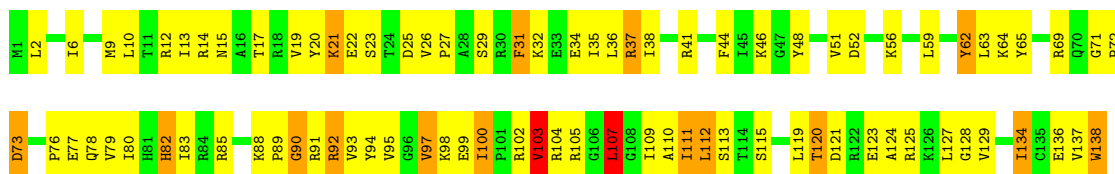
• Molecule 6: 30S ribosomal protein S7

Chain G:



• Molecule 7: 30S ribosomal protein S8

Chain H:



• Molecule 8: 30S ribosomal protein S9

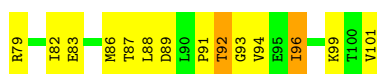
Chain I:





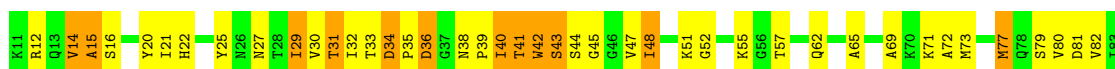
• Molecule 9: 30S ribosomal protein S10

Chain J:



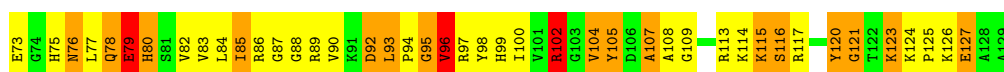
• Molecule 10: 30S ribosomal protein S11

Chain K:



• Molecule 11: 30S ribosomal protein S12

Chain L:



• Molecule 12: 30S ribosomal protein S13

Chain M:



• Molecule 13: 30S ribosomal protein S14 type Z

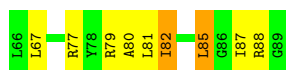
Chain N:



• Molecule 14: 30S ribosomal protein S15

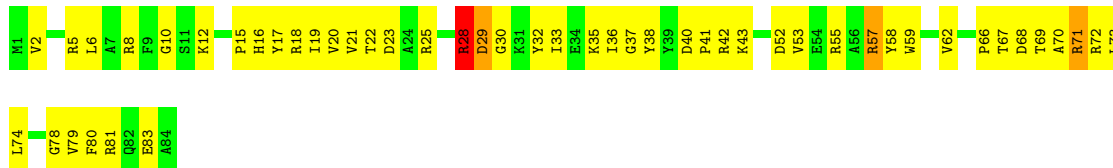
Chain O:





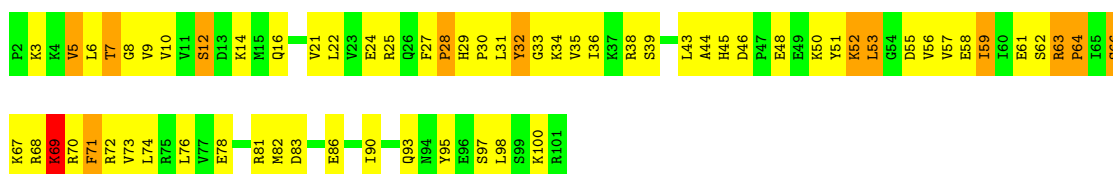
- Molecule 15: 30S ribosomal protein S16

Chain P:



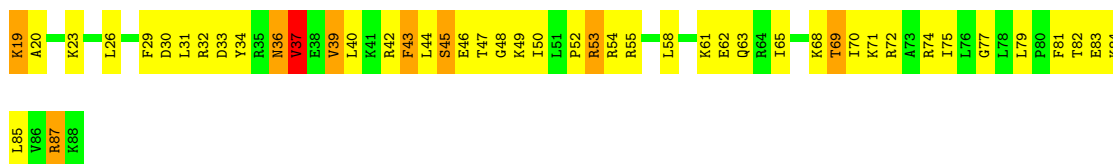
- Molecule 16: 30S ribosomal protein S17

Chain Q:



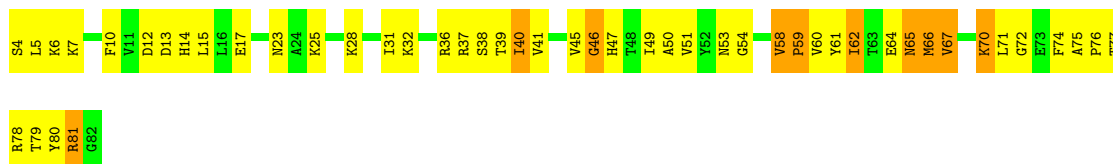
- Molecule 17: 30S ribosomal protein S18

Chain R:



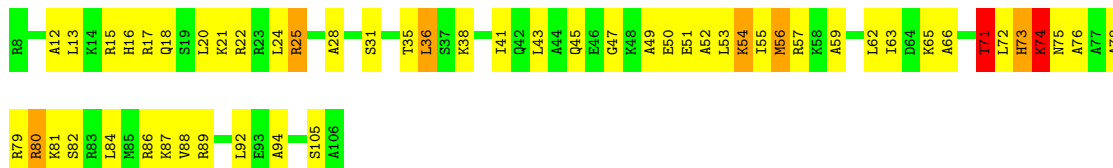
- Molecule 18: 30S ribosomal protein S19

Chain S:



- Molecule 19: 30S ribosomal protein S20

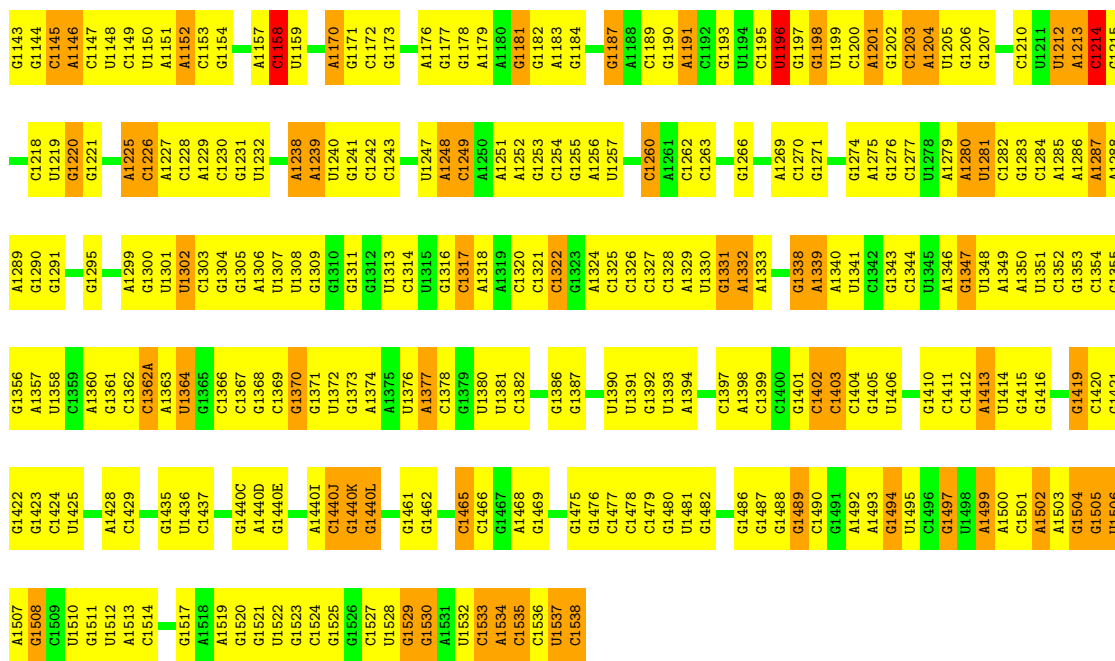
Chain T:



- Molecule 20: ribosomal RNA 16S

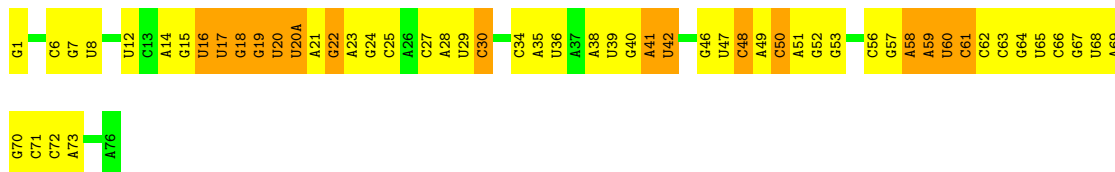
Chain A:

C1075	C1076	C1077	U1077	A1004	U1012	G1013	A1014	A1015	A1016	G1017	G1018	C1019	C1019	U1020	G1021	U1025	G1026	A1035	G1036	C1037	C1038	G1039	U1040	A1041	G1042	C1043	A1044	C1045	A1046	A1047	G1048	U1049	G1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	A1058	C1059	C1060	G1061	U1062	C1063	U1064	C1065	C1066	A1067	G1068	C1069	G1070	C1071	U1072	U1073	G1074													
G939	C940	G941	G942	U943	G944	G945	A946	G947	A948	A949	U950	G951	U952	G953	G954	U955	U956	U957	A989	G990	U991	C992	G993	A994	U997	G998	C999	U999	G976	A977	A978	C979	A980	U981	U982	G983	C984	A985	C986	G987	G988	C989	C990	U991	U992	G993	A994	U997	G998	C999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999							
A865	C866	G867	C868	G869	U870	G871	A872	G873	G874	G875	G876	G877	G878	C879	C880	G881	G882	G883	A889	G890	U891	A892	C893	A964	G965	A966	A967	A968	A969	G970	G971	C972	G973	A974	A975	G976	A977	A978	C979	A980	G981	U982	G983	C984	A985	C986	G987	G988	C989	C990	U991	U992	G993	A994	U997	G998	C999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999	U999
A777	G778	C779	A780	G781	U782	G783	G784	G785	G791	U792	U793	A794	G800	U801	A802	G803	A807	C810	C811	C812	U813	A814	A815	A816	C817	G818	A819	U820	G821	C822	G823	U827	A828	G829	G830	U831	C832	U833	C834	U835	G836	U838A	U838B	U838C	C848	G851	A859	A860	G861	C862	G776																			
U705	A706	C707	G708	G709	G713	G714	A715	A716	G717	G718	G719	G720	G721	A722	U723	G724	G725	A728	A729	G730	G731	G732	A733	G734	C735	G736	A737	C738	C739	U740	G741	G742	C745	A746	G747	G748	C749	G750	A753	C754	G755	C756	U757	G758	A759	G760	C764	G765	A766	A767	A768	G769	G776																	
G637	G638	G639	A640	U641	A642	C643	G644	C651	U652	A653	G658	U659	G660	G661	G662	A663	A665	G666	G667	G668	U669	G670	U671	U672	G673	G674	A675	A676	U677	U678	C679	C680	C681	G682	A684	G685	U686	A687	G688	C689	G690	G691	U692	G693	A694	A695	A696	U697	G698	G699	G700	G703	A704																	
G570	U571	A572	A573	A574	G575	G576	G577	C578	U580	C581	U582	A583	G584	G585	G588	C589	U590	U591	G592	C596	G597	U598	C599	C600	G601	A602	U603	G604	U605	C606	A607	A608	A609	G610	A611	C612	C613	A614	C615	G616	G617	U618	U619	C620	A621	A622	C623	C624	G625	U626	G627	U628	G629	G633	C634															
A509	A510	C511	U512	C513	C514	G515	U516	C517	C518	C519	A520	G521	C522	A523	U524	C525	C526	C527	C528	U531	A532	A533	C534	C535	C536	C537	A538	G539	A540	C541	G542	C543	C544	C545	C546	A547	G548	C549	U550	U551	U552	A553	C554	C555	C556	G557	U558	A559	U560	U561	C562	A563	U564	U565	G566	G567	C568	C569												
U367	U368	C369	A370	G371	C372	A373	A374	U375	G376	G377	A382	A383	G384	C385	C386	U387	C388	A389	C390	G391	C395	G396	A397	C398	G399	C400	C401	G402	C403	U404	U405	A406	G407	A408	A409	G410	A411	A412	C413	A414	A415	G416	C417	C418	C419	U420	U421	C422	C423	G424	G425	C426	U427	G428	U429	A430	A431													
A432	C433	U434	C435	C436	U437	C438	A440	A441	C442	C443	C444	G447	A448	C449	A452	A453	C454	C455	C456	C457	C458	A458A	A458B	G458C	A458E	G476	A477	U478	C479	U480	G481	G484	U485	A486	A487	C488	C489	G490	G491	G492	C493	U494	A495	A497	U498	C501	G502	U503	C504	U505	G506	G507	C508																	
C295	U296	A297	C298	G299	A300	G301	G302	U303	C304	G305	C306	C307	C308	G309	C310	C311	C312	C313	C314	A315	G316	G317	G318	G319	C320	A321	U322	G323	C324	G325	U326	A327	U328	C329	G332	A338	C339	U340	C344	C345	G346	G347	C352	A353	G354	C355	C356	G357	U358	G362	A363	A364	U365	C366																
G68D	G68E	G68F	G68G	G68H	G68I	G68J	U68K	U68L	U68M	U68N	A68O	C68P	U68Q	C68R	U68U	U68V	U68W	U68X	C68Y	A101	G102	C106	G107	G108	C109	C110	G111	G112	G113	U114	G115	C116	G117	U118	A119	A120	C121	G122	C123	G124	U125	G126	G127	C128	U129	A130	C131	U132	U133	A134	C135	C136	G137	G138	G139	G227														
A228	U229	G230	G231	G232	G233	C234	C235	G236	G237	G238	C241	C242	A243	U244	C245	A246	G247	G251	U252	U253	G254	G255	U256	G257	G258	G259	C260	U261	A262	A263	U264	G265	G266	C267	C268	C269	A270	C271	C272	A273	C277	G278	A279	G199	U201C	G216	C217	C218	U219	C220	G221	U222	C291	G226	U294															



• Molecule 21: transfer RNA

Chain W:



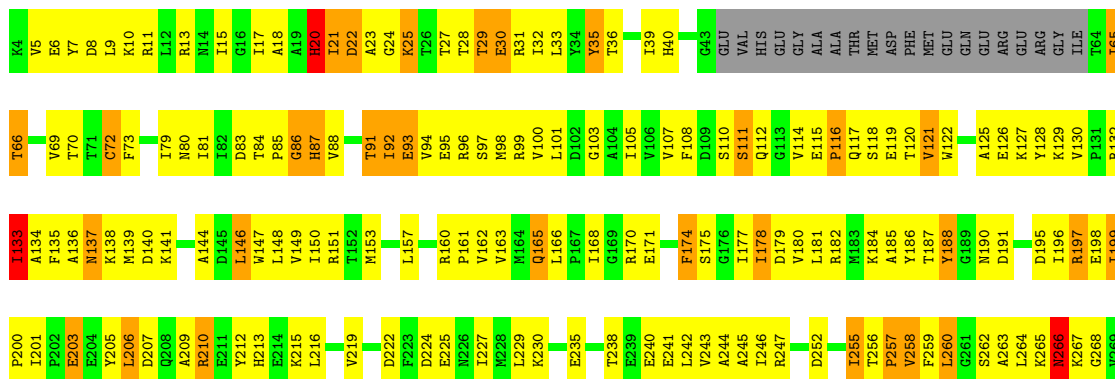
• Molecule 22: messenger RNA

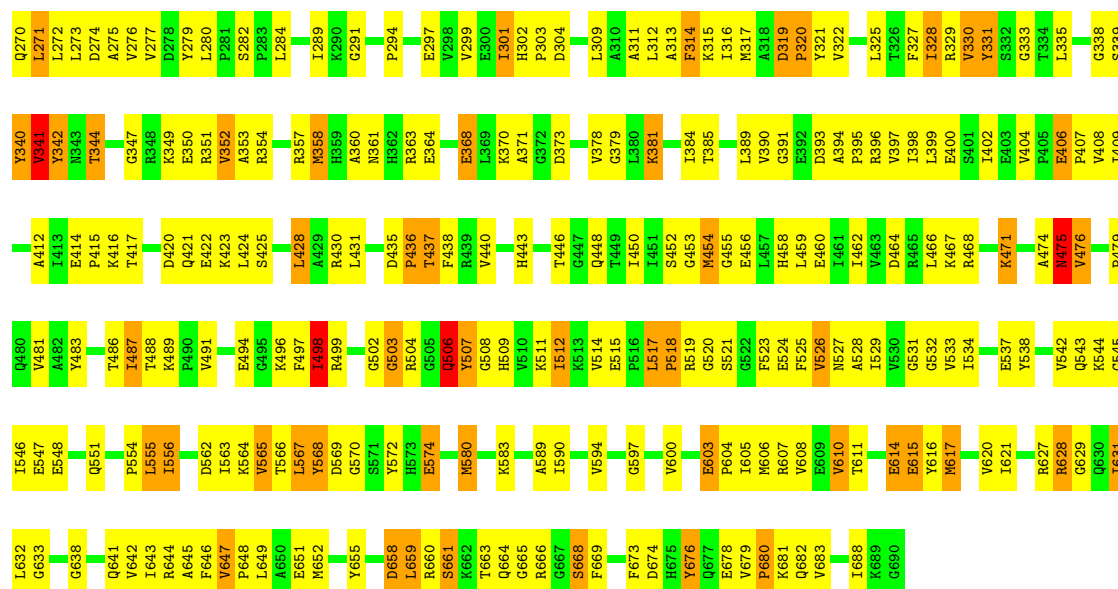
Chain V:



• Molecule 23: Elongation factor G

Chain Y:





- Molecule 24: VIOMYCIN

Chain U: _____

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Xtriage (Phenix) failed to run properly; EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	308.96Å 670.66Å 347.77Å 90.00° 92.52° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.284 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	58959	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, DPP, KBE, UAL, FUA, 5OH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	B	0.38	0/1945	0.72	1/2621 (0.0%)
2	C	0.28	0/1645	0.53	0/2216
3	D	0.30	0/1733	0.58	0/2318
4	E	0.32	0/1172	0.58	1/1576 (0.1%)
5	F	0.31	0/856	0.59	0/1154
6	G	0.29	0/1276	0.51	0/1709
7	H	0.30	0/1136	0.57	0/1527
8	I	0.29	0/1029	0.53	0/1379
9	J	0.27	0/815	0.54	0/1095
10	K	0.33	0/900	0.61	0/1213
11	L	0.40	0/992	0.83	2/1327 (0.2%)
12	M	0.29	0/1008	0.59	1/1347 (0.1%)
13	N	0.30	0/501	0.52	0/664
14	O	0.31	0/745	0.52	0/992
15	P	0.28	0/722	0.50	0/970
16	Q	0.36	0/848	0.65	0/1131
17	R	0.31	0/579	0.59	0/768
18	S	0.31	0/647	0.60	0/870
19	T	0.33	0/765	0.56	0/1007
20	A	0.37	0/36351	1.02	61/56736 (0.1%)
21	W	0.33	0/1827	1.03	0/2845
22	V	0.27	0/568	0.81	0/886
23	Y	0.34	1/5317 (0.0%)	0.66	7/7198 (0.1%)
24	U	0.95	0/11	1.28	0/13
All	All	0.35	1/63388 (0.0%)	0.89	73/93562 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
23	Y	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	506	GLN	C-N	-5.48	1.21	1.34

The worst 5 of 73 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	506	GLN	O-C-N	-12.49	102.72	122.70
20	A	815	A	C5-C6-N6	11.75	133.10	123.70
20	A	815	A	N1-C6-N6	-11.03	111.98	118.60
20	A	1508	G	N1-C2-N3	8.68	129.11	123.90
20	A	1158	C	C2-N1-C1'	8.16	127.78	118.80

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	ILE	Peptide
1	B	170	GLU	Peptide
1	B	185	ILE	Peptide
23	Y	133	ILE	Peptide
23	Y	503	GLY	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1910	0	1957	135	0
2	C	1621	0	1688	87	0
3	D	1703	0	1763	104	0
4	E	1156	0	1213	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	843	0	857	42	0
6	G	1257	0	1296	54	0
7	H	1116	0	1177	67	0
8	I	1010	0	1037	78	0
9	J	802	0	849	44	0
10	K	885	0	904	54	0
11	L	976	0	1062	113	0
12	M	997	0	1072	67	0
13	N	492	0	529	37	0
14	O	734	0	771	47	0
15	P	706	0	725	45	0
16	Q	835	0	904	64	0
17	R	574	0	644	36	0
18	S	634	0	655	34	0
19	T	763	0	861	38	0
20	A	32474	0	16393	994	0
21	W	1635	0	831	60	0
22	V	503	0	252	12	0
23	Y	5219	0	5290	313	0
24	U	48	0	39	0	0
25	Y	37	0	47	6	0
26	Y	28	0	12	12	0
27	Y	1	0	0	0	0
All	All	58959	0	42828	2304	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 2304 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:W:15:G:N2	21:W:48:C:H42	1.36	1.24
21:W:15:G:H22	21:W:48:C:N4	1.38	1.21
20:A:815:A:N1	20:A:1508:G:N2	1.93	1.15
20:A:815:A:H2	20:A:1527:C:O2	1.29	1.15
21:W:50:C:N4	21:W:64:G:H1	1.50	1.08

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	233/235 (99%)	154 (66%)	51 (22%)	28 (12%)	1	11
2	C	205/207 (99%)	154 (75%)	32 (16%)	19 (9%)	1	18
3	D	206/208 (99%)	149 (72%)	31 (15%)	26 (13%)	0	10
4	E	149/151 (99%)	117 (78%)	22 (15%)	10 (7%)	2	28
5	F	99/101 (98%)	75 (76%)	15 (15%)	9 (9%)	1	18
6	G	153/155 (99%)	121 (79%)	25 (16%)	7 (5%)	4	39
7	H	136/138 (99%)	97 (71%)	27 (20%)	12 (9%)	1	19
8	I	125/127 (98%)	93 (74%)	27 (22%)	5 (4%)	5	44
9	J	97/99 (98%)	75 (77%)	13 (13%)	9 (9%)	1	18
10	K	117/119 (98%)	82 (70%)	21 (18%)	14 (12%)	1	11
11	L	123/125 (98%)	38 (31%)	52 (42%)	33 (27%)	0	1
12	M	123/125 (98%)	93 (76%)	20 (16%)	10 (8%)	1	21
13	N	58/60 (97%)	44 (76%)	7 (12%)	7 (12%)	1	11
14	O	86/88 (98%)	65 (76%)	14 (16%)	7 (8%)	1	21
15	P	82/84 (98%)	66 (80%)	15 (18%)	1 (1%)	19	75
16	Q	98/100 (98%)	70 (71%)	18 (18%)	10 (10%)	1	14
17	R	68/70 (97%)	51 (75%)	10 (15%)	7 (10%)	1	14
18	S	77/79 (98%)	41 (53%)	23 (30%)	13 (17%)	0	4
19	T	97/99 (98%)	82 (84%)	11 (11%)	4 (4%)	4	44
23	Y	663/687 (96%)	451 (68%)	138 (21%)	74 (11%)	1	13
24	U	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	2997/3063 (98%)	2119 (71%)	573 (19%)	305 (10%)	1	14

5 of 305 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	GLU

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Mol	Chain	Res	Type
1	B	76	GLN
1	B	165	VAL
1	B	194	PRO
2	C	4	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	203/203 (100%)	164 (81%)	39 (19%)	2	12
2	C	161/161 (100%)	132 (82%)	29 (18%)	2	15
3	D	180/180 (100%)	145 (81%)	35 (19%)	2	12
4	E	116/116 (100%)	93 (80%)	23 (20%)	2	11
5	F	90/90 (100%)	78 (87%)	12 (13%)	6	31
6	G	126/126 (100%)	113 (90%)	13 (10%)	10	47
7	H	119/119 (100%)	98 (82%)	21 (18%)	3	16
8	I	98/98 (100%)	82 (84%)	16 (16%)	3	21
9	J	89/89 (100%)	75 (84%)	14 (16%)	4	23
10	K	90/90 (100%)	71 (79%)	19 (21%)	1	9
11	L	104/104 (100%)	77 (74%)	27 (26%)	1	5
12	M	100/100 (100%)	83 (83%)	17 (17%)	3	18
13	N	49/49 (100%)	43 (88%)	6 (12%)	7	36
14	O	79/79 (100%)	71 (90%)	8 (10%)	11	48
15	P	72/72 (100%)	66 (92%)	6 (8%)	16	59
16	Q	95/95 (100%)	81 (85%)	14 (15%)	4	26
17	R	61/61 (100%)	51 (84%)	10 (16%)	3	20
18	S	69/69 (100%)	55 (80%)	14 (20%)	2	11
19	T	76/76 (100%)	64 (84%)	12 (16%)	4	23
23	Y	563/579 (97%)	470 (84%)	93 (16%)	3	20
24	U	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2542/2558 (99%)	2114 (83%)	428 (17%)	3 19

5 of 428 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	J	55	LYS
11	L	85	ILE
23	Y	428	LEU
9	J	83	GLU
10	K	116	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
10	K	93	GLN
10	K	116	HIS
23	Y	20	HIS
8	I	117	HIS
10	K	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	A	1510/1511 (99%)	305 (20%)	17 (1%)
21	W	76/77 (98%)	23 (30%)	1 (1%)
22	V	22/23 (95%)	8 (36%)	1 (4%)
All	All	1608/1611 (99%)	336 (20%)	19 (1%)

5 of 336 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	A	6	G
20	A	9	G
20	A	13	U
20	A	15	G
20	A	29	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	A	739	C
20	A	992	U
20	A	1532	U
20	A	687	A
20	A	1537	U

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

4 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$
24	KBE	U	1	24	8,8,9	8.27	1 (12%)	6,8,10	0.70	0
24	DPP	U	2	24	5,5,6	6.96	1 (20%)	3,5,7	2.10	1 (33%)
24	UAL	U	5	24	7,8,9	1.32	1 (14%)	6,9,11	1.44	1 (16%)
24	5OH	U	6	24	12,12,13	5.61	4 (33%)	13,16,18	2.23	3 (23%)

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
24	KBE	U	1	24	-	0/6/7/8	0/0/0/0
24	DPP	U	2	24	-	0/2/4/6	0/0/0/0
24	UAL	U	5	24	-	0/3/7/9	0/0/0/0
24	5OH	U	6	24	-	0/2/18/20	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	1	KBE	O-C	23.33	1.27	1.11
24	U	6	5OH	O-C	17.99	1.23	1.11
24	U	2	DPP	O-C	15.46	1.22	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	6	5OH	CQ-NP	5.73	1.40	1.34
24	U	6	5OH	CA-C	3.71	1.55	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	U	6	5OH	CR-CB-CA	4.35	117.65	112.53
24	U	6	5OH	CR-CS-NR	4.28	120.78	108.18
24	U	6	5OH	CR-CB-NP	3.93	114.43	108.69
24	U	2	DPP	CB-CA-N	-2.62	102.70	111.50
24	U	5	UAL	CB-CA-N	2.15	128.00	123.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
25	FUA	Y	701	-	40,40,40	1.80	8 (20%)	64,64,64	1.88	13 (20%)
26	GDP	Y	702	-	30,30,30	1.20	2 (6%)	44,47,47	2.06	10 (22%)

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
25	FUA	Y	701	-	-	1/18/92/92	0/0/4/4
26	GDP	Y	702	-	-	0/16/32/32	0/1/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	701	FUA	C17-C22	4.57	1.39	1.34
25	Y	701	FUA	C29-C22	4.50	1.53	1.47
25	Y	701	FUA	C23-C22	-4.09	1.40	1.51
25	Y	701	FUA	C23-C24	-4.01	1.39	1.53
25	Y	701	FUA	C24-C25	-3.72	1.39	1.50

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	702	GDP	C6-C5-N7	-6.72	133.24	134.14
25	Y	701	FUA	C13-C12-C11	-5.87	103.73	112.00
25	Y	701	FUA	C24-C23-C22	5.55	125.63	111.93
26	Y	702	GDP	C2-N3-C4	4.54	121.47	115.09
26	Y	702	GDP	O4'-C1'-N9	4.30	112.44	108.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	Y	701	FUA	C16-C17-C22-C29

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.