



# wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 06:00 PM BST

PDB ID : 3SFS  
Title : Crystal Structure of Release Factor RF3 Trapped in the GTP State on a Rotated Conformation of the Ribosome  
Authors : Zhou, J.; Lancaster, L.; Trakhanov, S.; Noller, H.F.  
Deposited on : 2011-06-13  
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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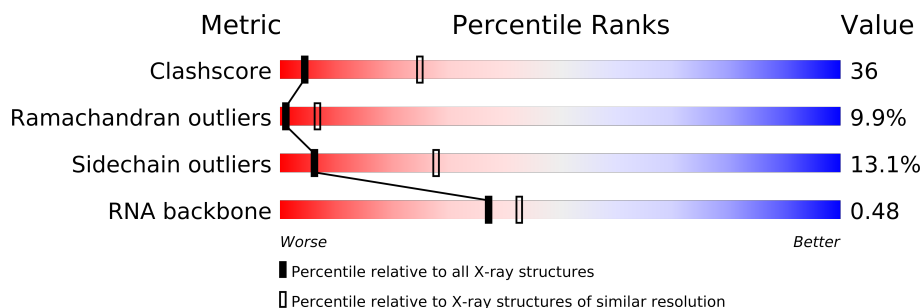
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
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 3.20 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	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RNA backbone	1838	1002 (3.72-2.68)


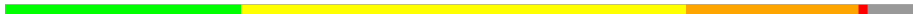
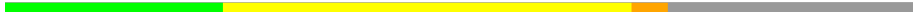

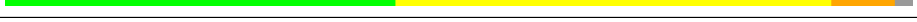

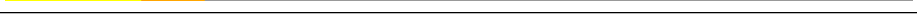

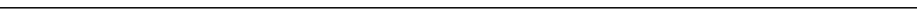
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	A	1533	
2	B	241	
3	C	233	
4	D	206	
5	E	167	
6	F	131	
7	G	156	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	

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Mol	Chain	Length	Quality of chain
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	V	27	
23	W	529	
24	Y	6	

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55876 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1532	Total	C	N	O	P	0	0	0
			32873	14661	6031	10649	1532			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 15 is a protein called 30S ribosomal protein S15 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a protein called Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	525	Total	C	N	O	S	0	0	0
			4144	2617	722	783	22			

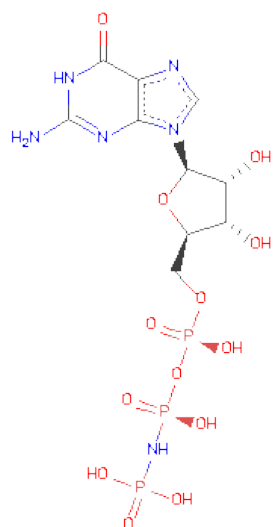
- Molecule 24 is a protein called Viomycin.

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

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	H	1	Total	Mg	0	0
			1	1		
25	W	1	Total	Mg	0	0
			1	1		
25	A	99	Total	Mg	0	0
			99	99		
25	L	2	Total	Mg	0	0
			2	2		
25	F	1	Total	Mg	0	0
			1	1		
25	M	1	Total	Mg	0	0
			1	1		

- Molecule 26 is PHOSPHOAMINOPHOSPHONICACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	W	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	W	2	Total	O	0	0
			2	2		



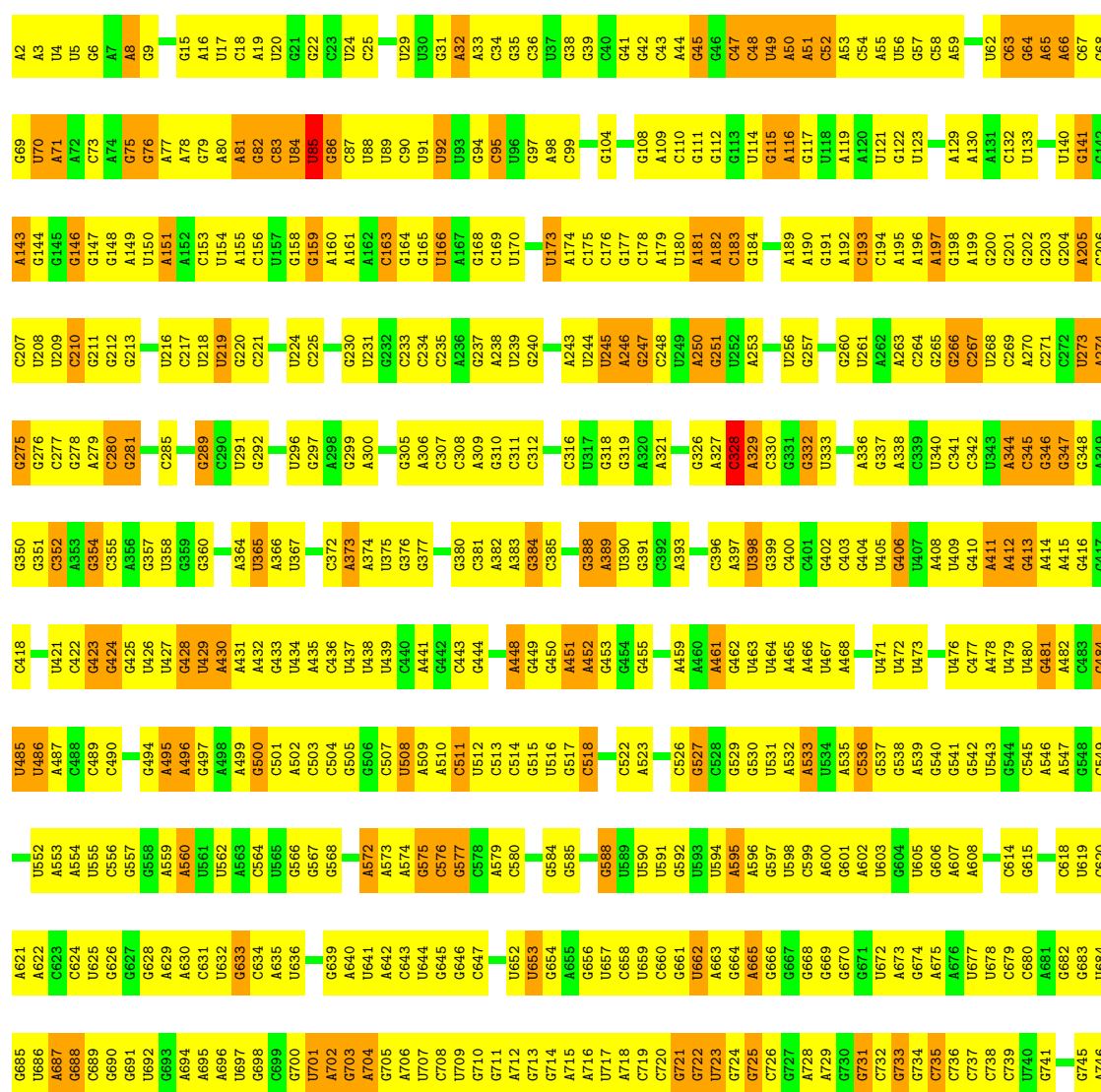
### 3 Residue-property plots

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.

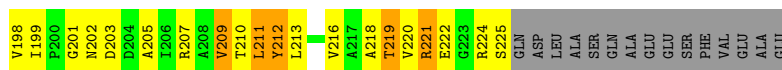
Note EDS was not executed.

#### • Molecule 1: 16S rRNA

Chain A:

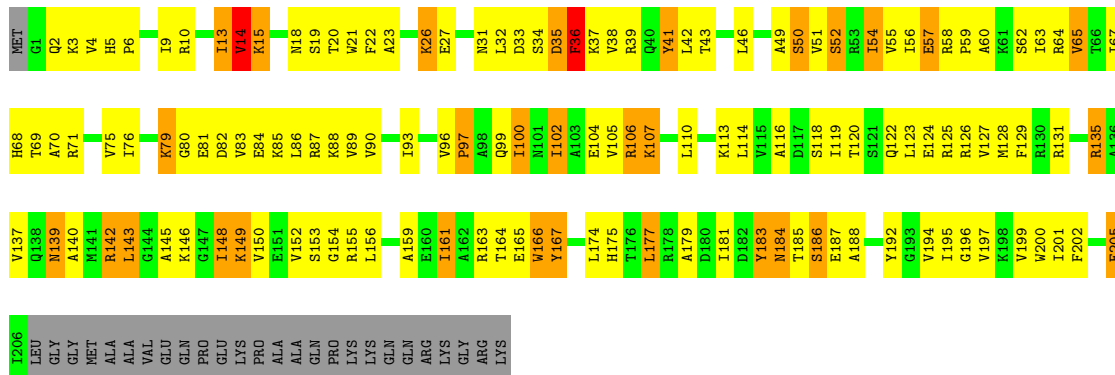


G126	K127	L128	M129	N130	O131	P132	Q133	R134	S135	T136	U137	V138	W139	X140	Y141	Z142	A143	B144	C145	D146	E147	F148	G149	H150	I151	J152	K153	L154	M155	N156	O157	P158	Q159	R160	S161	T162	U163	V164	W165	X166	Y167	Z168	A169	B170	C171	D172	E173	F174	G175	H176	I177	J178	K179	L180	M181	N182	O183	P184	Q185	R186	S187	T188	U189	V190	W191	X192	Y193	Z194	A195	B196	C197	D198	E199	F200	G201	H202	I203	J204	K205	L206	M207	N208	O209	P210	Q211	R212	S213	T214	U215	V216	W217	X218	Y219	Z220	A221	B222	C223	D224	E225	F226	G227	H228	I229	J230	K231	L232	M233	N234	O235	P236	Q237	R238	S239	T240	U241	V242	W243	X244	Y245	Z246	A247	B248	C249	D250	E251	F252	G253	H254	I255	J256	K257	L258	M259	N260	O261	P262	Q263	R264	S265	T266	U267	V268	W269	X270	Y271	Z272	A273	B274	C275	D276	E277	F278	G279	H280	I281	J282	K283	L284	M285	N286	O287	P288	Q289	R290	S291	T292	U293	V294	W295	X296	Y297	Z298	A299	B300	C301	D302	E303	F304	G305	H306	I307	J308	K309	L310	M311	N312	O313	P314	Q315	R316	S317	T318	U319	V320	W321	X322	Y323	Z324	A325	B326	C327	D328	E329	F330	G331	H332	I333	J334	K335	L336	M337	N338	O339	P340	Q341	R342	S343	T344	U345	V346	W347	X348	Y349	Z350	A351	B352	C353	D354	E355	F356	G357	H358	I359	J360	K361	L362	M363	N364	O365	P366	Q367	R368	S369	T370	U371	V372	W373	X374	Y375	Z376	A377	B378	C379	D380	E381	F382	G383	H384	I385	J386	K387	L388	M389	N390	O391	P392	Q393	R394	S395	T396	U397	V398	W399	X400	Y401	Z402	A403	B404	C405	D406	E407	F408	G409	H410	I411	J412	K413	L414	M415	N416	O417	P418	Q419	R420	S421	T422	U423	V424	W425	X426	Y427	Z428	A429	B430	C431	D432	E433	F434	G435	H436	I437	J438	K439	L440	M441	N442	O443	P444	Q445	R446	S447	T448	U449	V450	W451	X452	Y453	Z454	A455	B456	C457	D458	E459	F460	G461	H462	I463	J464	K465	L466	M467	N468	O469	P470	Q471	R472	S473	T474	U475	V476	W477	X478	Y479	Z480	A481	B482	C483	D484	E485	F486	G487	H488	I489	J490	K491	L492	M493	N494	O495	P496	Q497	R498	S499	T500	U501	V502	W503	X504	Y505	Z506	A507	B508	C509	D510	E511	F512	G513	H514	I515	J516	K517	L518	M519	N520	O521	P522	Q523	R524	S525	T526	U527	V528	W529	X530	Y531	Z532	A533	B534	C535	D536	E537	F538	G539	H540	I541	J542	K543	L544	M545	N546	O547	P548	Q549	R550	S551	T552	U553	V554	W555	X556	Y557	Z558	A559	B560	C561	D562	E563	F564	G565	H566	I567	J568	K569	L570	M571	N572	O573	P574	Q575	R576	S577	T578	U579	V580	W581	X582	Y583	Z584	A585	B586	C587	D588	E589	F590	G591	H592	I593	J594	K595	L596	M597	N598	O599	P600	Q601	R602	S603	T604	U605	V606	W607	X608	Y609	Z610	A611	B612	C613	D614	E615	F616	G617	H618	I619	J620	K621	L622	M623	N624	O625	P626	Q627	R628	S629	T630	U631	V632	W633	X634	Y635	Z636	A637	B638	C639	D640	E641	F642	G643	H644	I645	J646	K647	L648	M649	N650	O651	P652	Q653	R654	S655	T656	U657	V658	W659	X660	Y661	Z662	A663	B664	C665	D666	E667	F668	G669	H670	I671	J672	K673	L674	M675	N676	O677	P678	Q679	R680	S681	T682	U683	V684	W685	X686	Y687	Z688	A689	B690	C691	D692	E693	F694	G695	H696	I697	J698	K699	L700	M701	N702	O703	P704	Q705	R706	S707	T708	U709	V710	W711	X712	Y713	Z714	A715	B716	C717	D718	E719	F720	G721	H722	I723	J724	K725	L726	M727	N728	O729	P730	Q731	R732	S733	T734	U735	V736	W737	X738	Y739	Z740	A741	B742	C743	D744	E745	F746	G747	H748	I749	J750	K751	L752	M753	N754	O755	P756	Q757	R758	S759	T760	U761	V762	W763	X764	Y765	Z766	A767	B768	C769	D770	E771	F772	G773	H774	I775	J776	K777	L778	M779	N780	O781	P782	Q783	R784	S785	T786	U787	V788	W789	X790	Y791	Z792	A793	B794	C795	D796	E797	F798	G799	H800	I801	J802	K803	L804	M805	N806	O807	P808	Q809	R810	S811	T812	U813	V814	W815	X816	Y817	Z818	A819	B820	C821	D822	E823	F824	G825	H826	I827	J828	K829	L830	M831	N832	O833	P834	Q835	R836	S837	T838	U839	V840	W841	X842	Y843	Z844	A845	B846	C847	D848	E849	F850	G851	H852	I853	J854	K855	L856	M857	N858	O859	P860	Q861	R862	S863	T864	U865	V866	W867	X868	Y869	Z870	A871	B872	C873	D874	E875	F876	G877	H878	I879	J880	K881	L882	M883	N884	O885	P886	Q887	R888	S889	T890	U891	V892	W893	X894	Y895	Z896	A897	B898	C899	D900	E901	F902	G903	H904	I905	J906	K907	L908	M909	N910	O911	P912	Q913	R914	S915	T916	U917	V918	W919	X920	Y921	Z922	A923	B924	C925	D926	E927	F928	G929	H930	I931	J932	K933	L934	M935	N936	O937	P938	Q939	R940	S941	T942	U943	V944	W945	X946	Y947	Z948	A949	B950	C951	D952	E953	F954	G955	H956	I957	J958	K959	L960	M961	N962	O963	P964	Q965	R966	S967	T968	U969	V970	W971	X972	Y973	Z974	A975	B976	C977	D978	E979	F980	G981	H982	I983	J984	K985	L986	M987	N988	O989	P990	Q991	R992	S993	T994	U995	V996	W997	X998	Y999	Z1000	A1001	B1002	C1003	D1004	E1005	F1006	G1007	H1008	I1009	J1010	K1011	L1012	M1013	N1014	O1015	P1016	Q1017	R1018	S1019	T1020	U1021	V1022	W1023	X1024	Y1025	Z1026	A1027	B1028	C1029	D1030	E1031	F1032	G1033	H1034	I1035	J1036	K1037	L1038	M1039	N1040	O1041	P1042	Q1043	R1044	S1045	T1046	U1047	V1048	W1049	X1050	Y1051	Z1052	A1053	B1054	C1055	D1056	E1057	F1058	G1059	H1060	I1061	J1062	K1063	L1064	M1065	N1066	O1067	P1068	Q1069	R1070	S1071	T1072	U1073	V1074	W1075	X1076	Y1077	Z1078	A1079	B1080	C1081	D1082	E1083	F1084	G1085	H1086	I1087	J1088	K1089	L1090	M1091	N1092	O1093	P1094	Q1095	R1096	S1097	T1098	U1099	V1100	W1101	X1102	Y1103	Z1104	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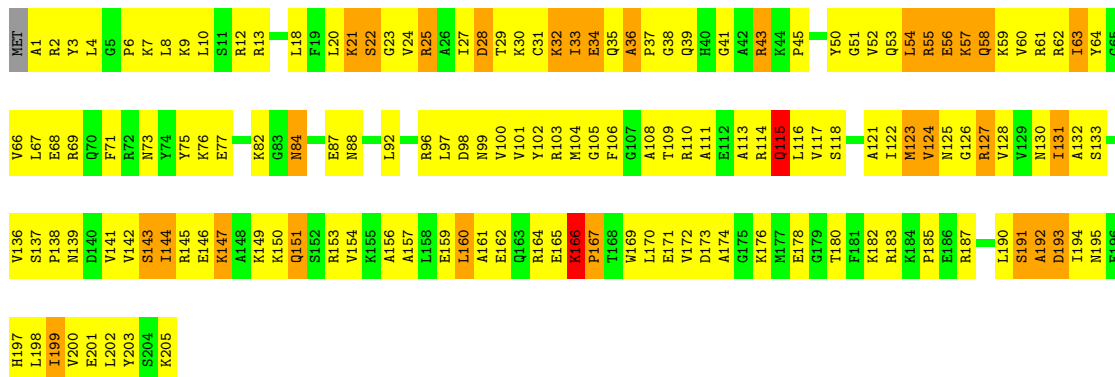
• Molecule 3: 30S ribosomal protein S3

Chain C:



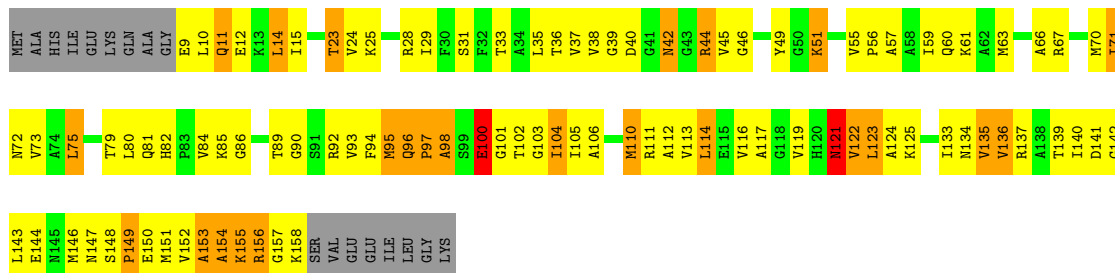
• Molecule 4: 30S ribosomal protein S4

Chain D:



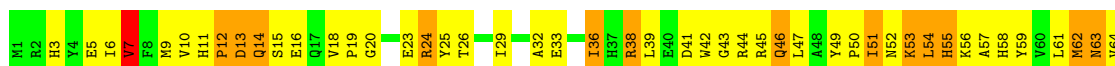
• Molecule 5: 30S ribosomal protein S5

Chain E:



• Molecule 6: 30S ribosomal protein S6 1

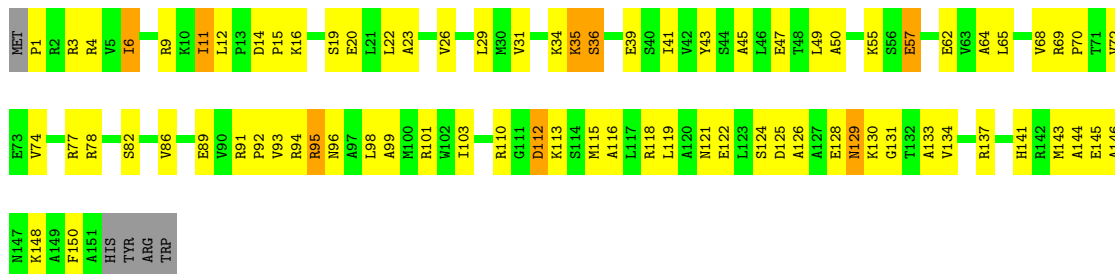
Chain F:





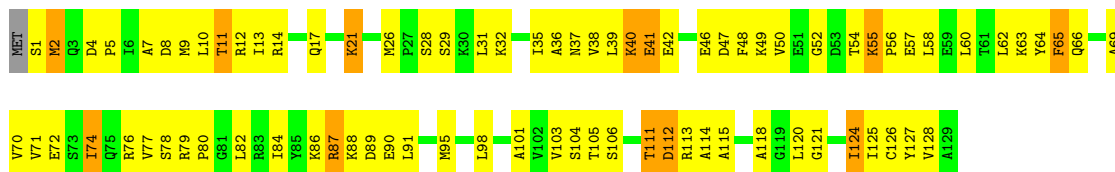
• Molecule 7: 30S ribosomal protein S7

Chain G:



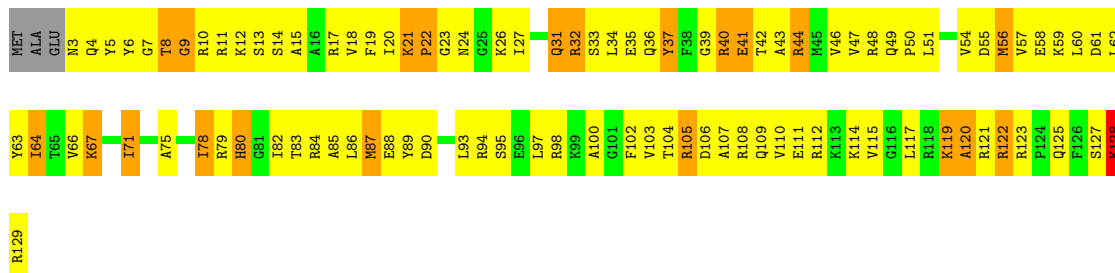
• Molecule 8: 30S ribosomal protein S8

Chain H:



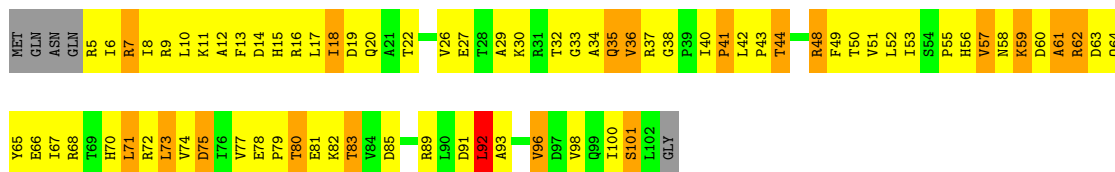
• Molecule 9: 30S ribosomal protein S9

Chain I:



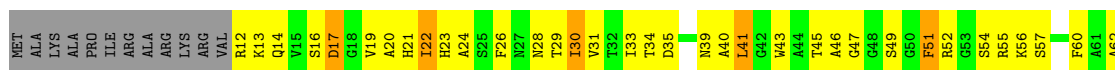
• Molecule 10: 30S ribosomal protein S10

Chain J:



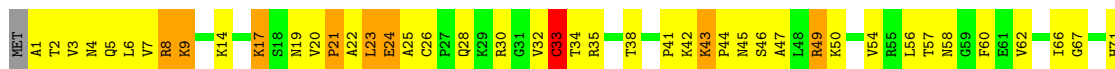
• Molecule 11: 30S ribosomal protein S11

Chain K:



- Molecule 12: 30S ribosomal protein S12 1

Chain L:



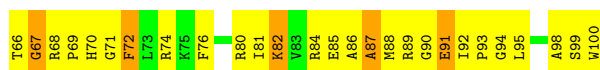
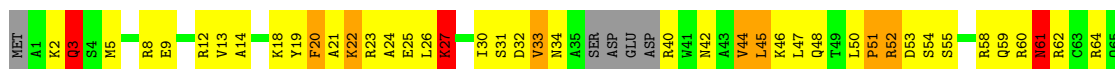
- Molecule 13: 30S ribosomal protein S13

Chain M:



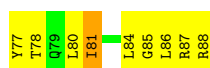
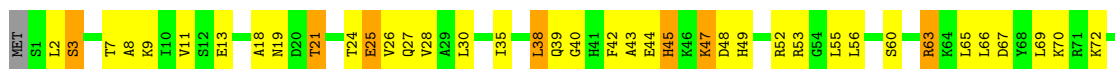
- Molecule 14: 30S ribosomal protein S14

Chain N:



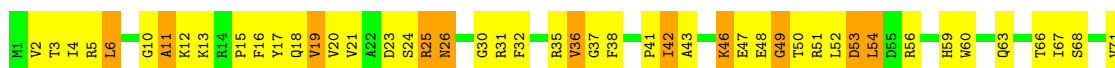
- Molecule 15: 30S ribosomal protein S15 1

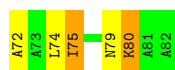
Chain O:



- Molecule 16: 30S ribosomal protein S16

Chain P:





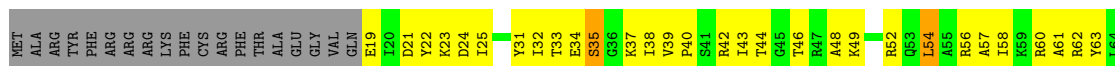
- Molecule 17: 30S ribosomal protein S17

Chain Q:



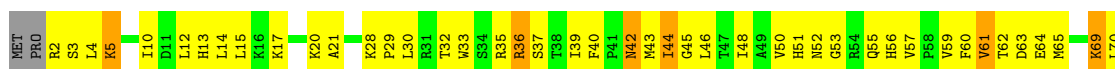
- Molecule 18: 30S ribosomal protein S18

Chain R:



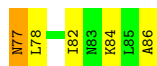
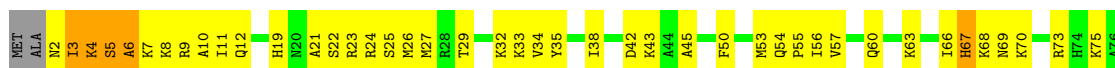
- Molecule 19: 30S ribosomal protein S19

Chain S:



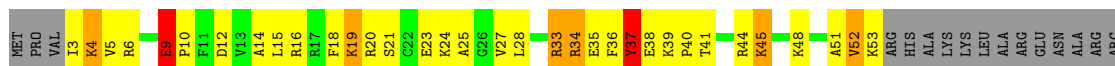
- Molecule 20: 30S ribosomal protein S20

Chain T:



- Molecule 21: 30S ribosomal protein S21

Chain U:



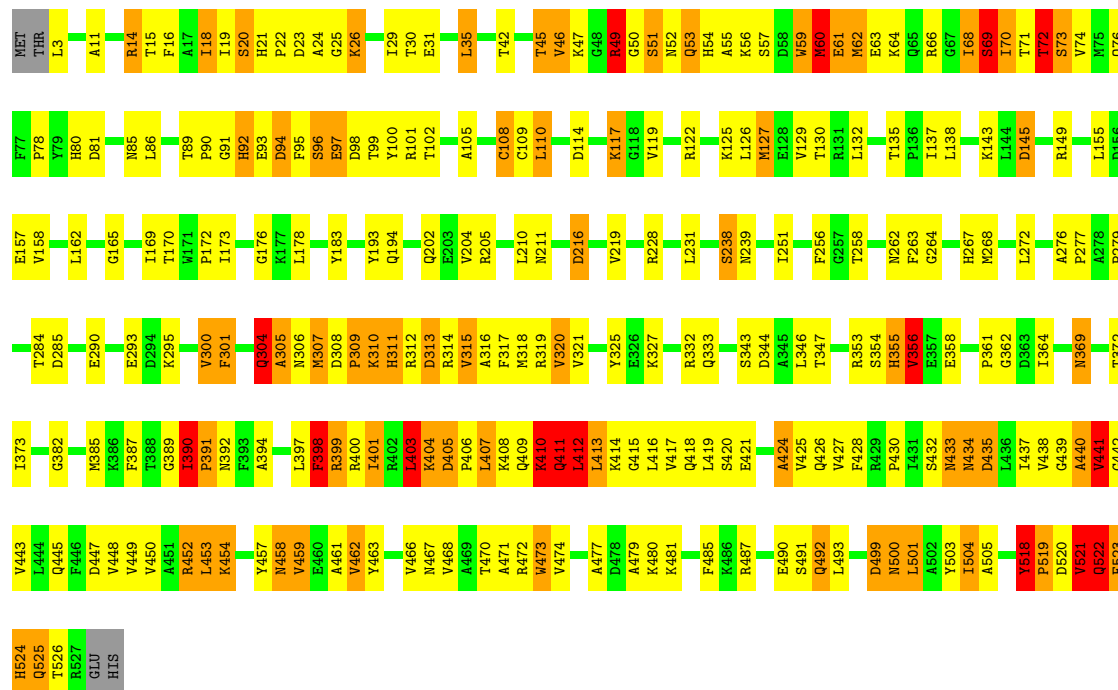
- Molecule 22: messenger RNA

Chain V:

G	G	C	A	A	G	G	A	G	G	G	U	U	A	A	A	A15	A16	U17	G18	U19	A20	A	A	A	A	A	A	A
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	-----	-----	-----	-----	-----	-----	---	---	---	---	---	---	---

• Molecule 23: Peptide chain release factor 3

Chain W:



• Molecule 24: Viomycin

Chain Y:

?1	A2	S3	S4	?5	?6
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## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	257.60Å 312.90Å 328.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2, phenix	Depositor
R, $R_{free}$	0.210 , 0.250	Depositor
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.241	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 524622 reflections	Xtriage
Total number of atoms	55876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, DPP, MG, KBE, UAL, 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	A	0.44	0/36809	0.81	26/57423 (0.0%)
2	B	0.29	0/1735	0.48	0/2338
3	C	0.29	0/1651	0.51	0/2225
4	D	0.29	0/1665	0.50	0/2227
5	E	0.34	0/1118	0.58	0/1504
6	F	0.27	0/835	0.49	0/1128
7	G	0.23	0/1195	0.41	0/1602
8	H	0.30	0/989	0.50	0/1326
9	I	0.26	0/1034	0.49	0/1375
10	J	0.30	0/796	0.54	0/1077
11	K	0.29	0/893	0.51	0/1205
12	L	0.38	0/969	0.65	0/1300
13	M	0.21	0/892	0.42	0/1193
14	N	0.28	0/785	0.47	0/1043
15	O	0.28	0/722	0.49	0/964
16	P	0.30	0/659	0.48	0/884
17	Q	0.30	0/657	0.52	0/881
18	R	0.30	0/462	0.49	0/621
19	S	0.23	0/652	0.42	0/877
20	T	0.31	0/671	0.53	0/888
21	U	0.31	0/430	0.46	0/570
22	V	0.53	0/144	0.91	0/222
23	W	0.47	2/4221 (0.0%)	0.73	5/5702 (0.1%)
24	Y	0.97	0/11	0.62	0/13
All	All	0.40	2/59995 (0.0%)	0.73	31/88588 (0.0%)

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
12	L	0	1
23	W	0	2
24	Y	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	72	THR	C-O	6.02	1.34	1.23
23	W	73	SER	CB-OG	5.44	1.49	1.42

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1499	A	C8-N9-C4	6.80	108.52	105.80
1	A	912	C	C6-N1-C2	6.34	122.84	120.30
1	A	1099	G	C5-C6-O6	6.28	132.37	128.60
1	A	49	U	C6-N1-C2	6.25	124.75	121.00
23	W	26	LYS	CA-C-N	-6.17	103.63	117.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	22	ALA	Peptide
23	W	410	LYS	Peptide
23	W	411	GLN	Peptide
24	Y	1	KBE	Mainchain
24	Y	2	DPP	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	A	32873	0	16542	1443	0
2	B	1704	0	1732	189	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1624	0	1699	162	0
4	D	1643	0	1710	196	0
5	E	1105	0	1148	135	0
6	F	817	0	808	102	0
7	G	1181	0	1240	70	0
8	H	979	0	1034	91	0
9	I	1022	0	1070	126	0
10	J	786	0	828	97	0
11	K	877	0	887	104	0
12	L	955	0	1019	123	0
13	M	883	0	944	96	0
14	N	774	0	827	90	0
15	O	714	0	737	45	0
16	P	649	0	666	63	0
17	Q	648	0	691	62	0
18	R	455	0	478	41	0
19	S	637	0	665	70	0
20	T	665	0	714	60	0
21	U	425	0	449	67	0
22	V	129	0	65	9	0
23	W	4144	0	4127	278	0
24	Y	48	0	40	29	0
25	A	99	0	0	0	0
25	F	1	0	0	0	0
25	H	1	0	0	0	0
25	L	2	0	0	0	0
25	M	1	0	0	0	0
25	W	1	0	0	0	0
26	W	32	0	13	6	0
27	W	2	0	0	2	0
All	All	55876	0	40133	3415	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 36.

The worst 5 of 3415 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1495:U:O4	24:Y:1:KBE:CE	1.84	1.26
1:A:1494:G:N7	24:Y:1:KBE:HGA	1.52	1.24
1:A:1494:G:O6	24:Y:1:KBE:HG	1.35	1.22
1:A:1495:U:C4	24:Y:1:KBE:HE	1.75	1.20
1:A:877:G:H21	8:H:1:SER:HB2	1.13	1.14

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	
2	B	216/241 (90%)	130 (60%)	52 (24%)	34 (16%)	0	1
3	C	204/233 (88%)	156 (76%)	32 (16%)	16 (8%)	1	11
4	D	203/206 (98%)	134 (66%)	45 (22%)	24 (12%)	1	4
5	E	148/167 (89%)	97 (66%)	31 (21%)	20 (14%)	0	2
6	F	98/131 (75%)	66 (67%)	19 (19%)	13 (13%)	0	2
7	G	149/156 (96%)	112 (75%)	28 (19%)	9 (6%)	2	20
8	H	127/130 (98%)	96 (76%)	27 (21%)	4 (3%)	7	41
9	I	125/130 (96%)	83 (66%)	25 (20%)	17 (14%)	0	2
10	J	96/103 (93%)	68 (71%)	18 (19%)	10 (10%)	1	5
11	K	115/129 (89%)	82 (71%)	25 (22%)	8 (7%)	2	13
12	L	121/124 (98%)	89 (74%)	22 (18%)	10 (8%)	1	9
13	M	112/118 (95%)	78 (70%)	27 (24%)	7 (6%)	2	18
14	N	92/101 (91%)	55 (60%)	24 (26%)	13 (14%)	0	2
15	O	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	6	37
16	P	80/82 (98%)	57 (71%)	16 (20%)	7 (9%)	1	8
17	Q	78/84 (93%)	57 (73%)	10 (13%)	11 (14%)	0	2
18	R	53/75 (71%)	38 (72%)	12 (23%)	3 (6%)	3	22
19	S	77/92 (84%)	60 (78%)	14 (18%)	3 (4%)	5	33
20	T	83/87 (95%)	59 (71%)	20 (24%)	4 (5%)	4	27
21	U	49/71 (69%)	24 (49%)	19 (39%)	6 (12%)	1	3
23	W	523/529 (99%)	381 (73%)	82 (16%)	60 (12%)	1	4
24	Y	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	2837/3084 (92%)	1991 (70%)	564 (20%)	282 (10%)	1	7

5 of 282 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	TYR
2	B	22	TRP
2	B	33	ALA
2	B	40	ILE
2	B	75	ALA

### 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	
2	B	180/199 (90%)	145 (81%)	35 (19%)	2	10
3	C	170/190 (90%)	146 (86%)	24 (14%)	5	23
4	D	172/173 (99%)	152 (88%)	20 (12%)	8	34
5	E	113/126 (90%)	95 (84%)	18 (16%)	4	16
6	F	87/112 (78%)	73 (84%)	14 (16%)	3	16
7	G	124/129 (96%)	121 (98%)	3 (2%)	61	91
8	H	104/105 (99%)	94 (90%)	10 (10%)	12	44
9	I	105/107 (98%)	92 (88%)	13 (12%)	7	30
10	J	86/90 (96%)	70 (81%)	16 (19%)	2	11
11	K	90/99 (91%)	74 (82%)	16 (18%)	2	13
12	L	103/104 (99%)	89 (86%)	14 (14%)	5	25
13	M	92/96 (96%)	87 (95%)	5 (5%)	31	75
14	N	79/84 (94%)	71 (90%)	8 (10%)	11	41
15	O	76/77 (99%)	66 (87%)	10 (13%)	6	27
16	P	65/65 (100%)	57 (88%)	8 (12%)	7	31
17	Q	74/78 (95%)	61 (82%)	13 (18%)	3	13
18	R	48/65 (74%)	44 (92%)	4 (8%)	16	55
19	S	70/79 (89%)	64 (91%)	6 (9%)	15	52
20	T	65/66 (98%)	60 (92%)	5 (8%)	18	59
21	U	44/61 (72%)	37 (84%)	7 (16%)	4	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W	447/453 (99%)	381 (85%)	66 (15%)	4	20
24	Y	2/2 (100%)	2 (100%)	0	100	100
All	All	2396/2560 (94%)	2081 (87%)	315 (13%)	6	28

5 of 315 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	48	ARG
12	L	73	LEU
23	W	390	ILE
10	J	73	LEU
11	K	69	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	24	ASN
10	J	99	GLN
21	U	8	ASN
9	I	49	GLN
10	J	35	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1531/1533 (99%)	298 (19%)	45 (2%)
22	V	5/27 (18%)	3 (60%)	0
All	All	1536/1560 (98%)	301 (19%)	45 (2%)

5 of 301 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	9	G
1	A	19	A
1	A	22	G
1	A	31	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	495	A
1	A	812	G
1	A	1297	G
1	A	687	A
1	A	815	A

## 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	Y	1	24	8,8,9	8.20	1 (12%)	6,8,10	0.69	0
24	DPP	Y	2	24	5,5,6	10.94	2 (40%)	3,5,7	2.68	1 (33%)
24	UAL	Y	5	24	7,8,9	1.30	1 (14%)	6,9,11	0.96	0
24	5OH	Y	6	24	12,12,13	5.41	4 (33%)	13,16,18	0.83	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	KBE	Y	1	24	-	0/6/7/8	0/0/0/0
24	DPP	Y	2	24	-	0/2/4/6	0/0/0/0
24	UAL	Y	5	24	-	0/3/7/9	0/0/0/0
24	5OH	Y	6	24	-	0/2/18/20	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	2	DPP	O-C	24.19	1.28	1.11
24	Y	1	KBE	O-C	23.13	1.27	1.11
24	Y	6	5OH	O-C	17.41	1.23	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	6	5OH	CQ-NP	5.53	1.40	1.34
24	Y	2	DPP	CA-C	3.39	1.54	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	2	DPP	C-CA-N	4.34	118.16	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates i

There are no carbohydrates in this entry.

## 5.6 Ligand geometry i

Of 106 ligands modelled in this entry, 105 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
26	GNP	W	843	25	34,34,34	1.72	6 (17%)	50,54,54	5.60	14 (28%)

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
26	GNP	W	843	25	-	0/18/38/38	0/1/3/3



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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	W	843	GNP	PG-O1G	6.16	1.53	1.46
26	W	843	GNP	PB-N3B	-4.48	1.60	1.64
26	W	843	GNP	PA-O3A	-2.74	1.54	1.59
26	W	843	GNP	PB-O3A	-2.23	1.56	1.59
26	W	843	GNP	PA-O2A	-2.16	1.45	1.55

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	W	843	GNP	C6-C5-N7	-37.38	129.11	134.14
26	W	843	GNP	PA-O3A-PB	-4.61	116.08	131.81
26	W	843	GNP	C2-N3-C4	-3.73	109.85	115.09
26	W	843	GNP	C4'-O4'-C1'	-3.66	105.77	109.75
26	W	843	GNP	C4-C5-N7	3.56	112.57	109.52

There are no chirality outliers.

There are no torsion outliers.

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.