



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 05:51 PM BST

PDB ID : 4B8F
Title : Crystal Structure of 70S Ribosome with Both Cognate tRNAs in the E and P Sites Representing an Authentic Elongation Complex.
Authors : Gao, Y.G.; Feng, S.; Chen, Y.
Deposited on : 2012-08-28
Resolution : 3.70 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>

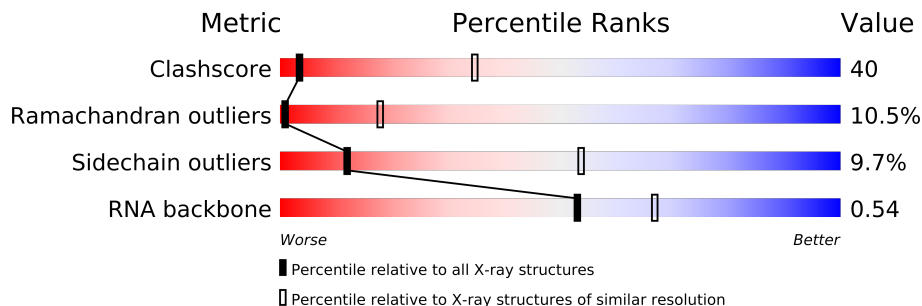
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	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 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RNA backbone	1838	1008 (4.52-2.80)

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. 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	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	

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Mol	Chain	Length	Quality of chain
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	76	
23	W	77	
24	X	25	
25	Y	691	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 60287 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 RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- 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
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- 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	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

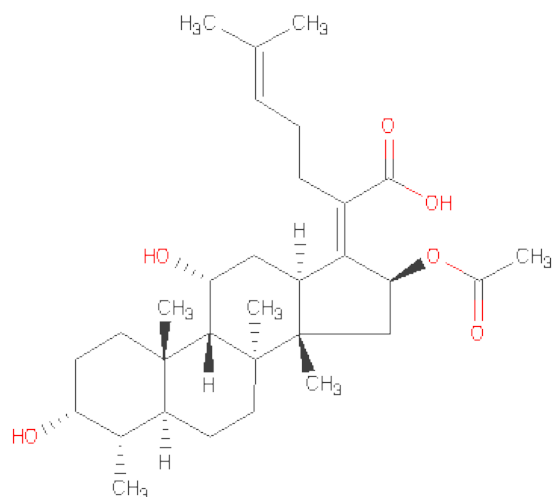
- Molecule 24 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	12	Total	C	N	O	P	0	0	0
			257	116	49	80	12			

- Molecule 25 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			

- Molecule 26 is FUSIDIC ACID (three-letter code: FUA) (formula: C₃₁H₄₈O₆).

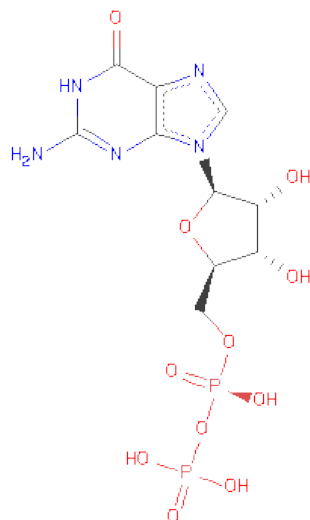


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	F	1	Total	C	O	0	0
			37	31	6		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	I	4	Total	Zn	0	0
			4	4		

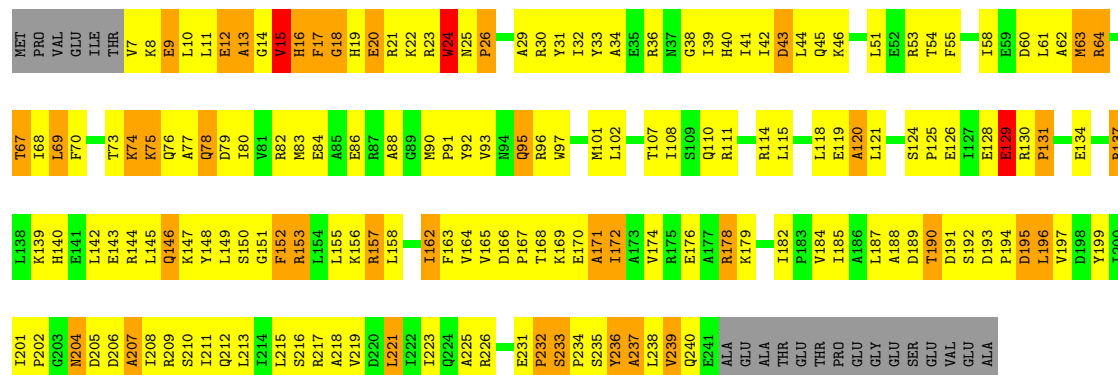
- Molecule 28 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

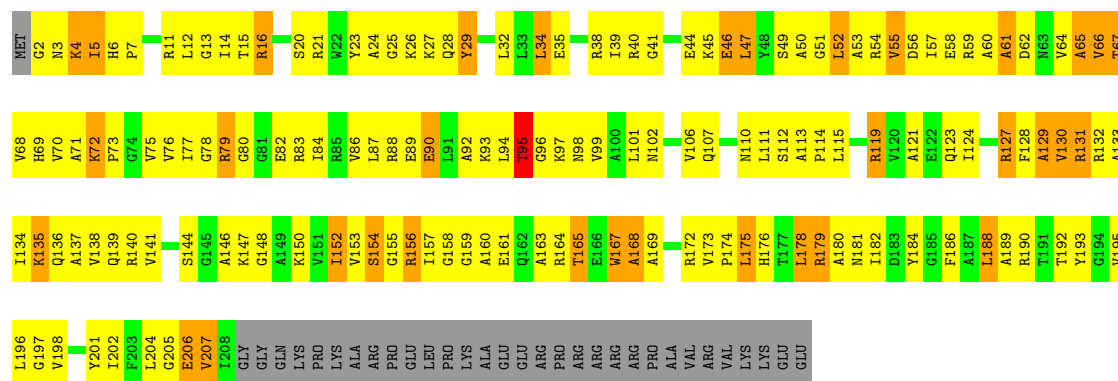
- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



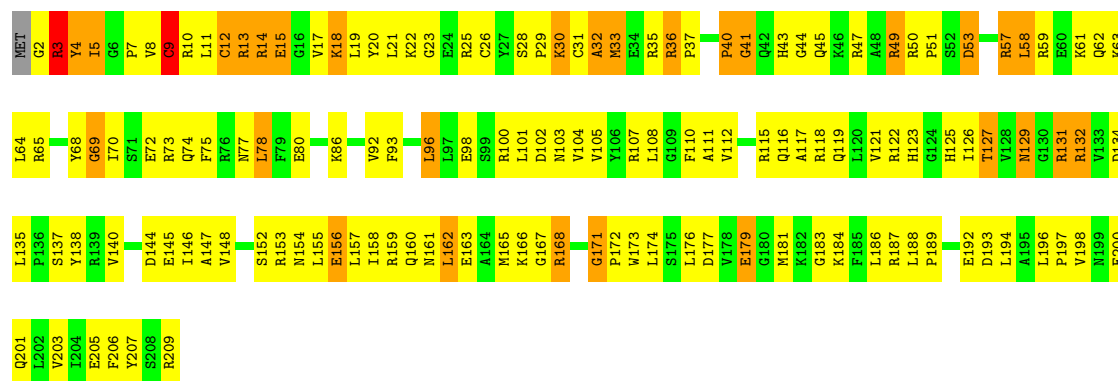
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



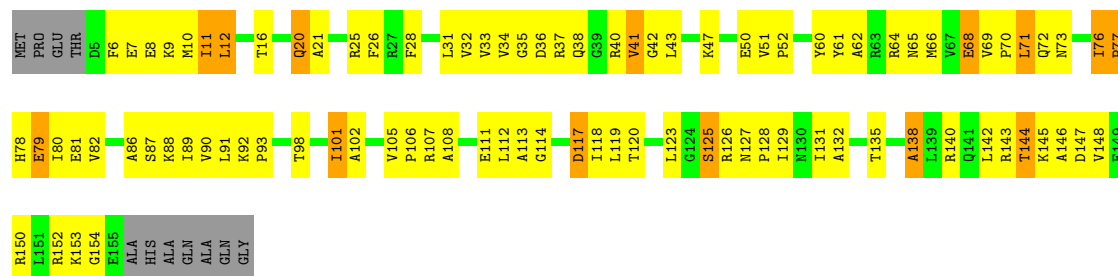
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



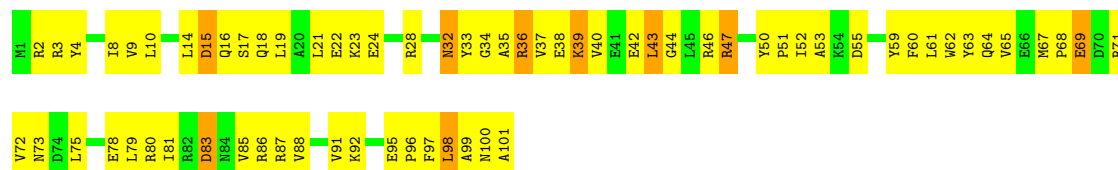
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



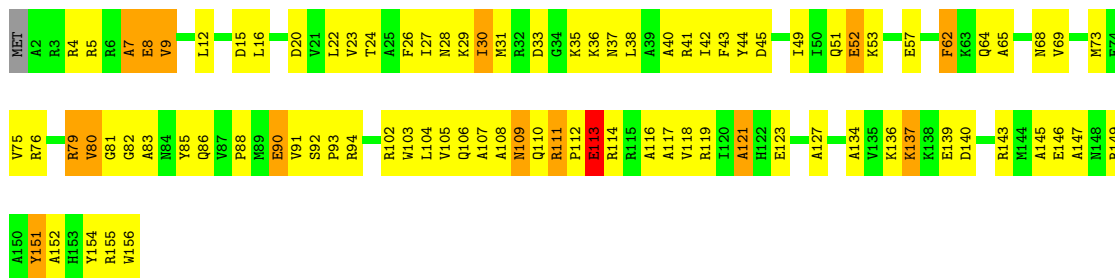
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:



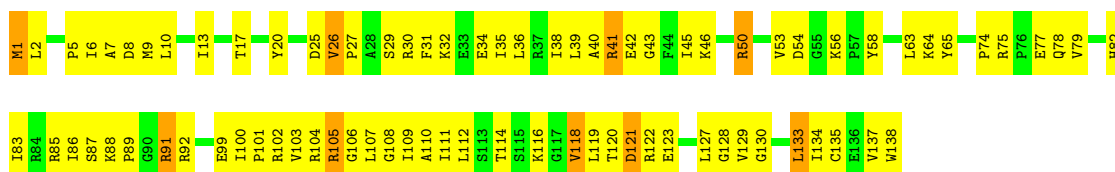
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



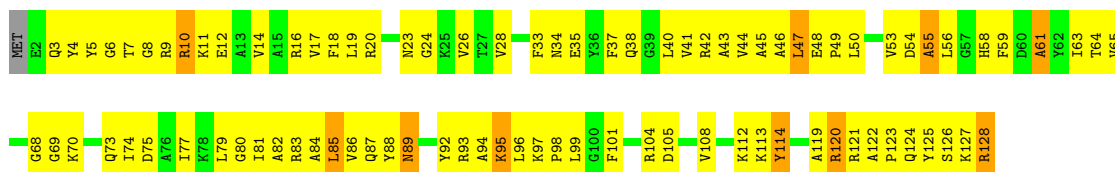
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



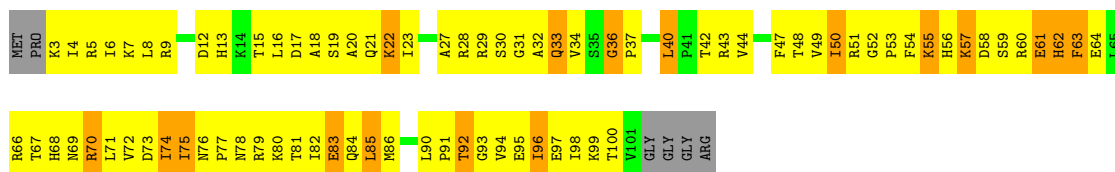
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



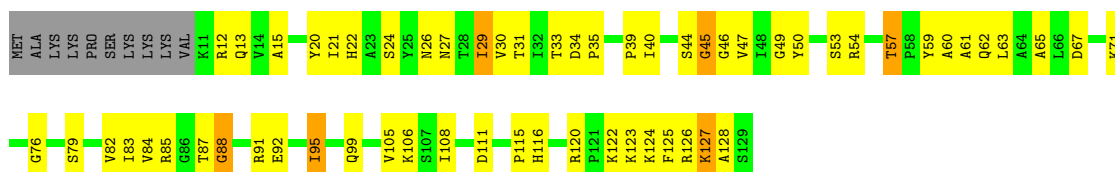
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:



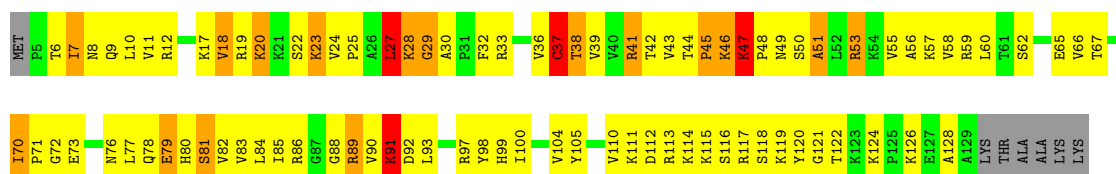
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



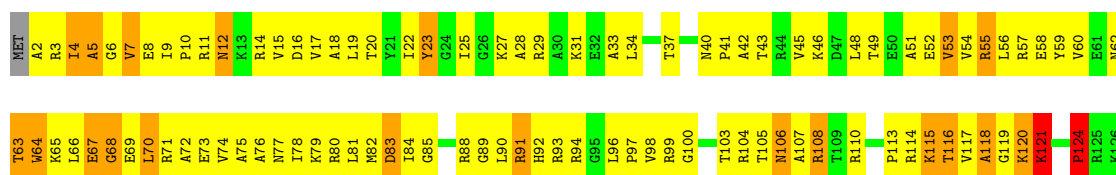
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



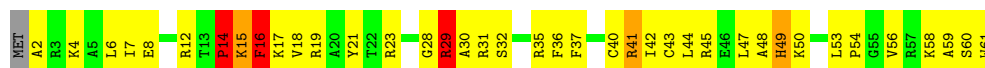
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



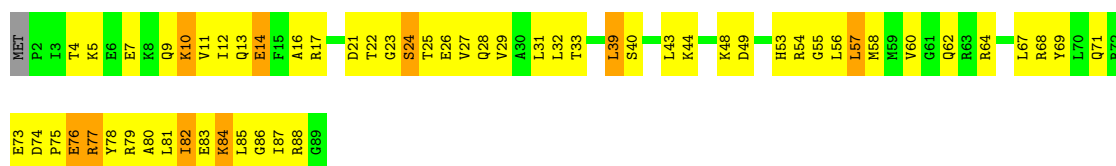
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain N:



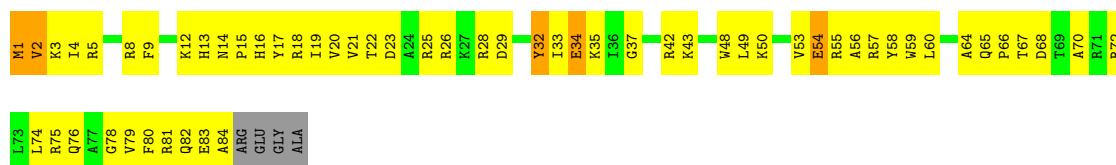
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O:



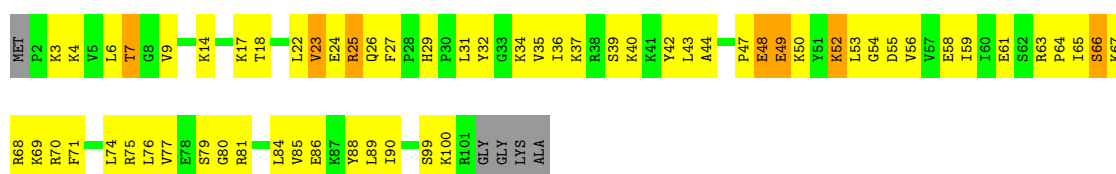
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P:



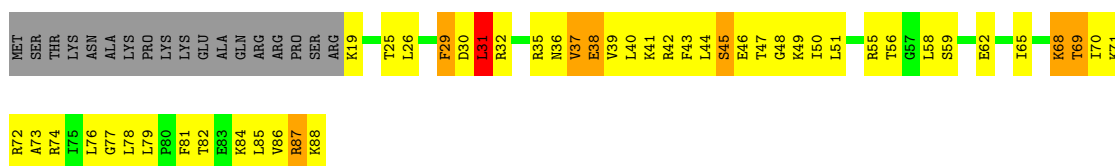
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q:



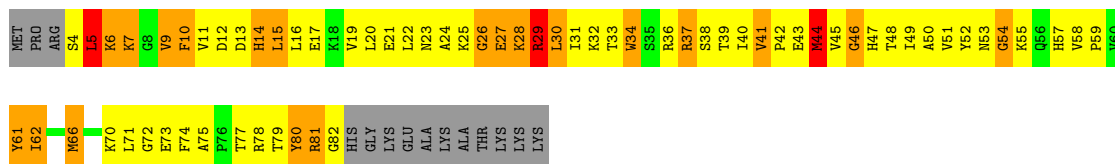
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



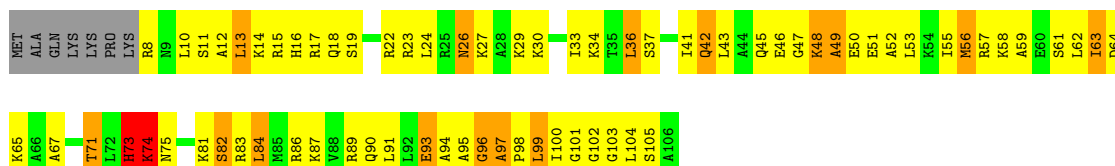
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:



• Molecule 22: MRNA

Chain V:



• Molecule 23: RNA

Chain W:



• Molecule 24: RNA

Chain X:

G	G	A	A	G	G	A	A	A	A11	A12	A13	U14	G15	U16	U17	C18	A19	A20	A21	A22
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• Molecule 25: ELONGATION FACTOR G

Chain Y:

MET	ALA	VAL	K4	V5	E6	Y7	D8	L9	K10	R11	L12	R13	N14	I15	G16	I17	A18	A19	H20	I21	D22	A23	G24	K25	T26	T27	T28	T29	E30	R31	I32	L33	Y34	Y35	T36	G37	R38	I39	H40	K41	I42	G43	GLU	VAL	HIS	GLU	GLY	ALA	THR	MET	ASP	PHE	MET	GLU	GLN	ARG	GLU		
ARG	GLY	ILE	T64	T65	T66	A67	T70	T71	C72	F73			R78	I79	N80	I81	I82	D83	T84	P85	G86	H87	H88	D89	F90	T91	I92	E93	V94	E95	A159	S97	R98	R99	V100	L101	D102		I105	V106		D109	S110	Q111	Q112	G113	V114	E115	P116	Q117	S118	E119	T120	V121	W122	R123	Q124		K127
Y128	K129	P130	P131	I133	A134	F135	A136	R137	K138	M139	D140	K141	T142	G143	A144	D145	L146	W147	L148	V149	I150	R151	T152	M153	E154	E155	R156	L157	G158	A159	S160	P161	V162	M164	Q165	L166	P167	I168	G169	R170	E171	D172	D173	S175	F174	G176	I177	L178	D179	V180	L181	W182	A185	T186	T187	Y188			
D191	L192	G193	T194	D195	T196	R197	E198	P199	T200	T201	P202	E203	E204	Y205	L206	D207	G208	A209	R210	E211	Y212	H213	E214	K215	L216	V217	E218	V219	A220	A221	D222	F223	D224	E225	W226	K228	L229	K230	Y231	L232	E233	G234	E235	E236	T237	T238	E239	E240	E241	L242	A243	A244	A245	T246	R247	K248	G249		
T250	I251	D252	L253	K254	T255	T256	V257	V258	F259	L260	G261	S262	A263	L264	K265	N266	K267	G268	V269		L272	L273	D274	A275	V276	V277	D278	Y279	L280	P281	S282	L284	D285	L286	P287	P288	L289		T292	T293	P294	E295	G296	E297	I301	H302	P303	D304	P305	N306	L309	A311	L312	A313	F314				
K315	I316	K317	A318	D319	V322	L325	T326	F327	L328	R329	V330	S332	S333	L335	T336	S337	G338	S339	Y340	Y341	Y342	K343	T344	T345	Y346	G347	E350	R351	V352		L355	L356	R357	K358	H359	A360	K361	H362	S363	E364	E365	V366	E367	L368	K369	A370	A371	G372	D373	L374	G375	A376	V377	A378	G379				
L380	K381	E382	T383	I384	T385	G386	D387	L388	L389	V390	G391	P395	R396	V397	L398	L399	E400	S401	L402	E403	V404	P405	E406	P407	V408	L409	D410	V411	A412	I413	E414	P415	K416	T417	K418	D419	Q421	K422	K423	L424	S425	Q426	A427	L428	L431	E434	D435	P436	T437	F438	R439	V440	S441	T442	H443				
R444	E445	T446	G447	Q448	T449	L450	L451	S452	G453	H454	L457	H458	L459	E460	L461	L462	V463	D464	R465	L466	K467	R468	E469	F470	V471	V472	D473	A474	V481	A482	Y483	R484	E485	T486	L487	T488	K489	P490	V491	D492	G495	K496	F497	L498	R499	O500	T501	G502	O503	R504	G505	O506	Y507	G508	H509	V510			
K511	I512	K513	S514	E515	P516	L517	P518	R519	G520	S521	V526	N527	A528	I529	V530	G531	G532	V533	I534	P535	K536	E537	Y538	I539	P540	A541	V542	Q543	K544	G545	I546	E547	E548	A549	M550	Q551	S552	P553	P554	L555	I556	G557	F558	P559	V560	N561	D562	L563	K564	V565	T566	L567	Y568	G569	Q570	S571	Y572	H573	
E574	V575	P576	S577	S578	E579	N580	A581	F582	K583	L584	S587	N588	A589	I590	K591	E592	A593	V594	Q595	K596	G597	D598	P599	V600	L601	L602	E603	P604	L605	M606	R607	E608	E609	V610	P613	E614	E615	Y616	M617	V620	I621	L624	N625	A626	R627	R628	G629	Q630	I631	L632	G633	N634	E635	P636	R637				
Q641	V642	I643	A644	A645	F646	V647	P648	L649	A650	E651	G654	Y655	A656	T657	D658	L659	R660	S661	K662	T663	Q664	G665	R666	F669	V670	M671	F672	F673	D674	H675	Y676	G677	E678	V679	P680	K681	Q682	V683	Q684	L687	I688	K689	G690	GLN															

4 Data and refinement statistics i

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	291.36Å 269.43Å 401.95Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	49.75 – 3.70	Depositor
% Data completeness (in resolution range)	99.9 (49.75-3.70)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.249	Depositor
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.051	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 846438 reflections	Xtriage
Total number of atoms	60287	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GDP, 5MU, ZN, MG, FUA

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	0.54	0/36190	0.74	23/56486 (0.0%)
2	B	0.44	0/1934	0.67	0/2609
3	C	0.48	0/1637	0.64	0/2207
4	D	0.39	0/1733	0.65	0/2318
5	E	0.49	0/1163	0.68	0/1566
6	F	0.40	0/856	0.63	0/1154
7	G	0.40	0/1276	0.60	0/1709
8	H	0.45	0/1136	0.71	0/1527
9	I	0.42	0/1027	0.67	0/1373
10	J	0.45	0/808	0.69	0/1087
11	K	0.45	0/900	0.70	0/1213
12	L	0.47	0/987	0.71	0/1322
13	M	0.39	0/999	0.67	0/1338
14	N	0.47	0/501	0.67	0/664
15	O	0.40	0/745	0.62	0/992
16	P	0.39	0/717	0.63	0/965
17	Q	0.47	0/837	0.66	0/1119
18	R	0.45	0/579	0.67	0/768
19	S	0.43	0/643	0.68	1/867 (0.1%)
20	T	0.38	0/765	0.64	0/1007
21	U	0.47	0/213	0.61	0/279
22	V	0.52	0/1809	0.70	0/2819
23	W	0.36	0/1810	0.70	0/2821
24	X	0.38	0/288	0.72	0/446
25	Y	0.47	0/5313	0.69	0/7195
All	All	0.50	0/64866	0.71	24/95851 (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
1	A	1	26
22	V	0	1
All	All	1	27

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.73	130.91	109.50
1	A	115	G	C2'-C3'-O3'	8.39	127.96	109.50
1	A	1502	A	N9-C1'-C2'	7.98	124.38	114.00
1	A	60	A	C2'-C3'-O3'	7.36	125.69	109.50
1	A	533	A	C2'-C3'-O3'	7.29	125.54	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1498	U	C3'

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	118	U	Sidechain
1	A	202	U	Sidechain
1	A	250	A	Sidechain
1	A	436	C	Sidechain

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	32329	0	16318	1155	0
2	B	1901	0	1941	221	0
3	C	1613	0	1677	185	0
4	D	1703	0	1763	171	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1147	0	1207	115	0
6	F	843	0	857	76	0
7	G	1257	0	1296	89	0
8	H	1116	0	1177	89	0
9	I	1010	0	1035	139	0
10	J	795	0	840	154	0
11	K	885	0	904	56	0
12	L	971	0	1057	142	0
13	M	988	0	1059	151	0
14	N	492	0	529	64	0
15	O	734	0	771	69	0
16	P	701	0	720	66	0
17	Q	824	0	891	57	0
18	R	574	0	644	79	0
19	S	630	0	652	101	0
20	T	763	0	861	97	0
21	U	209	0	221	18	0
22	V	1619	0	822	59	0
23	W	1641	0	839	123	0
24	X	257	0	130	45	0
25	Y	5215	0	5288	849	0
26	F	37	0	47	15	0
27	I	4	0	0	0	0
28	Y	28	0	12	13	0
29	Y	1	0	0	0	0
All	All	60287	0	43558	4094	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 40.

The worst 5 of 4094 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:34:C:C3'	23:W:35:A:H5''	1.42	1.44
24:X:11:A:H4'	24:X:12:A:C5'	1.69	1.21
23:W:34:C:C2'	23:W:35:A:H5''	1.71	1.20
24:X:11:A:H4'	24:X:12:A:H5'	1.24	1.17
10:J:75:ILE:HG13	10:J:76:ASN:H	1.10	1.17

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	233/256 (91%)	148 (64%)	52 (22%)	33 (14%)	0	10
3	C	205/239 (86%)	146 (71%)	32 (16%)	27 (13%)	0	12
4	D	206/209 (99%)	138 (67%)	47 (23%)	21 (10%)	1	19
5	E	149/162 (92%)	117 (78%)	26 (17%)	6 (4%)	5	50
6	F	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	5	50
7	G	153/156 (98%)	112 (73%)	27 (18%)	14 (9%)	1	24
8	H	136/138 (99%)	106 (78%)	26 (19%)	4 (3%)	7	60
9	I	121/128 (94%)	85 (70%)	27 (22%)	9 (7%)	2	31
10	J	97/105 (92%)	67 (69%)	19 (20%)	11 (11%)	1	16
11	K	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	29
12	L	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	7
13	M	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	10
14	N	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	25
15	O	86/89 (97%)	55 (64%)	24 (28%)	7 (8%)	1	27
16	P	82/88 (93%)	62 (76%)	15 (18%)	5 (6%)	2	37
17	Q	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	7	59
18	R	68/88 (77%)	47 (69%)	13 (19%)	8 (12%)	1	15
19	S	77/93 (83%)	42 (54%)	17 (22%)	18 (23%)	0	2
20	T	97/106 (92%)	57 (59%)	28 (29%)	12 (12%)	1	14
21	U	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	13
25	Y	663/691 (96%)	458 (69%)	126 (19%)	79 (12%)	1	15
All	All	3014/3229 (93%)	2089 (69%)	609 (20%)	316 (10%)	1	18

5 of 316 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	GLU

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Mol	Chain	Res	Type
2	B	13	ALA
2	B	15	VAL
2	B	74	LYS
2	B	75	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	
2	B	200/220 (91%)	182 (91%)	18 (9%)	14	58
3	C	160/188 (85%)	139 (87%)	21 (13%)	6	37
4	D	180/181 (99%)	160 (89%)	20 (11%)	9	46
5	E	115/123 (94%)	104 (90%)	11 (10%)	12	54
6	F	90/90 (100%)	83 (92%)	7 (8%)	18	65
7	G	126/127 (99%)	117 (93%)	9 (7%)	21	70
8	H	119/119 (100%)	110 (92%)	9 (8%)	19	67
9	I	98/99 (99%)	91 (93%)	7 (7%)	21	70
10	J	88/92 (96%)	77 (88%)	11 (12%)	7	40
11	K	90/99 (91%)	87 (97%)	3 (3%)	50	89
12	L	104/109 (95%)	93 (89%)	11 (11%)	10	49
13	M	99/101 (98%)	90 (91%)	9 (9%)	14	57
14	N	49/50 (98%)	44 (90%)	5 (10%)	11	51
15	O	79/80 (99%)	73 (92%)	6 (8%)	19	67
16	P	72/74 (97%)	68 (94%)	4 (6%)	30	78
17	Q	94/97 (97%)	89 (95%)	5 (5%)	32	80
18	R	61/77 (79%)	58 (95%)	3 (5%)	35	82
19	S	69/80 (86%)	60 (87%)	9 (13%)	6	37
20	T	76/82 (93%)	66 (87%)	10 (13%)	6	36
21	U	19/22 (86%)	18 (95%)	1 (5%)	32	80
25	Y	563/582 (97%)	495 (88%)	68 (12%)	7	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2551/2692 (95%)	2304 (90%)	247 (10%)	12 54

5 of 247 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	92	THR
14	N	29	ARG
25	Y	512	ILE
11	K	92	GLU
12	L	85	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
10	J	13	HIS
12	L	8	ASN
25	Y	458	HIS
10	J	56	HIS
10	J	78	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	254 (16%)	36 (2%)
22	V	75/76 (98%)	13 (17%)	1 (1%)
23	W	76/77 (98%)	27 (35%)	1 (1%)
24	X	12/25 (48%)	8 (66%)	2 (16%)
All	All	1666/1700 (98%)	302 (18%)	40 (2%)

5 of 302 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	33	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	748	C
1	A	1049	U
22	V	17	C
1	A	913	A
1	A	1065	U

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
23	5MU	W	54	23	20,22,23	0.88	2 (10%)	25,32,35	1.36	3 (12%)

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
23	5MU	W	54	23	-	0/6/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	54	5MU	P-OP1	2.16	1.49	1.46
23	W	54	5MU	C6-C5	-2.07	1.34	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	54	5MU	C6-N1-C2	-4.94	121.00	122.41
23	W	54	5MU	C5-C6-N1	2.25	123.77	121.59
23	W	54	5MU	C5M-C5-C6	2.02	122.88	118.59

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 7 ligands modelled in this entry, 5 are 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$
26	FUA	F	1102	-	40,40,40	1.80	8 (20%)	64,64,64	1.62	10 (15%)
28	GDP	Y	1690	29	30,30,30	1.35	4 (13%)	44,47,47	2.43	9 (20%)

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	FUA	F	1102	-	-	0/18/92/92	0/0/4/4
28	GDP	Y	1690	29	-	0/16/32/32	0/1/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	F	1102	FUA	C17-C22	4.70	1.39	1.34
26	F	1102	FUA	C29-C22	4.52	1.53	1.47
26	F	1102	FUA	C23-C22	-4.16	1.39	1.51
26	F	1102	FUA	C23-C24	-3.98	1.39	1.53
28	Y	1690	GDP	C4-N9	-3.82	1.32	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	1690	GDP	C6-C5-N7	-11.74	132.56	134.14
26	F	1102	FUA	C24-C23-C22	4.94	124.11	111.93
28	Y	1690	GDP	C2-N3-C4	4.53	121.45	115.09
26	F	1102	FUA	C13-C12-C11	-4.37	105.84	112.00
28	Y	1690	GDP	C5-C4-N3	-3.91	120.28	125.94

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.