



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2026 – 10:19 PM UTC

PDB ID : 2E5L / pdb_00002e5l
Title : A snapshot of the 30S ribosomal subunit capturing mRNA via the Shine-Dalgarno interaction
Authors : Kaminishi, T.; Wilson, D.N.; Takemoto, C.; Harms, J.M.; Kawazoe, M.; Schlunzen, F.; Hanawa-Suetsugu, K.; Shirouzu, M.; Fucini, P.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-12-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

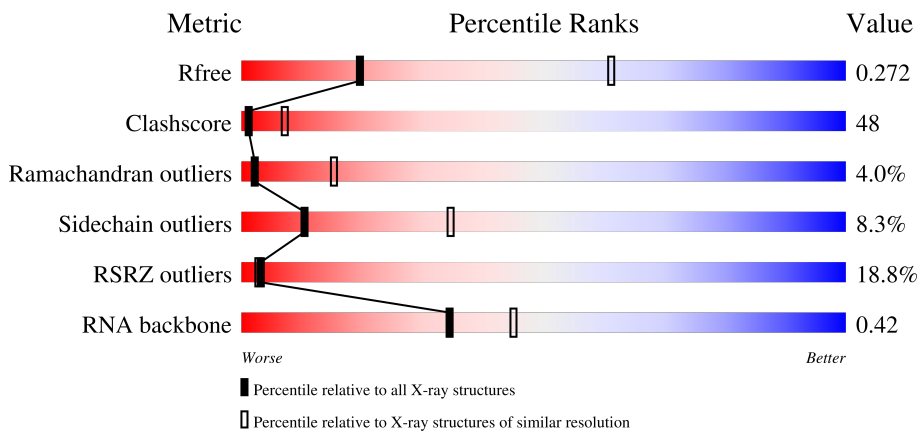
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1520	Upper red bar: 7% Lower bar segments: 10% (red), 59% (yellow), 20% (orange), 10% (red)
2	1	6	Upper red bar: 67% Lower bar segments: 17% (green), 50% (yellow), 33% (orange)
2	2	6	Lower bar segments: 33% (red), 50% (yellow), 33% (orange), 33% (grey)
3	B	227	Lower bar segments: 30% (red), 43% (green), 44% (yellow), 10% (orange), 10% (grey)

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Mol	Chain	Length	Quality of chain
4	C	238	
5	D	208	
6	E	161	
7	F	101	
8	G	155	
9	H	138	
10	I	128	
11	J	104	
12	K	128	
13	L	131	
14	M	125	
15	N	60	
16	O	88	
17	P	88	
18	Q	104	
19	R	87	
20	S	92	
21	T	105	
22	V	26	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 51895 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1517	32594	14508	6027	10542	1517	0	0	0

- Molecule 2 is a RNA chain called 5'-R(*GP*AP*AP*AP*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	1	6	131	60	30	36	5	0	0	0
2	2	4	86	40	20	23	3	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	222	1811	1154	328	324	5	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	206	1612	1016	314	281	1	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

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

- Molecule 6 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	150	1146	724	217	201	4	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S6.

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

- Molecule 8 is a protein called 30S ribosomal protein S7.

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

- Molecule 9 is a protein called 30S ribosomal protein S8.

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

- Molecule 10 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	127	1011	639	198	174	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	98	794	499	156	138	1	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	115	853	531	160	159	3	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	124	970	611	195	163	1	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	M	122	969	600	200	167	2	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S14.

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

- Molecule 16 is a protein called 30S ribosomal protein S15.

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

- Molecule 17 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	P	83	700	443	139	117	1	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Q	104	857	547	161	147	2	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
19	R	73	597	380	118	99	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 21 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 22 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

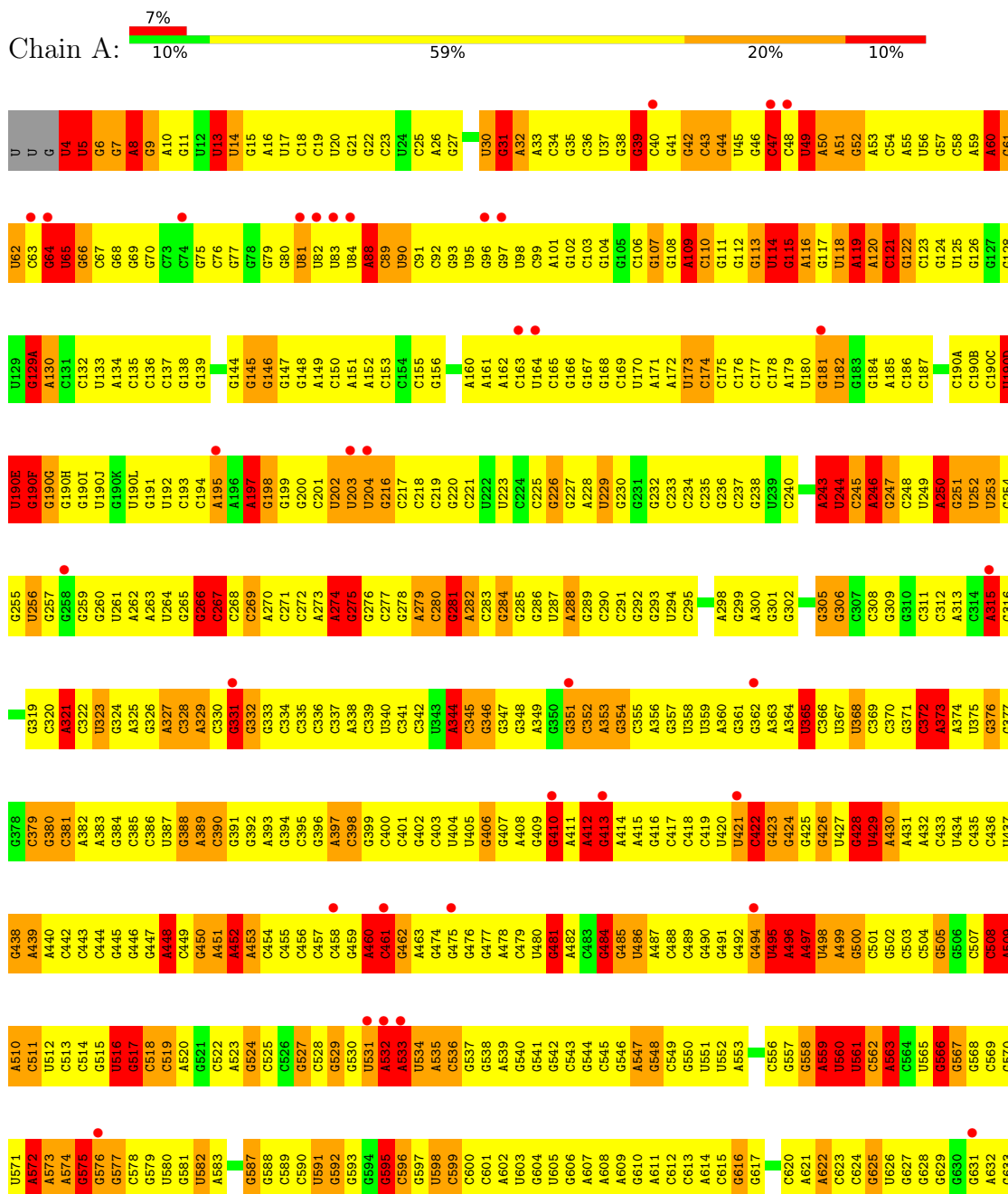
- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

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

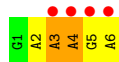
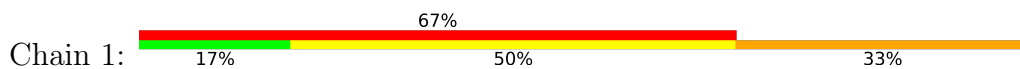
- Molecule 1: 16S ribosomal RNA



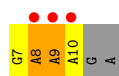
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G1373	A1374	A1375	A1376	A1377	A1378	A1379	G1380	G1381	G1382	G1385	G1386	G1387	G1388	G1389	G1390	G1391	G1392	G1393	G1394	G1395	G1396	G1397	G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434		
C1314	U1315	C1316	C1317	C1318	C1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	
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G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	C1018	C1019	G1020	G1021	G1022	G1023	G1024	U1025	G1026	G1027	C1028	C1029	G1030	G1030A	C1030B	G1030C	A1030D	G1031	G1032	G1033	G1034	A1035	G1036	C1037	C1038	C1039	U1040	A1044	C1045	A1046	G1047	G1048	U1049	G1050	C1051	U1052	G1053	A1054	A1055	U1056	G1057	G1058	C1059	G1060	G1061	U1062	C1063	G1064	U1065	C1066	
C948	A949	U950	G951	U952	G953	G954	U955	U956	U957	U958	U959	U960	U961	G962	G963	U964	G965	G966	G967	U968	A969	U970	C971	G972	G973	A974	A975	U976	U977	A978	C979	U980	U981	A982	A983	C984	C985	U986	G987	G988	C989	G990	U991	U992	G993	A994	A995	U996	U997	G998	G1002	G1003	G1004	U1005	C1006	C1007	C1008		
U820	G821	C822	G823	C824	G825	C826	U827	A828	C829	G830	U831	C832	U833	C836	G837	C838	U839	C840	U841	C848	C849	U850	U851	G852	A782	C783	C784	G785	C786	U787	U788	U789	A790	G791	A792	U793	C866	C867	C868	C869	U870	U871	A872	U873	U874	C875	C876	C877	G878	C879	C880	C881	C882	C883	U884	C885	C886	C887	
G888	A889	G890	U891	C892	G893	G894	C895	C896	G897	G898	G899	A900	A901	G902	G903	C904	U905	G906	G907	A908	A909	C910	U911	C912	A913	A914	A915	G916	G917	G918	A919	U920	G921	A922	U923	U924	G925	G926	G927	G928	G929	C930	C931	C932	A933	A934	A935	C936	U937	G938	G939	C940	U941	C942	U943	U944	G945	A946	G947
A694	A695	A696	U697	G698	G699	G700	C701	A702	G703	A704	U705	A706	C707	A648	G649	G650	G651	A652	A653	G654	A655	G656	G657	G658	U659	G660	G661	A662	A663	G664	A665	G666	G667	U668	G669	G670	G671	U672	G673	G674	A675	A676	U677	U678	C679	G741	G742	U743	U744	C745	A746	U686	A687	G688	C689	G690	U691	U692	G693



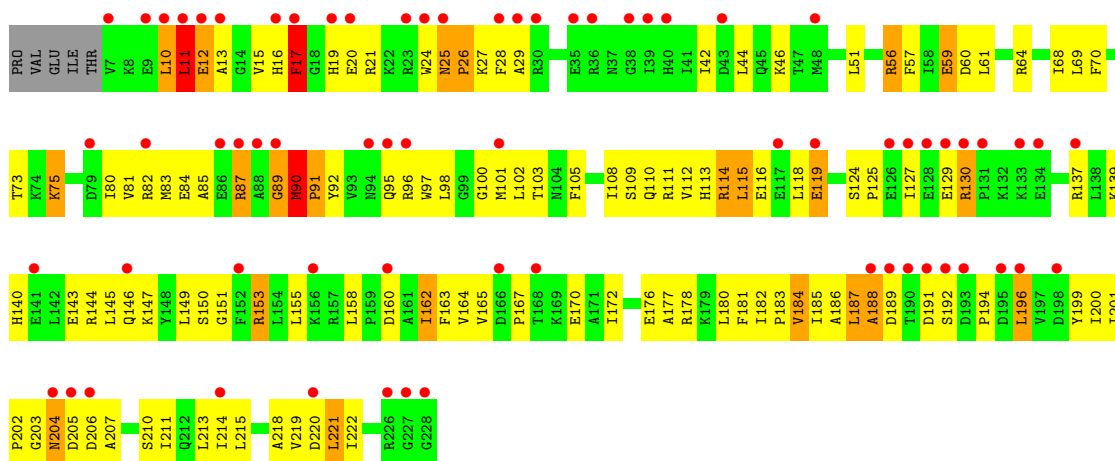
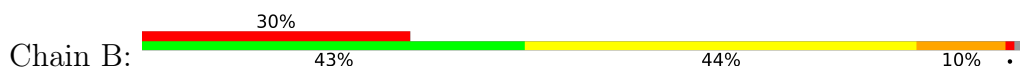
- Molecule 2: 5'-R(*GP*AP*AP*AP*GP*A)-3'



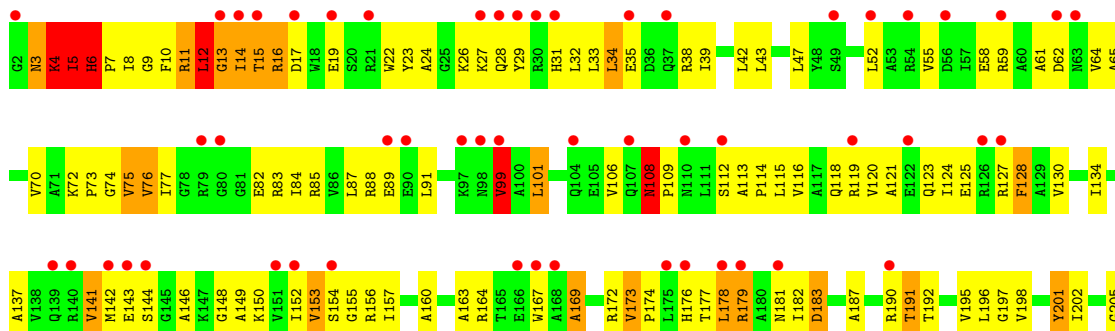
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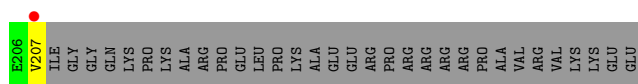


- Molecule 3: 30S ribosomal protein S2

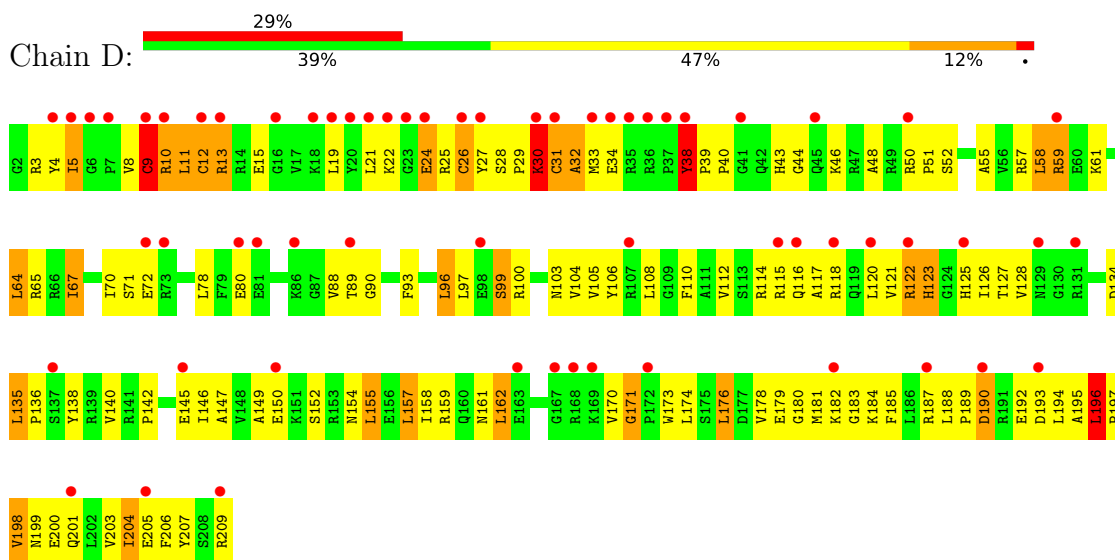


- Molecule 4: 30S ribosomal protein S3

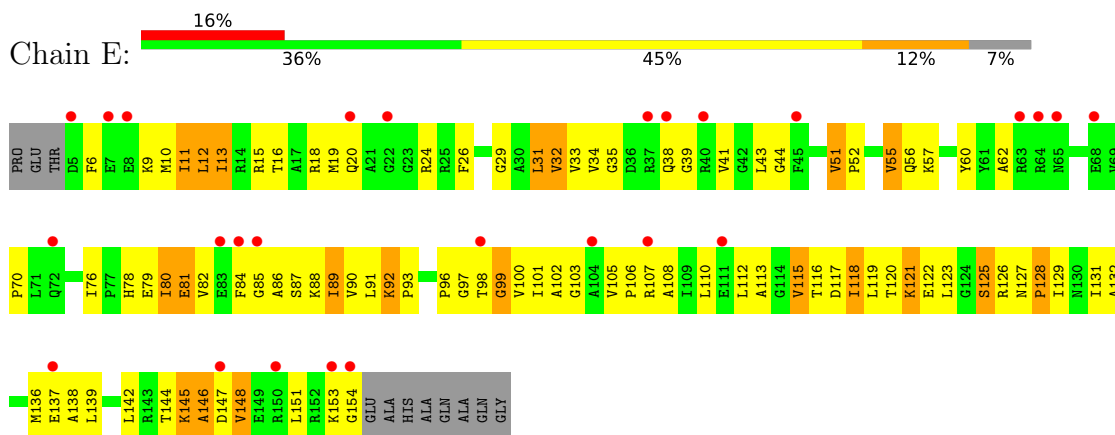




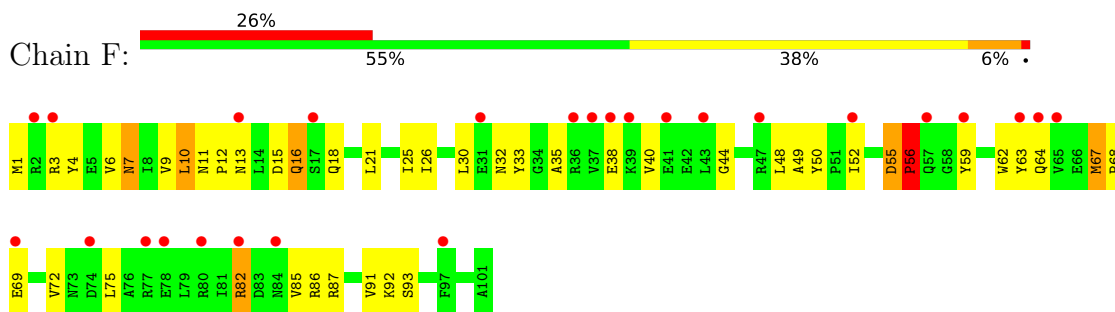
- Molecule 5: 30S ribosomal protein S4



- Molecule 6: 30S ribosomal protein S5

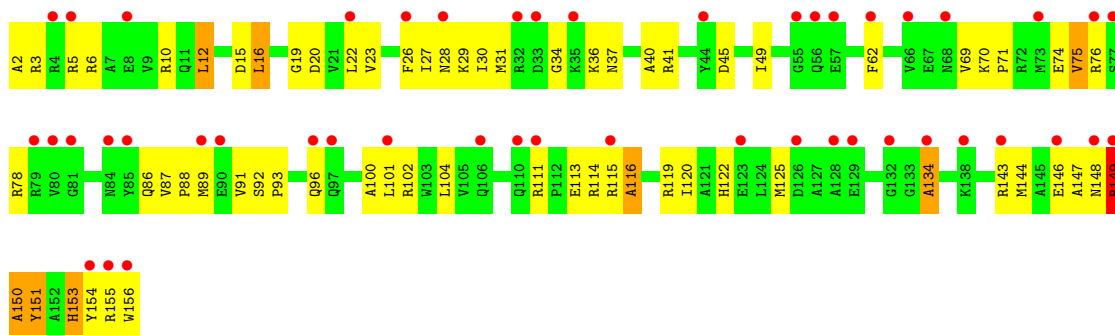


- Molecule 7: 30S ribosomal protein S6

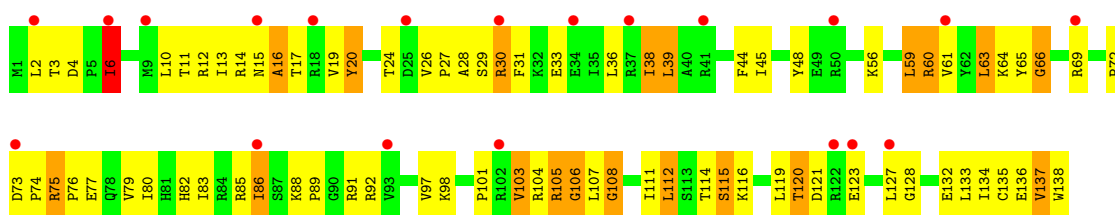
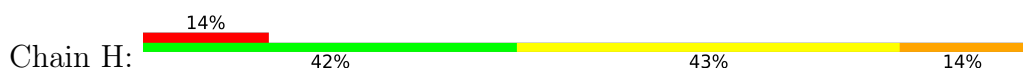


- Molecule 8: 30S ribosomal protein S7

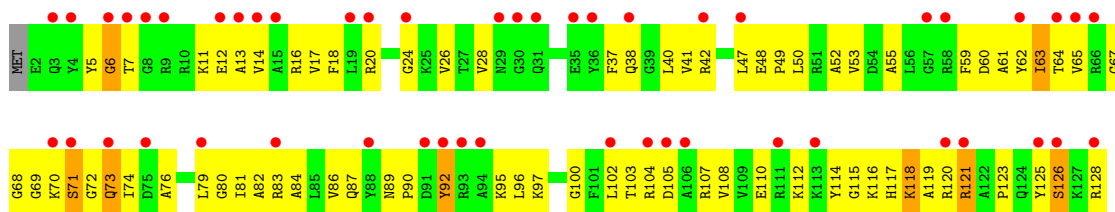




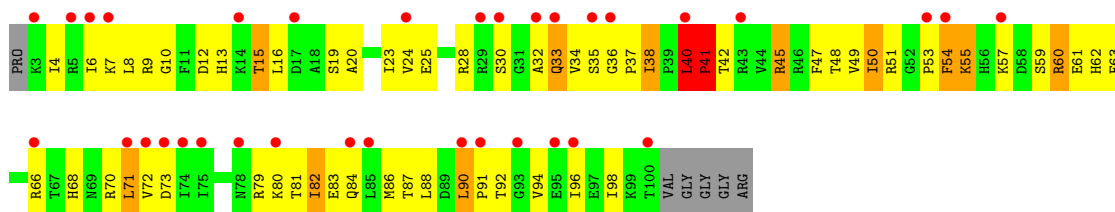
- Molecule 9: 30S ribosomal protein S8



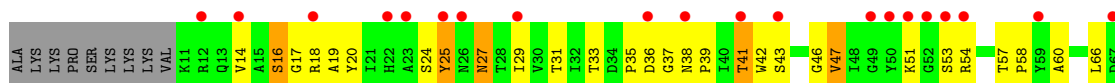
- Molecule 10: 30S ribosomal protein S9

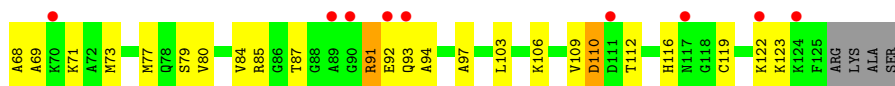


- Molecule 11: 30S ribosomal protein S10



- Molecule 12: 30S ribosomal protein S11

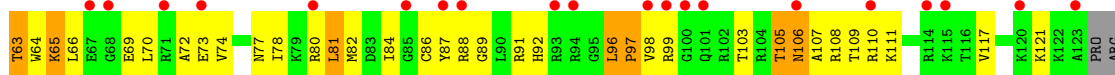
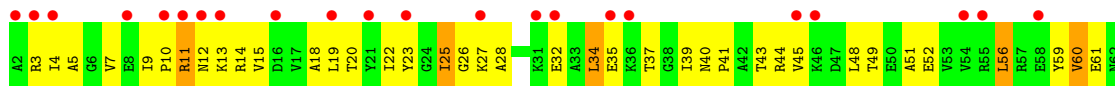




- Molecule 13: 30S ribosomal protein S12

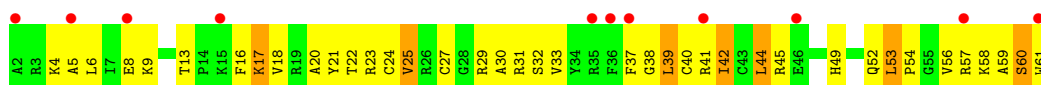


- Molecule 14: 30S ribosomal protein S13

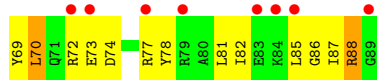
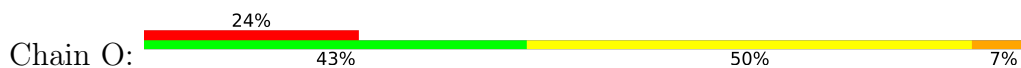


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- Molecule 15: 30S ribosomal protein S14

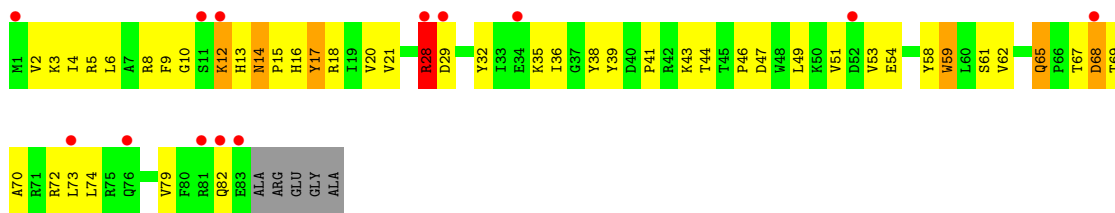


- Molecule 16: 30S ribosomal protein S15

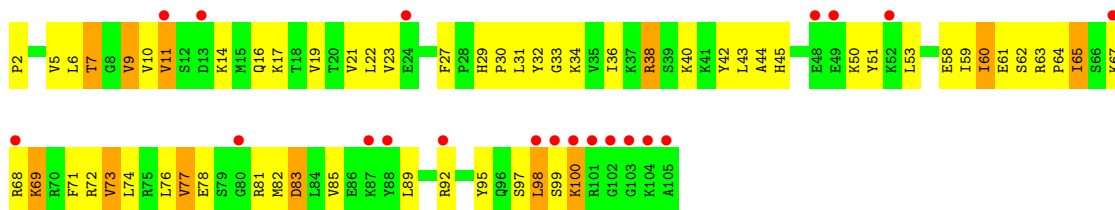
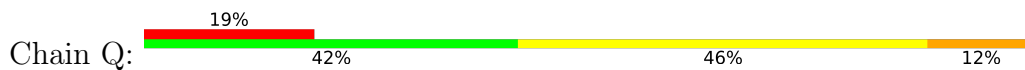


- Molecule 17: 30S ribosomal protein S16

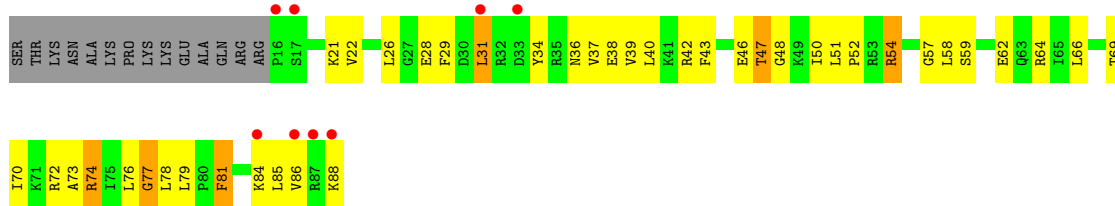




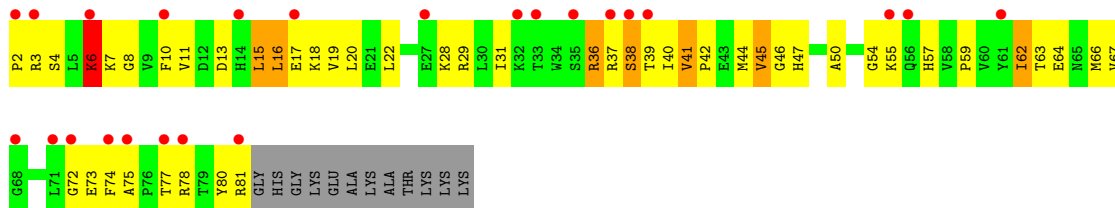
- Molecule 18: 30S ribosomal protein S17



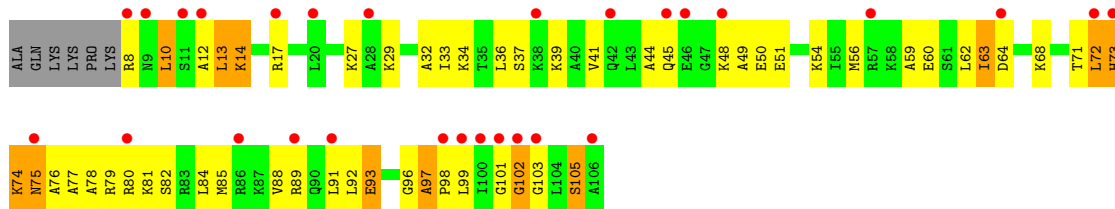
- Molecule 19: 30S ribosomal protein S18



- Molecule 20: 30S ribosomal protein S19

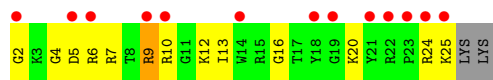


- Molecule 21: 30S ribosomal protein S20



● Molecule 22: 30S ribosomal protein Thx

Chain V: 50%
42% 46% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	411.79Å 411.79Å 173.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	148.83 – 3.30 148.83 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (148.83-3.30) 97.1 (148.83-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.33Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.301 0.230 , 0.272	Depositor DCC
R_{free} test set	10897 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	96.4	Xtrriage
Anisotropy	0.310	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	51895	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.64	0/36482	1.06	224/56937 (0.4%)
2	1	0.51	0/148	0.90	0/230
2	2	0.38	0/97	0.81	0/150
3	B	0.89	2/1843 (0.1%)	1.33	25/2479 (1.0%)
4	C	0.83	0/1636	1.26	22/2205 (1.0%)
5	D	1.02	7/1733 (0.4%)	1.36	25/2318 (1.1%)
6	E	1.12	4/1162 (0.3%)	1.43	18/1564 (1.2%)
7	F	0.66	0/856	1.23	8/1154 (0.7%)
8	G	0.63	0/1276	1.07	6/1709 (0.4%)
9	H	1.00	2/1136 (0.2%)	1.55	19/1527 (1.2%)
10	I	0.65	0/1029	1.16	6/1378 (0.4%)
11	J	0.74	0/807	1.24	8/1085 (0.7%)
12	K	0.71	0/868	1.21	8/1173 (0.7%)
13	L	0.84	2/986 (0.2%)	1.23	8/1320 (0.6%)
14	M	0.67	0/979	1.23	14/1310 (1.1%)
15	N	0.85	0/501	1.30	7/664 (1.1%)
16	O	0.87	0/745	1.29	4/992 (0.4%)
17	P	0.82	0/716	1.22	8/963 (0.8%)
18	Q	1.01	4/870 (0.5%)	1.32	8/1159 (0.7%)
19	R	0.79	0/603	1.25	7/799 (0.9%)
20	S	0.65	1/661 (0.2%)	1.20	5/890 (0.6%)
21	T	0.64	0/764	1.12	5/1006 (0.5%)
22	V	0.65	0/212	0.93	0/277
All	All	0.72	22/56110 (0.0%)	1.13	435/83289 (0.5%)

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	127

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	12	CYS	CA-CB	12.18	1.73	1.53
5	D	12	CYS	CA-C	8.85	1.65	1.52
18	Q	77	VAL	CA-CB	-8.18	1.46	1.55
3	B	182	ILE	CA-CB	-7.81	1.44	1.54
13	L	26	ALA	CA-CB	7.20	1.62	1.53

The worst 5 of 435 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	75	ARG	CA-C-N	12.91	135.98	119.84
9	H	75	ARG	C-N-CA	12.91	135.98	119.84
5	D	31	CYS	N-CA-C	-12.23	98.60	113.15
5	D	12	CYS	CA-CB-SG	11.09	139.90	114.40
3	B	158	LEU	CA-C-N	10.78	130.86	119.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	511	C	C1'

5 of 127 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	30	U	Sidechain
1	A	39	G	Sidechain
1	A	47	C	Sidechain
1	A	49	U	Sidechain
1	A	60	A	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32594	0	16454	3163	0
2	1	131	0	68	14	0
2	2	86	0	46	9	0
3	B	1811	0	1861	103	0
4	C	1612	0	1677	139	0
5	D	1703	0	1763	133	0
6	E	1146	0	1207	97	0
7	F	843	0	857	37	0
8	G	1257	0	1296	82	0
9	H	1116	0	1177	99	0
10	I	1011	0	1043	109	0
11	J	794	0	840	83	0
12	K	853	0	868	55	0
13	L	970	0	1057	76	0
14	M	969	0	1039	81	0
15	N	492	0	529	53	0
16	O	734	0	771	50	0
17	P	700	0	720	53	0
18	Q	857	0	930	55	0
19	R	597	0	668	46	0
20	S	647	0	673	64	0
21	T	762	0	859	49	0
22	V	208	0	221	14	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51895	0	36624	4218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

The worst 5 of 4218 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:C:C2'	1:A:1028:C:H5''	1.48	1.40
1:A:390:C:H4'	17:P:28:ARG:NH2	1.46	1.28
1:A:1027:C:H2'	1:A:1028:C:C5'	1.65	1.25
1:A:243:A:H4'	1:A:244:U:C5'	1.65	1.24
1:A:839:U:H5'	1:A:840:C:C5	1.71	1.24

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	220/227 (97%)	169 (77%)	39 (18%)	12 (6%)	1	10
4	C	204/238 (86%)	149 (73%)	42 (21%)	13 (6%)	1	8
5	D	206/208 (99%)	165 (80%)	31 (15%)	10 (5%)	1	12
6	E	148/161 (92%)	113 (76%)	30 (20%)	5 (3%)	3	18
7	F	99/101 (98%)	83 (84%)	14 (14%)	2 (2%)	6	27
8	G	153/155 (99%)	129 (84%)	23 (15%)	1 (1%)	18	49
9	H	136/138 (99%)	113 (83%)	21 (15%)	2 (2%)	8	32
10	I	125/128 (98%)	94 (75%)	25 (20%)	6 (5%)	2	12
11	J	96/104 (92%)	75 (78%)	14 (15%)	7 (7%)	1	6
12	K	113/128 (88%)	88 (78%)	22 (20%)	3 (3%)	4	22
13	L	122/131 (93%)	96 (79%)	21 (17%)	5 (4%)	2	15
14	M	120/125 (96%)	89 (74%)	26 (22%)	5 (4%)	2	14
15	N	58/60 (97%)	45 (78%)	13 (22%)	0	100	100
16	O	86/88 (98%)	70 (81%)	14 (16%)	2 (2%)	5	25
17	P	81/88 (92%)	64 (79%)	16 (20%)	1 (1%)	10	37
18	Q	102/104 (98%)	86 (84%)	11 (11%)	5 (5%)	1	12
19	R	71/87 (82%)	57 (80%)	13 (18%)	1 (1%)	9	33
20	S	78/92 (85%)	63 (81%)	11 (14%)	4 (5%)	1	11
21	T	97/105 (92%)	72 (74%)	17 (18%)	8 (8%)	0	5
22	V	22/26 (85%)	19 (86%)	1 (4%)	2 (9%)	0	3
All	All	2337/2494 (94%)	1839 (79%)	404 (17%)	94 (4%)	2	15

5 of 94 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	12	GLU

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Mol	Chain	Res	Type
3	B	21	ARG
3	B	24	TRP
3	B	130	ARG
4	C	4	LYS

5.3.2 Protein sidechains [i](#)

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	
3	B	191/196 (97%)	172 (90%)	19 (10%)	7	27
4	C	160/187 (86%)	143 (89%)	17 (11%)	6	24
5	D	180/180 (100%)	161 (89%)	19 (11%)	6	24
6	E	115/122 (94%)	101 (88%)	14 (12%)	5	19
7	F	90/90 (100%)	84 (93%)	6 (7%)	15	42
8	G	126/126 (100%)	121 (96%)	5 (4%)	28	56
9	H	119/119 (100%)	107 (90%)	12 (10%)	7	26
10	I	98/99 (99%)	95 (97%)	3 (3%)	35	60
11	J	88/91 (97%)	82 (93%)	6 (7%)	14	42
12	K	87/98 (89%)	80 (92%)	7 (8%)	11	36
13	L	104/108 (96%)	99 (95%)	5 (5%)	23	52
14	M	97/100 (97%)	90 (93%)	7 (7%)	13	40
15	N	49/49 (100%)	41 (84%)	8 (16%)	2	11
16	O	79/79 (100%)	70 (89%)	9 (11%)	5	21
17	P	72/74 (97%)	68 (94%)	4 (6%)	19	47
18	Q	96/96 (100%)	87 (91%)	9 (9%)	8	30
19	R	64/76 (84%)	62 (97%)	2 (3%)	35	60
20	S	71/79 (90%)	65 (92%)	6 (8%)	10	33
21	T	76/81 (94%)	69 (91%)	7 (9%)	8	30
22	V	19/21 (90%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1981/2071 (96%)	1816 (92%)	165 (8%)	10 34

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	M	63	THR
18	Q	11	VAL
14	M	117	VAL
16	O	39	LEU
19	R	31	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
9	H	82	HIS
12	K	38	ASN
20	S	47	HIS
10	I	31	GLN
11	J	13	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1517/1520 (99%)	338 (22%)	187 (12%)
2	1	5/6 (83%)	1 (20%)	1 (20%)
2	2	3/6 (50%)	2 (66%)	0
All	All	1525/1532 (99%)	341 (22%)	188 (12%)

5 of 341 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G

5 of 188 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	975	A
1	A	1214	C
1	A	993	G
1	A	1129	C
1	A	1257	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1517/1520 (99%)	0.44	113 (7%) 20 15	44, 89, 178, 199	0
2	1	6/6 (100%)	2.43	4 (66%) 0 0	199, 199, 199, 199	0
2	2	4/6 (66%)	2.40	3 (75%) 0 0	185, 193, 195, 198	0
3	B	222/227 (97%)	1.42	68 (30%) 1 1	46, 104, 169, 199	0
4	C	206/238 (86%)	1.28	54 (26%) 1 1	49, 107, 172, 198	0
5	D	208/208 (100%)	1.29	61 (29%) 1 1	32, 90, 156, 199	0
6	E	150/161 (93%)	0.82	26 (17%) 4 4	32, 72, 151, 195	0
7	F	101/101 (100%)	1.43	26 (25%) 1 1	63, 116, 167, 182	0
8	G	155/155 (100%)	1.61	47 (30%) 1 1	70, 133, 184, 199	0
9	H	138/138 (100%)	0.68	20 (14%) 6 5	31, 72, 145, 181	0
10	I	127/128 (99%)	1.84	49 (38%) 1 1	55, 147, 191, 199	0
11	J	98/104 (94%)	1.74	34 (34%) 1 1	64, 138, 198, 199	0
12	K	115/128 (89%)	1.18	29 (25%) 1 1	59, 111, 172, 190	0
13	L	124/131 (94%)	1.09	19 (15%) 5 5	46, 104, 165, 199	0
14	M	122/125 (97%)	1.57	42 (34%) 1 1	71, 127, 180, 198	0
15	N	60/60 (100%)	0.97	11 (18%) 3 3	56, 89, 158, 190	0
16	O	88/88 (100%)	1.21	21 (23%) 2 1	45, 100, 167, 185	0
17	P	83/88 (94%)	1.04	13 (15%) 5 4	38, 91, 146, 185	0
18	Q	104/104 (100%)	0.95	20 (19%) 3 3	49, 90, 172, 199	0
19	R	73/87 (83%)	0.75	8 (10%) 10 9	46, 103, 175, 199	0
20	S	80/92 (86%)	1.39	24 (30%) 1 1	74, 136, 187, 199	0
21	T	99/105 (94%)	1.44	28 (28%) 1 1	69, 122, 182, 199	0
22	V	24/26 (92%)	2.17	13 (54%) 0 0	72, 120, 168, 199	0
All	All	3904/4026 (96%)	0.96	733 (18%) 3 3	31, 99, 178, 199	0

The worst 5 of 733 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	C	107	GLN	9.4
1	A	1129	C	9.4
6	E	154	GLY	9.0
4	C	143	GLU	8.9
3	B	19	HIS	8.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	ZN	D	210	1/1	0.91	0.23	85,85,85,85	0
23	ZN	N	62	1/1	1.00	0.02	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.