



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:00 PM GMT

PDB ID : 4IO9
Title : Crystal structure of compound 4d bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

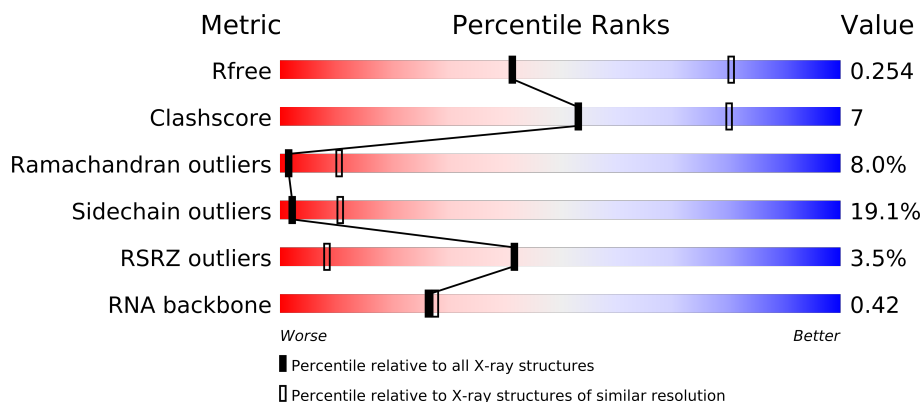
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

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))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
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 ≥ 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.

Mol	Chain	Length	Quality of chain
1	X	2880	
2	Y	123	
3	A	274	
4	B	211	
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	

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Mol	Chain	Length	Quality of chain
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	
30	4	37	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
31	MG	J	201	-	X
31	MG	M	201	-	X
31	MG	X	2901	-	X
31	MG	X	2902	-	X
31	MG	X	2903	-	X
31	MG	X	2904	-	X
31	MG	X	2905	-	X
31	MG	X	2906	-	X
31	MG	X	2907	-	X
31	MG	X	2908	-	X
31	MG	X	2909	-	X
31	MG	X	2910	-	X
31	MG	X	2911	-	X
31	MG	X	2912	-	X
31	MG	X	2913	-	X
31	MG	X	2915	-	X
31	MG	X	2916	-	X
31	MG	X	2917	-	X
31	MG	X	2918	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
31	MG	X	2919	-	X
31	MG	X	2920	-	X
31	MG	X	2921	-	X
31	MG	X	2922	-	X
31	MG	X	2923	-	X
31	MG	X	2924	-	X
31	MG	X	2925	-	X
31	MG	X	2926	-	X
31	MG	X	2927	-	X
31	MG	X	2928	-	X
31	MG	Y	201	-	X
31	MG	Y	202	-	X
31	MG	Y	203	-	X
31	MG	Y	204	-	X
31	MG	Y	205	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83875 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

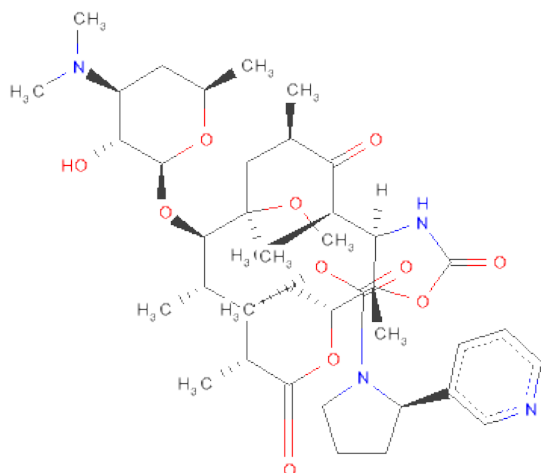
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	J	1	Total Mg 1 1	0	0
31	Y	5	Total Mg 5 5	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3AS,4R,7R,8S,9S,10R,11R,13R,15R,15AR)-4-ETHYL-11-METHOXY-3A,7,9,11,13,15-HEXAMETHYL-2,6,14-TRIOXO-10-{{3,4,6-TRIDEOXY-3-(DIMETHYLAMINO)-BETA-D-XYLO-HEXOPYRANOSYL}OXY}TETRADECAHYDRO-2H-OXACYCLO TETRADECINO[4,3-D][1,3]OXAZOL-8-YL(2R)-2-(PYRIDIN-3-YL)PYRROLIDINE-1-CARBOXYLATE (three-letter code: 1F2) (formula: C₄₁H₆₄N₄O₁₁).



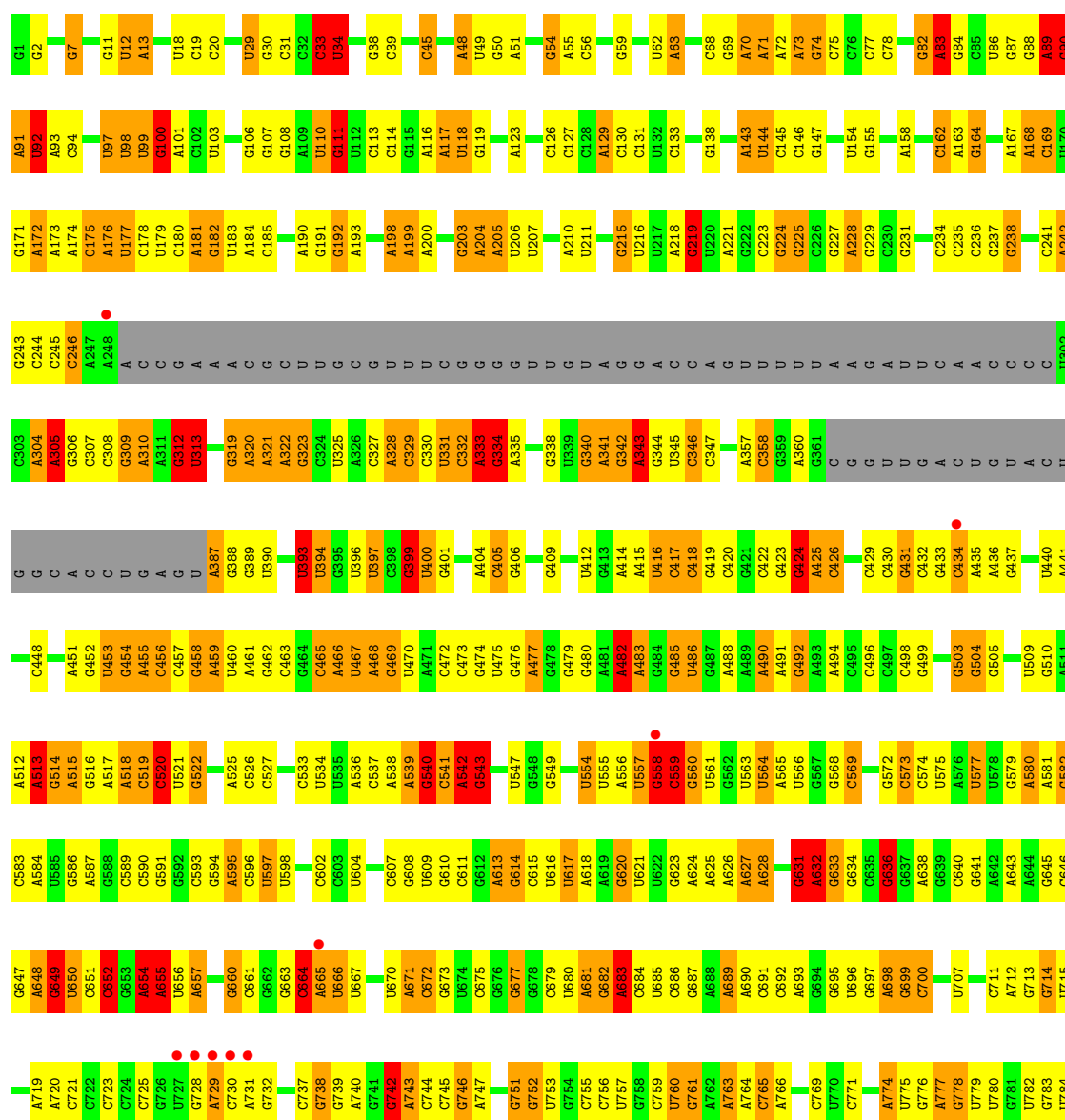
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	X	1	56	41	4	11	0	0

3 Residue-property plots

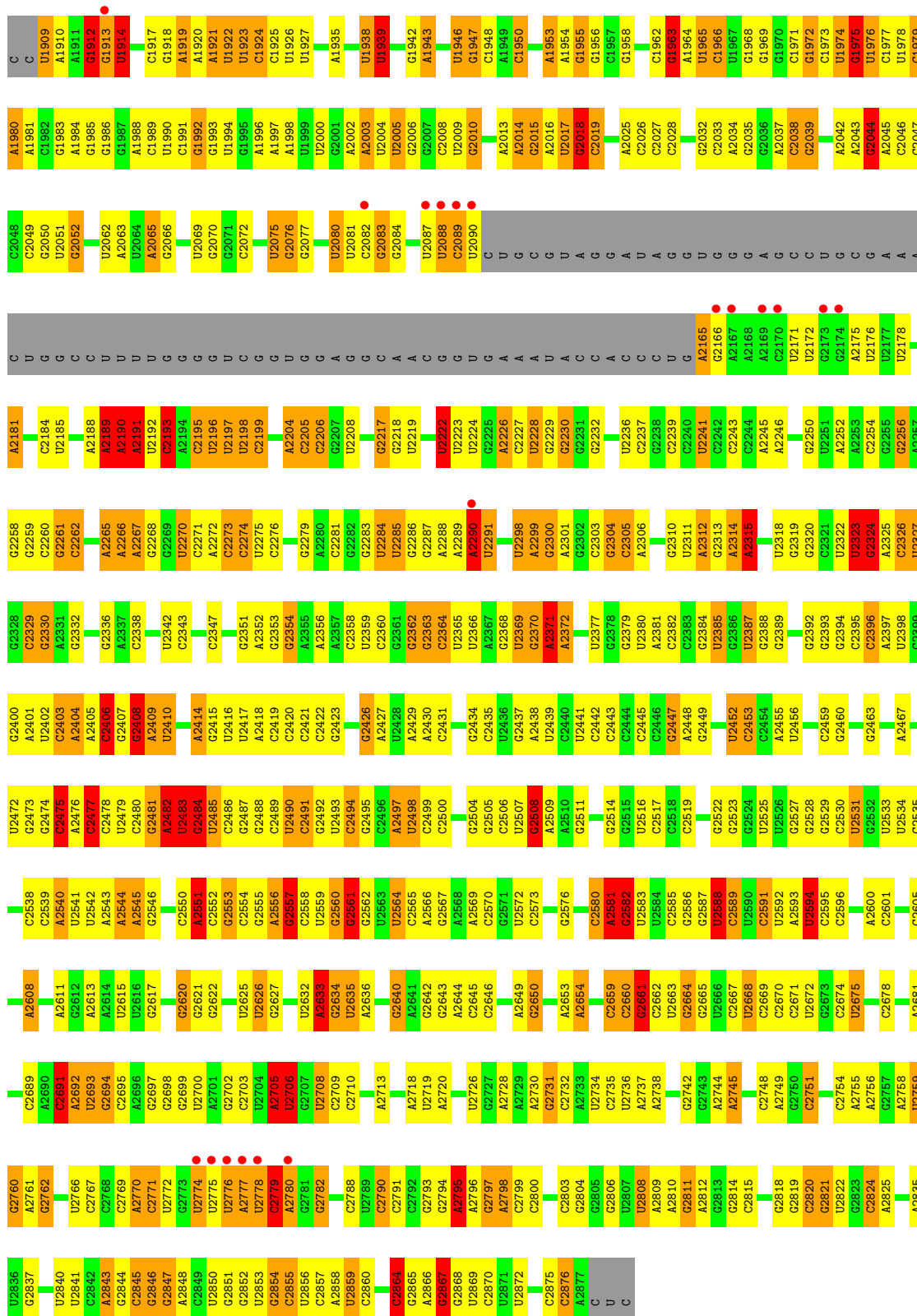
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

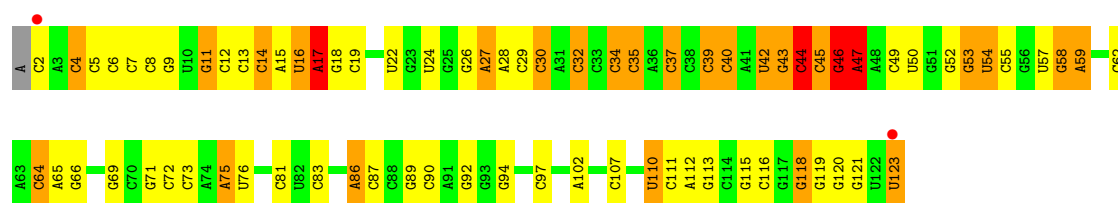
• Molecule 1: 23S ribosomal RNA

Chain X: 



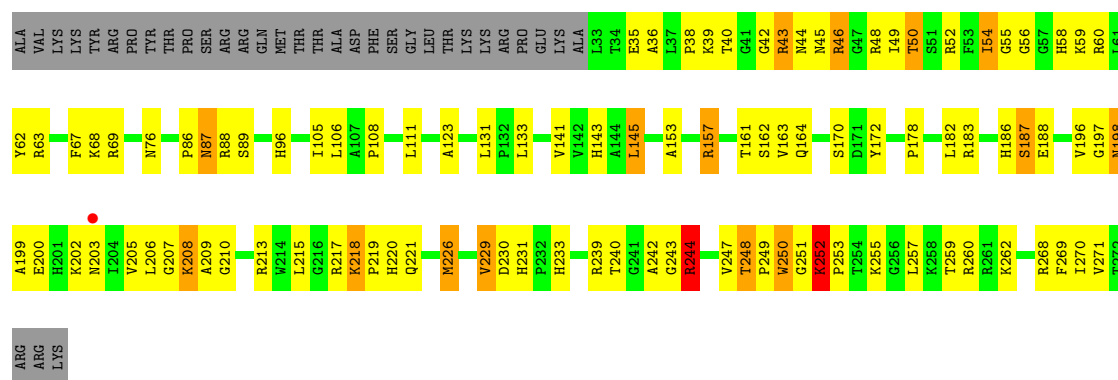






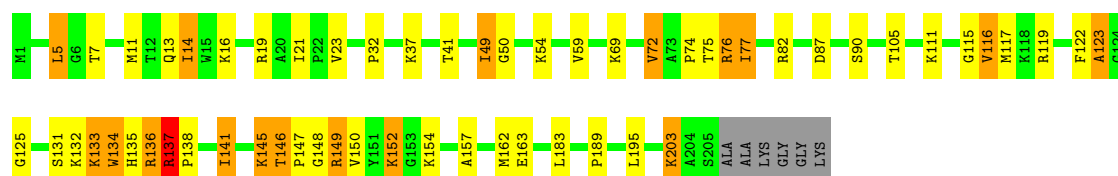
• Molecule 3: 50S ribosomal protein L2

Chain A:



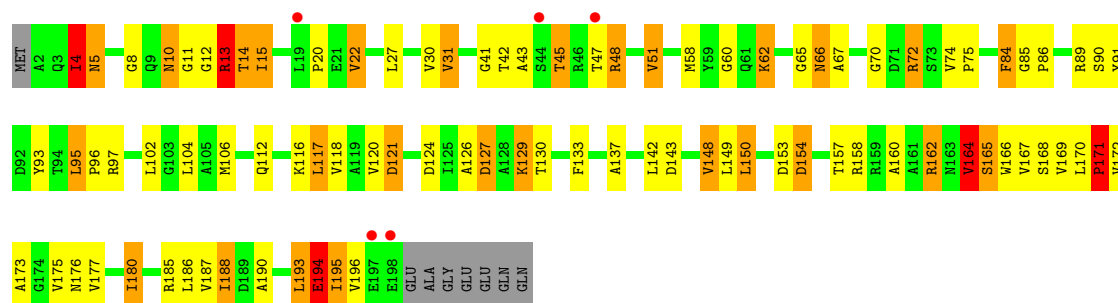
• Molecule 4: 50S ribosomal protein L3

Chain B:



• Molecule 5: 50S ribosomal protein L4

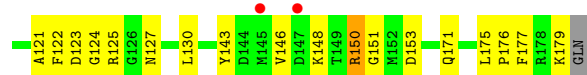
Chain C:



• Molecule 6: 50S ribosomal protein L5

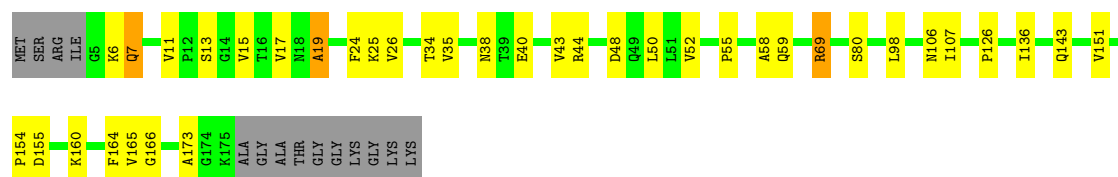
Chain D:

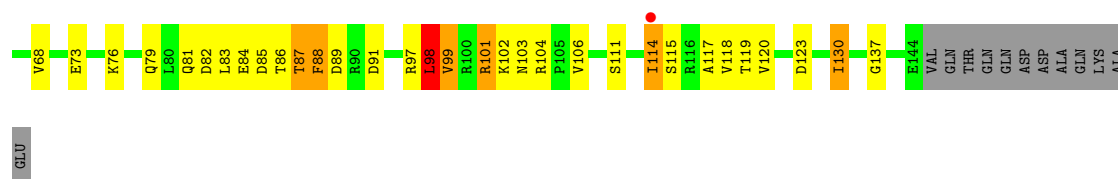




• Molecule 7: 50S ribosomal protein L6

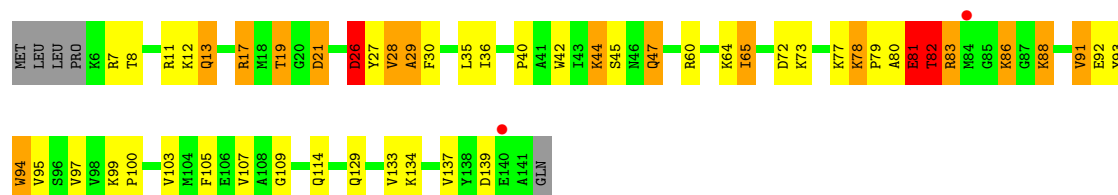
Chain E:





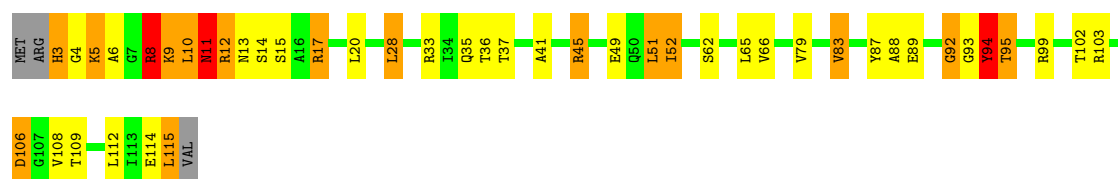
- Molecule 12: 50S ribosomal protein L16

Chain J:



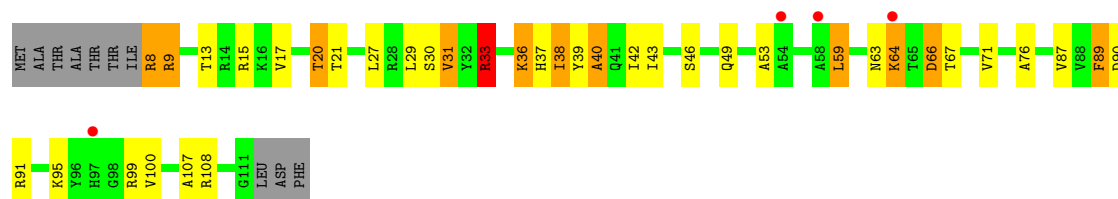
- Molecule 13: 50S ribosomal protein L17

Chain K:



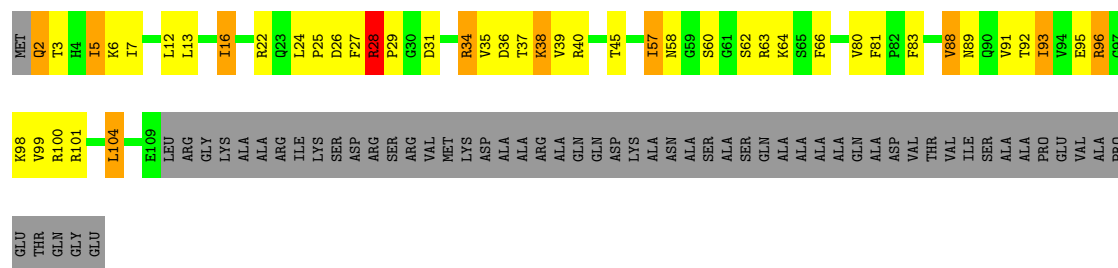
- Molecule 14: 50S ribosomal protein L18

Chain L:



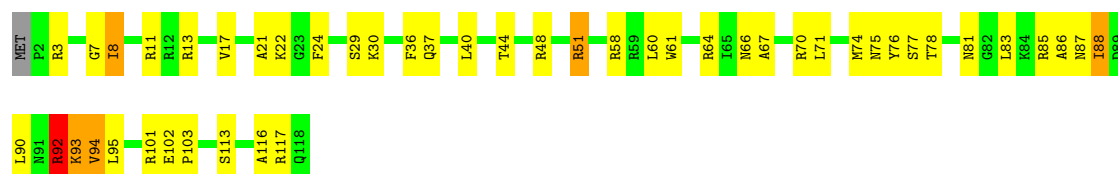
- Molecule 15: 50S ribosomal protein L19

Chain M:



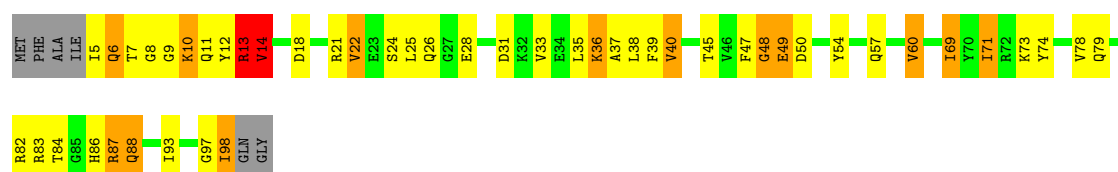
- Molecule 16: 50S ribosomal protein L20

Chain N:



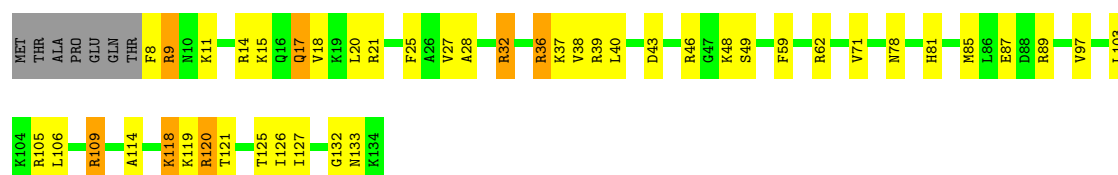
- Molecule 17: 50S ribosomal protein L21

Chain O:



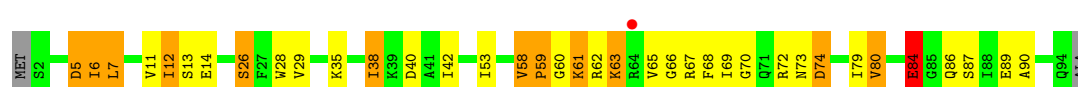
- Molecule 18: 50S ribosomal protein L22

Chain P:



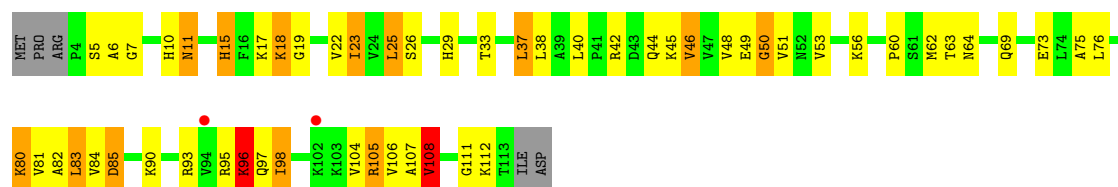
- Molecule 19: 50S ribosomal protein L23

Chain Q:



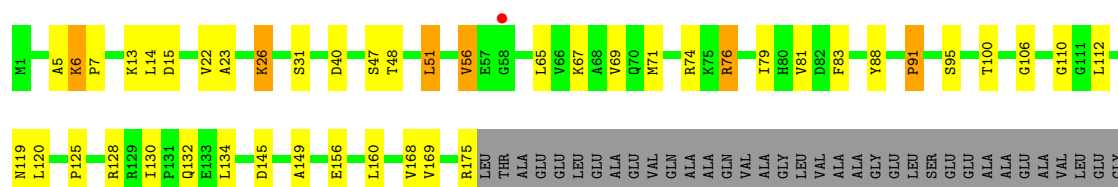
- Molecule 20: 50S ribosomal protein L24

Chain R:



- Molecule 21: 50S ribosomal protein L25

Chain S:



ASP
ALA
SER
LEU
GLU
GLU
VAL
LYS
ALA
GLU
ALA
SER
GLU
ASP
ASN
ALA
GLY
THR
ASP
SER
GLU
ASP
ASN
SER
ASP
ALA
GLN

- Molecule 22: 50S ribosomal protein L27

Chain T:

MET A2 H3 K4 K5 G8 S9 S10 M11 M12 G13 S16 M17 P18 P19 Y20 Y21 L21 L22 G23 G27 L37 L38 V38 R39 Q40 R41 G42 T43 K46 Q49 Q50 L62 S63 D64 G73 K74 F78 Q85 THR GLU VAL ALA ASP

- Molecule 23: 50S ribosomal protein L28

Chain U:

MET SER ARG GLU CYS TYR LEU T8 G9 K10 K11 V14 V15 M16 M17 S17 M18 V19 R20 R21 G22 G23 K23 D27 D28 G29 Y30 G31 G32 R33 K34 T35 G36 G37 I37 K39 R40 R41 V41 Q42 R43 A44 N45 L46 H47 K48 K49 A50 I51 R52 E53 Q56 T59 V60 W61 L62 S63 N65
A66 L67 P74 Y75 I78 E79 LEU ILE

- Molecule 24: 50S ribosomal protein L29

Chain V:

M1 K2 P3 R7 F14 D19 A20 R21 L25 L28 Q36 L37 R44 R47 L53 V56 R57 A58 E59 L60 E65 Q66 GLN

- Molecule 25: 50S ribosomal protein L30

Chain W:

M1 K2 I3 K4 V9 I10 G11 R12 R26 D30 S31 R32 E33 V34 T37 V40 M43 V44 K45 T46 V47 L50 L51 E55

- Molecule 26: 50S ribosomal protein L32

Chain Z:

MET A2 K3 H4 P5 V6 P7 K8 T11 R16 D17 M18 R19 R20 L25 Q35 C36 H37 K40 L41 S42 H43 H44 T45 C49 D53 G54 R55 Q56 V57 L58 A59 VAL

- Molecule 27: 50S ribosomal protein L33

Chain 1:

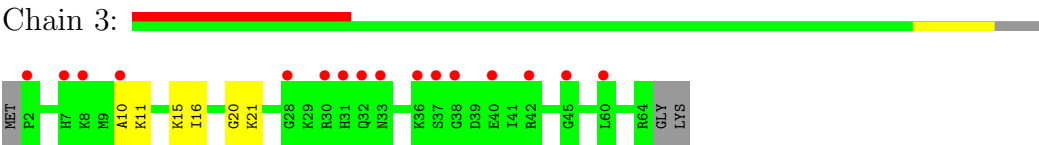
MET A2 R7 K26 Y40 D41 P42 V43 A44 K54 VAL

- Molecule 28: 50S ribosomal protein L34

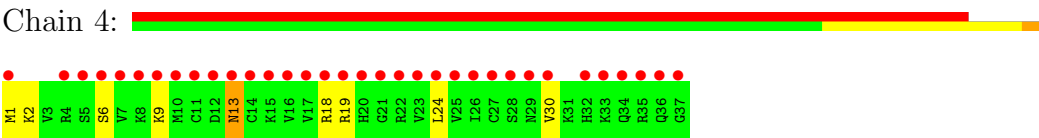
Chain 2:

M1 K2 R3 T4 Y5 Q6 P7 N8 N9 R10 K11 K14 T15 H16 A20 R21 M22 K23 T24 K25 S26 G27 R28 N29 I30 L31 A32 R33 R34 R35 A36 K37 G38 R39 H40 Q41 D46 GLU

● Molecule 29: 50S ribosomal protein L35



● Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.94Å 409.69Å 694.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.20 – 3.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 94.1 (30.20-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 3.24Å)	Xtriage
Refinement program	autobuster	Depositor
R, R_{free}	0.199 , 0.235 0.215 , 0.254	Depositor DCC
R_{free} test set	18481 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 56.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 367392 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83875	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: MG, 1F2

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	X	1.00	46/64561 (0.1%)	1.87	1961/100708 (1.9%)
2	Y	1.05	0/2904	1.78	84/4525 (1.9%)
3	A	0.61	0/1862	0.92	1/2510 (0.0%)
4	B	0.57	0/1567	0.94	1/2105 (0.0%)
5	C	0.62	0/1529	0.98	2/2070 (0.1%)
6	D	0.45	0/1419	0.66	0/1903
7	E	0.45	0/1308	0.67	0/1771
8	F	0.46	0/508	0.64	0/683
9	G	0.58	0/1138	0.94	1/1539 (0.1%)
10	H	0.55	0/1007	0.88	1/1352 (0.1%)
11	I	0.73	1/1081 (0.1%)	1.12	6/1448 (0.4%)
12	J	0.68	1/1113 (0.1%)	0.95	1/1486 (0.1%)
13	K	0.77	2/886 (0.2%)	1.02	3/1188 (0.3%)
14	L	0.53	0/785	0.88	1/1048 (0.1%)
15	M	0.64	0/884	0.98	1/1186 (0.1%)
16	N	0.51	0/994	0.77	0/1323
17	O	0.52	0/750	0.95	1/1000 (0.1%)
18	P	0.56	0/1027	0.85	0/1373
19	Q	0.60	0/737	1.03	5/988 (0.5%)
20	R	0.61	0/835	0.99	0/1121
21	S	0.48	0/1370	0.73	0/1862
22	T	0.55	0/633	0.82	0/838
23	U	0.75	0/556	1.10	1/741 (0.1%)
24	V	0.47	0/537	0.71	0/714
25	W	0.48	0/426	0.81	0/568
26	Z	0.62	0/469	0.97	0/629
30	4	0.44	0/298	0.62	0/390
All	All	0.91	50/91184 (0.1%)	1.69	2070/137069 (1.5%)

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	X	0	6

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1688	U	C4-O4	9.12	1.30	1.23
1	X	774	A	C5-C4	8.90	1.45	1.38
1	X	1685	A	C3'-O3'	7.74	1.52	1.42
1	X	1468	A	N9-C4	7.70	1.42	1.37
1	X	1333	G	N9-C4	-7.09	1.32	1.38

The worst 5 of 2070 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1631	C	C1'-O4'-C4'	-33.72	82.92	109.90
1	X	1288	A	C1'-O4'-C4'	-32.93	83.55	109.90
1	X	1288	A	C5'-C4'-O4'	20.68	133.91	109.10
1	X	1288	A	O4'-C1'-N9	20.52	124.61	108.20
1	X	1019	U	P-O3'-C3'	19.59	143.21	119.70

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1143	A	Sidechain
1	X	474	G	Sidechain
1	X	671	A	Sidechain
1	X	683	A	Sidechain
1	X	805	G	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	X	57651	0	29049	404	0
2	Y	2598	0	1328	17	0
3	A	1826	0	1885	61	0
4	B	1539	0	1600	61	0
5	C	1506	0	1525	49	0
6	D	1400	0	1481	22	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	68	0
10	H	997	0	1046	31	0
11	I	1067	0	1103	37	0
12	J	1090	0	1125	36	0
13	K	878	0	930	36	0
14	L	779	0	820	25	0
15	M	871	0	894	25	0
16	N	978	0	1020	33	0
17	O	741	0	756	34	0
18	P	1014	0	1096	20	0
19	Q	726	0	753	15	0
20	R	825	0	881	27	0
21	S	1345	0	1372	18	0
22	T	625	0	655	11	0
23	U	552	0	604	26	0
24	V	533	0	558	5	0
25	W	424	0	470	8	0
26	Z	457	0	462	12	0
27	1	53	0	0	1	0
28	2	46	0	0	2	0
29	3	63	0	0	3	0
30	4	297	0	330	5	0
31	J	1	0	0	0	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	5	0	0	0	0
32	X	56	0	64	3	0
All	All	83875	0	54807	954	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 7.

The worst 5 of 954 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:M:57:ILE:CD1	15:M:57:ILE:CG1	1.79	1.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.95	1.45
11:I:57:ILE:CD1	11:I:57:ILE:CG1	1.92	1.45
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.66	1.08
11:I:62:LYS:HE2	11:I:64:GLY:HA2	1.34	1.03

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	
3	A	238/274 (87%)	178 (75%)	39 (16%)	21 (9%)	1	8
4	B	203/211 (96%)	171 (84%)	24 (12%)	8 (4%)	5	33
5	C	195/205 (95%)	129 (66%)	45 (23%)	21 (11%)	1	5
6	D	175/180 (97%)	141 (81%)	27 (15%)	7 (4%)	5	32
7	E	169/185 (91%)	139 (82%)	20 (12%)	10 (6%)	2	20
8	F	69/144 (48%)	57 (83%)	10 (14%)	2 (3%)	7	43
9	G	140/174 (80%)	105 (75%)	21 (15%)	14 (10%)	1	6
10	H	132/134 (98%)	115 (87%)	11 (8%)	6 (4%)	4	29
11	I	139/156 (89%)	85 (61%)	28 (20%)	26 (19%)	0	0
12	J	134/141 (95%)	101 (75%)	19 (14%)	14 (10%)	1	5
13	K	111/116 (96%)	92 (83%)	11 (10%)	8 (7%)	2	13
14	L	102/114 (90%)	75 (74%)	19 (19%)	8 (8%)	1	11
15	M	106/166 (64%)	89 (84%)	13 (12%)	4 (4%)	5	34
16	N	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	3	25
17	O	92/100 (92%)	67 (73%)	13 (14%)	12 (13%)	0	3
18	P	125/134 (93%)	108 (86%)	12 (10%)	5 (4%)	5	32
19	Q	91/95 (96%)	64 (70%)	14 (15%)	13 (14%)	0	2
20	R	108/115 (94%)	66 (61%)	24 (22%)	18 (17%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	173/237 (73%)	135 (78%)	28 (16%)	10 (6%)	3	21
22	T	82/91 (90%)	64 (78%)	11 (13%)	7 (8%)	1	9
23	U	70/81 (86%)	43 (61%)	16 (23%)	11 (16%)	0	1
24	V	64/67 (96%)	58 (91%)	4 (6%)	2 (3%)	7	41
25	W	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
26	Z	56/60 (93%)	48 (86%)	5 (9%)	3 (5%)	3	24
30	4	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	7	43
All	All	2977/3390 (88%)	2303 (77%)	437 (15%)	237 (8%)	1	10

5 of 237 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	56	GLY
3	A	89	SER
3	A	198	ASN
3	A	199	ALA
3	A	249	PRO

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	
3	A	185/215 (86%)	151 (82%)	34 (18%)	2	11
4	B	155/157 (99%)	128 (83%)	27 (17%)	3	13
5	C	157/163 (96%)	120 (76%)	37 (24%)	1	4
6	D	153/156 (98%)	133 (87%)	20 (13%)	6	28
7	E	136/144 (94%)	125 (92%)	11 (8%)	17	56
8	F	51/107 (48%)	49 (96%)	2 (4%)	43	84
9	G	118/146 (81%)	93 (79%)	25 (21%)	1	8
10	H	103/103 (100%)	87 (84%)	16 (16%)	4	17
11	I	108/121 (89%)	76 (70%)	32 (30%)	0	1
12	J	110/115 (96%)	88 (80%)	22 (20%)	2	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	K	90/93 (97%)	68 (76%)	22 (24%)	1	3
14	L	74/82 (90%)	56 (76%)	18 (24%)	1	3
15	M	94/134 (70%)	66 (70%)	28 (30%)	0	1
16	N	96/97 (99%)	81 (84%)	15 (16%)	4	17
17	O	75/79 (95%)	57 (76%)	18 (24%)	1	4
18	P	109/115 (95%)	89 (82%)	20 (18%)	2	12
19	Q	75/76 (99%)	62 (83%)	13 (17%)	3	13
20	R	91/96 (95%)	70 (77%)	21 (23%)	1	5
21	S	149/192 (78%)	130 (87%)	19 (13%)	6	28
22	T	62/67 (92%)	53 (86%)	9 (14%)	5	22
23	U	57/66 (86%)	37 (65%)	20 (35%)	0	0
24	V	54/55 (98%)	46 (85%)	8 (15%)	4	20
25	W	48/48 (100%)	35 (73%)	13 (27%)	1	2
26	Z	51/53 (96%)	39 (76%)	12 (24%)	1	5
30	4	35/35 (100%)	31 (89%)	4 (11%)	8	35
All	All	2436/2715 (90%)	1970 (81%)	466 (19%)	2	11

5 of 466 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	45	SER
14	L	89	PHE
24	V	7	ARG
12	J	82	THR
13	K	51	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	31	GLN
17	O	88	GLN
26	Z	29	ASN
16	N	91	ASN
18	P	78	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	672 (25%)	252 (9%)
2	Y	121/123 (98%)	26 (21%)	7 (5%)
All	All	2804/3003 (93%)	698 (24%)	259 (9%)

5 of 698 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	34	U
1	X	45	C
1	X	48	A

5 of 259 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1142	G
1	X	1442	C
1	X	2738	A
1	X	1186	G
1	X	1333	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 35 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	$\# Z > 2$
32	1F2	X	2929	-	60,60,60	1.94	14 (23%)	90,90,90	2.53	33 (36%)

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
32	1F2	X	2929	-	-	0/74/115/115	0/3/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F2	C30-N29	8.88	1.46	1.33
32	X	2929	1F2	C8-C10	4.10	1.59	1.52
32	X	2929	1F2	O11-C12	-3.56	1.26	1.34
32	X	2929	1F2	C2-C5	-3.35	1.50	1.54
32	X	2929	1F2	C10-C9	-3.24	1.46	1.55

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F2	C25-C6-C5	-9.69	109.41	117.03
32	X	2929	1F2	C5-N29-C30	-9.13	103.55	112.50
32	X	2929	1F2	O1-C44-N45	7.46	119.70	111.02
32	X	2929	1F2	C24-C7-C6	-5.59	107.76	115.53
32	X	2929	1F2	C48-C47-N45	4.99	107.56	101.74

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 ⓘ

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	X	2686/2880 (93%)	-0.31	71 (2%) 53 11	43, 92, 197, 276	0
2	Y	122/123 (99%)	-0.18	2 (1%) 68 20	83, 136, 170, 192	0
3	A	240/274 (87%)	-0.01	1 (0%) 90 51	69, 116, 146, 173	0
4	B	205/211 (97%)	-0.23	0 100 100	45, 73, 106, 154	0
5	C	197/205 (96%)	0.04	5 (2%) 54 12	57, 114, 155, 187	0
6	D	177/180 (98%)	0.24	5 (2%) 50 11	146, 183, 216, 227	0
7	E	171/185 (92%)	-0.16	0 100 100	92, 143, 192, 206	0
8	F	71/144 (49%)	1.21	9 (12%) 4 1	211, 236, 252, 257	0
9	G	142/174 (81%)	-0.01	3 (2%) 60 15	73, 97, 145, 161	0
10	H	134/134 (100%)	-0.32	0 100 100	50, 70, 96, 120	0
11	I	141/156 (90%)	0.42	13 (9%) 9 2	67, 129, 174, 204	0
12	J	136/141 (96%)	0.02	2 (1%) 70 21	74, 103, 149, 184	0
13	K	113/116 (97%)	-0.31	0 100 100	35, 60, 79, 91	0
14	L	104/114 (91%)	0.16	4 (3%) 38 7	98, 134, 156, 169	0
15	M	108/166 (65%)	-0.29	0 100 100	50, 73, 111, 144	0
16	N	117/118 (99%)	-0.23	0 100 100	60, 90, 127, 160	0
17	O	94/100 (94%)	-0.20	0 100 100	67, 115, 156, 173	0
18	P	127/134 (94%)	-0.28	0 100 100	50, 67, 108, 158	0
19	Q	93/95 (97%)	-0.06	1 (1%) 77 27	73, 106, 162, 195	0
20	R	110/115 (95%)	0.05	2 (1%) 65 18	88, 117, 170, 178	0
21	S	175/237 (73%)	0.04	1 (0%) 86 41	121, 155, 175, 190	0
22	T	84/91 (92%)	0.22	5 (5%) 21 5	80, 108, 186, 199	0
23	U	72/81 (88%)	0.24	3 (4%) 35 7	92, 128, 153, 162	0
24	V	66/67 (98%)	0.28	4 (6%) 21 4	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	-0.29	0 100 100	81, 98, 126, 152	0
26	Z	58/60 (96%)	-0.18	1 (1%) 67 19	49, 71, 105, 113	0
27	1	53/55 (96%)	0.38	5 (9%) 9 2	8, 32, 61, 96	0
28	2	46/47 (97%)	2.13	25 (54%) 0 0	3, 16, 37, 59	0
29	3	63/66 (95%)	1.30	16 (25%) 1 1	3, 25, 40, 60	0
30	4	37/37 (100%)	4.29	34 (91%) 0 0	227, 254, 265, 269	0
All	All	5997/6561 (91%)	-0.08	212 (3%) 42 8	3, 100, 196, 276	0

The worst 5 of 212 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	24	LEU	12.1
27	1	7	ARG	9.0
30	4	25	VAL	8.9
30	4	17	VAL	8.7
24	V	1	MET	7.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
31	MG	X	2908	1/1	0.87	111.52	37,37,37,37	0
31	MG	X	2921	1/1	0.40	58.00	81,81,81,81	0
31	MG	X	2926	1/1	0.92	32.92	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
31	MG	Y	203	1/1	0.70	30.49	87,87,87,87	0
31	MG	X	2918	1/1	0.66	28.04	42,42,42,42	0
31	MG	X	2924	1/1	1.19	25.73	69,69,69,69	0
31	MG	X	2922	1/1	0.66	23.81	44,44,44,44	0
31	MG	X	2919	1/1	0.43	23.69	30,30,30,30	0
31	MG	X	2903	1/1	0.69	22.35	89,89,89,89	0
31	MG	X	2912	1/1	0.49	22.16	71,71,71,71	0
31	MG	X	2911	1/1	0.22	21.86	68,68,68,68	0
31	MG	X	2907	1/1	0.63	21.46	51,51,51,51	0
31	MG	Y	204	1/1	0.25	19.50	82,82,82,82	0
31	MG	X	2909	1/1	0.54	18.56	96,96,96,96	0
31	MG	X	2923	1/1	0.33	18.18	34,34,34,34	0
31	MG	M	201	1/1	0.51	18.17	23,23,23,23	0
31	MG	X	2928	1/1	0.47	17.77	62,62,62,62	0
31	MG	X	2913	1/1	0.57	17.22	61,61,61,61	0
31	MG	X	2915	1/1	0.59	17.16	57,57,57,57	0
31	MG	X	2917	1/1	0.52	16.51	55,55,55,55	0
31	MG	X	2916	1/1	0.60	16.49	37,37,37,37	0
31	MG	Y	202	1/1	0.51	16.30	58,58,58,58	0
31	MG	Y	201	1/1	0.77	13.50	89,89,89,89	0
31	MG	X	2910	1/1	0.44	13.08	42,42,42,42	0
31	MG	Y	205	1/1	0.35	12.06	79,79,79,79	0
31	MG	X	2901	1/1	0.36	11.30	50,50,50,50	0
31	MG	X	2927	1/1	0.53	11.22	62,62,62,62	0
31	MG	X	2902	1/1	0.70	10.73	94,94,94,94	0
31	MG	X	2906	1/1	0.37	9.00	58,58,58,58	0
31	MG	X	2925	1/1	0.45	7.65	122,122,122,122	0
31	MG	X	2904	1/1	0.30	7.37	107,107,107,107	0
31	MG	X	2905	1/1	0.25	6.78	65,65,65,65	0
31	MG	J	201	1/1	0.31	5.34	100,100,100,100	0
31	MG	X	2920	1/1	0.21	3.58	115,115,115,115	0
31	MG	X	2914	1/1	0.37	1.32	27,27,27,27	0
32	1F2	X	2929	56/56	0.19	-0.26	42,68,77,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.