wwPDB X-ray Structure Validation Summary Report (i)

Oct 6, 2024 – 01:31 AM EDT

PDB ID	:	2F4V
Title	:	30S ribosome + designer antibiotic
Authors	:	Murray, J.B.; Meroueh, S.O.; Russell, R.J.; Lentzen, G.; Haddad, J.; Mobashery, S.
Deposited on	:	2005-11-24
Resolution	:	3.80 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 (i) 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 (1)) were used in the production of this report:

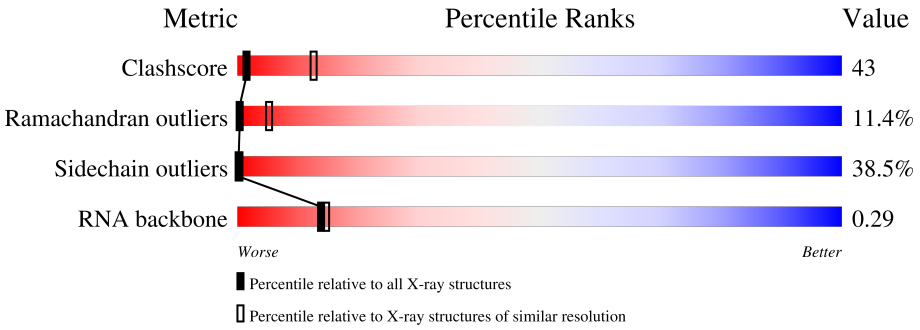
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.80 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	180529	1005 (3.96-3.64)
Ramachandran outliers	177936	1044 (3.98-3.62)
Sidechain outliers	177891	1039 (3.98-3.62)
RNA backbone	3690	1131 (4.60-3.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1511	11% 37% 36% 17%
2	Z	4	100%
3	B	256	20% 45% 24% • 7%
4	C	239	20% 37% 24% 5% 14%
5	D	209	21% 45% 28% 5%
6	E	162	20% 40% 31% • 7%

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Mol	Chain	Length	Quality of chain
7	F	101	36% 46% 19%
8	G	156	32% 44% 21%
9	H	138	33% 43% 20%
10	I	128	19% 48% 27% 5%
11	J	105	22% 32% 32% 7% 7%
12	K	129	27% 47% 16% 8%
13	L	132	20% 36% 31% 8% 5%
14	M	126	21% 44% 29% 6%
15	N	61	20% 43% 23% 13%
16	O	89	22% 49% 22%
17	P	88	20% 48% 22% 5% 6%
18	Q	105	25% 54% 17%
19	R	88	19% 39% 23% 17%
20	S	93	29% 40% 18% 10%
21	T	106	18% 51% 20% 5% 7%

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 51728 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	1507	32391	14418	6002	10465	1506	22	0	0

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Z	4	80	36	9	31	4	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	237	1923	1226	344	348	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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	199	GLN	ASN	conflict	UNP P80373
D	201	ASN	GLN	conflict	UNP P80373

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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			

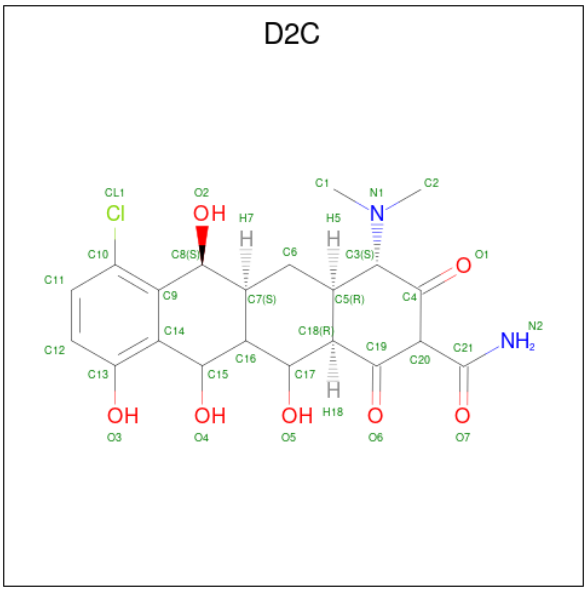
- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	98	Total	Mg	0	0
			98	98		
22	Z	1	Total	Mg	0	0
			1	1		
22	D	1	Total	Mg	0	0
			1	1		
22	M	1	Total	Mg	0	0
			1	1		

- Molecule 23 is POTASSIUM ION (three-letter code: K) (formula: K).

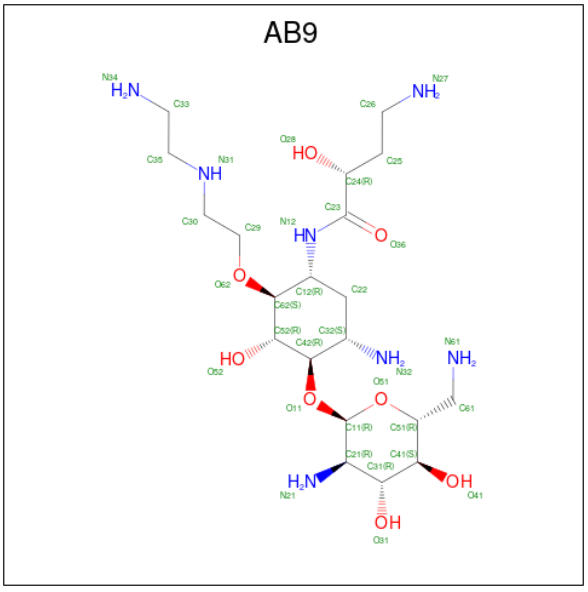
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	12	Total	K	0	0
			12	12		

- Molecule 24 is (2S,4S,4AR,5AS,6S,11R,11AS,12R,12AR)-7-CHLORO-4-(DIMETHYLAMINO)-6,10,11,12-TETRAHYDROXY-1,3-DIOXO-1,2,3,4,4A,5,5A,6,11,11A,12,12A-DODECAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: D2C) (formula: $C_{21}H_{25}ClN_2O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Cl	N	O	0	0
			31	21	1	2	7		

- Molecule 25 is (2R)-4-AMINO-N-{(1R,2S,3R,4R,5S)-5-AMINO-2-{2-[(2-AMINOETHYL)AMINO]ETHOXY}-4-[(2,6-DIAMINO-2,6-DIDEOXY-ALPHA-D-GLUCOPYRANOSYL)OXY]-3-HYDROXYCYCLOHEXYL}-2-HYDROXYBUTANAMIDE (three-letter code: AB9) (formula: $C_{20}H_{43}N_7O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			35	20	7	8		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

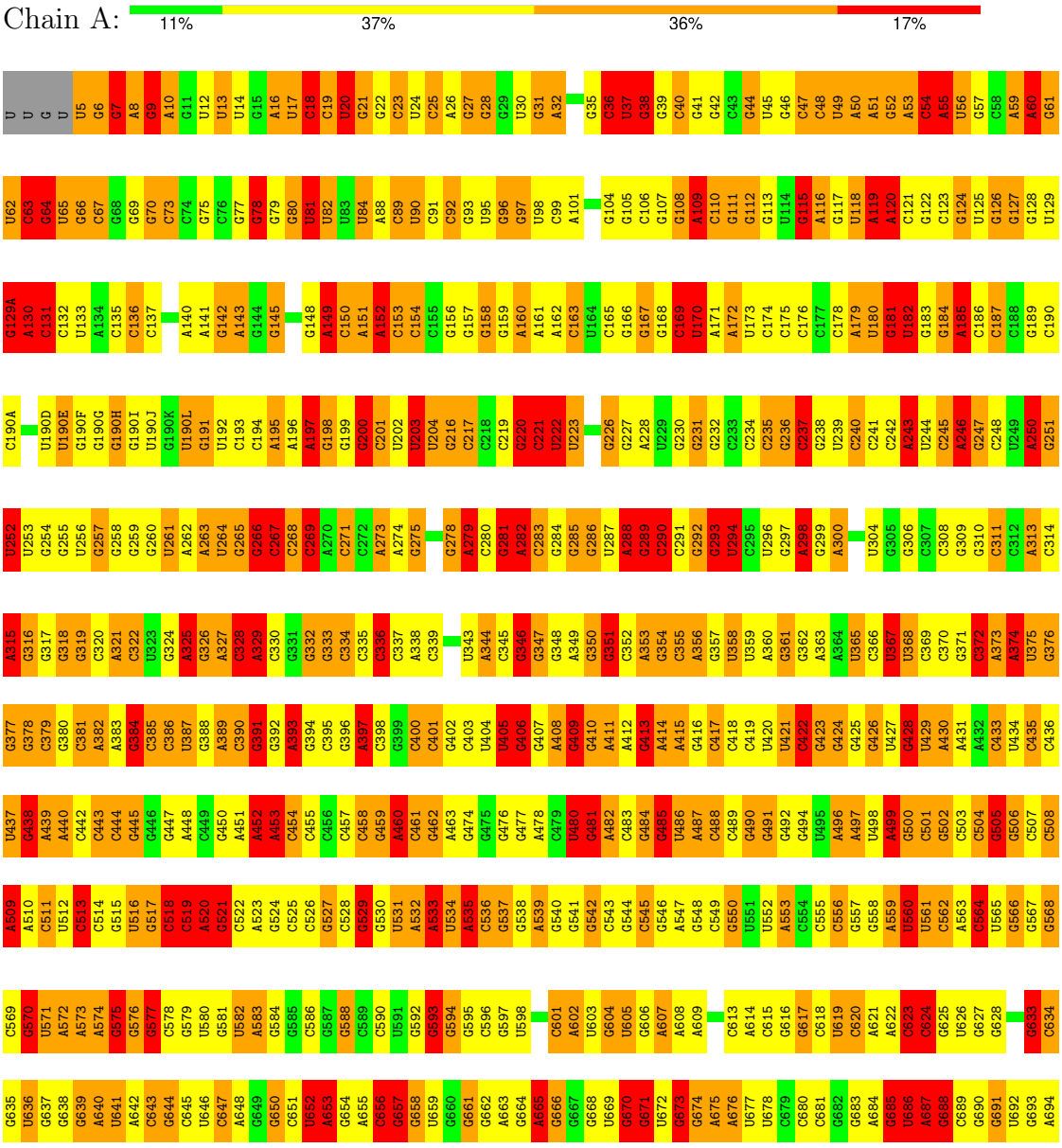
3 Residue-property plots (i)

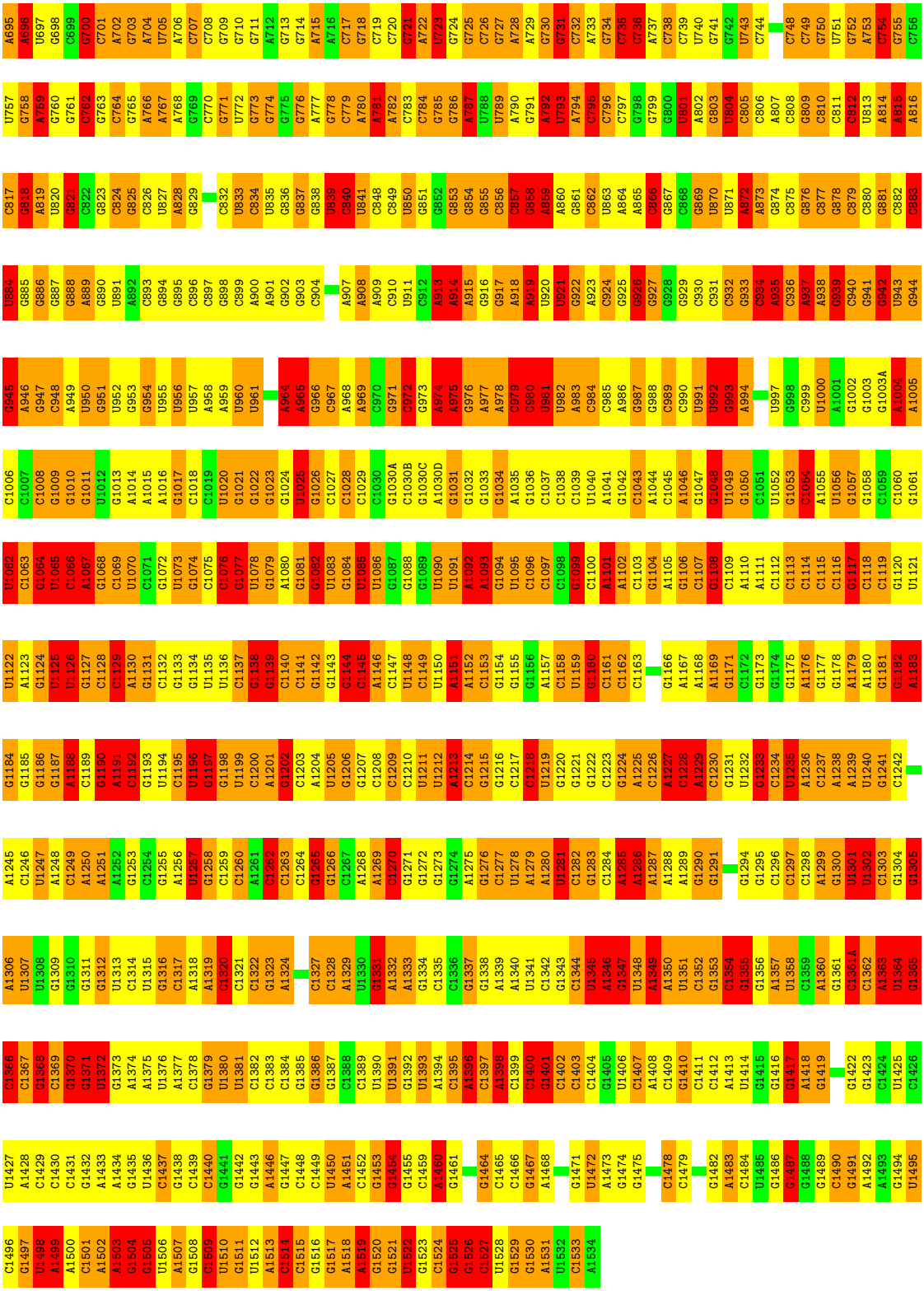
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: 16S ribosomal RNA

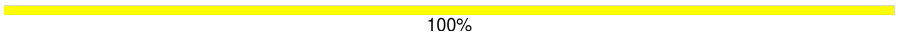
Chain A:





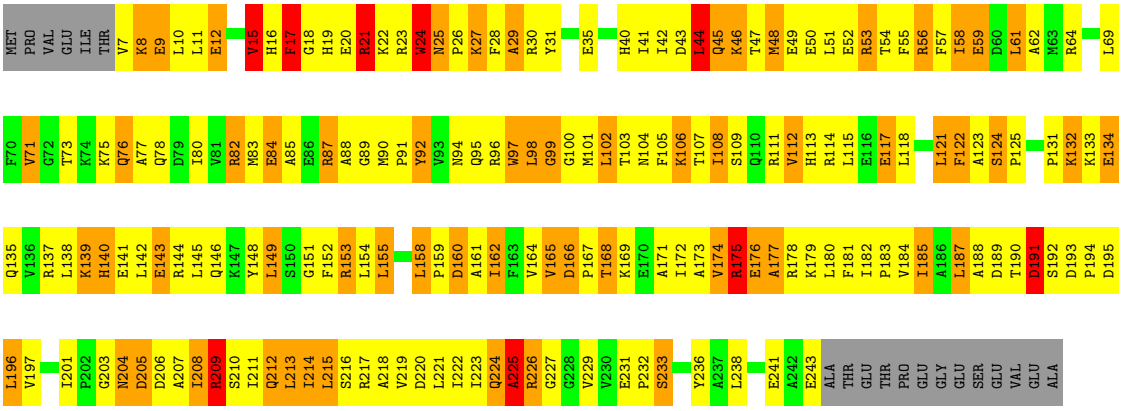
• Molecule 2: 5'-R(P*UP*UP*CP*U)-3'

Chain Z:



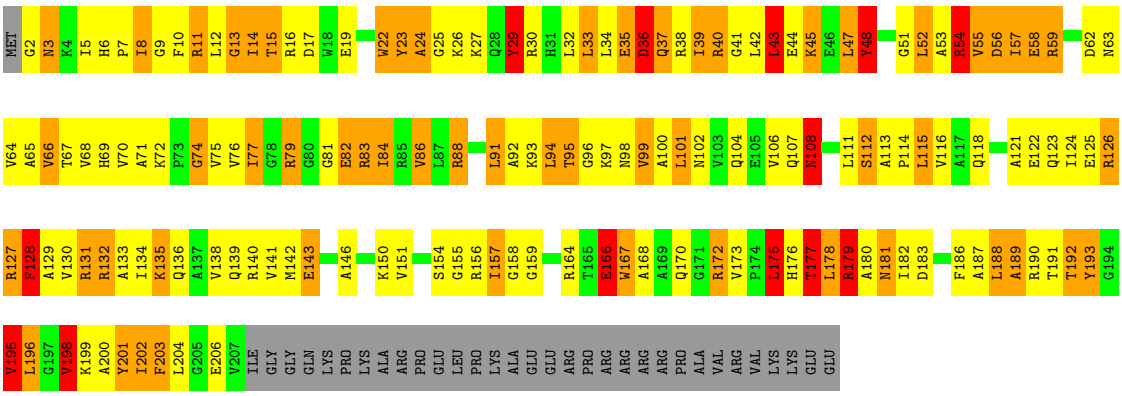
• Molecule 3: 30S ribosomal protein S2

Chain B:



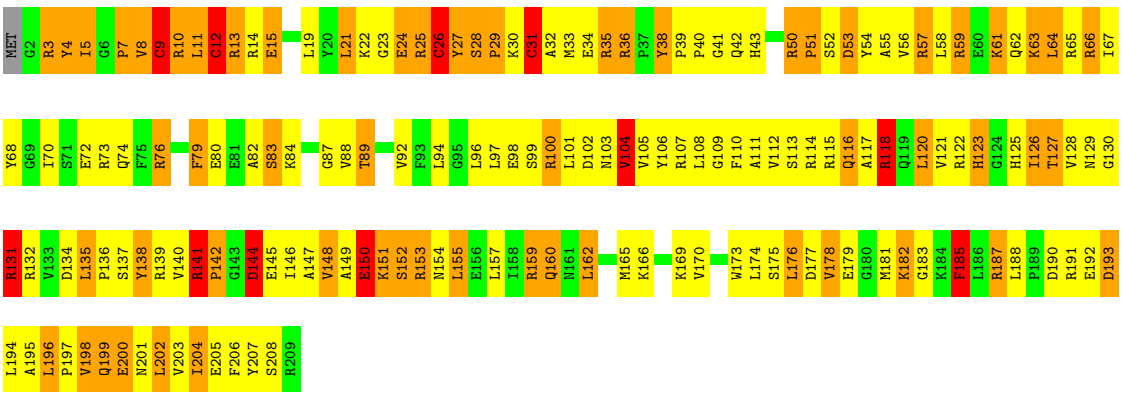
• Molecule 4: 30S ribosomal protein S3

Chain C:



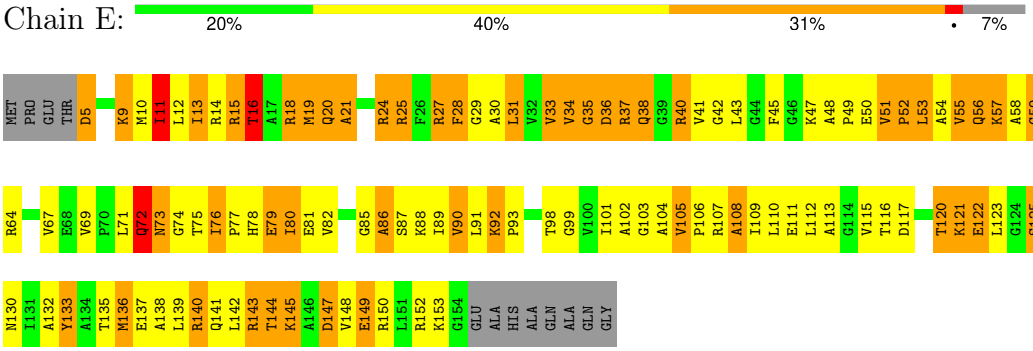
• Molecule 5: 30S ribosomal protein S4

Chain D:



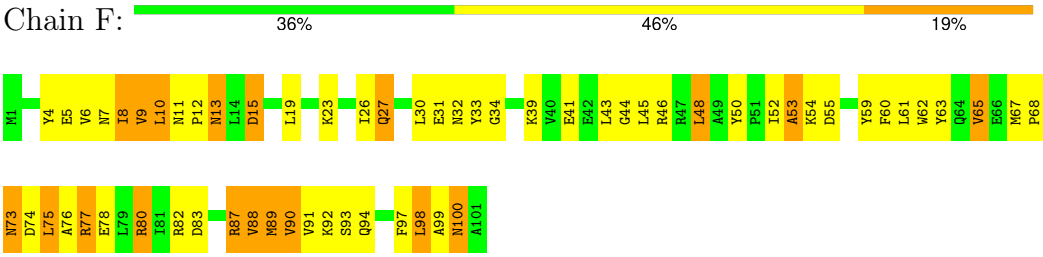
• Molecule 6: 30S ribosomal protein S5

Chain E:



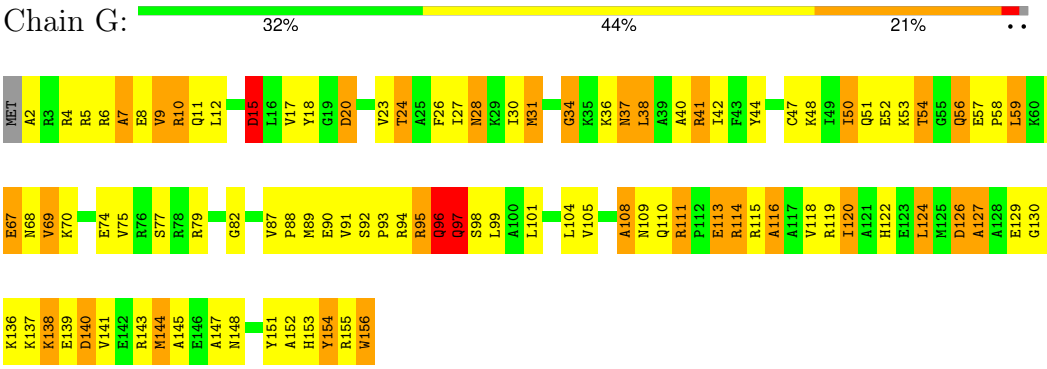
• Molecule 7: 30S ribosomal protein S6

Chain F:



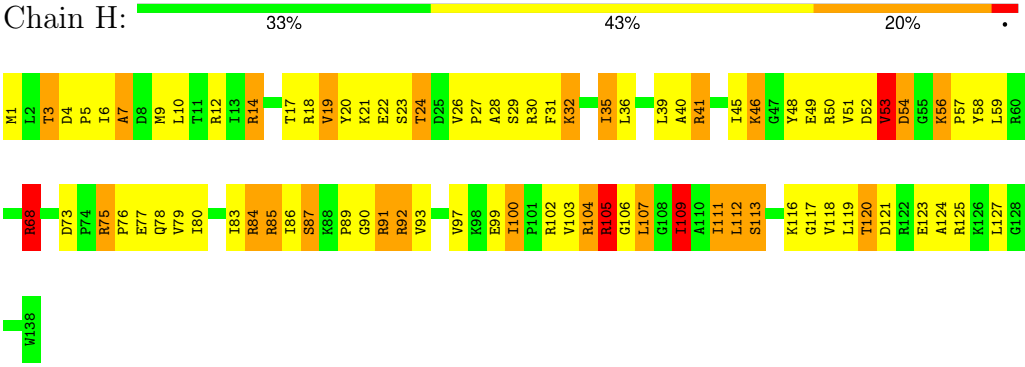
• Molecule 8: 30S ribosomal protein S7

Chain G:



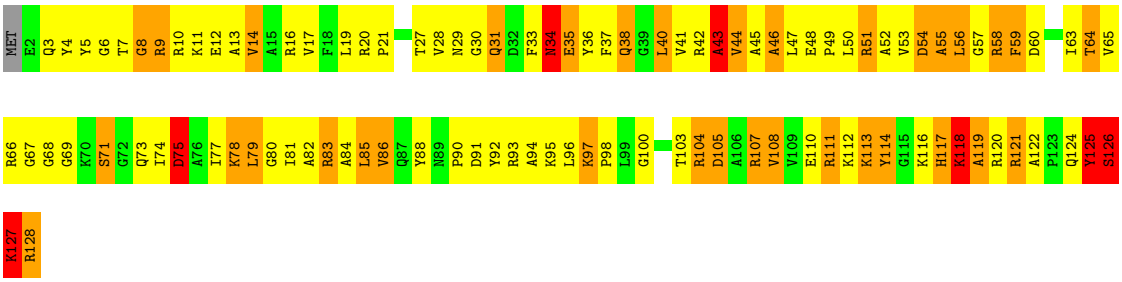
• Molecule 9: 30S ribosomal protein S8

Chain H:



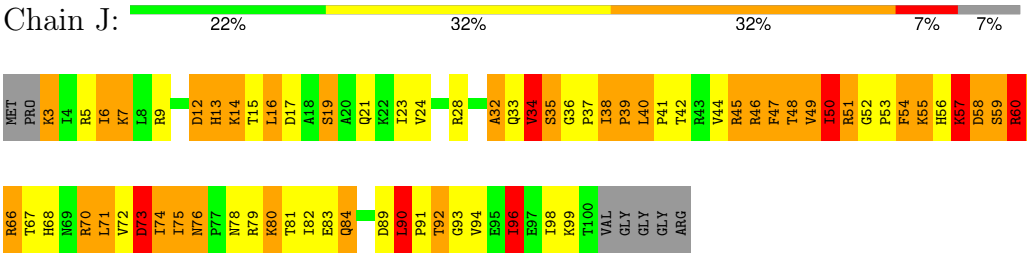
• Molecule 10: 30S ribosomal protein S9

Chain I:



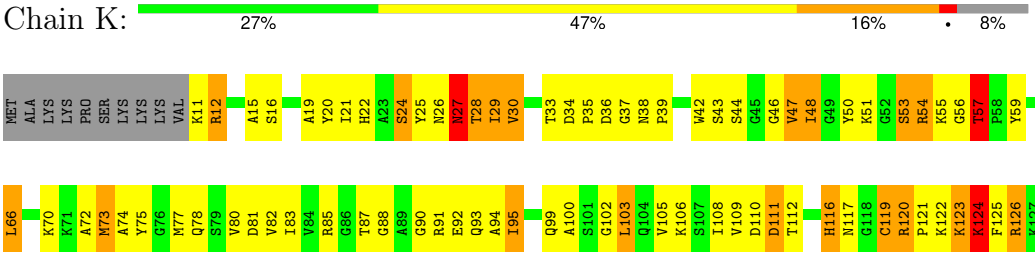
• Molecule 11: 30S ribosomal protein S10

Chain J:



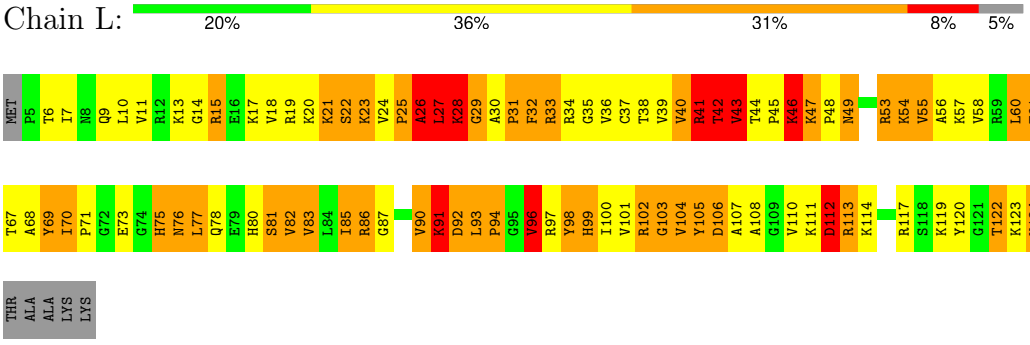
• Molecule 12: 30S ribosomal protein S11

Chain K:



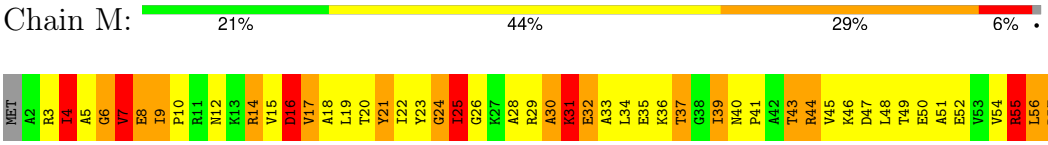
• Molecule 13: 30S ribosomal protein S12

Chain L:



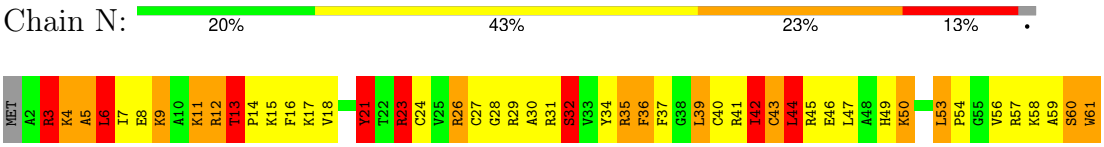
• Molecule 14: 30S ribosomal protein S13

Chain M:



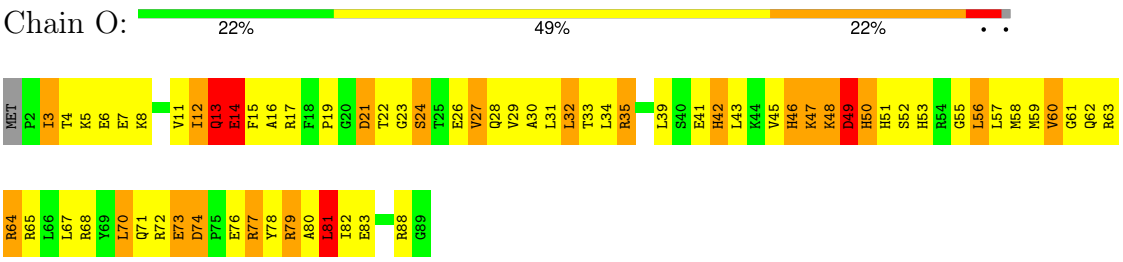
• Molecule 15: 30S ribosomal protein S14

Chain N:



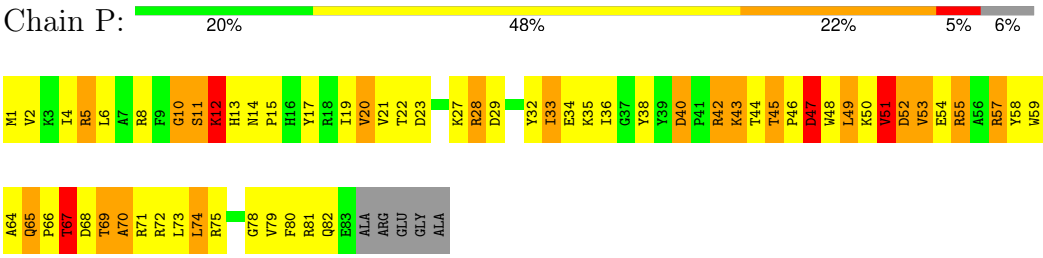
• Molecule 16: 30S ribosomal protein S15

Chain O:



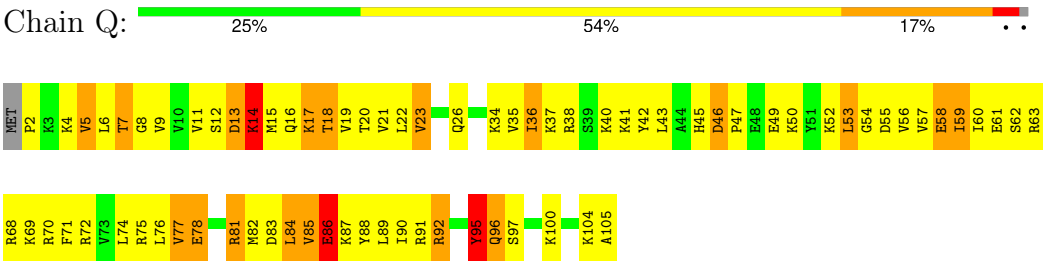
• Molecule 17: 30S ribosomal protein S16

Chain P:



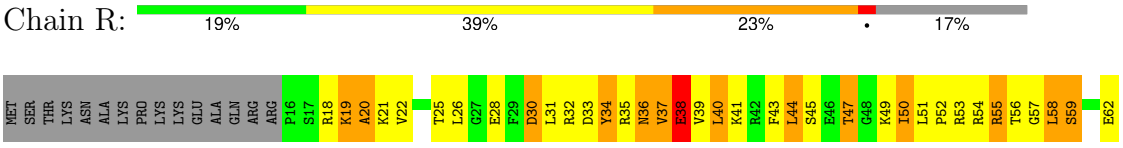
• Molecule 18: 30S ribosomal protein S17

Chain Q:



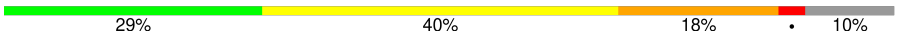
• Molecule 19: 30S ribosomal protein S18

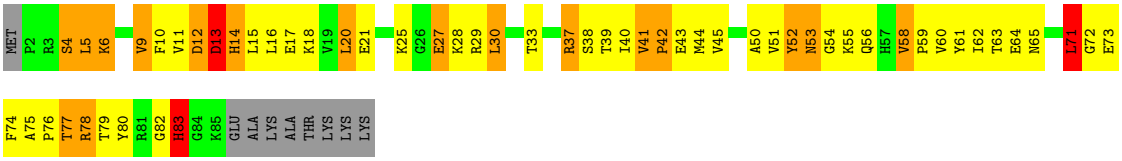
Chain R:



• Molecule 20: 30S ribosomal protein S19

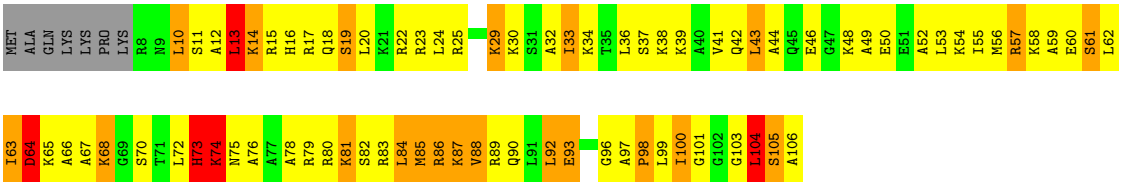
Chain S:





• Molecule 21: 30S ribosomal protein S20

Chain T:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	403.32Å 403.32Å 176.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80	Depositor
% Data completeness (in resolution range)	97.2 (30.00-3.80)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.259 , 0.315	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51728	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, AB9, D2C, MG, 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	1.70	440/36247 (1.2%)	1.64	607/56545 (1.1%)
2	Z	2.01	1/87 (1.1%)	1.60	0/132
3	B	0.84	1/1958 (0.1%)	0.69	5/2640 (0.2%)
4	C	0.91	1/1636 (0.1%)	0.66	3/2205 (0.1%)
5	D	0.81	1/1733 (0.1%)	0.66	5/2318 (0.2%)
6	E	1.14	1/1162 (0.1%)	0.75	3/1564 (0.2%)
7	F	0.73	0/856	0.65	2/1154 (0.2%)
8	G	0.89	1/1276 (0.1%)	0.64	4/1709 (0.2%)
9	H	1.18	1/1136 (0.1%)	0.80	2/1527 (0.1%)
10	I	0.79	0/1029	0.67	5/1378 (0.4%)
11	J	0.81	1/805 (0.1%)	0.75	3/1082 (0.3%)
12	K	0.99	0/900	0.73	2/1213 (0.2%)
13	L	0.87	0/991	0.67	3/1327 (0.2%)
14	M	0.87	1/1008 (0.1%)	0.69	3/1347 (0.2%)
15	N	0.86	0/501	0.63	0/664
16	O	0.88	0/745	0.67	3/992 (0.3%)
17	P	1.16	1/716 (0.1%)	0.82	2/963 (0.2%)
18	Q	1.01	0/870	0.71	3/1159 (0.3%)
19	R	0.92	0/603	0.72	1/799 (0.1%)
20	S	0.70	0/689	0.66	2/926 (0.2%)
21	T	1.07	0/764	0.68	0/1006
All	All	1.47	450/55712 (0.8%)	1.41	658/82650 (0.8%)

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
3	B	0	2
4	C	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	D	0	6
6	E	0	5
7	F	0	1
9	H	0	5
10	I	0	4
11	J	0	6
12	K	0	5
13	L	0	8
14	M	0	4
15	N	0	8
17	P	0	4
18	Q	0	1
20	S	0	5
21	T	0	4
All	All	0	74

The worst 5 of 450 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1169	A	O3'-P	35.46	2.03	1.61
1	A	1227	A	N9-C4	-13.10	1.29	1.37
1	A	1346	A	C3'-O3'	11.14	1.57	1.42
1	A	1224	G	C3'-O3'	10.61	1.57	1.42
1	A	1129	C	C1'-N1	10.46	1.64	1.48

The worst 5 of 658 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1169	A	P-O3'-C3'	29.86	155.53	119.70
1	A	1525	G	C4'-C3'-C2'	-12.91	89.69	102.60
1	A	1346	A	P-O3'-C3'	11.99	134.09	119.70
1	A	1345	U	C1'-O4'-C4'	-11.81	100.45	109.90
1	A	1025	U	C1'-O4'-C4'	-11.60	100.62	109.90

There are no chirality outliers.

5 of 74 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	133	LYS	Peptide
3	B	225	ALA	Peptide
4	C	13	GLY	Peptide

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Mol	Chain	Res	Type	Group
4	C	166	GLU	Peptide
4	C	48	TYR	Peptide

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	32391	0	16359	1894	0
2	Z	80	0	42	4	0
3	B	1923	0	1968	218	0
4	C	1612	0	1677	175	0
5	D	1703	0	1763	198	0
6	E	1146	0	1207	161	0
7	F	843	0	857	58	0
8	G	1257	0	1296	105	0
9	H	1116	0	1177	93	0
10	I	1011	0	1043	122	0
11	J	792	0	835	125	0
12	K	885	0	904	80	0
13	L	975	0	1062	129	0
14	M	997	0	1072	111	0
15	N	492	0	530	84	0
16	O	734	0	771	70	0
17	P	700	0	720	72	0
18	Q	857	0	930	70	0
19	R	597	0	668	68	0
20	S	674	0	699	56	0
21	T	762	0	859	97	0
22	A	98	0	0	0	0
22	D	1	0	0	0	0
22	M	1	0	0	0	0
22	Z	1	0	0	0	0
23	A	12	0	0	0	0
24	A	31	0	19	4	0
25	A	35	0	43	1	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	51728	0	36501	3715	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 43.

The worst 5 of 3715 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)
8:G:89:MET:CE	8:G:89:MET:SD	2.02	1.45
1:A:492:G:H3'	1:A:494:G:OP2	1.29	1.32
6:E:80:ILE:CD1	6:E:91:LEU:HB2	1.62	1.29
1:A:70:G:H3'	1:A:73:C:P	1.72	1.27
15:N:40:CYS:O	15:N:43:CYS:HB2	1.23	1.27

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	235/256 (92%)	153 (65%)	48 (20%)	34 (14%)	0 3
4	C	204/239 (85%)	120 (59%)	51 (25%)	33 (16%)	0 2
5	D	206/209 (99%)	145 (70%)	37 (18%)	24 (12%)	0 5
6	E	148/162 (91%)	110 (74%)	24 (16%)	14 (10%)	0 8
7	F	99/101 (98%)	76 (77%)	17 (17%)	6 (6%)	1 15
8	G	153/156 (98%)	103 (67%)	36 (24%)	14 (9%)	0 9
9	H	136/138 (99%)	103 (76%)	26 (19%)	7 (5%)	1 17
10	I	125/128 (98%)	79 (63%)	33 (26%)	13 (10%)	0 7
11	J	96/105 (91%)	63 (66%)	20 (21%)	13 (14%)	0 3
12	K	117/129 (91%)	79 (68%)	25 (21%)	13 (11%)	0 6
13	L	123/132 (93%)	76 (62%)	29 (24%)	18 (15%)	0 3
14	M	123/126 (98%)	75 (61%)	31 (25%)	17 (14%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	N	58/61 (95%)	43 (74%)	8 (14%)	7 (12%)	0 5
16	O	86/89 (97%)	56 (65%)	22 (26%)	8 (9%)	0 9
17	P	81/88 (92%)	55 (68%)	17 (21%)	9 (11%)	0 6
18	Q	102/105 (97%)	73 (72%)	21 (21%)	8 (8%)	1 11
19	R	71/88 (81%)	50 (70%)	14 (20%)	7 (10%)	0 7
20	S	82/93 (88%)	58 (71%)	17 (21%)	7 (8%)	0 9
21	T	97/106 (92%)	60 (62%)	21 (22%)	16 (16%)	0 2
All	All	2342/2511 (93%)	1577 (67%)	497 (21%)	268 (11%)	0 5

5 of 268 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	17	PHE
3	B	29	ALA
3	B	99	GLY
3	B	106	LYS
3	B	131	PRO

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	204/220 (93%)	125 (61%)	79 (39%)	0 0
4	C	160/188 (85%)	90 (56%)	70 (44%)	0 0
5	D	180/181 (99%)	105 (58%)	75 (42%)	0 0
6	E	115/123 (94%)	70 (61%)	45 (39%)	0 0
7	F	90/90 (100%)	63 (70%)	27 (30%)	0 1
8	G	126/127 (99%)	80 (64%)	46 (36%)	0 0
9	H	119/119 (100%)	78 (66%)	41 (34%)	0 1
10	I	98/99 (99%)	61 (62%)	37 (38%)	0 0
11	J	87/92 (95%)	51 (59%)	36 (41%)	0 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	K	90/99 (91%)	62 (69%)	28 (31%)	0 1
13	L	104/109 (95%)	53 (51%)	51 (49%)	0 0
14	M	100/101 (99%)	59 (59%)	41 (41%)	0 0
15	N	49/50 (98%)	26 (53%)	23 (47%)	0 0
16	O	79/80 (99%)	48 (61%)	31 (39%)	0 0
17	P	72/74 (97%)	45 (62%)	27 (38%)	0 0
18	Q	96/97 (99%)	69 (72%)	27 (28%)	0 2
19	R	64/77 (83%)	37 (58%)	27 (42%)	0 0
20	S	73/80 (91%)	47 (64%)	26 (36%)	0 0
21	T	76/82 (93%)	50 (66%)	26 (34%)	0 1
All	All	1982/2088 (95%)	1219 (62%)	763 (38%)	0 0

5 of 763 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	30	VAL
14	M	121	LYS
12	K	93	GLN
12	K	29	ILE
13	L	85	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	99	HIS
20	S	65	ASN
14	M	40	ASN
18	Q	16	GLN
21	T	73	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1494/1511 (98%)	656 (43%)	162 (10%)
2	Z	3/4 (75%)	0	0
All	All	1497/1515 (98%)	656 (43%)	162 (10%)

5 of 656 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	16	A

5 of 162 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1192	C
1	A	1337	G
1	A	1212	U
1	A	1263	C
1	A	1396	A

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 117 ligands modelled in this entry, 115 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	$\#\|Z\| > 2$
24	D2C	A	1636	22	31,34,34	4.34	11 (35%)	37,54,54	2.47	16 (43%)
25	AB9	A	1637	-	35,36,36	2.20	3 (8%)	43,49,49	1.65	3 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	D2C	A	1636	22	-	6/6/64/64	0/4/4/4
25	AB9	A	1637	-	-	11/24/64/64	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1636	D2C	C16-C15	-15.94	1.40	1.53
24	A	1636	D2C	C16-C17	-12.35	1.37	1.53
25	A	1637	AB9	O36-C23	10.63	1.43	1.23
24	A	1636	D2C	C18-C5	-7.06	1.44	1.54
24	A	1636	D2C	C14-C15	-6.64	1.43	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1637	AB9	O36-C23-N12	-7.27	109.94	122.96
25	A	1637	AB9	O36-C23-C24	-6.29	111.32	120.61
24	A	1636	D2C	O5-C17-C18	5.18	121.55	109.80
24	A	1636	D2C	O4-C15-C14	5.09	122.53	110.56
24	A	1636	D2C	C18-C17-C16	4.88	118.55	110.45

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1636	D2C	C4-C3-N1-C1
24	A	1636	D2C	C5-C3-N1-C1
24	A	1636	D2C	C4-C3-N1-C2
24	A	1636	D2C	C4-C20-C21-O7
24	A	1636	D2C	C19-C20-C21-O7

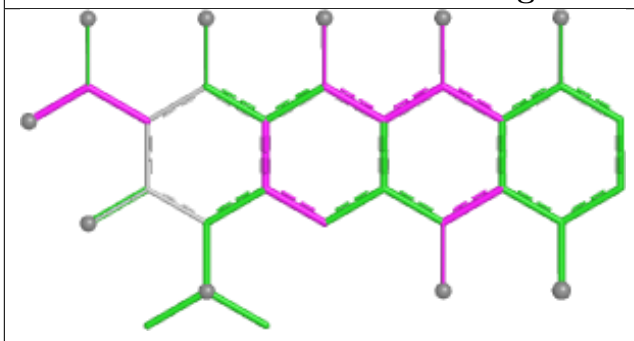
There are no ring outliers.

2 monomers are involved in 5 short contacts:

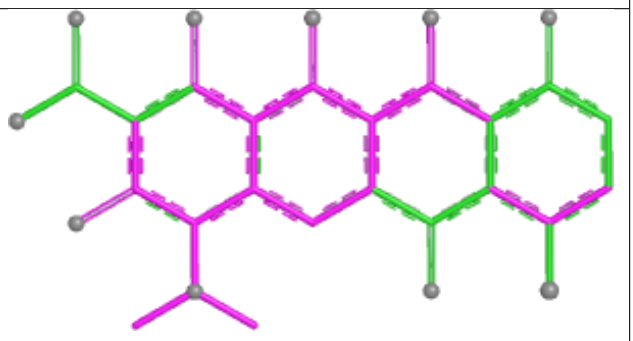
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1636	D2C	4	0
25	A	1637	AB9	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

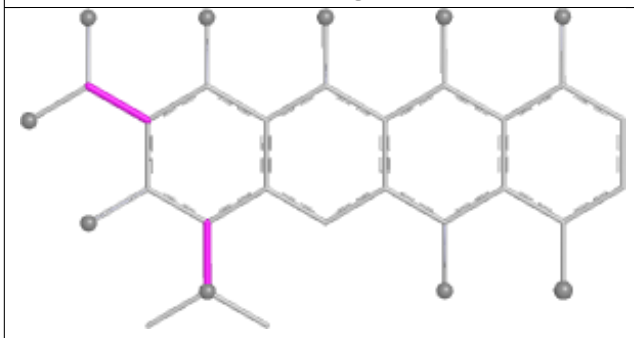
Ligand D2C A 1636



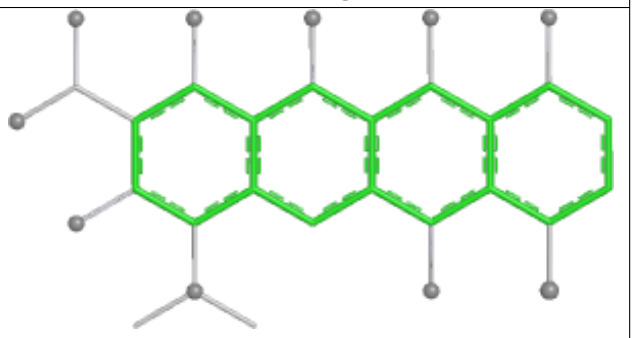
Bond lengths



Bond angles

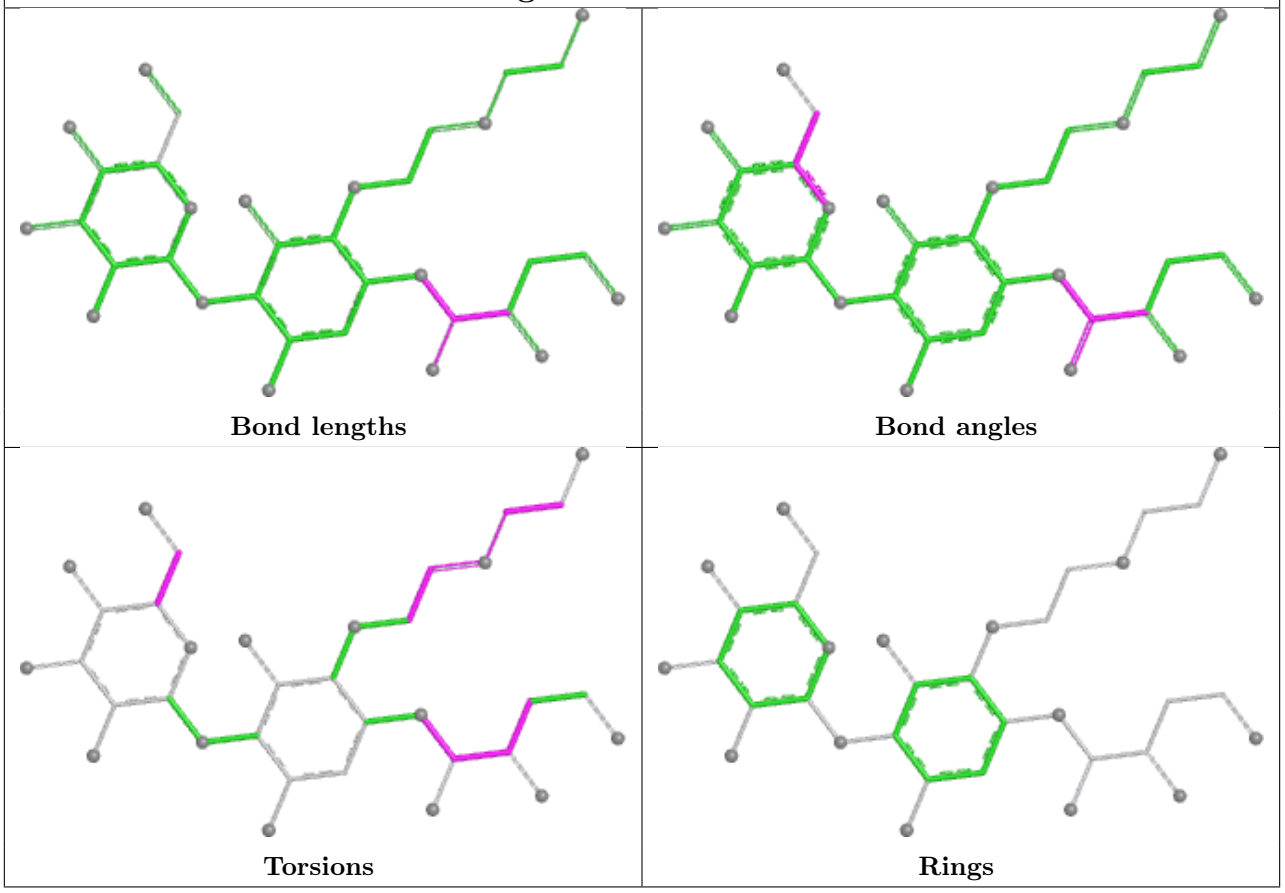


Torsions



Rings

Ligand AB9 A 1637



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	13

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	841:U	O3'	848:C	P	5.02
1	A	84:U	O3'	88:A	P	3.79
1	A	1533:C	O3'	1534:A	P	3.45
1	A	70:G	O3'	73:C	P	3.36
1	A	204:U	O3'	216:G	P	3.36

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.