wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 06:25 am GMT

PDB ID	:	5NRG
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with RB02
Authors	:	Yonath, A.; Matzov, D.; Eyal, Z.; Ben Hamou, R.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Fridman, M.
Deposited on	:	2017-04-23
Resolution	:	3.44 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 (i)) were used in the production of this report:

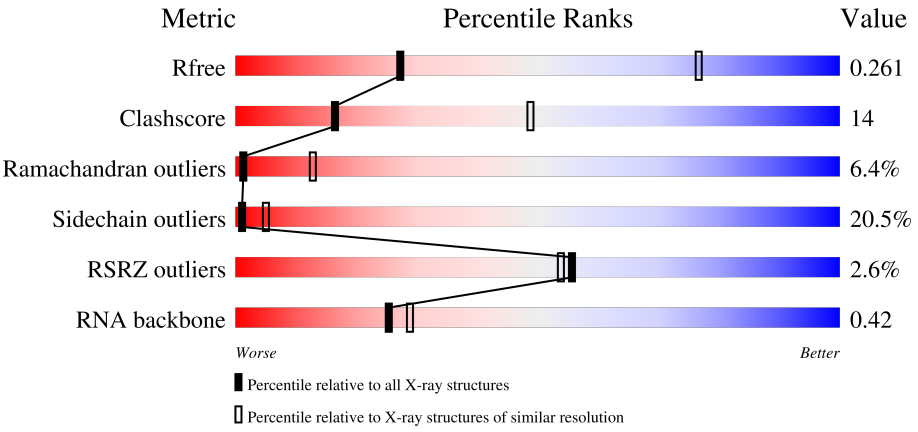
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.44 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}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

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% 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	X	2923	34% 38% 18% 7%
2	Y	114	2% 42% 39% 18%
3	A	277	4% 51% 33% 10% 6%

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Mol	Chain	Length	Quality of chain
4	B	220	57% 34% 7%
5	C	207	43% 37% 16%
6	D	179	18% 51% 18% 7% 23%
7	E	178	5% 54% 24% 5% 17%
8	G	145	55% 36% 7%
9	H	122	50% 40% 10%
10	I	140	5% 44% 35% 12% 9%
11	J	144	62% 28% 6%
12	K	122	52% 39% 7%
13	L	119	8% 67% 21% 8%
14	M	116	56% 31% 9%
15	N	118	57% 33% 8%
16	O	102	54% 32% 13%
17	P	117	53% 38%
18	Q	91	10% 49% 38% 11%
19	R	105	10% 58% 30% 9%
20	S	217	6% 45% 30% 6% 20%
21	T	94	56% 21% 19%
22	V	69	41% 38% 16% 6%
23	W	59	49% 41% 7%
24	Z	58	38% 31% 7% 24%
25	2	45	16% 56% 33% 9%
26	3	66	74% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	MN	X	3062	-	-	-	X
29	MN	X	3075	-	-	-	X
30	MG	3	104	-	-	-	X
30	MG	J	201	-	-	-	X
30	MG	X	3202	-	-	-	X
30	MG	X	3242	-	-	-	X
30	MG	X	3260	-	-	-	X
30	MG	X	3264	-	-	-	X
30	MG	X	3266	-	-	-	X
30	MG	X	3271	-	-	-	X
30	MG	X	3274	-	-	-	X
30	MG	X	3279	-	-	-	X
30	MG	X	3280	-	-	-	X
30	MG	X	3283	-	-	-	X

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 80800 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2710	58141	25956	10658	18816	2711	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	114	2430	1086	436	794	114	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	260	1641	1008	314	315	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	215	1534	961	287	281	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	198	1365	852	256	255	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	137	926	580	165	177	4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	147	Total	C	N	O	0	0	0
			793	481	154	158			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1062	664	194	201	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			902	561	173	166	2			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	0	0	0
			780	467	162	151			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1011	651	184	172	4			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			883	539	176	167	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			672	410	126	136			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	111	Total 779	C 492	N 147	O 140	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total 937	C 590	N 186	O 157	S 4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	101	Total 700	C 445	N 128	O 127	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total 852	C 532	N 161	O 156	S 3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total 656	C 411	N 111	O 132	S 2	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	102	Total 596	C 365	N 111	O 120	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	174	Total 1145	C 722	N 204	O 217	S 2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	76	Total	C	N	O	0	0	0
			561	349	107	105			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	0	0	0
			519	319	96	104			

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	57	Total	C	N	O	0	0	0
			437	272	83	82			

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	44	Total	C	N	O	S	0	0	0
			337	205	75	54	3			

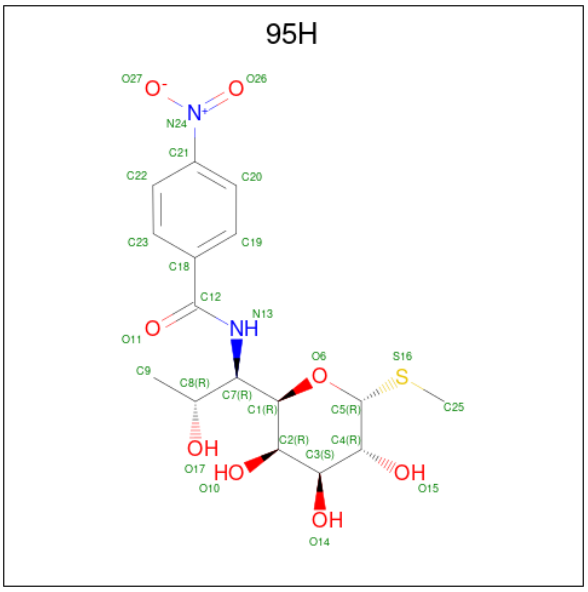
- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			360	219	87	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

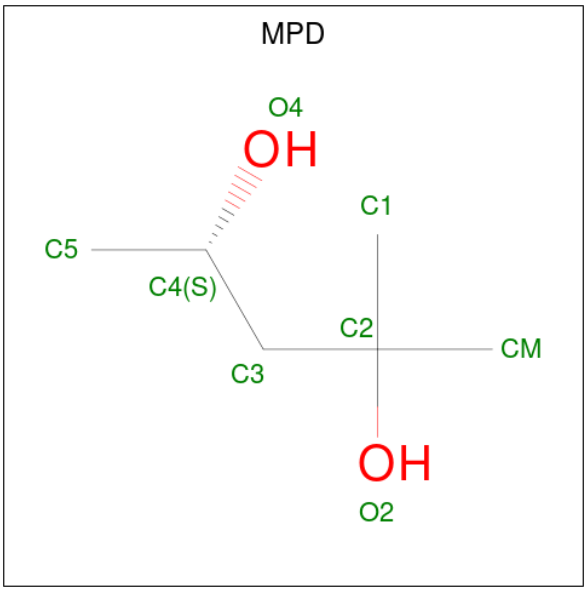
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	65	Total	C	N	O	S	0	0	0
			419	257	83	78	1			

- Molecule 27 is {N}-[(1 {R},2 {R})-1-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-methylsulfanyl-3,4,5-tris(oxidanyl)oxan-2-yl]-2-oxidanyl-propy l]-4-nitro-benzamide (three-letter code: 95H) (formula: $C_{16}H_{22}N_2O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	X	1	Total	C	N	O	S	1	0
			27	16	2	8	1		

- Molecule 28 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		

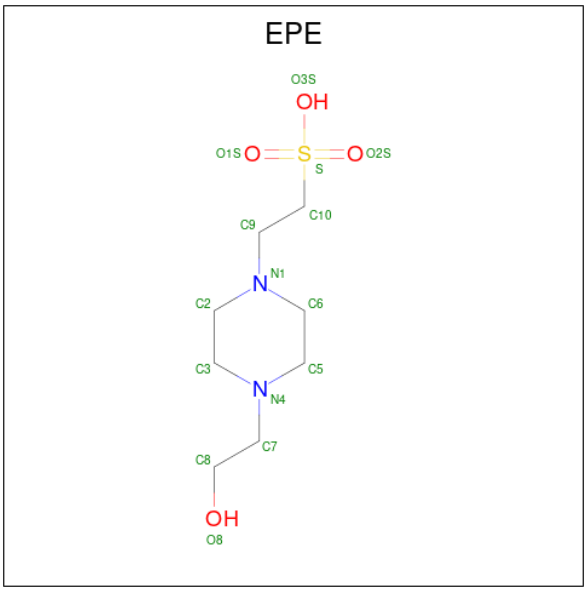
- Molecule 29 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	X	203	Total Mn 203 203	0	0
29	Y	1	Total Mn 1 1	0	0
29	E	1	Total Mn 1 1	0	0
29	I	1	Total Mn 1 1	0	0
29	Z	1	Total Mn 1 1	0	0
29	3	3	Total Mn 3 3	0	0

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

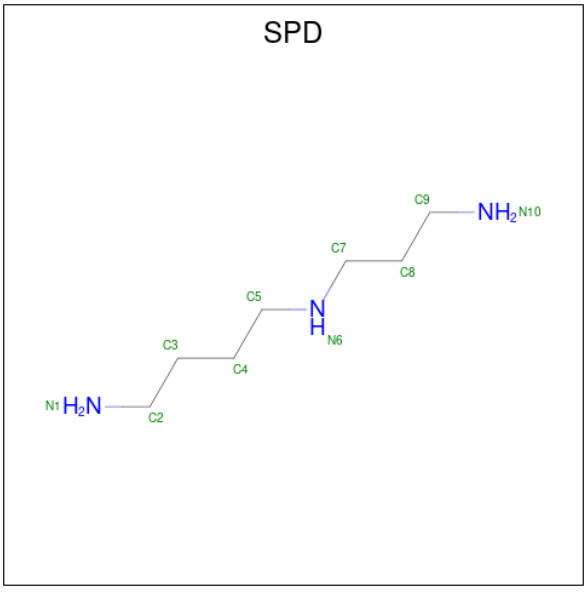
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	78	Total Mg 78 78	0	0
30	Y	2	Total Mg 2 2	0	0
30	C	1	Total Mg 1 1	0	0
30	G	1	Total Mg 1 1	0	0
30	J	1	Total Mg 1 1	0	0
30	3	1	Total Mg 1 1	0	0

- Molecule 31 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 32 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



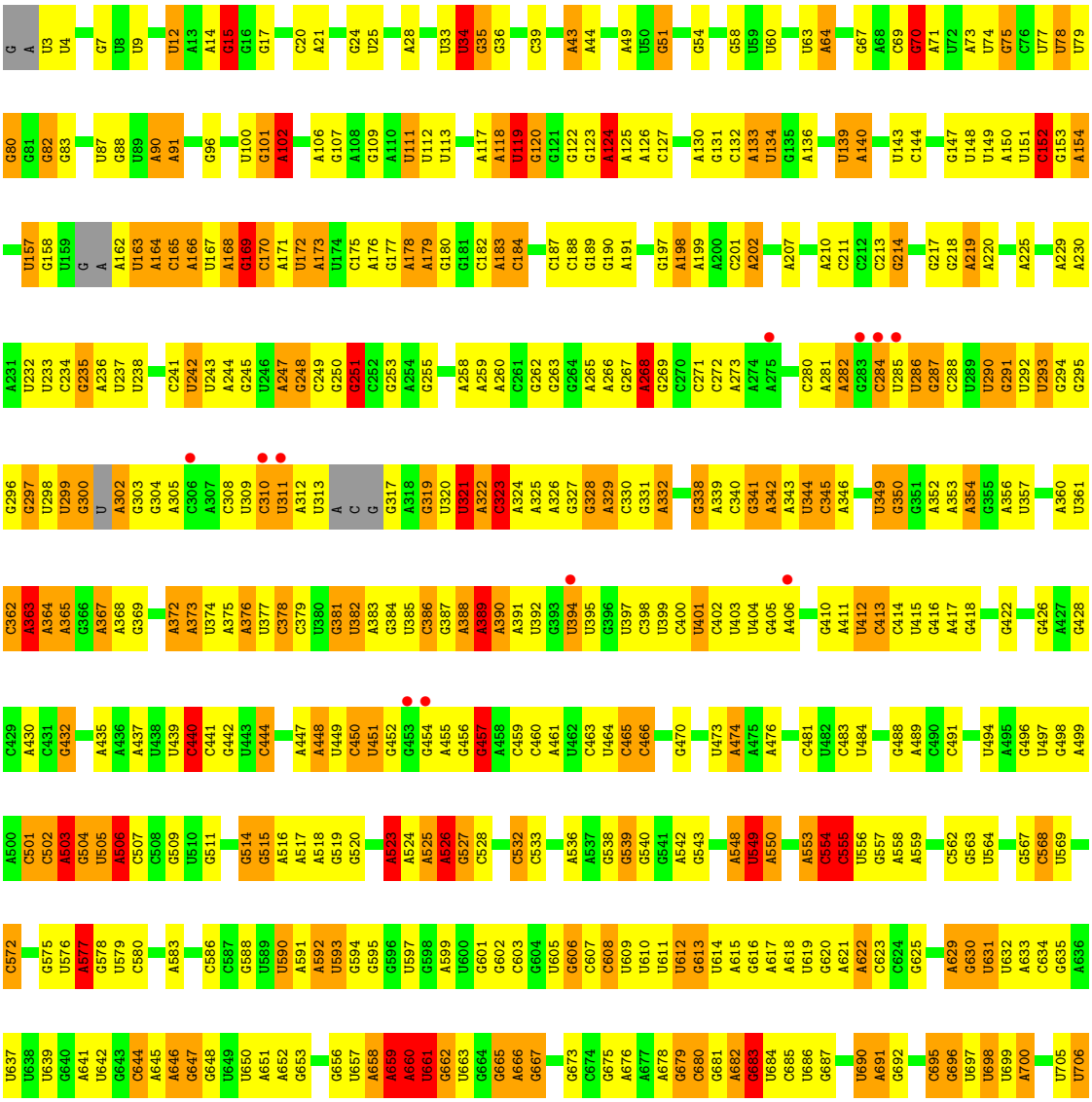
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N		0	0
			10	7	3			

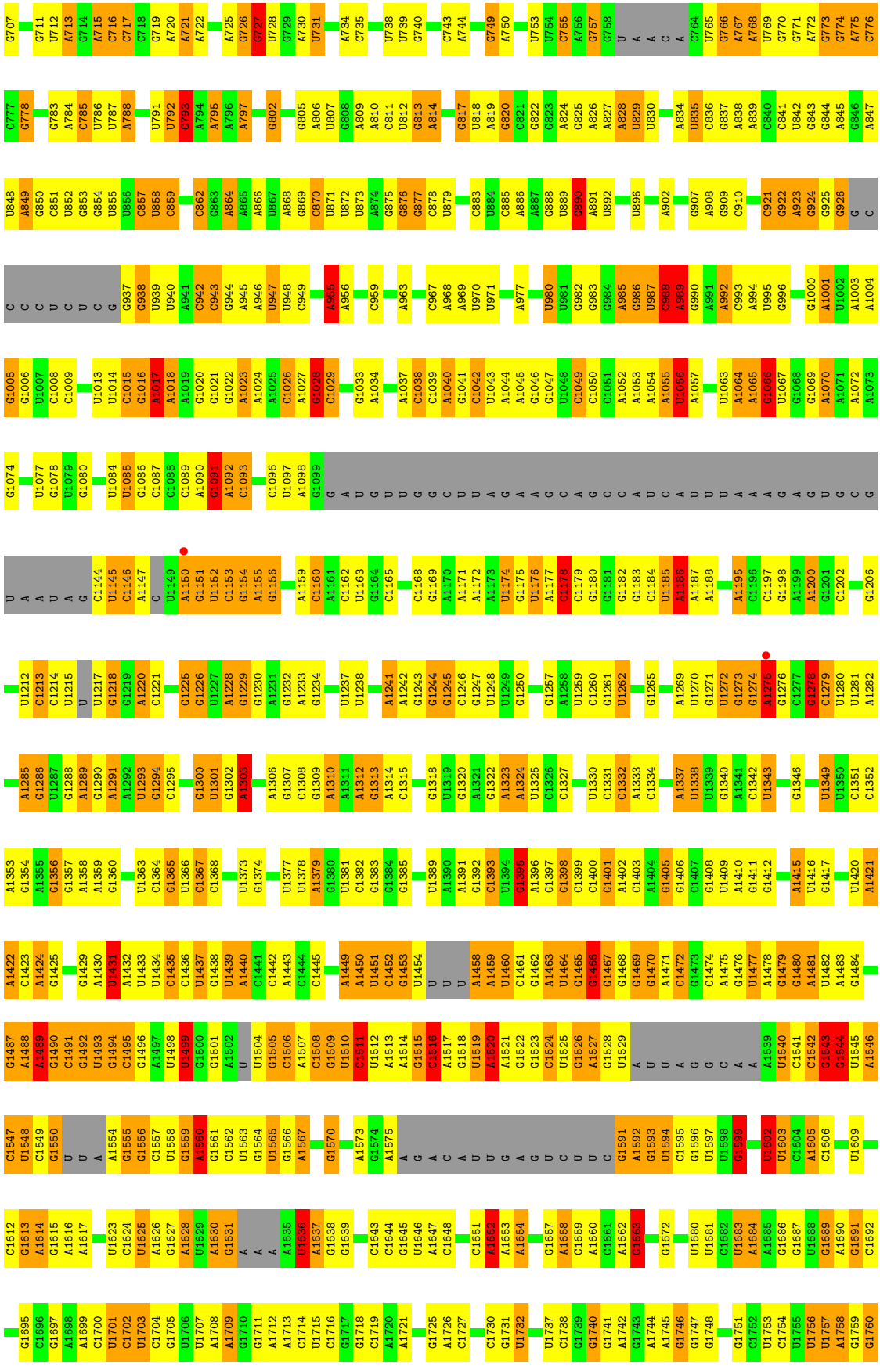
3 Residue-property plots (i)

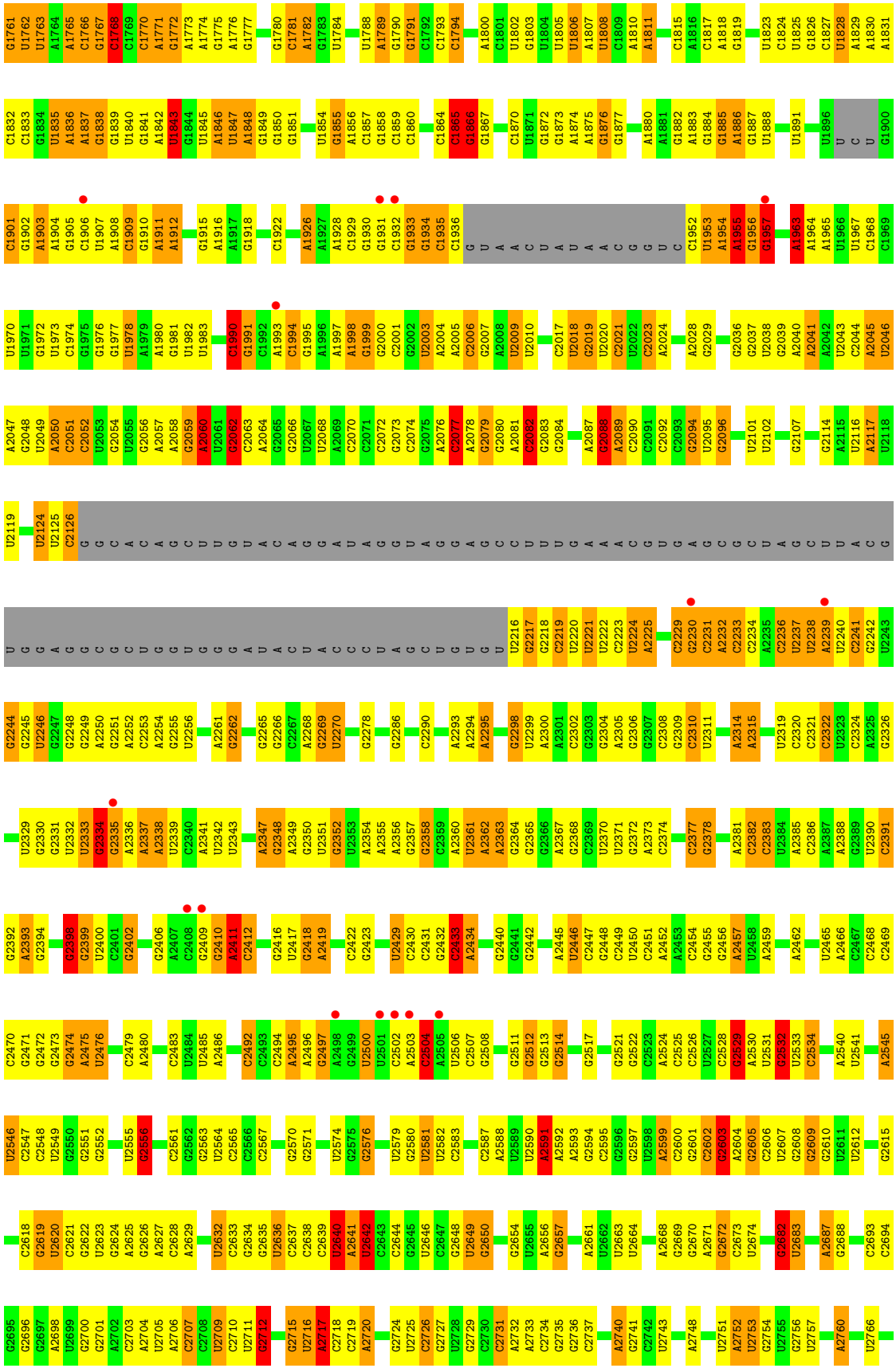
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

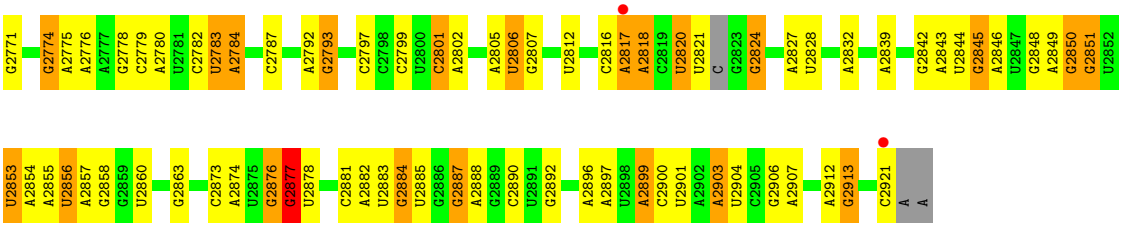
- Molecule 1: 23S ribosomal RNA

Chain X:



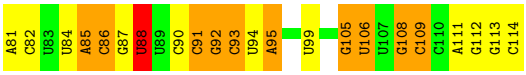






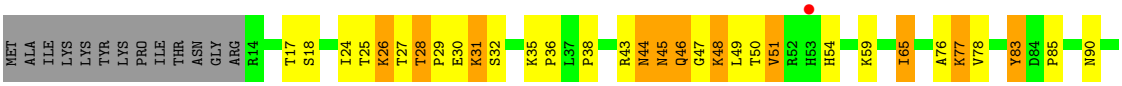
• Molecule 2: 5S ribosomal RNA

Chain Y:



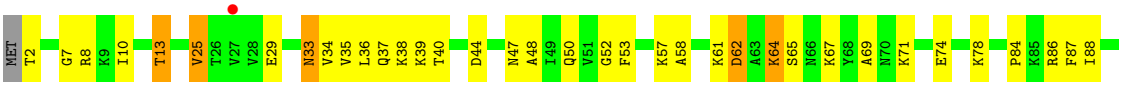
• Molecule 3: 50S ribosomal protein L2

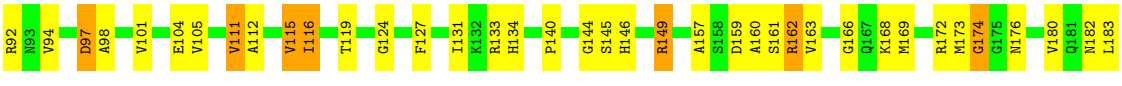
Chain A:



• Molecule 4: 50S ribosomal protein L3

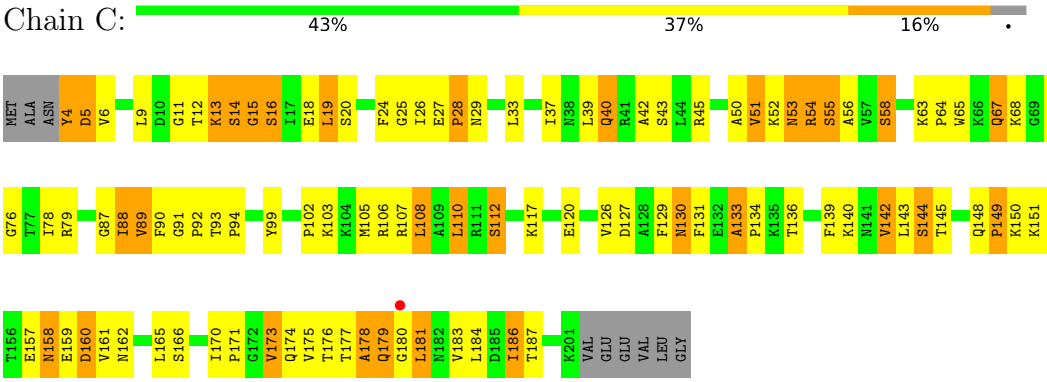
Chain B:





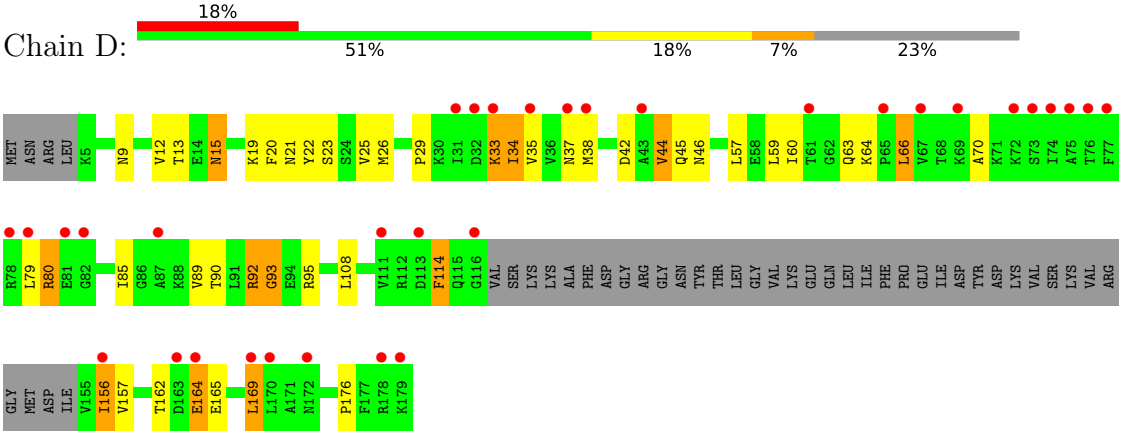
• Molecule 5: 50S ribosomal protein L4

Chain C:



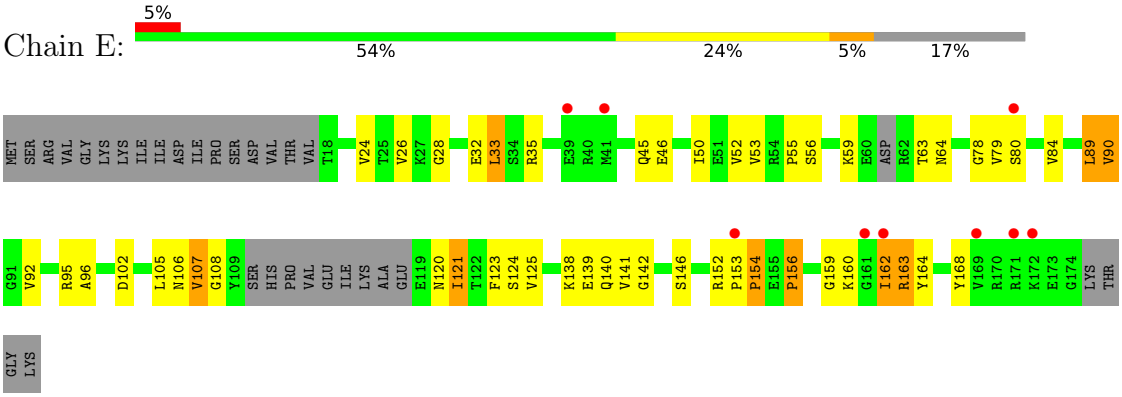
• Molecule 6: 50S ribosomal protein L5

Chain D:



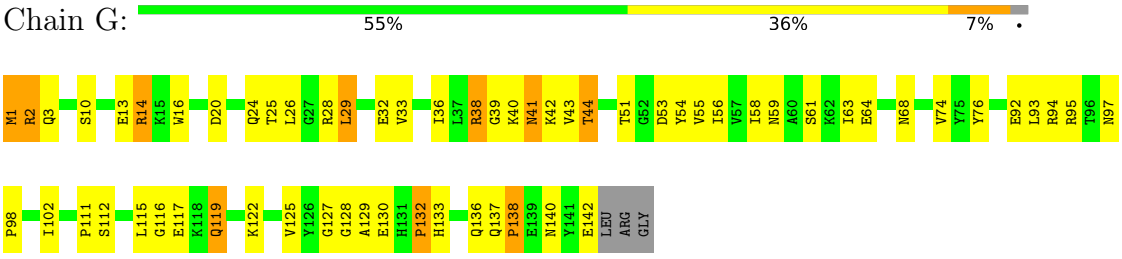
• Molecule 7: 50S ribosomal protein L6

Chain E:



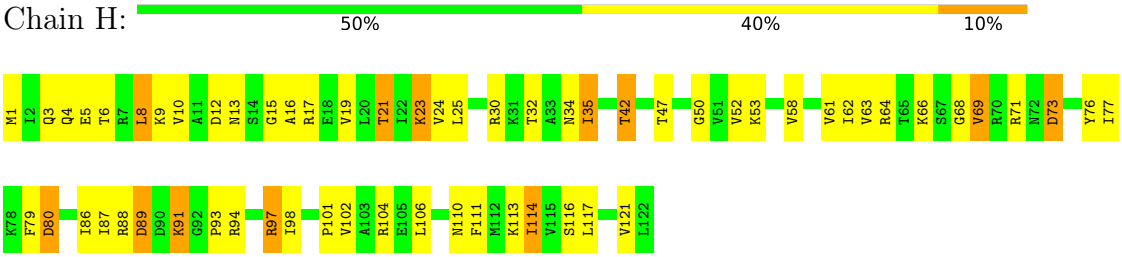
• Molecule 8: 50S ribosomal protein L13

Chain G:



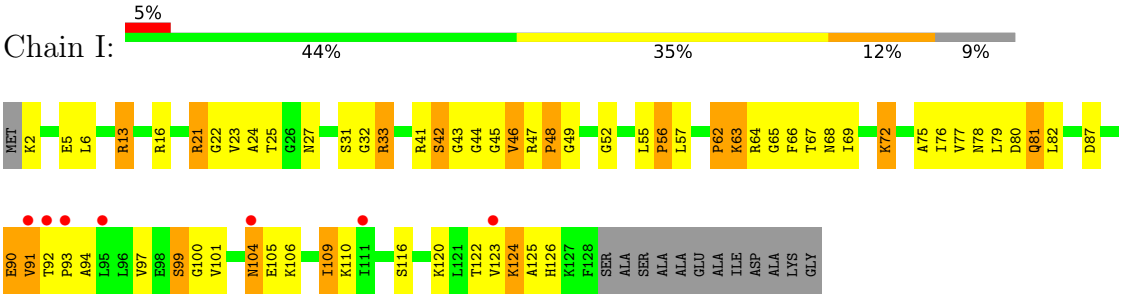
• Molecule 9: 50S ribosomal protein L14

Chain H:



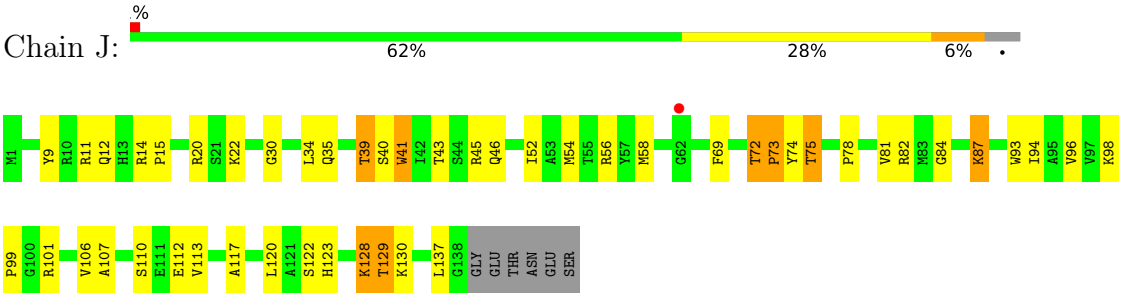
• Molecule 10: 50S ribosomal protein L15

Chain I:



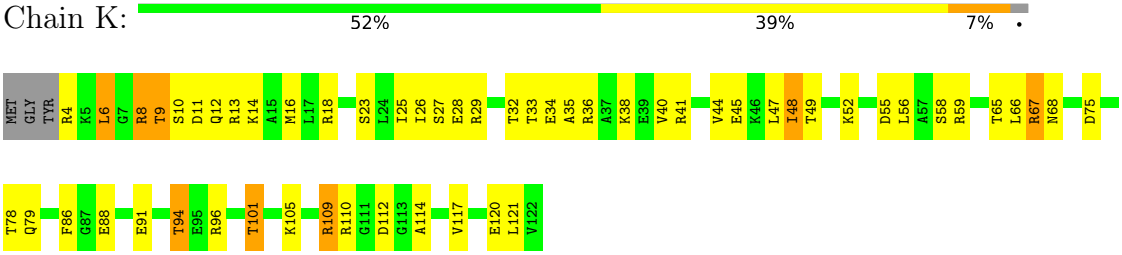
• Molecule 11: 50S ribosomal protein L16

Chain J:



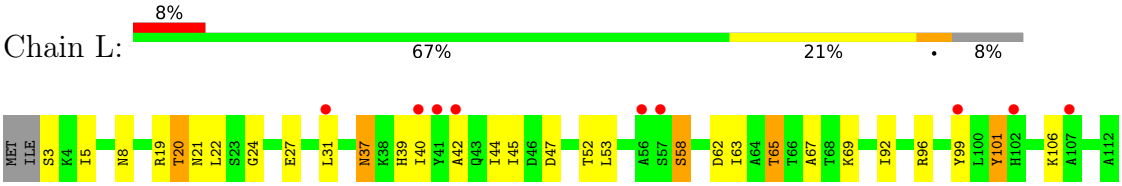
• Molecule 12: 50S ribosomal protein L17

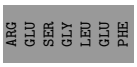
Chain K:



• Molecule 13: 50S ribosomal protein L18

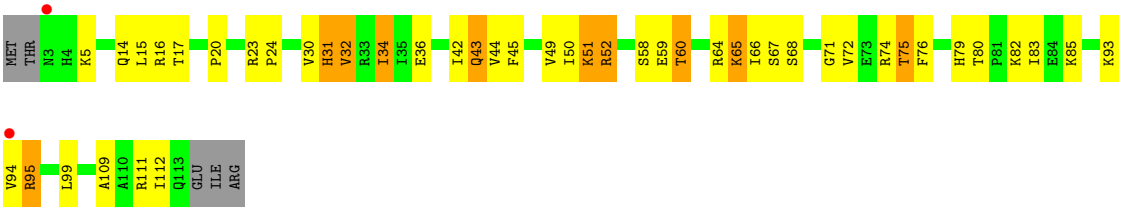
Chain L:





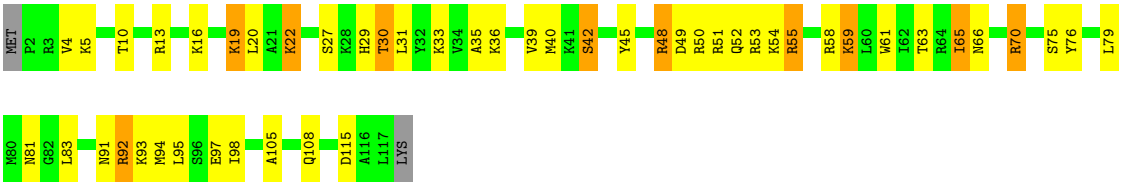
• Molecule 14: 50S ribosomal protein L19

Chain M:



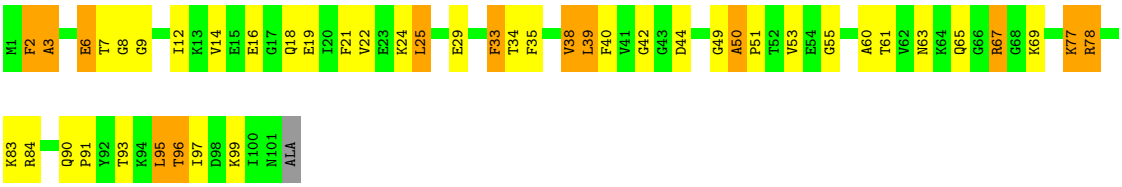
• Molecule 15: 50S ribosomal protein L20

Chain N:



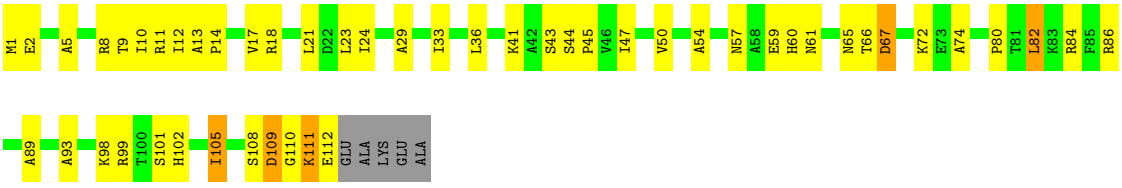
• Molecule 16: 50S ribosomal protein L21

Chain O:



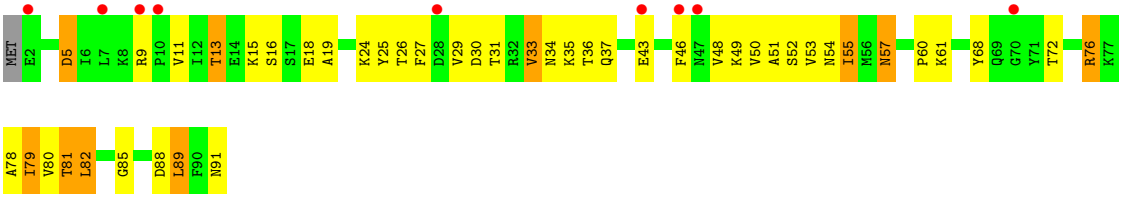
• Molecule 17: 50S ribosomal protein L22

Chain P:



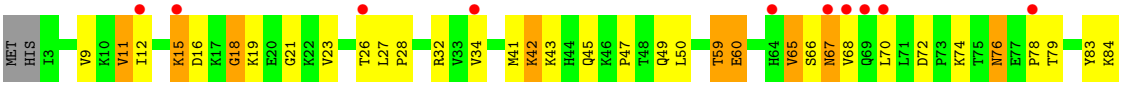
• Molecule 18: 50S ribosomal protein L23

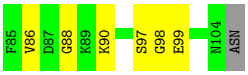
Chain Q:



• Molecule 19: 50S ribosomal protein L24

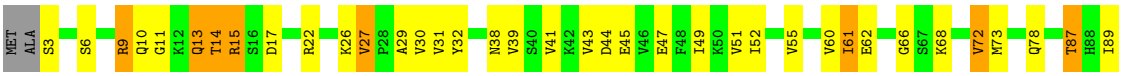
Chain R:

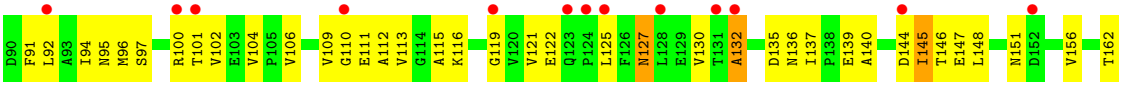


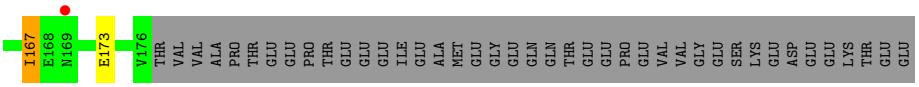


• Molecule 20: 50S ribosomal protein L25

Chain S:

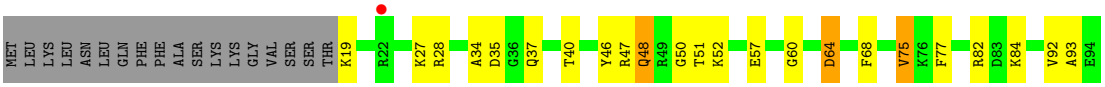






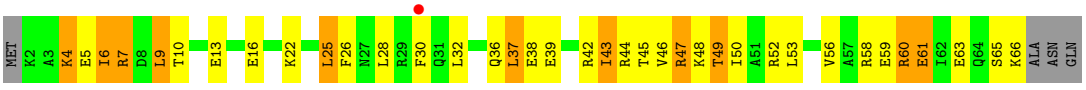
• Molecule 21: 50S ribosomal protein L27

Chain T:



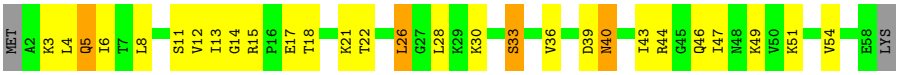
• Molecule 22: 50S ribosomal protein L29

Chain V:

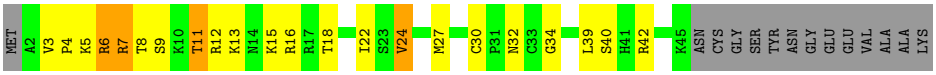


• Molecule 23: 50S ribosomal protein L30

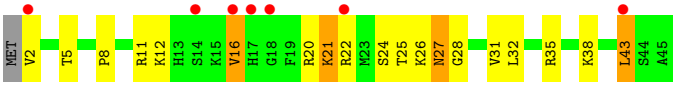
Chain W:



• Molecule 24: 50S ribosomal protein L32



• Molecule 25: 50S ribosomal protein L34



• Molecule 26: 50S ribosomal protein L35

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	279.80Å 279.80Å 873.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.37 – 3.44 49.77 – 3.44	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.37-3.44) 96.1 (49.77-3.44)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.219 , 0.261 0.219 , 0.261	Depositor DCC
R_{free} test set	12721 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	99.6	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 72.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	80800	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, EPE, MG, MN, MPD, 95H

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	0.86	66/65104 (0.1%)	1.53	1119/101503 (1.1%)
2	Y	0.76	1/2717 (0.0%)	1.41	46/4232 (1.1%)
3	A	0.49	0/1665	0.73	0/2275
4	B	0.58	0/1557	0.71	0/2102
5	C	0.60	0/1386	0.82	1/1890 (0.1%)
6	D	0.45	1/934 (0.1%)	0.53	0/1273
7	E	0.29	0/798	0.58	0/1102
8	G	0.47	0/1083	0.67	0/1466
9	H	0.49	0/908	0.71	0/1221
10	I	0.45	0/789	0.77	0/1073
11	J	0.57	1/1034 (0.1%)	0.65	1/1401 (0.1%)
12	K	0.40	0/885	0.62	0/1185
13	L	0.35	0/678	0.58	0/934
14	M	0.53	0/790	0.80	0/1071
15	N	0.62	0/949	0.79	0/1258
16	O	0.62	1/710 (0.1%)	0.84	1/962 (0.1%)
17	P	0.64	0/860	0.73	0/1159
18	Q	0.46	0/662	0.62	0/898
19	R	0.44	0/601	0.67	0/830
20	S	0.43	0/1158	0.58	0/1588
21	T	0.49	0/567	0.70	0/756
22	V	0.43	0/520	0.61	0/694
23	W	0.56	0/439	0.67	0/592
24	Z	0.59	0/342	0.73	0/456
25	2	0.66	0/363	0.73	0/475
26	3	0.41	0/424	0.70	0/578
All	All	0.79	70/87923 (0.1%)	1.39	1168/132974 (0.9%)

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	A	0	3
4	B	0	5
5	C	0	5
7	E	0	1
8	G	0	5
9	H	0	1
10	I	0	4
11	J	0	1
14	M	0	1
16	O	0	2
18	Q	0	1
19	R	0	2
All	All	0	31

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2088	G	C8-N7	15.26	1.40	1.30
1	X	2474	G	C8-N7	15.10	1.40	1.30
1	X	2059	G	C5-C4	12.16	1.46	1.38
1	X	1000	G	C5-C4	-11.92	1.30	1.38
1	X	1931	G	N3-C4	10.72	1.43	1.35

The worst 5 of 1168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2474	G	C5-N7-C8	-23.23	92.68	104.30
1	X	2088	G	C5-N7-C8	-21.74	93.43	104.30
1	X	2059	G	C6-C5-N7	20.68	142.81	130.40
1	X	2059	G	C4-C5-C6	-20.37	106.58	118.80
1	X	2845	G	N3-C4-C5	18.55	137.88	128.60

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	156	ARG	Peptide
3	A	195	VAL	Peptide
3	A	50	THR	Peptide
4	B	58	ALA	Peptide
4	B	97	ASP	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	X	58141	0	29232	1120	0
2	Y	2430	0	1229	57	0
3	A	1641	0	1415	71	0
4	B	1534	0	1495	52	0
5	C	1365	0	1258	88	0
6	D	926	0	824	33	0
7	E	793	0	475	17	0
8	G	1062	0	1000	34	0
9	H	902	0	956	39	0
10	I	780	0	621	38	0
11	J	1011	0	988	30	0
12	K	883	0	890	41	0
13	L	672	0	515	13	0
14	M	779	0	726	28	0
15	N	937	0	1003	47	0
16	O	700	0	629	32	0
17	P	852	0	905	32	0
18	Q	656	0	615	33	0
19	R	596	0	450	23	0
20	S	1145	0	991	40	0
21	T	561	0	555	16	0
22	V	519	0	530	24	0
23	W	437	0	474	18	0
24	Z	337	0	343	19	0
25	2	360	0	402	16	0
26	3	419	0	323	10	0
27	X	27	0	0	2	0
28	X	16	0	28	2	0
29	3	3	0	0	0	0
29	E	1	0	0	0	0
29	I	1	0	0	0	0
29	X	203	0	0	0	0
29	Y	1	0	0	0	0
29	Z	1	0	0	0	0
30	3	1	0	0	0	0
30	C	1	0	0	0	0
30	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	J	1	0	0	0	0
30	X	78	0	0	0	0
30	Y	2	0	0	0	0
31	X	15	0	17	0	0
32	X	10	0	19	3	0
All	All	80800	0	48908	1794	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 14.

The worst 5 of 1794 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)
5:C:40:GLN:HE22	5:C:178:ALA:HB2	1.24	1.00
1:X:1835:U:H2'	1:X:1836:A:H5"	1.45	0.98
1:X:1515:G:H1	1:X:1564:G:H1	1.11	0.96
1:X:2850:G:OP2	4:B:86:ARG:NH2	2.00	0.93
1:X:630:G:OP2	10:I:21:ARG:NH2	2.03	0.92

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	A	258/277 (93%)	189 (73%)	47 (18%)	22 (8%)	1 8
4	B	213/220 (97%)	180 (84%)	22 (10%)	11 (5%)	2 17
5	C	196/207 (95%)	147 (75%)	30 (15%)	19 (10%)	0 6
6	D	133/179 (74%)	115 (86%)	14 (10%)	4 (3%)	4 29
7	E	141/178 (79%)	79 (56%)	35 (25%)	27 (19%)	0 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	G	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	4 30
9	H	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9 41
10	I	125/140 (89%)	65 (52%)	34 (27%)	26 (21%)	0 1
11	J	136/144 (94%)	121 (89%)	11 (8%)	4 (3%)	4 30
12	K	117/122 (96%)	105 (90%)	7 (6%)	5 (4%)	2 21
13	L	108/119 (91%)	83 (77%)	15 (14%)	10 (9%)	0 7
14	M	109/116 (94%)	88 (81%)	14 (13%)	7 (6%)	1 13
15	N	114/118 (97%)	111 (97%)	2 (2%)	1 (1%)	17 54
16	O	99/102 (97%)	81 (82%)	14 (14%)	4 (4%)	3 23
17	P	110/117 (94%)	103 (94%)	6 (6%)	1 (1%)	17 54
18	Q	88/91 (97%)	75 (85%)	12 (14%)	1 (1%)	14 50
19	R	100/105 (95%)	71 (71%)	19 (19%)	10 (10%)	0 6
20	S	172/217 (79%)	133 (77%)	25 (14%)	14 (8%)	1 9
21	T	74/94 (79%)	61 (82%)	11 (15%)	2 (3%)	5 32
22	V	63/69 (91%)	59 (94%)	3 (5%)	1 (2%)	9 42
23	W	55/59 (93%)	52 (94%)	3 (6%)	0	100 100
24	Z	42/58 (72%)	37 (88%)	4 (10%)	1 (2%)	6 34
25	2	42/45 (93%)	39 (93%)	2 (5%)	1 (2%)	6 34
26	3	63/66 (96%)	49 (78%)	11 (18%)	3 (5%)	2 19
All	All	2818/3110 (91%)	2280 (81%)	358 (13%)	180 (6%)	1 13

5 of 180 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	35	LYS
3	A	36	PRO
3	A	38	PRO
3	A	51	VAL
3	A	77	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	A	125/224 (56%)	93 (74%)	32 (26%)	0 2
4	B	146/177 (82%)	119 (82%)	27 (18%)	1 7
5	C	118/169 (70%)	92 (78%)	26 (22%)	1 4
6	D	78/158 (49%)	61 (78%)	17 (22%)	1 4
7	E	26/155 (17%)	20 (77%)	6 (23%)	1 3
8	G	103/123 (84%)	86 (84%)	17 (16%)	2 11
9	H	95/100 (95%)	74 (78%)	21 (22%)	1 4
10	I	51/108 (47%)	36 (71%)	15 (29%)	0 2
11	J	92/119 (77%)	78 (85%)	14 (15%)	3 15
12	K	84/102 (82%)	69 (82%)	15 (18%)	2 8
13	L	40/95 (42%)	31 (78%)	9 (22%)	1 3
14	M	68/102 (67%)	52 (76%)	16 (24%)	1 3
15	N	95/98 (97%)	81 (85%)	14 (15%)	3 16
16	O	56/86 (65%)	41 (73%)	15 (27%)	0 2
17	P	89/94 (95%)	77 (86%)	12 (14%)	4 19
18	Q	64/82 (78%)	48 (75%)	16 (25%)	0 3
19	R	36/90 (40%)	28 (78%)	8 (22%)	1 4
20	S	91/190 (48%)	71 (78%)	20 (22%)	1 4
21	T	53/75 (71%)	46 (87%)	7 (13%)	4 20
22	V	55/62 (89%)	38 (69%)	17 (31%)	0 2
23	W	50/53 (94%)	40 (80%)	10 (20%)	1 5
24	Z	35/51 (69%)	27 (77%)	8 (23%)	1 3
25	2	37/40 (92%)	31 (84%)	6 (16%)	2 12
26	3	26/57 (46%)	23 (88%)	3 (12%)	5 25
All	All	1713/2610 (66%)	1362 (80%)	351 (20%)	1 5

5 of 351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	O	18	GLN
20	S	27	VAL
16	O	67	ARG

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Mol	Chain	Res	Type
18	Q	33	VAL
21	T	19	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	91	ASN
20	S	38	ASN
20	S	78	GLN
10	I	78	ASN
8	G	3	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2690/2923 (92%)	711 (26%)	31 (1%)
2	Y	113/114 (99%)	17 (15%)	0
All	All	2803/3037 (92%)	728 (25%)	31 (1%)

5 of 728 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	12	U
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1323	A
1	X	2433	C
1	X	1520	A
1	X	2783	U
1	X	2062	G

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 299 ligands modelled in this entry, 294 are monoatomic - leaving 5 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	SPD	X	3286	-	9,9,9	0.34	0	8,8,8	0.30	0
27	95H	X	3001	-	25,28,28	1.86	5 (20%)	32,40,40	2.67	9 (28%)
28	MPD	X	3002	-	7,7,7	0.34	0	9,10,10	0.15	0
28	MPD	X	3003	-	7,7,7	1.65	1 (14%)	9,10,10	0.68	0
31	EPE	X	3285	-	15,15,15	0.54	0	18,20,20	0.74	1 (5%)

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	SPD	X	3286	-	-	0/7/7/7	-
27	95H	X	3001	-	-	5/20/42/42	0/2/2/2
28	MPD	X	3002	-	-	2/5/5/5	-
28	MPD	X	3003	-	-	1/5/5/5	-
31	EPE	X	3285	-	-	5/9/19/19	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	3001	95H	C12-N13	6.46	1.48	1.34
28	X	3003	MPD	C3-C2	3.80	1.64	1.53
27	X	3001	95H	C18-C12	-3.27	1.43	1.50
27	X	3001	95H	C21-N24	2.94	1.52	1.45
27	X	3001	95H	O10-C2	-2.55	1.37	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	3001	95H	C22-C21-N24	-9.15	112.49	119.38
27	X	3001	95H	C20-C21-N24	7.11	124.73	119.38
27	X	3001	95H	C20-C19-C18	-4.25	115.83	120.78
27	X	3001	95H	C23-C18-C19	4.03	124.32	118.59
27	X	3001	95H	C18-C12-N13	-3.05	111.21	117.06

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	X	3001	95H	O6-C5-S16-C25
31	X	3285	EPE	C10-C9-N1-C6
31	X	3285	EPE	C9-C10-S-O2S
27	X	3001	95H	C18-C12-N13-C7
27	X	3001	95H	O11-C12-N13-C7

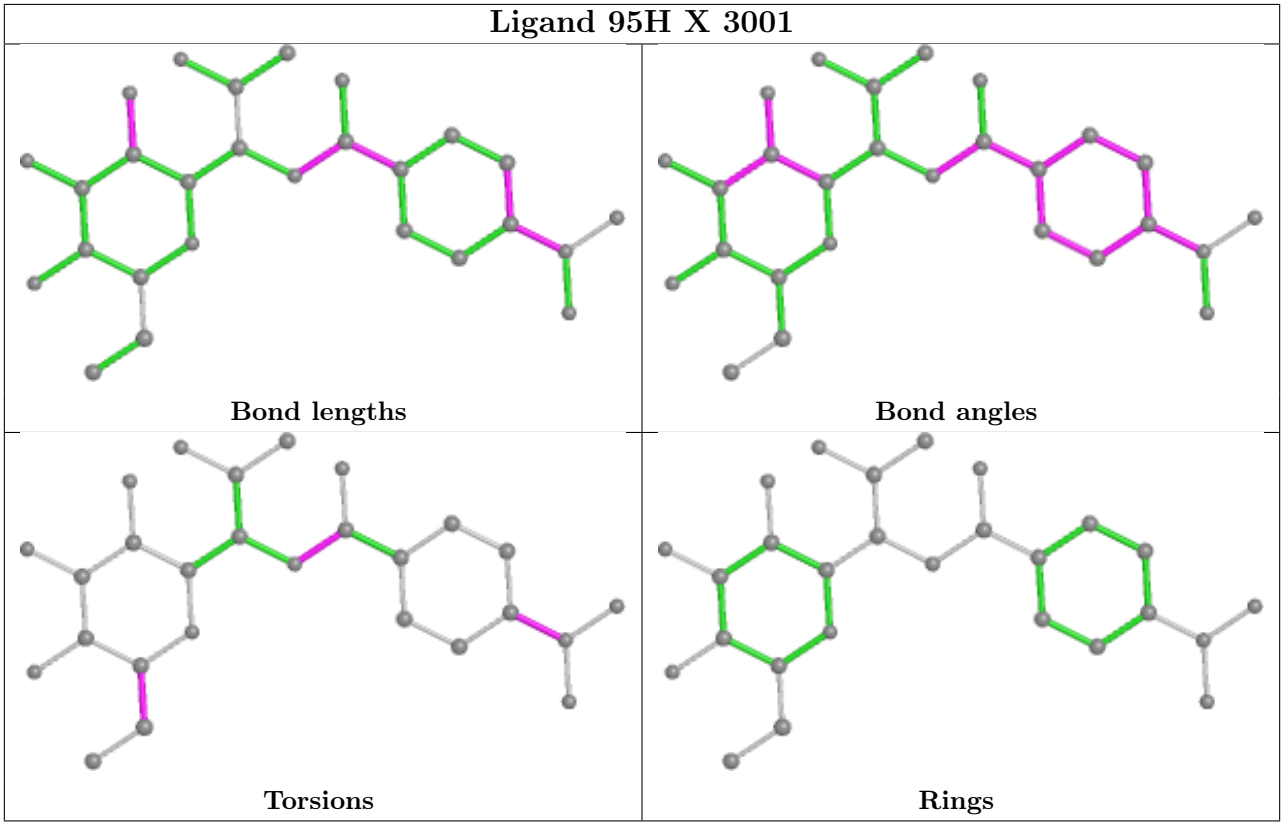
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	3286	SPD	3	0
27	X	3001	95H	2	0
28	X	3002	MPD	1	0
28	X	3003	MPD	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.



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
11	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	69:PHE	C	70:PRO	N	1.16

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, 95^{th} 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	2710/2923 (92%)	-0.12	30 (1%) 80 77	46, 97, 197, 300	0
2	Y	114/114 (100%)	0.10	2 (1%) 68 66	68, 128, 188, 250	0
3	A	260/277 (93%)	0.18	10 (3%) 40 39	87, 134, 168, 183	0
4	B	215/220 (97%)	-0.22	1 (0%) 91 89	50, 74, 96, 119	0
5	C	198/207 (95%)	-0.15	1 (0%) 91 89	63, 92, 113, 140	0
6	D	137/179 (76%)	1.23	33 (24%) 0 1	162, 186, 212, 219	0
7	E	147/178 (82%)	0.00	9 (6%) 21 23	122, 156, 181, 185	0
8	G	142/145 (97%)	-0.22	0 100 100	58, 70, 87, 95	0
9	H	122/122 (100%)	-0.03	0 100 100	75, 93, 118, 125	0
10	I	127/140 (90%)	0.25	7 (5%) 25 26	49, 108, 135, 139	0
11	J	138/144 (95%)	-0.05	1 (0%) 87 85	69, 89, 116, 141	0
12	K	119/122 (97%)	-0.15	0 100 100	63, 81, 115, 135	0
13	L	110/119 (92%)	0.26	9 (8%) 11 14	106, 120, 143, 152	0
14	M	111/116 (95%)	-0.02	2 (1%) 68 66	77, 91, 127, 151	0
15	N	116/118 (98%)	-0.18	0 100 100	49, 65, 90, 102	0
16	O	101/102 (99%)	-0.40	0 100 100	47, 79, 98, 115	0
17	P	112/117 (95%)	-0.00	0 100 100	59, 70, 103, 129	0
18	Q	90/91 (98%)	0.44	9 (10%) 7 9	100, 123, 152, 170	0
19	R	102/105 (97%)	0.30	10 (9%) 7 10	95, 115, 171, 180	0
20	S	174/217 (80%)	0.17	14 (8%) 12 15	75, 102, 184, 192	0
21	T	76/94 (80%)	0.00	1 (1%) 77 74	76, 88, 113, 155	0
22	V	65/69 (94%)	0.04	1 (1%) 73 71	119, 136, 160, 164	0
23	W	57/59 (96%)	0.22	0 100 100	59, 71, 95, 103	0
24	Z	44/58 (75%)	0.02	0 100 100	55, 86, 144, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	2	44/45 (97%)	1.09	7 (15%) 1 3	80, 89, 96, 104	0
26	3	65/66 (98%)	-0.02	1 (1%) 73 71	70, 81, 95, 100	0
All	All	5696/6147 (92%)	-0.01	148 (2%) 56 54	46, 96, 186, 300	0

The worst 5 of 148 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	73	SER	12.7
6	D	74	ILE	11.5
6	D	75	ALA	9.1
6	D	179	LYS	7.7
6	D	32	ASP	5.6

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 monosaccharides 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
30	MG	X	3255	1/1	-0.21	0.34	112,112,112,112	0
30	MG	J	201	1/1	0.17	2.12	107,107,107,107	0
30	MG	X	3268	1/1	0.21	0.31	134,134,134,134	0
30	MG	X	3240	1/1	0.28	0.30	87,87,87,87	0
29	MN	X	3145	1/1	0.37	0.32	144,144,144,144	0
30	MG	X	3224	1/1	0.38	0.28	97,97,97,97	0
30	MG	X	3271	1/1	0.42	0.67	90,90,90,90	0
30	MG	X	3246	1/1	0.43	0.27	131,131,131,131	0
30	MG	X	3261	1/1	0.46	0.36	163,163,163,163	0
30	MG	C	301	1/1	0.50	0.37	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3222	1/1	0.52	0.27	142,142,142,142	0
29	MN	X	3214	1/1	0.54	0.35	125,125,125,125	0
30	MG	X	3260	1/1	0.55	0.89	73,73,73,73	0
30	MG	X	3227	1/1	0.57	0.19	93,93,93,93	0
29	MN	X	3062	1/1	0.62	0.41	135,135,135,135	0
30	MG	X	3202	1/1	0.64	0.44	64,64,64,64	0
29	MN	X	3172	1/1	0.67	0.10	126,126,126,126	0
29	MN	X	3203	1/1	0.67	0.18	141,141,141,141	0
29	MN	X	3156	1/1	0.67	0.34	104,104,104,104	0
30	MG	X	3266	1/1	0.67	0.41	119,119,119,119	0
29	MN	X	3169	1/1	0.68	0.40	98,98,98,98	0
29	MN	X	3179	1/1	0.70	0.19	110,110,110,110	0
30	MG	X	3267	1/1	0.70	0.19	91,91,91,91	0
30	MG	X	3247	1/1	0.70	0.33	69,69,69,69	0
29	MN	X	3191	1/1	0.70	0.11	126,126,126,126	0
30	MG	X	3280	1/1	0.70	0.53	66,66,66,66	0
29	MN	X	3194	1/1	0.70	0.25	140,140,140,140	0
29	MN	X	3229	1/1	0.70	0.14	144,144,144,144	0
30	MG	3	104	1/1	0.70	0.47	56,56,56,56	0
29	MN	X	3234	1/1	0.71	0.22	137,137,137,137	0
29	MN	X	3075	1/1	0.73	0.45	102,102,102,102	0
29	MN	X	3142	1/1	0.73	0.11	111,111,111,111	0
30	MG	X	3283	1/1	0.73	0.42	59,59,59,59	0
29	MN	X	3187	1/1	0.74	0.15	112,112,112,112	0
30	MG	X	3242	1/1	0.74	0.41	60,60,60,60	0
29	MN	X	3141	1/1	0.74	0.29	104,104,104,104	0
29	MN	3	101	1/1	0.74	0.21	96,96,96,96	0
29	MN	X	3205	1/1	0.75	0.13	143,143,143,143	0
29	MN	X	3231	1/1	0.75	0.17	125,125,125,125	0
30	MG	X	3265	1/1	0.75	0.24	73,73,73,73	0
30	MG	X	3274	1/1	0.76	0.86	69,69,69,69	0
30	MG	X	3181	1/1	0.76	0.36	89,89,89,89	0
30	MG	X	3279	1/1	0.77	0.54	66,66,66,66	0
29	MN	X	3131	1/1	0.77	0.35	114,114,114,114	0
30	MG	X	3257	1/1	0.77	0.04	156,156,156,156	0
30	MG	X	3112	1/1	0.78	0.38	84,84,84,84	0
30	MG	X	3228	1/1	0.78	0.24	65,65,65,65	0
30	MG	X	3264	1/1	0.78	0.47	102,102,102,102	0
29	MN	X	3198	1/1	0.80	0.34	100,100,100,100	0
29	MN	X	3171	1/1	0.80	0.18	117,117,117,117	0
29	MN	X	3092	1/1	0.81	0.24	87,87,87,87	0
30	MG	X	3276	1/1	0.81	0.82	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3196	1/1	0.81	0.50	78,78,78,78	0
29	MN	X	3096	1/1	0.81	0.46	98,98,98,98	0
30	MG	X	3204	1/1	0.81	0.28	67,67,67,67	0
29	MN	X	3189	1/1	0.81	0.14	123,123,123,123	0
29	MN	X	3051	1/1	0.81	0.22	100,100,100,100	0
29	MN	X	3150	1/1	0.81	0.22	98,98,98,98	0
29	MN	3	102	1/1	0.82	0.31	101,101,101,101	0
29	MN	X	3165	1/1	0.82	0.12	109,109,109,109	0
29	MN	X	3192	1/1	0.82	0.10	106,106,106,106	0
30	MG	X	3182	1/1	0.82	0.81	53,53,53,53	0
29	MN	X	3199	1/1	0.83	0.23	131,131,131,131	0
28	MPD	X	3003	8/8	0.83	0.30	80,80,80,80	0
29	MN	3	103	1/1	0.83	0.48	129,129,129,129	0
30	MG	X	3217	1/1	0.83	0.66	64,64,64,64	0
30	MG	X	3223	1/1	0.83	0.79	71,71,71,71	0
29	MN	X	3176	1/1	0.84	0.13	128,128,128,128	0
30	MG	X	3277	1/1	0.84	0.51	59,59,59,59	0
29	MN	X	3162	1/1	0.84	0.10	110,110,110,110	0
29	MN	X	3170	1/1	0.84	0.22	103,103,103,103	0
30	MG	X	3258	1/1	0.85	0.23	64,64,64,64	0
29	MN	X	3147	1/1	0.85	0.10	113,113,113,113	0
29	MN	X	3074	1/1	0.86	0.16	129,129,129,129	0
29	MN	Z	101	1/1	0.86	0.32	109,109,109,109	0
30	MG	X	3158	1/1	0.86	0.33	48,48,48,48	0
30	MG	X	3256	1/1	0.86	0.39	91,91,91,91	0
30	MG	X	3263	1/1	0.86	0.46	81,81,81,81	0
29	MN	X	3235	1/1	0.87	0.10	118,118,118,118	0
29	MN	X	3225	1/1	0.87	0.23	101,101,101,101	0
30	MG	X	3168	1/1	0.87	0.18	73,73,73,73	0
29	MN	X	3212	1/1	0.87	0.19	117,117,117,117	0
29	MN	X	3157	1/1	0.87	0.18	87,87,87,87	0
30	MG	X	3251	1/1	0.87	0.16	65,65,65,65	0
29	MN	X	3006	1/1	0.87	0.14	49,49,49,49	0
30	MG	X	3259	1/1	0.88	0.57	61,61,61,61	0
29	MN	X	3029	1/1	0.88	0.17	82,82,82,82	0
29	MN	X	3178	1/1	0.88	0.27	108,108,108,108	0
29	MN	X	3151	1/1	0.88	0.10	97,97,97,97	0
29	MN	E	201	1/1	0.88	0.17	125,125,125,125	0
29	MN	X	3185	1/1	0.88	0.14	100,100,100,100	0
30	MG	X	3281	1/1	0.88	0.46	69,69,69,69	0
29	MN	X	3164	1/1	0.88	0.24	110,110,110,110	0
30	MG	X	3195	1/1	0.88	0.47	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3135	1/1	0.88	0.17	108,108,108,108	0
30	MG	X	3269	1/1	0.88	0.61	104,104,104,104	0
30	MG	X	3239	1/1	0.89	0.33	46,46,46,46	0
29	MN	X	3123	1/1	0.89	0.19	109,109,109,109	0
29	MN	X	3155	1/1	0.89	0.19	105,105,105,105	0
29	MN	X	3018	1/1	0.89	0.30	86,86,86,86	0
29	MN	X	3016	1/1	0.89	0.17	87,87,87,87	0
30	MG	X	3197	1/1	0.89	0.35	54,54,54,54	0
30	MG	X	3253	1/1	0.89	0.27	90,90,90,90	0
29	MN	X	3037	1/1	0.89	0.20	78,78,78,78	0
32	SPD	X	3286	10/10	0.89	0.25	65,65,65,65	0
30	MG	X	3218	1/1	0.90	0.29	74,74,74,74	0
29	MN	X	3052	1/1	0.90	0.14	121,121,121,121	0
29	MN	X	3154	1/1	0.90	0.25	114,114,114,114	0
29	MN	X	3206	1/1	0.90	0.21	127,127,127,127	0
29	MN	X	3073	1/1	0.90	0.17	120,120,120,120	0
30	MG	X	3232	1/1	0.90	0.10	67,67,67,67	0
30	MG	Y	203	1/1	0.90	0.07	122,122,122,122	0
30	MG	X	3238	1/1	0.90	0.76	58,58,58,58	0
29	MN	X	3163	1/1	0.90	0.14	99,99,99,99	0
29	MN	X	3215	1/1	0.90	0.18	119,119,119,119	0
29	MN	X	3190	1/1	0.90	0.21	117,117,117,117	0
30	MG	X	3254	1/1	0.91	0.38	67,67,67,67	0
30	MG	X	3152	1/1	0.91	0.33	57,57,57,57	0
29	MN	X	3184	1/1	0.91	0.09	126,126,126,126	0
29	MN	X	3082	1/1	0.91	0.19	59,59,59,59	0
29	MN	X	3233	1/1	0.91	0.13	59,59,59,59	0
29	MN	X	3008	1/1	0.91	0.13	50,50,50,50	0
30	MG	X	3193	1/1	0.91	0.51	78,78,78,78	0
29	MN	X	3071	1/1	0.91	0.23	83,83,83,83	0
29	MN	X	3208	1/1	0.91	0.15	77,77,77,77	0
29	MN	X	3026	1/1	0.91	0.21	94,94,94,94	0
29	MN	X	3174	1/1	0.91	0.16	115,115,115,115	0
29	MN	X	3130	1/1	0.91	0.17	94,94,94,94	0
29	MN	X	3053	1/1	0.91	0.13	96,96,96,96	0
29	MN	X	3061	1/1	0.91	0.07	119,119,119,119	0
30	MG	X	3250	1/1	0.92	0.63	66,66,66,66	0
29	MN	X	3033	1/1	0.92	0.34	90,90,90,90	0
29	MN	X	3139	1/1	0.92	0.07	102,102,102,102	0
30	MG	X	3160	1/1	0.92	0.15	69,69,69,69	0
29	MN	X	3219	1/1	0.92	0.07	118,118,118,118	0
30	MG	X	3241	1/1	0.92	0.07	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3226	1/1	0.92	0.30	74,74,74,74	0
30	MG	X	3243	1/1	0.92	0.29	54,54,54,54	0
30	MG	X	3072	1/1	0.92	0.35	41,41,41,41	0
30	MG	X	3273	1/1	0.92	0.07	57,57,57,57	0
29	MN	X	3125	1/1	0.92	0.10	86,86,86,86	0
30	MG	X	3036	1/1	0.93	0.16	55,55,55,55	0
29	MN	X	3031	1/1	0.93	0.18	80,80,80,80	0
29	MN	X	3013	1/1	0.93	0.41	67,67,67,67	0
30	MG	X	3201	1/1	0.93	0.38	66,66,66,66	0
30	MG	X	3126	1/1	0.93	0.44	58,58,58,58	0
28	MPD	X	3002	8/8	0.93	0.32	96,96,96,96	0
29	MN	X	3047	1/1	0.93	0.10	87,87,87,87	0
29	MN	X	3132	1/1	0.93	0.22	101,101,101,101	0
29	MN	X	3067	1/1	0.93	0.18	103,103,103,103	0
29	MN	X	3017	1/1	0.93	0.04	90,90,90,90	0
29	MN	X	3109	1/1	0.93	0.21	87,87,87,87	0
30	MG	X	3252	1/1	0.93	0.39	60,60,60,60	0
30	MG	X	3183	1/1	0.93	0.34	72,72,72,72	0
29	MN	X	3188	1/1	0.93	0.29	117,117,117,117	0
29	MN	X	3133	1/1	0.94	0.18	85,85,85,85	0
27	95H	X	3001	27/27	0.94	0.24	52,52,52,52	19
29	MN	X	3138	1/1	0.94	0.18	102,102,102,102	0
29	MN	I	201	1/1	0.94	0.31	95,95,95,95	0
29	MN	X	3039	1/1	0.94	0.16	94,94,94,94	0
30	MG	X	3270	1/1	0.94	0.26	68,68,68,68	0
29	MN	X	3159	1/1	0.94	0.18	104,104,104,104	0
29	MN	X	3161	1/1	0.94	0.07	130,130,130,130	0
29	MN	X	3209	1/1	0.94	0.13	105,105,105,105	0
29	MN	X	3120	1/1	0.94	0.14	72,72,72,72	0
30	MG	X	3058	1/1	0.94	0.49	63,63,63,63	0
29	MN	X	3186	1/1	0.94	0.17	104,104,104,104	0
29	MN	X	3055	1/1	0.94	0.11	129,129,129,129	0
29	MN	X	3144	1/1	0.94	0.13	80,80,80,80	0
30	MG	X	3282	1/1	0.94	0.20	63,63,63,63	0
29	MN	X	3221	1/1	0.94	0.07	141,141,141,141	0
30	MG	Y	202	1/1	0.94	0.16	54,54,54,54	0
29	MN	X	3076	1/1	0.94	0.14	93,93,93,93	0
29	MN	X	3167	1/1	0.94	0.08	110,110,110,110	0
29	MN	X	3081	1/1	0.94	0.17	57,57,57,57	0
29	MN	X	3068	1/1	0.94	0.17	84,84,84,84	0
29	MN	X	3059	1/1	0.94	0.15	92,92,92,92	0
29	MN	X	3065	1/1	0.95	0.12	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3007	1/1	0.95	0.30	61,61,61,61	0
29	MN	X	3102	1/1	0.95	0.32	77,77,77,77	0
29	MN	X	3021	1/1	0.95	0.11	68,68,68,68	0
29	MN	X	3230	1/1	0.95	0.10	126,126,126,126	0
29	MN	X	3111	1/1	0.95	0.13	80,80,80,80	0
29	MN	X	3117	1/1	0.95	0.09	66,66,66,66	0
29	MN	X	3005	1/1	0.95	0.30	53,53,53,53	0
29	MN	X	3038	1/1	0.95	0.18	73,73,73,73	0
30	MG	X	3245	1/1	0.95	0.23	63,63,63,63	0
29	MN	X	3056	1/1	0.95	0.19	94,94,94,94	0
29	MN	X	3057	1/1	0.95	0.16	93,93,93,93	0
30	MG	X	3248	1/1	0.95	0.42	66,66,66,66	0
30	MG	X	3249	1/1	0.95	0.16	89,89,89,89	0
29	MN	X	3207	1/1	0.95	0.09	92,92,92,92	0
29	MN	X	3028	1/1	0.95	0.23	90,90,90,90	0
29	MN	X	3045	1/1	0.95	0.13	88,88,88,88	0
29	MN	X	3210	1/1	0.95	0.23	107,107,107,107	0
30	MG	X	3213	1/1	0.95	0.26	47,47,47,47	0
30	MG	X	3216	1/1	0.95	0.20	43,43,43,43	0
29	MN	X	3012	1/1	0.95	0.29	72,72,72,72	0
29	MN	X	3088	1/1	0.95	0.22	68,68,68,68	0
30	MG	G	201	1/1	0.95	0.24	25,25,25,25	0
30	MG	X	3069	1/1	0.95	0.42	52,52,52,52	0
29	MN	X	3136	1/1	0.95	0.26	106,106,106,106	0
31	EPE	X	3285	15/15	0.95	0.20	72,72,72,72	0
29	MN	X	3090	1/1	0.95	0.18	69,69,69,69	0
29	MN	X	3066	1/1	0.96	0.12	91,91,91,91	0
29	MN	X	3103	1/1	0.96	0.47	81,81,81,81	0
29	MN	X	3105	1/1	0.96	0.17	71,71,71,71	0
29	MN	X	3106	1/1	0.96	0.21	99,99,99,99	0
29	MN	X	3140	1/1	0.96	0.07	100,100,100,100	0
29	MN	X	3107	1/1	0.96	0.24	68,68,68,68	0
29	MN	X	3046	1/1	0.96	0.12	94,94,94,94	0
29	MN	X	3023	1/1	0.96	0.21	70,70,70,70	0
29	MN	X	3173	1/1	0.96	0.44	112,112,112,112	0
29	MN	X	3084	1/1	0.96	0.28	71,71,71,71	0
30	MG	X	3032	1/1	0.96	0.59	31,31,31,31	0
29	MN	X	3175	1/1	0.96	0.11	103,103,103,103	0
29	MN	X	3119	1/1	0.96	0.08	77,77,77,77	0
29	MN	X	3054	1/1	0.96	0.34	82,82,82,82	0
29	MN	X	3048	1/1	0.96	0.07	117,117,117,117	0
29	MN	X	3091	1/1	0.96	0.13	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3127	1/1	0.96	0.15	79,79,79,79	0
29	MN	X	3064	1/1	0.96	0.37	124,124,124,124	0
29	MN	X	3035	1/1	0.96	0.43	104,104,104,104	0
30	MG	X	3237	1/1	0.96	0.17	93,93,93,93	0
29	MN	X	3098	1/1	0.96	0.41	70,70,70,70	0
29	MN	X	3100	1/1	0.96	0.18	59,59,59,59	0
29	MN	X	3134	1/1	0.96	0.11	84,84,84,84	0
29	MN	X	3093	1/1	0.97	0.14	61,61,61,61	0
29	MN	X	3236	1/1	0.97	0.06	104,104,104,104	0
29	MN	X	3278	1/1	0.97	0.14	99,99,99,99	0
30	MG	X	3244	1/1	0.97	0.23	57,57,57,57	0
29	MN	X	3094	1/1	0.97	0.12	83,83,83,83	0
29	MN	X	3110	1/1	0.97	0.20	65,65,65,65	0
29	MN	X	3027	1/1	0.97	0.15	89,89,89,89	0
29	MN	X	3113	1/1	0.97	0.09	75,75,75,75	0
29	MN	X	3114	1/1	0.97	0.20	65,65,65,65	0
30	MG	X	3275	1/1	0.97	0.25	57,57,57,57	0
29	MN	X	3137	1/1	0.97	0.18	72,72,72,72	0
29	MN	X	3116	1/1	0.97	0.31	78,78,78,78	0
29	MN	X	3097	1/1	0.97	0.15	79,79,79,79	0
29	MN	X	3087	1/1	0.97	0.18	63,63,63,63	0
29	MN	X	3020	1/1	0.97	0.15	78,78,78,78	0
29	MN	X	3220	1/1	0.97	0.06	112,112,112,112	0
29	MN	X	3089	1/1	0.97	0.14	69,69,69,69	0
29	MN	X	3166	1/1	0.97	0.11	95,95,95,95	0
29	MN	X	3063	1/1	0.97	0.17	140,140,140,140	0
29	MN	X	3015	1/1	0.97	0.38	63,63,63,63	0
29	MN	X	3146	1/1	0.97	0.09	101,101,101,101	0
29	MN	X	3060	1/1	0.97	0.10	84,84,84,84	0
30	MG	X	3262	1/1	0.97	0.28	82,82,82,82	0
29	MN	X	3148	1/1	0.97	0.39	91,91,91,91	0
29	MN	X	3200	1/1	0.97	0.11	136,136,136,136	0
29	MN	X	3101	1/1	0.98	0.19	60,60,60,60	0
29	MN	X	3034	1/1	0.98	0.11	94,94,94,94	0
29	MN	X	3049	1/1	0.98	0.23	81,81,81,81	0
29	MN	X	3070	1/1	0.98	0.27	97,97,97,97	0
29	MN	X	3050	1/1	0.98	0.19	98,98,98,98	0
29	MN	X	3040	1/1	0.98	0.16	79,79,79,79	0
29	MN	X	3108	1/1	0.98	0.21	70,70,70,70	0
29	MN	X	3041	1/1	0.98	0.09	75,75,75,75	0
29	MN	X	3177	1/1	0.98	0.43	110,110,110,110	0
29	MN	Y	201	1/1	0.98	0.07	95,95,95,95	0

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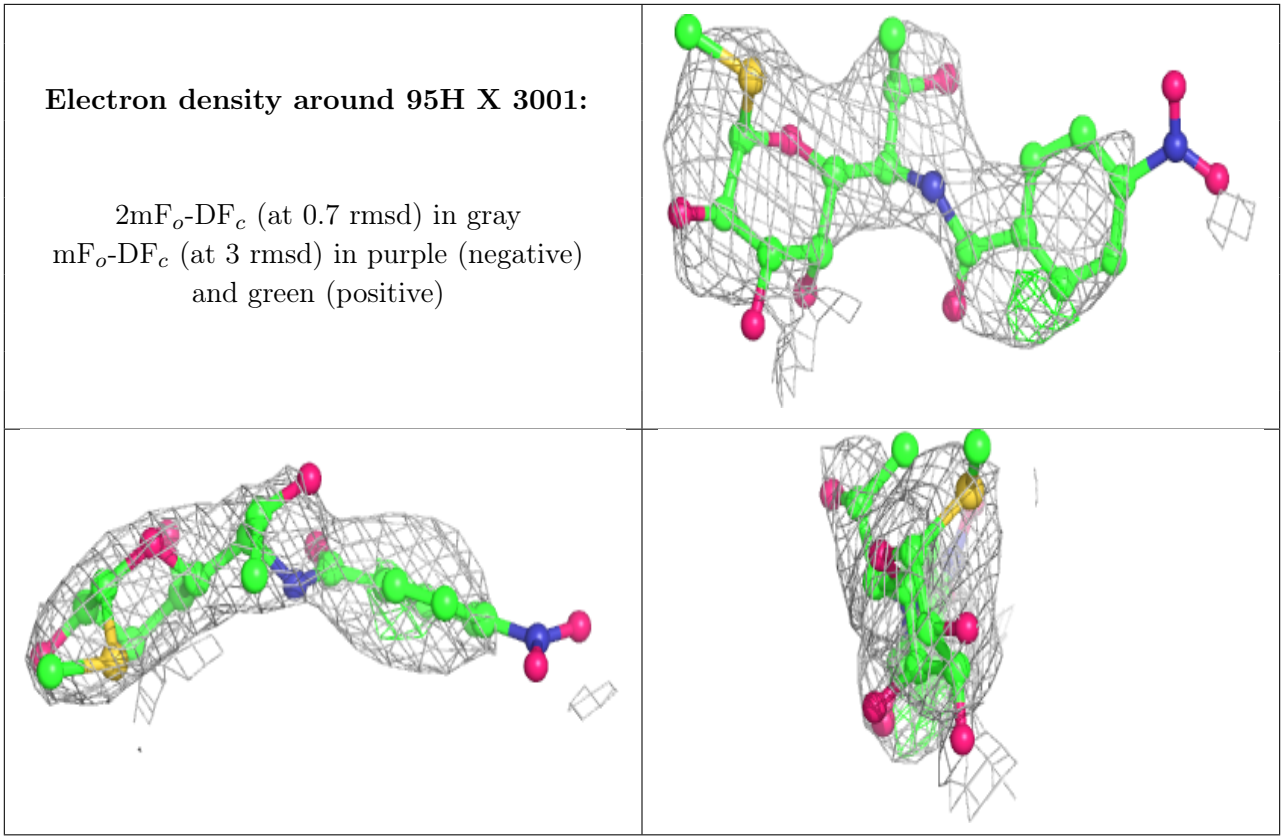
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3044	1/1	0.98	0.18	93,93,93,93	0
29	MN	X	3030	1/1	0.98	0.06	89,89,89,89	0
29	MN	X	3079	1/1	0.98	0.12	70,70,70,70	0
29	MN	X	3095	1/1	0.98	0.12	69,69,69,69	0
29	MN	X	3115	1/1	0.98	0.19	63,63,63,63	0
29	MN	X	3080	1/1	0.98	0.21	59,59,59,59	0
29	MN	X	3024	1/1	0.98	0.23	74,74,74,74	0
29	MN	X	3025	1/1	0.98	0.12	79,79,79,79	0
29	MN	X	3143	1/1	0.98	0.22	44,44,44,44	0
29	MN	X	3083	1/1	0.98	0.19	56,56,56,56	0
29	MN	X	3077	1/1	0.99	0.18	88,88,88,88	0
29	MN	X	3104	1/1	0.99	0.26	86,86,86,86	0
29	MN	X	3121	1/1	0.99	0.07	67,67,67,67	0
29	MN	X	3122	1/1	0.99	0.19	82,82,82,82	0
29	MN	X	3022	1/1	0.99	0.14	74,74,74,74	0
29	MN	X	3124	1/1	0.99	0.22	76,76,76,76	0
30	MG	X	3272	1/1	0.99	0.10	60,60,60,60	0
29	MN	X	3011	1/1	0.99	0.28	40,40,40,40	0
29	MN	X	3004	1/1	0.99	0.29	60,60,60,60	0
29	MN	X	3128	1/1	0.99	0.14	62,62,62,62	0
29	MN	X	3149	1/1	0.99	0.12	102,102,102,102	0
29	MN	X	3129	1/1	0.99	0.25	74,74,74,74	0
29	MN	X	3009	1/1	0.99	0.28	59,59,59,59	0
29	MN	X	3211	1/1	0.99	0.12	100,100,100,100	0
29	MN	X	3153	1/1	0.99	0.17	99,99,99,99	0
29	MN	X	3042	1/1	0.99	0.14	80,80,80,80	0
29	MN	X	3180	1/1	0.99	0.17	70,70,70,70	0
30	MG	X	3284	1/1	0.99	0.06	56,56,56,56	0
29	MN	X	3043	1/1	0.99	0.18	79,79,79,79	0
29	MN	X	3085	1/1	0.99	0.25	61,61,61,61	0
29	MN	X	3086	1/1	0.99	0.09	62,62,62,62	0
29	MN	X	3099	1/1	0.99	0.19	73,73,73,73	0
29	MN	X	3019	1/1	0.99	0.11	73,73,73,73	0
29	MN	X	3014	1/1	0.99	0.19	56,56,56,56	0
29	MN	X	3010	1/1	0.99	0.31	59,59,59,59	0
29	MN	X	3118	1/1	0.99	0.14	69,69,69,69	0
29	MN	X	3078	1/1	1.00	0.18	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 95H X 3001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.