wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2025 – 02:50 PM EST

PDB ID	:	4DV1
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, U20G, bound with streptomycin
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-22
Resolution	:	3.85 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:

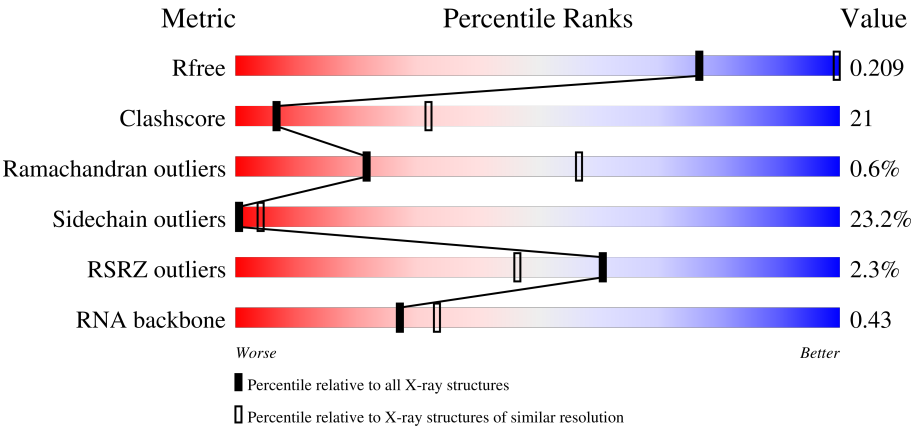
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

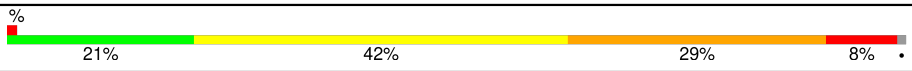
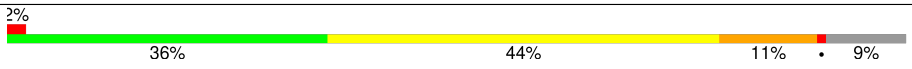
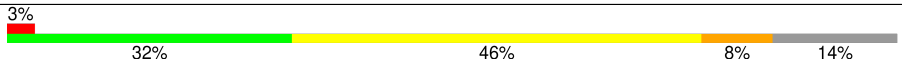
The reported resolution of this entry is 3.85 Å.

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}	164625	1056 (4.00-3.68)
Clashscore	180529	1117 (4.00-3.68)
Ramachandran outliers	177936	1080 (4.00-3.68)
Sidechain outliers	177891	1073 (4.00-3.68)
RSRZ outliers	164620	1056 (4.00-3.68)
RNA backbone	3690	1133 (4.68-3.00)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	

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Mol	Chain	Length	Quality of chain
4	D	209	4% 39% 49% 11%
5	E	162	42% 39% 11% 7%
6	F	101	37% 53% 10%
7	G	156	% 44% 44% 10%
8	H	138	% 46% 41% 13%
9	I	128	4% 44% 45% 11%
10	J	105	6% 43% 39% 11% 7%
11	K	129	2% 47% 35% 8% 10%
12	L	135	3% 40% 36% 16% 8%
13	M	126	6% 44% 40% 10% 6%
14	N	61	3% 39% 49% 10%
15	O	89	% 37% 44% 17%
16	P	88	3% 36% 44% 11% 6%
17	Q	105	3% 35% 44% 14% 6%
18	R	88	34% 36% 9% 20%
19	S	93	8% 34% 37% 15% 14%
20	T	106	2% 31% 50% 12% 7%
21	U	27	4% 41% 37% 11% 11%

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
23	MG	A	1712	-	-	-	X
23	MG	A	1730	-	-	-	X
23	MG	A	1757	-	-	-	X
23	MG	P	101	-	-	-	X

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 52297 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32510	14478	6014	10506	1512	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	G	U	engineered mutation	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

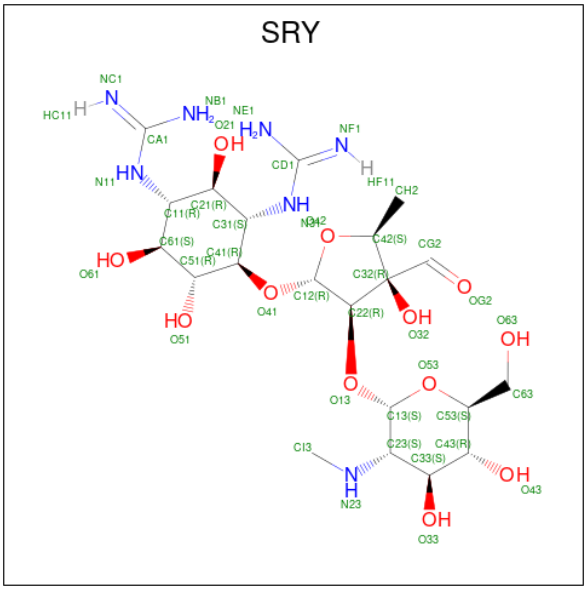
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			40	21	7	12		

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	230	Total Mg 230 230	0	0
23	B	1	Total Mg 1 1	0	0
23	D	1	Total Mg 1 1	0	0
23	E	1	Total Mg 1 1	0	0
23	H	2	Total Mg 2 2	0	0
23	I	1	Total Mg 1 1	0	0
23	J	1	Total Mg 1 1	0	0
23	K	1	Total Mg 1 1	0	0
23	M	2	Total Mg 2 2	0	0
23	N	2	Total Mg 2 2	0	0
23	P	1	Total Mg 1 1	0	0
23	S	2	Total Mg 2 2	0	0
23	T	2	Total Mg 2 2	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	396	Total O 396 396	0	0
25	E	6	Total O 6 6	0	0

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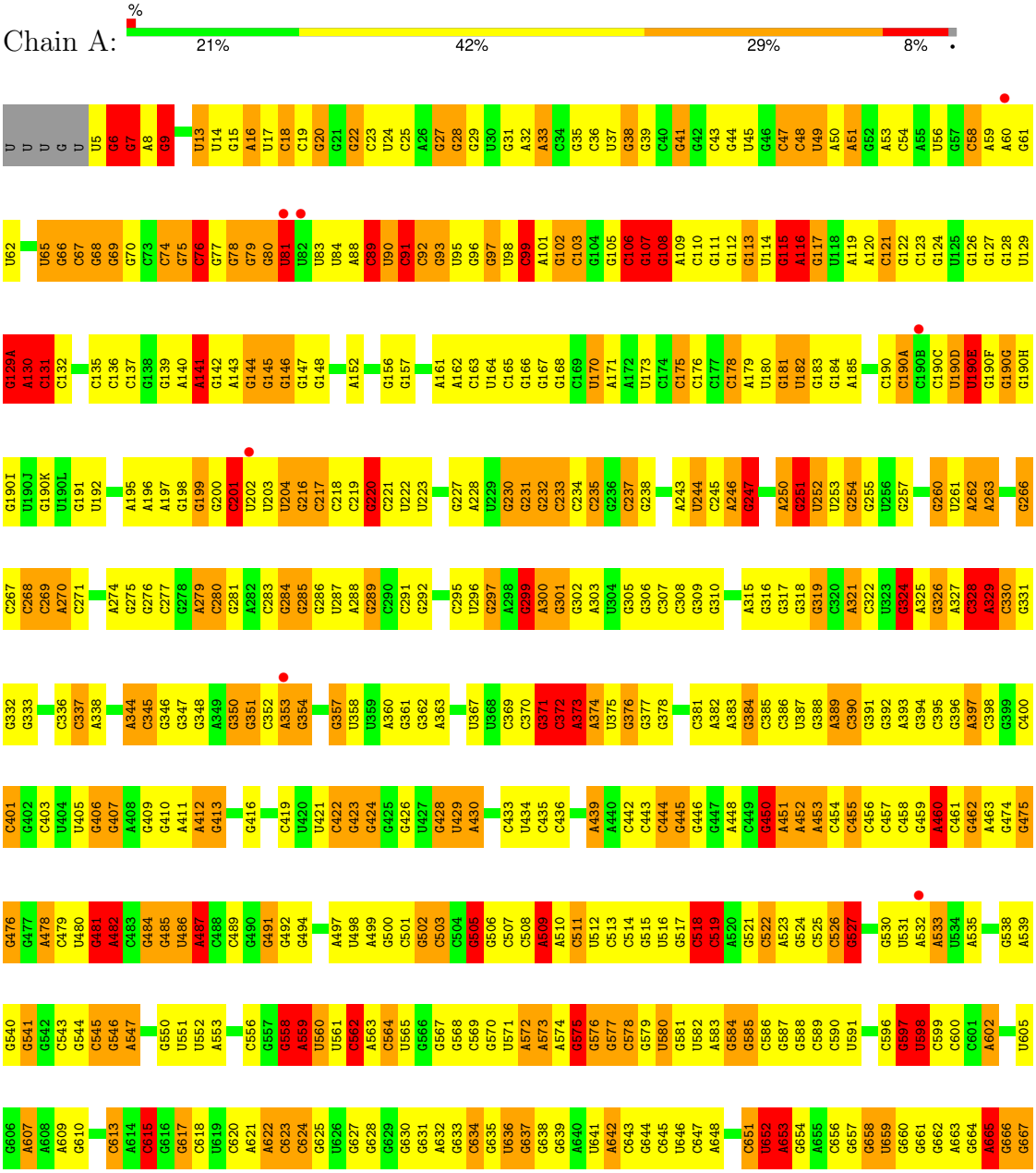
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	G	1	Total O 1 1	0	0
25	J	1	Total O 1 1	0	0
25	N	1	Total O 1 1	0	0
25	Q	1	Total O 1 1	0	0
25	T	3	Total O 3 3	0	0
25	U	1	Total O 1 1	0	0

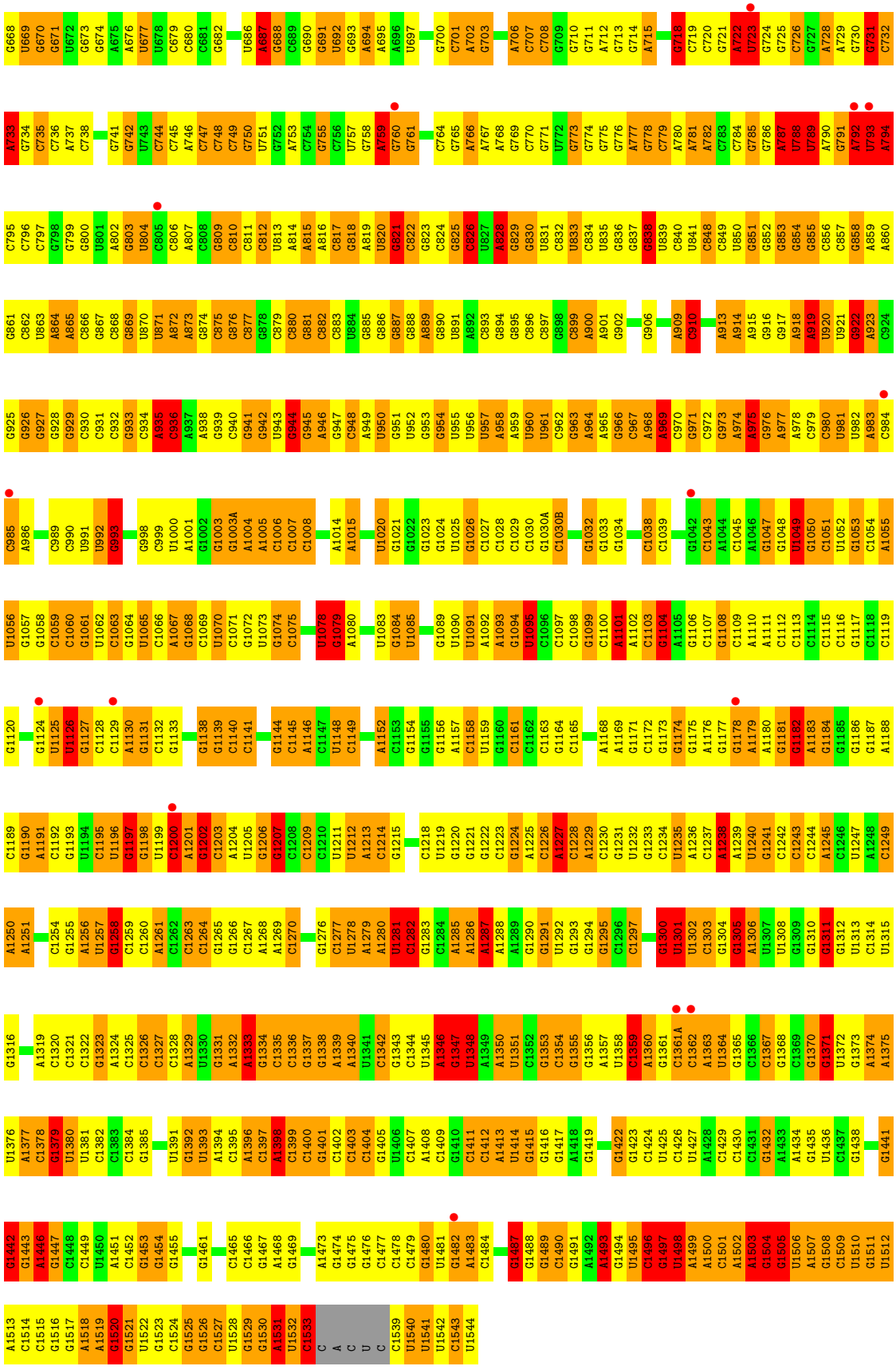
3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 16S rRNA

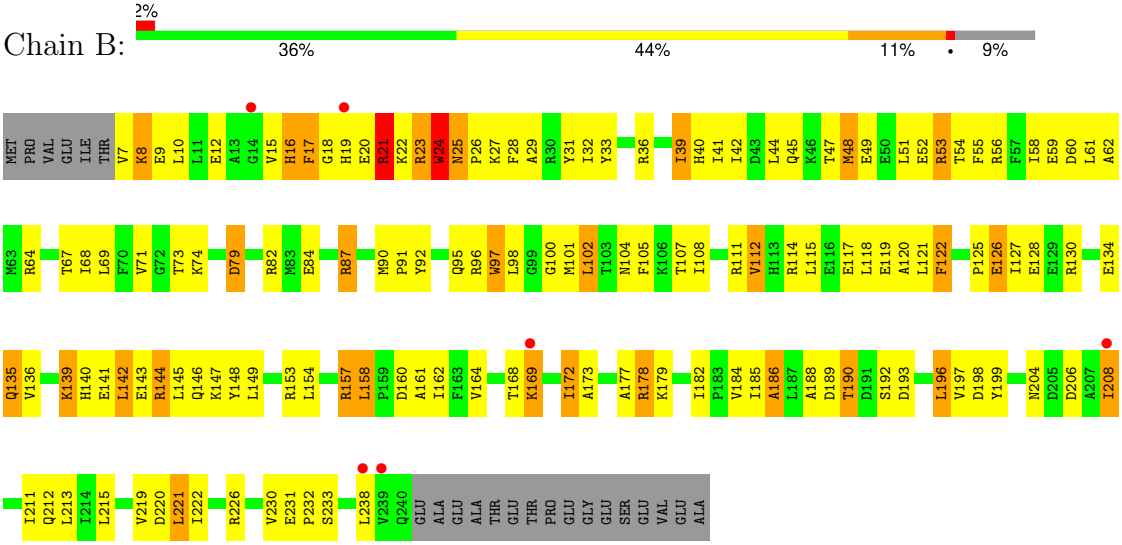
Chain A:





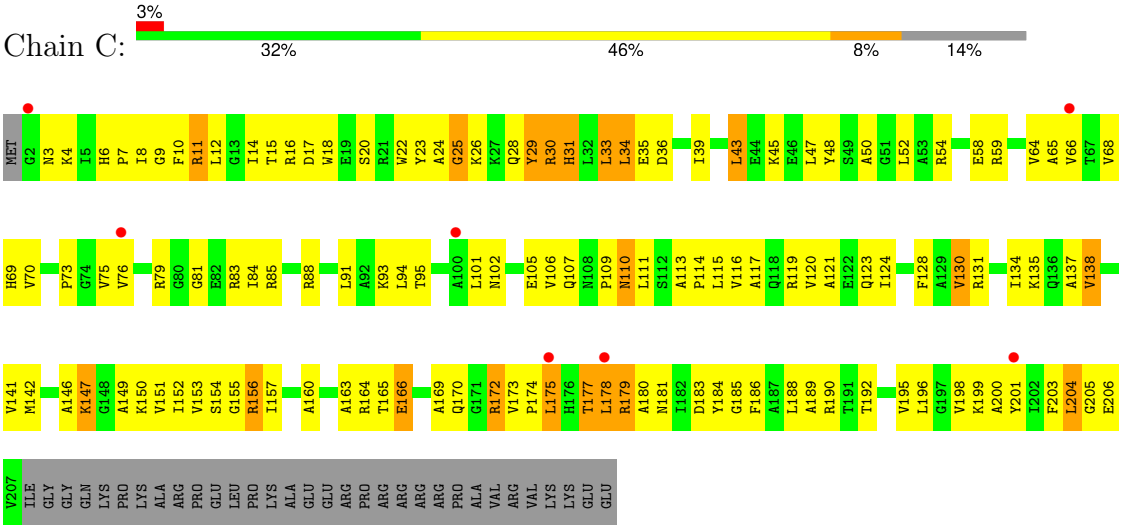
• Molecule 2: ribosomal protein S2

Chain B:



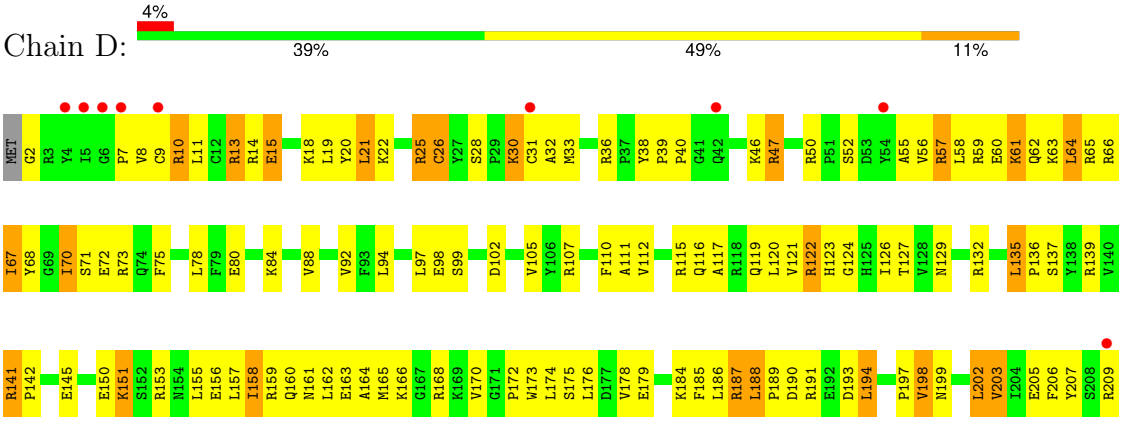
• Molecule 3: ribosomal protein S3

Chain C:



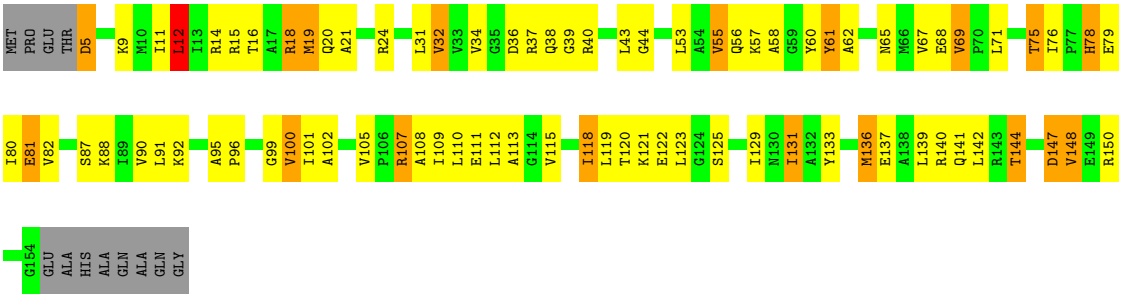
• Molecule 4: ribosomal protein S4

Chain D:



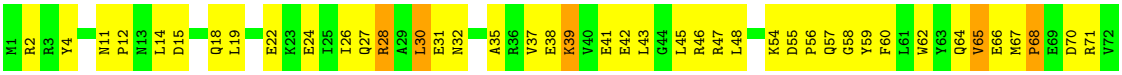
• Molecule 5: ribosomal protein S5

Chain E:



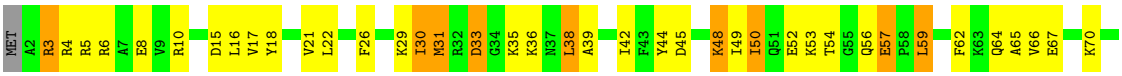
• Molecule 6: ribosomal protein S6

Chain F:



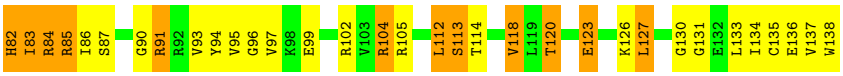
• Molecule 7: ribosomal protein S7

Chain G:



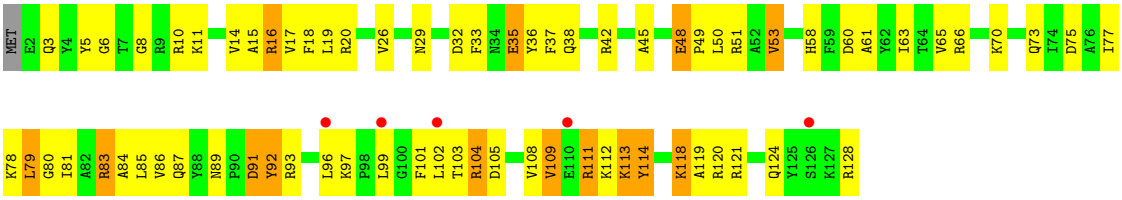
• Molecule 8: ribosomal protein S8

Chain H:



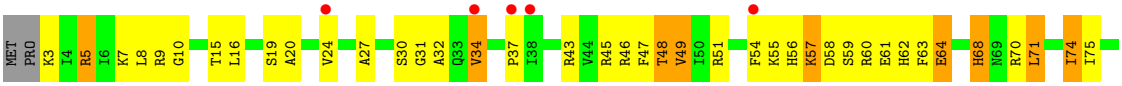
• Molecule 9: ribosomal protein S9

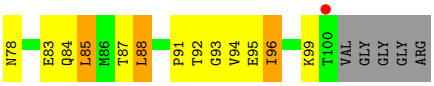
Chain I:



• Molecule 10: ribosomal protein S10

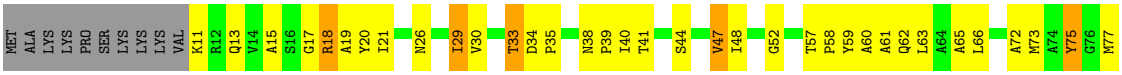
Chain J:

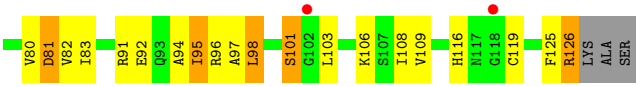




• Molecule 11: ribosomal protein S11

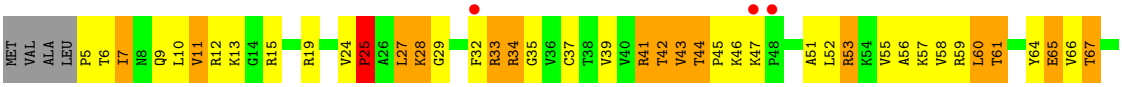
Chain K:





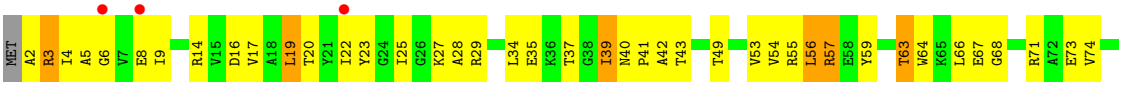
• Molecule 12: ribosomal protein S12

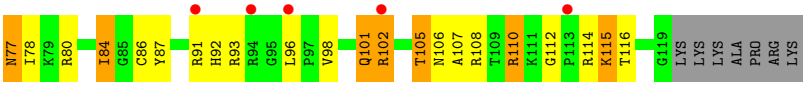
Chain L:



• Molecule 13: ribosomal protein S13

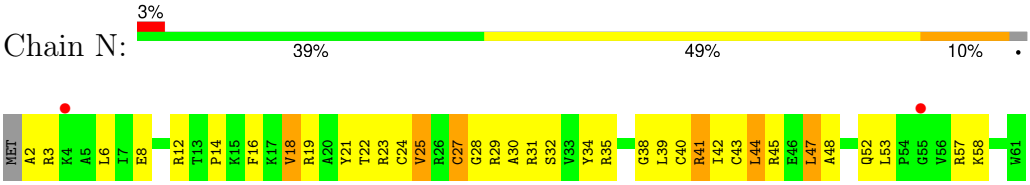
Chain M:





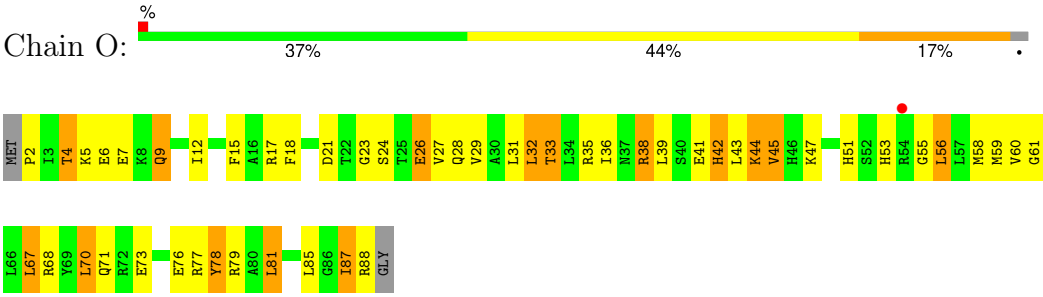
• Molecule 14: ribosomal protein S14

Chain N:



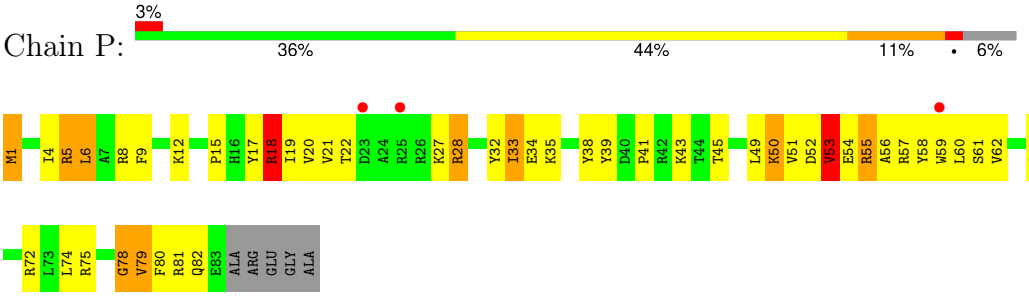
• Molecule 15: ribosomal protein S15

Chain O:



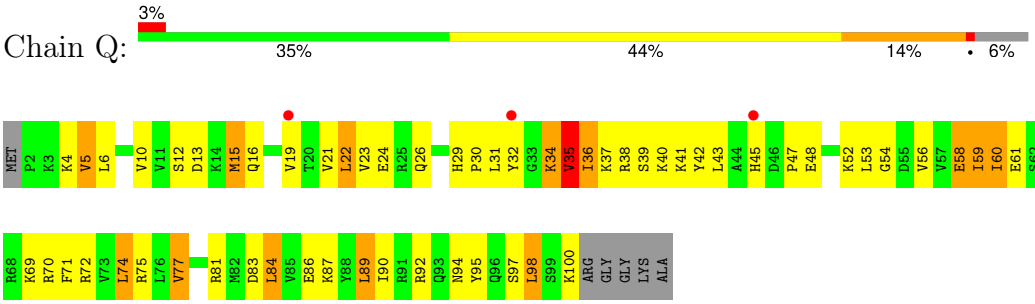
• Molecule 16: ribosomal protein S16

Chain P:



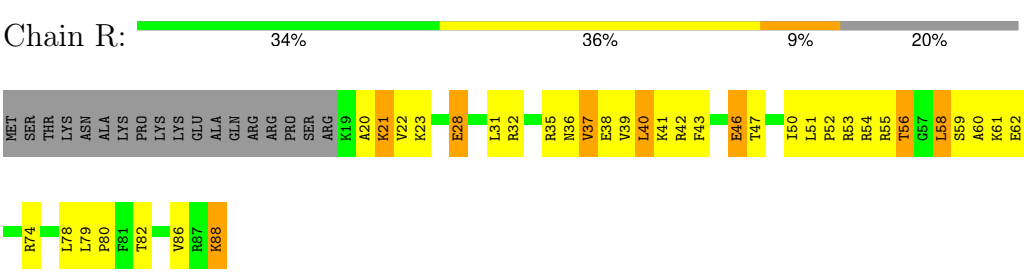
• Molecule 17: ribosomal protein S17

Chain Q:



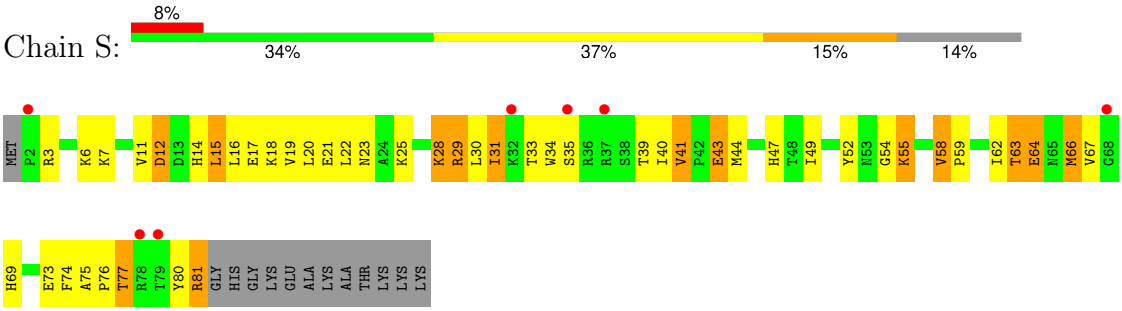
• Molecule 18: ribosomal protein S18

Chain R:



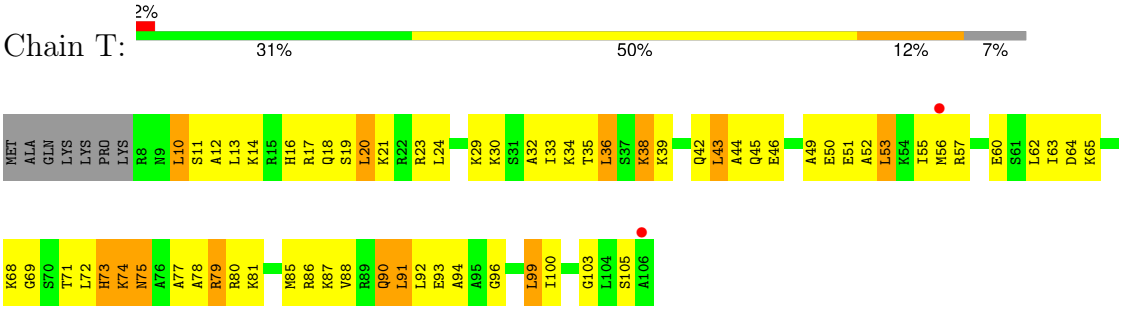
• Molecule 19: ribosomal protein S19

Chain S:



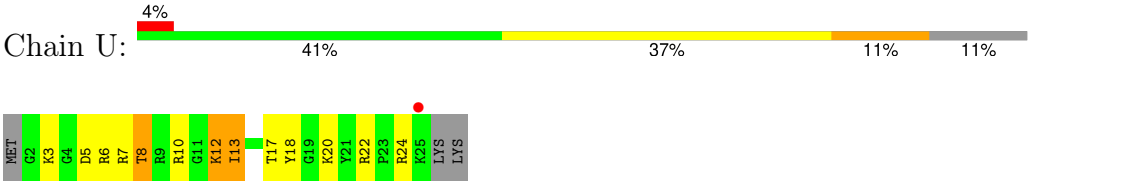
• Molecule 20: ribosomal protein S20

Chain T:



• Molecule 21: ribosomal protein THX

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	403.45Å 403.45Å 173.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.85 34.93 – 3.85	Depositor EDS
% Data completeness (in resolution range)	97.3 (34.93-3.85) 96.9 (34.93-3.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.87Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.150 , 0.212 0.150 , 0.209	Depositor DCC
R_{free} test set	6514 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	161.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 153.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52297	wwPDB-VP
Average B, all atoms (Å^2)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: 7MG, 0TD, UR3, M2G, MG, ZN, 4OC, PSU, MA6, 2MG, 5MC, SRY

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	1.12	108/36044 (0.3%)	1.81	1604/56250 (2.9%)
2	B	0.63	0/1935	0.79	0/2609
3	C	0.59	0/1636	0.78	1/2205 (0.0%)
4	D	0.69	0/1733	0.89	2/2318 (0.1%)
5	E	0.88	0/1162	1.05	3/1564 (0.2%)
6	F	0.61	0/856	0.79	1/1154 (0.1%)
7	G	0.64	0/1276	0.84	0/1709
8	H	1.01	1/1136 (0.1%)	1.12	2/1527 (0.1%)
9	I	0.61	0/1029	0.82	0/1379
10	J	0.56	0/805	0.80	0/1082
11	K	0.68	0/879	0.89	0/1187
12	L	0.77	0/977	1.01	1/1306 (0.1%)
13	M	0.66	0/947	0.85	0/1270
14	N	0.64	0/501	0.83	0/664
15	O	0.73	0/740	0.91	0/987
16	P	0.77	0/716	1.00	2/963 (0.2%)
17	Q	0.97	0/836	1.14	6/1117 (0.5%)
18	R	0.70	0/579	0.87	1/768 (0.1%)
19	S	0.55	0/661	0.75	0/890
20	T	0.74	0/765	1.00	1/1007 (0.1%)
21	U	0.64	0/212	0.78	0/277
All	All	1.00	109/55425 (0.2%)	1.58	1624/82233 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	1
13	M	0	1
16	P	0	2
20	T	0	1
All	All	0	9

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1509	C	N3-C4	-10.95	1.26	1.33
1	A	279	A	N9-C4	-10.62	1.31	1.37
1	A	573	A	N7-C5	-8.71	1.34	1.39
1	A	1523	G	N7-C5	-8.10	1.34	1.39
1	A	715	A	N9-C4	-8.01	1.33	1.37

The worst 5 of 1624 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	573	A	C8-N9-C4	-18.34	98.46	105.80
1	A	1505	G	C8-N9-C4	-15.18	100.33	106.40
1	A	372	C	C6-N1-C2	13.96	125.89	120.30
1	A	279	A	C5-N7-C8	-13.43	97.18	103.90
1	A	481	G	N3-C4-N9	13.26	133.96	126.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	186	ALA	Peptide
2	B	8	LYS	Peptide
8	H	90	GLY	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	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	32510	0	16434	862	0
2	B	1900	0	1951	98	0
3	C	1612	0	1677	122	0
4	D	1703	0	1763	105	0
5	E	1146	0	1207	59	0
6	F	843	0	857	47	0
7	G	1257	0	1296	69	0
8	H	1116	0	1177	60	0
9	I	1010	0	1037	75	0
10	J	792	0	835	49	0
11	K	864	0	881	37	0
12	L	972	0	1058	67	0
13	M	937	0	995	51	0
14	N	492	0	529	49	0
15	O	729	0	768	37	0
16	P	700	0	720	49	0
17	Q	823	0	893	52	0
18	R	574	0	644	41	0
19	S	647	0	673	34	0
20	T	763	0	861	49	0
21	U	208	0	221	15	0
22	A	40	0	37	7	0
23	A	230	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	2	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0
23	K	1	0	0	0	0
23	M	2	0	0	0	0
23	N	2	0	0	0	0
23	P	1	0	0	0	0
23	S	2	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	396	0	0	4	0
25	E	6	0	0	0	0
25	G	1	0	0	1	0
25	J	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	3	0	0	1	0
25	U	1	0	0	0	0
All	All	52297	0	36514	1832	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 21.

The worst 5 of 1832 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:H5"	1:A:1446:A:H5'	1.37	1.01
1:A:103:C:OP1	20:T:17:ARG:NH1	1.98	0.95
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.50	0.91
1:A:279:A:OP2	17:Q:95:TYR:OH	1.89	0.90
4:D:68:TYR:OH	4:D:98:GLU:OE1	1.91	0.89

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
2	B	232/256 (91%)	200 (86%)	30 (13%)	2 (1%)	14 48
3	C	204/239 (85%)	179 (88%)	25 (12%)	0	100 100
4	D	206/209 (99%)	186 (90%)	20 (10%)	0	100 100
5	E	148/162 (91%)	136 (92%)	11 (7%)	1 (1%)	19 54
6	F	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	13 46
7	G	153/156 (98%)	136 (89%)	16 (10%)	1 (1%)	19 54
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100 100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	13 46
11	K	114/129 (88%)	103 (90%)	11 (10%)	0	100 100
12	L	121/135 (90%)	107 (88%)	12 (10%)	2 (2%)	7 36
13	M	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	14 48
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100 100
15	O	85/89 (96%)	80 (94%)	4 (5%)	1 (1%)	11 43
16	P	81/88 (92%)	75 (93%)	5 (6%)	1 (1%)	11 43
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100 100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100 100
19	S	78/93 (84%)	67 (86%)	10 (13%)	1 (1%)	10 41
20	T	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	13 46
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100 100
All	All	2336/2541 (92%)	2089 (89%)	233 (10%)	14 (1%)	22 57

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
12	L	28	LYS
2	B	21	ARG
2	B	24	TRP
9	I	119	ALA

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
2	B	202/220 (92%)	158 (78%)	44 (22%)	1 5
3	C	160/188 (85%)	129 (81%)	31 (19%)	1 7
4	D	180/181 (99%)	136 (76%)	44 (24%)	0 4
5	E	115/123 (94%)	83 (72%)	32 (28%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	F	90/90 (100%)	70 (78%)	20 (22%)	1 5
7	G	126/127 (99%)	96 (76%)	30 (24%)	0 4
8	H	119/119 (100%)	91 (76%)	28 (24%)	0 4
9	I	98/99 (99%)	76 (78%)	22 (22%)	1 5
10	J	87/92 (95%)	71 (82%)	16 (18%)	1 9
11	K	88/99 (89%)	71 (81%)	17 (19%)	1 7
12	L	103/110 (94%)	75 (73%)	28 (27%)	0 3
13	M	94/101 (93%)	74 (79%)	20 (21%)	1 5
14	N	49/50 (98%)	39 (80%)	10 (20%)	1 6
15	O	79/80 (99%)	56 (71%)	23 (29%)	0 2
16	P	72/74 (97%)	57 (79%)	15 (21%)	1 5
17	Q	94/97 (97%)	71 (76%)	23 (24%)	0 3
18	R	61/77 (79%)	47 (77%)	14 (23%)	0 4
19	S	71/80 (89%)	51 (72%)	20 (28%)	0 2
20	T	76/82 (93%)	55 (72%)	21 (28%)	0 2
21	U	19/22 (86%)	16 (84%)	3 (16%)	2 13
All	All	1983/2111 (94%)	1522 (77%)	461 (23%)	0 4

5 of 461 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	16	ARG
20	T	36	LEU
12	L	27	LEU
20	T	13	LEU
17	Q	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
15	O	46	HIS
9	I	73	GLN
6	F	100	ASN
6	F	73	ASN
7	G	110	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	390 (25%)	45 (2%)

5 of 390 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	19	C
1	A	22	G

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1049	U
1	A	1201	A
1	A	1065	U
1	A	1145	C
1	A	1257	U

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PSU	A	1540	1	18,21,22	1.41	1 (5%)	21,30,33	1.64	4 (19%)
1	5MC	A	1404	1	19,22,23	1.54	4 (21%)	26,32,35	1.45	5 (19%)
1	5MC	A	967	1	19,22,23	1.09	2 (10%)	26,32,35	0.90	1 (3%)
1	MA6	A	1519	1	19,26,27	2.25	5 (26%)	18,38,41	0.94	0
1	2MG	A	1207	1	18,26,27	1.70	4 (22%)	16,38,41	1.31	2 (12%)
1	PSU	A	1541	1	18,21,22	1.27	1 (5%)	21,30,33	1.91	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	7MG	A	527	1	23,26,27	3.80	7 (30%)	27,39,42	2.62	9 (33%)
1	5MC	A	1407	1	19,22,23	2.27	5 (26%)	26,32,35	1.29	4 (15%)
1	UR3	A	1498	1	19,22,23	1.18	1 (5%)	26,32,35	1.14	1 (3%)
1	4OC	A	1402	1	20,23,24	1.25	1 (5%)	25,32,35	0.72	0
12	0TD	L	92	12	8,9,10	1.02	0	6,11,13	3.36	3 (50%)
1	MA6	A	1518	1	19,26,27	1.70	3 (15%)	18,38,41	1.41	2 (11%)
1	5MC	A	1400	1	19,22,23	1.56	4 (21%)	26,32,35	1.09	4 (15%)
1	PSU	A	516	1	18,21,22	1.39	3 (16%)	21,30,33	1.39	4 (19%)
1	M2G	A	966	1	20,27,28	1.40	4 (20%)	19,40,43	1.34	2 (10%)

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
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	5/7/29/30	0/3/3/3
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	PSU	A	1541	1	-	2/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
12	0TD	L	92	12	-	4/7/12/14	-
1	MA6	A	1518	1	-	5/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-16.09	1.35	1.45
1	A	1407	5MC	C5-C4	6.98	1.49	1.44
1	A	1519	MA6	C6-N1	6.11	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C5-N7	5.84	1.43	1.35
1	A	1540	PSU	C6-C5	5.05	1.40	1.35

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	7MG	C5-C6-N1	6.42	122.24	110.94
12	L	92	0TD	CSB-SB-CB	-6.04	91.51	102.36
1	A	527	7MG	N9-C4-N3	5.74	133.87	125.46
1	A	1541	PSU	N1-C2-N3	5.03	120.48	115.17
1	A	1518	MA6	C1'-N9-C4	-4.96	117.92	126.64

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C9

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1540	PSU	1	0
1	A	1404	5MC	3	0
1	A	967	5MC	1	0
1	A	1519	MA6	4	0
1	A	1207	2MG	1	0
1	A	1541	PSU	1	0
1	A	527	7MG	1	0
1	A	1498	UR3	3	0
12	L	92	0TD	2	0
1	A	1518	MA6	2	0
1	A	1400	5MC	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 250 ligands modelled in this entry, 249 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	$\#\|Z\| > 2$
22	SRY	A	1601	-	40,42,42	2.42	13 (32%)	49,63,63	2.32	11 (22%)

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
22	SRY	A	1601	-	-	5/20/87/87	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.49	1.49	1.33
22	A	1601	SRY	CA1-N11	6.03	1.43	1.33
22	A	1601	SRY	C11-N11	-3.42	1.40	1.45
22	A	1601	SRY	O53-C53	-3.38	1.36	1.44
22	A	1601	SRY	CA1-NB1	3.10	1.45	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	SRY	C13-O13-C22	-6.04	105.98	116.26
22	A	1601	SRY	C61-C11-N11	-6.02	99.52	110.62
22	A	1601	SRY	C12-O42-C42	-5.83	99.07	108.48
22	A	1601	SRY	O41-C12-O42	-4.52	106.75	111.37
22	A	1601	SRY	CI3-N23-C23	-4.51	108.41	114.23

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C41-C31-N31-CD1
22	A	1601	SRY	C21-C31-N31-CD1
22	A	1601	SRY	C21-C11-N11-CA1
22	A	1601	SRY	C61-C11-N11-CA1

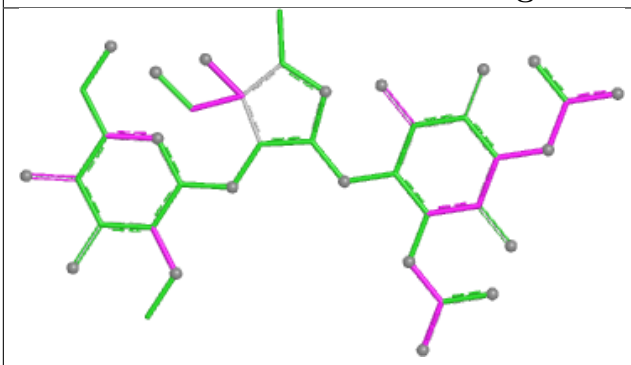
There are no ring outliers.

1 monomer is involved in 7 short contacts:

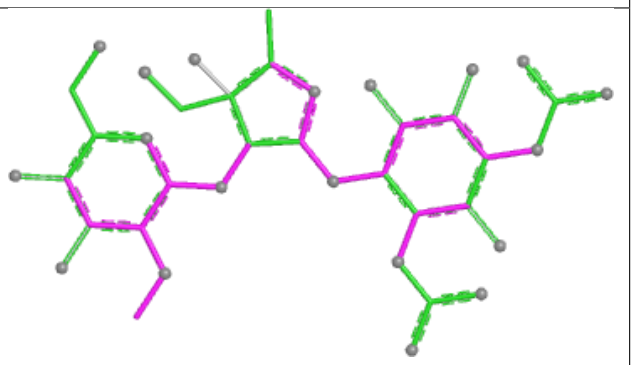
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	7	0

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.

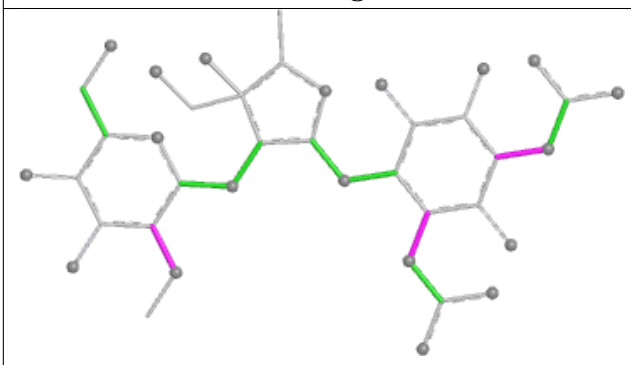
Ligand SRY A 1601



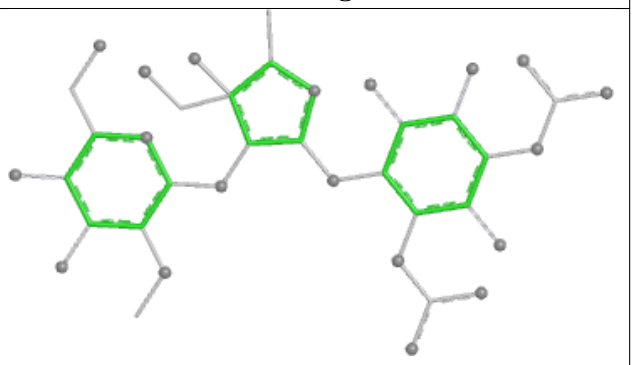
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	1498/1522 (98%)	-0.19	22 (1%)	71	55	106, 179, 327, 407	0
2	B	234/256 (91%)	-0.32	6 (2%)	57	44	145, 211, 332, 358	0
3	C	206/239 (86%)	-0.07	7 (3%)	48	39	181, 265, 316, 365	0
4	D	208/209 (99%)	0.04	9 (4%)	40	34	124, 193, 249, 283	0
5	E	150/162 (92%)	-0.47	0	100	100	104, 150, 199, 232	0
6	F	101/101 (100%)	-0.43	0	100	100	155, 212, 246, 277	0
7	G	155/156 (99%)	-0.19	2 (1%)	74	58	172, 228, 288, 335	0
8	H	138/138 (100%)	-0.42	1 (0%)	84	71	94, 135, 187, 218	0
9	I	127/128 (99%)	-0.07	5 (3%)	44	36	201, 250, 303, 322	0
10	J	98/105 (93%)	0.28	6 (6%)	28	25	220, 277, 355, 391	0
11	K	116/129 (89%)	-0.33	2 (1%)	69	52	130, 171, 224, 258	0
12	L	123/135 (91%)	0.02	4 (3%)	49	39	107, 175, 218, 248	0
13	M	118/126 (93%)	0.10	8 (6%)	25	23	162, 214, 254, 309	0
14	N	60/61 (98%)	-0.01	2 (3%)	49	39	187, 249, 314, 329	0
15	O	87/89 (97%)	-0.09	1 (1%)	77	63	113, 171, 213, 232	0
16	P	83/88 (94%)	-0.12	3 (3%)	46	38	130, 180, 220, 274	0
17	Q	99/105 (94%)	-0.10	3 (3%)	52	41	116, 150, 201, 232	0
18	R	70/88 (79%)	-0.26	0	100	100	116, 183, 244, 259	0
19	S	80/93 (86%)	0.36	7 (8%)	17	17	234, 284, 341, 352	0
20	T	99/106 (93%)	-0.24	2 (2%)	64	49	124, 172, 240, 267	0
21	U	24/27 (88%)	0.35	1 (4%)	41	34	198, 248, 286, 302	0
All	All	3874/4063 (95%)	-0.16	91 (2%)	61	46	94, 194, 306, 407	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	4	TYR	5.5
20	T	106	ALA	5.2
7	G	154	TYR	5.0
3	C	2	GLY	4.7
1	A	532	A	4.5

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	PSU	A	1541	20/21	0.73	0.18	297,305,321,325	0
1	PSU	A	1540	20/21	0.75	0.21	235,263,334,335	0
1	MA6	A	1518	24/25	0.92	0.10	151,187,221,227	0
1	M2G	A	966	25/26	0.93	0.11	177,182,207,211	0
1	PSU	A	516	20/21	0.93	0.10	163,188,214,220	0
1	7MG	A	527	24/25	0.94	0.13	125,146,165,180	0
1	MA6	A	1519	24/25	0.96	0.13	144,181,202,206	0
1	5MC	A	1407	21/22	0.96	0.09	171,191,202,207	0
1	5MC	A	1400	21/22	0.96	0.11	142,169,178,182	0
12	0TD	L	92	10/11	0.96	0.10	121,166,173,350	0
1	UR3	A	1498	21/22	0.97	0.09	160,183,204,223	0
1	4OC	A	1402	22/23	0.97	0.11	150,156,180,192	0
1	2MG	A	1207	24/25	0.97	0.15	231,289,310,316	0
1	5MC	A	1404	21/22	0.98	0.08	166,182,196,204	0
1	5MC	A	967	21/22	0.98	0.07	182,192,200,205	0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1681	1/1	0.36	0.20	243,243,243,243	0
23	MG	A	1831	1/1	0.40	0.18	484,484,484,484	0
23	MG	K	201	1/1	0.44	0.23	181,181,181,181	0
23	MG	S	102	1/1	0.52	0.33	156,156,156,156	0
23	MG	B	301	1/1	0.60	0.27	181,181,181,181	0
23	MG	N	103	1/1	0.60	0.25	156,156,156,156	0
23	MG	E	201	1/1	0.60	0.14	435,435,435,435	0
23	MG	A	1757	1/1	0.62	1.04	143,143,143,143	0
23	MG	A	1659	1/1	0.64	0.32	142,142,142,142	0
23	MG	P	101	1/1	0.67	0.44	122,122,122,122	0
23	MG	A	1778	1/1	0.71	0.33	156,156,156,156	0
23	MG	A	1712	1/1	0.72	0.55	138,138,138,138	0
23	MG	A	1788	1/1	0.72	0.27	156,156,156,156	0
23	MG	A	1773	1/1	0.72	0.32	162,162,162,162	0
23	MG	A	1817	1/1	0.73	0.10	197,197,197,197	0
23	MG	A	1763	1/1	0.74	0.37	181,181,181,181	0
23	MG	A	1696	1/1	0.74	0.12	245,245,245,245	0
23	MG	A	1710	1/1	0.74	0.23	161,161,161,161	0
23	MG	A	1693	1/1	0.78	0.35	179,179,179,179	0
23	MG	A	1730	1/1	0.79	0.70	134,134,134,134	0
23	MG	A	1695	1/1	0.80	0.63	245,245,245,245	0
23	MG	A	1714	1/1	0.80	0.22	143,143,143,143	0
23	MG	A	1736	1/1	0.81	0.53	125,125,125,125	0
23	MG	H	201	1/1	0.81	0.21	131,131,131,131	0
23	MG	A	1751	1/1	0.81	0.43	133,133,133,133	0
23	MG	A	1692	1/1	0.81	0.62	142,142,142,142	0
23	MG	A	1728	1/1	0.81	0.16	150,150,150,150	0
23	MG	A	1668	1/1	0.81	0.49	173,173,173,173	0
23	MG	A	1784	1/1	0.82	0.32	145,145,145,145	0
23	MG	A	1819	1/1	0.82	0.22	483,483,483,483	0
23	MG	A	1765	1/1	0.83	0.16	372,372,372,372	0
23	MG	A	1782	1/1	0.83	0.34	131,131,131,131	0
23	MG	A	1787	1/1	0.84	0.40	102,102,102,102	0
23	MG	M	202	1/1	0.84	0.31	148,148,148,148	0
23	MG	A	1739	1/1	0.84	0.27	162,162,162,162	0
23	MG	A	1770	1/1	0.84	0.41	141,141,141,141	0
23	MG	A	1718	1/1	0.84	0.64	144,144,144,144	0
23	MG	A	1783	1/1	0.85	0.32	133,133,133,133	0
23	MG	A	1755	1/1	0.85	0.54	190,190,190,190	0
23	MG	A	1727	1/1	0.85	0.27	138,138,138,138	0
23	MG	A	1744	1/1	0.85	0.17	176,176,176,176	0
23	MG	A	1623	1/1	0.85	0.32	170,170,170,170	0
23	MG	A	1771	1/1	0.86	0.43	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1785	1/1	0.86	0.55	142,142,142,142	0
23	MG	A	1758	1/1	0.86	0.52	128,128,128,128	0
23	MG	A	1774	1/1	0.86	0.37	128,128,128,128	0
23	MG	A	1802	1/1	0.86	0.14	457,457,457,457	0
23	MG	A	1738	1/1	0.86	0.45	123,123,123,123	0
23	MG	A	1636	1/1	0.86	0.29	186,186,186,186	0
23	MG	A	1706	1/1	0.86	0.41	163,163,163,163	0
23	MG	A	1704	1/1	0.87	0.20	118,118,118,118	0
23	MG	A	1746	1/1	0.87	0.21	282,282,282,282	0
23	MG	A	1720	1/1	0.87	0.34	139,139,139,139	0
23	MG	M	201	1/1	0.87	0.43	163,163,163,163	0
23	MG	A	1750	1/1	0.88	0.18	125,125,125,125	0
23	MG	A	1822	1/1	0.88	0.25	374,374,374,374	0
23	MG	A	1795	1/1	0.88	0.38	457,457,457,457	0
23	MG	A	1672	1/1	0.89	0.26	102,102,102,102	0
23	MG	A	1661	1/1	0.89	0.49	124,124,124,124	0
23	MG	A	1626	1/1	0.89	0.57	118,118,118,118	0
23	MG	A	1772	1/1	0.89	0.14	121,121,121,121	0
23	MG	A	1667	1/1	0.90	0.47	143,143,143,143	0
23	MG	D	302	1/1	0.90	0.15	186,186,186,186	0
23	MG	A	1777	1/1	0.90	0.25	107,107,107,107	0
23	MG	A	1768	1/1	0.90	0.06	550,550,550,550	0
23	MG	A	1781	1/1	0.90	0.21	145,145,145,145	0
23	MG	A	1813	1/1	0.90	0.58	146,146,146,146	0
23	MG	A	1643	1/1	0.90	0.27	135,135,135,135	0
23	MG	A	1618	1/1	0.90	0.22	152,152,152,152	0
23	MG	A	1679	1/1	0.90	0.64	133,133,133,133	0
23	MG	A	1637	1/1	0.90	0.39	143,143,143,143	0
23	MG	A	1747	1/1	0.91	0.15	296,296,296,296	0
23	MG	A	1725	1/1	0.91	0.21	153,153,153,153	0
23	MG	A	1737	1/1	0.91	0.24	140,140,140,140	0
23	MG	A	1794	1/1	0.91	0.23	206,206,206,206	0
23	MG	A	1658	1/1	0.91	0.13	146,146,146,146	0
23	MG	I	201	1/1	0.91	0.16	204,204,204,204	0
23	MG	A	1656	1/1	0.92	0.27	173,173,173,173	0
23	MG	A	1682	1/1	0.92	0.08	365,365,365,365	0
23	MG	A	1754	1/1	0.92	0.07	177,177,177,177	0
23	MG	A	1697	1/1	0.92	0.29	135,135,135,135	0
23	MG	A	1701	1/1	0.92	0.22	129,129,129,129	0
23	MG	A	1721	1/1	0.92	0.20	135,135,135,135	0
23	MG	A	1760	1/1	0.92	0.06	130,130,130,130	0
23	MG	A	1779	1/1	0.92	0.52	146,146,146,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1677	1/1	0.92	0.24	191,191,191,191	0
23	MG	A	1818	1/1	0.92	0.42	483,483,483,483	0
23	MG	A	1638	1/1	0.92	0.18	170,170,170,170	0
23	MG	A	1694	1/1	0.92	0.22	180,180,180,180	0
23	MG	A	1769	1/1	0.93	0.15	209,209,209,209	0
23	MG	A	1732	1/1	0.93	0.53	131,131,131,131	0
23	MG	A	1715	1/1	0.93	0.33	151,151,151,151	0
23	MG	A	1759	1/1	0.93	0.16	161,161,161,161	0
23	MG	A	1651	1/1	0.93	0.49	140,140,140,140	0
23	MG	A	1647	1/1	0.93	0.23	180,180,180,180	0
23	MG	A	1820	1/1	0.93	0.13	265,265,265,265	0
23	MG	A	1776	1/1	0.93	0.26	111,111,111,111	0
23	MG	A	1700	1/1	0.93	0.12	134,134,134,134	0
23	MG	A	1731	1/1	0.93	0.42	148,148,148,148	0
23	MG	A	1713	1/1	0.94	0.10	133,133,133,133	0
23	MG	A	1829	1/1	0.94	0.09	323,323,323,323	0
23	MG	A	1752	1/1	0.94	0.32	147,147,147,147	0
23	MG	A	1699	1/1	0.94	0.11	135,135,135,135	0
23	MG	A	1735	1/1	0.94	0.22	155,155,155,155	0
23	MG	A	1676	1/1	0.94	0.32	133,133,133,133	0
23	MG	A	1654	1/1	0.94	0.30	201,201,201,201	0
23	MG	A	1702	1/1	0.94	0.09	126,126,126,126	0
23	MG	A	1811	1/1	0.94	0.16	346,346,346,346	0
23	MG	A	1621	1/1	0.94	0.17	166,166,166,166	0
23	MG	A	1648	1/1	0.94	0.14	230,230,230,230	0
23	MG	A	1707	1/1	0.94	0.56	120,120,120,120	0
23	MG	A	1633	1/1	0.94	0.22	125,125,125,125	0
23	MG	A	1683	1/1	0.94	0.11	422,422,422,422	0
23	MG	A	1660	1/1	0.95	0.06	194,194,194,194	0
23	MG	A	1745	1/1	0.95	0.44	235,235,235,235	0
23	MG	A	1723	1/1	0.95	0.25	109,109,109,109	0
23	MG	A	1734	1/1	0.95	0.29	163,163,163,163	0
23	MG	A	1809	1/1	0.95	0.22	281,281,281,281	0
23	MG	A	1724	1/1	0.95	0.34	176,176,176,176	0
23	MG	A	1670	1/1	0.95	0.28	173,173,173,173	0
23	MG	A	1645	1/1	0.95	0.09	146,146,146,146	0
23	MG	A	1673	1/1	0.95	0.12	118,118,118,118	0
22	SRY	A	1601	40/40	0.95	0.09	123,154,201,206	0
23	MG	A	1756	1/1	0.95	0.10	213,213,213,213	0
23	MG	A	1741	1/1	0.95	0.15	145,145,145,145	0
23	MG	A	1827	1/1	0.95	0.13	391,391,391,391	0
23	MG	T	201	1/1	0.95	0.09	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1786	1/1	0.96	0.76	145,145,145,145	0
23	MG	A	1663	1/1	0.96	0.15	138,138,138,138	0
23	MG	A	1825	1/1	0.96	0.12	377,377,377,377	0
23	MG	A	1616	1/1	0.96	0.22	107,107,107,107	0
23	MG	A	1789	1/1	0.96	0.11	152,152,152,152	0
23	MG	A	1790	1/1	0.96	0.16	148,148,148,148	0
23	MG	A	1619	1/1	0.96	0.19	253,253,253,253	0
23	MG	A	1617	1/1	0.96	0.08	129,129,129,129	0
23	MG	A	1764	1/1	0.96	0.14	308,308,308,308	0
23	MG	A	1803	1/1	0.96	0.14	342,342,342,342	0
23	MG	A	1807	1/1	0.96	0.15	427,427,427,427	0
23	MG	A	1639	1/1	0.96	0.23	126,126,126,126	0
23	MG	A	1686	1/1	0.96	0.11	150,150,150,150	0
23	MG	A	1641	1/1	0.96	0.05	134,134,134,134	0
23	MG	A	1816	1/1	0.96	0.04	262,262,262,262	0
23	MG	A	1652	1/1	0.96	0.09	141,141,141,141	0
23	MG	A	1742	1/1	0.96	0.05	134,134,134,134	0
23	MG	A	1703	1/1	0.96	0.10	180,180,180,180	0
23	MG	A	1666	1/1	0.97	0.39	187,187,187,187	0
23	MG	A	1603	1/1	0.97	0.10	128,128,128,128	0
23	MG	A	1740	1/1	0.97	0.27	123,123,123,123	0
23	MG	A	1622	1/1	0.97	0.06	138,138,138,138	0
23	MG	A	1716	1/1	0.97	0.10	121,121,121,121	0
23	MG	A	1653	1/1	0.97	0.11	185,185,185,185	0
23	MG	A	1604	1/1	0.97	0.19	133,133,133,133	0
23	MG	A	1775	1/1	0.97	0.09	123,123,123,123	0
23	MG	A	1624	1/1	0.97	0.16	210,210,210,210	0
23	MG	A	1675	1/1	0.97	0.18	121,121,121,121	0
23	MG	A	1749	1/1	0.97	0.35	126,126,126,126	0
23	MG	A	1657	1/1	0.97	0.22	177,177,177,177	0
23	MG	A	1780	1/1	0.97	0.11	111,111,111,111	0
23	MG	A	1608	1/1	0.97	0.15	118,118,118,118	0
23	MG	A	1726	1/1	0.97	0.32	130,130,130,130	0
23	MG	A	1628	1/1	0.97	0.28	191,191,191,191	0
23	MG	A	1632	1/1	0.97	0.07	91,91,91,91	0
23	MG	A	1610	1/1	0.97	0.23	193,193,193,193	0
23	MG	A	1705	1/1	0.97	0.24	153,153,153,153	0
23	MG	A	1635	1/1	0.97	0.13	214,214,214,214	0
23	MG	H	202	1/1	0.97	0.04	137,137,137,137	0
23	MG	A	1733	1/1	0.97	0.07	126,126,126,126	0
23	MG	A	1684	1/1	0.97	0.15	124,124,124,124	0
23	MG	A	1709	1/1	0.97	0.13	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1791	1/1	0.97	0.05	144,144,144,144	0
23	MG	N	102	1/1	0.97	0.16	214,214,214,214	0
23	MG	A	1793	1/1	0.97	0.06	302,302,302,302	0
23	MG	A	1665	1/1	0.97	0.12	247,247,247,247	0
23	MG	S	101	1/1	0.97	0.11	138,138,138,138	0
23	MG	A	1691	1/1	0.97	0.10	187,187,187,187	0
23	MG	A	1800	1/1	0.97	0.34	400,400,400,400	0
23	MG	A	1640	1/1	0.98	0.17	129,129,129,129	0
23	MG	A	1743	1/1	0.98	0.17	183,183,183,183	0
23	MG	A	1805	1/1	0.98	0.25	426,426,426,426	0
23	MG	A	1806	1/1	0.98	0.19	392,392,392,392	0
23	MG	A	1606	1/1	0.98	0.40	126,126,126,126	0
23	MG	A	1808	1/1	0.98	0.15	444,444,444,444	0
23	MG	A	1722	1/1	0.98	0.09	116,116,116,116	0
23	MG	A	1810	1/1	0.98	0.05	117,117,117,117	0
23	MG	A	1629	1/1	0.98	0.06	125,125,125,125	0
23	MG	A	1812	1/1	0.98	0.06	226,226,226,226	0
23	MG	A	1631	1/1	0.98	0.33	127,127,127,127	0
23	MG	A	1814	1/1	0.98	0.20	128,128,128,128	0
23	MG	A	1815	1/1	0.98	0.15	190,190,190,190	0
23	MG	A	1611	1/1	0.98	0.07	223,223,223,223	0
23	MG	A	1662	1/1	0.98	0.13	162,162,162,162	0
23	MG	A	1620	1/1	0.98	0.42	197,197,197,197	0
23	MG	A	1664	1/1	0.98	0.22	226,226,226,226	0
23	MG	A	1753	1/1	0.98	0.13	118,118,118,118	0
23	MG	A	1685	1/1	0.98	0.09	263,263,263,263	0
23	MG	A	1823	1/1	0.98	0.08	194,194,194,194	0
23	MG	A	1708	1/1	0.98	0.14	119,119,119,119	0
23	MG	A	1650	1/1	0.98	0.13	155,155,155,155	0
23	MG	A	1613	1/1	0.98	0.11	126,126,126,126	0
23	MG	A	1830	1/1	0.98	0.13	494,494,494,494	0
23	MG	A	1711	1/1	0.98	0.14	187,187,187,187	0
23	MG	A	1614	1/1	0.98	0.08	94,94,94,94	0
23	MG	A	1615	1/1	0.98	0.08	129,129,129,129	0
23	MG	A	1761	1/1	0.98	0.20	158,158,158,158	0
23	MG	A	1762	1/1	0.98	0.10	109,109,109,109	0
23	MG	A	1669	1/1	0.98	0.27	138,138,138,138	0
23	MG	A	1607	1/1	0.98	0.10	161,161,161,161	0
23	MG	J	201	1/1	0.98	0.14	138,138,138,138	0
23	MG	A	1655	1/1	0.98	0.29	181,181,181,181	0
23	MG	A	1766	1/1	0.98	0.04	220,220,220,220	0
23	MG	A	1717	1/1	0.98	0.09	110,110,110,110	0

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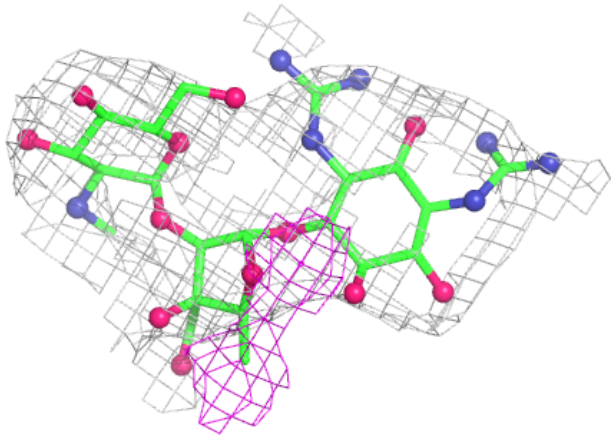
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1796	1/1	0.98	0.23	372,372,372,372	0
23	MG	A	1797	1/1	0.98	0.15	429,429,429,429	0
23	MG	A	1798	1/1	0.98	0.11	454,454,454,454	0
23	MG	A	1799	1/1	0.98	0.12	242,242,242,242	0
23	MG	A	1605	1/1	0.98	0.10	148,148,148,148	0
23	MG	A	1801	1/1	0.98	0.29	423,423,423,423	0
23	MG	T	202	1/1	0.98	0.13	450,450,450,450	0
23	MG	A	1821	1/1	0.99	0.09	236,236,236,236	0
23	MG	A	1687	1/1	0.99	0.04	96,96,96,96	0
23	MG	A	1729	1/1	0.99	0.34	123,123,123,123	0
23	MG	A	1824	1/1	0.99	0.10	366,366,366,366	0
23	MG	A	1688	1/1	0.99	0.20	301,301,301,301	0
23	MG	A	1826	1/1	0.99	0.16	458,458,458,458	0
23	MG	A	1689	1/1	0.99	0.12	151,151,151,151	0
23	MG	A	1828	1/1	0.99	0.19	356,356,356,356	0
23	MG	A	1690	1/1	0.99	0.10	216,216,216,216	0
23	MG	A	1649	1/1	0.99	0.05	192,192,192,192	0
23	MG	A	1602	1/1	0.99	0.20	180,180,180,180	0
23	MG	A	1804	1/1	0.99	0.14	420,420,420,420	0
23	MG	A	1674	1/1	0.99	0.14	112,112,112,112	0
23	MG	A	1627	1/1	0.99	0.12	160,160,160,160	0
23	MG	A	1634	1/1	0.99	0.02	112,112,112,112	0
23	MG	A	1642	1/1	0.99	0.11	107,107,107,107	0
23	MG	A	1678	1/1	0.99	0.07	136,136,136,136	0
23	MG	A	1698	1/1	0.99	0.11	131,131,131,131	0
23	MG	A	1609	1/1	0.99	0.13	155,155,155,155	0
23	MG	A	1680	1/1	0.99	0.11	306,306,306,306	0
23	MG	A	1644	1/1	0.99	0.11	175,175,175,175	0
23	MG	A	1612	1/1	0.99	0.07	123,123,123,123	0
23	MG	A	1767	1/1	0.99	0.09	327,327,327,327	0
23	MG	A	1646	1/1	0.99	0.05	131,131,131,131	0
23	MG	A	1630	1/1	0.99	0.11	92,92,92,92	0
23	MG	A	1625	1/1	0.99	0.11	134,134,134,134	0
23	MG	A	1748	1/1	0.99	0.18	204,204,204,204	0
23	MG	A	1671	1/1	0.99	0.16	208,208,208,208	0
24	ZN	D	301	1/1	0.99	0.20	159,159,159,159	0
24	ZN	N	101	1/1	0.99	0.08	336,336,336,336	0
23	MG	A	1719	1/1	1.00	0.17	105,105,105,105	0
23	MG	A	1792	1/1	1.00	0.08	127,127,127,127	0

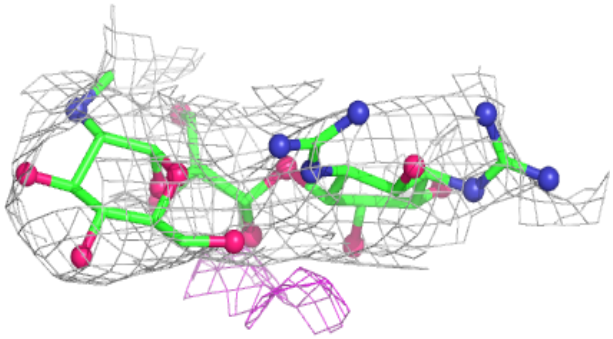
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

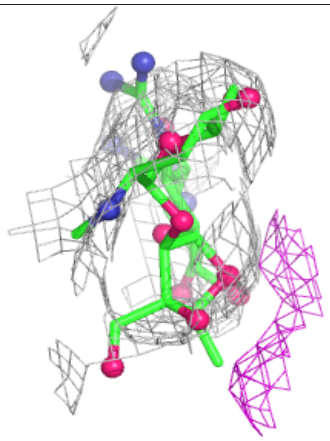
orientation to approximate a three-dimensional view.

Electron density around SRY A 1601:

$2mF_o$-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

There are no such residues in this entry.