wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2025 – 01:52 PM EST

PDB ID	:	4DR7
Title	:	Crystal structure of the Thermus thermophilus (HB8) 30S ribosomal subunit with codon, crystallographically disordered near-cognate transfer RNA anti-codon stem-loop mismatched at the second codon position, and streptomycin bound
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-16
Resolution	:	3.75 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:

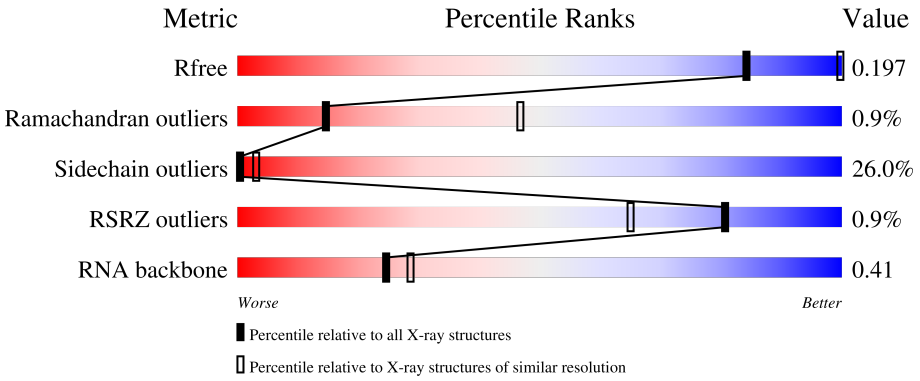
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber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

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 3.75 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	1256 (3.92-3.60)
Ramachandran outliers	177936	1293 (3.92-3.60)
Sidechain outliers	177891	1288 (3.92-3.60)
RSRZ outliers	164620	1256 (3.92-3.60)
RNA backbone	3690	1130 (4.52-3.00)

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	41% 45% 13%
2	B	256	70% 23% 8%
3	C	239	% 68% 18% 13%

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

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Mol	Chain	Length	Quality of chain
4	D	209	3% 76% 23%
5	E	162	% 65% 28% 7%
6	F	101	70% 30%
7	G	156	% 78% 22%
8	H	138	70% 28%
9	I	128	2% 78% 21%
10	J	105	% 71% 23% 6%
11	K	129	% 78% 13% 9%
12	L	135	% 69% 23% 7%
13	M	126	70% 23% 6%
14	N	61	3% 74% 25%
15	O	89	76% 20%
16	P	88	69% 26% 5%
17	Q	105	71% 24% 5%
18	R	88	64% 17% 19%
19	S	93	% 69% 16% 13%
20	T	106	% 67% 24% 7%
21	U	27	15% 78% 15% 7%
22	V	4	25% 75% 25%
23	W	11	27% 73% 27%
24	a	8	12% 38% 25% 38%
25	b	3	67% 33%

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
26	MG	A	1728	-	-	-	X

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 53659 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	1513	32707	14570	6056	10561	1520	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1896	1211	337	343	5	0	0	1

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called 30S 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 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called 30S 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 30S 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 30S 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 30S 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 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

- Molecule 13 is a protein called 30S 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 30S 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 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	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 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	71	Total	C	N	O	0	0	0
			585	373	116	96			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 23 is a RNA chain called 5'-R(*GP*CP*CP*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	11	Total	C	N	O	P	0	0	0
			235	106	45	74	10			

- Molecule 24 is a RNA chain called 5'-R(P*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	a	8	Total	C	N	O	P	0	0	0
			175	78	34	55	8			

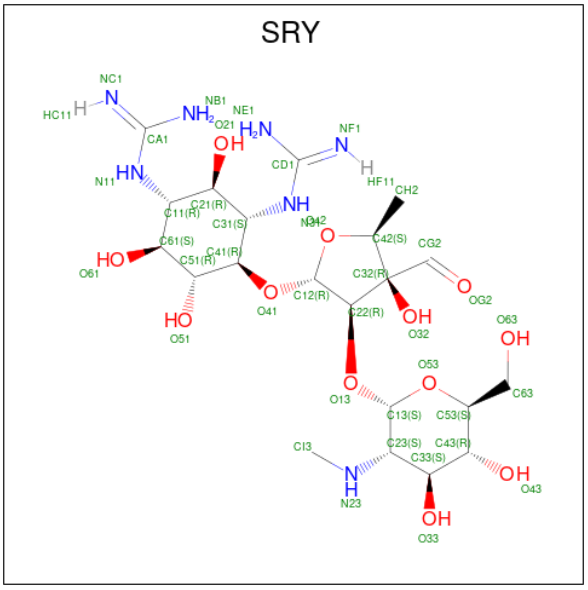
- Molecule 25 is a RNA chain called 5'-R(P*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	b	3	Total	C	N	O	P	0	0	0
			60	27	6	24	3			

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	326	Total Mg 326 326	0	0
26	D	3	Total Mg 3 3	0	0
26	E	4	Total Mg 4 4	0	0
26	F	1	Total Mg 1 1	0	0
26	G	1	Total Mg 1 1	0	0
26	H	1	Total Mg 1 1	0	0
26	J	1	Total Mg 1 1	0	0
26	N	1	Total Mg 1 1	0	0
26	P	3	Total Mg 3 3	0	0
26	Q	1	Total Mg 1 1	0	0
26	S	2	Total Mg 2 2	0	0

- Molecule 27 is STREPTOMYCIN (three-letter code: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



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

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

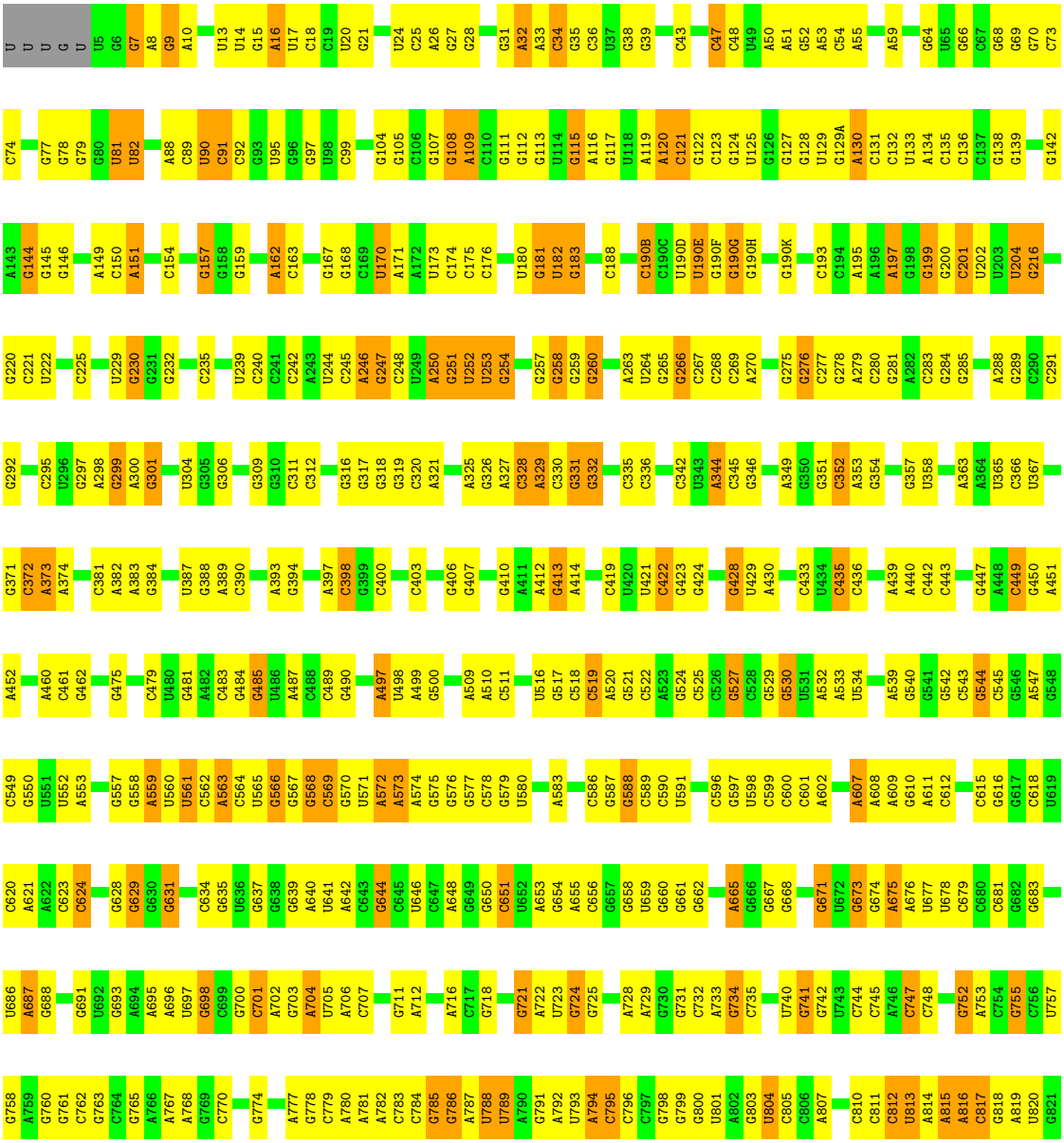
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	866	Total O 866 866	0	0
29	C	1	Total O 1 1	0	0
29	D	7	Total O 7 7	0	0
29	E	5	Total O 5 5	0	0
29	L	1	Total O 1 1	0	0
29	N	1	Total O 1 1	0	0
29	P	1	Total O 1 1	0	0
29	Q	2	Total O 2 2	0	0
29	T	3	Total O 3 3	0	0
29	U	4	Total O 4 4	0	0
29	W	1	Total O 1 1	0	0

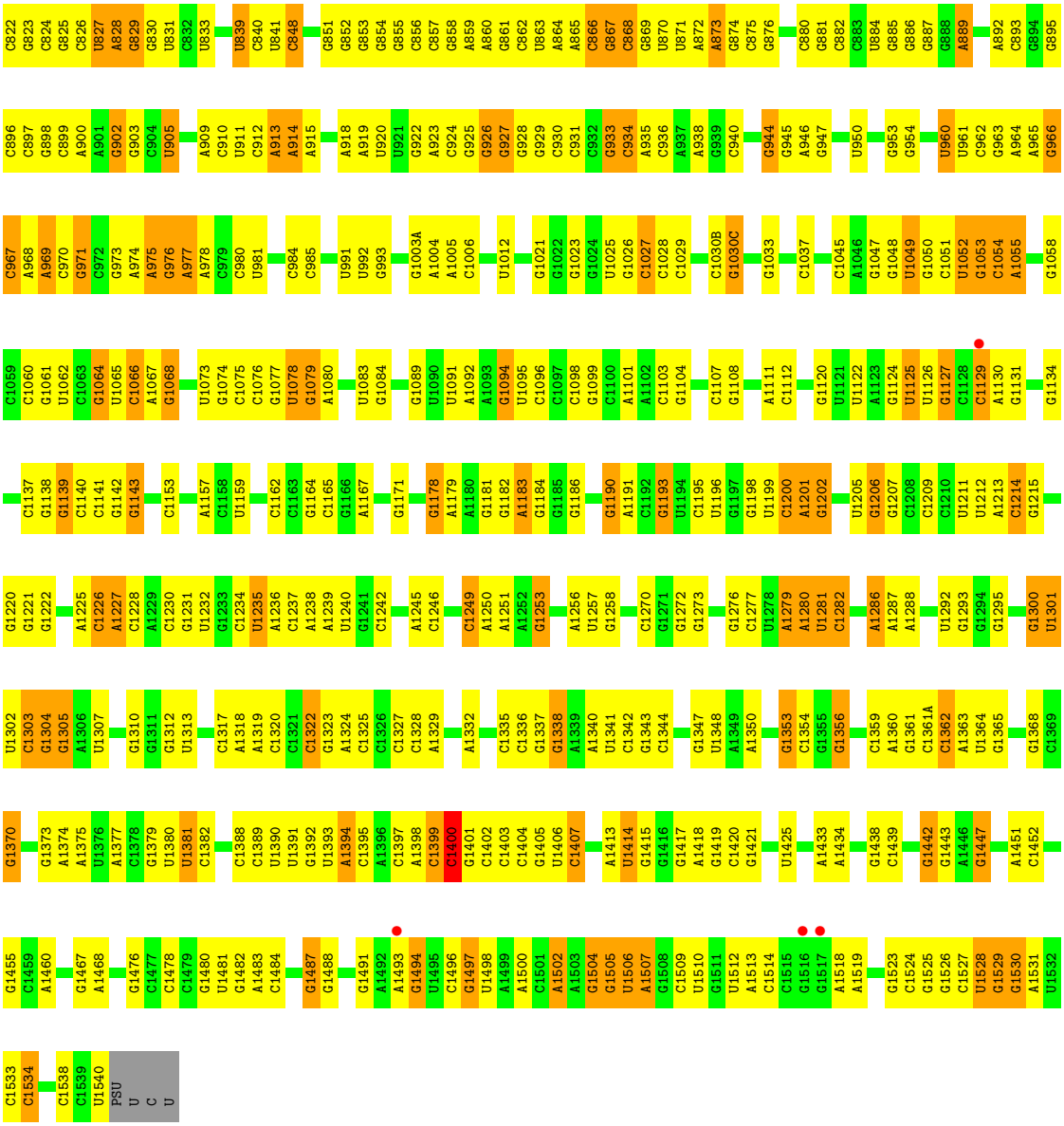
3 Residue-property plots (i)

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

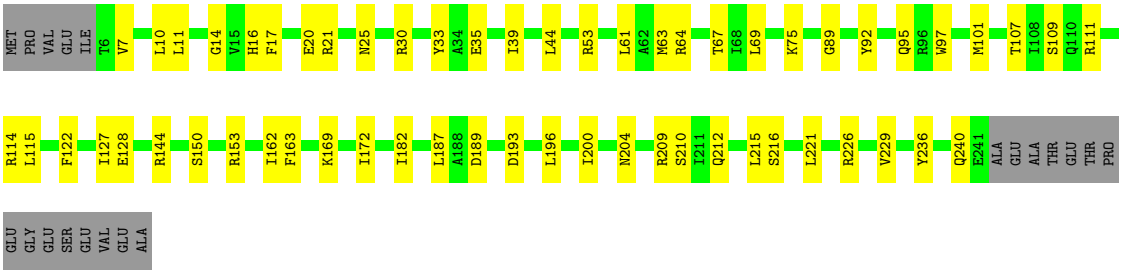
Chain A:





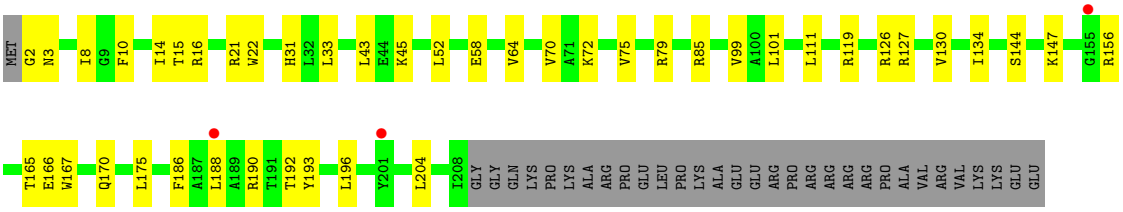
• Molecule 2: 30S ribosomal protein S2

Chain B:

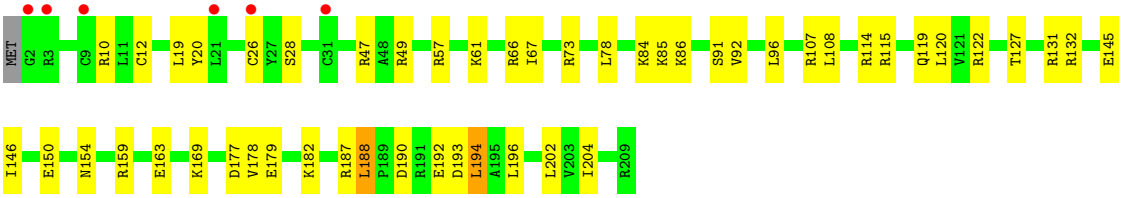


• Molecule 3: 30S ribosomal protein S3

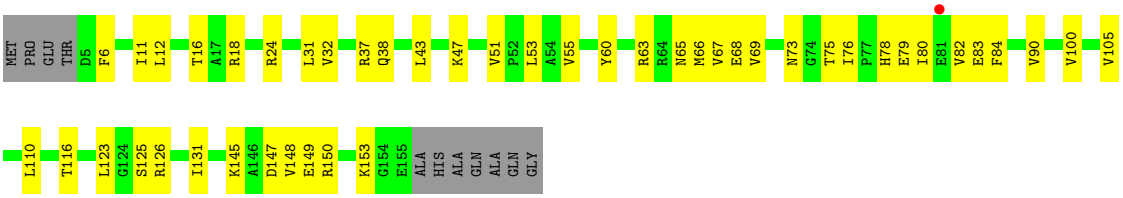
Chain C:



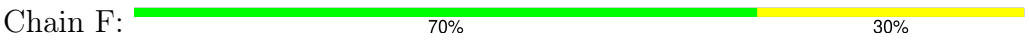
• Molecule 4: 30S ribosomal protein S4

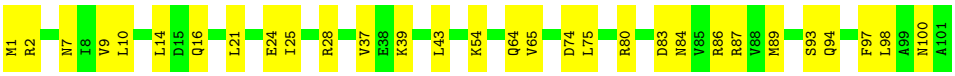


• Molecule 5: 30S ribosomal protein S5

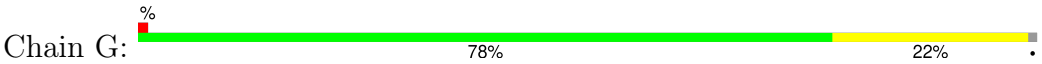


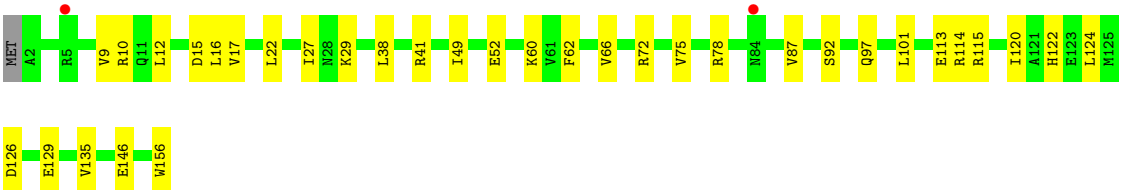
• Molecule 6: 30S ribosomal protein S6





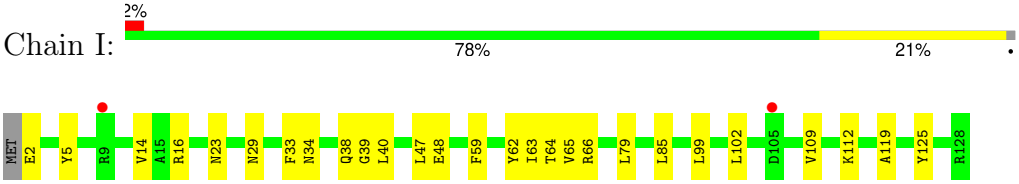
• Molecule 7: 30S ribosomal protein S7



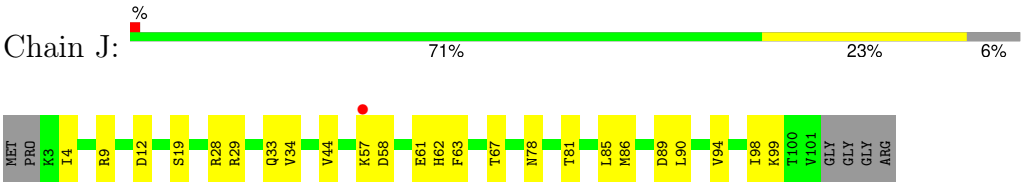


• Molecule 8: 30S ribosomal protein S8

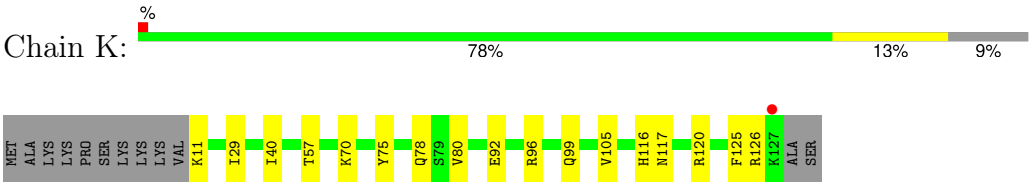
• Molecule 9: 30S ribosomal protein S9



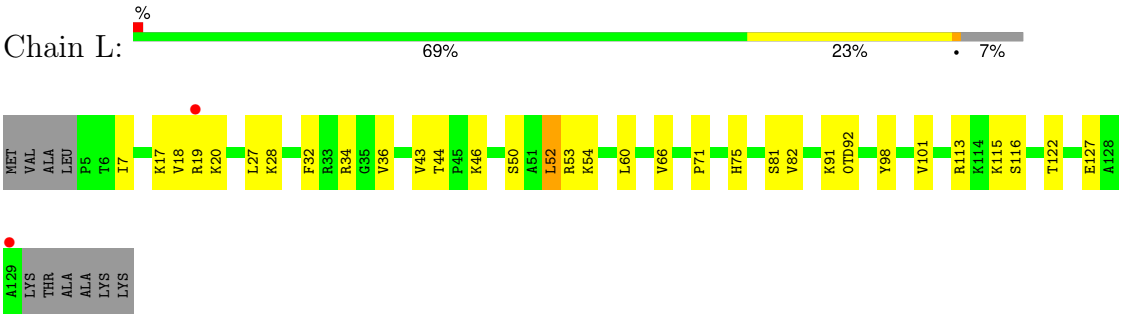
• Molecule 10: 30S ribosomal protein S10



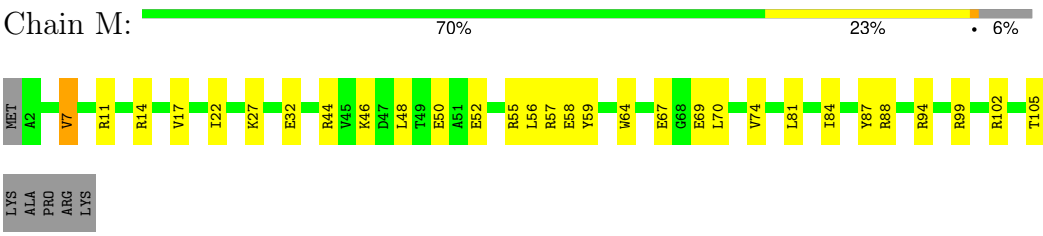
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12

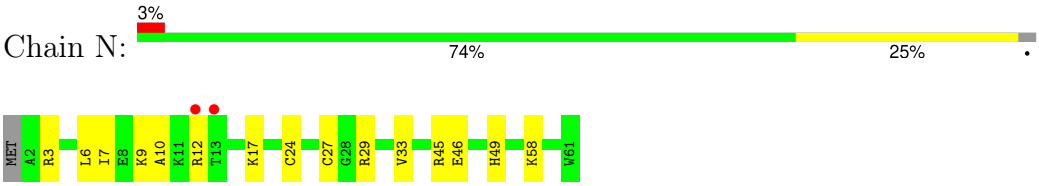


• Molecule 13: 30S ribosomal protein S13



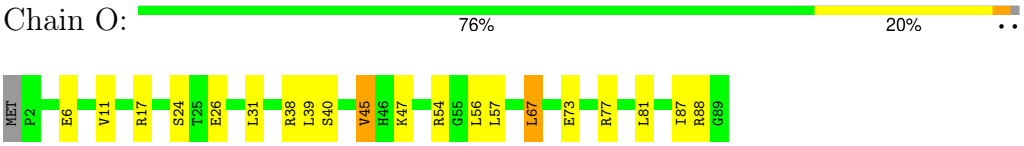
• Molecule 14: 30S ribosomal protein S14

Chain N:



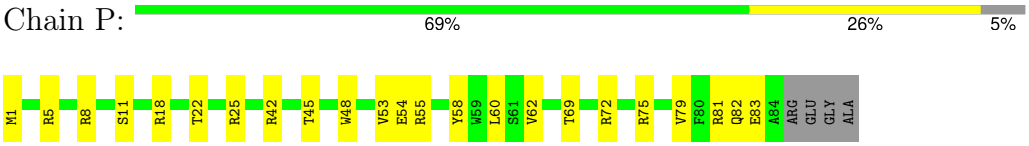
• Molecule 15: 30S ribosomal protein S15

Chain O:



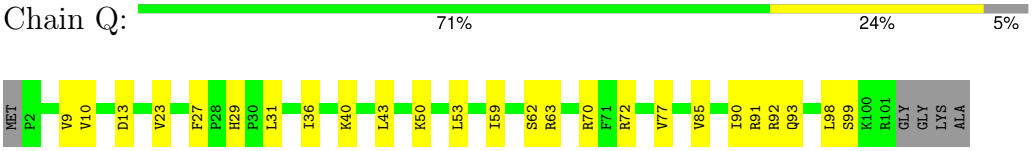
• Molecule 16: 30S ribosomal protein S16

Chain P:



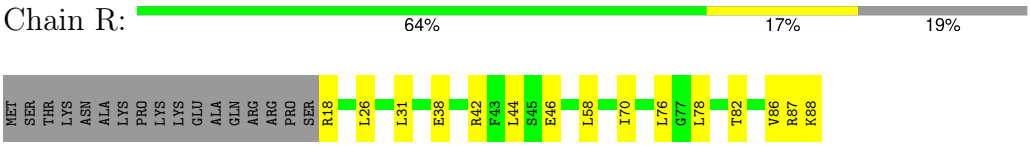
• Molecule 17: 30S ribosomal protein S17

Chain Q:



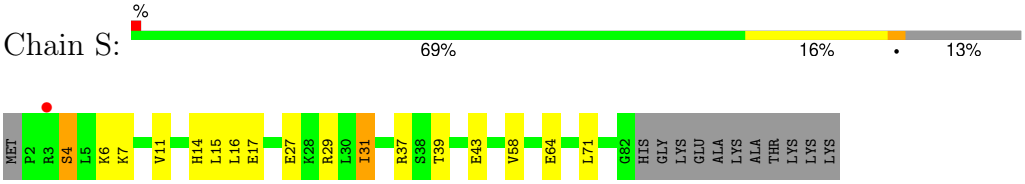
• Molecule 18: 30S ribosomal protein S18

Chain R:



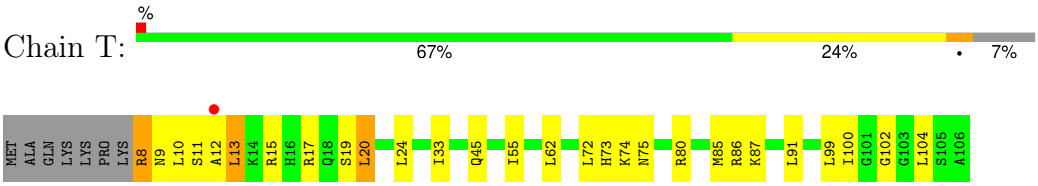
• Molecule 19: 30S ribosomal protein S19

Chain S:



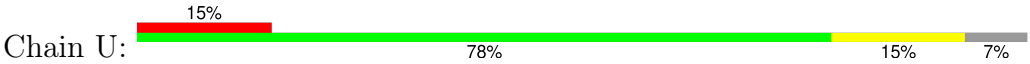
• Molecule 20: 30S ribosomal protein S20

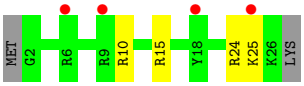
Chain T:



• Molecule 21: 30S ribosomal protein THX

Chain U:



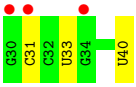


• Molecule 22: 5'-R(*UP*UP*UP*U)-3'

Chain V:

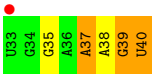
• Molecule 23: 5'-R(*GP*CP*CP*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'

Chain W:



• Molecule 24: 5'-R(P*UP*GP*GP*AP*AP*AP*GP*(PSU))-3'

Chain a:



• Molecule 25: 5'-R(P*UP*UP*U)-3'

Chain b:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.49Å 402.49Å 174.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 3.75 48.91 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.91-3.75) 99.9 (48.91-3.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.77Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.148 , 0.201 0.146 , 0.197	Depositor DCC
R_{free} test set	7304 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	130.7	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 98.5	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	0.97	EDS
Total number of atoms	53659	wwPDB-VP
Average B, all atoms (Å^2)	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M2G, MG, PSU, MA6, 7MG, 0TD, ZN, 5MC, 2MG, 4OC, SRY, UR3

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	1.21	135/36234 (0.4%)	1.90	1769/56547 (3.1%)
2	B	0.74	0/1931	0.93	2/2607 (0.1%)
3	C	0.62	0/1637	0.83	0/2207
4	D	0.73	1/1733 (0.1%)	0.93	4/2318 (0.2%)
5	E	1.04	1/1163 (0.1%)	1.17	3/1566 (0.2%)
6	F	0.65	0/856	0.86	0/1154
7	G	0.68	0/1276	0.87	0/1709
8	H	1.11	2/1136 (0.2%)	1.18	4/1527 (0.3%)
9	I	0.65	0/1029	0.88	2/1379 (0.1%)
10	J	0.71	1/806 (0.1%)	0.95	2/1084 (0.2%)
11	K	0.76	0/888	0.97	0/1198
12	L	0.90	0/978	1.08	3/1308 (0.2%)
13	M	0.68	0/947	0.94	0/1270
14	N	0.68	0/501	0.85	1/664 (0.2%)
15	O	0.86	0/745	1.02	3/992 (0.3%)
16	P	0.93	0/717	1.08	3/965 (0.3%)
17	Q	1.08	1/847 (0.1%)	1.25	4/1131 (0.4%)
18	R	0.76	0/590	1.00	1/782 (0.1%)
19	S	0.57	0/662	0.77	0/892
20	T	0.87	0/765	1.18	4/1007 (0.4%)
21	U	0.69	0/213	0.87	0/279
22	V	0.53	0/84	0.98	0/128
23	W	0.62	0/241	0.92	0/375
24	a	0.85	0/174	1.89	10/270 (3.7%)
25	b	0.76	0/65	1.31	2/98 (2.0%)
All	All	1.08	141/56218 (0.3%)	1.66	1817/83457 (2.2%)

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	3
3	C	0	2
4	D	0	1
8	H	0	2
9	I	0	1
10	J	0	2
12	L	0	2
16	P	0	1
19	S	0	1
20	T	0	2
21	U	0	1
All	All	0	18

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	828	A	N9-C4	-10.24	1.31	1.37
1	A	1513	A	N9-C4	-9.49	1.32	1.37
1	A	266	G	N7-C5	-9.34	1.33	1.39
1	A	573	A	N7-C5	-9.28	1.33	1.39
8	H	135	CYS	CB-SG	-9.04	1.66	1.82

The worst 5 of 1817 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	266	G	C6-C5-N7	-19.86	118.48	130.40
1	A	366	C	N1-C2-O2	17.84	129.60	118.90
1	A	117	G	N1-C6-O6	15.21	129.03	119.90
1	A	1200	C	C2-N1-C1'	15.12	135.43	118.80
1	A	573	A	C8-N9-C4	-15.02	99.79	105.80

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	75	LYS	Peptide
2	B	89	GLY	Peptide
3	C	166	GLU	Peptide
3	C	2	GLY	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	234/256 (91%)	197 (84%)	34 (14%)	3 (1%)	10 41
3	C	205/239 (86%)	169 (82%)	35 (17%)	1 (0%)	25 58
4	D	206/209 (99%)	180 (87%)	25 (12%)	1 (0%)	25 58
5	E	149/162 (92%)	137 (92%)	11 (7%)	1 (1%)	19 52
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
7	G	153/156 (98%)	132 (86%)	21 (14%)	0	100 100
8	H	136/138 (99%)	128 (94%)	7 (5%)	1 (1%)	19 52
9	I	125/128 (98%)	107 (86%)	17 (14%)	1 (1%)	16 49
10	J	97/105 (92%)	77 (79%)	17 (18%)	3 (3%)	3 27
11	K	115/129 (89%)	98 (85%)	17 (15%)	0	100 100
12	L	122/135 (90%)	110 (90%)	8 (7%)	4 (3%)	3 26
13	M	116/126 (92%)	99 (85%)	16 (14%)	1 (1%)	14 47
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100 100
15	O	86/89 (97%)	72 (84%)	14 (16%)	0	100 100
16	P	82/88 (93%)	74 (90%)	7 (8%)	1 (1%)	11 42
17	Q	98/105 (93%)	93 (95%)	5 (5%)	0	100 100
18	R	69/88 (78%)	60 (87%)	9 (13%)	0	100 100
19	S	79/93 (85%)	68 (86%)	9 (11%)	2 (2%)	4 30
20	T	97/106 (92%)	80 (82%)	16 (16%)	1 (1%)	13 45
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
All	All	2349/2541 (92%)	2046 (87%)	283 (12%)	20 (1%)	14 47

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	15	THR
9	I	119	ALA
12	L	28	LYS
16	P	83	GLU
19	S	31	ILE

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	201/220 (91%)	151 (75%)	50 (25%)	0	4
3	C	160/188 (85%)	119 (74%)	41 (26%)	0	3
4	D	180/181 (99%)	134 (74%)	46 (26%)	0	3
5	E	115/123 (94%)	75 (65%)	40 (35%)	0	1
6	F	90/90 (100%)	60 (67%)	30 (33%)	0	1
7	G	126/127 (99%)	92 (73%)	34 (27%)	0	2
8	H	119/119 (100%)	83 (70%)	36 (30%)	0	2
9	I	98/99 (99%)	75 (76%)	23 (24%)	0	4
10	J	87/92 (95%)	70 (80%)	17 (20%)	1	7
11	K	89/99 (90%)	72 (81%)	17 (19%)	1	7
12	L	103/110 (94%)	80 (78%)	23 (22%)	1	5
13	M	94/101 (93%)	64 (68%)	30 (32%)	0	1
14	N	49/50 (98%)	35 (71%)	14 (29%)	0	2
15	O	79/80 (99%)	60 (76%)	19 (24%)	0	4
16	P	72/74 (97%)	54 (75%)	18 (25%)	0	3
17	Q	95/97 (98%)	74 (78%)	21 (22%)	1	5
18	R	62/77 (80%)	48 (77%)	14 (23%)	1	5
19	S	71/80 (89%)	55 (78%)	16 (22%)	1	5
20	T	76/82 (93%)	51 (67%)	25 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	U	19/22 (86%)	16 (84%)	3 (16%)	2 13
All	All	1985/2111 (94%)	1468 (74%)	517 (26%)	0 3

5 of 517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	R	42	ARG
19	S	14	HIS
18	R	38	GLU
6	F	74	ASP
6	F	39	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	101	GLN
15	O	42	HIS
20	T	9	ASN
19	S	23	ASN
19	S	57	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	377 (25%)	48 (3%)
22	V	3/4 (75%)	1 (33%)	0
23	W	10/11 (90%)	2 (20%)	0
24	a	7/8 (87%)	4 (57%)	0
25	b	2/3 (66%)	0	0
All	All	1525/1548 (98%)	384 (25%)	48 (3%)

5 of 384 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	16	A
1	A	31	G
1	A	32	A

5 of 48 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1026	G
1	A	1201	A
1	A	1049	U
1	A	1137	C
1	A	1256	A

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

18 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	516	1	18,21,22	1.52	2 (11%)	21,30,33	1.71	6 (28%)
1	5MC	A	1404	1	19,22,23	1.09	2 (10%)	26,32,35	1.26	5 (19%)
24	PSU	a	40	24,1	18,21,22	1.39	3 (16%)	21,30,33	1.99	6 (28%)
1	MA6	A	1518[B]	1	19,26,27	1.31	2 (10%)	18,38,41	0.72	0
1	M2G	A	966	1	20,27,28	0.93	1 (5%)	19,40,43	1.40	2 (10%)
1	MA6	A	1519[A]	1	19,26,27	1.15	2 (10%)	18,38,41	0.99	0
1	PSU	A	1540	1	18,21,22	1.22	1 (5%)	21,30,33	1.69	3 (14%)
1	MA6	A	1518[A]	1	19,26,27	1.27	3 (15%)	18,38,41	0.73	0
23	PSU	W	40	23	18,21,22	1.12	1 (5%)	21,30,33	1.84	5 (23%)
1	4OC	A	1402	1	20,23,24	1.73	4 (20%)	25,32,35	1.11	2 (8%)
1	MA6	A	1519[B]	1	19,26,27	2.15	5 (26%)	18,38,41	0.77	0
1	5MC	A	1400	1	19,22,23	2.10	7 (36%)	26,32,35	1.13	3 (11%)
1	UR3	A	1498	1	19,22,23	0.89	1 (5%)	26,32,35	1.09	1 (3%)
1	7MG	A	527	1	23,26,27	4.96	7 (30%)	27,39,42	2.65	9 (33%)
1	5MC	A	1407	1	19,22,23	2.47	3 (15%)	26,32,35	1.33	2 (7%)
1	5MC	A	967	1	19,22,23	1.35	3 (15%)	26,32,35	0.73	1 (3%)
12	0TD	L	92	12	8,9,10	1.39	1 (12%)	6,11,13	3.62	3 (50%)
1	2MG	A	1207	1	18,26,27	2.14	4 (22%)	16,38,41	1.60	3 (18%)

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	516	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
24	PSU	a	40	24,1	-	3/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	1/7/29/30	0/3/3/3
1	M2G	A	966	1	-	4/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	4/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	2/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	4/7/29/30	0/3/3/3
23	PSU	W	40	23	-	3/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	4/9/29/30	0/2/2/2
1	MA6	A	1519[B]	1	-	4/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	1/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1407	1	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	3/7/25/26	0/2/2/2
12	0TD	L	92	12	-	3/7/12/14	-
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-20.99	1.32	1.45
1	A	1407	5MC	C5-C4	8.60	1.50	1.44
1	A	527	7MG	C5-N7	8.43	1.46	1.35
1	A	1519[B]	MA6	C6-N1	5.67	1.40	1.32
1	A	1400	5MC	C2-N1	5.62	1.51	1.40

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	L	92	0TD	CB-CA-N	-6.30	96.33	109.10
1	A	527	7MG	C6-C5-N7	6.25	141.62	131.93
1	A	527	7MG	C5-C6-N1	5.77	121.09	110.94
1	A	527	7MG	C2-N3-C4	5.49	121.76	112.30
12	L	92	0TD	CSB-SB-CB	-4.90	93.56	102.36

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	0	1

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 347 ligands modelled in this entry, 346 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	$\#\|Z\| > 2$
27	SRY	A	1928	-	40,42,42	2.36	11 (27%)	49,63,63	2.54	16 (32%)

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
27	SRY	A	1928	-	-	6/20/87/87	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1928	SRY	CD1-N31	9.40	1.49	1.33
27	A	1928	SRY	CA1-N11	5.81	1.43	1.33
27	A	1928	SRY	O53-C53	-3.58	1.35	1.44
27	A	1928	SRY	C23-N23	-3.11	1.42	1.47
27	A	1928	SRY	C32-CG2	-3.04	1.47	1.52

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	A	1928	SRY	C43-C33-C23	-7.61	99.32	110.40
27	A	1928	SRY	C61-C11-N11	-6.57	98.51	110.62
27	A	1928	SRY	C12-O42-C42	-6.05	98.71	108.48
27	A	1928	SRY	C13-O13-C22	-5.57	106.79	116.26
27	A	1928	SRY	O53-C13-C23	4.53	119.15	110.59

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

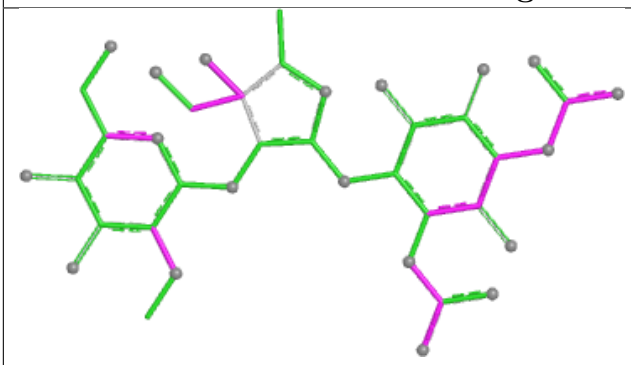
Mol	Chain	Res	Type	Atoms
27	A	1928	SRY	O53-C53-C63-O63
27	A	1928	SRY	C43-C53-C63-O63
27	A	1928	SRY	O42-C12-O41-C41
27	A	1928	SRY	C51-C41-O41-C12
27	A	1928	SRY	C13-C23-N23-CI3

There are no ring outliers.

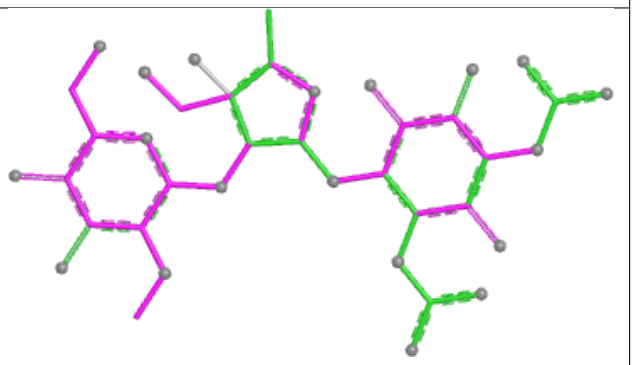
No monomer is involved in short contacts.

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.

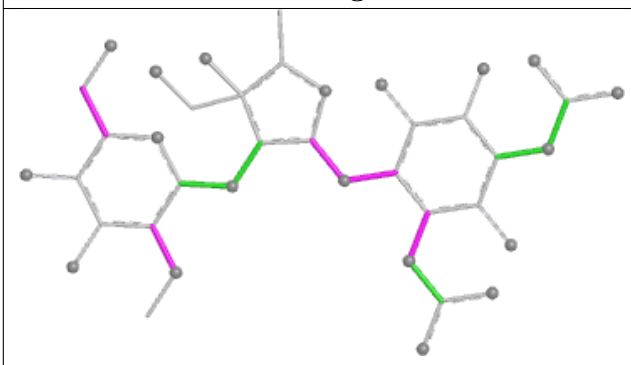
Ligand SRY A 1928



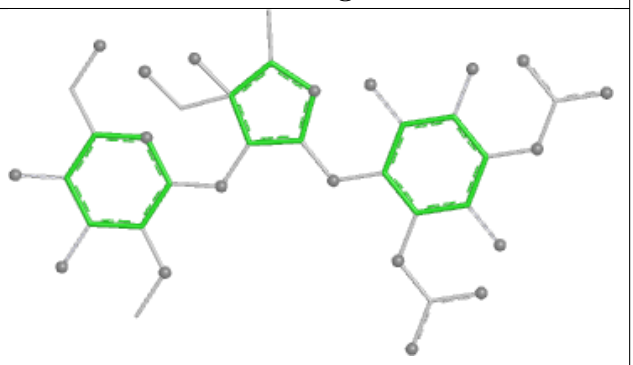
Bond lengths



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	1500/1522 (98%)	-0.80	4 (0%) 90 80	55, 129, 232, 327	6 (0%)
2	B	236/256 (92%)	-0.49	0 100 100	62, 153, 220, 247	0
3	C	207/239 (86%)	-0.52	3 (1%) 73 55	94, 191, 226, 244	0
4	D	208/209 (99%)	-0.39	6 (2%) 54 40	105, 149, 198, 214	0
5	E	151/162 (93%)	-0.71	1 (0%) 84 70	80, 114, 166, 193	0
6	F	101/101 (100%)	-0.79	0 100 100	110, 150, 182, 226	0
7	G	155/156 (99%)	-0.56	2 (1%) 74 57	121, 160, 223, 238	0
8	H	138/138 (100%)	-0.65	0 100 100	75, 104, 138, 155	0
9	I	127/128 (99%)	-0.33	2 (1%) 70 52	125, 184, 217, 240	0
10	J	99/105 (94%)	-0.25	1 (1%) 79 63	81, 203, 272, 295	0
11	K	117/129 (90%)	-0.58	1 (0%) 81 65	88, 130, 160, 167	0
12	L	124/135 (91%)	-0.35	2 (1%) 70 52	97, 136, 168, 247	0
13	M	118/126 (93%)	-0.51	0 100 100	127, 158, 192, 211	0
14	N	60/61 (98%)	-0.10	2 (3%) 49 37	144, 169, 210, 246	0
15	O	88/89 (98%)	-0.64	0 100 100	94, 127, 182, 225	0
16	P	84/88 (95%)	-0.28	0 100 100	96, 126, 164, 239	0
17	Q	100/105 (95%)	-0.58	0 100 100	83, 111, 150, 189	0
18	R	71/88 (80%)	-0.77	0 100 100	95, 132, 178, 229	0
19	S	81/93 (87%)	-0.47	1 (1%) 76 58	84, 184, 228, 234	0
20	T	99/106 (93%)	-0.34	1 (1%) 79 63	95, 126, 167, 212	0
21	U	25/27 (92%)	0.52	4 (16%) 6 8	77, 163, 192, 220	0
22	V	4/4 (100%)	1.68	1 (25%) 2 3	252, 267, 272, 275	0
23	W	10/11 (90%)	1.24	3 (30%) 1 3	173, 279, 296, 387	5 (50%)
24	a	7/8 (87%)	0.75	1 (14%) 7 10	200, 217, 282, 330	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	b	3/3 (100%)	0.53	0 100 100	160, 160, 206, 218	0
All	All	3913/4089 (95%)	-0.60	35 (0%) 81 65	55, 140, 221, 387	11 (0%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1517[A]	G	6.8
11	K	127	LYS	4.8
21	U	25	LYS	4.6
12	L	129	ALA	4.5
1	A	1516[A]	G	4.1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	PSU	W	40	20/21	0.36	0.12	291,301,325,326	0
1	PSU	A	1540	20/21	0.71	0.18	253,269,289,293	0
24	PSU	a	40	20/21	0.86	0.24	208,236,258,262	0
1	2MG	A	1207	24/25	0.93	0.09	154,167,200,202	0
1	UR3	A	1498	21/22	0.94	0.12	111,124,183,193	0
1	5MC	A	1407	21/22	0.94	0.07	127,152,158,162	0
1	PSU	A	516	20/21	0.95	0.05	123,147,168,168	0
1	MA6	A	1518[A]	24/25	0.95	0.28	110,122,127,131	24
1	MA6	A	1518[B]	24/25	0.95	0.28	107,122,137,148	24
1	5MC	A	1400	21/22	0.97	0.08	103,130,148,159	0
1	4OC	A	1402	22/23	0.97	0.08	104,119,127,142	0
1	M2G	A	966	25/26	0.97	0.09	122,137,142,145	0
1	MA6	A	1519[A]	24/25	0.98	0.17	100,115,125,126	24
1	MA6	A	1519[B]	24/25	0.98	0.17	101,116,129,130	24
1	7MG	A	527	24/25	0.98	0.07	91,114,123,126	0
1	5MC	A	1404	21/22	0.98	0.09	102,129,148,149	0
1	5MC	A	967	21/22	0.98	0.06	117,131,145,146	0
12	0TD	L	92	10/11	0.99	0.06	113,121,127,289	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
26	MG	A	1797	1/1	0.37	0.09	502,502,502,502	0
26	MG	A	1808	1/1	0.42	0.13	498,498,498,498	0
26	MG	A	1814	1/1	0.42	0.14	440,440,440,440	0
26	MG	A	1875	1/1	0.48	0.07	460,460,460,460	0
26	MG	A	1926	1/1	0.48	0.38	116,116,116,116	0
26	MG	A	1801	1/1	0.50	0.08	464,464,464,464	0
26	MG	A	1839	1/1	0.54	0.10	467,467,467,467	0
26	MG	A	1863	1/1	0.55	0.07	409,409,409,409	0
26	MG	A	1683	1/1	0.59	0.17	154,154,154,154	0
26	MG	A	1819	1/1	0.60	0.15	493,493,493,493	0
26	MG	A	1884	1/1	0.61	0.23	119,119,119,119	0
26	MG	A	1837	1/1	0.62	0.06	469,469,469,469	0
26	MG	A	1917	1/1	0.62	0.13	128,128,128,128	0
26	MG	A	1675	1/1	0.62	0.34	122,122,122,122	0
26	MG	A	1845	1/1	0.63	0.11	410,410,410,410	0
26	MG	A	1925	1/1	0.63	0.14	114,114,114,114	0
26	MG	A	1820	1/1	0.63	0.08	373,373,373,373	0
26	MG	A	1830	1/1	0.65	0.08	480,480,480,480	0
26	MG	A	1728	1/1	0.65	0.43	114,114,114,114	0
26	MG	A	1618	1/1	0.66	0.09	130,130,130,130	0
26	MG	A	1717	1/1	0.67	0.17	152,152,152,152	0
26	MG	A	1700	1/1	0.67	0.10	302,302,302,302	0
26	MG	A	1910	1/1	0.68	0.19	120,120,120,120	0
26	MG	A	1614	1/1	0.68	0.18	285,285,285,285	0
26	MG	A	1916	1/1	0.69	0.13	119,119,119,119	0
26	MG	A	1826	1/1	0.69	0.10	395,395,395,395	0
26	MG	A	1719	1/1	0.69	0.14	262,262,262,262	0
26	MG	A	1674	1/1	0.69	0.09	260,260,260,260	0
26	MG	A	1766	1/1	0.70	0.19	105,105,105,105	0
26	MG	A	1853	1/1	0.70	0.13	502,502,502,502	0
26	MG	A	1886	1/1	0.70	0.14	121,121,121,121	0
26	MG	A	1792	1/1	0.70	0.08	415,415,415,415	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1841	1/1	0.71	0.07	496,496,496,496	0
26	MG	A	1724	1/1	0.71	0.21	117,117,117,117	0
26	MG	S	101	1/1	0.71	0.21	115,115,115,115	0
26	MG	A	1865	1/1	0.72	0.07	457,457,457,457	0
26	MG	A	1729	1/1	0.72	0.18	101,101,101,101	0
26	MG	A	1898	1/1	0.72	0.26	89,89,89,89	0
26	MG	A	1871	1/1	0.74	0.14	392,392,392,392	0
26	MG	A	1897	1/1	0.74	0.15	114,114,114,114	0
26	MG	A	1756	1/1	0.74	0.12	126,126,126,126	0
26	MG	A	1901	1/1	0.74	0.08	101,101,101,101	0
26	MG	A	1678	1/1	0.74	0.09	217,217,217,217	0
26	MG	A	1699	1/1	0.75	0.11	414,414,414,414	0
26	MG	G	201	1/1	0.75	0.18	117,117,117,117	0
26	MG	A	1794	1/1	0.75	0.08	518,518,518,518	0
26	MG	A	1740	1/1	0.76	0.13	93,93,93,93	0
26	MG	A	1799	1/1	0.76	0.06	426,426,426,426	0
26	MG	A	1877	1/1	0.76	0.11	456,456,456,456	1
26	MG	A	1768	1/1	0.77	0.28	107,107,107,107	0
26	MG	A	1665	1/1	0.77	0.21	117,117,117,117	0
26	MG	A	1846	1/1	0.77	0.10	449,449,449,449	0
26	MG	A	1805	1/1	0.78	0.06	331,331,331,331	0
26	MG	A	1790	1/1	0.78	0.08	444,444,444,444	0
26	MG	A	1844	1/1	0.79	0.09	420,420,420,420	0
26	MG	A	1777	1/1	0.79	0.08	94,94,94,94	0
26	MG	A	1787	1/1	0.79	0.19	496,496,496,496	0
26	MG	A	1878	1/1	0.79	0.10	346,346,346,346	0
26	MG	A	1873	1/1	0.80	0.13	361,361,361,361	0
26	MG	E	204	1/1	0.80	0.09	128,128,128,128	0
26	MG	F	601	1/1	0.80	0.12	102,102,102,102	0
26	MG	A	1912	1/1	0.80	0.22	104,104,104,104	0
26	MG	A	1913	1/1	0.80	0.23	108,108,108,108	0
26	MG	A	1706	1/1	0.81	0.09	190,190,190,190	0
26	MG	A	1755	1/1	0.81	0.27	74,74,74,74	0
26	MG	A	1684	1/1	0.81	0.20	109,109,109,109	0
26	MG	A	1784	1/1	0.81	0.08	122,122,122,122	0
26	MG	A	1800	1/1	0.82	0.12	415,415,415,415	1
26	MG	A	1923	1/1	0.82	0.43	86,86,86,86	0
26	MG	A	1915	1/1	0.82	0.24	117,117,117,117	0
26	MG	A	1908	1/1	0.82	0.23	81,81,81,81	0
26	MG	A	1673	1/1	0.83	0.23	91,91,91,91	0
26	MG	A	1904	1/1	0.83	0.22	97,97,97,97	0
26	MG	A	1679	1/1	0.83	0.10	369,369,369,369	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1696	1/1	0.83	0.09	263,263,263,263	0
26	MG	A	1730	1/1	0.83	0.21	97,97,97,97	0
26	MG	A	1772	1/1	0.83	0.06	93,93,93,93	0
26	MG	A	1796	1/1	0.83	0.08	416,416,416,416	0
26	MG	A	1682	1/1	0.83	0.08	242,242,242,242	0
26	MG	A	1779	1/1	0.84	0.17	102,102,102,102	0
26	MG	A	1894	1/1	0.84	0.17	94,94,94,94	0
26	MG	A	1813	1/1	0.84	0.13	471,471,471,471	0
26	MG	A	1823	1/1	0.84	0.10	422,422,422,422	0
26	MG	A	1629	1/1	0.84	0.27	223,223,223,223	0
26	MG	A	1681	1/1	0.85	0.07	256,256,256,256	0
26	MG	A	1628	1/1	0.85	0.19	152,152,152,152	0
26	MG	A	1860	1/1	0.85	0.08	460,460,460,460	0
26	MG	A	1757	1/1	0.85	0.39	88,88,88,88	0
26	MG	A	1909	1/1	0.85	0.06	93,93,93,93	0
26	MG	A	1660	1/1	0.85	0.07	224,224,224,224	0
26	MG	A	1744	1/1	0.85	0.18	82,82,82,82	0
26	MG	A	1895	1/1	0.85	0.06	106,106,106,106	0
26	MG	A	1812	1/1	0.85	0.25	444,444,444,444	0
26	MG	A	1743	1/1	0.86	0.26	105,105,105,105	0
26	MG	A	1767	1/1	0.86	0.24	111,111,111,111	0
26	MG	A	1902	1/1	0.86	0.11	119,119,119,119	0
26	MG	A	1671	1/1	0.86	0.15	96,96,96,96	0
26	MG	A	1670	1/1	0.86	0.17	234,234,234,234	0
26	MG	A	1891	1/1	0.86	0.14	127,127,127,127	0
26	MG	A	1804	1/1	0.86	0.14	447,447,447,447	0
26	MG	A	1680	1/1	0.86	0.29	214,214,214,214	0
26	MG	A	1742	1/1	0.86	0.14	97,97,97,97	0
26	MG	P	102	1/1	0.86	0.06	101,101,101,101	0
26	MG	A	1914	1/1	0.86	0.23	99,99,99,99	0
26	MG	A	1907	1/1	0.87	0.26	120,120,120,120	0
26	MG	A	1921	1/1	0.87	0.11	84,84,84,84	0
26	MG	A	1849	1/1	0.87	0.22	471,471,471,471	0
26	MG	A	1793	1/1	0.87	0.12	483,483,483,483	0
26	MG	A	1874	1/1	0.87	0.24	467,467,467,467	0
26	MG	D	302	1/1	0.87	0.09	104,104,104,104	0
26	MG	A	1856	1/1	0.87	0.25	478,478,478,478	0
26	MG	A	1650	1/1	0.87	0.14	151,151,151,151	0
26	MG	A	1791	1/1	0.87	0.11	283,283,283,283	0
26	MG	A	1789	1/1	0.87	0.12	378,378,378,378	0
26	MG	A	1870	1/1	0.87	0.15	406,406,406,406	0
26	MG	A	1855	1/1	0.88	0.10	401,401,401,401	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1739	1/1	0.88	0.08	78,78,78,78	0
26	MG	A	1892	1/1	0.88	0.27	92,92,92,92	0
26	MG	A	1722	1/1	0.88	0.31	95,95,95,95	0
26	MG	A	1872	1/1	0.88	0.14	359,359,359,359	0
26	MG	A	1788	1/1	0.88	0.06	285,285,285,285	0
26	MG	S	102	1/1	0.88	0.08	106,106,106,106	0
26	MG	A	1859	1/1	0.89	0.17	427,427,427,427	0
26	MG	A	1918	1/1	0.89	0.11	75,75,75,75	0
26	MG	A	1741	1/1	0.89	0.06	105,105,105,105	0
26	MG	A	1809	1/1	0.89	0.10	494,494,494,494	0
26	MG	A	1824	1/1	0.89	0.18	503,503,503,503	0
26	MG	A	1890	1/1	0.89	0.09	112,112,112,112	0
26	MG	A	1769	1/1	0.89	0.17	127,127,127,127	0
26	MG	A	1781	1/1	0.89	0.08	104,104,104,104	0
26	MG	A	1758	1/1	0.89	0.33	101,101,101,101	0
26	MG	A	1838	1/1	0.89	0.27	538,538,538,538	0
26	MG	A	1785	1/1	0.89	0.05	108,108,108,108	0
26	MG	Q	201	1/1	0.89	0.16	145,145,145,145	0
26	MG	A	1857	1/1	0.89	0.28	308,308,308,308	0
26	MG	A	1900	1/1	0.89	0.11	93,93,93,93	0
26	MG	A	1817	1/1	0.90	0.18	419,419,419,419	0
26	MG	A	1887	1/1	0.90	0.22	102,102,102,102	0
26	MG	A	1644	1/1	0.90	0.25	127,127,127,127	0
26	MG	A	1734	1/1	0.90	0.64	124,124,124,124	0
26	MG	A	1811	1/1	0.90	0.37	468,468,468,468	0
26	MG	D	304	1/1	0.90	0.17	455,455,455,455	0
26	MG	A	1858	1/1	0.90	0.23	355,355,355,355	0
26	MG	A	1802	1/1	0.90	0.21	355,355,355,355	0
26	MG	A	1798	1/1	0.90	0.07	464,464,464,464	0
26	MG	A	1829	1/1	0.90	0.23	489,489,489,489	0
26	MG	A	1880	1/1	0.90	0.11	508,508,508,508	0
26	MG	A	1881	1/1	0.90	0.12	414,414,414,414	0
26	MG	A	1666	1/1	0.90	0.10	149,149,149,149	0
26	MG	A	1668	1/1	0.91	0.21	173,173,173,173	0
26	MG	A	1654	1/1	0.91	0.10	161,161,161,161	0
26	MG	A	1861	1/1	0.91	0.25	443,443,443,443	0
26	MG	A	1711	1/1	0.91	0.14	133,133,133,133	0
26	MG	N	102	1/1	0.91	0.19	107,107,107,107	0
26	MG	A	1889	1/1	0.91	0.08	95,95,95,95	0
26	MG	P	103	1/1	0.91	0.17	96,96,96,96	0
26	MG	A	1726	1/1	0.91	0.30	98,98,98,98	0
26	MG	A	1646	1/1	0.91	0.09	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1718	1/1	0.91	0.10	326,326,326,326	0
26	MG	A	1639	1/1	0.92	0.17	87,87,87,87	0
26	MG	A	1899	1/1	0.92	0.15	68,68,68,68	0
26	MG	A	1832	1/1	0.92	0.09	278,278,278,278	0
26	MG	A	1879	1/1	0.92	0.15	438,438,438,438	0
26	MG	A	1727	1/1	0.92	0.26	84,84,84,84	0
26	MG	A	1664	1/1	0.92	0.19	154,154,154,154	0
26	MG	A	1677	1/1	0.92	0.19	235,235,235,235	0
26	MG	A	1759	1/1	0.92	0.23	86,86,86,86	0
26	MG	A	1642	1/1	0.92	0.07	78,78,78,78	0
26	MG	A	1609	1/1	0.92	0.06	157,157,157,157	0
26	MG	A	1825	1/1	0.92	0.14	436,436,436,436	0
26	MG	A	1848	1/1	0.92	0.24	407,407,407,407	0
26	MG	A	1748	1/1	0.92	0.10	110,110,110,110	0
26	MG	A	1851	1/1	0.92	0.13	328,328,328,328	0
26	MG	A	1828	1/1	0.92	0.15	432,432,432,432	0
26	MG	A	1753	1/1	0.92	0.17	109,109,109,109	0
26	MG	A	1655	1/1	0.93	0.13	125,125,125,125	0
26	MG	A	1613	1/1	0.93	0.07	202,202,202,202	0
26	MG	A	1721	1/1	0.93	0.18	92,92,92,92	0
26	MG	A	1746	1/1	0.93	0.19	104,104,104,104	0
26	MG	A	1661	1/1	0.93	0.24	244,244,244,244	0
26	MG	A	1687	1/1	0.93	0.07	106,106,106,106	0
26	MG	A	1688	1/1	0.93	0.19	186,186,186,186	0
26	MG	A	1663	1/1	0.93	0.16	160,160,160,160	0
26	MG	A	1807	1/1	0.93	0.47	517,517,517,517	1
26	MG	A	1621	1/1	0.93	0.07	131,131,131,131	0
26	MG	A	1834	1/1	0.93	0.34	412,412,412,412	1
26	MG	A	1927	1/1	0.93	0.28	112,112,112,112	0
26	MG	A	1622	1/1	0.93	0.08	81,81,81,81	0
26	MG	A	1810	1/1	0.93	0.12	474,474,474,474	0
26	MG	A	1604	1/1	0.93	0.10	91,91,91,91	0
26	MG	A	1709	1/1	0.93	0.17	245,245,245,245	0
26	MG	A	1617	1/1	0.93	0.18	85,85,85,85	0
26	MG	J	201	1/1	0.93	0.16	109,109,109,109	0
26	MG	A	1712	1/1	0.93	0.10	170,170,170,170	0
26	MG	P	101	1/1	0.93	0.20	58,58,58,58	0
26	MG	A	1905	1/1	0.93	0.08	105,105,105,105	0
26	MG	A	1815	1/1	0.93	0.24	506,506,506,506	0
26	MG	A	1847	1/1	0.93	0.20	441,441,441,441	0
26	MG	A	1816	1/1	0.93	0.13	454,454,454,454	0
26	MG	A	1636	1/1	0.93	0.15	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1840	1/1	0.94	0.21	467,467,467,467	1
26	MG	A	1760	1/1	0.94	0.11	88,88,88,88	0
26	MG	A	1842	1/1	0.94	0.11	488,488,488,488	0
26	MG	A	1919	1/1	0.94	0.20	78,78,78,78	0
26	MG	A	1920	1/1	0.94	0.07	138,138,138,138	0
26	MG	A	1896	1/1	0.94	0.08	114,114,114,114	0
26	MG	A	1761	1/1	0.94	0.09	105,105,105,105	0
26	MG	A	1732	1/1	0.94	0.11	100,100,100,100	0
26	MG	A	1691	1/1	0.94	0.17	186,186,186,186	0
26	MG	A	1806	1/1	0.94	0.42	505,505,505,505	0
26	MG	A	1735	1/1	0.94	0.07	106,106,106,106	0
26	MG	A	1737	1/1	0.94	0.17	89,89,89,89	0
26	MG	A	1827	1/1	0.94	0.09	251,251,251,251	0
26	MG	A	1852	1/1	0.94	0.26	450,450,450,450	0
26	MG	A	1906	1/1	0.94	0.10	64,64,64,64	0
26	MG	A	1659	1/1	0.94	0.18	90,90,90,90	0
26	MG	A	1774	1/1	0.94	0.34	109,109,109,109	0
26	MG	A	1624	1/1	0.94	0.33	147,147,147,147	0
26	MG	A	1669	1/1	0.94	0.06	123,123,123,123	0
26	MG	A	1780	1/1	0.94	0.27	119,119,119,119	0
26	MG	A	1716	1/1	0.94	0.08	132,132,132,132	0
26	MG	A	1783	1/1	0.94	0.04	110,110,110,110	0
26	MG	A	1723	1/1	0.94	0.14	117,117,117,117	0
26	MG	A	1692	1/1	0.95	0.07	182,182,182,182	0
26	MG	A	1782	1/1	0.95	0.22	87,87,87,87	0
26	MG	A	1626	1/1	0.95	0.19	245,245,245,245	0
26	MG	A	1633	1/1	0.95	0.07	118,118,118,118	0
26	MG	A	1610	1/1	0.95	0.11	81,81,81,81	0
26	MG	A	1720	1/1	0.95	0.12	74,74,74,74	0
26	MG	A	1702	1/1	0.95	0.07	279,279,279,279	0
26	MG	A	1831	1/1	0.95	0.34	395,395,395,395	0
26	MG	A	1762	1/1	0.95	0.15	82,82,82,82	0
26	MG	A	1705	1/1	0.95	0.12	74,74,74,74	0
26	MG	A	1835	1/1	0.95	0.22	309,309,309,309	0
26	MG	A	1685	1/1	0.95	0.22	126,126,126,126	0
26	MG	A	1866	1/1	0.95	0.17	434,434,434,434	0
26	MG	A	1868	1/1	0.95	0.39	380,380,380,380	0
26	MG	A	1707	1/1	0.95	0.06	135,135,135,135	0
26	MG	A	1708	1/1	0.95	0.28	152,152,152,152	0
26	MG	A	1770	1/1	0.95	0.73	106,106,106,106	0
26	MG	A	1795	1/1	0.95	0.30	359,359,359,359	0
26	MG	A	1637	1/1	0.95	0.11	228,228,228,228	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1747	1/1	0.95	0.27	115,115,115,115	0
26	MG	A	1710	1/1	0.95	0.12	253,253,253,253	0
26	MG	A	1649	1/1	0.95	0.14	84,84,84,84	0
26	MG	A	1821	1/1	0.95	0.25	428,428,428,428	0
26	MG	A	1822	1/1	0.95	0.13	293,293,293,293	0
26	MG	A	1667	1/1	0.95	0.06	119,119,119,119	0
26	MG	A	1885	1/1	0.96	0.10	84,84,84,84	0
26	MG	A	1775	1/1	0.96	0.10	79,79,79,79	0
26	MG	A	1776	1/1	0.96	0.18	96,96,96,96	0
26	MG	A	1657	1/1	0.96	0.17	220,220,220,220	0
26	MG	A	1836	1/1	0.96	0.25	416,416,416,416	1
26	MG	A	1694	1/1	0.96	0.12	87,87,87,87	0
26	MG	A	1632	1/1	0.96	0.29	248,248,248,248	0
26	MG	A	1893	1/1	0.96	0.32	114,114,114,114	0
26	MG	A	1818	1/1	0.96	0.05	189,189,189,189	0
26	MG	A	1922	1/1	0.96	0.13	110,110,110,110	0
26	MG	A	1605	1/1	0.96	0.07	254,254,254,254	0
26	MG	A	1924	1/1	0.96	0.17	131,131,131,131	0
26	MG	A	1652	1/1	0.96	0.05	72,72,72,72	0
26	MG	A	1765	1/1	0.96	0.07	104,104,104,104	0
26	MG	A	1751	1/1	0.96	0.20	76,76,76,76	0
26	MG	A	1752	1/1	0.96	0.11	91,91,91,91	0
26	MG	A	1786	1/1	0.96	0.05	109,109,109,109	0
26	MG	A	1686	1/1	0.96	0.13	184,184,184,184	0
26	MG	A	1754	1/1	0.96	0.11	85,85,85,85	0
26	MG	A	1615	1/1	0.96	0.07	147,147,147,147	0
26	MG	A	1876	1/1	0.96	0.28	463,463,463,463	1
26	MG	A	1850	1/1	0.96	0.07	236,236,236,236	0
26	MG	A	1771	1/1	0.96	0.10	102,102,102,102	0
26	MG	A	1620	1/1	0.96	0.10	166,166,166,166	0
26	MG	A	1773	1/1	0.96	0.08	103,103,103,103	0
26	MG	A	1854	1/1	0.96	0.18	418,418,418,418	0
26	MG	A	1911	1/1	0.96	0.08	100,100,100,100	0
26	MG	A	1656	1/1	0.96	0.10	236,236,236,236	0
26	MG	A	1612	1/1	0.97	0.25	281,281,281,281	0
26	MG	A	1714	1/1	0.97	0.05	108,108,108,108	0
26	MG	A	1764	1/1	0.97	0.05	78,78,78,78	0
26	MG	A	1697	1/1	0.97	0.06	135,135,135,135	0
26	MG	A	1608	1/1	0.97	0.10	73,73,73,73	0
26	MG	E	201	1/1	0.97	0.12	95,95,95,95	0
26	MG	E	202	1/1	0.97	0.04	124,124,124,124	0
26	MG	A	1745	1/1	0.97	0.20	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1864	1/1	0.97	0.16	393,393,393,393	0
26	MG	A	1778	1/1	0.97	0.04	119,119,119,119	1
26	MG	H	201	1/1	0.97	0.21	67,67,67,67	0
26	MG	A	1882	1/1	0.97	0.22	315,315,315,315	0
26	MG	A	1725	1/1	0.97	0.06	92,92,92,92	0
26	MG	A	1867	1/1	0.97	0.16	413,413,413,413	1
26	MG	A	1693	1/1	0.97	0.05	108,108,108,108	0
26	MG	A	1803	1/1	0.97	0.09	345,345,345,345	0
26	MG	A	1672	1/1	0.97	0.09	166,166,166,166	0
26	MG	A	1695	1/1	0.97	0.06	176,176,176,176	0
26	MG	A	1843	1/1	0.97	0.29	357,357,357,357	0
26	MG	A	1640	1/1	0.98	0.24	172,172,172,172	0
26	MG	A	1738	1/1	0.98	0.04	68,68,68,68	0
26	MG	A	1627	1/1	0.98	0.06	141,141,141,141	0
26	MG	A	1653	1/1	0.98	0.15	96,96,96,96	0
26	MG	A	1869	1/1	0.98	0.15	431,431,431,431	0
26	MG	A	1630	1/1	0.98	0.08	158,158,158,158	0
26	MG	A	1645	1/1	0.98	0.12	227,227,227,227	0
26	MG	A	1763	1/1	0.98	0.04	120,120,120,120	0
26	MG	A	1631	1/1	0.98	0.12	158,158,158,158	0
26	MG	A	1698	1/1	0.98	0.08	124,124,124,124	0
26	MG	A	1713	1/1	0.98	0.07	211,211,211,211	0
26	MG	A	1647	1/1	0.98	0.10	104,104,104,104	0
26	MG	A	1715	1/1	0.98	0.13	229,229,229,229	0
26	MG	A	1648	1/1	0.98	0.08	93,93,93,93	0
26	MG	E	203	1/1	0.98	0.06	101,101,101,101	0
26	MG	A	1833	1/1	0.98	0.28	335,335,335,335	0
26	MG	A	1749	1/1	0.98	0.06	84,84,84,84	0
26	MG	A	1750	1/1	0.98	0.07	74,74,74,74	0
26	MG	A	1731	1/1	0.98	0.09	68,68,68,68	0
26	MG	A	1883	1/1	0.98	0.22	443,443,443,443	0
26	MG	A	1701	1/1	0.98	0.07	108,108,108,108	0
26	MG	A	1733	1/1	0.98	0.10	70,70,70,70	0
26	MG	A	1689	1/1	0.98	0.06	126,126,126,126	0
26	MG	A	1862	1/1	0.98	0.08	268,268,268,268	0
26	MG	A	1888	1/1	0.98	0.06	89,89,89,89	0
26	MG	A	1606	1/1	0.98	0.11	87,87,87,87	0
26	MG	A	1736	1/1	0.98	0.07	123,123,123,123	0
28	ZN	D	301	1/1	0.98	0.20	138,138,138,138	0
26	MG	A	1603	1/1	0.99	0.10	277,277,277,277	0
26	MG	A	1676	1/1	0.99	0.08	158,158,158,158	0
26	MG	D	303	1/1	0.99	0.09	104,104,104,104	0

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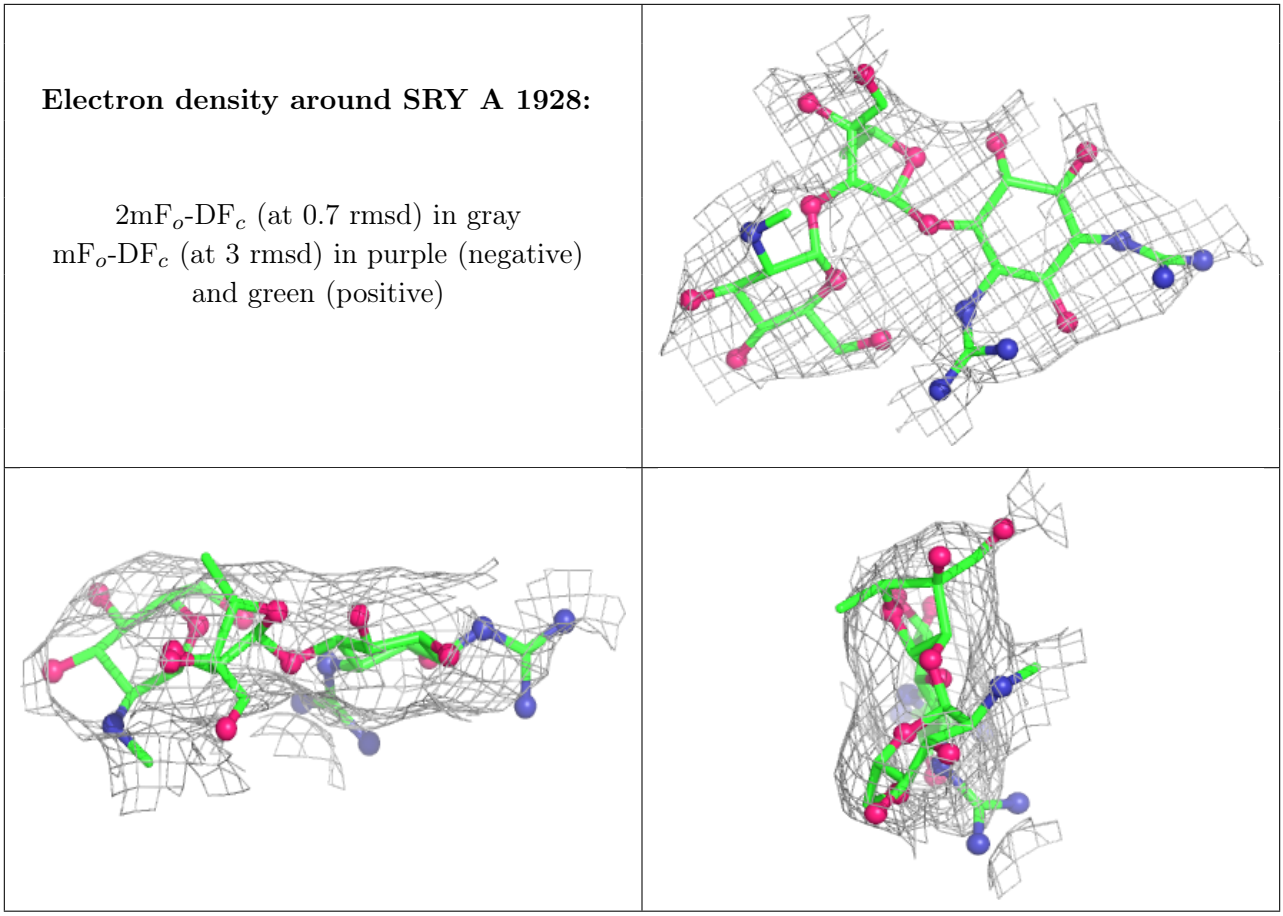
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	MG	A	1662	1/1	0.99	0.04	123,123,123,123	0
26	MG	A	1638	1/1	0.99	0.03	86,86,86,86	0
26	MG	A	1602	1/1	0.99	0.13	66,66,66,66	1
26	MG	A	1651	1/1	0.99	0.05	110,110,110,110	0
26	MG	A	1625	1/1	0.99	0.03	113,113,113,113	0
26	MG	A	1641	1/1	0.99	0.04	102,102,102,102	0
26	MG	A	1619	1/1	0.99	0.03	64,64,64,64	0
26	MG	A	1643	1/1	0.99	0.02	71,71,71,71	0
26	MG	A	1607	1/1	0.99	0.04	154,154,154,154	0
26	MG	A	1634	1/1	0.99	0.04	107,107,107,107	0
26	MG	A	1703	1/1	0.99	0.04	97,97,97,97	0
26	MG	A	1704	1/1	0.99	0.07	104,104,104,104	0
26	MG	A	1903	1/1	0.99	0.06	78,78,78,78	0
26	MG	A	1658	1/1	0.99	0.04	115,115,115,115	0
26	MG	A	1635	1/1	0.99	0.05	74,74,74,74	0
26	MG	A	1611	1/1	0.99	0.05	113,113,113,113	0
27	SRY	A	1928	40/40	0.99	0.05	70,100,124,130	0
26	MG	A	1690	1/1	0.99	0.04	114,114,114,114	0
28	ZN	N	101	1/1	0.99	0.04	164,164,164,164	0
26	MG	A	1623	1/1	1.00	0.03	67,67,67,67	0
26	MG	A	1616	1/1	1.00	0.05	63,63,63,63	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 1928:

$2mF_o$-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.