



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 07:44 am GMT

PDB ID : 1J5E
Title : Structure of the Thermus thermophilus 30S Ribosomal Subunit
Authors : Wimberly, B.T.; Brodersen, D.E.; Clemons Jr., W.M.; Morgan-Warren, R.;
Carter, A.P.; Vornrhein, C.; Hartsch, T.; Ramakrishnan, V.
Deposited on : 2002-04-08
Resolution : 3.05 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

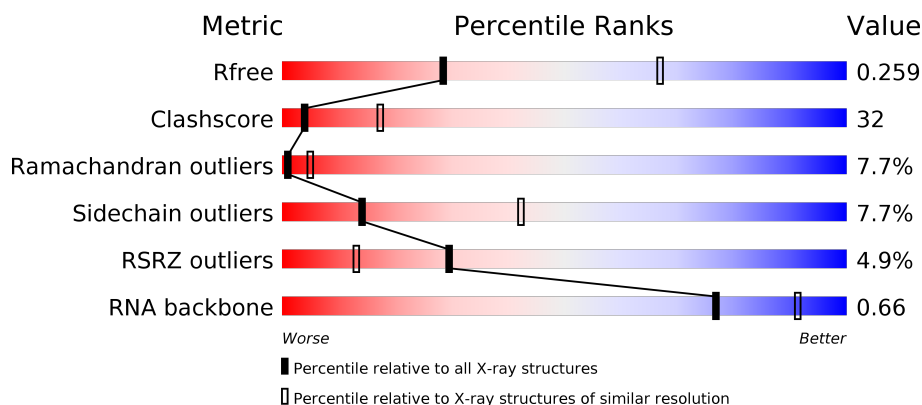
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


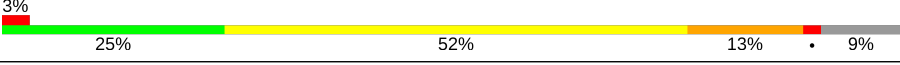
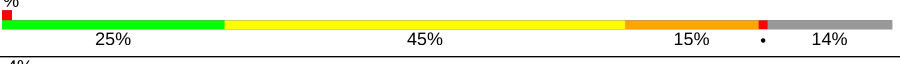
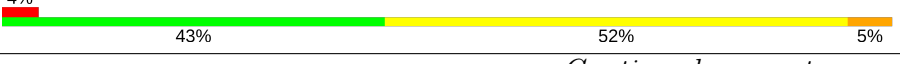
The reported resolution of this entry is 3.05 Å.

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}	111664	1497 (3.10-3.02)
Clashscore	122126	1601 (3.10-3.02)
Ramachandran outliers	120053	1548 (3.10-3.02)
Sidechain outliers	120020	1547 (3.10-3.02)
RSRZ outliers	108989	1462 (3.10-3.02)
RNA backbone	2636	1006 (3.40-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	
4	D	208	

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Mol	Chain	Length	Quality of chain
5	E	161	
6	F	101	
7	G	155	
8	H	138	
9	I	128	
10	J	104	
11	K	129	
12	L	135	
13	M	126	
14	N	60	
15	O	88	
16	P	88	
17	Q	104	
18	R	88	
19	S	92	
20	T	106	
21	V	26	

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
22	UNX	A	100	-	-	-	X
22	UNX	A	1545	-	-	-	X
22	UNX	A	1546	-	-	-	X
22	UNX	A	1551	-	-	-	X
22	UNX	A	1557	-	-	-	X
22	UNX	A	1561	-	-	-	X
22	UNX	A	1565	-	-	-	X
22	UNX	A	1566	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	UNX	A	1568	-	-	-	X
22	UNX	A	1569	-	-	-	X
22	UNX	A	1570	-	-	-	X
22	UNX	A	1571	-	-	-	X
22	UNX	A	1572	-	-	-	X
22	UNX	A	1574	-	-	-	X
22	UNX	A	1575	-	-	-	X
22	UNX	A	1576	-	-	-	X
22	UNX	A	1579	-	-	-	X
22	UNX	A	1582	-	-	-	X
22	UNX	A	1583	-	-	-	X
22	UNX	A	1585	-	-	-	X
22	UNX	A	1588	-	-	-	X
22	UNX	A	1589	-	-	-	X
22	UNX	A	1593	-	-	-	X
22	UNX	A	1595	-	-	-	X
22	UNX	A	1597	-	-	-	X
22	UNX	A	1598	-	-	-	X
22	UNX	A	1600	-	-	-	X
22	UNX	A	1601	-	-	-	X
22	UNX	A	1602	-	-	-	X
22	UNX	A	1604	-	-	-	X
22	UNX	A	1606	-	-	-	X
22	UNX	A	1608	-	-	-	X
22	UNX	A	1609	-	-	-	X
22	UNX	A	1610	-	-	-	X
22	UNX	A	1611	-	-	-	X
22	UNX	A	1612	-	-	-	X
22	UNX	A	1613	-	-	-	X
22	UNX	A	1614	-	-	-	X
22	UNX	A	1615	-	-	-	X
22	UNX	A	1618	-	-	-	X
22	UNX	A	1619	-	-	-	X
22	UNX	A	1620	-	-	-	X
22	UNX	A	1621	-	-	-	X
22	UNX	A	1622	-	-	-	X
22	UNX	A	1625	-	-	-	X
22	UNX	A	1626	-	-	-	X
22	UNX	A	1628	-	-	-	X
22	UNX	A	1629	-	-	-	X
22	UNX	A	1632	-	-	-	X
22	UNX	A	1634	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	UNX	A	1635	-	-	-	X
22	UNX	A	1636	-	-	-	X
22	UNX	A	1637	-	-	-	X
22	UNX	A	1638	-	-	-	X
22	UNX	A	1639	-	-	-	X
22	UNX	A	1640	-	-	-	X
22	UNX	A	1641	-	-	-	X
22	UNX	A	1642	-	-	-	X
22	UNX	A	1643	-	-	-	X
22	UNX	A	1644	-	-	-	X
22	UNX	A	1645	-	-	-	X
22	UNX	A	1646	-	-	-	X
22	UNX	A	1647	-	-	-	X
22	UNX	A	1648	-	-	-	X
22	UNX	A	1650	-	-	-	X
22	UNX	A	1651	-	-	-	X
22	UNX	A	1652	-	-	-	X
22	UNX	A	1655	-	-	-	X
22	UNX	A	1656	-	-	-	X
22	UNX	A	1658	-	-	-	X
22	UNX	A	1659	-	-	-	X
22	UNX	A	1661	-	-	-	X
22	UNX	A	1663	-	-	-	X
22	UNX	A	1664	-	-	-	X
22	UNX	A	1665	-	-	-	X
22	UNX	A	1666	-	-	-	X
22	UNX	A	1667	-	-	-	X
22	UNX	A	1668	-	-	-	X
22	UNX	A	1669	-	-	-	X
22	UNX	A	1670	-	-	-	X
22	UNX	A	1671	-	-	-	X
22	UNX	A	1672	-	-	-	X
22	UNX	A	1673	-	-	-	X
22	UNX	A	1674	-	-	-	X
22	UNX	A	1675	-	-	-	X
22	UNX	A	1676	-	-	-	X
22	UNX	A	1677	-	-	-	X
22	UNX	A	1679	-	-	-	X
22	UNX	A	1680	-	-	-	X
22	UNX	A	1683	-	-	-	X
22	UNX	A	1684	-	-	-	X
22	UNX	A	1689	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	UNX	A	1690	-	-	-	X
22	UNX	A	1691	-	-	-	X
22	UNX	A	1694	-	-	-	X
22	UNX	A	1695	-	-	-	X
22	UNX	A	1696	-	-	-	X
22	UNX	A	1697	-	-	-	X
22	UNX	A	1698	-	-	-	X
22	UNX	A	1699	-	-	-	X
22	UNX	A	1700	-	-	-	X
22	UNX	A	1701	-	-	-	X
22	UNX	A	1702	-	-	-	X
22	UNX	A	1703	-	-	-	X
22	UNX	A	1704	-	-	-	X
22	UNX	A	1705	-	-	-	X
22	UNX	A	1711	-	-	-	X
22	UNX	A	1715	-	-	-	X
22	UNX	A	1716	-	-	-	X
22	UNX	A	1717	-	-	-	X
22	UNX	A	1718	-	-	-	X
22	UNX	A	1719	-	-	-	X
22	UNX	A	1720	-	-	-	X
22	UNX	A	1721	-	-	-	X
22	UNX	A	1722	-	-	-	X
22	UNX	A	1723	-	-	-	X
22	UNX	A	72	-	-	-	X
22	UNX	A	86	-	-	-	X
22	UNX	A	94	-	-	-	X
22	UNX	B	257	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 51933 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	66	0	0
			32514	14472	6016	10513	1513			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S 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 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	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S 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 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	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	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S 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 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	41	VAL	ILE	CONFLICT	EMBL 11125386

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	X	0	0
			1	1		
22	A	186	Total	X	0	0
			186	186		
22	M	1	Total	X	0	0
			1	1		

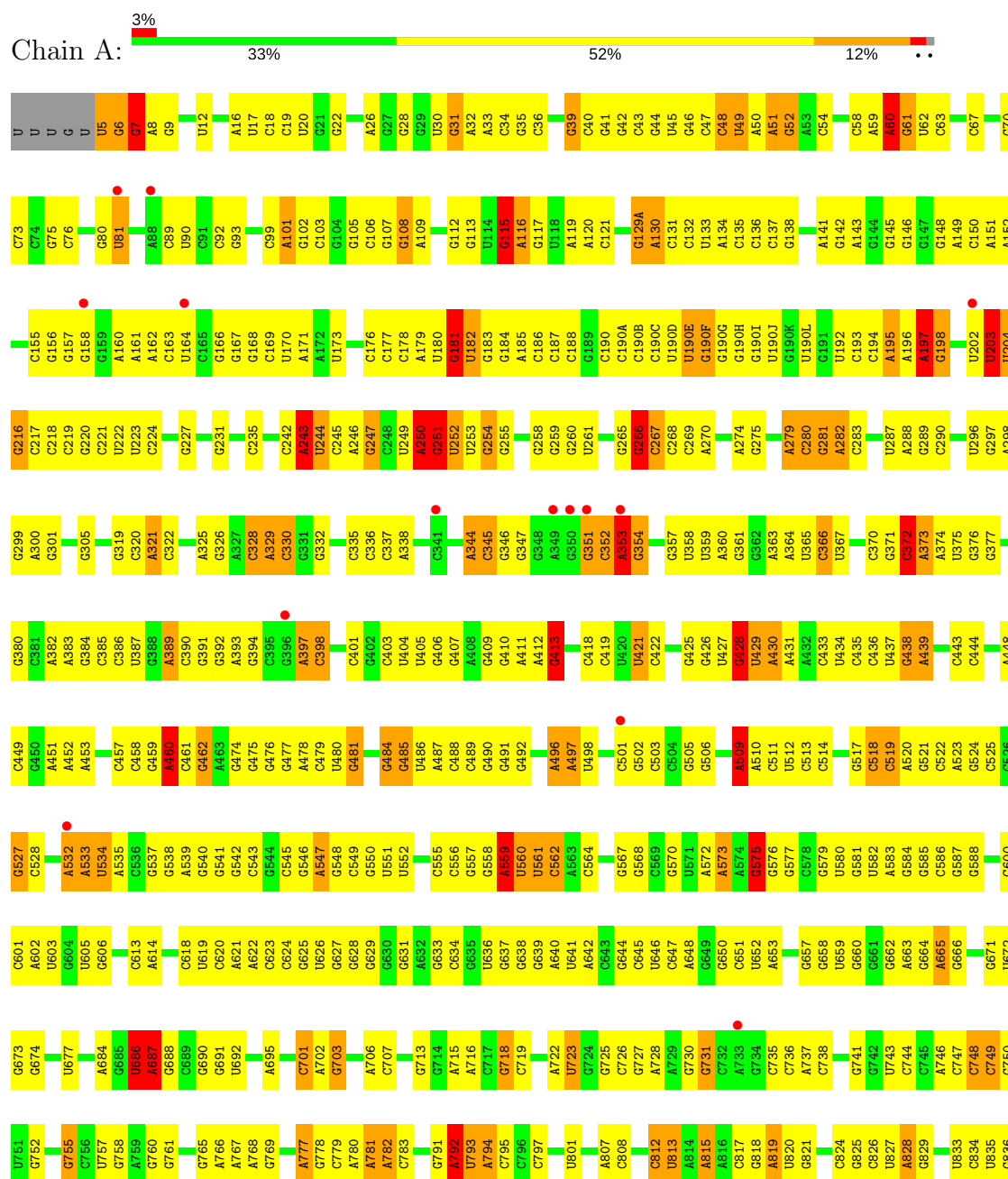
- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

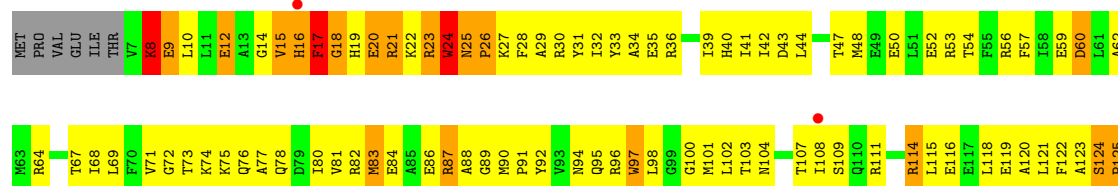
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	D	1	Total	Zn	0	0
			1	1		
23	N	1	Total	Zn	0	0
			1	1		

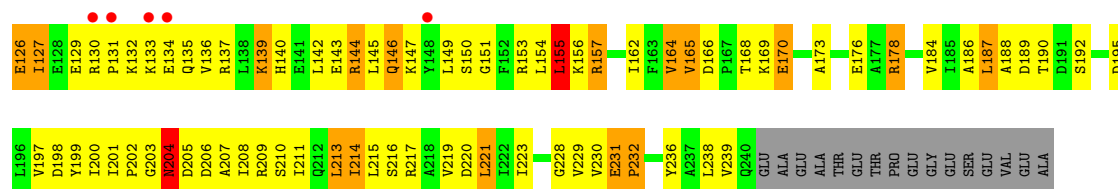
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

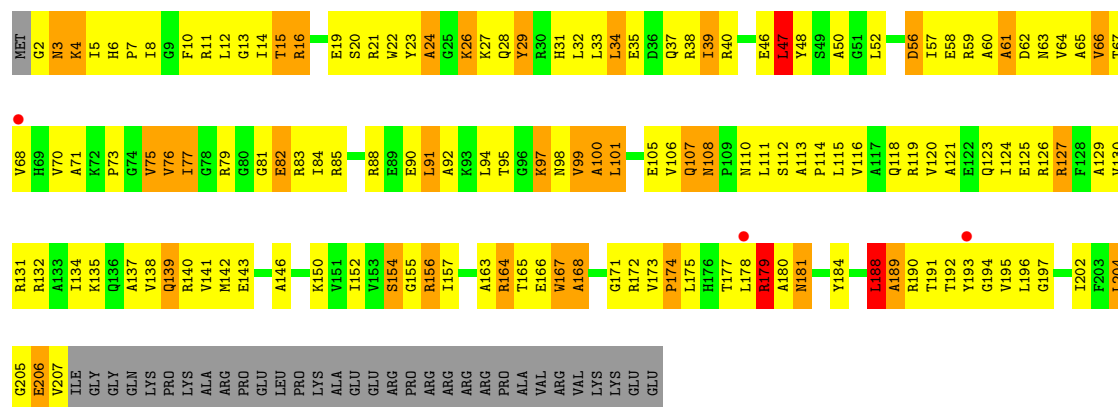
• Molecule 1: 16S ribosomal RNA



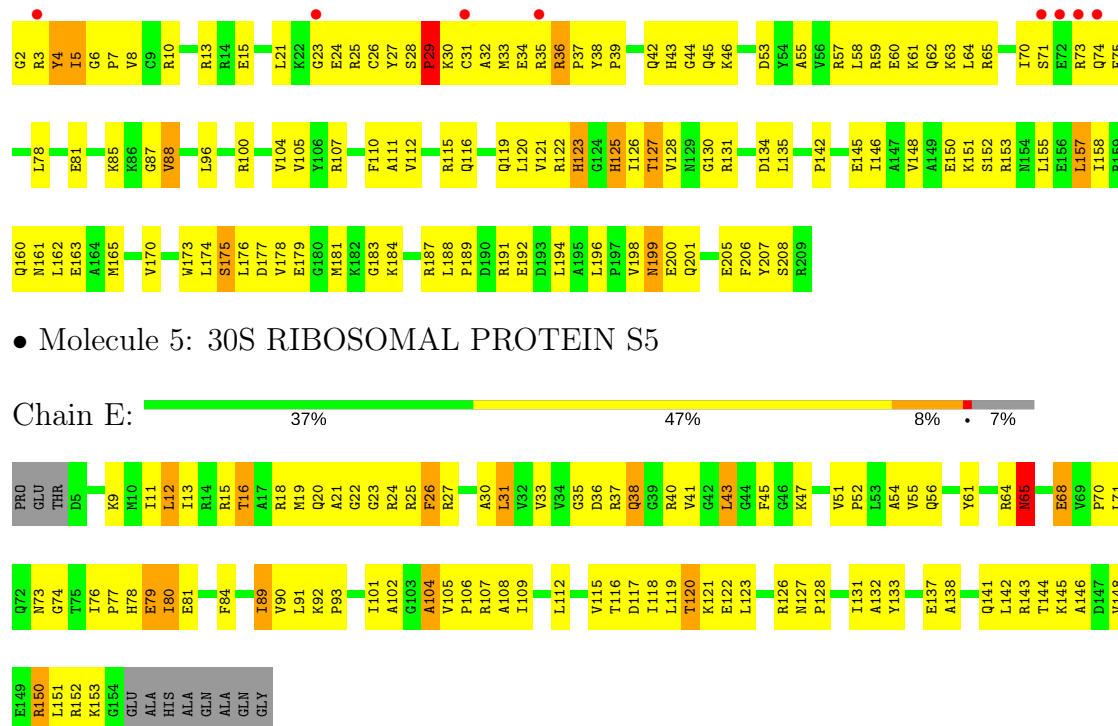
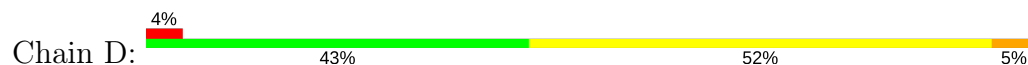




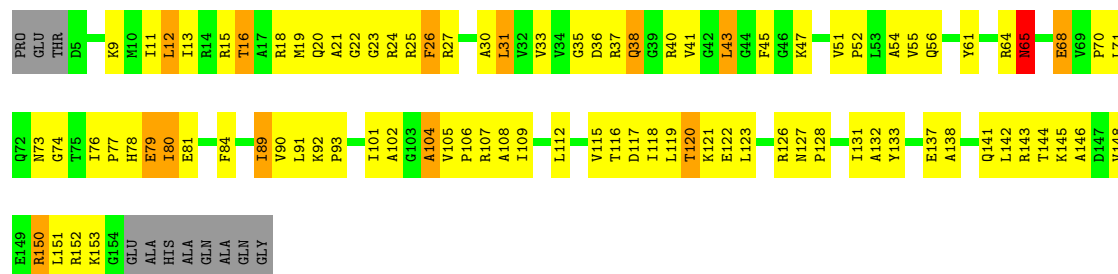
• Molecule 3: 30S RIBOSOMAL PROTEIN S3



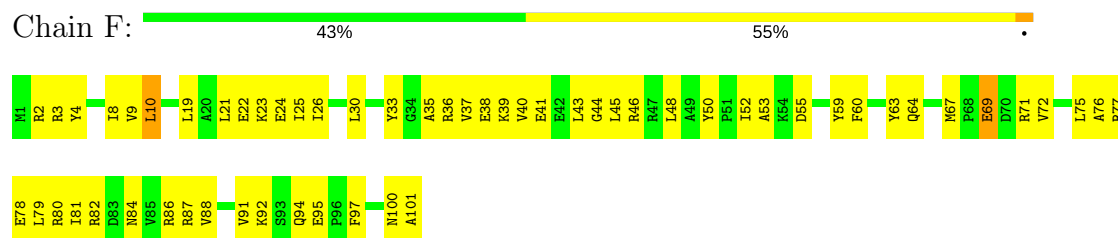
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



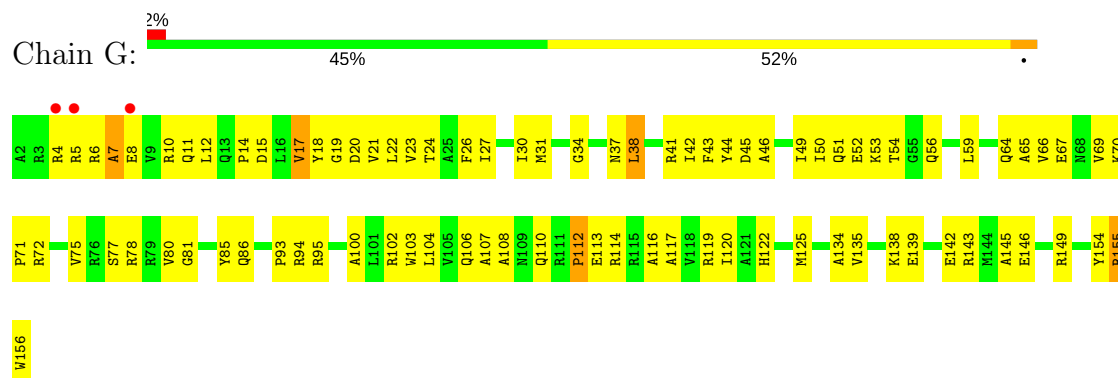
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



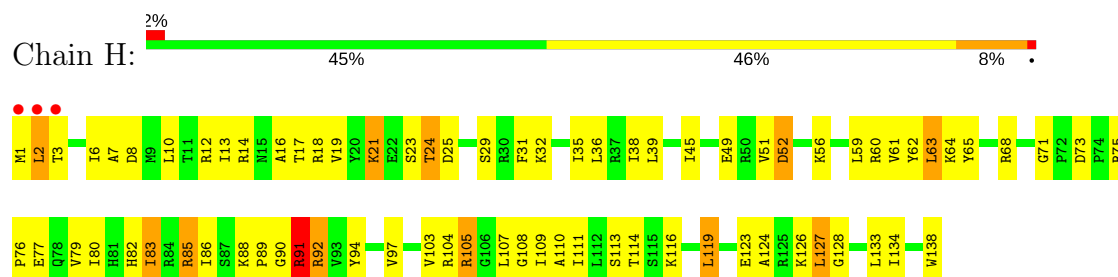
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



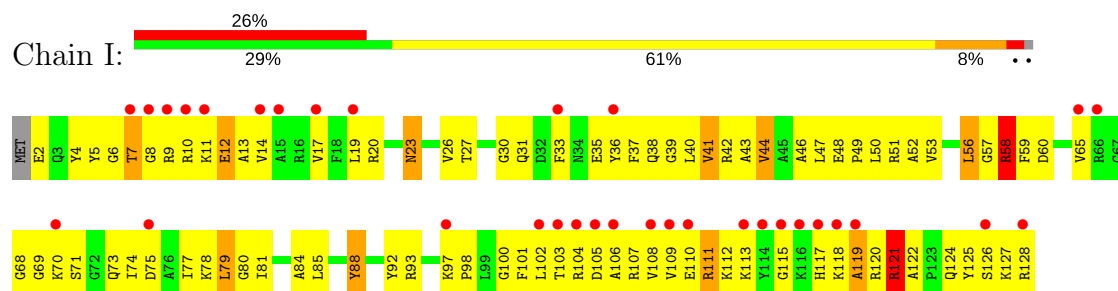
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



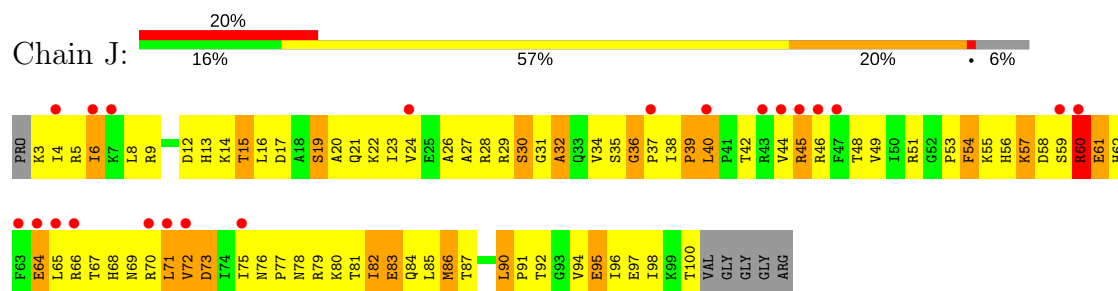
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



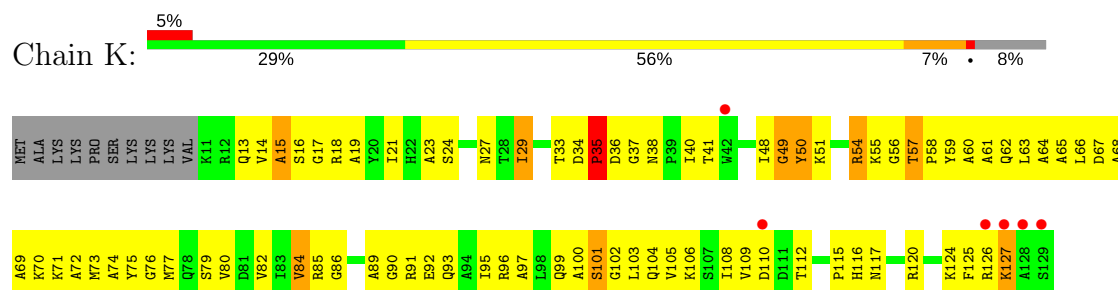
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



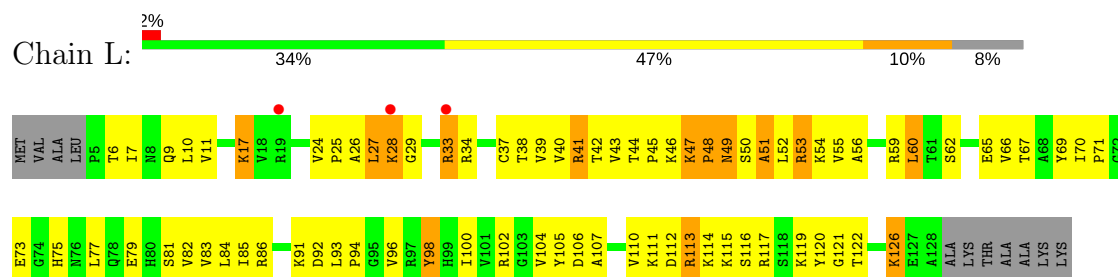
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



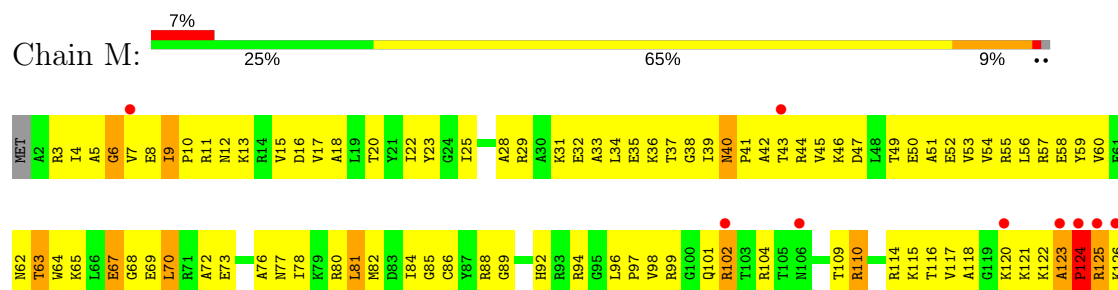
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



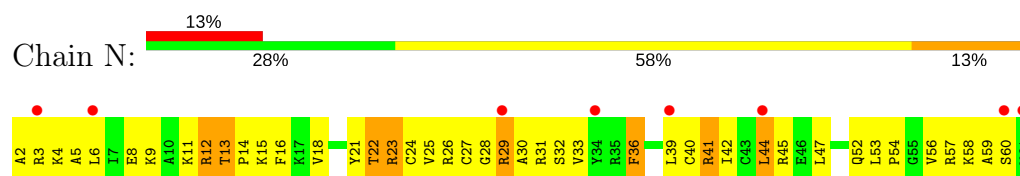
• Molecule 12: 30S RIBOSOMAL PROTEIN S12



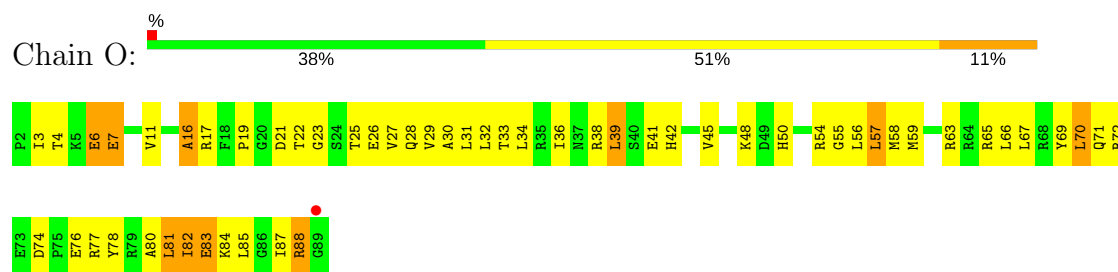
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 14: 30S RIBOSOMAL PROTEIN S14

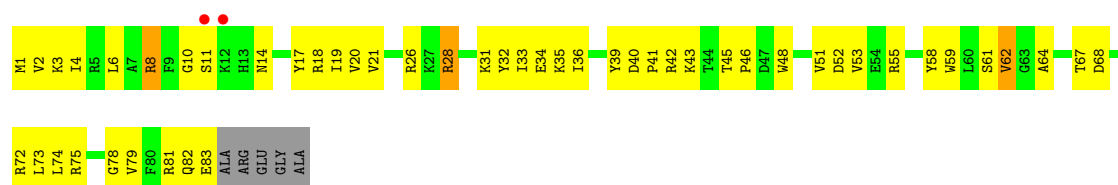


• Molecule 15: 30S RIBOSOMAL PROTEIN S15

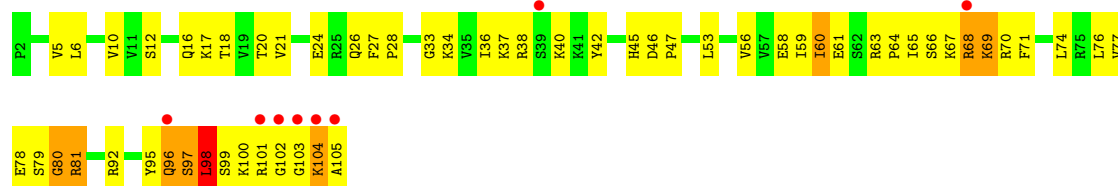
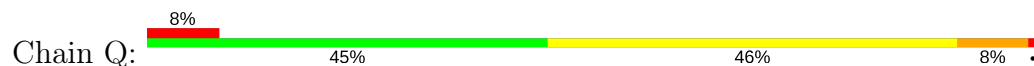


• Molecule 16: 30S RIBOSOMAL PROTEIN S16

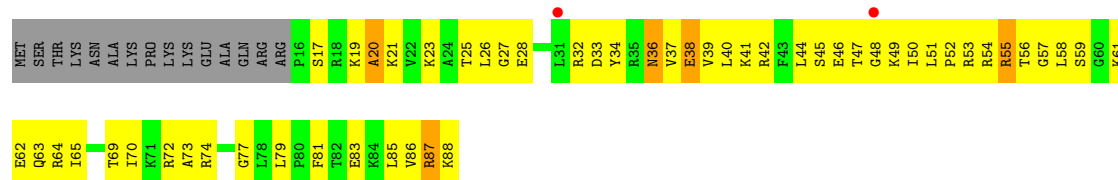




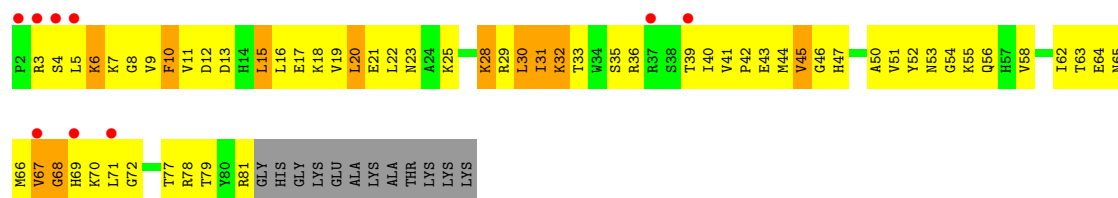
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



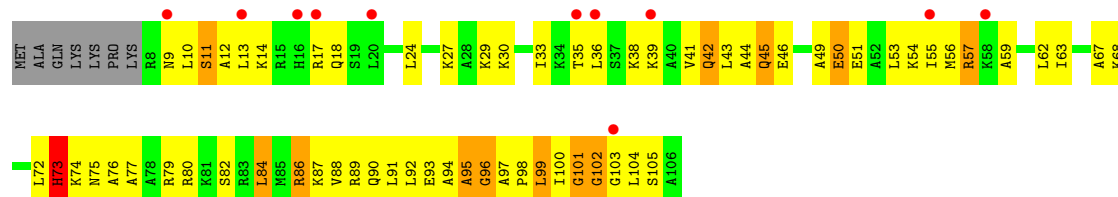
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	401.38Å 401.38Å 175.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.76 – 3.05 179.50 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.0 (59.76-3.05) 93.8 (179.50-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.07Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.208 , 0.252 0.229 , 0.259	Depositor DCC
R_{free} test set	12919 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	51933	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: UNX, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/36393	0.75	41/56797 (0.1%)
2	B	0.36	0/1935	0.67	1/2609 (0.0%)
3	C	0.37	0/1636	0.66	0/2205
4	D	0.37	0/1733	0.63	0/2318
5	E	0.48	0/1162	0.79	0/1564
6	F	0.33	0/856	0.62	0/1154
7	G	0.34	0/1276	0.61	0/1709
8	H	0.44	0/1136	0.74	0/1527
9	I	0.36	0/1029	0.62	0/1378
10	J	0.36	0/805	0.71	0/1082
11	K	0.39	0/900	0.70	0/1213
12	L	0.42	0/986	0.73	0/1320
13	M	0.35	0/1008	0.67	0/1347
14	N	0.40	0/501	0.78	0/664
15	O	0.36	0/745	0.63	1/992 (0.1%)
16	P	0.43	0/716	0.76	0/963
17	Q	0.44	0/870	0.75	0/1159
18	R	0.36	0/603	0.63	0/799
19	S	0.34	0/661	0.72	1/890 (0.1%)
20	T	0.39	0/764	0.73	0/1006
21	V	0.42	0/212	0.64	0/277
All	All	0.45	0/55927	0.73	44/82973 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	40

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.93	131.35	109.50
1	A	243	A	C2'-C3'-O3'	9.45	130.28	109.50
1	A	181	G	C2'-C3'-O3'	9.13	129.59	109.50
1	A	559	A	C2'-C3'-O3'	9.12	129.56	109.50
1	A	1299	A	N9-C1'-C2'	8.59	125.17	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	181	G	C3'
1	A	1528	U	C3'

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	U	Sidechain
1	A	197	A	Sidechain
1	A	203	U	Sidechain
1	A	231	G	Sidechain
1	A	249	U	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	32514	0	16410	1113	0
2	B	1900	0	1951	217	1
3	C	1612	0	1677	226	0
4	D	1703	0	1764	146	0
5	E	1146	0	1207	104	0
6	F	843	0	857	72	0
7	G	1257	0	1296	93	0
8	H	1116	0	1177	67	0
9	I	1011	0	1043	113	0
10	J	792	0	835	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	885	0	904	85	0
12	L	970	0	1057	118	0
13	M	997	0	1072	121	0
14	N	492	0	529	74	0
15	O	734	0	771	55	0
16	P	700	0	720	56	0
17	Q	857	0	930	84	0
18	R	597	0	668	68	0
19	S	647	0	673	81	0
20	T	762	0	859	78	0
21	V	208	0	221	26	0
22	A	186	0	0	0	0
22	B	1	0	0	0	0
22	M	1	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
All	All	51933	0	36621	2836	1

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 32.

The worst 5 of 2836 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)
12:L:41:ARG:HG2	12:L:42:THR:H	1.03	1.15
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.22	1.14
1:A:1443:G:H5''	1:A:1446:A:H5'	1.28	1.11
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.32	1.09
4:D:36:ARG:H	4:D:37:PRO:HD3	1.19	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:ARG:NH1	2:B:157:ARG:NH1[7_555]	1.70	0.50

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	232/256 (91%)	174 (75%)	34 (15%)	24 (10%)	0	3
3	C	204/239 (85%)	135 (66%)	40 (20%)	29 (14%)	0	1
4	D	206/208 (99%)	166 (81%)	31 (15%)	9 (4%)	3	14
5	E	148/161 (92%)	130 (88%)	13 (9%)	5 (3%)	4	19
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	17	49
7	G	153/155 (99%)	127 (83%)	16 (10%)	10 (6%)	1	7
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	5	23
9	I	125/128 (98%)	88 (70%)	27 (22%)	10 (8%)	1	5
10	J	96/104 (92%)	59 (62%)	20 (21%)	17 (18%)	0	0
11	K	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	5
12	L	122/135 (90%)	98 (80%)	15 (12%)	9 (7%)	1	5
13	M	123/126 (98%)	88 (72%)	27 (22%)	8 (6%)	1	7
14	N	58/60 (97%)	40 (69%)	11 (19%)	7 (12%)	0	1
15	O	86/88 (98%)	70 (81%)	11 (13%)	5 (6%)	2	9
16	P	81/88 (92%)	65 (80%)	15 (18%)	1 (1%)	14	44
17	Q	102/104 (98%)	84 (82%)	10 (10%)	8 (8%)	1	5
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	5	24
19	S	78/92 (85%)	49 (63%)	18 (23%)	11 (14%)	0	1
20	T	97/106 (92%)	65 (67%)	20 (21%)	12 (12%)	0	1
21	V	22/26 (85%)	19 (86%)	2 (9%)	1 (4%)	3	14
All	All	2356/2532 (93%)	1811 (77%)	363 (15%)	182 (8%)	1	5

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU

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Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	180 (89%)	22 (11%)	7	25
3	C	160/188 (85%)	142 (89%)	18 (11%)	6	23
4	D	180/180 (100%)	172 (96%)	8 (4%)	31	63
5	E	115/122 (94%)	100 (87%)	15 (13%)	4	17
6	F	90/90 (100%)	88 (98%)	2 (2%)	55	80
7	G	126/126 (100%)	122 (97%)	4 (3%)	42	73
8	H	119/119 (100%)	109 (92%)	10 (8%)	12	38
9	I	98/99 (99%)	90 (92%)	8 (8%)	12	39
10	J	87/91 (96%)	78 (90%)	9 (10%)	8	27
11	K	90/99 (91%)	84 (93%)	6 (7%)	18	48
12	L	104/111 (94%)	96 (92%)	8 (8%)	14	42
13	M	100/101 (99%)	90 (90%)	10 (10%)	8	28
14	N	49/49 (100%)	47 (96%)	2 (4%)	33	66
15	O	79/79 (100%)	72 (91%)	7 (9%)	11	35
16	P	72/74 (97%)	67 (93%)	5 (7%)	17	47
17	Q	96/96 (100%)	90 (94%)	6 (6%)	20	50
18	R	64/77 (83%)	61 (95%)	3 (5%)	29	61
19	S	71/79 (90%)	68 (96%)	3 (4%)	32	65
20	T	76/82 (93%)	69 (91%)	7 (9%)	10	33
21	V	19/21 (90%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1997/2103 (95%)	1844 (92%)	153 (8%)	14	42

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	2	LEU
9	I	111	ARG
18	R	38	GLU
8	H	52	ASP
8	H	105	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
6	F	64	GLN
9	I	73	GLN
18	R	36	ASN
6	F	94	GLN
7	G	37	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1512/1522 (99%)	220 (14%)	88 (5%)

5 of 220 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A

5 of 88 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	687	A
1	A	976	G
1	A	1397	C

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Mol	Chain	Res	Type
1	A	701	C
1	A	840	C

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 188 are unknown and 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1510/1522 (99%)	0.61	44 (2%)	51	26	28, 59, 140, 201	0
2	B	234/256 (91%)	0.12	7 (2%)	50	25	31, 77, 150, 191	0
3	C	206/239 (86%)	0.02	3 (1%)	73	51	35, 77, 131, 153	0
4	D	208/208 (100%)	0.31	8 (3%)	40	20	32, 64, 114, 169	0
5	E	150/161 (93%)	0.06	0	100	100	26, 48, 86, 139	0
6	F	101/101 (100%)	-0.25	0	100	100	47, 84, 120, 138	0
7	G	155/155 (100%)	-0.18	3 (1%)	66	43	38, 72, 122, 156	0
8	H	138/138 (100%)	0.17	3 (2%)	62	37	19, 45, 78, 131	0
9	I	127/128 (99%)	1.17	33 (25%)	0	0	36, 85, 129, 175	0
10	J	98/104 (94%)	0.88	21 (21%)	1	0	41, 106, 158, 190	0
11	K	119/129 (92%)	0.53	6 (5%)	29	12	34, 59, 105, 175	0
12	L	124/135 (91%)	0.34	3 (2%)	59	33	25, 60, 113, 162	0
13	M	125/126 (99%)	0.65	9 (7%)	15	6	46, 79, 138, 189	0
14	N	60/60 (100%)	1.02	8 (13%)	3	1	39, 72, 108, 148	0
15	O	88/88 (100%)	0.21	1 (1%)	80	61	31, 60, 114, 182	0
16	P	83/88 (94%)	0.47	2 (2%)	59	33	31, 53, 74, 138	0
17	Q	104/104 (100%)	1.06	8 (7%)	13	5	32, 55, 128, 201	0
18	R	73/88 (82%)	0.28	2 (2%)	54	28	37, 68, 137, 186	0
19	S	80/92 (86%)	0.56	9 (11%)	5	2	54, 95, 153, 187	0
20	T	99/106 (93%)	0.67	11 (11%)	5	2	29, 60, 115, 187	0
21	V	24/26 (92%)	2.32	12 (50%)	0	0	36, 66, 103, 129	0
All	All	3906/4054 (96%)	0.47	193 (4%)	29	13	19, 64, 135, 201	0

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	102	GLY	18.4
11	K	129	SER	17.2
19	S	3	ARG	15.3
17	Q	104	LYS	13.9
17	Q	105	ALA	11.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	UNX	A	1588	1/1	-0.47	1.00	57,57,57,57	1
22	UNX	A	1683	1/1	-0.17	2.50	57,57,57,57	1
22	UNX	A	1640	1/1	-0.03	1.00	57,57,57,57	1
22	UNX	A	1715	1/1	0.01	1.37	57,57,57,57	1
22	UNX	A	1675	1/1	0.06	1.04	57,57,57,57	1
22	UNX	A	1697	1/1	0.09	2.02	57,57,57,57	1
22	UNX	A	1582	1/1	0.13	0.82	57,57,57,57	1
22	UNX	A	1701	1/1	0.15	1.08	57,57,57,57	1
22	UNX	A	1632	1/1	0.17	0.92	57,57,57,57	1
22	UNX	A	1680	1/1	0.19	0.66	57,57,57,57	1
22	UNX	A	1670	1/1	0.26	0.74	57,57,57,57	1
22	UNX	A	1636	1/1	0.27	0.75	57,57,57,57	1
22	UNX	A	1664	1/1	0.28	0.79	57,57,57,57	1
22	UNX	A	1691	1/1	0.28	1.32	57,57,57,57	1
22	UNX	A	1694	1/1	0.32	0.75	57,57,57,57	1
22	UNX	A	1703	1/1	0.32	0.45	57,57,57,57	1
22	UNX	A	1673	1/1	0.33	1.06	57,57,57,57	1
22	UNX	A	1679	1/1	0.36	1.15	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	UNX	A	1579	1/1	0.36	1.20	57,57,57,57	1
22	UNX	A	1621	1/1	0.39	0.63	57,57,57,57	1
22	UNX	A	1698	1/1	0.39	0.94	57,57,57,57	1
22	UNX	A	1598	1/1	0.40	0.55	57,57,57,57	1
22	UNX	A	1661	1/1	0.41	0.85	57,57,57,57	1
22	UNX	A	1595	1/1	0.42	0.76	57,57,57,57	1
22	UNX	A	1570	1/1	0.42	0.81	57,57,57,57	1
22	UNX	A	1655	1/1	0.45	1.36	57,57,57,57	1
22	UNX	A	1561	1/1	0.45	0.94	57,57,57,57	1
22	UNX	A	72	1/1	0.46	1.49	57,57,57,57	1
22	UNX	A	1600	1/1	0.47	0.74	57,57,57,57	1
22	UNX	A	1696	1/1	0.47	1.48	57,57,57,57	1
22	UNX	A	1618	1/1	0.47	0.47	57,57,57,57	1
22	UNX	A	1613	1/1	0.47	0.91	57,57,57,57	1
22	UNX	A	1615	1/1	0.49	0.87	57,57,57,57	1
22	UNX	A	1676	1/1	0.49	0.83	57,57,57,57	1
22	UNX	A	1689	1/1	0.49	1.47	57,57,57,57	1
22	UNX	A	1722	1/1	0.50	0.87	55,55,55,55	1
22	UNX	A	1625	1/1	0.50	1.10	57,57,57,57	1
22	UNX	A	1677	1/1	0.51	0.68	57,57,57,57	1
22	UNX	A	1690	1/1	0.51	0.97	57,57,57,57	1
22	UNX	A	1637	1/1	0.52	0.86	57,57,57,57	1
22	UNX	A	1667	1/1	0.52	0.67	57,57,57,57	1
22	UNX	A	1700	1/1	0.53	0.53	57,57,57,57	1
22	UNX	A	1665	1/1	0.54	0.71	57,57,57,57	1
22	UNX	A	1643	1/1	0.54	0.53	57,57,57,57	1
22	UNX	A	1647	1/1	0.54	1.01	57,57,57,57	1
22	UNX	A	1717	1/1	0.56	0.69	57,57,57,57	1
22	UNX	A	1604	1/1	0.56	0.77	57,57,57,57	1
22	UNX	A	1638	1/1	0.56	1.06	57,57,57,57	1
22	UNX	A	1672	1/1	0.57	0.63	57,57,57,57	1
22	UNX	A	1626	1/1	0.57	2.35	57,57,57,57	1
22	UNX	A	1639	1/1	0.57	0.64	57,57,57,57	1
22	UNX	A	1593	1/1	0.57	0.68	57,57,57,57	1
22	UNX	A	1575	1/1	0.58	0.73	57,57,57,57	1
22	UNX	A	1583	1/1	0.58	1.44	57,57,57,57	1
22	UNX	A	1674	1/1	0.59	0.59	57,57,57,57	1
22	UNX	A	1716	1/1	0.59	0.71	57,57,57,57	1
22	UNX	A	1620	1/1	0.59	1.46	57,57,57,57	1
22	UNX	A	1571	1/1	0.60	0.99	57,57,57,57	1
22	UNX	A	1612	1/1	0.61	0.74	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	UNX	A	1629	1/1	0.61	0.54	57,57,57,57	1
22	UNX	A	1610	1/1	0.61	1.22	57,57,57,57	1
22	UNX	A	1565	1/1	0.61	1.42	57,57,57,57	1
22	UNX	A	86	1/1	0.62	0.79	57,57,57,57	1
22	UNX	A	1721	1/1	0.62	1.25	57,57,57,57	1
22	UNX	A	1684	1/1	0.63	0.94	57,57,57,57	1
22	UNX	A	1705	1/1	0.63	0.93	57,57,57,57	1
22	UNX	A	1645	1/1	0.63	0.58	57,57,57,57	1
22	UNX	A	1720	1/1	0.63	0.56	57,57,57,57	1
22	UNX	A	1695	1/1	0.64	0.76	57,57,57,57	1
22	UNX	A	1641	1/1	0.65	0.76	57,57,57,57	1
22	UNX	A	1644	1/1	0.66	2.17	57,57,57,57	1
22	UNX	A	1718	1/1	0.66	0.66	57,57,57,57	1
22	UNX	A	1585	1/1	0.66	1.08	57,57,57,57	1
22	UNX	A	1634	1/1	0.66	0.60	57,57,57,57	1
22	UNX	A	1551	1/1	0.66	0.82	57,57,57,57	1
22	UNX	A	1601	1/1	0.66	1.36	57,57,57,57	1
22	UNX	A	1569	1/1	0.67	0.76	57,57,57,57	1
22	UNX	A	1711	1/1	0.68	0.66	57,57,57,57	1
22	UNX	A	1546	1/1	0.68	0.73	57,57,57,57	0
22	UNX	A	1646	1/1	0.69	0.50	57,57,57,57	1
22	UNX	A	1685	1/1	0.69	0.40	57,57,57,57	1
22	UNX	A	1630	1/1	0.69	0.28	57,57,57,57	1
22	UNX	A	1611	1/1	0.69	0.79	57,57,57,57	1
22	UNX	A	1702	1/1	0.70	0.65	57,57,57,57	1
22	UNX	A	1609	1/1	0.70	0.68	57,57,57,57	1
22	UNX	A	100	1/1	0.70	0.72	57,57,57,57	1
22	UNX	A	1589	1/1	0.71	0.82	57,57,57,57	1
22	UNX	A	1635	1/1	0.71	0.57	57,57,57,57	1
22	UNX	A	1650	1/1	0.71	0.76	57,57,57,57	1
22	UNX	A	1614	1/1	0.71	1.03	57,57,57,57	1
22	UNX	A	1668	1/1	0.72	0.60	57,57,57,57	1
22	UNX	A	1719	1/1	0.73	0.85	57,57,57,57	1
22	UNX	A	1576	1/1	0.73	1.24	57,57,57,57	1
22	UNX	A	1628	1/1	0.74	1.34	57,57,57,57	1
22	UNX	A	1568	1/1	0.74	0.68	57,57,57,57	1
22	UNX	B	257	1/1	0.74	0.46	57,57,57,57	1
22	UNX	A	1659	1/1	0.74	1.14	57,57,57,57	1
22	UNX	A	1642	1/1	0.75	0.85	57,57,57,57	1
22	UNX	A	1557	1/1	0.75	1.04	57,57,57,57	1
22	UNX	A	1699	1/1	0.76	0.95	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	UNX	A	1723	1/1	0.76	1.06	55,55,55,55	1
22	UNX	A	1663	1/1	0.76	1.02	57,57,57,57	1
22	UNX	A	1669	1/1	0.76	0.46	57,57,57,57	1
22	UNX	A	1648	1/1	0.76	0.62	57,57,57,57	1
22	UNX	A	1572	1/1	0.76	1.08	57,57,57,57	1
22	UNX	A	1666	1/1	0.77	1.07	57,57,57,57	1
22	UNX	A	1662	1/1	0.77	0.37	57,57,57,57	1
22	UNX	A	1652	1/1	0.77	0.66	57,57,57,57	1
22	UNX	A	1704	1/1	0.77	0.99	57,57,57,57	1
22	UNX	A	1574	1/1	0.78	0.87	57,57,57,57	1
22	UNX	M	143	1/1	0.78	0.30	57,57,57,57	1
22	UNX	A	1671	1/1	0.78	1.11	57,57,57,57	1
22	UNX	A	1658	1/1	0.78	1.61	57,57,57,57	1
22	UNX	A	1566	1/1	0.79	1.02	57,57,57,57	1
22	UNX	A	1608	1/1	0.79	0.42	57,57,57,57	1
22	UNX	A	1651	1/1	0.79	0.99	57,57,57,57	1
22	UNX	A	1597	1/1	0.79	0.85	57,57,57,57	1
22	UNX	A	94	1/1	0.79	1.23	57,57,57,57	1
22	UNX	A	1606	1/1	0.79	0.73	57,57,57,57	1
22	UNX	A	1619	1/1	0.79	0.95	57,57,57,57	1
22	UNX	A	1545	1/1	0.79	0.78	57,57,57,57	0
22	UNX	A	1622	1/1	0.79	1.42	57,57,57,57	1
22	UNX	A	87	1/1	0.80	1.25	57,57,57,57	1
22	UNX	A	1602	1/1	0.80	0.99	57,57,57,57	1
22	UNX	A	1590	1/1	0.80	1.04	57,57,57,57	1
22	UNX	A	1656	1/1	0.80	1.06	57,57,57,57	1
22	UNX	A	1617	1/1	0.80	0.80	57,57,57,57	1
22	UNX	A	1708	1/1	0.81	1.15	57,57,57,57	1
22	UNX	A	1573	1/1	0.81	1.18	57,57,57,57	1
22	UNX	A	1549	1/1	0.81	0.99	57,57,57,57	1
22	UNX	A	1633	1/1	0.81	0.77	57,57,57,57	1
22	UNX	A	1592	1/1	0.81	0.70	57,57,57,57	0
22	UNX	A	1578	1/1	0.81	1.02	57,57,57,57	1
22	UNX	A	1558	1/1	0.82	0.93	57,57,57,57	1
22	UNX	A	1584	1/1	0.82	0.47	57,57,57,57	1
22	UNX	A	1687	1/1	0.82	1.06	57,57,57,57	1
22	UNX	A	1607	1/1	0.82	0.74	57,57,57,57	1
22	UNX	A	1596	1/1	0.82	0.93	57,57,57,57	1
22	UNX	A	1581	1/1	0.83	1.16	57,57,57,57	1
22	UNX	A	1562	1/1	0.83	0.99	57,57,57,57	1
22	UNX	A	1660	1/1	0.83	0.97	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	UNX	A	71	1/1	0.84	0.87	57,57,57,57	1
22	UNX	A	1713	1/1	0.84	1.24	57,57,57,57	1
22	UNX	A	1603	1/1	0.85	0.81	57,57,57,57	1
22	UNX	A	1710	1/1	0.85	1.00	57,57,57,57	1
22	UNX	A	1599	1/1	0.86	0.94	57,57,57,57	1
22	UNX	A	1653	1/1	0.86	0.56	57,57,57,57	1
22	UNX	A	1627	1/1	0.87	0.79	57,57,57,57	1
22	UNX	A	1580	1/1	0.87	0.80	57,57,57,57	1
22	UNX	A	1624	1/1	0.87	1.07	57,57,57,57	1
22	UNX	A	1709	1/1	0.88	0.99	57,57,57,57	1
22	UNX	A	1623	1/1	0.88	0.94	57,57,57,57	1
22	UNX	A	1563	1/1	0.89	0.90	57,57,57,57	1
22	UNX	A	1649	1/1	0.89	0.97	57,57,57,57	1
22	UNX	A	1654	1/1	0.89	1.17	57,57,57,57	1
22	UNX	A	1631	1/1	0.90	0.91	57,57,57,57	1
22	UNX	A	1556	1/1	0.90	0.93	57,57,57,57	1
22	UNX	A	1693	1/1	0.90	0.86	57,57,57,57	1
22	UNX	A	1567	1/1	0.90	0.82	57,57,57,57	1
22	UNX	A	1686	1/1	0.90	0.99	57,57,57,57	1
22	UNX	A	1548	1/1	0.90	0.82	57,57,57,57	0
22	UNX	A	1605	1/1	0.90	0.91	57,57,57,57	1
22	UNX	A	1564	1/1	0.91	0.99	57,57,57,57	1
22	UNX	A	1657	1/1	0.91	0.94	57,57,57,57	1
22	UNX	A	1692	1/1	0.91	1.06	57,57,57,57	1
22	UNX	A	1560	1/1	0.91	1.14	57,57,57,57	1
22	UNX	A	1555	1/1	0.91	0.77	57,57,57,57	0
22	UNX	A	1712	1/1	0.92	0.93	57,57,57,57	1
22	UNX	A	1559	1/1	0.92	0.90	57,57,57,57	0
22	UNX	A	1707	1/1	0.92	0.66	57,57,57,57	1
22	UNX	A	1706	1/1	0.92	1.08	57,57,57,57	1
22	UNX	A	1586	1/1	0.93	0.92	57,57,57,57	1
22	UNX	A	1591	1/1	0.93	1.17	57,57,57,57	1
22	UNX	A	1688	1/1	0.93	0.96	57,57,57,57	1
22	UNX	A	85	1/1	0.93	0.99	57,57,57,57	1
22	UNX	A	1682	1/1	0.93	0.86	57,57,57,57	1
22	UNX	A	1553	1/1	0.93	0.93	57,57,57,57	1
22	UNX	A	1714	1/1	0.93	1.07	57,57,57,57	1
22	UNX	A	1594	1/1	0.93	0.81	57,57,57,57	1
22	UNX	A	1552	1/1	0.94	0.89	57,57,57,57	1
22	UNX	A	1577	1/1	0.94	0.92	57,57,57,57	1
22	UNX	A	1678	1/1	0.94	0.99	57,57,57,57	1
22	UNX	A	1616	1/1	0.94	0.85	57,57,57,57	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
23	ZN	D	306	1/1	0.95	0.48	67,67,67,67	0
22	UNX	A	1547	1/1	0.95	0.88	57,57,57,57	0
22	UNX	A	1550	1/1	0.96	0.92	57,57,57,57	1
22	UNX	A	1554	1/1	0.96	0.81	57,57,57,57	0
22	UNX	A	1681	1/1	0.97	0.79	57,57,57,57	1
22	UNX	A	1587	1/1	0.97	1.11	57,57,57,57	1
23	ZN	N	307	1/1	0.99	0.17	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.