



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 26, 2016 – 12:13 AM EDT

PDB ID : 4YY3
Title : 30S ribosomal subunit- HigB complex
Authors : Schureck, M.A.; Maehigashi, T.; Dunham, C.M.
Deposited on : 2015-03-23
Resolution : 3.60 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

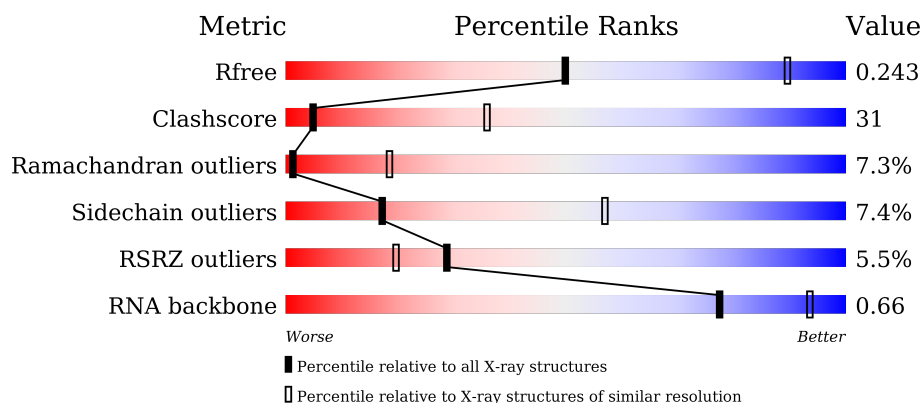
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)
RNA backbone	2183	1058 (4.40-2.80)

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	<div> <div>6%</div> <div> <div>34%</div> <div>51%</div> <div>12%</div> <div>••</div> </div> </div>
2	B	256	<div> <div>3%</div> <div> <div>25%</div> <div>52%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
3	C	239	<div> <div>5%</div> <div> <div>26%</div> <div>46%</div> <div>14%</div> <div>•</div> <div>14%</div> </div> </div>
4	D	209	<div> <div>5%</div> <div> <div>43%</div> <div>51%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	Y	118	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1603	-	-	-	X
23	MG	A	1621	-	-	-	X
23	MG	A	1623	-	-	-	X
23	MG	A	1627	-	-	-	X
23	MG	A	1637	-	-	-	X
23	MG	A	1648	-	-	-	X
23	MG	A	1652	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1658	-	-	-	X
23	MG	A	1661	-	-	-	X
23	MG	A	1665	-	-	-	X
23	MG	A	1670	-	-	-	X
23	MG	A	1676	-	-	-	X
23	MG	A	1685	-	-	-	X
23	MG	A	1689	-	-	-	X
23	MG	A	1692	-	-	-	X
23	MG	A	1697	-	-	-	X
23	MG	A	1704	-	-	-	X
23	MG	A	1719	-	-	-	X
23	MG	A	1720	-	-	-	X
23	MG	A	1723	-	-	-	X
23	MG	A	1727	-	-	-	X
23	MG	A	1733	-	-	-	X
23	MG	A	1751	-	-	-	X
23	MG	A	1753	-	-	-	X
23	MG	A	1755	-	-	-	X
23	MG	A	1756	-	-	-	X
23	MG	A	1757	-	-	-	X
23	MG	A	1766	-	-	-	X
23	MG	A	1770	-	-	-	X
23	MG	A	1773	-	-	-	X
23	MG	A	1774	-	-	-	X
23	MG	A	1776	-	-	-	X
23	MG	A	1780	-	-	-	X
23	MG	A	1782	-	-	-	X
23	MG	A	1786	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 52640 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
1	A	1513	Total	C	N	O	P	0	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	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	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	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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	100	Total	C	N	O	S	0	0	0
			834	534	155	143	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
			598	381	118	99			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	84	Total	C	N	O	S	0	0	0
			674	430	126	116	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	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 22 is a protein called Killer protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	Y	92	Total	C	N	O	0	0	0
			756	484	134	138			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	0	MET	-	initiating methionine	UNP Q7A225
Y	1	GLY	-	expression tag	UNP Q7A225
Y	93	LYS	-	expression tag	UNP Q7A225
Y	94	LEU	-	expression tag	UNP Q7A225
Y	95	GLY	-	expression tag	UNP Q7A225
Y	96	PRO	-	expression tag	UNP Q7A225
Y	97	GLU	-	expression tag	UNP Q7A225
Y	98	GLN	-	expression tag	UNP Q7A225
Y	99	LYS	-	expression tag	UNP Q7A225
Y	100	LEU	-	expression tag	UNP Q7A225
Y	101	ILE	-	expression tag	UNP Q7A225
Y	102	SER	-	expression tag	UNP Q7A225
Y	103	GLU	-	expression tag	UNP Q7A225
Y	104	GLU	-	expression tag	UNP Q7A225
Y	105	ASP	-	expression tag	UNP Q7A225
Y	106	LEU	-	expression tag	UNP Q7A225
Y	107	ASN	-	expression tag	UNP Q7A225
Y	108	SER	-	expression tag	UNP Q7A225
Y	109	ALA	-	expression tag	UNP Q7A225
Y	110	VAL	-	expression tag	UNP Q7A225
Y	111	ASP	-	expression tag	UNP Q7A225
Y	112	HIS	-	expression tag	UNP Q7A225
Y	113	HIS	-	expression tag	UNP Q7A225
Y	114	HIS	-	expression tag	UNP Q7A225
Y	115	HIS	-	expression tag	UNP Q7A225
Y	116	HIS	-	expression tag	UNP Q7A225
Y	117	HIS	-	expression tag	UNP Q7A225

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total 1	Mg 1	0	0
23	A	191	Total 191	Mg 191	0	0
23	D	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0

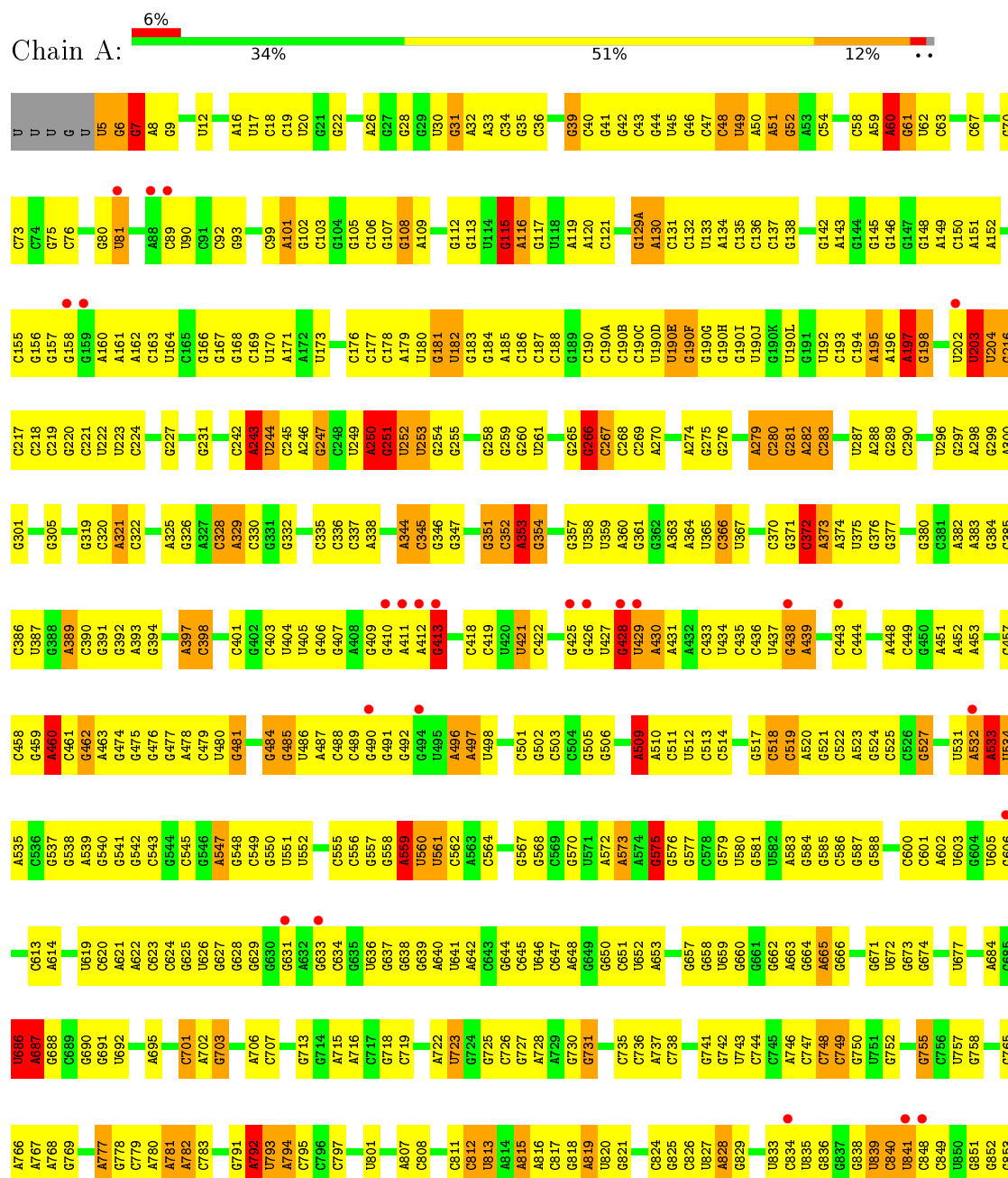
- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

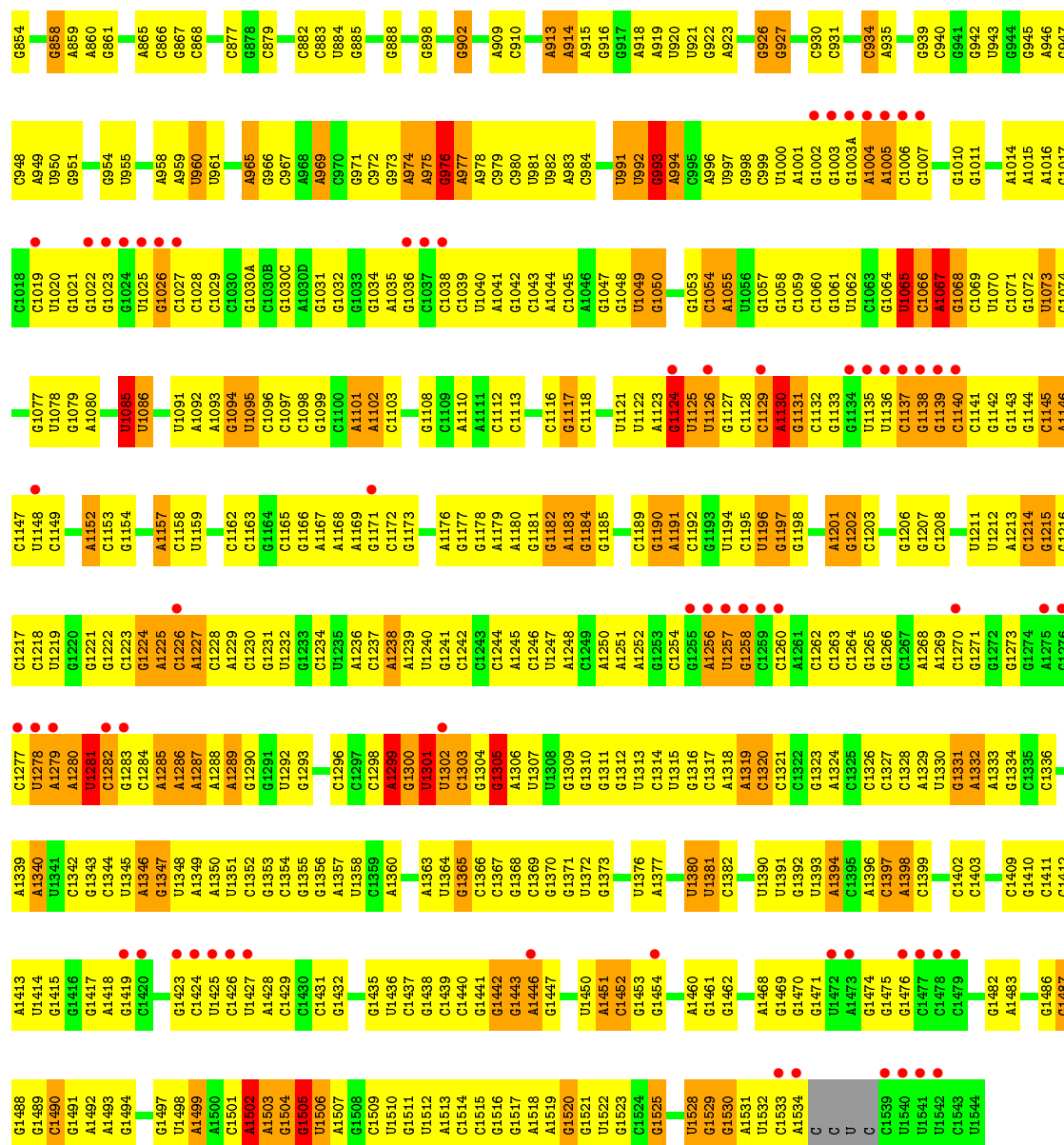
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	D	1	Total 1	Zn 1	0	0
24	N	1	Total 1	Zn 1	0	0

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 errors 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.

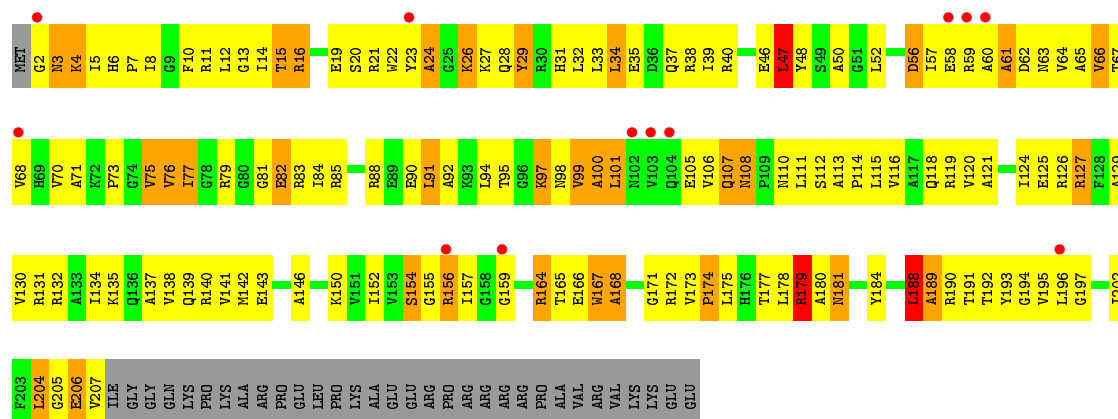
• Molecule 1: 16S rRNA



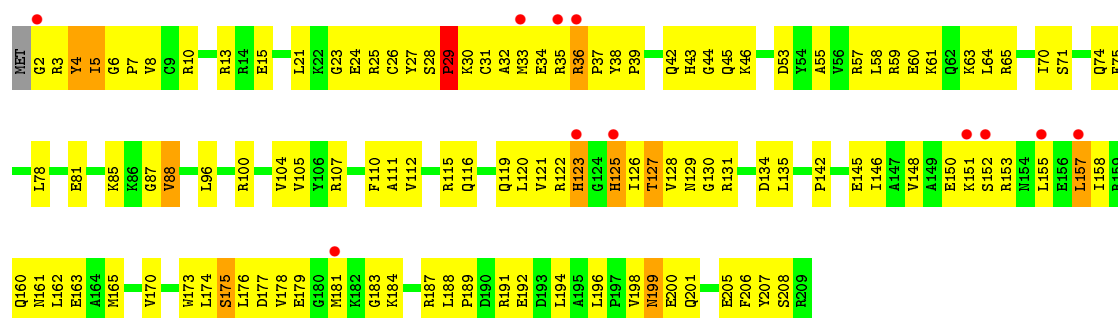
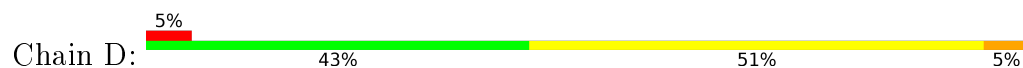




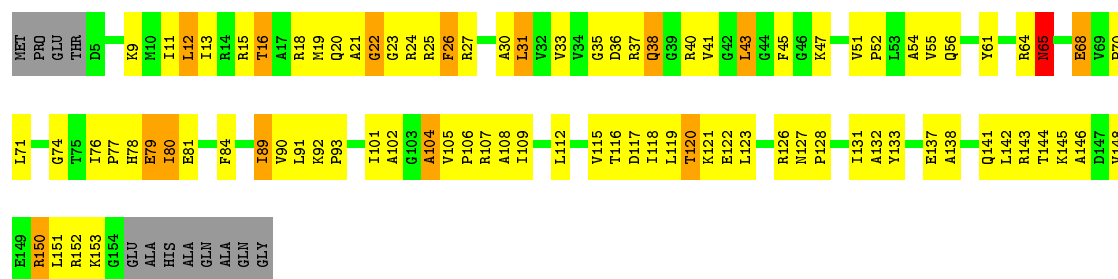
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

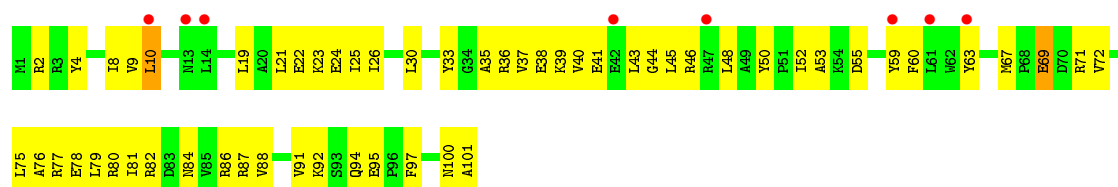


• Molecule 5: 30S ribosomal protein S5

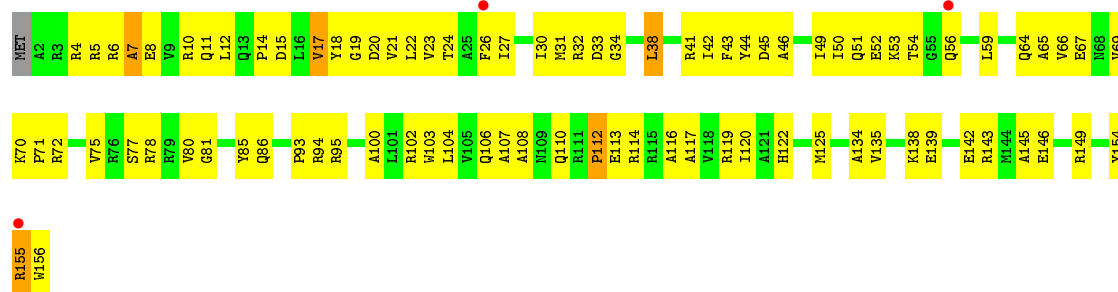
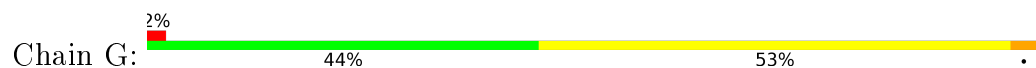


• Molecule 6: 30S ribosomal protein S6

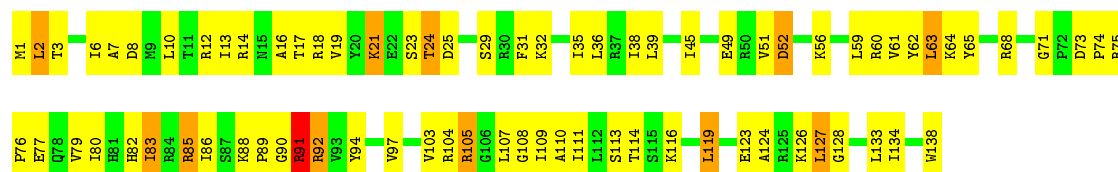




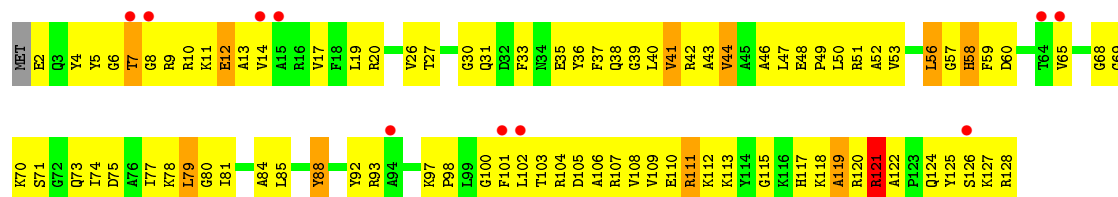
• Molecule 7: 30S ribosomal protein S7



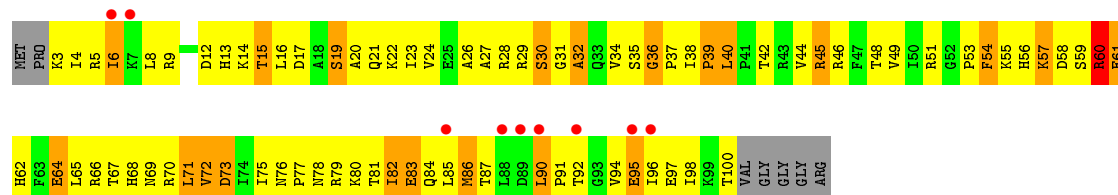
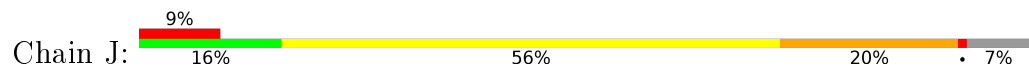
• Molecule 8: 30S ribosomal protein S8



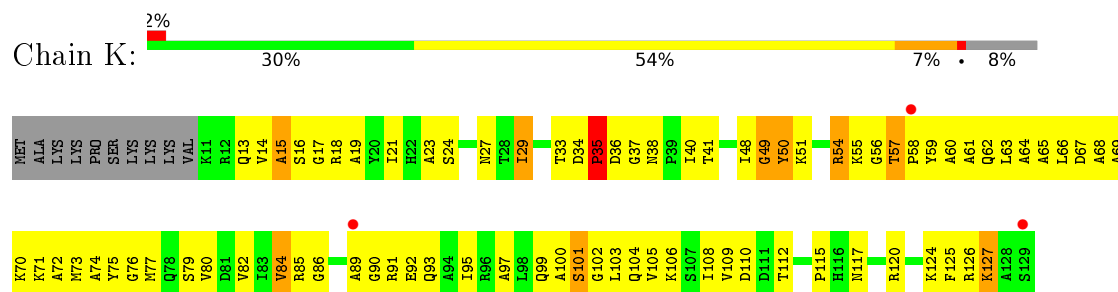
• Molecule 9: 30S ribosomal protein S9



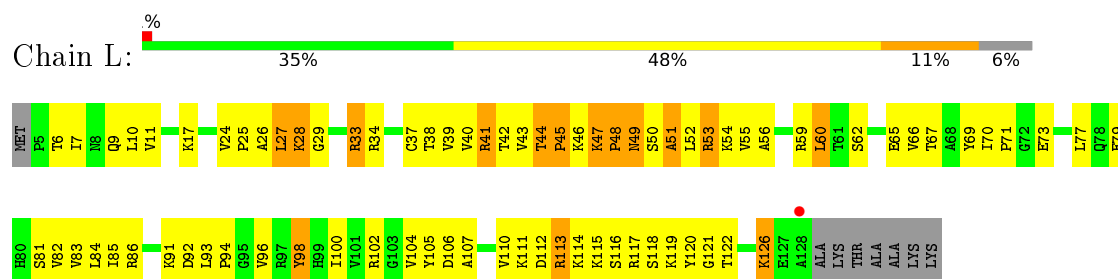
• Molecule 10: 30S ribosomal protein S10



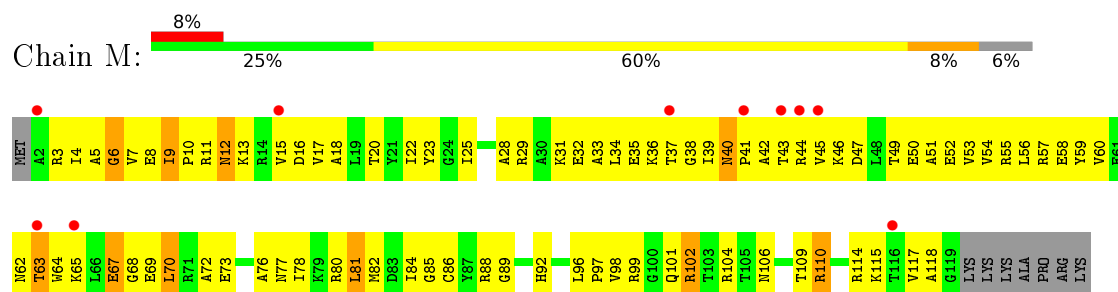
- Molecule 11: 30S ribosomal protein S11



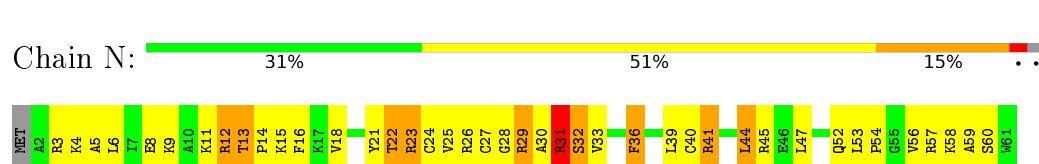
- Molecule 12: 30S ribosomal protein S12



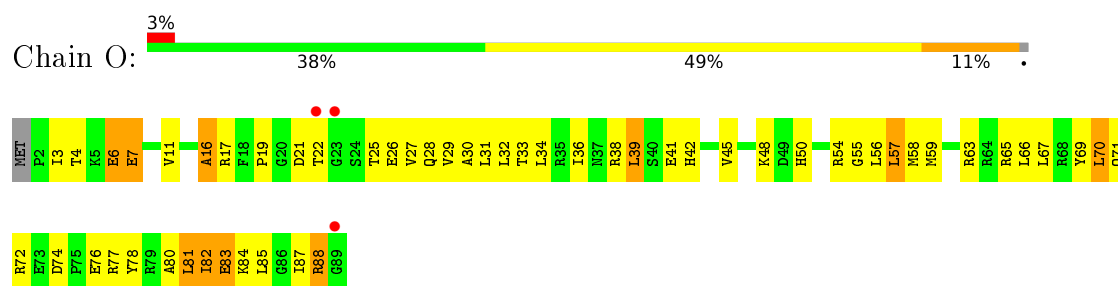
- Molecule 13: 30S ribosomal protein S13



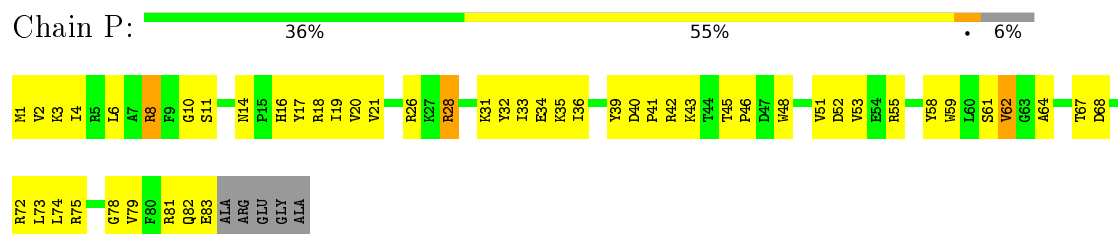
- Molecule 14: 30S ribosomal protein S14 type Z



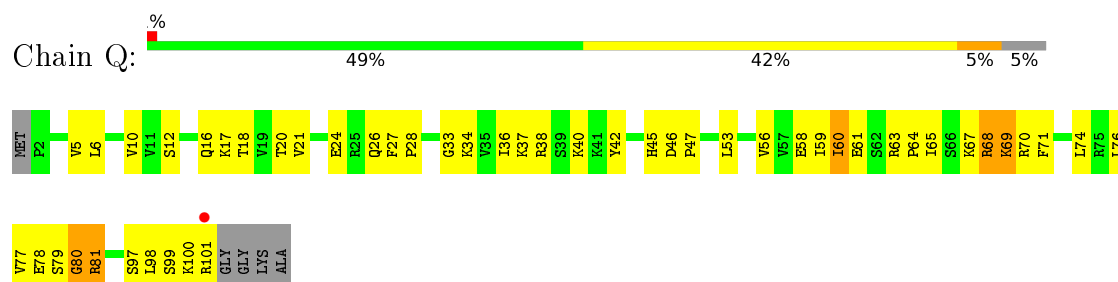
- Molecule 15: 30S ribosomal protein S15



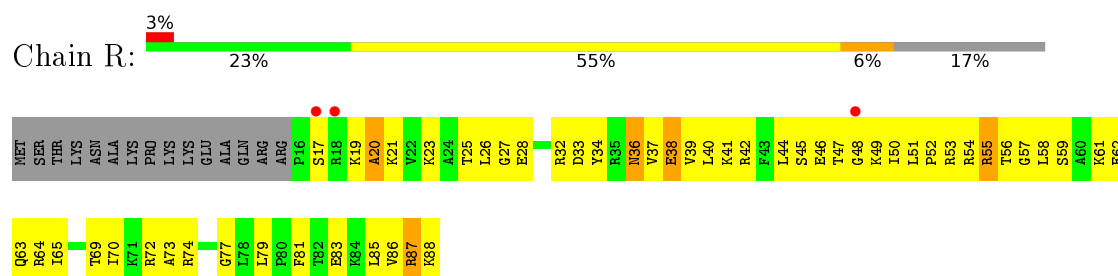
- Molecule 16: 30S ribosomal protein S16



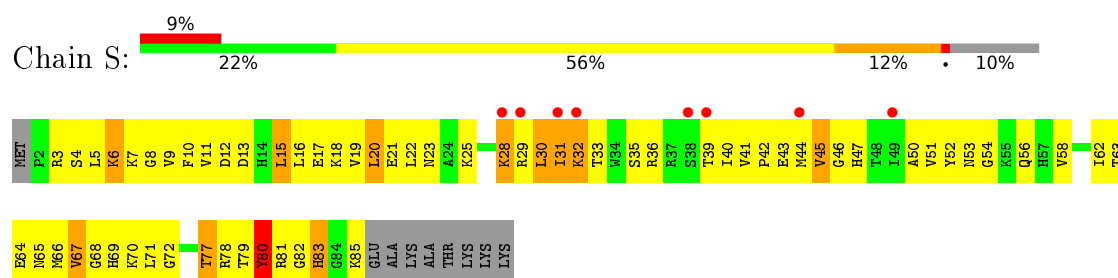
- Molecule 17: 30S ribosomal protein S17



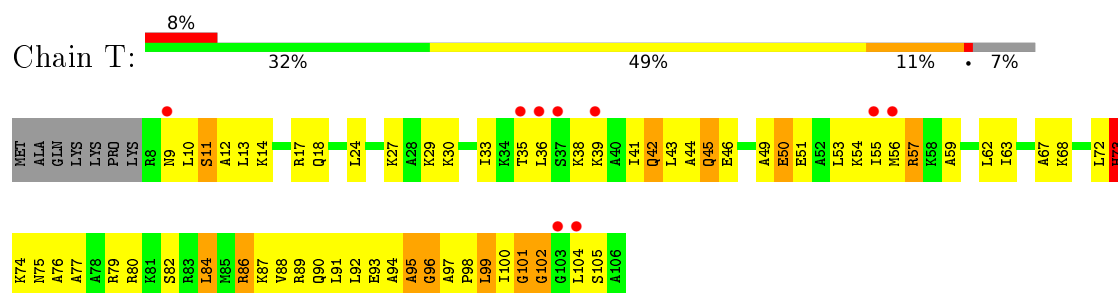
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



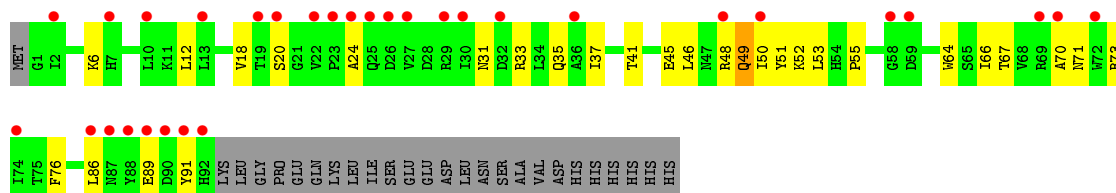
- Molecule 21: 30S ribosomal protein Thx

Chain V:  33% 52% 11%



- Molecule 22: Killer protein

Chain Y: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.59Å 402.59Å 176.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.16 – 3.60 49.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.16-3.60) 98.6 (49.91-3.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.214 , 0.239 0.217 , 0.243	Depositor DCC
R_{free} test set	7835 reflections (4.79%)	DCC
Wilson B-factor (Å ²)	110.0	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 89.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	52640	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: ZN, MG

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	38/56797 (0.1%)
2	B	0.36	0/1935	0.68	1/2609 (0.0%)
3	C	0.38	0/1636	0.66	0/2205
4	D	0.37	0/1733	0.63	0/2318
5	E	0.49	0/1162	0.79	0/1564
6	F	0.34	0/856	0.63	0/1154
7	G	0.35	0/1276	0.62	0/1709
8	H	0.44	0/1136	0.74	0/1527
9	I	0.36	0/1029	0.62	0/1379
10	J	0.35	0/805	0.70	0/1082
11	K	0.39	0/900	0.70	0/1213
12	L	0.46	1/986 (0.1%)	0.75	1/1320 (0.1%)
13	M	0.35	0/947	0.66	0/1270
14	N	0.41	0/501	0.77	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	0.45	0/847	0.73	0/1131
18	R	0.36	0/604	0.63	0/801
19	S	0.32	0/689	0.69	1/926 (0.1%)
20	T	0.39	0/765	0.73	0/1007
21	V	0.43	0/212	0.64	0/277
22	Y	0.33	0/773	0.46	0/1043
All	All	0.45	1/56646 (0.0%)	0.73	42/83951 (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	0	39

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	45	PRO	N-CD	5.02	1.54	1.47

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	A	C2'-C3'-O3'	9.49	130.38	109.50
1	A	559	A	C2'-C3'-O3'	9.13	129.59	109.50
1	A	1299	A	N9-C1'-C2'	8.60	125.18	114.00
1	A	366	C	C2'-C3'-O3'	7.85	126.77	109.50
1	A	687	A	C2'-C3'-O3'	7.74	126.54	109.50

There are no chirality outliers.

5 of 39 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	16412	1110	0
2	B	1900	0	1951	211	0
3	C	1612	0	1677	220	0
4	D	1703	0	1765	140	0
5	E	1146	0	1207	106	0
6	F	843	0	857	72	0
7	G	1257	0	1296	93	0
8	H	1116	0	1177	66	0
9	I	1010	0	1037	114	0
10	J	792	0	835	137	0
11	K	885	0	904	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	970	0	1057	116	0
13	M	937	0	995	108	0
14	N	492	0	529	73	0
15	O	734	0	771	54	0
16	P	700	0	720	58	0
17	Q	834	0	904	61	0
18	R	598	0	670	70	0
19	S	674	0	699	85	0
20	T	763	0	861	78	0
21	V	208	0	221	23	0
22	Y	756	0	749	18	0
23	A	191	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
All	All	52640	0	37294	2808	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 2808 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	1.14
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.22	1.14
1:A:1443:G:H5''	1:A:1446:A:H5'	1.29	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	174 (75%)	34 (15%)	24 (10%)	1	11
3	C	204/239 (85%)	135 (66%)	40 (20%)	29 (14%)	0	5
4	D	206/209 (99%)	166 (81%)	31 (15%)	9 (4%)	3	32
5	E	148/162 (91%)	130 (88%)	13 (9%)	5 (3%)	5	41
6	F	99/101 (98%)	79 (80%)	19 (19%)	1 (1%)	19	66
7	G	153/156 (98%)	127 (83%)	16 (10%)	10 (6%)	1	22
8	H	136/138 (99%)	125 (92%)	7 (5%)	4 (3%)	6	44
9	I	125/128 (98%)	88 (70%)	27 (22%)	10 (8%)	1	16
10	J	96/105 (91%)	59 (62%)	20 (21%)	17 (18%)	0	3
11	K	117/129 (91%)	88 (75%)	20 (17%)	9 (8%)	1	16
12	L	122/132 (92%)	98 (80%)	14 (12%)	10 (8%)	1	15
13	M	116/126 (92%)	85 (73%)	27 (23%)	4 (3%)	5	41
14	N	58/61 (95%)	39 (67%)	11 (19%)	8 (14%)	0	6
15	O	86/89 (97%)	70 (81%)	11 (13%)	5 (6%)	2	25
16	P	81/88 (92%)	65 (80%)	15 (18%)	1 (1%)	16	62
17	Q	98/105 (93%)	85 (87%)	9 (9%)	4 (4%)	3	34
18	R	71/88 (81%)	62 (87%)	7 (10%)	2 (3%)	6	45
19	S	82/93 (88%)	47 (57%)	22 (27%)	13 (16%)	0	4
20	T	97/106 (92%)	65 (67%)	20 (21%)	12 (12%)	0	8
21	V	22/27 (82%)	19 (86%)	2 (9%)	1 (4%)	3	31
22	Y	90/118 (76%)	82 (91%)	8 (9%)	0	100	100
All	All	2439/2656 (92%)	1888 (77%)	373 (15%)	178 (7%)	1	18

5 of 178 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	9	GLU
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%)	181 (90%)	21 (10%)	9	42
3	C	160/188 (85%)	143 (89%)	17 (11%)	8	40
4	D	180/181 (99%)	172 (96%)	8 (4%)	35	74
5	E	115/123 (94%)	101 (88%)	14 (12%)	6	32
6	F	90/90 (100%)	88 (98%)	2 (2%)	60	86
7	G	126/127 (99%)	123 (98%)	3 (2%)	57	85
8	H	119/119 (100%)	109 (92%)	10 (8%)	14	52
9	I	98/99 (99%)	92 (94%)	6 (6%)	23	65
10	J	87/92 (95%)	78 (90%)	9 (10%)	9	42
11	K	90/99 (91%)	84 (93%)	6 (7%)	20	62
12	L	104/109 (95%)	96 (92%)	8 (8%)	16	56
13	M	94/101 (93%)	85 (90%)	9 (10%)	10	45
14	N	49/50 (98%)	45 (92%)	4 (8%)	14	53
15	O	79/80 (99%)	72 (91%)	7 (9%)	12	50
16	P	72/74 (97%)	67 (93%)	5 (7%)	19	60
17	Q	95/97 (98%)	90 (95%)	5 (5%)	28	69
18	R	64/77 (83%)	61 (95%)	3 (5%)	32	72
19	S	73/80 (91%)	67 (92%)	6 (8%)	14	53
20	T	76/82 (93%)	69 (91%)	7 (9%)	11	48
21	V	19/22 (86%)	19 (100%)	0	100	100
22	Y	79/103 (77%)	75 (95%)	4 (5%)	29	70
All	All	2071/2213 (94%)	1917 (93%)	154 (7%)	17	57

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	85	ARG
10	J	71	LEU

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Mol	Chain	Res	Type
19	S	85	LYS
8	H	92	ARG
9	I	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	199	ASN
6	F	94	GLN
13	M	40	ASN
4	D	161	ASN
17	Q	16	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1512/1522 (99%)	229 (15%)	90 (5%)

5 of 229 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 90 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	575	G
1	A	965	A
1	A	1397	C
1	A	687	A
1	A	812	C

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

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 196 ligands modelled in this entry, 196 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	1513/1522 (99%)	0.57	91 (6%) 25 17	51, 88, 179, 307	0
2	B	234/256 (91%)	0.14	7 (2%) 54 38	64, 99, 175, 250	0
3	C	206/239 (86%)	0.07	12 (5%) 26 18	69, 115, 165, 205	0
4	D	208/209 (99%)	0.17	11 (5%) 30 21	61, 95, 141, 216	0
5	E	150/162 (92%)	0.06	0 100 100	40, 73, 120, 149	0
6	F	101/101 (100%)	0.23	8 (7%) 15 10	76, 116, 155, 175	0
7	G	155/156 (99%)	-0.10	3 (1%) 70 56	77, 110, 171, 198	0
8	H	138/138 (100%)	-0.32	0 100 100	45, 65, 97, 131	0
9	I	127/128 (99%)	0.13	10 (7%) 15 10	68, 119, 165, 185	0
10	J	98/105 (93%)	0.63	9 (9%) 11 8	74, 130, 216, 297	0
11	K	119/129 (92%)	0.05	3 (2%) 61 46	57, 93, 145, 228	0
12	L	124/132 (93%)	0.02	1 (0%) 87 78	49, 90, 128, 204	0
13	M	118/126 (93%)	0.54	10 (8%) 13 10	77, 116, 165, 200	0
14	N	60/61 (98%)	-0.07	0 100 100	77, 108, 155, 192	0
15	O	88/89 (98%)	-0.09	3 (3%) 49 35	56, 86, 143, 195	0
16	P	83/88 (94%)	-0.30	0 100 100	64, 84, 112, 165	0
17	Q	100/105 (95%)	0.17	1 (1%) 84 73	53, 81, 129, 186	0
18	R	73/88 (82%)	-0.03	3 (4%) 41 29	64, 97, 168, 223	0
19	S	84/93 (90%)	0.26	8 (9%) 10 8	97, 134, 168, 235	0
20	T	99/106 (93%)	0.34	9 (9%) 11 8	60, 96, 149, 227	0
21	V	24/27 (88%)	0.01	0 100 100	94, 117, 149, 157	0
22	Y	92/118 (77%)	1.52	31 (33%) 0 0	109, 178, 232, 276	0
All	All	3994/4178 (95%)	0.31	220 (5%) 29 20	40, 97, 175, 307	0

The worst 5 of 220 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1024	G	8.1
4	D	35	ARG	7.5
1	A	1129	C	7.3
1	A	1534	A	6.6
1	A	1006	C	6.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1637	1/1	0.79	1.21	79.95	48,48,48,48	0
23	MG	A	1661	1/1	0.98	0.64	45.84	33,33,33,33	0
23	MG	A	1719	1/1	0.86	1.00	36.72	76,76,76,76	0
23	MG	A	1774	1/1	0.75	0.78	34.84	79,79,79,79	0
23	MG	A	1727	1/1	0.95	0.58	30.93	40,40,40,40	0
23	MG	A	1623	1/1	0.65	1.40	29.59	96,96,96,96	0
23	MG	A	1676	1/1	0.90	0.70	26.94	25,25,25,25	0
23	MG	A	1627	1/1	0.94	0.55	16.16	53,53,53,53	0
23	MG	A	1689	1/1	0.67	1.12	16.04	50,50,50,50	0
23	MG	A	1755	1/1	0.98	0.37	14.99	50,50,50,50	0
23	MG	A	1652	1/1	0.97	0.59	14.64	17,17,17,17	0
23	MG	A	1621	1/1	0.69	0.33	11.45	69,69,69,69	0
23	MG	A	1782	1/1	0.78	0.43	9.96	58,58,58,58	0
23	MG	A	1757	1/1	0.97	0.50	9.78	24,24,24,24	0
23	MG	A	1720	1/1	0.90	0.61	9.04	40,40,40,40	0
23	MG	A	1665	1/1	0.60	0.52	8.77	60,60,60,60	0
23	MG	A	1756	1/1	0.76	0.37	6.56	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1770	1/1	0.91	0.42	6.51	52,52,52,52	0
23	MG	A	1658	1/1	0.94	0.37	5.85	20,20,20,20	0
23	MG	A	1776	1/1	0.63	0.50	5.81	91,91,91,91	0
23	MG	A	1751	1/1	0.64	0.36	5.32	89,89,89,89	0
23	MG	A	1603	1/1	0.48	0.47	4.61	68,68,68,68	0
23	MG	A	1685	1/1	0.96	0.33	4.59	38,38,38,38	0
23	MG	A	1697	1/1	0.90	0.25	4.55	83,83,83,83	0
23	MG	A	1723	1/1	0.90	0.33	4.47	37,37,37,37	0
23	MG	A	1648	1/1	0.94	0.41	3.72	25,25,25,25	0
23	MG	A	1786	1/1	0.86	0.39	3.38	56,56,56,56	0
23	MG	A	1704	1/1	0.94	0.30	3.34	68,68,68,68	0
23	MG	A	1780	1/1	0.93	0.23	3.02	48,48,48,48	0
23	MG	A	1733	1/1	0.81	0.34	2.70	56,56,56,56	0
23	MG	A	1773	1/1	0.90	0.34	2.54	31,31,31,31	0
23	MG	A	1670	1/1	0.71	0.26	2.51	43,43,43,43	0
23	MG	A	1766	1/1	0.91	0.32	2.02	44,44,44,44	0
23	MG	A	1753	1/1	0.70	0.27	2.02	77,77,77,77	0
23	MG	A	1688	1/1	0.96	0.29	1.27	65,65,65,65	0
23	MG	A	1692	1/1	0.96	0.43	1.11	50,50,50,50	0
23	MG	A	1750	1/1	0.92	0.25	0.46	51,51,51,51	0
23	MG	A	1691	1/1	0.92	0.26	0.44	36,36,36,36	0
23	MG	A	1646	1/1	0.95	0.27	0.12	22,22,22,22	0
23	MG	A	1731	1/1	0.87	0.20	-0.30	76,76,76,76	0
24	ZN	N	101	1/1	0.95	0.21	-0.49	123,123,123,123	0
23	MG	A	1625	1/1	0.96	0.21	-0.61	71,71,71,71	0
23	MG	A	1663	1/1	0.95	0.15	-0.86	42,42,42,42	0
23	MG	A	1680	1/1	0.63	0.17	-1.22	73,73,73,73	0
23	MG	A	1707	1/1	0.93	0.11	-1.67	43,43,43,43	0
23	MG	B	301	1/1	0.71	0.19	-1.81	108,108,108,108	0
23	MG	A	1758	1/1	0.78	0.17	-1.84	44,44,44,44	0
23	MG	A	1736	1/1	0.90	0.18	-2.80	39,39,39,39	0
23	MG	A	1662	1/1	0.97	0.13	-3.06	64,64,64,64	0
23	MG	A	1787	1/1	0.96	0.14	-3.41	34,34,34,34	0
23	MG	A	1788	1/1	0.95	0.14	-3.71	33,33,33,33	0
23	MG	A	1764	1/1	0.68	0.61	-	80,80,80,80	0
23	MG	A	1649	1/1	0.71	0.33	-	56,56,56,56	0
23	MG	A	1645	1/1	0.85	1.13	-	54,54,54,54	0
23	MG	A	1700	1/1	0.89	0.15	-	70,70,70,70	0
23	MG	A	1732	1/1	0.95	0.55	-	52,52,52,52	0
23	MG	A	1763	1/1	0.77	0.62	-	55,55,55,55	0
23	MG	A	1668	1/1	0.96	0.59	-	36,36,36,36	0
23	MG	A	1693	1/1	0.54	0.31	-	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1610	1/1	0.74	0.26	-	61,61,61,61	0
23	MG	A	1781	1/1	0.83	0.76	-	67,67,67,67	0
23	MG	A	1702	1/1	0.49	0.34	-	96,96,96,96	0
23	MG	A	1767	1/1	0.80	0.61	-	42,42,42,42	0
23	MG	A	1734	1/1	0.56	1.11	-	68,68,68,68	0
23	MG	A	1706	1/1	0.91	0.22	-	77,77,77,77	0
23	MG	A	1718	1/1	0.76	0.72	-	85,85,85,85	0
23	MG	A	1712	1/1	0.83	0.74	-	37,37,37,37	0
23	MG	D	302	1/1	0.71	1.32	-	94,94,94,94	0
23	MG	A	1655	1/1	0.87	0.52	-	57,57,57,57	0
23	MG	A	1728	1/1	0.95	0.45	-	59,59,59,59	0
23	MG	A	1626	1/1	0.92	0.44	-	98,98,98,98	0
23	MG	A	1695	1/1	0.86	0.39	-	67,67,67,67	0
23	MG	A	1675	1/1	0.92	1.01	-	58,58,58,58	0
23	MG	A	1674	1/1	0.86	1.15	-	56,56,56,56	0
23	MG	A	1641	1/1	0.85	0.95	-	33,33,33,33	0
23	MG	A	1724	1/1	0.98	0.39	-	47,47,47,47	0
23	MG	A	1611	1/1	0.95	0.52	-	20,20,20,20	0
23	MG	A	1620	1/1	0.84	0.74	-	62,62,62,62	0
23	MG	A	1769	1/1	0.75	1.07	-	106,106,106,106	0
23	MG	A	1619	1/1	0.61	0.36	-	75,75,75,75	0
23	MG	A	1772	1/1	0.81	0.34	-	94,94,94,94	0
23	MG	A	1785	1/1	0.75	0.65	-	90,90,90,90	0
23	MG	A	1726	1/1	0.80	0.62	-	40,40,40,40	0
23	MG	A	1672	1/1	0.95	0.38	-	21,21,21,21	0
23	MG	A	1735	1/1	0.77	0.97	-	87,87,87,87	0
23	MG	A	1775	1/1	0.70	0.41	-	74,74,74,74	0
23	MG	A	1752	1/1	0.53	0.28	-	76,76,76,76	0
23	MG	A	1687	1/1	0.99	0.27	-	34,34,34,34	0
23	MG	A	1684	1/1	0.85	0.34	-	49,49,49,49	0
23	MG	A	1681	1/1	0.81	0.20	-	74,74,74,74	0
23	MG	A	1711	1/1	0.90	0.29	-	31,31,31,31	0
23	MG	A	1618	1/1	0.90	0.62	-	59,59,59,59	0
23	MG	A	1664	1/1	0.95	0.32	-	58,58,58,58	0
23	MG	A	1608	1/1	0.85	0.65	-	94,94,94,94	0
23	MG	A	1739	1/1	0.65	0.24	-	94,94,94,94	0
23	MG	A	1666	1/1	0.71	0.24	-	8,8,8,8	0
23	MG	A	1790	1/1	0.44	0.61	-	81,81,81,81	0
23	MG	A	1771	1/1	0.87	0.40	-	51,51,51,51	0
23	MG	A	1606	1/1	0.89	0.72	-	49,49,49,49	0
23	MG	A	1789	1/1	0.79	0.69	-	50,50,50,50	0
23	MG	A	1708	1/1	0.97	0.26	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1624	1/1	0.15	0.42	-	102,102,102,102	0
23	MG	A	1696	1/1	0.60	0.47	-	67,67,67,67	0
23	MG	A	1638	1/1	0.69	0.19	-	83,83,83,83	0
23	MG	A	1698	1/1	0.93	0.34	-	33,33,33,33	0
23	MG	A	1737	1/1	0.89	0.24	-	60,60,60,60	0
23	MG	A	1615	1/1	0.92	0.48	-	24,24,24,24	0
23	MG	A	1679	1/1	0.82	0.64	-	37,37,37,37	0
23	MG	A	1647	1/1	0.96	0.38	-	23,23,23,23	0
23	MG	A	1613	1/1	0.87	0.40	-	95,95,95,95	0
23	MG	A	1643	1/1	0.73	0.53	-	69,69,69,69	0
23	MG	A	1678	1/1	0.89	0.98	-	40,40,40,40	0
23	MG	A	1631	1/1	0.89	0.32	-	57,57,57,57	0
23	MG	A	1738	1/1	0.84	0.85	-	62,62,62,62	0
23	MG	A	1653	1/1	0.89	0.46	-	24,24,24,24	0
23	MG	A	1602	1/1	0.81	0.12	-	74,74,74,74	0
23	MG	A	1629	1/1	0.51	0.84	-	80,80,80,80	0
23	MG	A	1703	1/1	0.81	0.52	-	72,72,72,72	0
23	MG	A	1791	1/1	0.96	0.58	-	41,41,41,41	0
23	MG	A	1709	1/1	0.86	0.49	-	32,32,32,32	0
23	MG	A	1714	1/1	0.65	0.70	-	65,65,65,65	0
23	MG	A	1730	1/1	0.65	0.42	-	69,69,69,69	0
23	MG	A	1747	1/1	0.62	0.42	-	44,44,44,44	0
23	MG	A	1654	1/1	0.63	0.17	-	63,63,63,63	0
23	MG	A	1612	1/1	0.93	0.69	-	35,35,35,35	0
23	MG	A	1694	1/1	0.68	0.24	-	87,87,87,87	0
23	MG	A	1713	1/1	0.51	1.00	-	84,84,84,84	0
23	MG	A	1671	1/1	0.80	0.46	-	33,33,33,33	0
23	MG	A	1669	1/1	0.69	0.29	-	63,63,63,63	0
23	MG	A	1725	1/1	0.81	0.37	-	83,83,83,83	0
23	MG	A	1768	1/1	0.71	0.27	-	66,66,66,66	0
23	MG	A	1632	1/1	0.72	1.74	-	79,79,79,79	0
23	MG	A	1749	1/1	0.88	0.47	-	41,41,41,41	0
23	MG	A	1777	1/1	0.66	0.72	-	79,79,79,79	0
23	MG	A	1701	1/1	0.48	0.56	-	92,92,92,92	0
23	MG	A	1746	1/1	0.80	0.52	-	44,44,44,44	0
23	MG	A	1743	1/1	0.74	0.66	-	38,38,38,38	0
23	MG	A	1604	1/1	0.67	0.63	-	69,69,69,69	0
23	MG	A	1784	1/1	0.76	0.70	-	63,63,63,63	0
23	MG	A	1759	1/1	0.91	0.42	-	53,53,53,53	0
23	MG	A	1717	1/1	0.95	0.30	-	34,34,34,34	0
23	MG	A	1636	1/1	0.91	0.52	-	65,65,65,65	0
23	MG	A	1744	1/1	0.83	0.55	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1710	1/1	0.59	0.39	-	46,46,46,46	0
23	MG	A	1748	1/1	0.28	0.86	-	80,80,80,80	0
24	ZN	D	301	1/1	0.85	0.37	-	72,72,72,72	0
23	MG	A	1754	1/1	0.82	0.81	-	41,41,41,41	0
23	MG	A	1616	1/1	0.68	0.69	-	70,70,70,70	0
23	MG	A	1605	1/1	0.43	0.79	-	79,79,79,79	0
23	MG	A	1683	1/1	0.94	0.51	-	38,38,38,38	0
23	MG	A	1609	1/1	0.80	0.39	-	45,45,45,45	0
23	MG	A	1741	1/1	0.97	0.07	-	32,32,32,32	0
23	MG	A	1690	1/1	0.86	0.39	-	81,81,81,81	0
23	MG	A	1729	1/1	0.91	0.36	-	71,71,71,71	0
23	MG	A	1622	1/1	0.69	1.57	-	89,89,89,89	0
23	MG	A	1778	1/1	0.89	0.38	-	64,64,64,64	0
23	MG	A	1673	1/1	0.93	0.49	-	25,25,25,25	0
23	MG	A	1650	1/1	0.59	0.38	-	70,70,70,70	0
23	MG	A	1699	1/1	0.60	1.40	-	78,78,78,78	0
23	MG	A	1705	1/1	0.78	0.55	-	51,51,51,51	0
23	MG	A	1659	1/1	0.88	0.70	-	32,32,32,32	0
23	MG	A	1686	1/1	0.84	0.77	-	68,68,68,68	0
23	MG	A	1783	1/1	0.82	0.38	-	61,61,61,61	0
23	MG	E	201	1/1	0.93	0.68	-	38,38,38,38	0
23	MG	A	1660	1/1	0.95	0.49	-	23,23,23,23	0
23	MG	A	1635	1/1	0.80	0.48	-	104,104,104,104	0
23	MG	A	1677	1/1	0.78	0.59	-	52,52,52,52	0
23	MG	A	1656	1/1	0.96	0.36	-	88,88,88,88	0
23	MG	A	1640	1/1	0.86	0.44	-	59,59,59,59	0
23	MG	A	1742	1/1	0.46	0.42	-	49,49,49,49	0
23	MG	A	1614	1/1	0.46	0.53	-	97,97,97,97	0
23	MG	A	1761	1/1	0.75	1.40	-	69,69,69,69	0
23	MG	A	1601	1/1	0.92	0.12	-	67,67,67,67	0
23	MG	A	1779	1/1	0.37	0.90	-	71,71,71,71	0
23	MG	A	1722	1/1	0.95	0.17	-	23,23,23,23	0
23	MG	A	1630	1/1	0.83	1.01	-	85,85,85,85	0
23	MG	A	1657	1/1	0.92	0.32	-	36,36,36,36	0
23	MG	A	1628	1/1	0.57	0.49	-	60,60,60,60	0
23	MG	A	1667	1/1	0.90	0.90	-	54,54,54,54	0
23	MG	A	1762	1/1	0.75	0.60	-	66,66,66,66	0
23	MG	A	1740	1/1	0.82	0.47	-	66,66,66,66	0
23	MG	A	1607	1/1	0.82	0.39	-	68,68,68,68	0
23	MG	A	1715	1/1	0.90	0.46	-	37,37,37,37	0
23	MG	A	1644	1/1	0.97	0.26	-	54,54,54,54	0
23	MG	A	1760	1/1	0.80	0.70	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
23	MG	A	1765	1/1	0.88	0.35	-	48,48,48,48	0
23	MG	A	1716	1/1	0.78	0.28	-	62,62,62,62	0
23	MG	A	1682	1/1	0.80	0.72	-	66,66,66,66	0
23	MG	A	1745	1/1	0.82	0.27	-	61,61,61,61	0
23	MG	A	1617	1/1	0.91	0.69	-	67,67,67,67	0
23	MG	A	1634	1/1	0.71	0.51	-	60,60,60,60	0
23	MG	A	1642	1/1	0.65	0.44	-	74,74,74,74	0
23	MG	A	1721	1/1	0.85	0.42	-	38,38,38,38	0
23	MG	A	1651	1/1	0.94	0.88	-	55,55,55,55	0
23	MG	A	1633	1/1	0.92	0.20	-	74,74,74,74	0
23	MG	A	1639	1/1	0.55	0.70	-	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.