



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 19, 2020 – 09:50 AM BST

PDB ID : 4WCE  
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus*  
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.  
Deposited on : 2014-09-04  
Resolution : 3.53 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.6

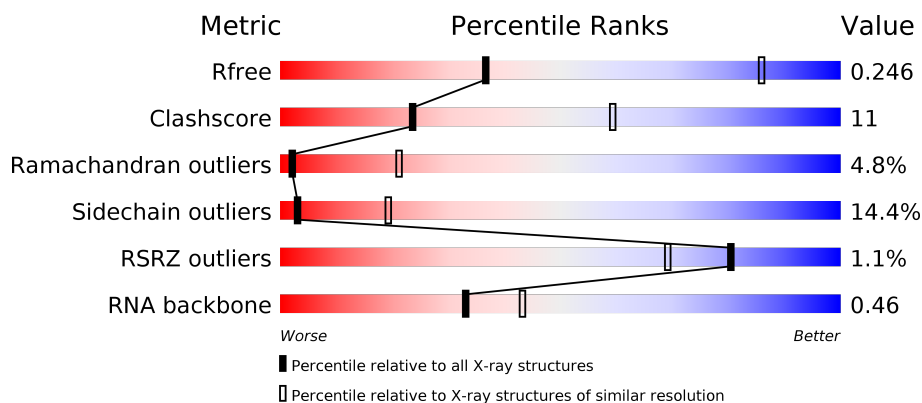
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.53 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.















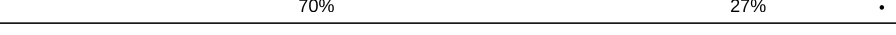









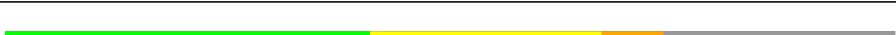
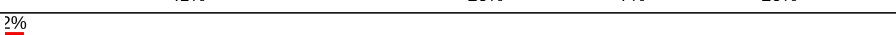
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)
RNA backbone	3102	1003 (4.02-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	X	2923	
2	Y	114	
3	A	277	
4	B	220	

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Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MN	B	303	-	-	-	X
30	MN	X	3050	-	-	-	X
30	MN	X	3053	-	-	-	X
30	MN	X	3308	-	-	-	X
31	MG	X	3013	-	-	-	X
31	MG	X	3113	-	-	-	X
31	MG	X	3173	-	-	-	X
34	EOH	X	3317	-	-	-	X

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 81909 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2708	Total	C	N	O	P	0	0	0
			58077	25928	10647	18794	2708			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	269	Total	C	N	O	S	0	0	0
			1686	1024	333	324	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1558	976	291	286	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1320	818	249	251	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			866	523	166	175	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			970	596	177	195	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1106	693	204	206	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			859	527	170	161	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1068	684	198	183	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			908	557	177	173	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O		0	0	0
			705	433	137	135				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O			
			826	521	164	141	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S			
			932	587	187	154	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S			
			751	477	138	135	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S			
			862	537	164	158	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total	C	N	O	S			
			626	394	113	116	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total	C	N	O	S			
			683	424	127	131	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S			
			1097	690	191	214	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			568	352	110	106			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	46	Total	C	N	O	0	0	0
			300	182	65	53			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			486	299	89	98			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

- Molecule 27 is a protein called 50S ribosomal protein L35.

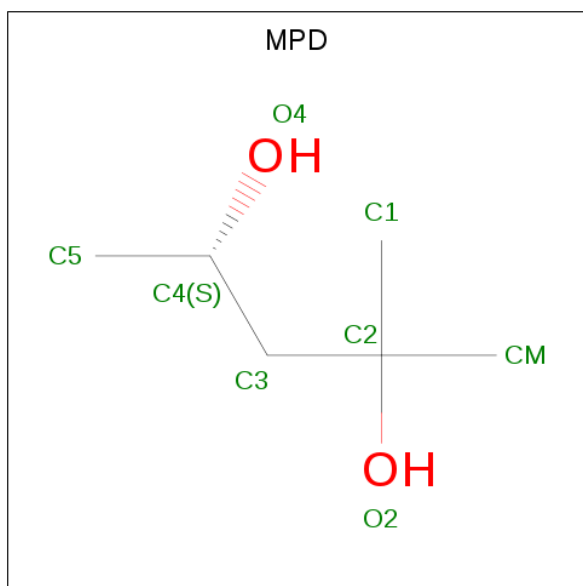
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			420	260	84	74	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	37	Total	C	N	O	S	0	0	0
			277	173	58	41	5			

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



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

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

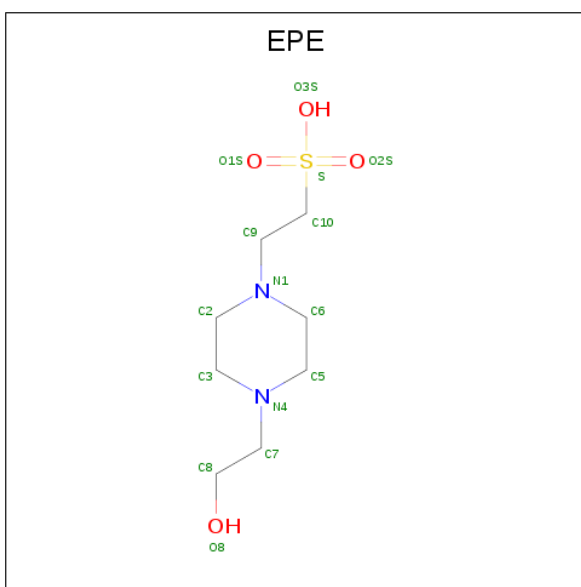
- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	1	Total	Mn	0	0
			1	1		
30	B	1	Total	Mn	0	0
			1	1		
30	I	2	Total	Mn	0	0
			2	2		
30	X	223	Total	Mn	0	0
			223	223		
30	R	2	Total	Mn	0	0
			2	2		
30	Y	2	Total	Mn	0	0
			2	2		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

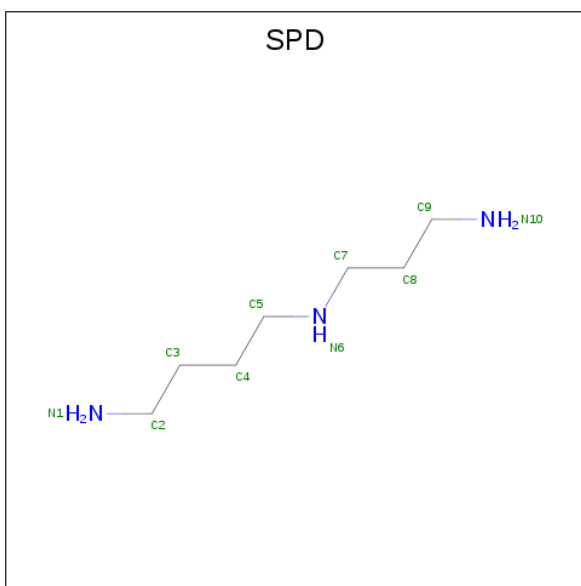
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	G	3	Total	Mg	0	0
			3	3		
31	B	2	Total	Mg	0	0
			2	2		
31	I	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	X	80	Total	Mg	0	0
			80	80		
31	O	1	Total	Mg	0	0
			1	1		
31	Y	3	Total	Mg	0	0
			3	3		

- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



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

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



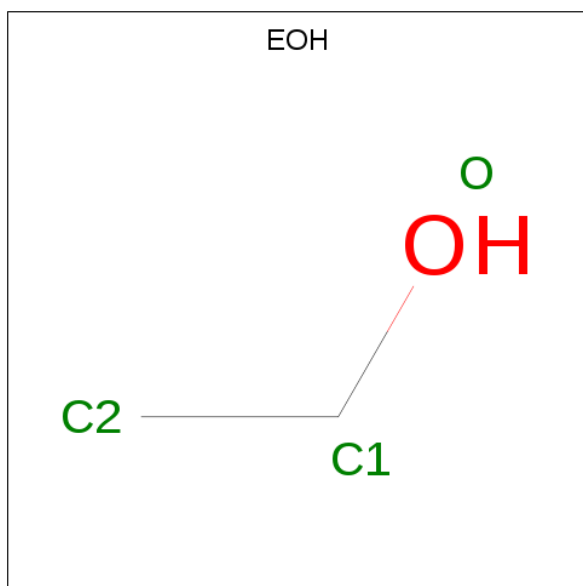
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		

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

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula:  $C_2H_6O$ ).

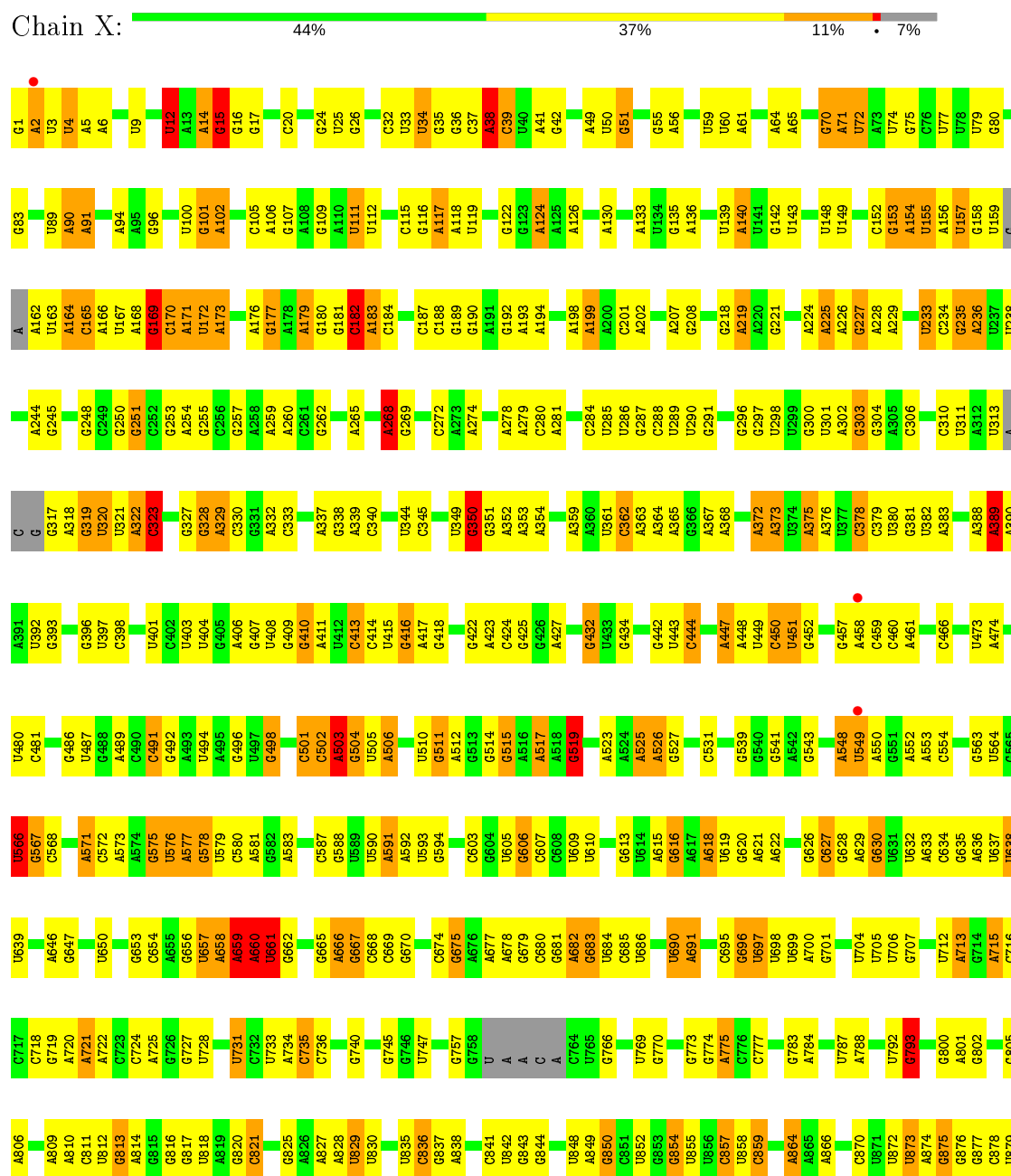


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		

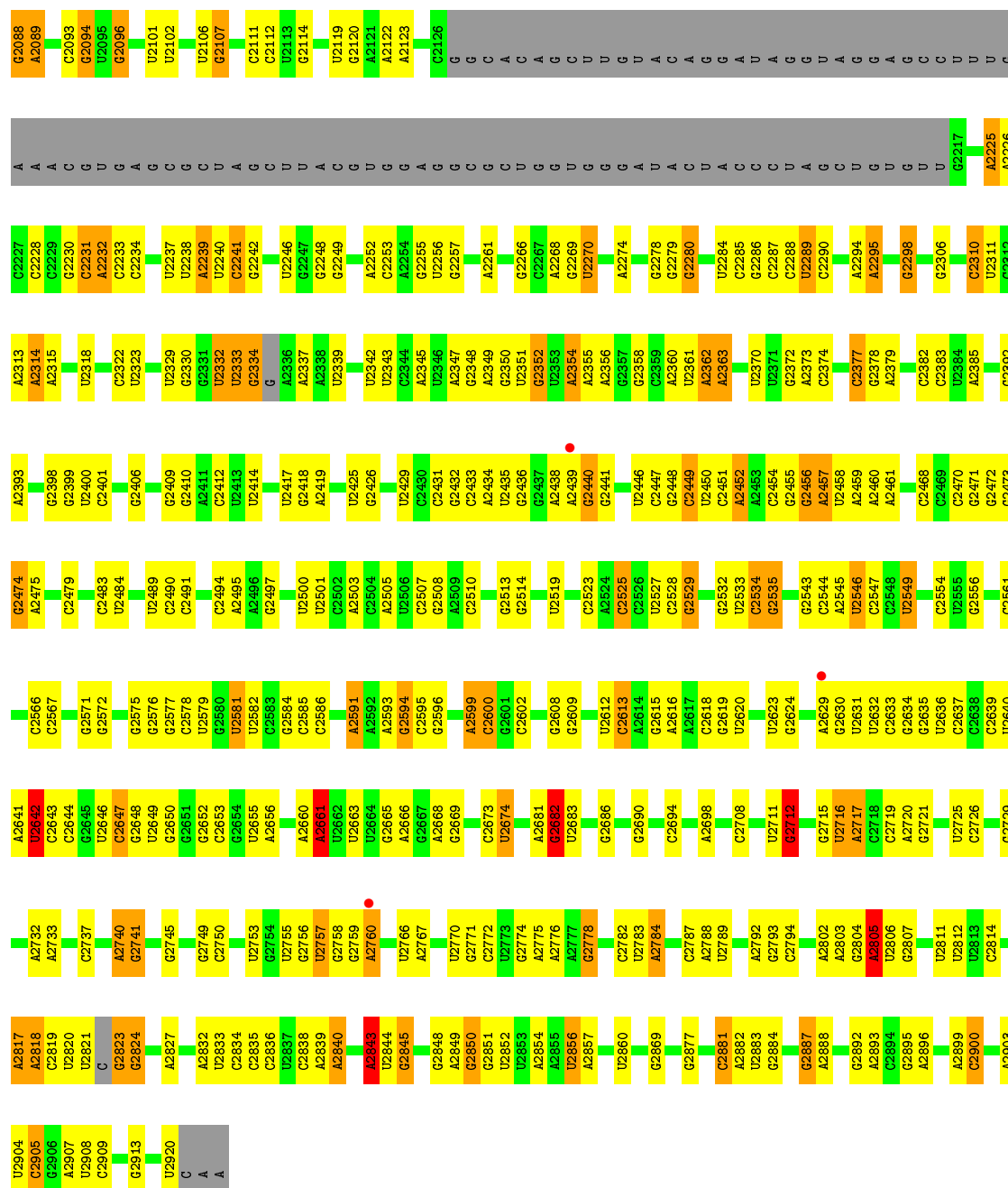
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

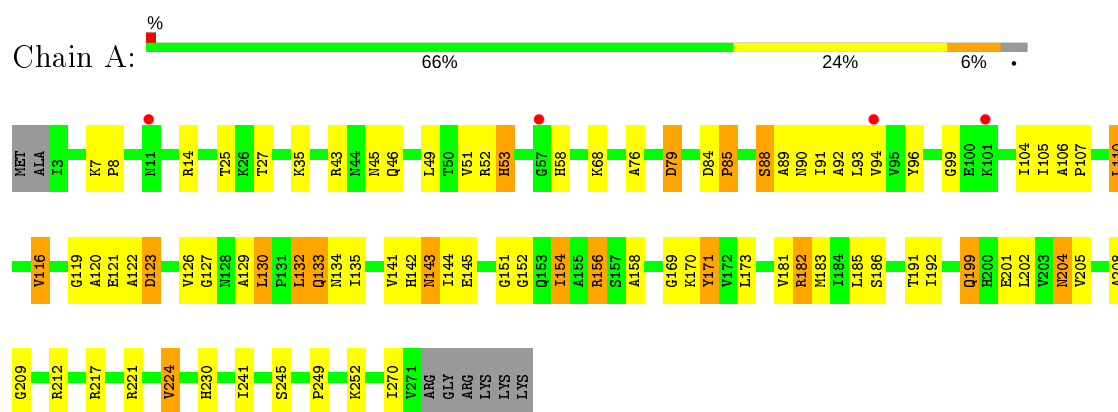
#### • Molecule 1: 23S rRNA



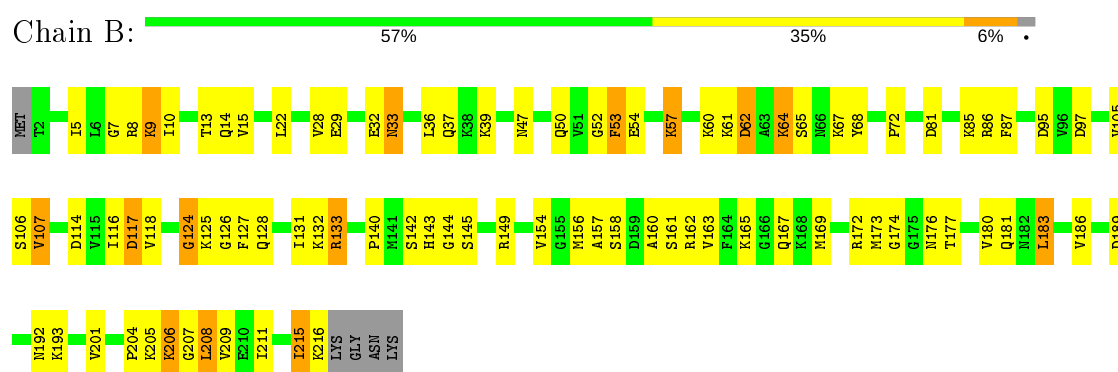




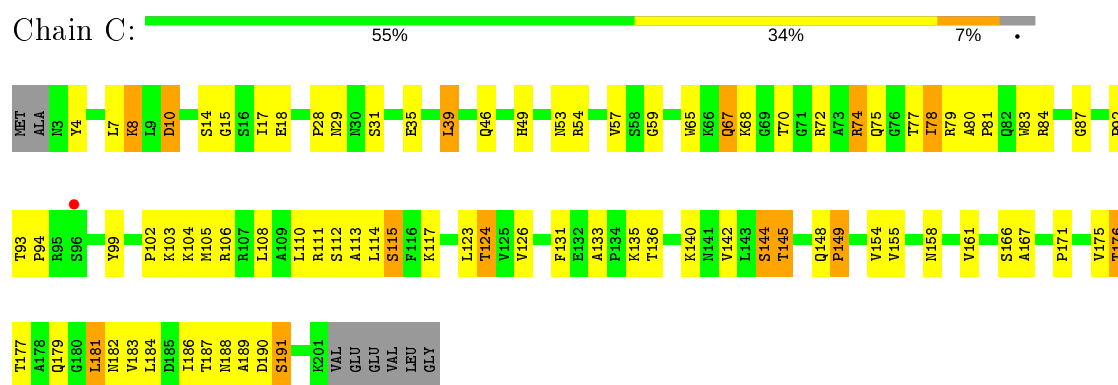
• Molecule 3: 50S ribosomal protein L2



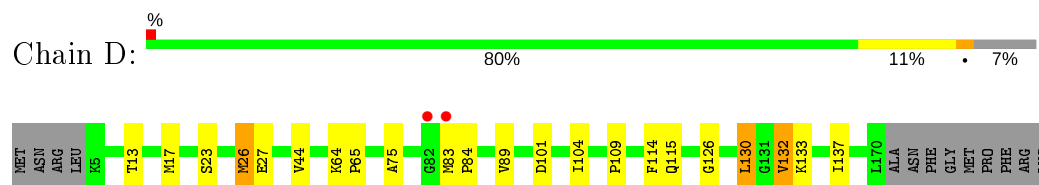
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4



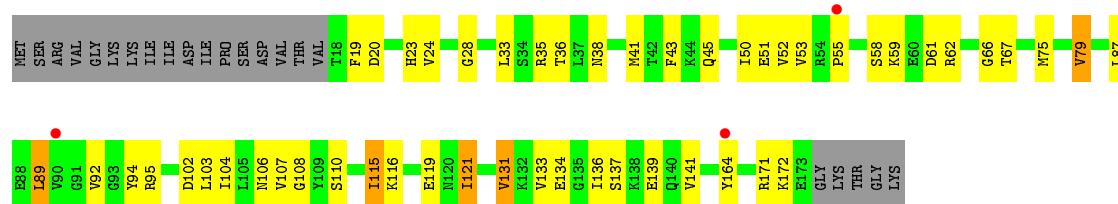
• Molecule 6: 50S ribosomal protein L5



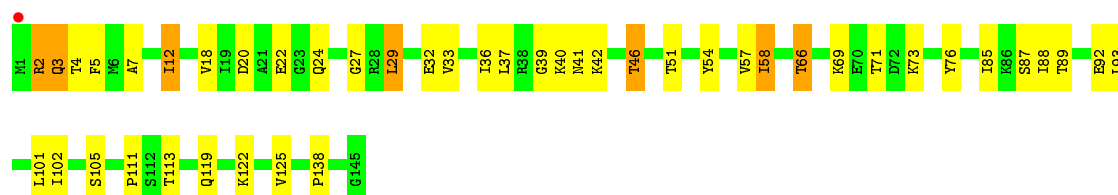
• Molecule 7: 50S ribosomal protein L6







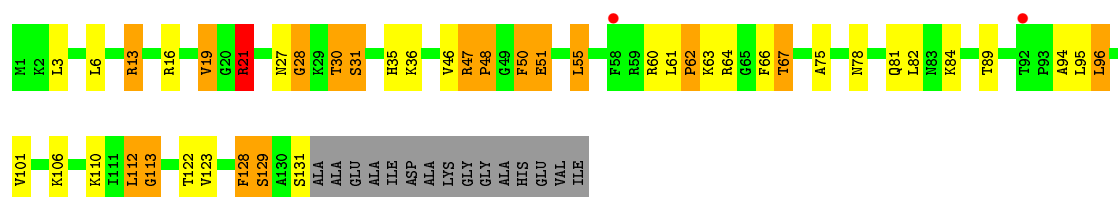
• Molecule 8: 50S ribosomal protein L13



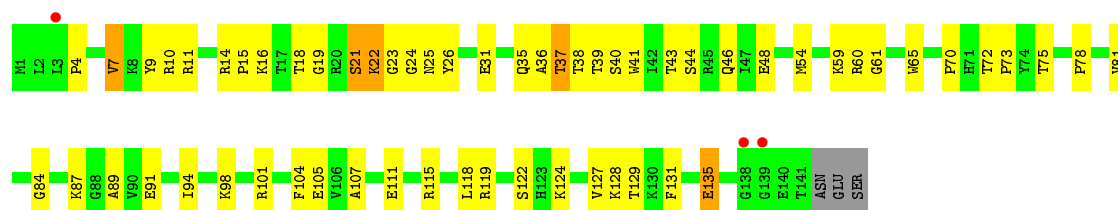
• Molecule 9: 50S ribosomal protein L14



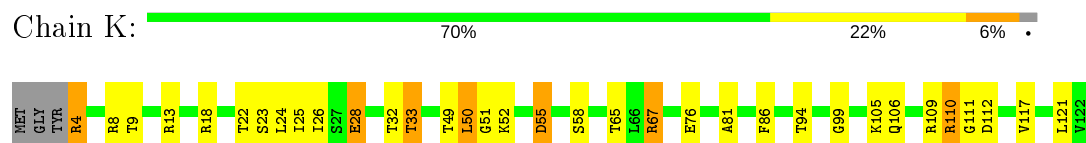
• Molecule 10: 50S ribosomal protein L15



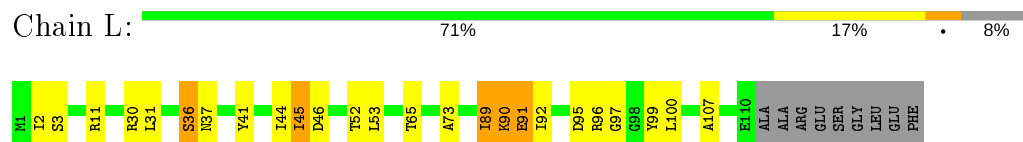
• Molecule 11: 50S ribosomal protein L16



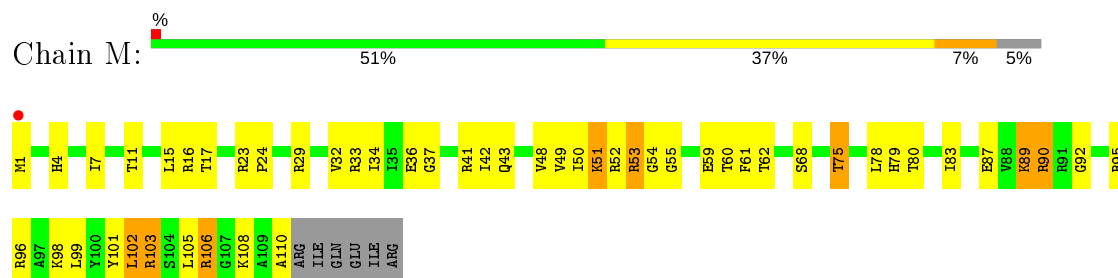
• Molecule 12: 50S ribosomal protein L17



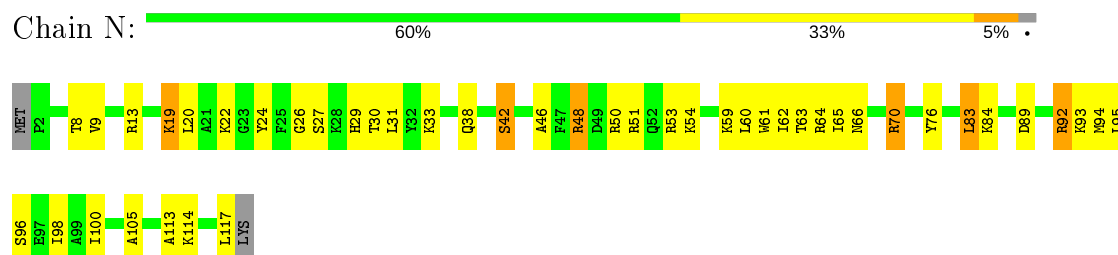
- Molecule 13: 50S ribosomal protein L18



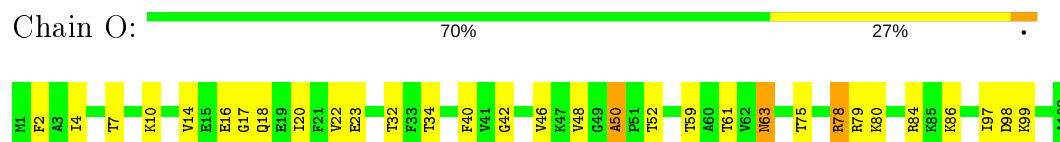
- Molecule 14: 50S ribosomal protein L19



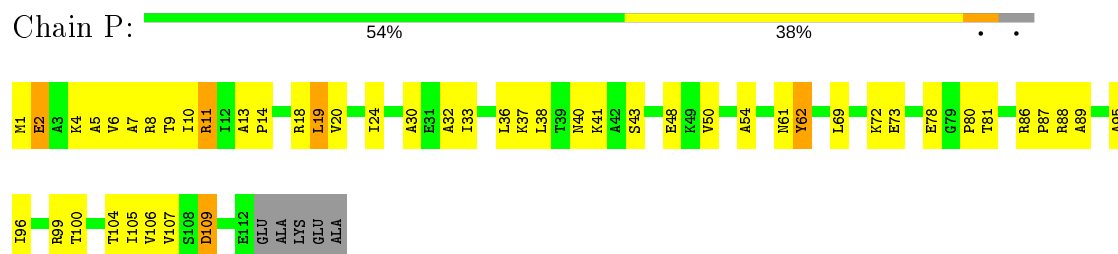
- Molecule 15: 50S ribosomal protein L20



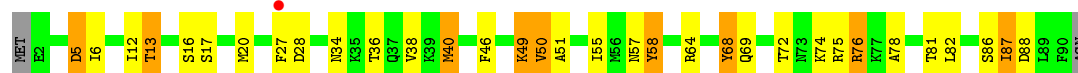
- Molecule 16: 50S ribosomal protein L21



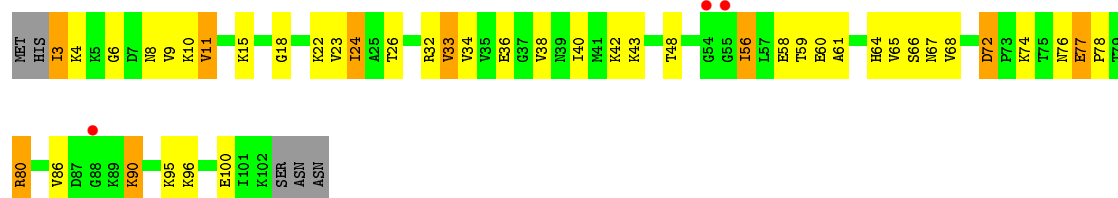
- Molecule 17: 50S ribosomal protein L22



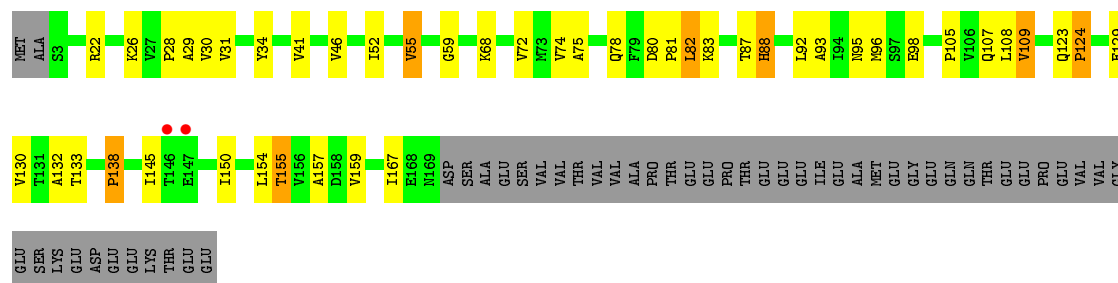
- Molecule 18: 50S ribosomal protein L23



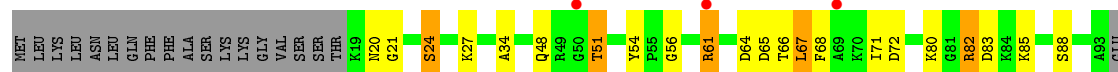
- Molecule 19: 50S ribosomal protein L24



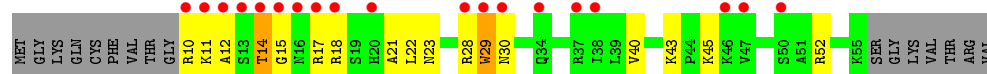
- Molecule 20: 50S ribosomal protein L25



- Molecule 21: 50S ribosomal protein L27



- Molecule 22: 50S ribosomal protein L28

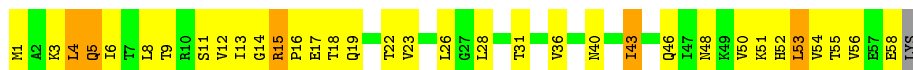


- Molecule 23: 50S ribosomal protein L29

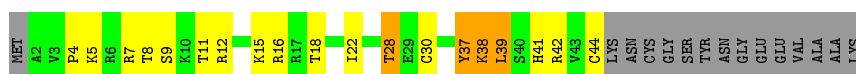




- Molecule 24: 50S ribosomal protein L30



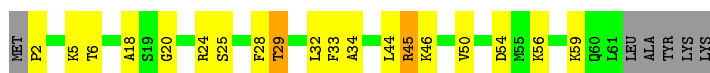
- Molecule 25: 50S ribosomal protein L32



- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 96.0 (49.74-3.53)	Depositor EDS
$R_{merge}$	0.25	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.202 , 0.246 0.202 , 0.246	Depositor DCC
$R_{free}$ test set	11858 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.21 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, MN, EOH, MPD, EPE, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	X	0.64	12/65032 (0.0%)	1.16	279/101388 (0.3%)
2	Y	0.56	0/2717	1.14	17/4232 (0.4%)
3	A	0.25	0/1717	0.55	0/2361
4	B	0.32	0/1581	0.62	0/2129
5	C	0.48	0/1338	0.72	0/1831
6	D	0.23	0/869	0.48	0/1205
7	E	0.27	0/982	0.51	0/1354
8	G	0.37	0/1128	0.58	0/1525
9	H	0.28	0/891	0.53	0/1203
10	I	0.58	0/868	0.91	1/1172 (0.1%)
11	J	0.30	0/1092	0.54	0/1473
12	K	0.31	0/911	0.59	0/1219
13	L	0.25	0/711	0.54	0/970
14	M	0.51	0/838	0.76	0/1132
15	N	0.38	0/944	0.59	0/1252
16	O	0.30	0/761	0.58	1/1022 (0.1%)
17	P	0.55	0/870	0.78	0/1171
18	Q	0.40	0/633	0.66	0/859
19	R	0.27	0/688	0.59	0/930
20	S	0.28	0/1109	0.58	0/1522
21	T	0.26	0/574	0.48	0/763
22	U	0.28	0/305	0.55	0/419
23	V	0.29	0/487	0.53	0/654
24	W	0.54	0/451	0.69	0/607
25	Z	0.48	0/345	0.67	0/460
26	2	0.47	0/366	0.65	0/480
27	3	0.32	0/424	0.66	0/566
28	4	0.39	0/280	0.63	0/371
All	All	0.59	12/88912 (0.0%)	1.07	298/134270 (0.2%)

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
3	A	0	1
7	E	0	1
27	3	0	1
All	All	0	3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-8.14	1.32	1.37
1	X	1065	A	N9-C4	-6.85	1.33	1.37
1	X	350	G	N9-C4	6.79	1.43	1.38
1	X	2845	G	N9-C4	-6.28	1.32	1.38
1	X	1186	A	N9-C4	-6.07	1.34	1.37

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2845	G	N3-C4-C5	11.31	134.26	128.60
1	X	955	A	N1-C6-N6	11.28	125.37	118.60
1	X	350	G	N3-C4-C5	-10.89	123.15	128.60
2	Y	86	C	N3-C2-O2	-10.49	114.56	121.90
1	X	1065	A	C2-N3-C4	-9.90	105.65	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	24	ARG	Peptide
3	A	52	ARG	Peptide
7	E	119	GLU	Peptide

## 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	X	58077	0	29209	849	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	60	0
5	C	1320	0	1171	54	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0
8	G	1106	0	1072	31	0
9	H	884	0	902	26	0
10	I	859	0	772	37	0
11	J	1068	0	1078	42	0
12	K	908	0	935	28	0
13	L	705	0	589	10	0
14	M	826	0	831	41	0
15	N	932	0	995	37	0
16	O	751	0	743	14	0
17	P	862	0	920	37	0
18	Q	626	0	567	21	0
19	R	683	0	661	21	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	9	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	19	0
26	2	362	0	398	14	0
27	3	420	0	405	7	0
28	4	277	0	301	17	0
29	X	88	0	154	14	0
29	Z	8	0	14	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	2	0	0	0	0
30	X	223	0	0	0	0
30	Y	2	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	G	3	0	0	0	0
31	I	1	0	0	0	0
31	O	1	0	0	0	0
31	X	80	0	0	0	0
31	Y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	15	0	17	0	0
33	X	40	0	76	0	0
34	X	21	0	42	0	0
All	All	81909	0	50258	1401	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 11.

The worst 5 of 1401 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2231:C:HO2'	1:X:2232:A:H8	1.06	0.97
2:Y:80:A:H61	2:Y:91:C:H42	1.05	0.94
2:Y:79:C:H42	2:Y:92:G:H1	1.06	0.94
1:X:1487:G:H1	1:X:1597:U:H3	1.17	0.93
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.52	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	15
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	1	16
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3	25
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1	15
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	0	8
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	11	47
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	5	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	0	7
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	2	23
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	17	57
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	2	22
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	3	28
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3	25
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100	100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	6	37
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3	25
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	0	8
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	11	47
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1	9
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	9	45
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100	100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	2	21
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0	4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4	33
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2	21

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	120	ALA
3	A	126	VAL
3	A	141	VAL

### 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	
3	A	120/224 (54%)	101 (84%)	19 (16%)	2	16
4	B	153/177 (86%)	136 (89%)	17 (11%)	6	29
5	C	106/169 (63%)	88 (83%)	18 (17%)	2	12
6	D	18/158 (11%)	17 (94%)	1 (6%)	21	55
7	E	67/155 (43%)	58 (87%)	9 (13%)	4	22
8	G	111/123 (90%)	101 (91%)	10 (9%)	9	38
9	H	91/100 (91%)	78 (86%)	13 (14%)	3	20
10	I	67/112 (60%)	52 (78%)	15 (22%)	1	5
11	J	103/119 (87%)	91 (88%)	12 (12%)	5	27
12	K	91/102 (89%)	81 (89%)	10 (11%)	6	30
13	L	47/95 (50%)	39 (83%)	8 (17%)	2	12
14	M	80/102 (78%)	66 (82%)	14 (18%)	2	11
15	N	93/98 (95%)	79 (85%)	14 (15%)	3	18
16	O	71/86 (83%)	60 (84%)	11 (16%)	2	17
17	P	91/94 (97%)	84 (92%)	7 (8%)	13	43
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0	3
19	R	63/90 (70%)	46 (73%)	17 (27%)	0	3
20	S	91/190 (48%)	83 (91%)	8 (9%)	10	39
21	T	56/75 (75%)	48 (86%)	8 (14%)	3	20
22	U	18/52 (35%)	17 (94%)	1 (6%)	21	55
23	V	47/62 (76%)	42 (89%)	5 (11%)	6	31
24	W	52/53 (98%)	40 (77%)	12 (23%)	1	5
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1	6
26	2	37/40 (92%)	32 (86%)	5 (14%)	4	21
27	3	37/57 (65%)	33 (89%)	4 (11%)	6	30
28	4	30/35 (86%)	27 (90%)	3 (10%)	7	33
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	3	19

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	33	THR
15	N	9	VAL
25	Z	5	LYS
12	K	76	GLU
14	M	17	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0
All	All	2804/3037 (92%)	640 (22%)	18 (0%)

5 of 640 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	U
1	X	9	U
1	X	12	U
1	X	14	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1503	U
1	X	1510	U
1	X	1576	A
1	X	1091	G
1	X	1490	G

## 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 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
29	MPD	X	3011	-	7,7,7	0.88	0	9,10,10	0.45	0
29	MPD	X	3003	-	7,7,7	0.30	0	9,10,10	0.37	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.66	0
32	EPE	X	3311	-	15,15,15	1.27	1 (6%)	18,20,20	0.45	0
29	MPD	X	3010	-	7,7,7	0.63	0	9,10,10	0.35	0
29	MPD	X	3001	-	7,7,7	0.33	0	9,10,10	0.45	0
29	MPD	X	3009	-	7,7,7	0.66	0	9,10,10	0.25	0
34	EOH	X	3320	-	2,2,2	0.58	0	1,1,1	0.63	0
29	MPD	X	3002	-	7,7,7	0.96	1 (14%)	9,10,10	0.53	0
34	EOH	X	3321	-	2,2,2	0.58	0	1,1,1	0.62	0
29	MPD	X	3008	-	7,7,7	0.69	0	9,10,10	0.32	0
33	SPD	X	3313	-	9,9,9	0.19	0	8,8,8	0.27	0
34	EOH	X	3322	-	2,2,2	0.54	0	1,1,1	0.66	0
29	MPD	X	3004	-	7,7,7	0.58	0	9,10,10	0.19	0
33	SPD	X	3314	-	9,9,9	0.14	0	8,8,8	0.22	0
29	MPD	X	3007	-	7,7,7	0.79	0	9,10,10	0.41	0
34	EOH	X	3316	-	2,2,2	0.67	0	1,1,1	0.41	0
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.76	0
29	MPD	X	3006	-	7,7,7	0.46	0	9,10,10	0.10	0
33	SPD	X	3315	-	9,9,9	0.23	0	8,8,8	0.23	0
33	SPD	X	3312	-	9,9,9	0.28	0	8,8,8	0.34	0
29	MPD	Z	101	-	7,7,7	0.30	0	9,10,10	0.36	0
29	MPD	X	3005	-	7,7,7	0.67	0	9,10,10	0.23	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.64	0

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
29	MPD	X	3009	-	-	1/5/5/5	-
29	MPD	X	3011	-	-	2/5/5/5	-
29	MPD	X	3003	-	-	3/5/5/5	-
29	MPD	X	3008	-	-	1/5/5/5	-
33	SPD	X	3313	-	-	2/7/7/7	-
29	MPD	X	3006	-	-	1/5/5/5	-
33	SPD	X	3315	-	-	2/7/7/7	-
33	SPD	X	3312	-	-	1/7/7/7	-
32	EPE	X	3311	-	-	6/9/19/19	0/1/1/1
29	MPD	Z	101	-	-	3/5/5/5	-
29	MPD	X	3005	-	-	3/5/5/5	-
29	MPD	X	3010	-	-	3/5/5/5	-
29	MPD	X	3004	-	-	0/5/5/5	-
29	MPD	X	3001	-	-	0/5/5/5	-
33	SPD	X	3314	-	-	2/7/7/7	-
29	MPD	X	3007	-	-	5/5/5/5	-
29	MPD	X	3002	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.67	1.70	1.77
29	X	3002	MPD	C3-C2	2.32	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3009	MPD	C2-C3-C4-C5
29	X	3011	MPD	C2-C3-C4-O4
29	X	3011	MPD	C2-C3-C4-C5
29	X	3007	MPD	C2-C3-C4-O4
29	X	3003	MPD	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3011	MPD	1	0
29	X	3003	MPD	4	0
29	X	3008	MPD	1	0
29	X	3007	MPD	4	0
29	X	3005	MPD	4	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	X	2708/2923 (92%)	-0.47	9 (0%) 94 89	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.66	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	-0.24	4 (1%) 73 61	43, 74, 106, 136	0
4	B	215/220 (97%)	-0.32	0 100 100	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.53	1 (0%) 91 84	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 79 67	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.26	3 (1%) 66 53	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 87 79	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.39	0 100 100	17, 41, 74, 102	0
10	I	131/146 (89%)	-0.11	2 (1%) 73 61	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.04	3 (2%) 63 50	25, 43, 97, 121	0
12	K	119/122 (97%)	-0.44	0 100 100	14, 37, 86, 97	0
13	L	110/119 (92%)	-0.50	0 100 100	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.48	1 (0%) 84 73	23, 43, 89, 115	0
15	N	116/118 (98%)	-0.54	0 100 100	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.57	0 100 100	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.35	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	-0.22	1 (1%) 80 69	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 50 37	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	2 (1%) 79 67	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 38 28	21, 39, 81, 102	0
22	U	46/62 (74%)	1.90	19 (41%) 0 0	60, 91, 122, 130	0
23	V	65/69 (94%)	-0.29	0 100 100	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.11	0 100 100	12, 24, 72, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Z	43/58 (74%)	-0.39	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	0.01	1 (2%) 60 46	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.43	0 100 100	10, 32, 69, 83	0
28	4	37/37 (100%)	1.54	10 (27%) 0 0	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.35	65 (1%) 80 69	6, 51, 123, 230	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	13	SER	6.3
22	U	12	ALA	6.1
22	U	14	THR	5.3
22	U	11	LYS	5.1
20	S	146	THR	4.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
30	MN	X	3308	1/1	0.39	0.74	92,92,92,92	0
31	MG	G	203	1/1	0.47	0.33	17,17,17,17	0
30	MN	X	3055	1/1	0.62	0.21	94,94,94,94	0
30	MN	X	3053	1/1	0.63	0.54	89,89,89,89	0
31	MG	X	3113	1/1	0.66	1.07	45,45,45,45	0
30	MN	X	3132	1/1	0.67	0.16	97,97,97,97	0
30	MN	X	3044	1/1	0.70	0.24	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	B	303	1/1	0.70	0.74	102,102,102,102	0
31	MG	X	3083	1/1	0.70	0.34	37,37,37,37	0
34	EOH	X	3317	3/3	0.71	0.51	46,46,46,46	0
31	MG	X	3173	1/1	0.71	1.13	26,26,26,26	0
30	MN	X	3213	1/1	0.71	0.23	95,95,95,95	0
30	MN	X	3057	1/1	0.71	0.20	71,71,71,71	0
30	MN	X	3133	1/1	0.72	0.31	98,98,98,98	0
30	MN	X	3222	1/1	0.73	0.35	71,71,71,71	0
30	MN	X	3168	1/1	0.73	0.21	74,74,74,74	0
31	MG	X	3034	1/1	0.73	0.39	18,18,18,18	0
30	MN	X	3015	1/1	0.74	0.38	75,75,75,75	0
30	MN	X	3050	1/1	0.74	0.47	99,99,99,99	0
31	MG	X	3016	1/1	0.74	0.39	23,23,23,23	0
30	MN	X	3148	1/1	0.75	0.25	79,79,79,79	0
31	MG	X	3084	1/1	0.76	0.14	14,14,14,14	0
31	MG	X	3013	1/1	0.76	0.83	30,30,30,30	0
33	SPD	X	3312	10/10	0.77	0.29	47,47,47,47	0
30	MN	X	3182	1/1	0.77	0.38	107,107,107,107	0
31	MG	X	3023	1/1	0.78	0.29	37,37,37,37	0
30	MN	X	3121	1/1	0.78	0.31	88,88,88,88	0
29	MPD	X	3008	8/8	0.79	0.35	70,70,70,70	0
30	MN	X	3128	1/1	0.79	0.16	84,84,84,84	0
30	MN	X	3066	1/1	0.79	0.12	56,56,56,56	0
30	MN	X	3143	1/1	0.79	0.18	94,94,94,94	0
30	MN	J	201	1/1	0.80	0.20	78,78,78,78	0
30	MN	X	3111	1/1	0.80	0.13	99,99,99,99	0
31	MG	X	3175	1/1	0.80	0.30	0,0,0,0	0
31	MG	X	3137	1/1	0.80	0.92	17,17,17,17	0
29	MPD	X	3010	8/8	0.81	0.33	87,87,87,87	0
30	MN	X	3293	1/1	0.81	0.19	70,70,70,70	0
30	MN	X	3220	1/1	0.81	0.43	68,68,68,68	0
30	MN	X	3124	1/1	0.81	0.11	77,77,77,77	0
30	MN	X	3126	1/1	0.81	0.24	77,77,77,77	0
31	MG	X	3298	1/1	0.82	1.02	23,23,23,23	0
31	MG	X	3114	1/1	0.82	0.57	36,36,36,36	0
30	MN	X	3130	1/1	0.82	0.13	102,102,102,102	0
30	MN	X	3140	1/1	0.82	0.17	71,71,71,71	0
30	MN	X	3076	1/1	0.83	0.09	74,74,74,74	0
30	MN	X	3135	1/1	0.83	0.14	94,94,94,94	0
34	EOH	X	3318	3/3	0.83	0.27	47,47,47,47	0
30	MN	X	3052	1/1	0.83	0.21	71,71,71,71	0
30	MN	X	3123	1/1	0.83	0.42	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3138	1/1	0.83	0.10	112,112,112,112	0
31	MG	X	3109	1/1	0.83	0.70	24,24,24,24	0
29	MPD	X	3002	8/8	0.83	0.32	45,45,45,45	0
30	MN	X	3254	1/1	0.83	0.23	48,48,48,48	0
31	MG	X	3093	1/1	0.84	0.27	21,21,21,21	0
30	MN	X	3059	1/1	0.84	0.10	61,61,61,61	0
30	MN	X	3122	1/1	0.84	0.50	89,89,89,89	0
30	MN	X	3090	1/1	0.84	0.35	96,96,96,96	0
31	MG	X	3095	1/1	0.84	0.34	26,26,26,26	0
31	MG	X	3079	1/1	0.84	0.74	27,27,27,27	0
30	MN	X	3042	1/1	0.84	0.11	104,104,104,104	0
33	SPD	X	3315	10/10	0.84	0.31	46,46,46,46	0
30	MN	X	3131	1/1	0.85	0.48	89,89,89,89	0
29	MPD	X	3011	8/8	0.85	0.24	39,39,39,39	0
30	MN	I	202	1/1	0.85	0.25	64,64,64,64	0
29	MPD	X	3006	8/8	0.85	0.18	88,88,88,88	0
34	EOH	X	3316	3/3	0.85	0.40	10,10,10,10	0
31	MG	X	3106	1/1	0.85	0.22	37,37,37,37	0
30	MN	X	3158	1/1	0.85	0.22	62,62,62,62	0
30	MN	X	3125	1/1	0.85	0.32	79,79,79,79	0
31	MG	X	3294	1/1	0.86	0.34	37,37,37,37	0
31	MG	G	201	1/1	0.86	0.20	19,19,19,19	0
30	MN	X	3268	1/1	0.86	0.29	27,27,27,27	0
33	SPD	X	3313	10/10	0.86	0.29	30,30,30,30	0
30	MN	X	3068	1/1	0.87	0.21	70,70,70,70	0
31	MG	X	3172	1/1	0.87	0.79	27,27,27,27	0
31	MG	Y	203	1/1	0.87	0.76	21,21,21,21	0
33	SPD	X	3314	10/10	0.87	0.48	26,26,26,26	0
30	MN	X	3118	1/1	0.87	0.31	101,101,101,101	0
31	MG	X	3302	1/1	0.87	0.30	20,20,20,20	0
30	MN	X	3183	1/1	0.88	0.15	41,41,41,41	0
34	EOH	X	3321	3/3	0.88	0.30	18,18,18,18	0
30	MN	X	3073	1/1	0.88	0.14	86,86,86,86	0
31	MG	Y	201	1/1	0.88	0.11	34,34,34,34	0
31	MG	X	3039	1/1	0.88	0.30	7,7,7,7	0
31	MG	Y	205	1/1	0.88	0.14	12,12,12,12	0
30	MN	Y	202	1/1	0.88	0.14	57,57,57,57	0
31	MG	X	3174	1/1	0.88	0.31	5,5,5,5	0
31	MG	X	3082	1/1	0.88	0.17	31,31,31,31	0
30	MN	X	3276	1/1	0.88	0.17	42,42,42,42	0
34	EOH	X	3320	3/3	0.88	0.28	28,28,28,28	0
30	MN	X	3216	1/1	0.89	0.19	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	X	3035	1/1	0.89	0.34	23,23,23,23	0
31	MG	X	3031	1/1	0.89	0.33	11,11,11,11	0
30	MN	X	3074	1/1	0.89	0.06	78,78,78,78	0
30	MN	X	3223	1/1	0.89	0.24	60,60,60,60	0
30	MN	X	3273	1/1	0.89	0.27	41,41,41,41	0
31	MG	B	301	1/1	0.89	0.14	0,0,0,0	0
30	MN	X	3169	1/1	0.89	0.67	78,78,78,78	0
34	EOH	X	3319	3/3	0.90	0.19	47,47,47,47	0
30	MN	X	3290	1/1	0.90	0.18	89,89,89,89	0
31	MG	C	301	1/1	0.90	0.25	2,2,2,2	0
31	MG	X	3305	1/1	0.90	0.91	15,15,15,15	0
31	MG	X	3028	1/1	0.90	0.30	34,34,34,34	0
30	MN	X	3127	1/1	0.90	0.13	44,44,44,44	0
30	MN	X	3155	1/1	0.90	0.38	87,87,87,87	0
29	MPD	Z	101	8/8	0.90	0.35	48,48,48,48	0
30	MN	X	3146	1/1	0.90	0.23	101,101,101,101	0
30	MN	X	3244	1/1	0.90	0.18	57,57,57,57	0
31	MG	X	3097	1/1	0.90	0.23	14,14,14,14	0
30	MN	X	3192	1/1	0.90	0.32	84,84,84,84	0
30	MN	X	3134	1/1	0.91	0.18	58,58,58,58	0
31	MG	X	3085	1/1	0.91	0.21	9,9,9,9	0
30	MN	X	3250	1/1	0.91	0.27	80,80,80,80	0
31	MG	X	3115	1/1	0.91	0.72	1,1,1,1	1
31	MG	X	3300	1/1	0.91	0.16	11,11,11,11	0
31	MG	X	3022	1/1	0.91	0.60	25,25,25,25	0
30	MN	X	3058	1/1	0.91	0.14	64,64,64,64	0
31	MG	X	3098	1/1	0.91	0.33	14,14,14,14	0
31	MG	X	3038	1/1	0.91	0.29	23,23,23,23	0
30	MN	X	3288	1/1	0.91	0.11	55,55,55,55	0
30	MN	X	3178	1/1	0.91	0.46	78,78,78,78	0
30	MN	X	3067	1/1	0.91	0.19	51,51,51,51	0
34	EOH	X	3322	3/3	0.91	0.47	34,34,34,34	0
30	MN	X	3041	1/1	0.91	0.22	84,84,84,84	0
31	MG	X	3026	1/1	0.91	0.61	18,18,18,18	0
29	MPD	X	3004	8/8	0.92	0.34	73,73,73,73	0
30	MN	X	3230	1/1	0.92	0.28	65,65,65,65	0
30	MN	X	3255	1/1	0.92	0.56	35,35,35,35	0
30	MN	X	3233	1/1	0.92	0.26	63,63,63,63	0
30	MN	X	3065	1/1	0.92	0.10	60,60,60,60	0
31	MG	O	201	1/1	0.92	0.28	7,7,7,7	0
31	MG	X	3297	1/1	0.92	0.31	5,5,5,5	0
30	MN	X	3186	1/1	0.92	0.29	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
29	MPD	X	3009	8/8	0.92	0.15	76,76,76,76	0
30	MN	X	3063	1/1	0.92	0.13	60,60,60,60	0
31	MG	X	3107	1/1	0.92	0.59	18,18,18,18	0
30	MN	X	3117	1/1	0.92	0.25	80,80,80,80	0
31	MG	I	201	1/1	0.92	0.26	0,0,0,0	0
30	MN	X	3226	1/1	0.92	0.33	89,89,89,89	0
30	MN	X	3227	1/1	0.92	0.17	57,57,57,57	0
31	MG	X	3103	1/1	0.92	0.45	3,3,3,3	0
30	MN	X	3207	1/1	0.92	0.44	62,62,62,62	0
30	MN	X	3199	1/1	0.92	0.36	51,51,51,51	0
31	MG	X	3299	1/1	0.93	0.26	5,5,5,5	0
30	MN	X	3072	1/1	0.93	0.17	80,80,80,80	0
30	MN	X	3269	1/1	0.93	0.24	36,36,36,36	0
31	MG	X	3018	1/1	0.93	0.47	15,15,15,15	0
30	MN	X	3061	1/1	0.93	0.12	63,63,63,63	0
31	MG	X	3019	1/1	0.93	0.25	15,15,15,15	0
30	MN	X	3202	1/1	0.93	0.23	54,54,54,54	0
31	MG	X	3309	1/1	0.93	0.24	20,20,20,20	0
31	MG	X	3100	1/1	0.93	0.21	17,17,17,17	0
31	MG	X	3136	1/1	0.93	0.34	27,27,27,27	0
30	MN	X	3119	1/1	0.93	0.15	63,63,63,63	0
30	MN	X	3231	1/1	0.93	0.24	74,74,74,74	0
30	MN	X	3149	1/1	0.93	0.27	94,94,94,94	0
31	MG	X	3304	1/1	0.93	0.78	15,15,15,15	0
30	MN	X	3291	1/1	0.93	0.52	94,94,94,94	0
30	MN	X	3229	1/1	0.93	0.13	79,79,79,79	0
30	MN	X	3211	1/1	0.93	0.20	60,60,60,60	0
30	MN	X	3046	1/1	0.93	0.30	94,94,94,94	0
31	MG	X	3099	1/1	0.94	0.14	26,26,26,26	0
30	MN	X	3218	1/1	0.94	0.31	65,65,65,65	0
31	MG	X	3108	1/1	0.94	0.10	12,12,12,12	0
30	MN	X	3187	1/1	0.94	0.28	74,74,74,74	0
30	MN	X	3160	1/1	0.94	0.18	45,45,45,45	0
29	MPD	X	3001	8/8	0.94	0.14	33,33,33,33	0
31	MG	X	3089	1/1	0.94	0.15	13,13,13,13	0
30	MN	X	3054	1/1	0.94	0.28	86,86,86,86	0
30	MN	X	3069	1/1	0.94	0.14	68,68,68,68	0
30	MN	X	3157	1/1	0.94	0.22	68,68,68,68	0
30	MN	X	3261	1/1	0.94	0.16	30,30,30,30	0
30	MN	X	3162	1/1	0.94	0.31	43,43,43,43	0
30	MN	X	3263	1/1	0.94	0.33	52,52,52,52	0
31	MG	X	3310	1/1	0.94	0.13	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3188	1/1	0.94	0.45	87,87,87,87	0
30	MN	X	3184	1/1	0.94	0.36	88,88,88,88	0
30	MN	X	3209	1/1	0.94	0.20	24,24,24,24	0
31	MG	X	3303	1/1	0.94	0.25	4,4,4,4	0
30	MN	X	3191	1/1	0.94	0.15	51,51,51,51	0
30	MN	X	3224	1/1	0.94	0.25	53,53,53,53	0
31	MG	G	202	1/1	0.94	0.37	12,12,12,12	0
31	MG	X	3295	1/1	0.94	0.68	18,18,18,18	0
31	MG	X	3021	1/1	0.94	0.18	21,21,21,21	0
30	MN	X	3208	1/1	0.94	0.25	37,37,37,37	0
30	MN	X	3267	1/1	0.94	0.31	48,48,48,48	0
30	MN	X	3221	1/1	0.94	0.12	46,46,46,46	0
31	MG	X	3027	1/1	0.94	0.19	29,29,29,29	0
31	MG	X	3032	1/1	0.94	0.25	21,21,21,21	0
30	MN	X	3177	1/1	0.95	0.21	82,82,82,82	0
30	MN	X	3040	1/1	0.95	0.19	74,74,74,74	0
31	MG	X	3036	1/1	0.95	0.14	8,8,8,8	0
30	MN	X	3049	1/1	0.95	0.39	82,82,82,82	0
30	MN	X	3265	1/1	0.95	0.24	43,43,43,43	0
29	MPD	X	3005	8/8	0.95	0.17	65,65,65,65	0
31	MG	X	3105	1/1	0.95	0.24	35,35,35,35	0
30	MN	X	3153	1/1	0.95	0.29	95,95,95,95	0
32	EPE	X	3311	15/15	0.95	0.18	57,57,57,57	0
30	MN	X	3156	1/1	0.95	0.22	53,53,53,53	0
30	MN	X	3179	1/1	0.95	0.21	83,83,83,83	0
30	MN	X	3129	1/1	0.95	0.07	73,73,73,73	0
31	MG	X	3176	1/1	0.95	0.16	14,14,14,14	0
30	MN	X	3070	1/1	0.95	0.10	78,78,78,78	0
31	MG	X	3087	1/1	0.95	0.32	51,51,51,51	0
30	MN	X	3048	1/1	0.95	0.10	59,59,59,59	0
30	MN	X	3142	1/1	0.95	0.39	72,72,72,72	0
30	MN	X	3110	1/1	0.95	0.13	96,96,96,96	0
30	MN	X	3171	1/1	0.95	0.15	86,86,86,86	0
31	MG	X	3104	1/1	0.96	0.32	28,28,28,28	0
30	MN	X	3112	1/1	0.96	0.06	54,54,54,54	0
31	MG	X	3102	1/1	0.96	0.34	6,6,6,6	0
30	MN	X	3120	1/1	0.96	0.17	55,55,55,55	0
30	MN	X	3225	1/1	0.96	0.41	41,41,41,41	0
30	MN	R	201	1/1	0.96	0.10	63,63,63,63	0
30	MN	X	3325	1/1	0.96	0.22	59,59,59,59	0
30	MN	X	3324	1/1	0.96	0.18	12,12,12,12	0
30	MN	X	3206	1/1	0.96	0.45	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	R	202	1/1	0.96	0.23	58,58,58,58	0
30	MN	X	3260	1/1	0.96	0.30	40,40,40,40	0
30	MN	X	3071	1/1	0.96	0.08	69,69,69,69	0
30	MN	X	3196	1/1	0.96	0.33	51,51,51,51	0
31	MG	X	3296	1/1	0.96	0.47	9,9,9,9	0
31	MG	X	3091	1/1	0.96	0.43	30,30,30,30	0
30	MN	X	3228	1/1	0.96	0.34	85,85,85,85	0
31	MG	X	3092	1/1	0.96	0.15	20,20,20,20	0
31	MG	X	3037	1/1	0.96	0.12	11,11,11,11	0
30	MN	X	3262	1/1	0.96	0.22	50,50,50,50	0
30	MN	X	3281	1/1	0.96	0.17	40,40,40,40	0
30	MN	X	3252	1/1	0.96	0.30	17,17,17,17	0
30	MN	X	3180	1/1	0.96	0.54	76,76,76,76	0
30	MN	X	3259	1/1	0.96	0.15	13,13,13,13	0
30	MN	X	3258	1/1	0.96	0.22	35,35,35,35	0
30	MN	X	3240	1/1	0.96	0.19	28,28,28,28	0
30	MN	X	3194	1/1	0.96	0.17	31,31,31,31	0
31	MG	X	3086	1/1	0.96	0.10	26,26,26,26	0
30	MN	X	3025	1/1	0.96	0.21	52,52,52,52	0
29	MPD	X	3007	8/8	0.96	0.28	9,9,9,9	0
31	MG	X	3307	1/1	0.96	0.04	21,21,21,21	0
30	MN	X	3014	1/1	0.97	0.20	12,12,12,12	0
31	MG	X	3029	1/1	0.97	0.39	19,19,19,19	0
30	MN	X	3075	1/1	0.97	0.11	76,76,76,76	0
31	MG	X	3088	1/1	0.97	0.13	36,36,36,36	0
30	MN	X	3282	1/1	0.97	0.21	49,49,49,49	0
30	MN	X	3152	1/1	0.97	0.29	68,68,68,68	0
31	MG	X	3306	1/1	0.97	0.06	29,29,29,29	0
30	MN	X	3323	1/1	0.97	0.15	42,42,42,42	0
30	MN	X	3212	1/1	0.97	0.27	56,56,56,56	0
30	MN	X	3278	1/1	0.97	0.30	35,35,35,35	0
31	MG	X	3080	1/1	0.97	0.19	33,33,33,33	0
30	MN	X	3287	1/1	0.97	0.31	78,78,78,78	0
30	MN	X	3166	1/1	0.97	0.23	62,62,62,62	0
31	MG	X	3020	1/1	0.97	0.25	20,20,20,20	0
30	MN	X	3165	1/1	0.97	0.16	63,63,63,63	0
30	MN	X	3024	1/1	0.97	0.43	107,107,107,107	0
30	MN	X	3151	1/1	0.97	0.17	44,44,44,44	0
30	MN	X	3219	1/1	0.97	0.31	53,53,53,53	0
30	MN	X	3289	1/1	0.97	0.28	57,57,57,57	0
30	MN	Y	204	1/1	0.97	0.11	63,63,63,63	0
30	MN	X	3239	1/1	0.97	0.36	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3078	1/1	0.97	0.19	78,78,78,78	0
30	MN	X	3141	1/1	0.97	0.35	69,69,69,69	0
30	MN	I	203	1/1	0.97	0.22	33,33,33,33	0
30	MN	X	3181	1/1	0.97	0.19	39,39,39,39	0
30	MN	X	3047	1/1	0.97	0.20	69,69,69,69	0
30	MN	X	3147	1/1	0.97	0.12	82,82,82,82	0
31	MG	X	3144	1/1	0.97	0.18	8,8,8,8	0
30	MN	X	3266	1/1	0.97	0.18	22,22,22,22	0
30	MN	X	3193	1/1	0.97	0.18	33,33,33,33	0
30	MN	X	3241	1/1	0.97	0.28	20,20,20,20	0
30	MN	X	3242	1/1	0.97	0.30	22,22,22,22	0
30	MN	X	3236	1/1	0.97	0.15	36,36,36,36	0
30	MN	X	3292	1/1	0.97	0.28	99,99,99,99	0
31	MG	X	3030	1/1	0.97	0.21	15,15,15,15	0
30	MN	X	3204	1/1	0.97	0.16	21,21,21,21	0
30	MN	X	3170	1/1	0.97	0.10	54,54,54,54	0
29	MPD	X	3003	8/8	0.97	0.19	21,21,21,21	0
30	MN	X	3159	1/1	0.97	0.15	42,42,42,42	0
30	MN	X	3012	1/1	0.97	0.31	19,19,19,19	0
30	MN	X	3253	1/1	0.97	0.34	26,26,26,26	0
30	MN	X	3256	1/1	0.98	0.22	13,13,13,13	0
30	MN	X	3251	1/1	0.98	0.19	8,8,8,8	0
31	MG	X	3096	1/1	0.98	0.24	9,9,9,9	0
30	MN	X	3214	1/1	0.98	0.11	81,81,81,81	0
30	MN	X	3203	1/1	0.98	0.37	27,27,27,27	0
30	MN	X	3077	1/1	0.98	0.20	78,78,78,78	0
30	MN	X	3280	1/1	0.98	0.27	39,39,39,39	0
31	MG	X	3033	1/1	0.98	0.19	19,19,19,19	0
30	MN	X	3277	1/1	0.98	0.17	35,35,35,35	0
30	MN	X	3238	1/1	0.98	0.22	34,34,34,34	0
30	MN	X	3195	1/1	0.98	0.21	30,30,30,30	0
30	MN	X	3043	1/1	0.98	0.11	61,61,61,61	0
30	MN	X	3274	1/1	0.98	0.10	36,36,36,36	0
30	MN	X	3285	1/1	0.98	0.21	85,85,85,85	0
31	MG	X	3101	1/1	0.98	0.35	9,9,9,9	0
31	MG	B	302	1/1	0.98	0.11	4,4,4,4	0
31	MG	X	3081	1/1	0.98	0.07	36,36,36,36	0
30	MN	X	3232	1/1	0.98	0.30	55,55,55,55	0
30	MN	X	3161	1/1	0.98	0.23	46,46,46,46	0
30	MN	X	3197	1/1	0.98	0.24	34,34,34,34	0
30	MN	X	3235	1/1	0.98	0.39	40,40,40,40	0
30	MN	X	3210	1/1	0.98	0.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3060	1/1	0.98	0.15	51,51,51,51	0
30	MN	X	3205	1/1	0.98	0.27	61,61,61,61	0
30	MN	X	3283	1/1	0.98	0.34	14,14,14,14	0
30	MN	X	3163	1/1	0.98	0.16	61,61,61,61	0
30	MN	X	3217	1/1	0.98	0.27	38,38,38,38	0
30	MN	X	3272	1/1	0.98	0.36	44,44,44,44	0
30	MN	X	3051	1/1	0.98	0.18	67,67,67,67	0
30	MN	X	3164	1/1	0.98	0.23	48,48,48,48	0
30	MN	X	3017	1/1	0.98	0.36	103,103,103,103	0
30	MN	X	3245	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3257	1/1	0.99	0.23	25,25,25,25	0
30	MN	X	3139	1/1	0.99	0.29	97,97,97,97	0
30	MN	X	3264	1/1	0.99	0.33	52,52,52,52	0
30	MN	X	3247	1/1	0.99	0.25	25,25,25,25	0
30	MN	X	3243	1/1	0.99	0.42	28,28,28,28	0
30	MN	X	3326	1/1	0.99	0.17	57,57,57,57	0
30	MN	X	3056	1/1	0.99	0.19	61,61,61,61	0
30	MN	X	3286	1/1	0.99	0.31	57,57,57,57	0
30	MN	X	3279	1/1	0.99	0.25	25,25,25,25	0
30	MN	X	3237	1/1	0.99	0.23	47,47,47,47	0
30	MN	X	3064	1/1	0.99	0.14	68,68,68,68	0
30	MN	X	3185	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3275	1/1	0.99	0.18	30,30,30,30	0
30	MN	X	3167	1/1	0.99	0.20	57,57,57,57	0
31	MG	X	3094	1/1	0.99	0.16	5,5,5,5	0
30	MN	X	3249	1/1	0.99	0.21	51,51,51,51	0
30	MN	X	3200	1/1	0.99	0.26	37,37,37,37	0
31	MG	X	3116	1/1	0.99	0.13	20,20,20,20	0
30	MN	X	3190	1/1	0.99	0.41	59,59,59,59	0
30	MN	X	3270	1/1	0.99	0.16	30,30,30,30	0
30	MN	X	3198	1/1	0.99	0.20	64,64,64,64	0
30	MN	X	3201	1/1	0.99	0.20	40,40,40,40	0
30	MN	X	3150	1/1	0.99	0.13	50,50,50,50	0
30	MN	X	3284	1/1	0.99	0.15	21,21,21,21	0
31	MG	X	3301	1/1	0.99	0.13	8,8,8,8	0
30	MN	X	3154	1/1	0.99	0.22	40,40,40,40	0
30	MN	X	3145	1/1	0.99	0.16	51,51,51,51	0
30	MN	X	3246	1/1	0.99	0.19	13,13,13,13	0
30	MN	X	3062	1/1	0.99	0.16	42,42,42,42	0
30	MN	X	3234	1/1	0.99	0.18	17,17,17,17	0
30	MN	X	3045	1/1	0.99	0.28	3,3,3,3	0
30	MN	X	3215	1/1	0.99	0.28	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	MN	X	3271	1/1	0.99	0.25	17,17,17,17	0
30	MN	X	3248	1/1	0.99	0.28	37,37,37,37	0
30	MN	X	3189	1/1	0.99	0.30	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.