wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2016 – 10:16 PM EST

PDB ID	:	5HL7
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with lefamulin
Authors	:	Eyal, Z.; Matzov, D.; Krupkin, M.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on	:	2016-01-14
Resolution	:	3.55 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

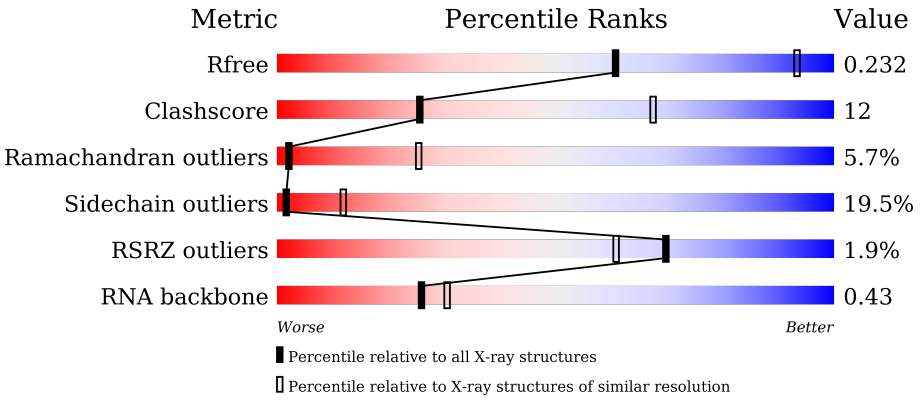
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.55 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	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)
RNA backbone	2183	1057 (4.30-2.80)

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 <=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	277	67% 24% 6%
2	X	2923	32% 41% 17% 7%
3	Y	114	34% 42% 23%
4	B	220	55% 34% 9%

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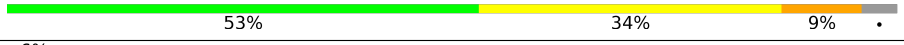
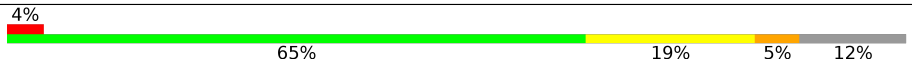
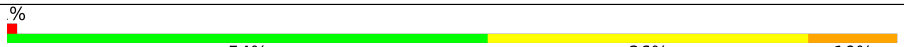
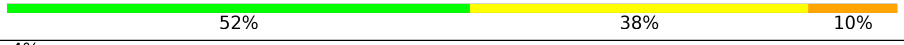
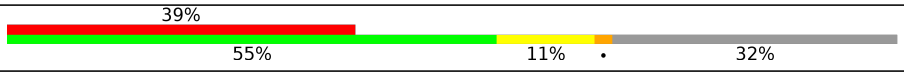
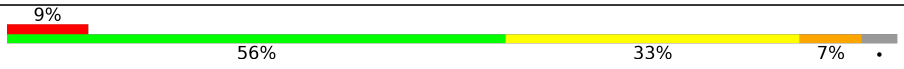
Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	140	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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
29	MN	A	301	-	-	-	X
29	MN	X	3001	-	-	-	X
29	MN	X	3013	-	-	-	X
29	MN	X	3026	-	-	-	X
29	MN	X	3028	-	-	-	X
29	MN	X	3029	-	-	-	X
29	MN	X	3034	-	-	-	X
29	MN	X	3036	-	-	-	X
29	MN	X	3040	-	-	-	X
29	MN	X	3043	-	-	-	X
29	MN	X	3045	-	-	-	X
29	MN	X	3047	-	-	-	X
29	MN	X	3049	-	-	-	X
29	MN	X	3053	-	-	-	X
29	MN	X	3054	-	-	-	X
29	MN	X	3058	-	-	-	X
29	MN	X	3063	-	-	-	X
29	MN	X	3066	-	-	-	X
29	MN	X	3067	-	-	-	X
29	MN	X	3068	-	-	-	X
29	MN	X	3073	-	-	-	X
29	MN	X	3081	-	-	-	X
29	MN	X	3083	-	-	-	X
29	MN	X	3085	-	-	-	X
29	MN	X	3096	-	-	-	X
29	MN	X	3099	-	-	-	X
29	MN	X	3122	-	-	-	X
29	MN	X	3139	-	-	-	X
29	MN	X	3164	-	-	-	X
29	MN	X	3168	-	-	-	X
29	MN	X	3173	-	-	-	X
29	MN	X	3194	-	-	-	X
29	MN	X	3202	-	-	-	X
29	MN	X	3320	-	-	-	X
29	MN	X	3439	-	-	-	X
30	MG	C	301	-	-	-	X
30	MG	I	201	-	-	-	X
30	MG	X	3002	-	-	-	X
30	MG	X	3123	-	-	-	X
30	MG	X	3144	-	-	-	X
30	MG	X	3233	-	-	-	X
30	MG	X	3239	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3279	-	-	-	X
30	MG	X	3293	-	-	-	X
30	MG	X	3295	-	-	-	X
30	MG	X	3329	-	-	-	X
30	MG	X	3335	-	-	-	X
30	MG	X	3340	-	-	-	X
30	MG	X	3354	-	-	-	X
30	MG	X	3390	-	-	-	X
30	MG	X	3420	-	-	-	X
30	MG	X	3435	-	-	-	X
30	MG	X	3501	-	-	-	X
30	MG	Y	207	-	-	-	X
31	62B	X	3003	-	-	-	X
32	MPD	X	3004	-	-	-	X
32	MPD	X	3005	-	-	-	X
32	MPD	X	3006	-	-	-	X
32	MPD	X	3007	-	-	-	X
32	MPD	X	3008	-	-	-	X
32	MPD	X	3009	-	-	-	X
32	MPD	X	3010	-	-	-	X
32	MPD	X	3011	-	-	-	X
33	SPD	X	3492	-	-	-	X
33	SPD	X	3494	-	-	-	X
33	SPD	X	3495	-	-	-	X
33	SPD	X	3496	-	-	-	X
33	SPD	X	3498	-	-	-	X
33	SPD	Y	213	-	-	-	X
35	EPE	N	201	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81462 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			1667	1007	331	324	5			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	2705	Total	C	N	O	P	0	0	0
			57983	25884	10620	18774	2705			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

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

- 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
			1547	967	289	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
			1324	823	250	249	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	165	Total	C	N	O	S	0	0	0
			853	512	165	174	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			915	559	172	182	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	174	LYS	GLY	conflict	UNP Q2FW21

- 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
			1090	682	202	203	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
			819	498	164	156	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1001	641	187	170	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
			906	556	175	174	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			673	411	134	128			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O	0	0	0
			807	510	162	135			

- 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	0	0	0
			922	581	183	154	4			

- 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	0	0	0
			751	477	138	135	1			

- 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	0	0	0
			853	531	161	158	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total	C	N	O	S	0	0	0
			583	365	103	112	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	102	Total	C	N	O	S	0	0	0
			627	382	120	124	1			

- 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	0	0	0
			1087	682	191	212	2			

- 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
			559	349	110	100			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	42	Total	C	N	O	0	0	0
			242	149	48	45			

- 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	57	Total	C	N	O	0	0	0
			437	271	82	84			

- 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	43	Total	C	N	O	S	0	0	0
			350	213	85	51	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
			405	248	81	74	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	36	Total	C	N	O	S	0	0	0
			181	107	36	36	2			

- Molecule 29 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Z	1	Total	Mn	0	0
			1	1		
29	A	1	Total	Mn	0	0
			1	1		
29	T	1	Total	Mn	0	0
			1	1		
29	X	268	Total	Mn	0	0
			268	268		
29	R	1	Total	Mn	0	0
			1	1		
29	Y	2	Total	Mn	0	0
			2	2		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	P	1	Total	Mg	0	0
			1	1		
30	G	2	Total	Mg	0	0
			2	2		
30	J	1	Total	Mg	0	0
			1	1		
30	I	1	Total	Mg	0	0
			1	1		
30	C	2	Total	Mg	0	0
			2	2		
30	A	3	Total	Mg	0	0
			3	3		
30	X	218	Total	Mg	0	0
			218	218		

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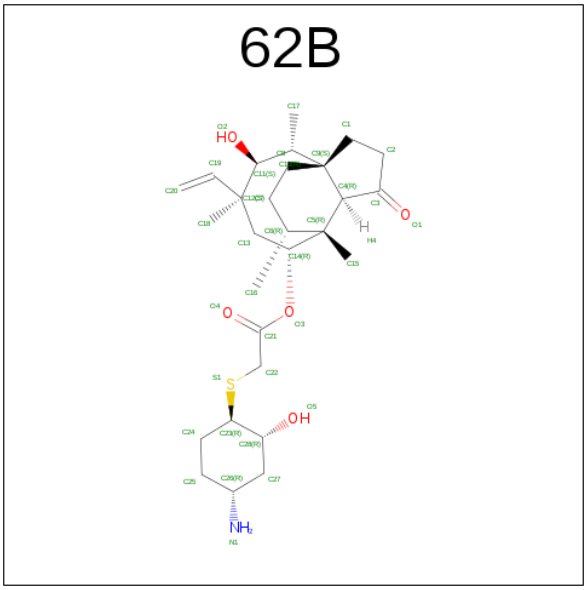
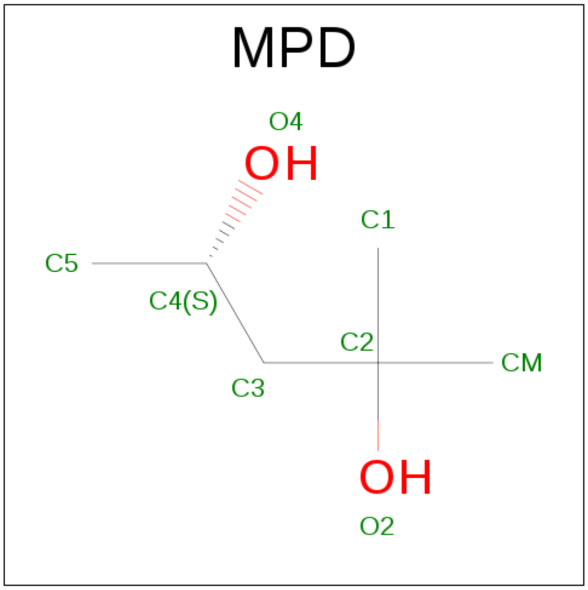
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	O	1	Total Mg 1 1	0	0
30	Y	10	Total Mg 10 10	0	0
30	M	1	Total Mg 1 1	0	0

- Molecule 31 is Lefamulin (three-letter code: 62B) (formula: $C_{28}H_{45}NO_5S$).



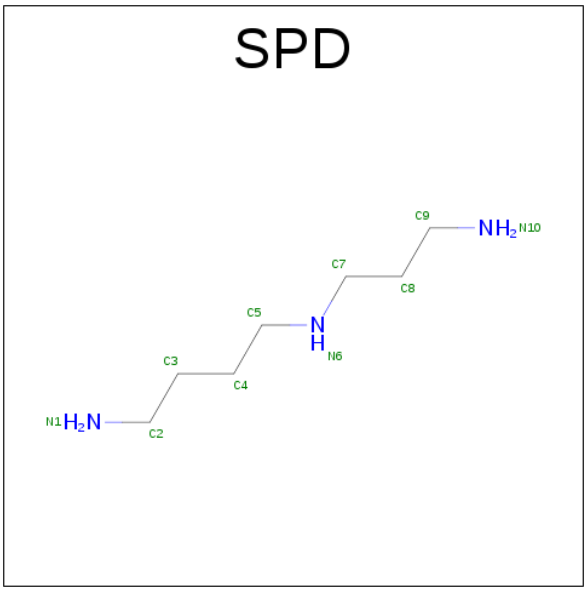
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	1	Total C N O S 35 28 1 5 1	0	0

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



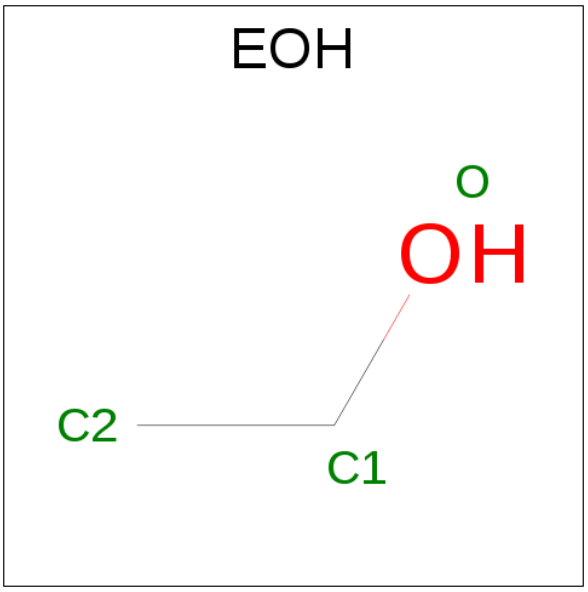
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	X	1	Total C O 8 6 2	0	0
32	J	1	Total C O 8 6 2	0	0
32	Q	1	Total C O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

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



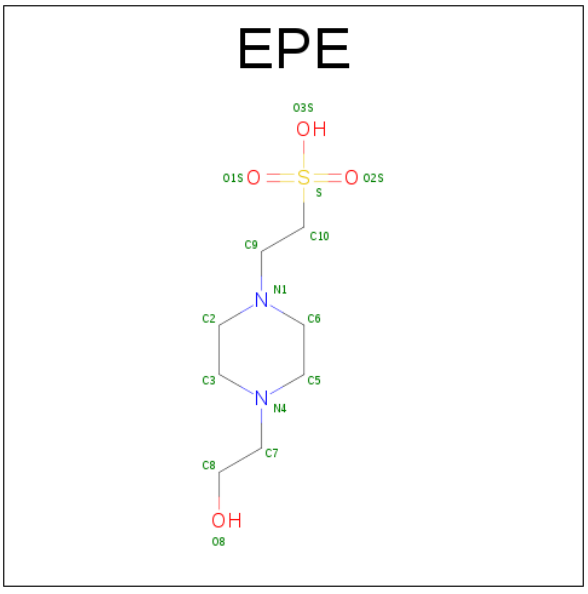
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	X	1	Total C N 10 7 3	0	0
33	Y	1	Total C N 10 7 3	0	0

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



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

- Molecule 35 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

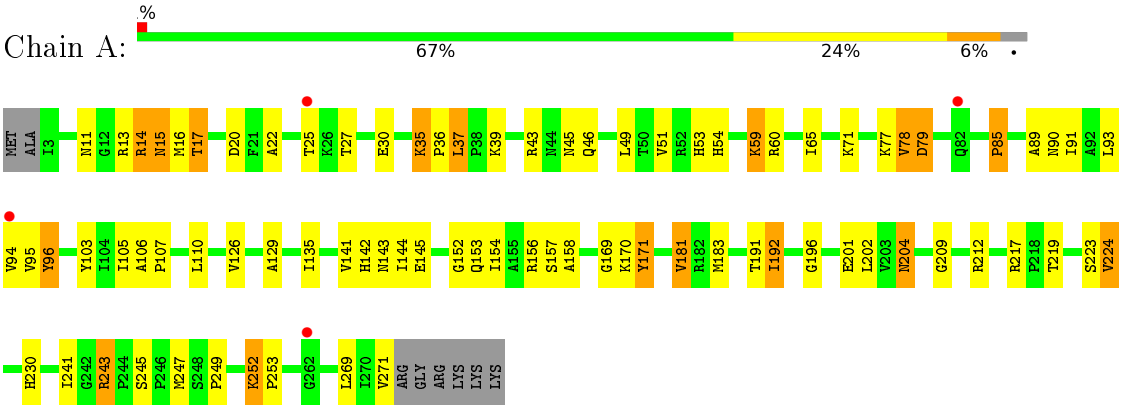


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	N	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

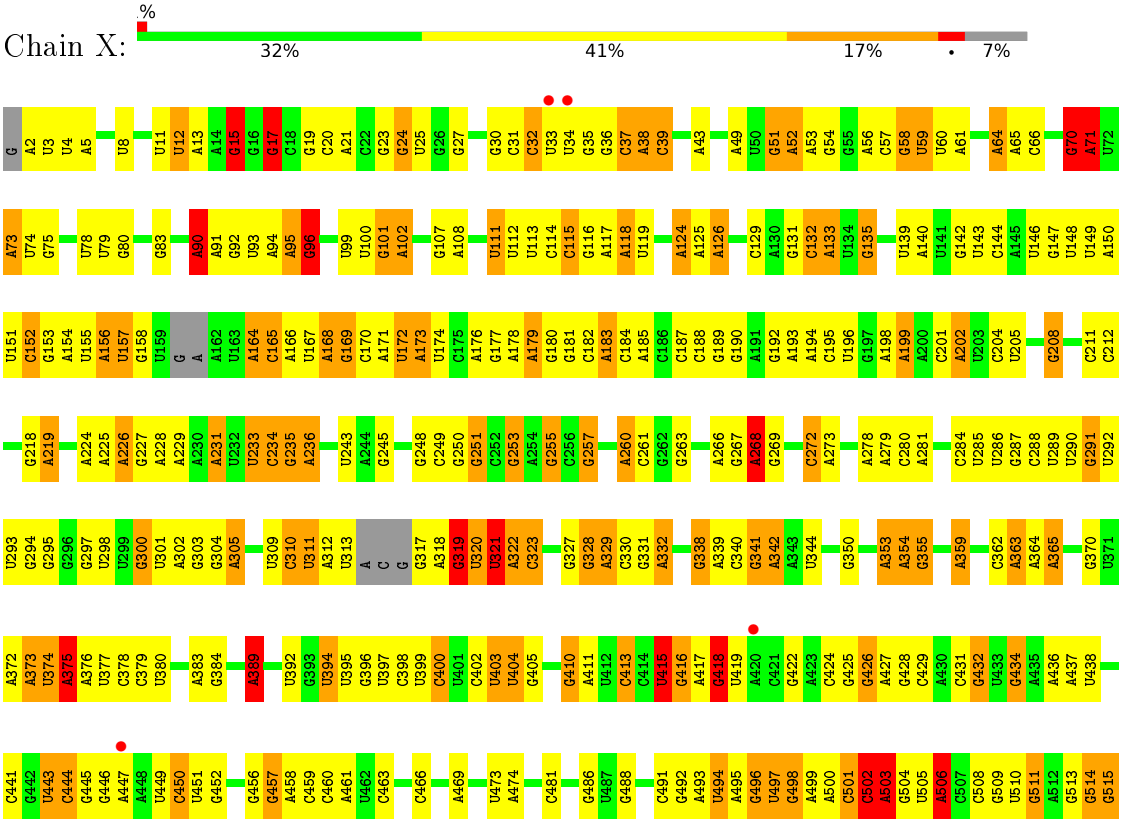
3 Residue-property plots (i)

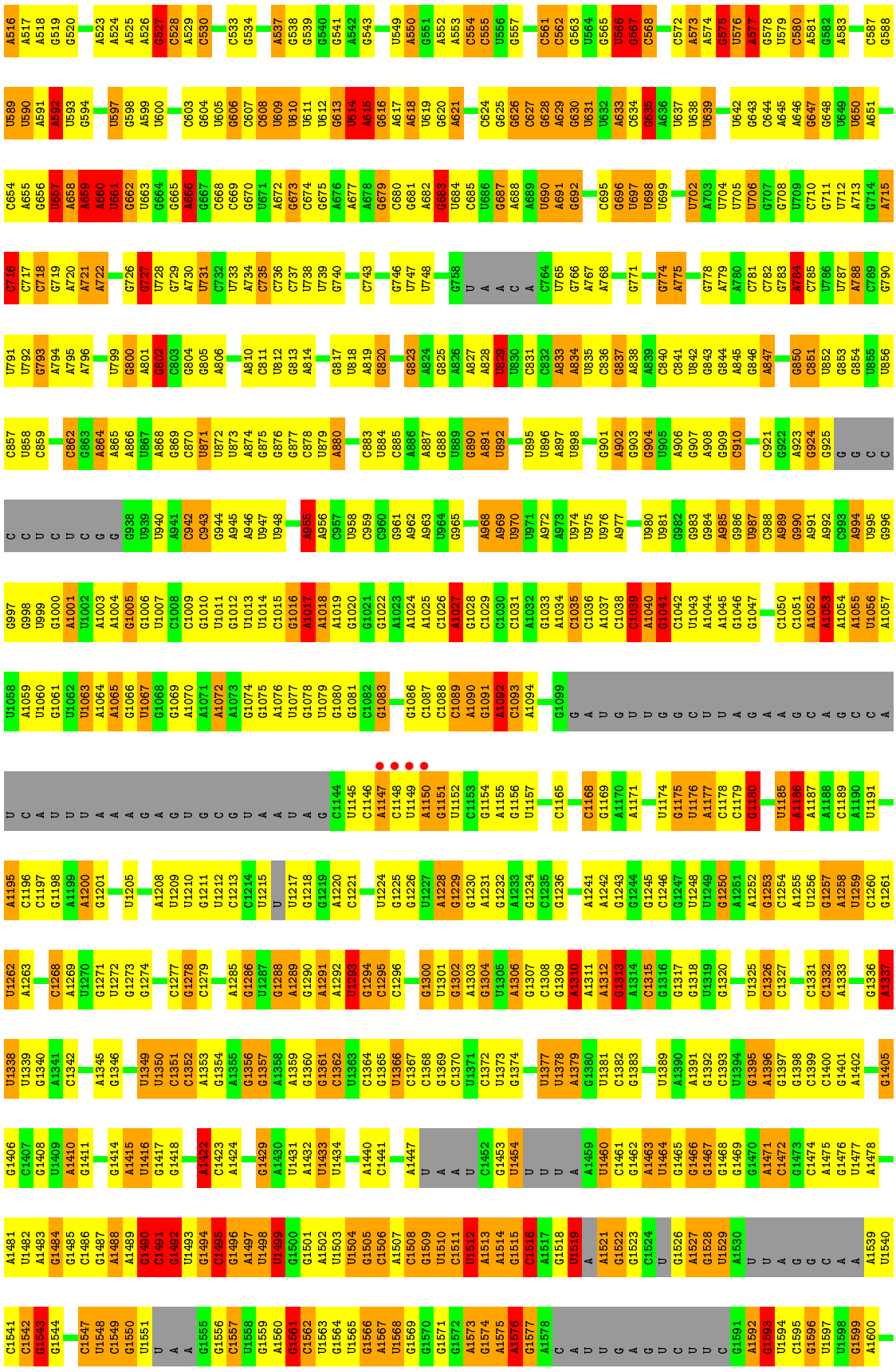
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

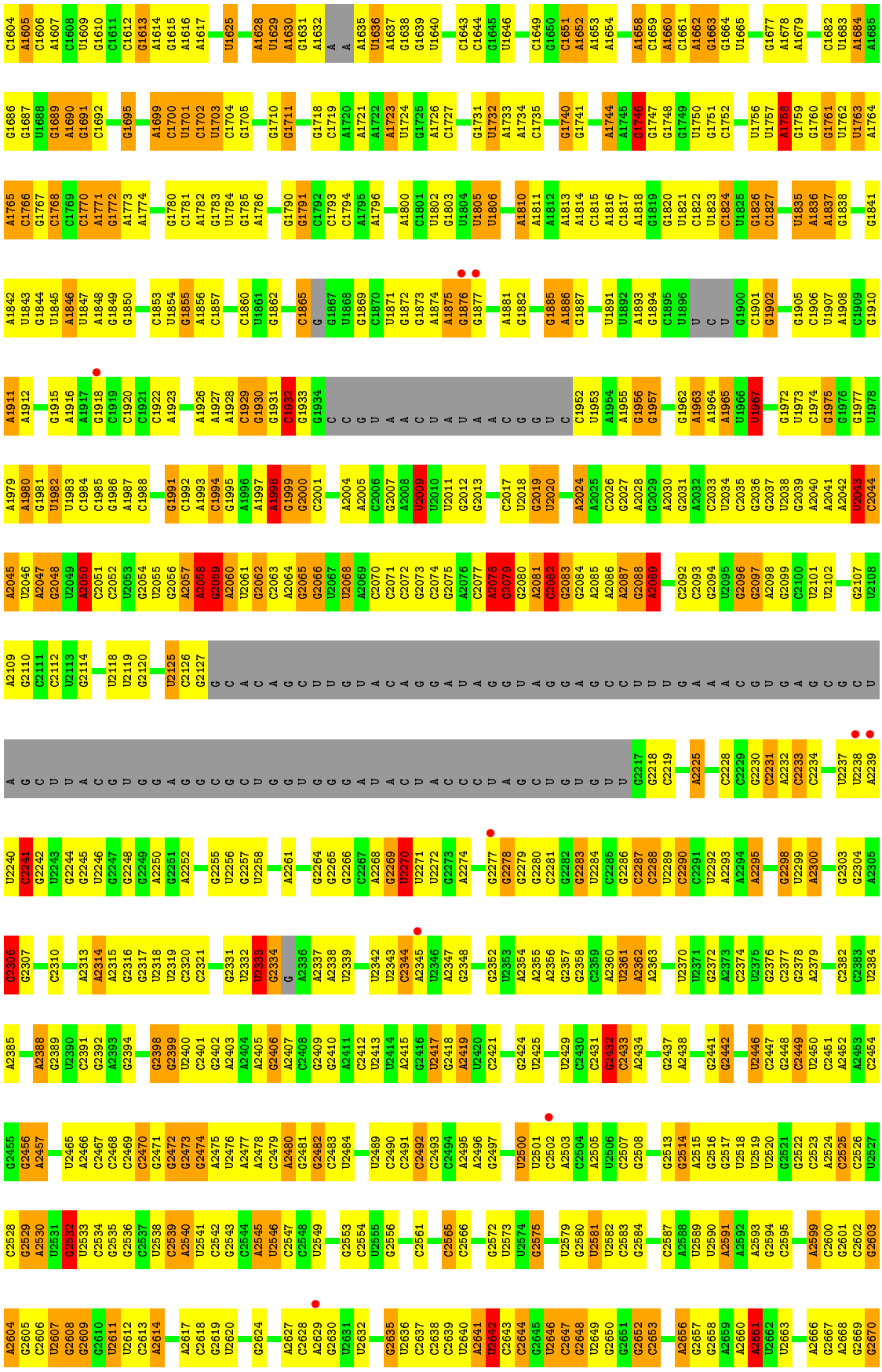
- Molecule 1: 50S ribosomal protein L2

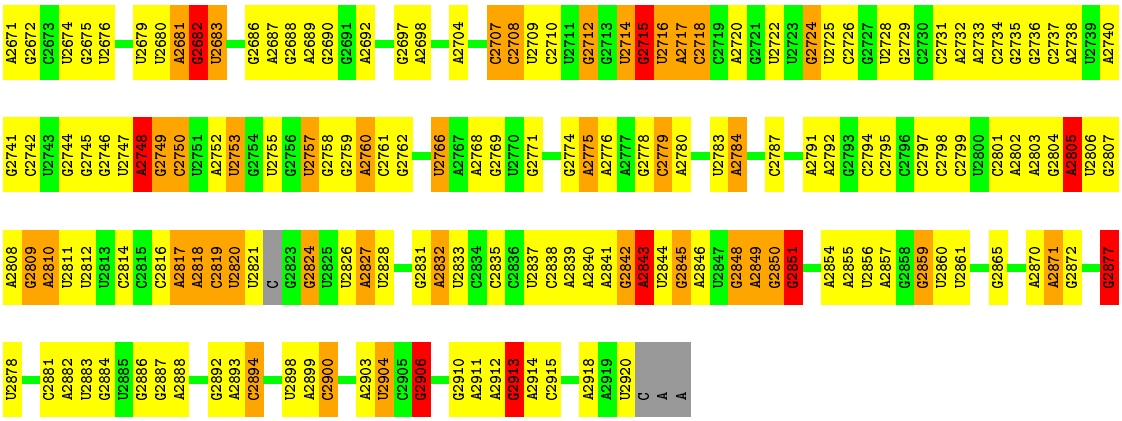


- Molecule 2: 23S ribosomal RNA



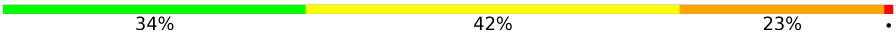


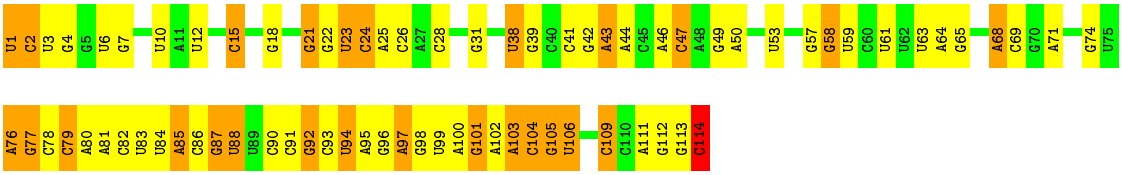




• Molecule 3: 5S ribosomal RNA

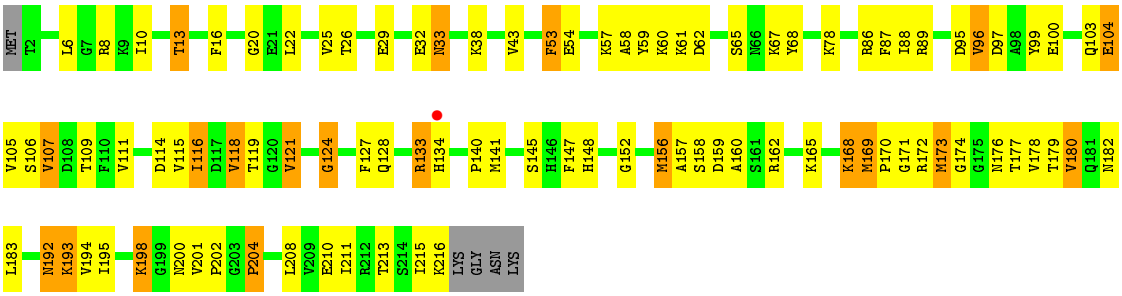
Chain Y:





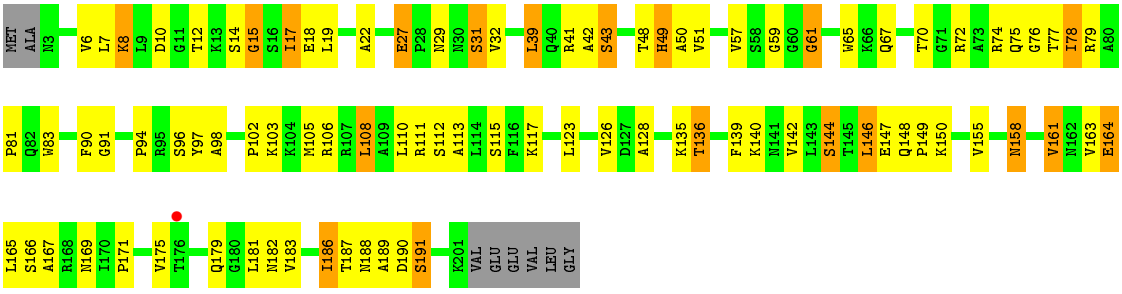
• Molecule 4: 50S ribosomal protein L3

Chain B:

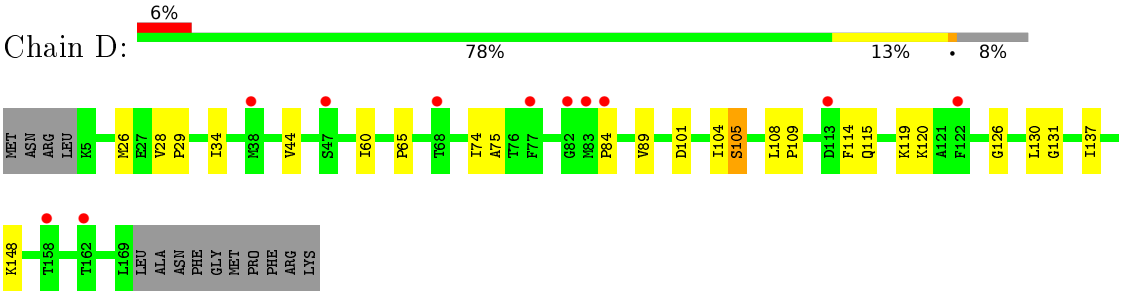


• Molecule 5: 50S ribosomal protein L4

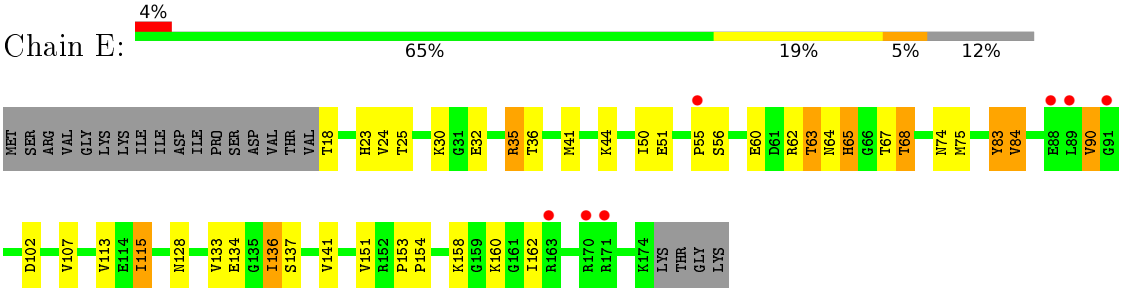
Chain C:



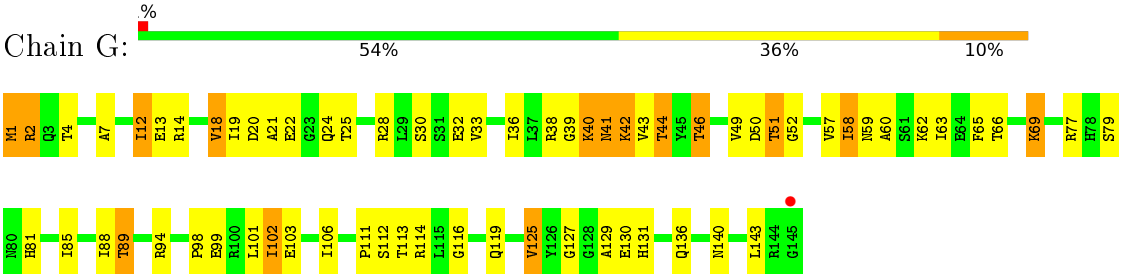
• Molecule 6: 50S ribosomal protein L5



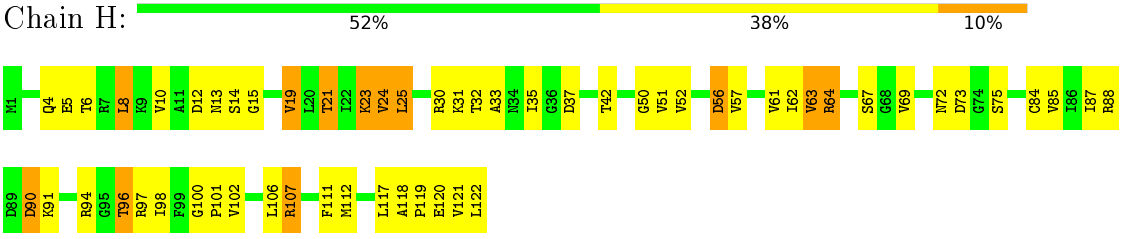
• Molecule 7: 50S ribosomal protein L6



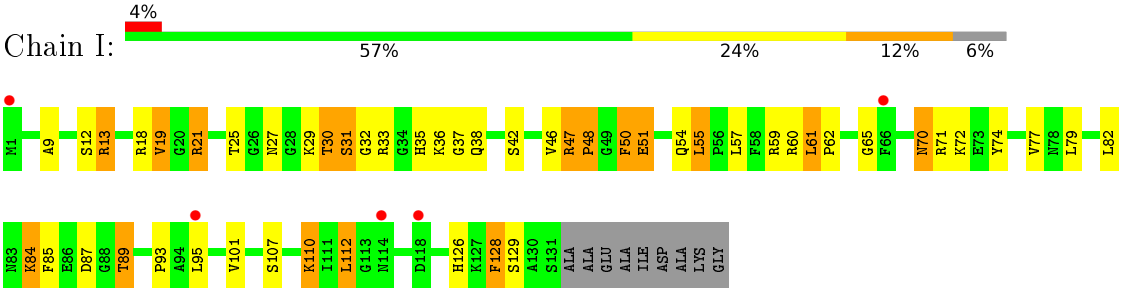
• Molecule 8: 50S ribosomal protein L13



• Molecule 9: 50S ribosomal protein L14

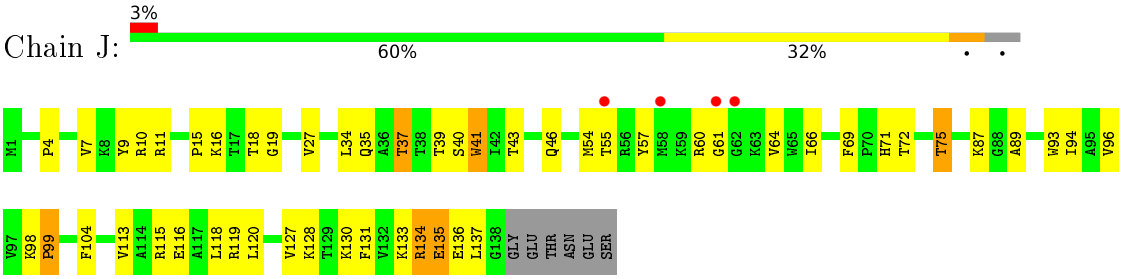


• Molecule 10: 50S ribosomal protein L15



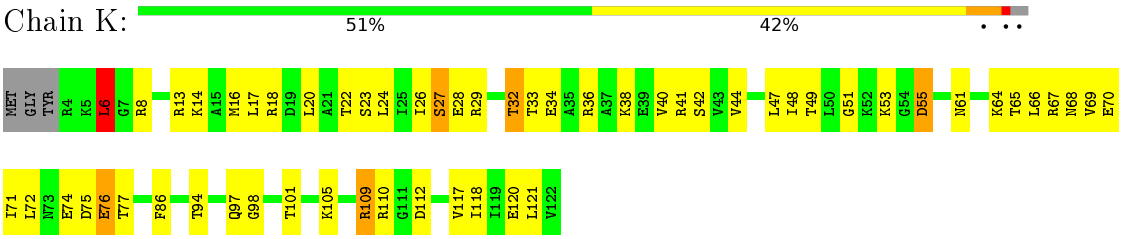
• Molecule 11: 50S ribosomal protein L16

Chain J:



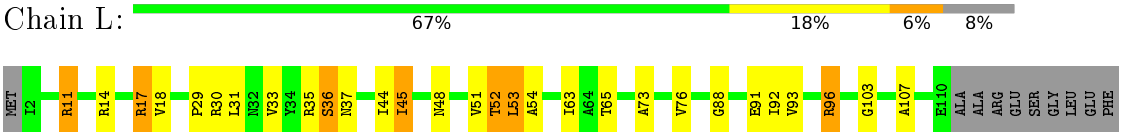
- Molecule 12: 50S ribosomal protein L17

Chain K:



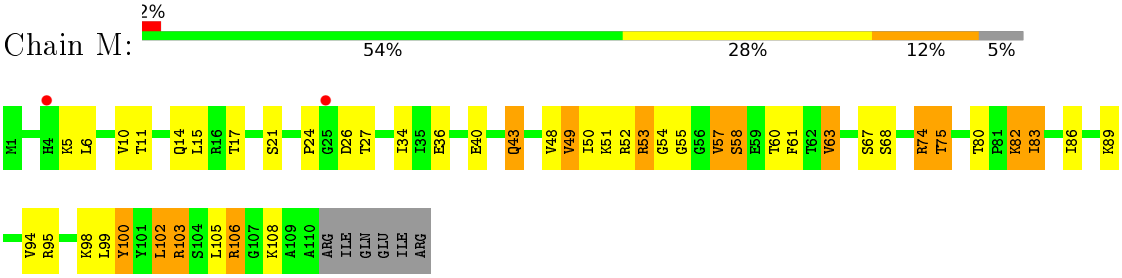
- Molecule 13: 50S ribosomal protein L18

Chain L:



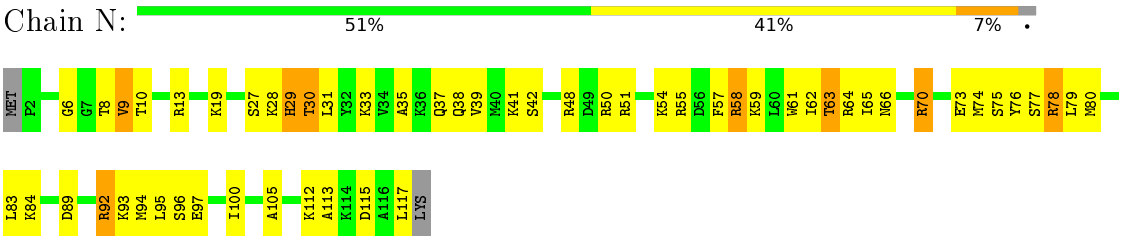
- Molecule 14: 50S ribosomal protein L19

Chain M:



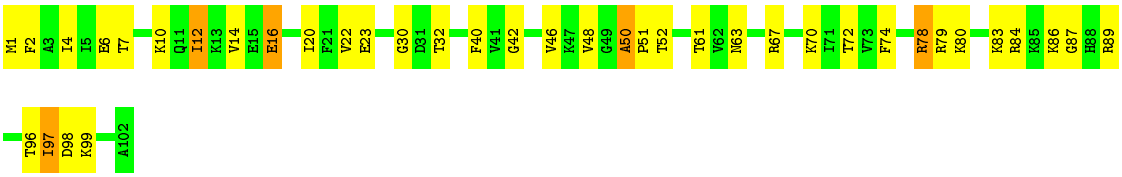
- Molecule 15: 50S ribosomal protein L20

Chain N:

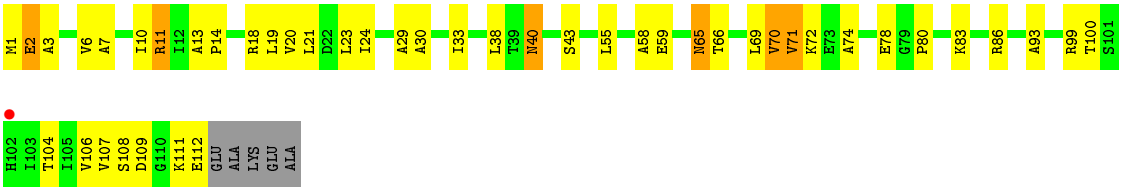


- Molecule 16: 50S ribosomal protein L21

Chain O:

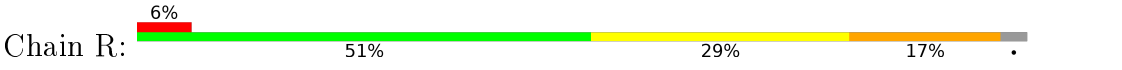


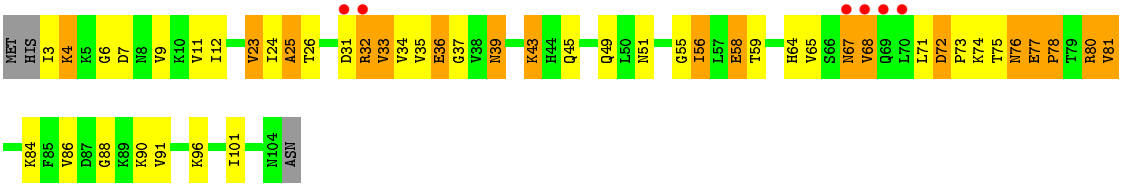
• Molecule 17: 50S ribosomal protein L22



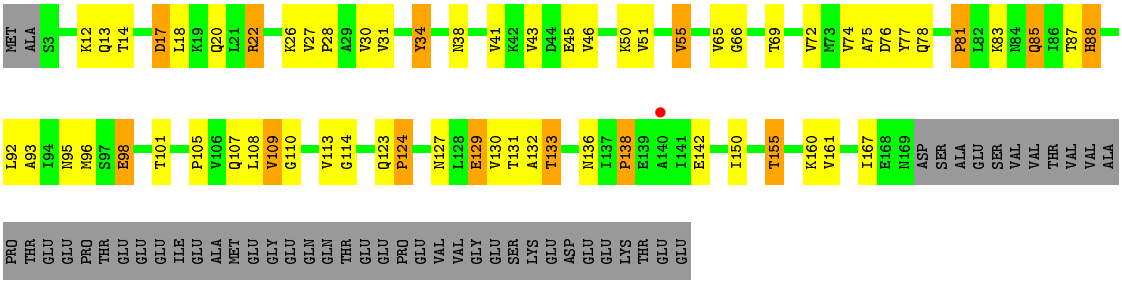
• Molecule 18: 50S ribosomal protein L23

• Molecule 19: 50S ribosomal protein L24

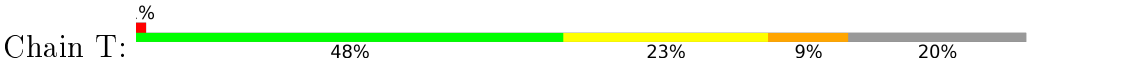


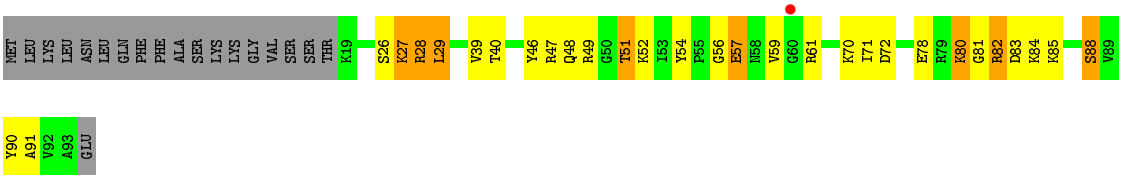


• Molecule 20: 50S ribosomal protein L25



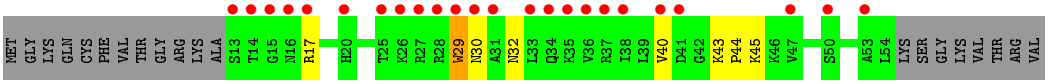
• Molecule 21: 50S ribosomal protein L27





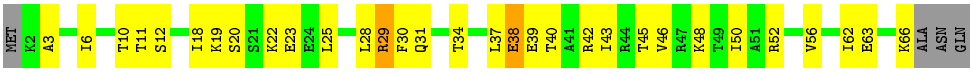
- Molecule 22: 50S ribosomal protein L28

Chain U:



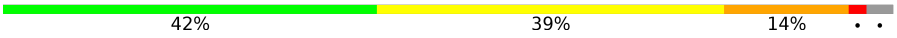
- Molecule 23: 50S ribosomal protein L29

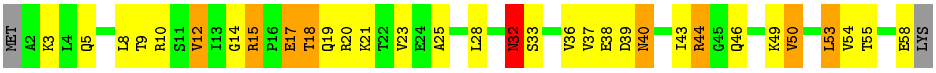
Chain V:



- Molecule 24: 50S ribosomal protein L30

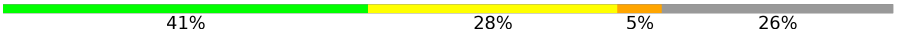
Chain W:

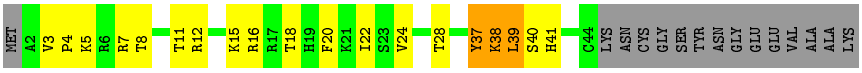




- Molecule 25: 50S ribosomal protein L32

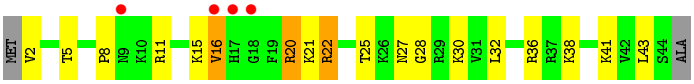
Chain Z:





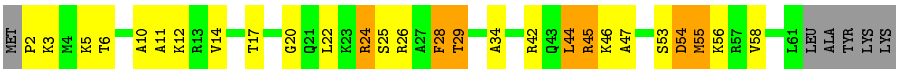
- Molecule 26: 50S ribosomal protein L34

Chain 2:



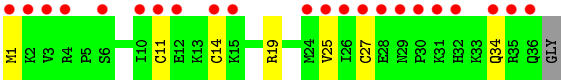
- Molecule 27: 50S ribosomal protein L35

Chain 3:



- Molecule 28: 50S ribosomal protein L36

Chain 4:


M1
K2
V3
R4
P5
S6
I10
C11
E12
K13
C14
K15
R19
M24
V25
I26
C27
E28
N29
P30
K31
H32
K33
Q34
R35
Q36
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	282.11Å 282.11Å 875.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.93 – 3.55 49.93 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.93-3.55) 95.4 (49.93-3.55)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.227 0.194 , 0.232	Depositor DCC
R_{free} test set	11840 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	105.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	81462	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MN, EOH, MPD, 62B, 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	A	0.26	0/1697	0.56	0/2332
2	X	0.96	108/64923 (0.2%)	1.63	1547/101215 (1.5%)
3	Y	0.90	10/2717 (0.4%)	1.73	90/4232 (2.1%)
4	B	0.68	0/1570	0.90	2/2117 (0.1%)
5	C	0.72	0/1343	0.98	1/1838 (0.1%)
6	D	0.33	0/855	0.56	0/1185
7	E	0.44	0/925	0.61	0/1279
8	G	0.78	0/1112	0.87	0/1507
9	H	0.62	0/891	0.80	0/1203
10	I	0.75	0/827	1.02	2/1121 (0.2%)
11	J	0.61	0/1023	0.80	0/1388
12	K	0.35	0/909	0.62	1/1217 (0.1%)
13	L	0.50	0/678	0.69	0/927
14	M	0.72	0/819	0.94	2/1107 (0.2%)
15	N	0.83	0/934	0.99	0/1241
16	O	0.84	1/761 (0.1%)	0.97	3/1022 (0.3%)
17	P	0.41	0/861	0.64	0/1160
18	Q	0.57	0/589	0.78	0/808
19	R	0.67	1/631 (0.2%)	0.85	0/863
20	S	0.60	0/1099	0.84	0/1509
21	T	0.59	0/565	0.79	0/751
22	U	0.37	0/247	0.57	0/344
23	V	0.50	0/487	0.64	0/654
24	W	0.73	0/439	0.93	0/593
25	Z	0.80	0/345	0.90	0/460
26	2	0.72	0/353	0.94	0/463
27	3	0.75	0/409	1.07	1/550 (0.2%)
28	4	0.41	0/180	0.66	0/249
All	All	0.89	120/88189 (0.1%)	1.50	1649/133335 (1.2%)

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
1	A	0	1
4	B	0	2
5	C	0	2
10	I	0	1
16	O	0	1
17	P	0	1
20	S	0	1
27	3	0	2
All	All	0	11

The worst 5 of 120 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1186	A	N9-C4	-12.81	1.30	1.37
2	X	1289	A	N9-C4	-11.75	1.30	1.37
2	X	2845	G	N9-C4	-9.65	1.30	1.38
2	X	1065	A	N9-C4	-9.16	1.32	1.37
2	X	2740	A	N9-C4	-8.95	1.32	1.37

The worst 5 of 1649 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	93	C	N3-C2-O2	-20.18	107.77	121.90
2	X	2845	G	N3-C4-C5	18.48	137.84	128.60
3	Y	93	C	N1-C2-O2	16.73	128.94	118.90
2	X	1395	G	N1-C6-O6	-16.42	110.05	119.90
2	X	1289	A	C2-N3-C4	-16.32	102.44	110.60

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	LYS	Peptide
4	B	104	GLU	Peptide
4	B	57	LYS	Peptide
5	C	161	VAL	Peptide
5	C	27	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1667	0	1292	51	0
2	X	57983	0	29161	923	0
3	Y	2430	0	1229	58	0
4	B	1547	0	1514	66	0
5	C	1324	0	1175	57	0
6	D	853	0	444	6	0
7	E	915	0	648	22	0
8	G	1090	0	1034	48	0
9	H	884	0	902	45	0
10	I	819	0	687	43	0
11	J	1001	0	971	37	0
12	K	906	0	930	36	0
13	L	673	0	538	19	0
14	M	807	0	803	32	0
15	N	922	0	973	61	0
16	O	751	0	743	22	0
17	P	853	0	900	30	0
18	Q	583	0	472	21	0
19	R	627	0	510	24	0
20	S	1087	0	934	26	0
21	T	559	0	569	24	0
22	U	242	0	141	4	0
23	V	486	0	469	10	0
24	W	437	0	467	26	0
25	Z	339	0	350	23	0
26	2	350	0	383	12	0
27	3	405	0	363	19	0
28	4	181	0	76	5	0
29	A	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	268	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
30	A	3	0	0	0	0
30	C	2	0	0	0	0
30	G	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	1	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	O	1	0	0	0	0
30	P	1	0	0	0	0
30	X	218	0	0	0	0
30	Y	10	0	0	0	0
31	X	35	0	0	1	0
32	J	8	0	14	1	0
32	Q	8	0	14	0	0
32	X	64	0	112	7	0
32	Z	8	0	14	0	0
33	X	70	0	133	9	0
33	Y	10	0	19	1	0
34	S	3	0	6	0	0
34	X	6	0	12	0	0
35	N	15	0	17	17	0
All	All	81462	0	49019	1574	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 12.

The worst 5 of 1574 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)
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.48	0.96
2:X:956:A:H2'	11:J:11:ARG:HH11	1.30	0.96
2:X:83:G:H21	2:X:102:A:H2	1.15	0.93
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.53	0.91
3:Y:21:G:H1	3:Y:58:G:H1	1.08	0.91

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
1	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1 21
4	B	213/220 (97%)	187 (88%)	17 (8%)	9 (4%)	3 34
5	C	197/207 (95%)	155 (79%)	31 (16%)	11 (6%)	2 26
6	D	163/179 (91%)	131 (80%)	17 (10%)	15 (9%)	1 12
7	E	155/178 (87%)	120 (77%)	26 (17%)	9 (6%)	2 25
8	G	143/145 (99%)	131 (92%)	8 (6%)	4 (3%)	6 45
9	H	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	11 56
10	I	129/140 (92%)	91 (70%)	25 (19%)	13 (10%)	1 11
11	J	136/144 (94%)	110 (81%)	15 (11%)	11 (8%)	1 15
12	K	117/122 (96%)	101 (86%)	9 (8%)	7 (6%)	2 24
13	L	107/119 (90%)	86 (80%)	16 (15%)	5 (5%)	3 30
14	M	108/116 (93%)	85 (79%)	18 (17%)	5 (5%)	3 31
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100 100
16	O	100/102 (98%)	90 (90%)	5 (5%)	5 (5%)	3 29
17	P	110/117 (94%)	101 (92%)	8 (7%)	1 (1%)	21 67
18	Q	88/91 (97%)	74 (84%)	9 (10%)	5 (6%)	2 25
19	R	100/105 (95%)	71 (71%)	17 (17%)	12 (12%)	0 8
20	S	165/217 (76%)	121 (73%)	23 (14%)	21 (13%)	0 7
21	T	73/94 (78%)	63 (86%)	10 (14%)	0	100 100
22	U	40/62 (64%)	32 (80%)	6 (15%)	2 (5%)	3 29
23	V	63/69 (91%)	55 (87%)	5 (8%)	3 (5%)	3 30
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	11 54
25	Z	41/58 (71%)	36 (88%)	4 (10%)	1 (2%)	7 49
26	2	41/45 (91%)	39 (95%)	1 (2%)	1 (2%)	7 49
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0 8
28	4	34/37 (92%)	26 (76%)	8 (24%)	0	100 100
All	All	2937/3209 (92%)	2430 (83%)	339 (12%)	168 (6%)	2 25

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	35	LYS
1	A	36	PRO
1	A	51	VAL
1	A	78	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	112/224 (50%)	97 (87%)	15 (13%)	5 29
4	B	150/177 (85%)	121 (81%)	29 (19%)	2 12
5	C	106/169 (63%)	84 (79%)	22 (21%)	1 10
6	D	15/158 (10%)	13 (87%)	2 (13%)	5 29
7	E	51/156 (33%)	39 (76%)	12 (24%)	1 7
8	G	106/123 (86%)	87 (82%)	19 (18%)	2 15
9	H	91/100 (91%)	74 (81%)	17 (19%)	2 13
10	I	56/108 (52%)	39 (70%)	17 (30%)	0 3
11	J	90/119 (76%)	80 (89%)	10 (11%)	8 38
12	K	91/102 (89%)	77 (85%)	14 (15%)	3 23
13	L	40/95 (42%)	30 (75%)	10 (25%)	1 6
14	M	75/102 (74%)	53 (71%)	22 (29%)	0 3
15	N	91/98 (93%)	70 (77%)	21 (23%)	1 7
16	O	71/86 (83%)	63 (89%)	8 (11%)	7 37
17	P	89/94 (95%)	77 (86%)	12 (14%)	5 29
18	Q	41/82 (50%)	34 (83%)	7 (17%)	2 17
19	R	44/90 (49%)	26 (59%)	18 (41%)	0 1
20	S	88/190 (46%)	73 (83%)	15 (17%)	2 18
21	T	53/75 (71%)	40 (76%)	13 (24%)	1 6
22	U	8/52 (15%)	7 (88%)	1 (12%)	6 31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	V	47/62 (76%)	35 (74%)	12 (26%)	1 5
24	W	50/53 (94%)	38 (76%)	12 (24%)	1 6
25	Z	38/51 (74%)	32 (84%)	6 (16%)	3 22
26	2	35/40 (88%)	29 (83%)	6 (17%)	2 17
27	3	33/57 (58%)	27 (82%)	6 (18%)	2 14
28	4	2/35 (6%)	1 (50%)	1 (50%)	0 0
All	All	1673/2698 (62%)	1346 (80%)	327 (20%)	2 12

5 of 327 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	36	ARG
14	M	82	LYS
24	W	40	ASN
12	K	94	THR
13	L	96	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
14	M	14	GLN
16	O	63	ASN
17	P	40	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	2685/2923 (91%)	645 (24%)	36 (1%)
3	Y	113/114 (99%)	18 (15%)	0
All	All	2798/3037 (92%)	663 (23%)	36 (1%)

5 of 663 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	8	U
2	X	15	G
2	X	17	G
2	X	34	U

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Mol	Chain	Res	Type
2	X	38	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	X	1149	U
2	X	1369	G
2	X	2457	A
2	X	1303	A
2	X	1490	G

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 538 ligands modelled in this entry, 514 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	$\#\|Z\| > 2$
32	MPD	J	201	-	6,7,7	0.76	0	6,10,10	0.47	0
35	EPE	N	201	-	15,15,15	1.09	1 (6%)	19,20,20	1.56	3 (15%)
32	MPD	Q	101	-	6,7,7	0.49	0	6,10,10	0.19	0
34	EOH	S	301	-	2,2,2	0.70	0	1,1,1	0.30	0
31	62B	X	3003	-	32,38,38	0.50	0	26,60,60	1.84	6 (23%)
32	MPD	X	3004	-	6,7,7	0.60	0	6,10,10	0.55	0
32	MPD	X	3005	-	6,7,7	0.70	0	6,10,10	0.43	0
32	MPD	X	3006	-	6,7,7	0.49	0	6,10,10	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	MPD	X	3007	-	6,7,7	0.39	0	6,10,10	0.18	0
32	MPD	X	3008	-	6,7,7	0.65	0	6,10,10	0.63	0
32	MPD	X	3009	-	6,7,7	0.43	0	6,10,10	0.22	0
32	MPD	X	3010	-	6,7,7	0.62	0	6,10,10	0.28	0
32	MPD	X	3011	-	6,7,7	0.81	0	6,10,10	0.27	0
33	SPD	X	3492	-	9,9,9	0.40	0	8,8,8	0.42	0
33	SPD	X	3493	-	9,9,9	0.35	0	8,8,8	0.52	0
33	SPD	X	3494	-	9,9,9	0.23	0	8,8,8	0.31	0
33	SPD	X	3495	-	9,9,9	0.26	0	8,8,8	0.37	0
33	SPD	X	3496	-	9,9,9	0.28	0	8,8,8	0.21	0
33	SPD	X	3497	-	9,9,9	0.15	0	8,8,8	0.33	0
33	SPD	X	3498	-	9,9,9	0.39	0	8,8,8	0.61	0
34	EOH	X	3499	-	2,2,2	0.61	0	1,1,1	0.48	0
34	EOH	X	3500	-	2,2,2	0.61	0	1,1,1	0.50	0
33	SPD	Y	213	-	9,9,9	0.22	0	8,8,8	0.15	0
32	MPD	Z	101	-	6,7,7	0.42	0	6,10,10	0.12	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
32	MPD	J	201	-	-	0/5/5/5	0/0/0/0
35	EPE	N	201	-	-	0/9/19/19	0/1/1/1
32	MPD	Q	101	-	-	0/5/5/5	0/0/0/0
34	EOH	S	301	-	-	0/0/0/0	0/0/0/0
31	62B	X	3003	-	-	0/10/86/86	0/2/4/4
32	MPD	X	3004	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3005	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3006	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3007	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3008	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3009	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3010	-	-	0/5/5/5	0/0/0/0
32	MPD	X	3011	-	-	0/5/5/5	0/0/0/0
33	SPD	X	3492	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3493	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3494	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3495	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3496	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3497	-	-	0/7/7/7	0/0/0/0
33	SPD	X	3498	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	EOH	X	3499	-	-	0/0/0/0	0/0/0/0
34	EOH	X	3500	-	-	0/0/0/0	0/0/0/0
33	SPD	Y	213	-	-	0/7/7/7	0/0/0/0
32	MPD	Z	101	-	-	0/5/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	201	EPE	C10-S	-3.56	1.72	1.77

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	3003	62B	C13-C12-C19	-5.58	98.31	109.73
31	X	3003	62B	C28-C23-S1	-4.61	103.18	111.13
31	X	3003	62B	C15-C5-C14	-3.27	100.50	107.59
35	N	201	EPE	O3S-S-C10	-2.92	98.92	104.99
31	X	3003	62B	C7-C6-C5	-2.60	108.62	111.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	J	201	MPD	1	0
35	N	201	EPE	17	0
31	X	3003	62B	1	0
32	X	3004	MPD	2	0
32	X	3005	MPD	1	0
32	X	3006	MPD	2	0
32	X	3008	MPD	1	0
32	X	3010	MPD	1	0
33	X	3493	SPD	2	0
33	X	3494	SPD	1	0
33	X	3495	SPD	2	0
33	X	3497	SPD	3	0
33	X	3498	SPD	1	0
33	Y	213	SPD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	269/277 (97%)	-0.31	4 (1%) 76 68	92, 138, 160, 172	0
2	X	2705/2923 (92%)	-0.49	17 (0%) 90 85	53, 101, 188, 280	0
3	Y	114/114 (100%)	-0.63	0 100 100	76, 125, 175, 180	0
4	B	215/220 (97%)	-0.31	1 (0%) 91 88	62, 81, 99, 116	0
5	C	199/207 (96%)	-0.43	1 (0%) 91 88	64, 96, 113, 138	0
6	D	165/179 (92%)	0.02	11 (6%) 21 16	166, 193, 231, 239	0
7	E	157/178 (88%)	-0.25	7 (4%) 37 29	133, 172, 206, 212	0
8	G	145/145 (100%)	-0.20	1 (0%) 89 83	64, 79, 91, 96	0
9	H	122/122 (100%)	-0.37	0 100 100	84, 102, 123, 128	0
10	I	131/140 (93%)	-0.02	5 (3%) 44 36	58, 116, 136, 142	0
11	J	138/144 (95%)	0.24	4 (2%) 55 45	77, 103, 135, 152	0
12	K	119/122 (97%)	-0.54	0 100 100	67, 84, 108, 141	0
13	L	109/119 (91%)	-0.83	0 100 100	121, 130, 157, 189	0
14	M	110/116 (94%)	-0.39	2 (1%) 71 62	85, 99, 132, 156	0
15	N	116/118 (98%)	-0.43	0 100 100	54, 70, 90, 96	0
16	O	102/102 (100%)	-0.56	0 100 100	54, 88, 103, 109	0
17	P	112/117 (95%)	-0.01	1 (0%) 85 79	64, 75, 114, 139	0
18	Q	90/91 (98%)	-0.19	0 100 100	98, 122, 138, 170	0
19	R	102/105 (97%)	0.30	6 (5%) 26 20	98, 121, 189, 206	0
20	S	167/217 (76%)	-0.27	1 (0%) 90 85	87, 109, 199, 218	0
21	T	75/94 (79%)	-0.00	1 (1%) 79 71	85, 97, 115, 129	0
22	U	42/62 (67%)	2.37	24 (57%) 0 0	160, 172, 203, 213	0
23	V	65/69 (94%)	-0.06	0 100 100	134, 145, 159, 163	0
24	W	57/59 (96%)	0.22	0 100 100	63, 77, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Z	43/58 (74%)	-0.26	0 100 100	54, 76, 131, 136	0
26	2	43/45 (95%)	0.42	4 (9%) 11 9	83, 92, 102, 105	0
27	3	60/66 (90%)	-0.23	0 100 100	80, 89, 105, 109	0
28	4	36/37 (97%)	2.41	22 (61%) 0 0	159, 164, 174, 178	0
All	All	5808/6246 (92%)	-0.32	112 (1%) 70 61	53, 103, 190, 280	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	16	ASN	5.6
22	U	30	ASN	5.4
28	4	32	HIS	5.1
22	U	27	ARG	5.1
28	4	30	PRO	5.0

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(Å^2)	Q<0.9
30	MG	X	3354	1/1	0.82	0.72	70.58	75,75,75,75	0
32	MPD	X	3007	8/8	0.92	0.36	32.06	132,132,132,132	0
32	MPD	X	3011	8/8	0.92	0.30	31.14	75,75,75,75	0
30	MG	X	3335	1/1	0.63	0.70	23.50	61,61,61,61	0
29	MN	X	3034	1/1	0.90	0.26	22.00	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3058	1/1	0.87	0.40	17.41	101,101,101,101	0
30	MG	X	3002	1/1	0.85	1.01	17.39	100,100,100,100	0
30	MG	X	3293	1/1	0.72	0.46	16.47	117,117,117,117	0
30	MG	X	3420	1/1	0.88	0.47	15.87	75,75,75,75	0
30	MG	X	3390	1/1	0.94	0.57	15.78	63,63,63,63	0
33	SPD	X	3496	10/10	0.81	0.48	14.55	102,102,102,102	0
30	MG	Y	207	1/1	0.81	0.28	13.21	78,78,78,78	0
30	MG	X	3340	1/1	0.45	0.64	13.14	84,84,84,84	0
30	MG	X	3123	1/1	0.84	0.49	12.26	69,69,69,69	0
29	MN	X	3194	1/1	0.87	0.21	12.01	138,138,138,138	0
29	MN	X	3139	1/1	0.84	0.45	9.65	117,117,117,117	0
29	MN	X	3073	1/1	0.90	0.36	9.64	95,95,95,95	0
30	MG	X	3329	1/1	0.86	0.53	9.62	63,63,63,63	0
33	SPD	X	3494	10/10	0.86	0.27	9.45	87,87,87,87	0
29	MN	X	3096	1/1	0.95	0.38	9.15	100,100,100,100	0
33	SPD	Y	213	10/10	0.78	0.38	8.99	101,101,101,101	0
29	MN	X	3029	1/1	0.96	0.39	8.90	69,69,69,69	0
29	MN	X	3036	1/1	0.95	0.30	8.73	86,86,86,86	0
29	MN	X	3045	1/1	0.91	0.27	8.63	96,96,96,96	0
30	MG	X	3279	1/1	0.98	0.34	8.26	67,67,67,67	0
29	MN	X	3063	1/1	0.97	0.30	8.01	70,70,70,70	0
30	MG	X	3144	1/1	0.88	0.32	7.70	71,71,71,71	0
30	MG	X	3295	1/1	0.87	0.45	7.08	100,100,100,100	0
29	MN	X	3040	1/1	0.99	0.36	6.66	81,81,81,81	0
29	MN	X	3173	1/1	0.92	0.25	6.36	129,129,129,129	0
32	MPD	X	3009	8/8	0.93	0.39	5.99	129,129,129,129	0
29	MN	X	3043	1/1	0.99	0.34	5.88	81,81,81,81	0
33	SPD	X	3498	10/10	0.69	0.41	5.72	93,93,93,93	0
29	MN	X	3320	1/1	0.89	0.31	5.67	107,107,107,107	0
30	MG	C	301	1/1	0.97	0.40	5.66	64,64,64,64	0
30	MG	X	3501	1/1	0.95	0.83	5.60	64,64,64,64	0
33	SPD	X	3495	10/10	0.87	0.24	5.49	83,83,83,83	0
29	MN	X	3081	1/1	0.96	0.28	5.27	109,109,109,109	0
29	MN	X	3054	1/1	0.96	0.35	5.06	97,97,97,97	0
32	MPD	X	3004	8/8	0.79	0.30	4.81	135,135,135,135	0
30	MG	I	201	1/1	0.93	0.57	4.76	80,80,80,80	0
29	MN	X	3439	1/1	0.91	0.28	4.73	94,94,94,94	0
31	62B	X	3003	35/35	0.95	0.29	4.69	65,65,65,65	0
29	MN	X	3085	1/1	1.00	0.27	4.62	59,59,59,59	0
29	MN	X	3067	1/1	0.97	0.42	4.34	104,104,104,104	0
29	MN	X	3066	1/1	0.99	0.24	4.31	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3068	1/1	0.96	0.35	4.23	94,94,94,94	0
29	MN	X	3099	1/1	0.98	0.28	4.21	82,82,82,82	0
29	MN	X	3028	1/1	0.98	0.25	4.10	53,53,53,53	0
29	MN	X	3001	1/1	0.97	0.38	3.89	97,97,97,97	0
29	MN	X	3202	1/1	0.66	0.22	3.79	173,173,173,173	0
29	MN	X	3049	1/1	0.96	0.30	3.78	93,93,93,93	0
30	MG	X	3239	1/1	0.94	0.38	3.76	91,91,91,91	0
29	MN	X	3026	1/1	0.97	0.29	3.75	66,66,66,66	0
29	MN	X	3168	1/1	0.84	0.29	3.55	115,115,115,115	0
29	MN	X	3164	1/1	0.99	0.28	3.52	111,111,111,111	0
29	MN	A	301	1/1	0.91	0.39	3.43	138,138,138,138	0
32	MPD	X	3006	8/8	0.92	0.22	3.39	82,82,82,82	0
32	MPD	X	3005	8/8	0.95	0.23	3.20	78,78,78,78	0
29	MN	X	3083	1/1	0.99	0.31	3.13	73,73,73,73	0
32	MPD	X	3010	8/8	0.88	0.22	2.99	113,113,113,113	0
29	MN	X	3013	1/1	0.95	0.25	2.94	70,70,70,70	0
33	SPD	X	3492	10/10	0.84	0.27	2.83	105,105,105,105	0
29	MN	X	3047	1/1	0.94	0.26	2.78	70,70,70,70	0
32	MPD	X	3008	8/8	0.85	0.26	2.53	94,94,94,94	0
30	MG	X	3233	1/1	0.86	0.34	2.48	68,68,68,68	0
30	MG	X	3435	1/1	0.68	0.28	2.44	153,153,153,153	0
29	MN	X	3122	1/1	0.93	0.23	2.42	99,99,99,99	0
29	MN	X	3053	1/1	0.98	0.22	2.22	58,58,58,58	0
29	MN	X	3097	1/1	0.96	0.26	1.99	109,109,109,109	0
29	MN	X	3095	1/1	0.95	0.20	1.90	79,79,79,79	0
30	MG	X	3299	1/1	0.95	0.22	1.87	149,149,149,149	0
29	MN	X	3075	1/1	0.98	0.23	1.83	71,71,71,71	0
29	MN	X	3463	1/1	0.84	0.17	1.66	134,134,134,134	0
29	MN	X	3199	1/1	0.92	0.20	1.63	143,143,143,143	0
29	MN	X	3126	1/1	0.99	0.21	1.63	74,74,74,74	0
30	MG	X	3434	1/1	0.93	0.20	1.60	64,64,64,64	0
29	MN	X	3263	1/1	0.66	0.35	1.47	166,166,166,166	0
29	MN	X	3503	1/1	0.98	0.25	1.34	68,68,68,68	0
30	MG	A	303	1/1	0.63	0.31	1.26	94,94,94,94	0
29	MN	X	3198	1/1	0.90	0.18	1.05	125,125,125,125	0
29	MN	X	3050	1/1	0.99	0.25	0.95	98,98,98,98	0
35	EPE	N	201	15/15	0.91	0.20	0.95	73,73,73,73	0
29	MN	X	3103	1/1	0.95	0.21	0.86	85,85,85,85	0
29	MN	X	3177	1/1	0.92	0.16	0.75	125,125,125,125	0
29	MN	X	3152	1/1	0.98	0.16	0.66	75,75,75,75	0
30	MG	X	3397	1/1	0.88	0.21	0.55	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3127	1/1	0.99	0.17	0.52	94,94,94,94	0
29	MN	X	3105	1/1	0.97	0.19	0.49	97,97,97,97	0
33	SPD	X	3493	10/10	0.89	0.28	0.34	83,83,83,83	0
32	MPD	J	201	8/8	0.78	0.30	0.32	125,125,125,125	0
29	MN	X	3181	1/1	0.70	0.12	0.30	142,142,142,142	0
29	MN	X	3146	1/1	0.81	0.20	0.14	122,122,122,122	0
29	MN	X	3109	1/1	0.92	0.14	0.13	92,92,92,92	0
30	MG	X	3356	1/1	0.83	0.13	0.01	83,83,83,83	0
29	MN	X	3409	1/1	0.97	0.17	0.00	87,87,87,87	0
29	MN	X	3160	1/1	0.96	0.15	-0.07	100,100,100,100	0
29	MN	X	3200	1/1	0.97	0.19	-0.22	123,123,123,123	0
30	MG	X	3353	1/1	0.93	0.17	-0.30	79,79,79,79	0
29	MN	X	3091	1/1	0.98	0.16	-0.34	92,92,92,92	0
29	MN	X	3219	1/1	0.99	0.15	-0.41	85,85,85,85	0
29	MN	T	101	1/1	0.92	0.18	-0.49	121,121,121,121	0
30	MG	J	202	1/1	0.88	0.18	-0.65	92,92,92,92	0
29	MN	X	3185	1/1	0.81	0.16	-0.70	101,101,101,101	0
29	MN	X	3217	1/1	0.99	0.14	-0.85	86,86,86,86	0
29	MN	X	3104	1/1	0.93	0.14	-1.04	94,94,94,94	0
29	MN	X	3270	1/1	0.99	0.12	-1.06	110,110,110,110	0
29	MN	X	3106	1/1	0.98	0.14	-1.15	100,100,100,100	0
29	MN	X	3022	1/1	0.98	0.11	-1.30	92,92,92,92	0
30	MG	X	3218	1/1	0.96	0.17	-2.02	75,75,75,75	0
29	MN	X	3234	1/1	0.97	0.05	-2.25	144,144,144,144	0
29	MN	X	3215	1/1	0.99	0.14	-2.32	87,87,87,87	0
29	MN	X	3220	1/1	0.96	0.08	-2.69	103,103,103,103	0
29	MN	X	3318	1/1	0.94	0.08	-2.82	128,128,128,128	0
29	MN	X	3192	1/1	0.95	0.09	-3.77	138,138,138,138	0
29	MN	X	3015	1/1	0.96	0.09	-4.78	80,80,80,80	0
29	MN	X	3016	1/1	0.96	0.12	-6.28	75,75,75,75	0
30	MG	X	3221	1/1	0.97	0.12	-	89,89,89,89	0
30	MG	X	3429	1/1	0.83	0.22	-	102,102,102,102	0
29	MN	X	3118	1/1	0.98	0.19	-	65,65,65,65	0
29	MN	X	3322	1/1	0.92	0.15	-	137,137,137,137	0
29	MN	X	3059	1/1	0.90	0.24	-	111,111,111,111	0
29	MN	Y	202	1/1	0.95	0.15	-	105,105,105,105	0
29	MN	X	3115	1/1	0.94	0.32	-	116,116,116,116	0
30	MG	X	3430	1/1	0.98	0.40	-	74,74,74,74	0
30	MG	X	3204	1/1	0.95	0.14	-	100,100,100,100	0
30	MG	Y	201	1/1	0.97	0.28	-	66,66,66,66	0
30	MG	X	3438	1/1	0.95	0.20	-	84,84,84,84	0
32	MPD	Q	101	8/8	0.83	0.20	-	137,137,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MG	X	3448	1/1	0.91	0.66	-	72,72,72,72	0
29	MN	X	3062	1/1	0.95	0.14	-	87,87,87,87	0
29	MN	X	3455	1/1	0.91	0.43	-	116,116,116,116	0
30	MG	X	3306	1/1	0.42	0.43	-	95,95,95,95	0
29	MN	X	3071	1/1	0.93	0.21	-	98,98,98,98	0
30	MG	X	3196	1/1	0.72	0.52	-	89,89,89,89	0
30	MG	X	3309	1/1	0.94	0.34	-	105,105,105,105	0
29	MN	X	3437	1/1	0.49	0.13	-	153,153,153,153	0
29	MN	X	3223	1/1	0.95	0.17	-	119,119,119,119	0
30	MG	X	3386	1/1	0.68	0.41	-	88,88,88,88	0
29	MN	X	3128	1/1	0.95	0.24	-	93,93,93,93	0
30	MG	X	3378	1/1	0.82	0.59	-	83,83,83,83	0
30	MG	X	3291	1/1	0.89	0.47	-	86,86,86,86	0
30	MG	X	3367	1/1	0.92	0.39	-	83,83,83,83	0
29	MN	X	3325	1/1	0.95	0.16	-	187,187,187,187	0
29	MN	X	3088	1/1	0.97	0.28	-	101,101,101,101	0
30	MG	X	3327	1/1	0.57	1.12	-	126,126,126,126	0
29	MN	X	3470	1/1	0.93	0.18	-	148,148,148,148	0
29	MN	X	3172	1/1	0.97	0.14	-	114,114,114,114	0
30	MG	X	3423	1/1	0.81	0.32	-	79,79,79,79	0
30	MG	X	3385	1/1	0.81	1.06	-	88,88,88,88	0
30	MG	X	3485	1/1	0.90	0.23	-	102,102,102,102	0
29	MN	X	3084	1/1	0.90	0.14	-	123,123,123,123	0
30	MG	X	3298	1/1	0.89	0.40	-	95,95,95,95	0
29	MN	X	3069	1/1	0.97	0.29	-	103,103,103,103	0
30	MG	X	3443	1/1	0.91	0.24	-	118,118,118,118	0
30	MG	X	3489	1/1	0.84	0.70	-	62,62,62,62	0
29	MN	X	3453	1/1	0.91	0.33	-	126,126,126,126	0
29	MN	X	3110	1/1	0.91	0.19	-	117,117,117,117	0
34	EOH	X	3499	3/3	0.93	0.40	-	80,80,80,80	0
30	MG	Y	211	1/1	0.90	0.43	-	115,115,115,115	0
30	MG	X	3408	1/1	0.82	1.49	-	97,97,97,97	0
30	MG	X	3249	1/1	0.89	0.97	-	109,109,109,109	0
29	MN	X	3197	1/1	0.96	0.26	-	138,138,138,138	0
30	MG	X	3282	1/1	0.88	0.25	-	85,85,85,85	0
30	MG	X	3285	1/1	0.91	0.21	-	75,75,75,75	0
29	MN	X	3446	1/1	0.66	0.46	-	142,142,142,142	0
30	MG	X	3389	1/1	0.96	0.38	-	94,94,94,94	0
30	MG	X	3334	1/1	0.87	0.72	-	89,89,89,89	0
29	MN	X	3132	1/1	0.99	0.20	-	104,104,104,104	0
29	MN	X	3076	1/1	0.98	0.30	-	90,90,90,90	0
29	MN	X	3112	1/1	0.77	0.25	-	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3042	1/1	0.99	0.23	-	74,74,74,74	0
30	MG	G	202	1/1	0.72	0.37	-	77,77,77,77	0
29	MN	X	3466	1/1	0.37	0.38	-	155,155,155,155	0
30	MG	X	3250	1/1	0.21	1.65	-	89,89,89,89	0
29	MN	X	3201	1/1	0.99	0.15	-	88,88,88,88	0
30	MG	X	3375	1/1	0.81	0.25	-	76,76,76,76	0
30	MG	X	3410	1/1	0.97	0.16	-	95,95,95,95	0
30	MG	X	3290	1/1	0.88	0.58	-	98,98,98,98	0
30	MG	X	3143	1/1	0.96	0.44	-	59,59,59,59	0
30	MG	X	3444	1/1	0.85	0.40	-	100,100,100,100	0
30	MG	X	3268	1/1	0.91	0.36	-	62,62,62,62	0
29	MN	X	3257	1/1	0.98	0.06	-	93,93,93,93	0
29	MN	X	3245	1/1	0.97	0.21	-	129,129,129,129	0
30	MG	X	3300	1/1	0.85	0.24	-	94,94,94,94	0
30	MG	X	3346	1/1	0.78	0.47	-	68,68,68,68	0
30	MG	X	3341	1/1	0.60	0.64	-	96,96,96,96	0
29	MN	X	3480	1/1	0.91	0.57	-	175,175,175,175	0
30	MG	X	3271	1/1	0.98	0.26	-	92,92,92,92	0
34	EOH	S	301	3/3	0.74	0.35	-	90,90,90,90	0
30	MG	X	3441	1/1	0.75	0.59	-	96,96,96,96	0
30	MG	X	3451	1/1	0.96	0.30	-	115,115,115,115	0
30	MG	X	3213	1/1	0.83	1.49	-	86,86,86,86	0
29	MN	X	3134	1/1	0.97	0.17	-	121,121,121,121	0
29	MN	X	3195	1/1	0.97	0.22	-	139,139,139,139	0
29	MN	X	3461	1/1	0.87	0.26	-	149,149,149,149	0
30	MG	X	3504	1/1	0.87	0.57	-	74,74,74,74	0
29	MN	X	3018	1/1	1.00	0.12	-	86,86,86,86	0
29	MN	X	3460	1/1	0.52	0.36	-	182,182,182,182	0
32	MPD	Z	101	8/8	0.87	0.20	-	145,145,145,145	0
30	MG	X	3266	1/1	0.76	0.34	-	90,90,90,90	0
30	MG	X	3297	1/1	0.93	0.19	-	81,81,81,81	0
29	MN	X	3502	1/1	0.97	0.26	-	88,88,88,88	0
29	MN	X	3237	1/1	0.94	0.07	-	167,167,167,167	0
29	MN	X	3188	1/1	0.99	0.25	-	114,114,114,114	0
29	MN	X	3169	1/1	0.98	0.19	-	107,107,107,107	0
29	MN	X	3312	1/1	0.96	0.26	-	115,115,115,115	0
30	MG	X	3332	1/1	0.79	0.44	-	81,81,81,81	0
29	MN	X	3321	1/1	0.93	0.07	-	159,159,159,159	0
29	MN	X	3131	1/1	0.96	0.23	-	126,126,126,126	0
29	MN	X	3360	1/1	0.84	0.11	-	146,146,146,146	0
30	MG	X	3224	1/1	0.86	0.78	-	66,66,66,66	0
30	MG	X	3229	1/1	0.81	0.20	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3469	1/1	0.81	0.17	-	140,140,140,140	0
30	MG	X	3344	1/1	0.66	0.85	-	91,91,91,91	0
30	MG	X	3419	1/1	0.84	0.71	-	107,107,107,107	0
30	MG	X	3387	1/1	0.84	0.34	-	175,175,175,175	0
29	MN	X	3317	1/1	0.93	0.14	-	137,137,137,137	0
33	SPD	X	3497	10/10	0.85	0.19	-	96,96,96,96	0
29	MN	X	3403	1/1	0.98	0.11	-	114,114,114,114	0
29	MN	X	3452	1/1	0.91	0.08	-	120,120,120,120	0
30	MG	X	3214	1/1	0.90	0.76	-	86,86,86,86	0
29	MN	X	3326	1/1	0.89	0.21	-	145,145,145,145	0
29	MN	X	3210	1/1	0.73	0.22	-	201,201,201,201	0
29	MN	X	3405	1/1	0.92	0.17	-	103,103,103,103	0
30	MG	X	3280	1/1	0.85	0.32	-	159,159,159,159	0
30	MG	X	3482	1/1	0.95	0.26	-	90,90,90,90	0
30	MG	X	3412	1/1	0.88	0.53	-	106,106,106,106	0
30	MG	X	3351	1/1	0.46	0.63	-	116,116,116,116	0
29	MN	X	3030	1/1	0.98	0.37	-	69,69,69,69	0
29	MN	X	3019	1/1	0.89	0.32	-	109,109,109,109	0
29	MN	X	3468	1/1	0.81	0.25	-	104,104,104,104	0
29	MN	X	3330	1/1	0.95	0.15	-	104,104,104,104	0
29	MN	X	3077	1/1	0.92	0.33	-	100,100,100,100	0
29	MN	X	3407	1/1	0.95	0.20	-	83,83,83,83	0
29	MN	X	3017	1/1	0.95	0.09	-	92,92,92,92	0
30	MG	X	3260	1/1	0.82	0.14	-	123,123,123,123	0
30	MG	X	3416	1/1	0.90	0.27	-	90,90,90,90	0
30	MG	X	3364	1/1	0.96	0.73	-	83,83,83,83	0
30	MG	X	3294	1/1	0.67	0.46	-	108,108,108,108	0
29	MN	X	3314	1/1	0.81	0.30	-	147,147,147,147	0
29	MN	X	3157	1/1	0.93	0.24	-	108,108,108,108	0
30	MG	X	3310	1/1	0.56	0.22	-	129,129,129,129	0
30	MG	X	3328	1/1	0.86	0.54	-	103,103,103,103	0
30	MG	X	3361	1/1	0.75	0.37	-	86,86,86,86	0
30	MG	X	3388	1/1	0.93	0.86	-	85,85,85,85	0
29	MN	X	3100	1/1	0.95	0.25	-	96,96,96,96	0
29	MN	X	3251	1/1	0.99	0.12	-	81,81,81,81	0
30	MG	X	3382	1/1	0.79	0.66	-	126,126,126,126	0
29	MN	X	3315	1/1	0.91	0.18	-	104,104,104,104	0
30	MG	X	3307	1/1	0.83	0.51	-	71,71,71,71	0
30	MG	Y	203	1/1	0.55	0.60	-	96,96,96,96	0
29	MN	X	3086	1/1	0.97	0.47	-	92,92,92,92	0
29	MN	X	3392	1/1	0.96	0.11	-	89,89,89,89	0
30	MG	X	3222	1/1	0.73	0.21	-	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MG	X	3395	1/1	0.72	0.37	-	79,79,79,79	0
29	MN	X	3216	1/1	0.98	0.04	-	94,94,94,94	0
30	MG	X	3484	1/1	0.89	0.17	-	77,77,77,77	0
29	MN	X	3163	1/1	0.93	0.13	-	124,124,124,124	0
30	MG	X	3287	1/1	0.89	1.55	-	102,102,102,102	0
29	MN	X	3156	1/1	0.98	0.21	-	77,77,77,77	0
30	MG	X	3289	1/1	0.96	0.24	-	110,110,110,110	0
30	MG	X	3343	1/1	0.89	0.64	-	73,73,73,73	0
29	MN	X	3376	1/1	0.87	0.10	-	119,119,119,119	0
29	MN	X	3166	1/1	0.76	0.21	-	92,92,92,92	0
29	MN	X	3436	1/1	0.95	0.17	-	119,119,119,119	0
29	MN	X	3262	1/1	0.87	0.12	-	143,143,143,143	0
29	MN	X	3057	1/1	0.97	0.23	-	68,68,68,68	0
29	MN	X	3119	1/1	0.90	0.20	-	140,140,140,140	0
29	MN	X	3089	1/1	0.96	0.14	-	113,113,113,113	0
29	MN	X	3184	1/1	0.91	0.13	-	128,128,128,128	0
30	MG	X	3253	1/1	0.69	1.55	-	112,112,112,112	0
30	MG	Y	209	1/1	0.96	0.91	-	153,153,153,153	0
29	MN	X	3471	1/1	0.66	1.22	-	130,130,130,130	0
30	MG	X	3474	1/1	0.52	0.23	-	106,106,106,106	0
29	MN	X	3174	1/1	0.84	0.18	-	121,121,121,121	0
29	MN	X	3074	1/1	0.95	0.52	-	113,113,113,113	0
29	MN	X	3098	1/1	0.99	0.19	-	92,92,92,92	0
30	MG	X	3252	1/1	0.75	1.35	-	114,114,114,114	0
30	MG	X	3486	1/1	0.90	0.60	-	90,90,90,90	0
30	MG	X	3398	1/1	0.72	0.58	-	99,99,99,99	0
30	MG	X	3255	1/1	0.74	0.62	-	94,94,94,94	0
29	MN	X	3079	1/1	0.99	0.27	-	58,58,58,58	0
30	MG	X	3449	1/1	0.47	0.42	-	86,86,86,86	0
30	MG	X	3370	1/1	0.71	1.19	-	113,113,113,113	0
29	MN	X	3425	1/1	0.73	0.30	-	101,101,101,101	0
30	MG	X	3415	1/1	0.93	0.25	-	81,81,81,81	0
29	MN	X	3459	1/1	0.98	0.34	-	161,161,161,161	0
30	MG	X	3244	1/1	0.76	0.51	-	109,109,109,109	0
29	MN	X	3186	1/1	0.79	0.46	-	143,143,143,143	0
30	MG	X	3258	1/1	0.93	0.26	-	80,80,80,80	0
30	MG	M	201	1/1	0.91	0.42	-	68,68,68,68	0
30	MG	X	3165	1/1	0.92	0.79	-	84,84,84,84	0
29	MN	X	3120	1/1	0.95	0.21	-	166,166,166,166	0
29	MN	X	3070	1/1	0.96	0.33	-	129,129,129,129	0
30	MG	X	3440	1/1	0.84	0.41	-	79,79,79,79	0
30	MG	X	3281	1/1	0.97	0.71	-	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3051	1/1	0.97	0.24	-	97,97,97,97	0
30	MG	X	3339	1/1	0.77	1.67	-	108,108,108,108	0
30	MG	X	3481	1/1	0.91	0.23	-	82,82,82,82	0
30	MG	X	3338	1/1	0.87	0.34	-	82,82,82,82	0
30	MG	X	3350	1/1	0.87	0.39	-	100,100,100,100	0
30	MG	X	3277	1/1	0.95	0.61	-	97,97,97,97	0
30	MG	X	3087	1/1	0.65	0.66	-	55,55,55,55	0
29	MN	X	3211	1/1	0.61	0.35	-	144,144,144,144	0
30	MG	X	3428	1/1	0.73	0.12	-	105,105,105,105	0
29	MN	X	3048	1/1	0.97	0.43	-	93,93,93,93	0
29	MN	X	3145	1/1	0.99	0.19	-	69,69,69,69	0
29	MN	X	3478	1/1	0.76	0.20	-	132,132,132,132	0
30	MG	X	3399	1/1	0.91	0.47	-	79,79,79,79	0
29	MN	X	3191	1/1	0.97	0.06	-	138,138,138,138	0
30	MG	X	3303	1/1	0.92	0.71	-	101,101,101,101	0
30	MG	X	3278	1/1	0.96	0.23	-	82,82,82,82	0
29	MN	X	3060	1/1	0.89	0.23	-	90,90,90,90	0
30	MG	X	3384	1/1	0.95	0.26	-	102,102,102,102	0
29	MN	X	3193	1/1	0.94	0.09	-	110,110,110,110	0
30	MG	X	3259	1/1	0.92	0.49	-	122,122,122,122	0
30	MG	X	3483	1/1	0.92	0.29	-	91,91,91,91	0
29	MN	X	3161	1/1	0.93	0.23	-	93,93,93,93	0
30	MG	X	3362	1/1	0.55	0.37	-	114,114,114,114	0
29	MN	X	3147	1/1	0.89	0.11	-	119,119,119,119	0
30	MG	X	3417	1/1	0.47	0.92	-	82,82,82,82	0
29	MN	X	3187	1/1	0.97	0.09	-	137,137,137,137	0
29	MN	X	3044	1/1	0.92	0.37	-	116,116,116,116	0
29	MN	X	3447	1/1	0.80	0.24	-	128,128,128,128	0
29	MN	X	3116	1/1	0.87	0.42	-	111,111,111,111	0
30	MG	X	3296	1/1	0.97	0.21	-	45,45,45,45	0
29	MN	X	3041	1/1	0.94	0.18	-	77,77,77,77	0
29	MN	X	3033	1/1	0.99	0.27	-	78,78,78,78	0
30	MG	X	3393	1/1	0.67	1.22	-	104,104,104,104	0
29	MN	Y	208	1/1	0.86	0.20	-	164,164,164,164	0
29	MN	X	3189	1/1	0.95	0.07	-	154,154,154,154	0
30	MG	X	3226	1/1	0.87	0.82	-	102,102,102,102	0
30	MG	X	3363	1/1	0.82	0.36	-	82,82,82,82	0
30	MG	X	3359	1/1	0.88	0.51	-	91,91,91,91	0
29	MN	X	3154	1/1	0.82	0.36	-	124,124,124,124	0
29	MN	X	3031	1/1	0.97	0.24	-	68,68,68,68	0
30	MG	X	3236	1/1	0.73	0.72	-	88,88,88,88	0
30	MG	X	3400	1/1	0.60	0.63	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MG	X	3261	1/1	0.95	0.22	-	91,91,91,91	0
30	MG	X	3366	1/1	0.94	0.67	-	99,99,99,99	0
29	MN	X	3231	1/1	0.80	0.26	-	161,161,161,161	0
30	MG	X	3488	1/1	0.57	0.68	-	100,100,100,100	0
30	MG	X	3394	1/1	0.80	0.19	-	98,98,98,98	0
29	MN	X	3078	1/1	0.97	0.44	-	111,111,111,111	0
29	MN	X	3020	1/1	0.97	0.28	-	107,107,107,107	0
29	MN	X	3323	1/1	0.81	0.26	-	141,141,141,141	0
30	MG	X	3358	1/1	0.71	1.38	-	88,88,88,88	0
30	MG	X	3442	1/1	0.96	0.16	-	71,71,71,71	0
34	EOH	X	3500	3/3	0.90	0.34	-	99,99,99,99	0
29	MN	X	3101	1/1	0.92	0.48	-	131,131,131,131	0
29	MN	X	3456	1/1	0.81	0.24	-	113,113,113,113	0
30	MG	X	3141	1/1	0.96	0.24	-	85,85,85,85	0
30	MG	C	302	1/1	0.83	0.29	-	78,78,78,78	0
29	MN	X	3401	1/1	0.96	0.13	-	104,104,104,104	0
30	MG	Y	212	1/1	0.64	0.63	-	95,95,95,95	0
30	MG	X	3372	1/1	0.85	0.51	-	78,78,78,78	0
30	MG	X	3269	1/1	0.98	0.17	-	132,132,132,132	0
30	MG	X	3383	1/1	0.92	0.46	-	75,75,75,75	0
29	MN	X	3404	1/1	0.95	0.15	-	131,131,131,131	0
29	MN	X	3182	1/1	0.88	0.14	-	133,133,133,133	0
30	MG	X	3308	1/1	0.63	0.44	-	77,77,77,77	0
30	MG	X	3413	1/1	0.80	0.55	-	90,90,90,90	0
30	MG	X	3205	1/1	0.89	0.15	-	98,98,98,98	0
29	MN	X	3124	1/1	0.89	0.13	-	147,147,147,147	0
29	MN	X	3148	1/1	0.86	0.25	-	144,144,144,144	0
30	MG	X	3490	1/1	0.91	0.29	-	100,100,100,100	0
29	MN	X	3061	1/1	0.98	0.13	-	92,92,92,92	0
29	MN	X	3133	1/1	0.83	0.27	-	133,133,133,133	0
29	MN	X	3179	1/1	0.94	0.12	-	106,106,106,106	0
29	MN	X	3140	1/1	0.96	0.12	-	105,105,105,105	0
29	MN	X	3159	1/1	0.91	0.17	-	118,118,118,118	0
30	MG	X	3238	1/1	0.89	0.87	-	85,85,85,85	0
29	MN	X	3117	1/1	0.91	0.26	-	107,107,107,107	0
29	MN	X	3136	1/1	0.99	0.25	-	55,55,55,55	0
29	MN	X	3094	1/1	0.94	0.15	-	124,124,124,124	0
29	MN	X	3149	1/1	0.94	0.26	-	109,109,109,109	0
29	MN	X	3056	1/1	0.97	0.18	-	88,88,88,88	0
29	MN	X	3209	1/1	0.43	0.19	-	150,150,150,150	0
30	MG	X	3348	1/1	0.76	0.62	-	72,72,72,72	0
29	MN	X	3380	1/1	0.86	0.26	-	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MG	X	3424	1/1	0.88	1.45	-	89,89,89,89	0
29	MN	X	3151	1/1	0.88	0.25	-	97,97,97,97	0
30	MG	X	3274	1/1	0.94	0.34	-	99,99,99,99	0
30	MG	X	3286	1/1	0.79	0.46	-	77,77,77,77	0
30	MG	X	3305	1/1	0.82	0.44	-	123,123,123,123	0
30	MG	X	3377	1/1	0.96	0.43	-	121,121,121,121	0
30	MG	X	3129	1/1	0.87	0.59	-	79,79,79,79	0
30	MG	X	3138	1/1	0.90	0.53	-	72,72,72,72	0
30	MG	X	3227	1/1	0.96	0.72	-	95,95,95,95	0
29	MN	X	3037	1/1	0.94	0.27	-	90,90,90,90	0
29	MN	X	3102	1/1	0.96	0.57	-	124,124,124,124	0
29	MN	X	3162	1/1	0.82	0.24	-	118,118,118,118	0
29	MN	X	3316	1/1	0.84	0.10	-	173,173,173,173	0
29	MN	X	3176	1/1	0.88	0.31	-	128,128,128,128	0
29	MN	X	3418	1/1	0.95	0.13	-	124,124,124,124	0
30	MG	X	3391	1/1	0.58	1.00	-	107,107,107,107	0
30	MG	X	3288	1/1	0.83	0.32	-	81,81,81,81	0
30	MG	X	3342	1/1	0.78	0.53	-	80,80,80,80	0
29	MN	X	3203	1/1	0.71	0.19	-	145,145,145,145	0
30	MG	X	3373	1/1	0.93	0.33	-	97,97,97,97	0
30	MG	X	3355	1/1	0.89	0.19	-	91,91,91,91	0
29	MN	X	3243	1/1	0.93	0.18	-	114,114,114,114	0
29	MN	X	3190	1/1	0.93	0.20	-	124,124,124,124	0
30	MG	X	3473	1/1	0.89	0.19	-	82,82,82,82	0
29	MN	X	3111	1/1	0.92	0.32	-	130,130,130,130	0
30	MG	X	3167	1/1	0.83	0.34	-	62,62,62,62	0
29	MN	X	3454	1/1	0.79	0.49	-	126,126,126,126	0
30	MG	X	3301	1/1	0.94	0.19	-	72,72,72,72	0
30	MG	Y	206	1/1	0.91	0.87	-	104,104,104,104	0
29	MN	X	3080	1/1	0.98	0.23	-	78,78,78,78	0
29	MN	X	3072	1/1	0.74	0.21	-	123,123,123,123	0
30	MG	X	3411	1/1	0.87	0.42	-	82,82,82,82	0
29	MN	X	3479	1/1	0.82	0.23	-	171,171,171,171	0
29	MN	X	3158	1/1	0.79	0.30	-	117,117,117,117	0
29	MN	X	3462	1/1	0.91	0.28	-	152,152,152,152	0
30	MG	X	3477	1/1	0.82	0.32	-	80,80,80,80	0
29	MN	X	3225	1/1	0.73	0.52	-	157,157,157,157	0
30	MG	X	3241	1/1	0.87	1.24	-	78,78,78,78	0
29	MN	X	3027	1/1	0.90	0.36	-	68,68,68,68	0
30	MG	X	3242	1/1	0.86	0.69	-	65,65,65,65	0
30	MG	X	3371	1/1	0.85	0.50	-	88,88,88,88	0
30	MG	X	3347	1/1	0.88	1.25	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3422	1/1	0.87	0.24	-	154,154,154,154	0
30	MG	X	3304	1/1	0.91	0.46	-	117,117,117,117	0
30	MG	X	3267	1/1	0.97	0.26	-	72,72,72,72	0
30	MG	X	3247	1/1	0.95	0.54	-	85,85,85,85	0
30	MG	X	3381	1/1	0.90	0.72	-	97,97,97,97	0
29	MN	X	3374	1/1	0.97	0.11	-	104,104,104,104	0
29	MN	X	3171	1/1	0.95	0.22	-	114,114,114,114	0
30	MG	X	3137	1/1	0.93	1.13	-	63,63,63,63	0
30	MG	X	3406	1/1	0.82	0.29	-	71,71,71,71	0
30	MG	X	3396	1/1	0.91	0.60	-	108,108,108,108	0
29	MN	X	3038	1/1	0.98	0.31	-	106,106,106,106	0
30	MG	X	3368	1/1	0.88	0.54	-	87,87,87,87	0
29	MN	X	3457	1/1	0.99	0.46	-	135,135,135,135	0
30	MG	X	3180	1/1	0.56	1.16	-	78,78,78,78	0
30	MG	X	3207	1/1	0.91	0.28	-	66,66,66,66	0
30	MG	X	3333	1/1	0.92	0.77	-	97,97,97,97	0
29	MN	X	3046	1/1	0.96	0.29	-	91,91,91,91	0
30	MG	X	3254	1/1	0.73	0.77	-	66,66,66,66	0
29	MN	X	3012	1/1	0.97	0.38	-	79,79,79,79	0
30	MG	X	3228	1/1	0.81	0.30	-	150,150,150,150	0
30	MG	X	3275	1/1	0.99	0.16	-	71,71,71,71	0
30	MG	Y	204	1/1	0.92	0.38	-	78,78,78,78	0
30	MG	X	3450	1/1	0.95	0.74	-	132,132,132,132	0
29	MN	X	3311	1/1	0.93	0.17	-	124,124,124,124	0
29	MN	X	3125	1/1	0.95	0.13	-	123,123,123,123	0
29	MN	X	3032	1/1	0.99	0.33	-	64,64,64,64	0
29	MN	X	3052	1/1	0.96	0.31	-	90,90,90,90	0
30	MG	X	3283	1/1	0.84	0.22	-	129,129,129,129	0
29	MN	X	3235	1/1	0.97	0.11	-	155,155,155,155	0
30	MG	X	3142	1/1	0.94	0.51	-	72,72,72,72	0
30	MG	X	3433	1/1	0.60	0.34	-	124,124,124,124	0
29	MN	X	3107	1/1	0.98	0.29	-	73,73,73,73	0
30	MG	P	201	1/1	0.74	0.65	-	63,63,63,63	0
30	MG	X	3487	1/1	0.57	0.54	-	109,109,109,109	0
30	MG	X	3431	1/1	0.96	0.38	-	55,55,55,55	0
29	MN	X	3065	1/1	0.97	0.37	-	97,97,97,97	0
29	MN	X	3025	1/1	0.89	0.32	-	128,128,128,128	0
30	MG	G	201	1/1	0.76	0.57	-	89,89,89,89	0
30	MG	X	3276	1/1	0.97	0.23	-	67,67,67,67	0
29	MN	X	3324	1/1	0.62	0.16	-	164,164,164,164	0
30	MG	X	3491	1/1	0.98	0.15	-	86,86,86,86	0
29	MN	X	3082	1/1	0.94	0.20	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
29	MN	X	3113	1/1	0.88	0.23	-	96,96,96,96	0
29	MN	X	3035	1/1	0.97	0.23	-	74,74,74,74	0
30	MG	X	3426	1/1	0.97	0.26	-	104,104,104,104	0
29	MN	X	3021	1/1	0.96	0.21	-	91,91,91,91	0
29	MN	X	3465	1/1	0.90	0.23	-	117,117,117,117	0
29	MN	X	3064	1/1	0.97	0.18	-	84,84,84,84	0
29	MN	X	3114	1/1	0.71	0.57	-	122,122,122,122	0
30	MG	X	3273	1/1	0.98	0.47	-	124,124,124,124	0
29	MN	X	3206	1/1	0.97	0.07	-	95,95,95,95	0
30	MG	X	3331	1/1	0.95	0.36	-	86,86,86,86	0
29	MN	X	3023	1/1	0.99	0.27	-	92,92,92,92	0
30	MG	Y	205	1/1	0.85	0.82	-	94,94,94,94	0
30	MG	X	3427	1/1	0.94	0.15	-	59,59,59,59	0
30	MG	X	3256	1/1	0.98	0.37	-	69,69,69,69	0
29	MN	X	3175	1/1	0.77	0.28	-	122,122,122,122	0
30	MG	O	201	1/1	0.91	0.28	-	51,51,51,51	0
30	MG	X	3445	1/1	0.70	1.39	-	104,104,104,104	0
29	MN	X	3014	1/1	0.98	0.27	-	53,53,53,53	0
30	MG	X	3292	1/1	0.93	0.36	-	89,89,89,89	0
29	MN	X	3319	1/1	0.85	0.10	-	158,158,158,158	0
29	MN	X	3458	1/1	0.76	0.54	-	127,127,127,127	0
30	MG	X	3248	1/1	0.68	0.55	-	69,69,69,69	0
29	MN	X	3121	1/1	0.98	0.17	-	104,104,104,104	0
30	MG	X	3475	1/1	0.71	0.84	-	93,93,93,93	0
30	MG	X	3414	1/1	0.96	0.18	-	89,89,89,89	0
30	MG	X	3212	1/1	0.82	0.97	-	78,78,78,78	0
29	MN	X	3055	1/1	0.97	0.26	-	86,86,86,86	0
30	MG	X	3349	1/1	0.54	1.45	-	127,127,127,127	0
29	MN	R	201	1/1	0.90	0.28	-	123,123,123,123	0
29	MN	X	3135	1/1	0.96	0.15	-	115,115,115,115	0
29	MN	X	3464	1/1	0.95	0.56	-	149,149,149,149	0
30	MG	X	3365	1/1	0.78	0.69	-	76,76,76,76	0
30	MG	X	3246	1/1	0.84	0.91	-	72,72,72,72	0
30	MG	X	3272	1/1	0.92	0.45	-	104,104,104,104	0
29	MN	X	3402	1/1	0.97	0.13	-	108,108,108,108	0
29	MN	X	3170	1/1	0.98	0.17	-	104,104,104,104	0
29	MN	X	3092	1/1	0.99	0.22	-	90,90,90,90	0
29	MN	X	3379	1/1	0.79	0.19	-	158,158,158,158	0
30	MG	X	3240	1/1	0.94	0.67	-	78,78,78,78	0
30	MG	X	3130	1/1	0.79	0.37	-	72,72,72,72	0
29	MN	X	3093	1/1	0.96	0.22	-	81,81,81,81	0
30	MG	X	3345	1/1	0.84	0.29	-	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
30	MG	Y	210	1/1	0.17	1.31	-	105,105,105,105	0
30	MG	X	3284	1/1	0.96	0.17	-	72,72,72,72	0
30	MG	X	3336	1/1	0.79	0.93	-	99,99,99,99	0
30	MG	X	3352	1/1	0.76	0.52	-	94,94,94,94	0
30	MG	X	3337	1/1	0.55	0.47	-	89,89,89,89	0
29	MN	X	3313	1/1	0.96	0.10	-	117,117,117,117	0
30	MG	X	3432	1/1	0.95	0.23	-	71,71,71,71	0
30	MG	X	3476	1/1	0.95	0.15	-	64,64,64,64	0
30	MG	A	304	1/1	0.90	0.49	-	105,105,105,105	0
30	MG	X	3230	1/1	0.74	0.54	-	80,80,80,80	0
29	MN	X	3472	1/1	0.98	0.21	-	110,110,110,110	0
29	MN	X	3024	1/1	0.93	0.17	-	120,120,120,120	0
30	MG	X	3302	1/1	0.92	0.16	-	100,100,100,100	0
30	MG	X	3232	1/1	0.90	1.01	-	74,74,74,74	0
29	MN	X	3108	1/1	0.97	0.19	-	89,89,89,89	0
29	MN	X	3039	1/1	0.98	0.34	-	79,79,79,79	0
29	MN	X	3153	1/1	0.89	0.08	-	123,123,123,123	0
29	MN	Z	102	1/1	0.80	0.36	-	112,112,112,112	0
29	MN	X	3178	1/1	0.86	0.11	-	126,126,126,126	0
30	MG	X	3369	1/1	0.91	0.74	-	70,70,70,70	0
29	MN	X	3264	1/1	0.94	0.12	-	117,117,117,117	0
29	MN	X	3090	1/1	0.95	0.26	-	97,97,97,97	0
29	MN	X	3183	1/1	0.71	0.14	-	125,125,125,125	0
29	MN	X	3208	1/1	0.84	0.29	-	141,141,141,141	0
29	MN	X	3150	1/1	0.85	0.18	-	110,110,110,110	0
30	MG	X	3357	1/1	0.69	0.28	-	95,95,95,95	0
29	MN	X	3467	1/1	0.98	0.38	-	72,72,72,72	0
29	MN	X	3155	1/1	0.75	0.40	-	110,110,110,110	0
29	MN	X	3421	1/1	0.67	0.45	-	111,111,111,111	0
30	MG	A	302	1/1	0.79	0.57	-	92,92,92,92	0
30	MG	X	3265	1/1	0.75	0.64	-	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.