



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:17 PM GMT

PDB ID : 3D5B
Title : Structural basis for translation termination on the 70S ribosome. This file contains the 50S subunit of one 70S ribosome. The entire crystal structure contains two 70S ribosomes as described in remark 400.
Authors : Laurberg, M.; Asahara, H.; Korostelev, A.; Zhu, J.; Trakhanov, S.; Noller, H.F.
Deposited on : 2008-05-16
Resolution : 3.21 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

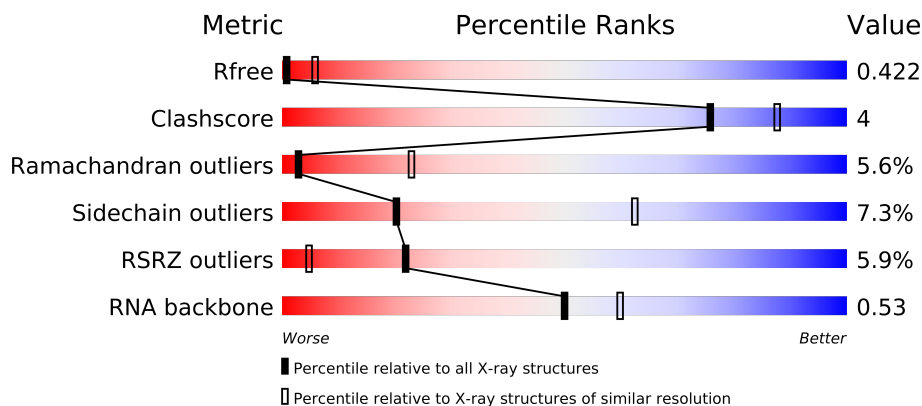
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.21 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2894	
2	B	124	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	J	173	
10	N	163	
11	O	122	

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Mol	Chain	Length	Quality of chain
12	P	150	
13	Q	141	
14	R	118	
15	S	112	
16	T	146	
17	U	118	
18	V	101	
19	W	113	
20	X	96	
21	Y	110	
22	Z	206	
23	0	85	
24	1	98	
25	2	72	
26	3	60	
27	4	97	
28	5	60	
29	6	54	
30	7	49	
31	8	65	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 91783 atoms, of which 0 are hydrogen and 0 are deuterium.

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	A	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

^ Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	A	-	INSERTION	GB 48271
B	120	U	-	INSERTION	GB 48271
B	121	U	-	INSERTION	GB 48271

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	202	Total	C	N	O	S	0	0	0
			1586	1011	297	275	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	INSERTION	UNP Q72I05
F	2	LYS	-	INSERTION	UNP Q72I05
F	3	GLU	-	INSERTION	UNP Q72I05
F	4	VAL	-	INSERTION	UNP Q72I05
F	5	ALA	-	INSERTION	UNP Q72I05

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1475	943	268	260	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	159	Total	C	N	O	S	0	0	0
			1222	773	228	220	1			

^ Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	145	Total	C	N	O	S	0	0	0
			1132	724	200	207	1			

^ Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	32	Total	C	N	O	0	0	0
			253	157	49	47			

^ Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	137	Total	C	N	O	S	0	0	0
			1096	707	205	181	3			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	2	VAL	-	INSERTION	UNP Q72IN1
N	3	LYS	-	INSERTION	UNP Q72IN1
N	4	SER	-	INSERTION	UNP Q72IN1
N	5	SER	-	INSERTION	UNP Q72IN1
N	6	LEU	-	INSERTION	UNP Q72IN1
N	7	ALA	-	INSERTION	UNP Q72IN1
N	8	PHE	-	INSERTION	UNP Q72IN1
N	9	LEU	-	INSERTION	UNP Q72IN1
N	10	ARG	-	INSERTION	UNP Q72IN1
N	11	GLY	-	INSERTION	UNP Q72IN1
N	12	PRO	-	INSERTION	UNP Q72IN1
N	13	PRO	-	INSERTION	UNP Q72IN1
N	14	ILE	-	INSERTION	UNP Q72IN1
N	15	PRO	-	INSERTION	UNP Q72IN1
N	16	ARG	-	INSERTION	UNP Q72IN1
N	17	GLN	-	INSERTION	UNP Q72IN1
N	18	GLU	-	INSERTION	UNP Q72IN1
N	19	GLN	-	INSERTION	UNP Q72IN1
N	20	ARG	-	INSERTION	UNP Q72IN1
N	21	ARG	-	INSERTION	UNP Q72IN1
N	22	ALA	-	INSERTION	UNP Q72IN1
N	23	LEU	-	INSERTION	UNP Q72IN1
N	24	VAL	-	INSERTION	UNP Q72IN1

^ Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	O	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

^ Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

^ Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Q	136	Total	C	N	O	S	0	0	0
			1079	688	204	182	5			

^ Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	R	117	Total	C	N	O	0	0	0
			960	599	202	159			

^ Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	S	98	Total	C	N	O	0	0	0
			770	486	154	130			

^ Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

^ Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	U	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

^ Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

^ Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	W	112	Total	C	N	O	S	0	0	0
			890	560	175	153	2			

^ Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	X	92	Total	C	N	O	0	0	0
			725	471	131	123			

^ Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Y	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

^ Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Z	188	Total	C	N	O	S	0	0	0
			1491	950	265	274	2			

^ Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

^ Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	1	88	Total	C	N	O		0	0	0
			694	435	141	118				

^ Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	72	Total	C	N	O	S	0	0	0
			605	375	122	106	2			

^ Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

^ Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	2	PRO	-	INSERTION	UNP Q72JR0
4	3	LEU	-	INSERTION	UNP Q72JR0
4	4	GLY	-	INSERTION	UNP Q72JR0
4	5	VAL	-	INSERTION	UNP Q72JR0
4	6	HIS	-	INSERTION	UNP Q72JR0
4	7	PRO	-	INSERTION	UNP Q72JR0
4	8	LEU	-	INSERTION	UNP Q72JR0
4	9	TYR	-	INSERTION	UNP Q72JR0
4	10	THR	-	INSERTION	UNP Q72JR0
4	11	LYS	-	INSERTION	UNP Q72JR0
4	12	ARG	-	INSERTION	UNP Q72JR0
4	13	TRP	-	INSERTION	UNP Q72JR0
4	14	LEU	-	INSERTION	UNP Q72JR0
4	15	ALA	-	INSERTION	UNP Q72JR0
4	16	HIS	-	INSERTION	UNP Q72JR0
4	17	GLY	-	INSERTION	UNP Q72JR0
4	18	GLN	-	INSERTION	UNP Q72JR0
4	19	ASP	-	INSERTION	UNP Q72JR0
4	20	ARG	-	INSERTION	UNP Q72JR0
4	21	ALA	-	INSERTION	UNP Q72JR0
4	22	LYS	-	INSERTION	UNP Q72JR0
4	23	LYS	-	INSERTION	UNP Q72JR0
4	24	GLU	-	INSERTION	UNP Q72JR0
4	25	ALA	-	INSERTION	UNP Q72JR0
4	26	ASN	-	INSERTION	UNP Q72JR0
4	27	VAL	-	INSERTION	UNP Q72JR0

^ Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

^ Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

^ Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

^ Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

^ Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	B	26	Total	Mg	0	0
			26	26		
32	W	2	Total	Mg	0	0
			2	2		
32	N	2	Total	Mg	0	0
			2	2		
32	2	3	Total	Mg	0	0
			3	3		
32	J	1	Total	Mg	0	0
			1	1		
32	E	1	Total	Mg	0	0
			1	1		
32	V	1	Total	Mg	0	0
			1	1		
32	A	807	Total	Mg	0	0
			807	807		
32	5	1	Total	Mg	0	0
			1	1		
32	R	3	Total	Mg	0	0
			3	3		
32	1	1	Total	Mg	0	0
			1	1		
32	D	2	Total	Mg	0	0
			2	2		
32	I	3	Total	Mg	0	0
			3	3		
32	Z	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		

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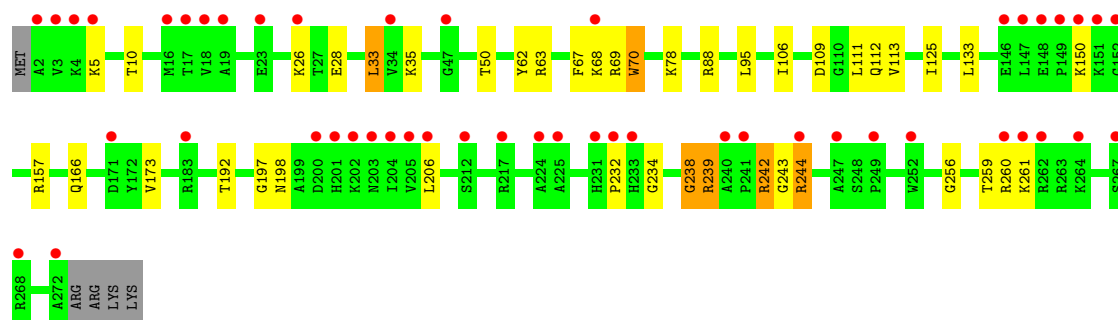
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	G	3	Total 3	Mg 3	0	0
32	Q	3	Total 3	Mg 3	0	0
32	H	2	Total 2	Mg 2	0	0
32	7	2	Total 2	Mg 2	0	0
32	T	2	Total 2	Mg 2	0	0
32	O	3	Total 3	Mg 3	0	0
32	Y	1	Total 1	Mg 1	0	0
32	F	5	Total 5	Mg 5	0	0





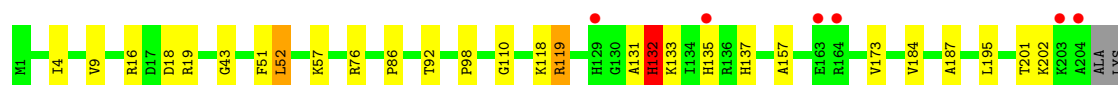
- Molecule 3: 50S ribosomal protein L2

Chain D:



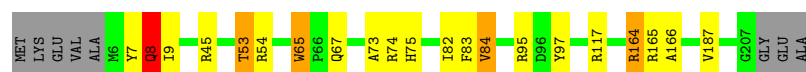
- Molecule 4: 50S ribosomal protein L3

Chain E:



- Molecule 5: 50S ribosomal protein L4

Chain F:



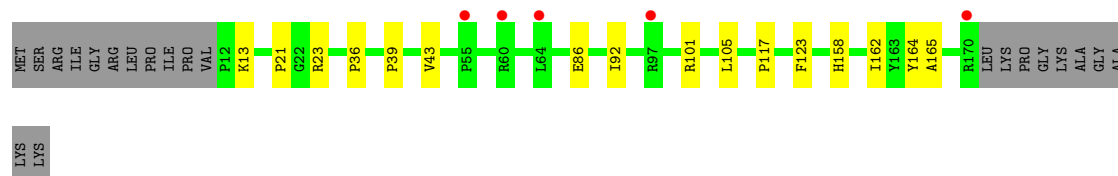
- Molecule 6: 50S ribosomal protein L5

Chain G:



- Molecule 7: 50S ribosomal protein L6

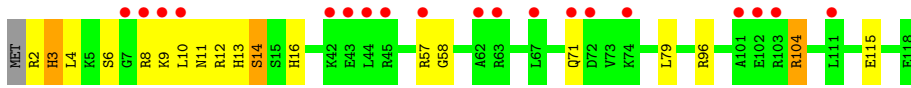
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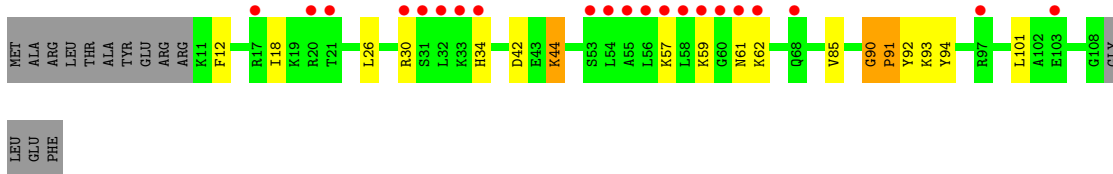
- Molecule 8: 50S ribosomal protein L9

Chain I:

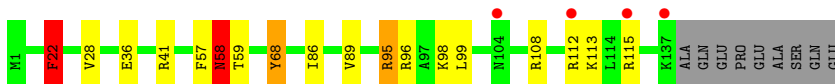
- Chain R:



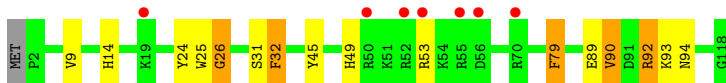
- Chain S:



- Chain T: 



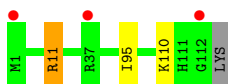
- Chain U:



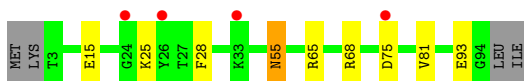
- Chain V: 



- Chain W: 

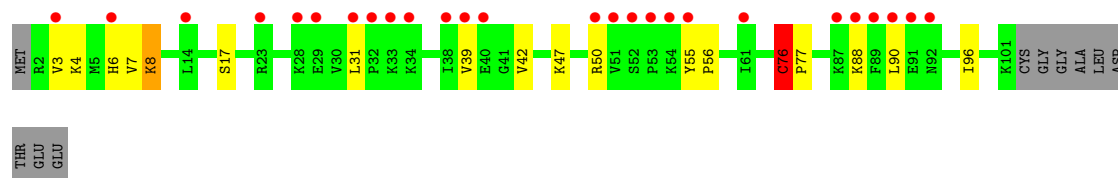


- Chain X:



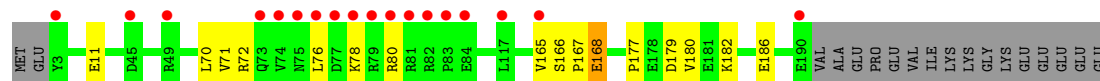
- WORLDWIDE
 PDB
PROTEIN DATA BANK

Chain Y:



- Molecule 22: 50S ribosomal protein L25

Chain Z:



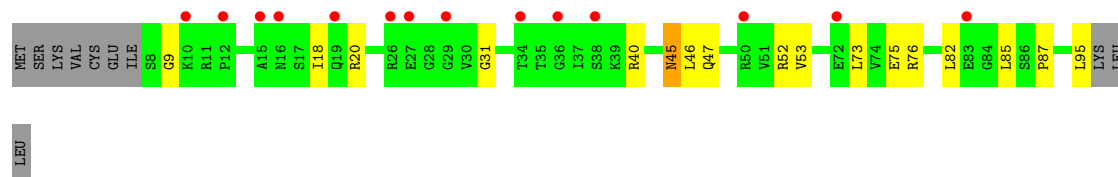
- Molecule 23: 50S ribosomal protein L27

Chain 0:



- Molecule 24: 50S ribosomal protein L28

Chain 1:



- Molecule 25: 50S ribosomal protein L29

Chain 2:



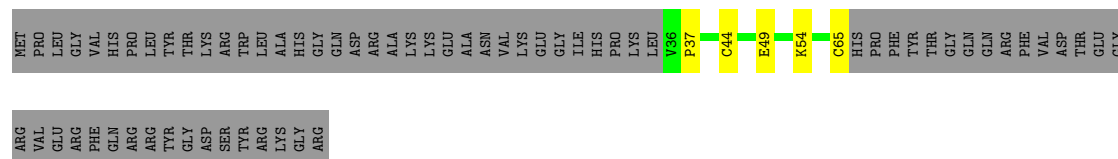
- Molecule 26: 50S ribosomal protein L30

Chain 3:



- Molecule 27: 50S ribosomal protein L31

Chain 4:



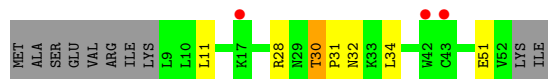
- Molecule 28: 50S ribosomal protein L32

Chain 5: 



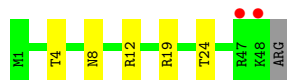
- Molecule 29: 50S ribosomal protein L33

Chain 6: 



- Molecule 30: 50S ribosomal protein L34

Chain 7: 



- Molecule 31: 50S ribosomal protein L35

Chain 8: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.13Å 454.39Å 616.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 3.21 87.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.90-3.21) 95.1 (87.17-3.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.292 , 0.319 0.415 , 0.422	Depositor DCC
R_{free} test set	8250 reflections (0.91%)	DCC
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , 4.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 952768 reflections	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	91783	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/69437	0.88	51/108401 (0.0%)
2	B	0.41	0/2853	0.85	1/4451 (0.0%)
3	D	0.25	0/2154	0.44	0/2905
4	E	0.24	0/1596	0.44	0/2153
5	F	0.23	0/1621	0.40	0/2194
6	G	0.21	0/1500	0.40	0/2017
7	H	0.20	0/1245	0.40	0/1682
8	I	0.21	0/1147	0.41	0/1552
9	J	0.21	0/251	0.38	0/333
10	N	0.22	0/1123	0.44	0/1515
11	O	0.25	0/942	0.42	0/1268
12	P	0.24	0/1131	0.45	0/1504
13	Q	0.24	0/1099	0.44	0/1468
14	R	0.23	0/974	0.45	1/1302 (0.1%)
15	S	0.21	0/778	0.38	0/1036
16	T	0.23	0/1157	0.40	0/1544
17	U	0.26	0/982	0.41	0/1306
18	V	0.23	0/790	0.40	0/1057
19	W	0.23	0/901	0.40	0/1209
20	X	0.24	0/739	0.41	0/993
21	Y	0.24	0/788	0.44	0/1051
22	Z	0.22	0/1523	0.42	0/2068
23	0	0.22	0/613	0.39	0/816
24	1	0.25	0/701	0.47	0/932
25	2	0.24	0/607	0.48	0/803
26	3	0.22	0/472	0.40	0/634
27	4	0.20	0/228	0.41	0/309
28	5	0.22	0/418	0.43	0/567
29	6	0.23	0/387	0.43	0/518
30	7	0.23	0/426	0.41	0/561
31	8	0.24	0/515	0.41	0/679
All	All	0.39	0/99098	0.79	53/148828 (0.0%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1379	A	C1'-O4'-C4'	-11.49	100.71	109.90
1	A	1091	G	P-O3'-C3'	10.65	132.48	119.70
1	A	1786	A	C1'-O4'-C4'	-9.75	102.10	109.90
1	A	1786	A	C3'-C2'-C1'	-8.72	94.53	101.50
1	A	1071	G	P-O3'-C3'	-8.37	109.65	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61997	0	0	252	0
2	B	2551	0	0	7	0
3	D	2104	0	0	9	0
4	E	1563	0	0	8	0
5	F	1586	0	0	8	0
6	G	1475	0	0	5	0
7	H	1222	0	0	0	0
8	I	1132	0	0	2	0
9	J	253	0	0	0	0
10	N	1096	0	0	6	0
11	O	932	0	0	4	0
12	P	1114	0	0	9	0
13	Q	1079	0	0	3	0
14	R	960	0	0	8	0
15	S	770	0	0	3	0
16	T	1143	0	0	5	0
17	U	964	0	0	12	0
18	V	779	0	0	3	0
19	W	890	0	0	0	0
20	X	725	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Y	775	0	0	3	0
22	Z	1491	0	0	2	0
23	0	605	0	0	1	0
24	1	694	0	0	2	0
25	2	605	0	0	7	0
26	3	467	0	0	0	0
27	4	225	0	0	0	0
28	5	404	0	0	2	0
29	6	380	0	0	1	0
30	7	418	0	0	2	0
31	8	507	0	0	2	0
32	1	1	0	0	0	0
32	2	3	0	0	0	0
32	5	1	0	0	0	0
32	7	2	0	0	0	0
32	A	807	0	0	0	0
32	B	26	0	0	0	0
32	D	2	0	0	0	0
32	E	1	0	0	0	0
32	F	5	0	0	0	0
32	G	3	0	0	0	0
32	H	2	0	0	0	0
32	I	3	0	0	0	0
32	J	1	0	0	0	0
32	N	2	0	0	0	0
32	O	3	0	0	0	0
32	P	1	0	0	0	0
32	Q	3	0	0	0	0
32	R	3	0	0	0	0
32	T	2	0	0	0	0
32	U	1	0	0	0	0
32	V	1	0	0	0	0
32	W	2	0	0	0	0
32	Y	1	0	0	0	0
32	Z	1	0	0	0	0
All	All	91783	0	0	342	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 342 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:U:31:SER:O	17:U:32:PHE:C	2.34	0.65
5:F:83:PHE:O	5:F:84:VAL:C	2.39	0.61
21:Y:8:LYS:N	21:Y:8:LYS:NZ	2.50	0.59
14:R:104:ARG:NH1	14:R:104:ARG:CG	2.65	0.59
1:A:1899:G:N2	1:A:1902:C:N4	2.50	0.58

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	269/276 (98%)	213 (79%)	40 (15%)	16 (6%)	2	20
4	E	202/206 (98%)	151 (75%)	41 (20%)	10 (5%)	3	26
5	F	200/210 (95%)	158 (79%)	35 (18%)	7 (4%)	6	37
6	G	179/182 (98%)	127 (71%)	42 (24%)	10 (6%)	3	23
7	H	157/180 (87%)	126 (80%)	24 (15%)	7 (4%)	4	29
8	I	143/148 (97%)	111 (78%)	25 (18%)	7 (5%)	3	26
9	J	28/173 (16%)	27 (96%)	1 (4%)	0	100	100
10	N	135/163 (83%)	100 (74%)	27 (20%)	8 (6%)	2	20
11	O	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	27	77
12	P	144/150 (96%)	82 (57%)	44 (31%)	18 (12%)	1	3
13	Q	134/141 (95%)	86 (64%)	36 (27%)	12 (9%)	1	8
14	R	115/118 (98%)	92 (80%)	18 (16%)	5 (4%)	4	30
15	S	96/112 (86%)	62 (65%)	24 (25%)	10 (10%)	1	5
16	T	135/146 (92%)	102 (76%)	29 (22%)	4 (3%)	7	42
17	U	115/118 (98%)	90 (78%)	21 (18%)	4 (4%)	6	37
18	V	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	8
19	W	110/113 (97%)	91 (83%)	17 (16%)	2 (2%)	13	60
20	X	90/96 (94%)	69 (77%)	20 (22%)	1 (1%)	21	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	Y	98/110 (89%)	65 (66%)	21 (21%)	12 (12%)	1	3
22	Z	186/206 (90%)	142 (76%)	34 (18%)	10 (5%)	3	24
23	0	74/85 (87%)	55 (74%)	14 (19%)	5 (7%)	2	15
24	1	86/98 (88%)	53 (62%)	27 (31%)	6 (7%)	2	13
25	2	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	1	8
26	3	57/60 (95%)	43 (75%)	13 (23%)	1 (2%)	13	60
27	4	28/97 (29%)	14 (50%)	11 (39%)	3 (11%)	1	5
28	5	50/60 (83%)	36 (72%)	12 (24%)	2 (4%)	5	32
29	6	42/54 (78%)	31 (74%)	8 (19%)	3 (7%)	2	13
30	7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
31	8	61/65 (94%)	42 (69%)	15 (25%)	4 (7%)	2	16
All	All	3269/3711 (88%)	2425 (74%)	661 (20%)	183 (6%)	3	23

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	33	LEU
3	D	35	LYS
3	D	244	ARG
4	E	16	ARG
4	E	86	PRO

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	D	213/218 (98%)	196 (92%)	17 (8%)	17	57
4	E	165/166 (99%)	153 (93%)	12 (7%)	20	62
5	F	161/166 (97%)	154 (96%)	7 (4%)	40	81
6	G	155/156 (99%)	142 (92%)	13 (8%)	16	53
7	H	132/148 (89%)	123 (93%)	9 (7%)	22	65
8	I	122/124 (98%)	113 (93%)	9 (7%)	20	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	27/135 (20%)	26 (96%)	1 (4%)	45	85
10	N	116/139 (84%)	106 (91%)	10 (9%)	15	52
11	O	100/100 (100%)	95 (95%)	5 (5%)	34	78
12	P	112/116 (97%)	92 (82%)	20 (18%)	2	12
13	Q	106/111 (96%)	95 (90%)	11 (10%)	10	39
14	R	100/101 (99%)	95 (95%)	5 (5%)	34	78
15	S	77/88 (88%)	70 (91%)	7 (9%)	14	47
16	T	121/128 (94%)	106 (88%)	15 (12%)	7	30
17	U	93/94 (99%)	90 (97%)	3 (3%)	51	87
18	V	82/82 (100%)	73 (89%)	9 (11%)	9	36
19	W	91/92 (99%)	89 (98%)	2 (2%)	64	91
20	X	74/78 (95%)	68 (92%)	6 (8%)	17	56
21	Y	84/91 (92%)	79 (94%)	5 (6%)	27	72
22	Z	163/179 (91%)	160 (98%)	3 (2%)	71	93
23	0	61/67 (91%)	59 (97%)	2 (3%)	50	87
24	1	73/83 (88%)	63 (86%)	10 (14%)	5	25
25	2	67/67 (100%)	64 (96%)	3 (4%)	38	81
26	3	51/52 (98%)	47 (92%)	4 (8%)	18	59
27	4	27/84 (32%)	25 (93%)	2 (7%)	20	62
28	5	45/52 (86%)	43 (96%)	2 (4%)	39	81
29	6	43/52 (83%)	40 (93%)	3 (7%)	21	64
30	7	41/42 (98%)	38 (93%)	3 (7%)	20	62
31	8	53/55 (96%)	51 (96%)	2 (4%)	44	84
All	All	2755/3066 (90%)	2555 (93%)	200 (7%)	20	62

5 of 200 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	P	61	ARG
13	Q	80	GLU
26	3	1	MET
12	P	70	GLN
12	P	148	LEU

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	A	2878/2894 (99%)	448 (15%)	101 (3%)
2	B	118/124 (95%)	12 (10%)	1 (0%)
All	All	2996/3018 (99%)	460 (15%)	102 (3%)

5 of 460 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	34	C
1	A	35	G
1	A	46	C
1	A	63	U

5 of 102 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1211	U
1	A	1458	C
1	A	2610	C
1	A	1253	A
1	A	1378	A

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 877 ligands modelled in this entry, 877 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2879/2894 (99%)	0.00	110 (3%) 38 7	65, 112, 248, 354	0
2	B	119/124 (95%)	0.72	20 (16%) 2 1	138, 171, 208, 265	0
3	D	271/276 (98%)	0.79	49 (18%) 2 1	98, 122, 149, 167	0
4	E	204/206 (99%)	0.03	6 (2%) 49 10	95, 126, 164, 180	0
5	F	202/210 (96%)	-0.17	0 100 100	97, 142, 175, 194	0
6	G	181/182 (99%)	0.01	7 (3%) 37 7	147, 198, 223, 252	0
7	H	159/180 (88%)	0.08	5 (3%) 47 10	141, 172, 206, 222	0
8	I	145/148 (97%)	0.41	9 (6%) 20 4	134, 211, 264, 286	0
9	J	32/173 (18%)	0.79	4 (12%) 5 1	203, 228, 245, 262	0
10	N	137/163 (84%)	0.42	11 (8%) 12 3	110, 142, 167, 219	0
11	O	122/122 (100%)	0.30	6 (4%) 28 6	104, 113, 133, 184	0
12	P	146/150 (97%)	0.55	20 (13%) 4 1	105, 145, 182, 203	0
13	Q	136/141 (96%)	0.99	31 (22%) 1 1	109, 142, 172, 226	0
14	R	117/118 (99%)	0.83	19 (16%) 2 1	102, 116, 153, 180	0
15	S	98/112 (87%)	1.02	21 (21%) 1 1	164, 192, 215, 232	0
16	T	137/146 (93%)	0.05	4 (2%) 49 10	107, 120, 163, 190	0
17	U	117/118 (99%)	0.23	7 (5%) 21 5	109, 144, 175, 196	0
18	V	101/101 (100%)	-0.00	4 (3%) 36 7	110, 160, 187, 202	0
19	W	112/113 (99%)	0.09	3 (2%) 52 11	95, 118, 156, 181	0
20	X	92/96 (95%)	0.30	4 (4%) 34 7	111, 129, 161, 179	0
21	Y	100/110 (90%)	1.18	26 (26%) 1 1	131, 150, 181, 216	0
22	Z	188/206 (91%)	0.34	18 (9%) 8 2	138, 180, 207, 229	0
23	0	76/85 (89%)	0.76	15 (19%) 2 1	116, 147, 174, 187	0
24	1	88/98 (89%)	0.78	14 (15%) 3 1	107, 128, 162, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
25	2	72/72 (100%)	-0.36	0	100 100	128, 148, 181, 208	0
26	3	59/60 (98%)	-0.19	0	100 100	127, 147, 180, 210	0
27	4	30/97 (30%)	0.01	0	100 100	204, 221, 244, 244	0
28	5	52/60 (86%)	0.36	2 (3%)	38 7	98, 120, 159, 188	0
29	6	44/54 (81%)	0.18	3 (6%)	17 4	132, 166, 195, 199	0
30	7	48/49 (97%)	0.14	2 (4%)	35 7	98, 105, 132, 171	0
31	8	63/65 (96%)	0.70	6 (9%)	8 2	115, 125, 158, 176	0
All	All	6327/6729 (94%)	0.21	426 (6%)	22 4	65, 131, 221, 354	0

The worst 5 of 426 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	615	G	11.1
22	Z	80	ARG	9.1
22	Z	81	ARG	8.7
22	Z	79	ARG	7.7
15	S	32	LEU	7.5

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	3299	1/1	0.12	-	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	U	798	1/1	0.38	-	35,35,35,35	0
32	MG	A	3278	1/1	0.18	-	38,38,38,38	0
32	MG	I	693	1/1	0.19	-	29,29,29,29	0
32	MG	A	3584	1/1	0.32	-	50,50,50,50	0
32	MG	A	3061	1/1	0.16	-	51,51,51,51	0
32	MG	A	3294	1/1	0.18	-	39,39,39,39	0
32	MG	A	3475	1/1	0.23	-	41,41,41,41	0
32	MG	A	3569	1/1	0.14	-	62,62,62,62	0
32	MG	A	2935	1/1	0.20	-	11,11,11,11	0
32	MG	A	3630	1/1	0.11	-	22,22,22,22	0
32	MG	A	3149	1/1	0.10	-	31,31,31,31	0
32	MG	A	3424	1/1	0.21	-	43,43,43,43	0
32	MG	A	3247	1/1	0.11	-	36,36,36,36	0
32	MG	A	3313	1/1	0.10	-	45,45,45,45	0
32	MG	D	674	1/1	0.18	-	2,2,2,2	0
32	MG	A	3391	1/1	0.42	-	60,60,60,60	0
32	MG	A	3589	1/1	0.18	-	67,67,67,67	0
32	MG	A	3161	1/1	0.15	-	10,10,10,10	0
32	MG	A	2968	1/1	0.13	-	18,18,18,18	0
32	MG	B	366	1/1	0.20	-	16,16,16,16	0
32	MG	A	368	1/1	0.10	-	4,4,4,4	0
32	MG	A	3383	1/1	0.06	-	17,17,17,17	0
32	MG	A	3526	1/1	0.16	-	38,38,38,38	0
32	MG	A	2980	1/1	0.07	-	8,8,8,8	0
32	MG	A	3131	1/1	0.08	-	6,6,6,6	0
32	MG	A	3230	1/1	0.06	-	4,4,4,4	0
32	MG	A	3342	1/1	0.27	-	51,51,51,51	0
32	MG	B	236	1/1	0.08	-	18,18,18,18	0
32	MG	A	3027	1/1	0.09	-	23,23,23,23	0
32	MG	A	3665	1/1	0.55	-	49,49,49,49	0
32	MG	A	3641	1/1	0.19	-	53,53,53,53	0
32	MG	A	2982	1/1	0.43	-	29,29,29,29	0
32	MG	A	3524	1/1	0.12	-	47,47,47,47	0
32	MG	P	469	1/1	0.23	-	34,34,34,34	0
32	MG	T	658	1/1	0.09	-	23,23,23,23	0
32	MG	A	3270	1/1	0.09	-	28,28,28,28	0
32	MG	A	3206	1/1	0.79	-	43,43,43,43	0
32	MG	A	3567	1/1	0.06	-	26,26,26,26	0
32	MG	A	3487	1/1	0.24	-	34,34,34,34	0
32	MG	A	3286	1/1	0.15	-	17,17,17,17	0
32	MG	A	3180	1/1	0.24	-	40,40,40,40	0
32	MG	A	3321	1/1	0.09	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2921	1/1	0.05	-	2,2,2,2	0
32	MG	A	3464	1/1	0.18	-	33,33,33,33	0
32	MG	A	3353	1/1	0.45	-	39,39,39,39	0
32	MG	A	3694	1/1	0.24	-	29,29,29,29	0
32	MG	A	3438	1/1	0.09	-	13,13,13,13	0
32	MG	A	3387	1/1	0.05	-	2,2,2,2	0
32	MG	A	3509	1/1	0.19	-	57,57,57,57	0
32	MG	A	3624	1/1	0.68	-	32,32,32,32	0
32	MG	A	3085	1/1	0.10	-	20,20,20,20	0
32	MG	A	2979	1/1	0.05	-	26,26,26,26	0
32	MG	O	659	1/1	0.06	-	19,19,19,19	0
32	MG	A	2948	1/1	0.15	-	40,40,40,40	0
32	MG	A	2923	1/1	0.13	-	2,2,2,2	0
32	MG	A	3446	1/1	0.12	-	54,54,54,54	0
32	MG	A	3102	1/1	0.07	-	27,27,27,27	0
32	MG	A	3298	1/1	0.09	-	42,42,42,42	0
32	MG	A	3491	1/1	0.40	-	26,26,26,26	0
32	MG	A	3189	1/1	0.12	-	43,43,43,43	0
32	MG	A	3445	1/1	0.26	-	59,59,59,59	0
32	MG	A	3273	1/1	0.12	-	2,2,2,2	0
32	MG	A	3671	1/1	0.92	-	54,54,54,54	0
32	MG	A	3418	1/1	0.12	-	32,32,32,32	0
32	MG	A	2991	1/1	0.11	-	10,10,10,10	0
32	MG	A	3007	1/1	0.11	-	36,36,36,36	0
32	MG	A	3127	1/1	0.10	-	25,25,25,25	0
32	MG	A	3306	1/1	0.20	-	24,24,24,24	0
32	MG	A	3642	1/1	0.17	-	30,30,30,30	0
32	MG	A	3673	1/1	0.23	-	29,29,29,29	0
32	MG	A	3655	1/1	0.12	-	36,36,36,36	0
32	MG	A	3684	1/1	0.28	-	12,12,12,12	0
32	MG	A	3291	1/1	0.10	-	17,17,17,17	0
32	MG	A	3588	1/1	0.30	-	35,35,35,35	0
32	MG	A	2963	1/1	0.19	-	37,37,37,37	0
32	MG	A	3473	1/1	0.09	-	20,20,20,20	0
32	MG	A	3339	1/1	0.13	-	45,45,45,45	0
32	MG	A	2998	1/1	0.14	-	27,27,27,27	0
32	MG	A	3236	1/1	0.13	-	26,26,26,26	0
32	MG	A	3676	1/1	0.11	-	56,56,56,56	0
32	MG	A	3077	1/1	0.44	-	64,64,64,64	0
32	MG	A	3623	1/1	0.17	-	43,43,43,43	0
32	MG	A	3679	1/1	0.13	-	35,35,35,35	0
32	MG	A	3261	1/1	0.17	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3636	1/1	0.28	-	65,65,65,65	0
32	MG	A	3518	1/1	0.28	-	41,41,41,41	0
32	MG	A	3450	1/1	0.22	-	29,29,29,29	0
32	MG	A	3364	1/1	0.13	-	35,35,35,35	0
32	MG	A	3397	1/1	0.16	-	29,29,29,29	0
32	MG	A	2959	1/1	0.07	-	3,3,3,3	0
32	MG	A	3489	1/1	0.31	-	33,33,33,33	0
32	MG	A	2957	1/1	0.11	-	27,27,27,27	0
32	MG	B	824	1/1	0.41	-	37,37,37,37	0
32	MG	A	3614	1/1	0.46	-	52,52,52,52	0
32	MG	A	3030	1/1	0.20	-	38,38,38,38	0
32	MG	A	3549	1/1	0.18	-	67,67,67,67	0
32	MG	A	2985	1/1	0.18	-	48,48,48,48	0
32	MG	A	3577	1/1	0.08	-	44,44,44,44	0
32	MG	A	3627	1/1	0.18	-	22,22,22,22	0
32	MG	A	3310	1/1	0.19	-	34,34,34,34	0
32	MG	A	3257	1/1	0.21	-	40,40,40,40	0
32	MG	A	3612	1/1	0.14	-	18,18,18,18	0
32	MG	A	3559	1/1	0.19	-	57,57,57,57	0
32	MG	A	3478	1/1	0.16	-	27,27,27,27	0
32	MG	A	3378	1/1	0.09	-	26,26,26,26	0
32	MG	A	3088	1/1	0.09	-	32,32,32,32	0
32	MG	A	3452	1/1	0.07	-	47,47,47,47	0
32	MG	A	3619	1/1	0.21	-	43,43,43,43	0
32	MG	A	3449	1/1	0.05	-	30,30,30,30	0
32	MG	A	3280	1/1	0.21	-	46,46,46,46	0
32	MG	A	2911	1/1	0.12	-	5,5,5,5	0
32	MG	A	3531	1/1	0.25	-	23,23,23,23	0
32	MG	A	3503	1/1	0.24	-	3,3,3,3	0
32	MG	A	3362	1/1	0.14	-	17,17,17,17	0
32	MG	A	3272	1/1	0.55	-	56,56,56,56	0
32	MG	A	3465	1/1	0.22	-	17,17,17,17	0
32	MG	A	3012	1/1	0.34	-	35,35,35,35	0
32	MG	A	3234	1/1	0.42	-	34,34,34,34	0
32	MG	A	3325	1/1	0.57	-	45,45,45,45	0
32	MG	A	2929	1/1	0.09	-	0,0,0,0	0
32	MG	A	3116	1/1	0.14	-	21,21,21,21	0
32	MG	A	3187	1/1	0.17	-	10,10,10,10	0
32	MG	A	3439	1/1	0.18	-	47,47,47,47	0
32	MG	A	3190	1/1	0.09	-	1,1,1,1	0
32	MG	A	3585	1/1	0.37	-	37,37,37,37	0
32	MG	A	3092	1/1	0.41	-	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3268	1/1	0.07	-	35,35,35,35	0
32	MG	A	2946	1/1	0.35	-	30,30,30,30	0
32	MG	A	3096	1/1	0.13	-	46,46,46,46	0
32	MG	A	3677	1/1	0.16	-	11,11,11,11	0
32	MG	G	740	1/1	0.16	-	54,54,54,54	0
32	MG	A	3441	1/1	0.12	-	24,24,24,24	0
32	MG	A	3550	1/1	0.48	-	40,40,40,40	0
32	MG	A	3099	1/1	0.16	-	21,21,21,21	0
32	MG	A	3368	1/1	0.20	-	10,10,10,10	0
32	MG	A	2944	1/1	0.09	-	25,25,25,25	0
32	MG	A	3182	1/1	0.12	-	27,27,27,27	0
32	MG	A	2964	1/1	0.11	-	26,26,26,26	0
32	MG	A	3650	1/1	0.28	-	40,40,40,40	0
32	MG	A	3154	1/1	0.13	-	27,27,27,27	0
32	MG	A	3609	1/1	0.10	-	30,30,30,30	0
32	MG	A	3333	1/1	0.37	-	26,26,26,26	0
32	MG	A	3433	1/1	0.10	-	25,25,25,25	0
32	MG	A	3522	1/1	0.10	-	18,18,18,18	0
32	MG	A	3561	1/1	0.05	-	46,46,46,46	0
32	MG	A	2989	1/1	0.12	-	23,23,23,23	0
32	MG	A	3578	1/1	0.65	-	38,38,38,38	0
32	MG	A	3179	1/1	0.07	-	12,12,12,12	0
32	MG	A	3629	1/1	0.09	-	37,37,37,37	0
32	MG	A	3158	1/1	0.07	-	0,0,0,0	0
32	MG	A	2952	1/1	0.06	-	4,4,4,4	0
32	MG	A	3431	1/1	0.34	-	19,19,19,19	0
32	MG	A	3024	1/1	0.27	-	50,50,50,50	0
32	MG	A	3403	1/1	0.08	-	24,24,24,24	0
32	MG	A	3686	1/1	0.10	-	27,27,27,27	0
32	MG	A	2972	1/1	0.11	-	11,11,11,11	0
32	MG	A	3065	1/1	0.07	-	63,63,63,63	0
32	MG	A	2999	1/1	0.11	-	16,16,16,16	0
32	MG	A	3358	1/1	0.17	-	35,35,35,35	0
32	MG	A	3252	1/1	0.08	-	17,17,17,17	0
32	MG	A	3635	1/1	0.21	-	39,39,39,39	0
32	MG	A	3035	1/1	0.14	-	48,48,48,48	0
32	MG	A	3408	1/1	0.09	-	9,9,9,9	0
32	MG	A	3138	1/1	0.15	-	14,14,14,14	0
32	MG	A	3428	1/1	0.34	-	23,23,23,23	0
32	MG	A	3605	1/1	0.11	-	28,28,28,28	0
32	MG	A	3649	1/1	0.15	-	41,41,41,41	0
32	MG	A	3126	1/1	0.21	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	713	1/1	0.14	-	63,63,63,63	0
32	MG	A	3670	1/1	0.61	-	56,56,56,56	0
32	MG	5	737	1/1	0.30	-	18,18,18,18	0
32	MG	2	771	1/1	0.30	-	38,38,38,38	0
32	MG	A	3309	1/1	0.09	-	25,25,25,25	0
32	MG	A	3494	1/1	0.23	-	54,54,54,54	0
32	MG	A	3005	1/1	0.19	-	35,35,35,35	0
32	MG	A	3573	1/1	0.26	-	37,37,37,37	0
32	MG	A	3412	1/1	0.23	-	0,0,0,0	0
32	MG	O	640	1/1	0.21	-	17,17,17,17	0
32	MG	A	3212	1/1	0.11	-	25,25,25,25	0
32	MG	A	3093	1/1	0.18	-	31,31,31,31	0
32	MG	A	3492	1/1	0.14	-	36,36,36,36	0
32	MG	A	3066	1/1	0.14	-	12,12,12,12	0
32	MG	A	3376	1/1	0.11	-	41,41,41,41	0
32	MG	A	3414	1/1	0.12	-	8,8,8,8	0
32	MG	A	3361	1/1	0.17	-	51,51,51,51	0
32	MG	A	3568	1/1	0.09	-	44,44,44,44	0
32	MG	A	2915	1/1	0.09	-	36,36,36,36	0
32	MG	A	3644	1/1	0.19	-	70,70,70,70	0
32	MG	B	792	1/1	0.38	-	52,52,52,52	0
32	MG	A	3167	1/1	0.15	-	15,15,15,15	0
32	MG	A	2997	1/1	0.07	-	23,23,23,23	0
32	MG	A	2912	1/1	0.12	-	0,0,0,0	0
32	MG	A	3231	1/1	0.07	-	38,38,38,38	0
32	MG	A	3134	1/1	0.14	-	22,22,22,22	0
32	MG	A	3033	1/1	0.17	-	30,30,30,30	0
32	MG	A	3382	1/1	0.08	-	47,47,47,47	0
32	MG	A	3643	1/1	0.23	-	28,28,28,28	0
32	MG	A	3275	1/1	0.24	-	29,29,29,29	0
32	MG	A	3002	1/1	0.10	-	1,1,1,1	0
32	MG	A	2934	1/1	0.07	-	11,11,11,11	0
32	MG	A	3211	1/1	0.17	-	12,12,12,12	0
32	MG	A	3026	1/1	0.11	-	33,33,33,33	0
32	MG	A	3245	1/1	0.17	-	32,32,32,32	0
32	MG	A	3265	1/1	0.15	-	24,24,24,24	0
32	MG	A	3626	1/1	0.08	-	39,39,39,39	0
32	MG	D	775	1/1	0.31	-	2,2,2,2	0
32	MG	A	3613	1/1	0.08	-	32,32,32,32	0
32	MG	A	3185	1/1	0.09	-	12,12,12,12	0
32	MG	A	3625	1/1	0.10	-	29,29,29,29	0
32	MG	A	2962	1/1	0.09	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3087	1/1	0.11	-	21,21,21,21	0
32	MG	A	3404	1/1	0.34	-	29,29,29,29	0
32	MG	A	3338	1/1	0.11	-	16,16,16,16	0
32	MG	A	3317	1/1	0.48	-	56,56,56,56	0
32	MG	A	3171	1/1	0.15	-	0,0,0,0	0
32	MG	A	3003	1/1	0.17	-	42,42,42,42	0
32	MG	A	3432	1/1	0.25	-	38,38,38,38	0
32	MG	A	3598	1/1	0.47	-	31,31,31,31	0
32	MG	A	3419	1/1	0.25	-	35,35,35,35	0
32	MG	A	3514	1/1	0.14	-	29,29,29,29	0
32	MG	A	3053	1/1	0.29	-	52,52,52,52	0
32	MG	A	3204	1/1	0.35	-	25,25,25,25	0
32	MG	A	3663	1/1	0.17	-	44,44,44,44	0
32	MG	A	3004	1/1	0.11	-	22,22,22,22	0
32	MG	A	3346	1/1	0.18	-	46,46,46,46	0
32	MG	A	3631	1/1	0.14	-	28,28,28,28	0
32	MG	A	3656	1/1	0.49	-	44,44,44,44	0
32	MG	A	3136	1/1	0.10	-	19,19,19,19	0
32	MG	A	160	1/1	0.09	-	18,18,18,18	0
32	MG	A	3084	1/1	0.28	-	41,41,41,41	0
32	MG	A	3535	1/1	0.26	-	20,20,20,20	0
32	MG	R	866	1/1	0.89	-	49,49,49,49	0
32	MG	A	3579	1/1	0.23	-	44,44,44,44	0
32	MG	A	3423	1/1	0.10	-	24,24,24,24	0
32	MG	A	3666	1/1	0.11	-	6,6,6,6	0
32	MG	A	3029	1/1	0.07	-	38,38,38,38	0
32	MG	A	3632	1/1	0.41	-	46,46,46,46	0
32	MG	A	3297	1/1	0.09	-	20,20,20,20	0
32	MG	A	3013	1/1	0.33	-	10,10,10,10	0
32	MG	A	3661	1/1	0.12	-	45,45,45,45	0
32	MG	A	2986	1/1	0.08	-	9,9,9,9	0
32	MG	A	3399	1/1	0.07	-	33,33,33,33	0
32	MG	A	2992	1/1	0.12	-	17,17,17,17	0
32	MG	A	3079	1/1	0.33	-	28,28,28,28	0
32	MG	A	3307	1/1	0.22	-	52,52,52,52	0
32	MG	A	3110	1/1	0.33	-	28,28,28,28	0
32	MG	A	3217	1/1	0.24	-	33,33,33,33	0
32	MG	A	3192	1/1	0.29	-	50,50,50,50	0
32	MG	A	3195	1/1	0.05	-	20,20,20,20	0
32	MG	A	3415	1/1	0.20	-	4,4,4,4	0
32	MG	A	3592	1/1	0.06	-	29,29,29,29	0
32	MG	A	3290	1/1	0.18	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3406	1/1	0.20	-	25,25,25,25	0
32	MG	A	3223	1/1	0.10	-	2,2,2,2	0
32	MG	B	122	1/1	0.11	-	35,35,35,35	0
32	MG	A	3337	1/1	0.13	-	39,39,39,39	0
32	MG	A	3392	1/1	0.28	-	38,38,38,38	0
32	MG	A	156	1/1	0.23	-	15,15,15,15	0
32	MG	A	3370	1/1	0.09	-	23,23,23,23	0
32	MG	B	585	1/1	0.14	-	29,29,29,29	0
32	MG	A	2971	1/1	0.10	-	14,14,14,14	0
32	MG	A	3678	1/1	0.31	-	49,49,49,49	0
32	MG	A	3693	1/1	0.42	-	55,55,55,55	0
32	MG	A	3246	1/1	0.78	-	39,39,39,39	0
32	MG	A	3311	1/1	0.09	-	29,29,29,29	0
32	MG	A	2996	1/1	0.28	-	34,34,34,34	0
32	MG	A	3571	1/1	0.08	-	18,18,18,18	0
32	MG	A	3183	1/1	0.32	-	8,8,8,8	0
32	MG	A	3458	1/1	0.30	-	21,21,21,21	0
32	MG	A	3572	1/1	0.10	-	46,46,46,46	0
32	MG	A	3282	1/1	0.17	-	33,33,33,33	0
32	MG	A	3277	1/1	0.47	-	18,18,18,18	0
32	MG	A	3360	1/1	0.16	-	28,28,28,28	0
32	MG	A	3543	1/1	0.17	-	47,47,47,47	0
32	MG	A	2945	1/1	0.12	-	12,12,12,12	0
32	MG	A	3264	1/1	0.15	-	38,38,38,38	0
32	MG	F	536	1/1	0.25	-	13,13,13,13	0
32	MG	A	2975	1/1	0.12	-	26,26,26,26	0
32	MG	A	3202	1/1	0.17	-	26,26,26,26	0
32	MG	A	3416	1/1	0.13	-	37,37,37,37	0
32	MG	A	3680	1/1	0.11	-	75,75,75,75	0
32	MG	A	3344	1/1	0.21	-	43,43,43,43	0
32	MG	A	3205	1/1	0.24	-	23,23,23,23	0
32	MG	A	3683	1/1	0.12	-	31,31,31,31	0
32	MG	A	3551	1/1	0.24	-	32,32,32,32	0
32	MG	A	3305	1/1	0.12	-	62,62,62,62	0
32	MG	A	3652	1/1	0.09	-	35,35,35,35	0
32	MG	A	3622	1/1	0.08	-	41,41,41,41	0
32	MG	A	3289	1/1	0.08	-	45,45,45,45	0
32	MG	A	3259	1/1	0.13	-	24,24,24,24	0
32	MG	A	3227	1/1	0.16	-	9,9,9,9	0
32	MG	A	3548	1/1	0.10	-	38,38,38,38	0
32	MG	A	2927	1/1	0.12	-	37,37,37,37	0
32	MG	A	3040	1/1	0.07	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3356	1/1	0.55	-	37,37,37,37	0
32	MG	A	2988	1/1	0.59	-	37,37,37,37	0
32	MG	A	3071	1/1	0.31	-	39,39,39,39	0
32	MG	A	3221	1/1	0.14	-	46,46,46,46	0
32	MG	A	3507	1/1	0.16	-	32,32,32,32	0
32	MG	A	3664	1/1	0.15	-	44,44,44,44	0
32	MG	A	3480	1/1	0.24	-	58,58,58,58	0
32	MG	A	3675	1/1	0.34	-	47,47,47,47	0
32	MG	A	3633	1/1	0.25	-	34,34,34,34	0
32	MG	A	3060	1/1	0.23	-	25,25,25,25	0
32	MG	A	3302	1/1	0.10	-	37,37,37,37	0
32	MG	A	3064	1/1	0.08	-	30,30,30,30	0
32	MG	A	3552	1/1	0.14	-	41,41,41,41	0
32	MG	A	3121	1/1	0.08	-	24,24,24,24	0
32	MG	A	3371	1/1	0.24	-	45,45,45,45	0
32	MG	A	3351	1/1	0.19	-	10,10,10,10	0
32	MG	A	2931	1/1	0.08	-	10,10,10,10	0
32	MG	A	2966	1/1	0.09	-	0,0,0,0	0
32	MG	A	3594	1/1	0.18	-	47,47,47,47	0
32	MG	A	2910	1/1	0.12	-	34,34,34,34	0
32	MG	A	3123	1/1	0.06	-	0,0,0,0	0
32	MG	B	124	1/1	0.09	-	22,22,22,22	0
32	MG	A	3151	1/1	0.07	-	13,13,13,13	0
32	MG	A	3112	1/1	0.07	-	0,0,0,0	0
32	MG	A	3409	1/1	0.13	-	38,38,38,38	0
32	MG	A	3326	1/1	0.50	-	43,43,43,43	0
32	MG	A	3078	1/1	0.27	-	5,5,5,5	0
32	MG	A	3495	1/1	0.15	-	23,23,23,23	0
32	MG	A	2970	1/1	0.17	-	27,27,27,27	0
32	MG	A	3314	1/1	0.12	-	24,24,24,24	0
32	MG	A	3168	1/1	0.10	-	17,17,17,17	0
32	MG	A	3200	1/1	0.16	-	5,5,5,5	0
32	MG	A	3164	1/1	0.20	-	37,37,37,37	0
32	MG	A	2920	1/1	0.10	-	18,18,18,18	0
32	MG	A	3525	1/1	0.06	-	14,14,14,14	0
32	MG	A	3094	1/1	0.14	-	20,20,20,20	0
32	MG	A	3352	1/1	0.09	-	23,23,23,23	0
32	MG	A	3139	1/1	0.35	-	34,34,34,34	0
32	MG	A	3394	1/1	0.10	-	12,12,12,12	0
32	MG	B	850	1/1	0.23	-	52,52,52,52	0
32	MG	G	664	1/1	0.29	-	47,47,47,47	0
32	MG	A	3587	1/1	0.14	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3389	1/1	0.12	-	18,18,18,18	0
32	MG	A	3479	1/1	0.11	-	50,50,50,50	0
32	MG	A	3274	1/1	0.18	-	33,33,33,33	0
32	MG	A	3435	1/1	0.11	-	26,26,26,26	0
32	MG	A	3654	1/1	0.36	-	36,36,36,36	0
32	MG	A	3267	1/1	0.11	-	14,14,14,14	0
32	MG	A	3447	1/1	0.06	-	15,15,15,15	0
32	MG	A	3660	1/1	0.36	-	30,30,30,30	0
32	MG	B	869	1/1	0.10	-	50,50,50,50	0
32	MG	A	3556	1/1	0.13	-	50,50,50,50	0
32	MG	A	3468	1/1	0.28	-	19,19,19,19	0
32	MG	A	3303	1/1	0.18	-	20,20,20,20	0
32	MG	A	3554	1/1	0.40	-	51,51,51,51	0
32	MG	A	3152	1/1	0.08	-	18,18,18,18	0
32	MG	A	3687	1/1	0.17	-	18,18,18,18	0
32	MG	A	3097	1/1	0.18	-	27,27,27,27	0
32	MG	A	3544	1/1	0.25	-	52,52,52,52	0
32	MG	A	3620	1/1	0.33	-	40,40,40,40	0
32	MG	A	3210	1/1	0.62	-	64,64,64,64	0
32	MG	A	3653	1/1	0.10	-	55,55,55,55	0
32	MG	A	3090	1/1	0.11	-	44,44,44,44	0
32	MG	A	2977	1/1	0.07	-	24,24,24,24	0
32	MG	B	172	1/1	0.18	-	36,36,36,36	0
32	MG	A	3388	1/1	0.14	-	19,19,19,19	0
32	MG	A	3045	1/1	0.12	-	40,40,40,40	0
32	MG	A	3237	1/1	0.12	-	36,36,36,36	0
32	MG	A	3107	1/1	0.13	-	24,24,24,24	0
32	MG	A	3014	1/1	0.28	-	26,26,26,26	0
32	MG	A	168	1/1	0.20	-	28,28,28,28	0
32	MG	A	3486	1/1	0.14	-	33,33,33,33	0
32	MG	A	3359	1/1	0.07	-	1,1,1,1	0
32	MG	A	3575	1/1	0.06	-	19,19,19,19	0
32	MG	A	3312	1/1	0.12	-	7,7,7,7	0
32	MG	A	3105	1/1	0.10	-	27,27,27,27	0
32	MG	A	3137	1/1	0.21	-	22,22,22,22	0
32	MG	A	3372	1/1	0.09	-	11,11,11,11	0
32	MG	A	3506	1/1	0.19	-	10,10,10,10	0
32	MG	A	3646	1/1	0.40	-	52,52,52,52	0
32	MG	A	3437	1/1	0.24	-	40,40,40,40	0
32	MG	A	3530	1/1	0.57	-	68,68,68,68	0
32	MG	A	3460	1/1	0.21	-	72,72,72,72	0
32	MG	A	3304	1/1	0.18	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3474	1/1	0.54	-	34,34,34,34	0
32	MG	A	3395	1/1	0.06	-	1,1,1,1	0
32	MG	A	3668	1/1	0.12	-	33,33,33,33	0
32	MG	A	3262	1/1	0.47	-	24,24,24,24	0
32	MG	A	3052	1/1	0.09	-	35,35,35,35	0
32	MG	A	3271	1/1	0.30	-	25,25,25,25	0
32	MG	B	796	1/1	0.14	-	60,60,60,60	0
32	MG	A	3039	1/1	0.12	-	47,47,47,47	0
32	MG	A	3240	1/1	0.12	-	37,37,37,37	0
32	MG	A	3658	1/1	1.08	-	46,46,46,46	0
32	MG	A	3249	1/1	0.14	-	19,19,19,19	0
32	MG	A	3243	1/1	0.15	-	9,9,9,9	0
32	MG	W	745	1/1	0.12	-	23,23,23,23	0
32	MG	A	3454	1/1	0.07	-	45,45,45,45	0
32	MG	A	2969	1/1	0.10	-	37,37,37,37	0
32	MG	B	699	1/1	0.35	-	51,51,51,51	0
32	MG	A	3292	1/1	0.22	-	35,35,35,35	0
32	MG	A	3607	1/1	0.14	-	33,33,33,33	0
32	MG	A	3219	1/1	0.12	-	33,33,33,33	0
32	MG	A	2947	1/1	0.20	-	18,18,18,18	0
32	MG	A	3407	1/1	0.17	-	40,40,40,40	0
32	MG	A	3162	1/1	0.07	-	21,21,21,21	0
32	MG	A	3010	1/1	0.12	-	24,24,24,24	0
32	MG	A	3651	1/1	0.24	-	15,15,15,15	0
32	MG	A	3621	1/1	0.40	-	45,45,45,45	0
32	MG	A	3332	1/1	0.25	-	28,28,28,28	0
32	MG	A	3016	1/1	0.17	-	47,47,47,47	0
32	MG	A	3173	1/1	0.07	-	37,37,37,37	0
32	MG	A	3207	1/1	0.21	-	7,7,7,7	0
32	MG	A	3163	1/1	0.21	-	6,6,6,6	0
32	MG	A	3132	1/1	0.08	-	28,28,28,28	0
32	MG	A	2936	1/1	0.13	-	24,24,24,24	0
32	MG	A	3367	1/1	0.19	-	31,31,31,31	0
32	MG	A	3417	1/1	0.09	-	9,9,9,9	0
32	MG	A	3555	1/1	0.16	-	63,63,63,63	0
32	MG	A	3122	1/1	0.10	-	36,36,36,36	0
32	MG	A	3541	1/1	0.18	-	38,38,38,38	0
32	MG	A	3119	1/1	0.23	-	52,52,52,52	0
32	MG	A	3130	1/1	0.18	-	21,21,21,21	0
32	MG	B	828	1/1	0.12	-	39,39,39,39	0
32	MG	A	3512	1/1	0.47	-	82,82,82,82	0
32	MG	A	2978	1/1	0.13	-	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3017	1/1	0.12	-	33,33,33,33	0
32	MG	A	3091	1/1	0.06	-	46,46,46,46	0
32	MG	A	3381	1/1	0.13	-	31,31,31,31	0
32	MG	A	3106	1/1	0.36	-	17,17,17,17	0
32	MG	A	3596	1/1	0.32	-	31,31,31,31	0
32	MG	A	3057	1/1	0.21	-	23,23,23,23	0
32	MG	A	159	1/1	0.07	-	44,44,44,44	0
32	MG	A	2938	1/1	0.11	-	38,38,38,38	0
32	MG	A	3565	1/1	0.82	-	63,63,63,63	0
32	MG	A	3043	1/1	0.13	-	39,39,39,39	0
32	MG	A	3258	1/1	0.07	-	10,10,10,10	0
32	MG	A	3086	1/1	0.11	-	2,2,2,2	0
32	MG	A	3083	1/1	0.14	-	36,36,36,36	0
32	MG	A	3497	1/1	0.32	-	10,10,10,10	0
32	MG	A	3038	1/1	0.07	-	32,32,32,32	0
32	MG	A	3640	1/1	0.10	-	24,24,24,24	0
32	MG	Q	647	1/1	0.34	-	45,45,45,45	0
32	MG	A	3484	1/1	0.21	-	8,8,8,8	0
32	MG	A	3330	1/1	0.13	-	7,7,7,7	0
32	MG	A	3648	1/1	0.26	-	24,24,24,24	0
32	MG	A	3175	1/1	0.17	-	26,26,26,26	0
32	MG	A	3411	1/1	0.09	-	0,0,0,0	0
32	MG	A	3276	1/1	0.19	-	1,1,1,1	0
32	MG	A	3226	1/1	0.12	-	10,10,10,10	0
32	MG	A	3256	1/1	0.17	-	60,60,60,60	0
32	MG	A	3546	1/1	0.59	-	56,56,56,56	0
32	MG	A	3117	1/1	0.09	-	13,13,13,13	0
32	MG	A	3380	1/1	0.11	-	22,22,22,22	0
32	MG	A	3301	1/1	0.10	-	22,22,22,22	0
32	MG	A	3098	1/1	0.12	-	41,41,41,41	0
32	MG	A	3000	1/1	0.12	-	16,16,16,16	0
32	MG	A	2965	1/1	0.12	-	24,24,24,24	0
32	MG	A	3674	1/1	0.14	-	36,36,36,36	0
32	MG	A	3533	1/1	0.21	-	25,25,25,25	0
32	MG	A	3166	1/1	0.28	-	0,0,0,0	0
32	MG	A	3058	1/1	0.26	-	25,25,25,25	0
32	MG	N	489	1/1	0.22	-	20,20,20,20	0
32	MG	A	3197	1/1	0.13	-	21,21,21,21	0
32	MG	B	851	1/1	0.08	-	25,25,25,25	0
32	MG	A	3193	1/1	0.10	-	5,5,5,5	0
32	MG	A	3451	1/1	0.36	-	55,55,55,55	0
32	MG	A	3354	1/1	0.30	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2994	1/1	0.20	-	39,39,39,39	0
32	MG	A	3213	1/1	0.12	-	39,39,39,39	0
32	MG	A	100	1/1	0.09	-	0,0,0,0	0
32	MG	A	3467	1/1	0.24	-	41,41,41,41	0
32	MG	A	2937	1/1	0.11	-	17,17,17,17	0
32	MG	A	3553	1/1	0.18	-	46,46,46,46	0
32	MG	A	3293	1/1	0.16	-	44,44,44,44	0
32	MG	A	3611	1/1	0.54	-	16,16,16,16	0
32	MG	A	3521	1/1	0.21	-	20,20,20,20	0
32	MG	A	3483	1/1	0.06	-	61,61,61,61	0
32	MG	A	3471	1/1	0.09	-	24,24,24,24	0
32	MG	A	3070	1/1	0.15	-	0,0,0,0	0
32	MG	A	3398	1/1	0.08	-	5,5,5,5	0
32	MG	A	2954	1/1	0.07	-	0,0,0,0	0
32	MG	B	261	1/1	0.07	-	26,26,26,26	0
32	MG	A	3520	1/1	0.12	-	50,50,50,50	0
32	MG	A	3430	1/1	0.19	-	13,13,13,13	0
32	MG	A	3379	1/1	0.13	-	46,46,46,46	0
32	MG	A	3639	1/1	0.14	-	30,30,30,30	0
32	MG	A	3574	1/1	0.21	-	30,30,30,30	0
32	MG	A	3072	1/1	0.21	-	26,26,26,26	0
32	MG	A	3269	1/1	0.17	-	4,4,4,4	0
32	MG	A	3022	1/1	0.08	-	1,1,1,1	0
32	MG	A	3146	1/1	0.17	-	43,43,43,43	0
32	MG	A	3685	1/1	0.10	-	35,35,35,35	0
32	MG	B	173	1/1	0.14	-	65,65,65,65	0
32	MG	A	3692	1/1	0.13	-	54,54,54,54	0
32	MG	A	2955	1/1	0.08	-	50,50,50,50	0
32	MG	A	3019	1/1	0.25	-	33,33,33,33	0
32	MG	A	3218	1/1	0.54	-	40,40,40,40	0
32	MG	A	158	1/1	0.08	-	8,8,8,8	0
32	MG	A	3315	1/1	0.09	-	22,22,22,22	0
32	MG	A	3536	1/1	0.13	-	4,4,4,4	0
32	MG	A	3599	1/1	0.23	-	13,13,13,13	0
32	MG	A	3448	1/1	0.12	-	27,27,27,27	0
32	MG	A	3374	1/1	0.07	-	23,23,23,23	0
32	MG	A	3036	1/1	0.17	-	61,61,61,61	0
32	MG	A	3001	1/1	0.07	-	28,28,28,28	0
32	MG	E	636	1/1	0.35	-	42,42,42,42	0
32	MG	A	3377	1/1	0.25	-	16,16,16,16	0
32	MG	A	3196	1/1	0.07	-	15,15,15,15	0
32	MG	A	2925	1/1	0.08	-	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3145	1/1	0.17	-	39,39,39,39	0
32	MG	A	3047	1/1	0.10	-	36,36,36,36	0
32	MG	A	3242	1/1	0.30	-	19,19,19,19	0
32	MG	A	2914	1/1	0.15	-	33,33,33,33	0
32	MG	A	3255	1/1	0.13	-	24,24,24,24	0
32	MG	A	3421	1/1	0.11	-	56,56,56,56	0
32	MG	A	3606	1/1	0.31	-	40,40,40,40	0
32	MG	A	3529	1/1	0.14	-	47,47,47,47	0
32	MG	A	3208	1/1	0.20	-	25,25,25,25	0
32	MG	A	3601	1/1	0.28	-	37,37,37,37	0
32	MG	A	3008	1/1	0.09	-	26,26,26,26	0
32	MG	F	211	1/1	0.16	-	39,39,39,39	0
32	MG	A	3075	1/1	0.12	-	22,22,22,22	0
32	MG	A	3528	1/1	0.19	-	34,34,34,34	0
32	MG	A	3427	1/1	0.17	-	77,77,77,77	0
32	MG	A	3028	1/1	0.10	-	37,37,37,37	0
32	MG	A	3562	1/1	0.11	-	52,52,52,52	0
32	MG	A	2919	1/1	0.12	-	0,0,0,0	0
32	MG	A	3108	1/1	0.21	-	33,33,33,33	0
32	MG	A	3172	1/1	0.17	-	54,54,54,54	0
32	MG	A	2976	1/1	0.08	-	23,23,23,23	0
32	MG	A	2974	1/1	0.11	-	34,34,34,34	0
32	MG	A	3288	1/1	0.13	-	57,57,57,57	0
32	MG	A	3153	1/1	0.10	-	30,30,30,30	0
32	MG	A	3209	1/1	0.06	-	10,10,10,10	0
32	MG	B	749	1/1	0.27	-	51,51,51,51	0
32	MG	A	3513	1/1	0.09	-	25,25,25,25	0
32	MG	B	588	1/1	0.11	-	47,47,47,47	0
32	MG	A	3461	1/1	0.21	-	30,30,30,30	0
32	MG	A	3669	1/1	0.53	-	47,47,47,47	0
32	MG	A	3617	1/1	0.26	-	36,36,36,36	0
32	MG	A	3523	1/1	0.13	-	32,32,32,32	0
32	MG	A	3284	1/1	0.27	-	27,27,27,27	0
32	MG	A	3050	1/1	0.30	-	17,17,17,17	0
32	MG	A	2993	1/1	0.10	-	56,56,56,56	0
32	MG	A	3647	1/1	0.29	-	45,45,45,45	0
32	MG	A	3426	1/1	0.17	-	17,17,17,17	0
32	MG	A	3466	1/1	0.33	-	19,19,19,19	0
32	MG	A	3455	1/1	0.08	-	11,11,11,11	0
32	MG	A	2981	1/1	0.09	-	22,22,22,22	0
32	MG	A	3089	1/1	0.24	-	46,46,46,46	0
32	MG	A	3125	1/1	0.07	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2987	1/1	0.11	-	1,1,1,1	0
32	MG	A	3390	1/1	0.12	-	16,16,16,16	0
32	MG	A	3560	1/1	0.16	-	45,45,45,45	0
32	MG	A	2953	1/1	0.08	-	16,16,16,16	0
32	MG	A	2990	1/1	0.10	-	30,30,30,30	0
32	MG	A	3063	1/1	0.08	-	18,18,18,18	0
32	MG	A	3011	1/1	0.13	-	25,25,25,25	0
32	MG	A	3515	1/1	0.14	-	49,49,49,49	0
32	MG	A	3025	1/1	0.17	-	34,34,34,34	0
32	MG	A	3144	1/1	0.17	-	41,41,41,41	0
32	MG	A	3018	1/1	0.16	-	68,68,68,68	0
32	MG	A	3080	1/1	0.06	-	65,65,65,65	0
32	MG	A	3500	1/1	0.13	-	31,31,31,31	0
32	MG	A	3662	1/1	0.13	-	57,57,57,57	0
32	MG	A	3413	1/1	0.32	-	36,36,36,36	0
32	MG	A	3593	1/1	0.14	-	42,42,42,42	0
32	MG	A	3657	1/1	0.13	-	20,20,20,20	0
32	MG	A	2941	1/1	0.10	-	37,37,37,37	0
32	MG	A	3224	1/1	0.08	-	49,49,49,49	0
32	MG	A	3357	1/1	0.08	-	22,22,22,22	0
32	MG	A	3101	1/1	0.36	-	31,31,31,31	0
32	MG	A	3041	1/1	0.10	-	33,33,33,33	0
32	MG	A	3681	1/1	0.14	-	54,54,54,54	0
32	MG	A	3538	1/1	0.14	-	33,33,33,33	0
32	MG	A	3323	1/1	0.18	-	53,53,53,53	0
32	MG	A	3582	1/1	0.16	-	51,51,51,51	0
32	MG	A	3481	1/1	0.76	-	55,55,55,55	0
32	MG	A	157	1/1	0.12	-	48,48,48,48	0
32	MG	A	3318	1/1	0.22	-	10,10,10,10	0
32	MG	A	3373	1/1	0.36	-	29,29,29,29	0
32	MG	A	3558	1/1	0.10	-	29,29,29,29	0
32	MG	A	3456	1/1	0.18	-	13,13,13,13	0
32	MG	A	3046	1/1	0.15	-	34,34,34,34	0
32	MG	A	2924	1/1	0.11	-	11,11,11,11	0
32	MG	A	3006	1/1	0.20	-	15,15,15,15	0
32	MG	A	3266	1/1	0.14	-	25,25,25,25	0
32	MG	A	3401	1/1	0.07	-	26,26,26,26	0
32	MG	A	3341	1/1	0.25	-	43,43,43,43	0
32	MG	A	2958	1/1	0.07	-	1,1,1,1	0
32	MG	A	3476	1/1	0.15	-	22,22,22,22	0
32	MG	V	795	1/1	0.12	-	21,21,21,21	0
32	MG	A	3156	1/1	0.21	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	379	1/1	0.09	-	35,35,35,35	0
32	MG	A	3281	1/1	0.22	-	33,33,33,33	0
32	MG	A	3343	1/1	0.06	-	18,18,18,18	0
32	MG	A	538	1/1	0.10	-	21,21,21,21	0
32	MG	A	3331	1/1	0.10	-	15,15,15,15	0
32	MG	A	3023	1/1	0.20	-	40,40,40,40	0
32	MG	A	3537	1/1	0.17	-	29,29,29,29	0
32	MG	A	3563	1/1	0.33	-	40,40,40,40	0
32	MG	A	369	1/1	0.20	-	44,44,44,44	0
32	MG	A	3120	1/1	0.11	-	21,21,21,21	0
32	MG	A	437	1/1	0.10	-	17,17,17,17	0
32	MG	A	3103	1/1	0.20	-	31,31,31,31	0
32	MG	A	3496	1/1	0.15	-	25,25,25,25	0
32	MG	A	3254	1/1	0.08	-	60,60,60,60	0
32	MG	A	3186	1/1	0.18	-	19,19,19,19	0
32	MG	A	2933	1/1	0.17	-	26,26,26,26	0
32	MG	A	3628	1/1	0.72	-	44,44,44,44	0
32	MG	A	3021	1/1	0.22	-	39,39,39,39	0
32	MG	A	3324	1/1	0.15	-	40,40,40,40	0
32	MG	A	3600	1/1	0.20	-	28,28,28,28	0
32	MG	A	3176	1/1	0.10	-	7,7,7,7	0
32	MG	A	3534	1/1	0.09	-	12,12,12,12	0
32	MG	A	3068	1/1	0.07	-	12,12,12,12	0
32	MG	A	3444	1/1	0.21	-	7,7,7,7	0
32	MG	A	3608	1/1	0.20	-	51,51,51,51	0
32	MG	A	3322	1/1	0.17	-	11,11,11,11	0
32	MG	A	3516	1/1	0.17	-	24,24,24,24	0
32	MG	A	3133	1/1	0.10	-	14,14,14,14	0
32	MG	A	3215	1/1	0.07	-	2,2,2,2	0
32	MG	A	3295	1/1	0.10	-	41,41,41,41	0
32	MG	A	3244	1/1	0.27	-	42,42,42,42	0
32	MG	A	3044	1/1	0.06	-	40,40,40,40	0
32	MG	A	3595	1/1	0.46	-	38,38,38,38	0
32	MG	A	3470	1/1	0.12	-	53,53,53,53	0
32	MG	A	3055	1/1	0.29	-	60,60,60,60	0
32	MG	A	3143	1/1	0.14	-	42,42,42,42	0
32	MG	A	2943	1/1	0.26	-	35,35,35,35	0
32	MG	A	3334	1/1	0.59	-	29,29,29,29	0
32	MG	A	3355	1/1	0.06	-	30,30,30,30	0
32	MG	A	3032	1/1	0.09	-	36,36,36,36	0
32	MG	A	3157	1/1	0.08	-	31,31,31,31	0
32	MG	A	3349	1/1	0.13	-	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	876	1/1	0.25	-	59,59,59,59	0
32	MG	A	3336	1/1	0.38	-	45,45,45,45	0
32	MG	A	3603	1/1	0.82	-	61,61,61,61	0
32	MG	R	781	1/1	0.49	-	61,61,61,61	0
32	MG	A	3691	1/1	0.13	-	45,45,45,45	0
32	MG	A	2961	1/1	0.06	-	11,11,11,11	0
32	MG	A	3198	1/1	0.08	-	22,22,22,22	0
32	MG	A	3287	1/1	0.06	-	34,34,34,34	0
32	MG	A	3031	1/1	0.11	-	34,34,34,34	0
32	MG	A	3340	1/1	0.12	-	31,31,31,31	0
32	MG	A	3615	1/1	0.06	-	36,36,36,36	0
32	MG	A	2922	1/1	0.10	-	5,5,5,5	0
32	MG	A	2930	1/1	0.06	-	20,20,20,20	0
32	MG	A	2956	1/1	0.09	-	6,6,6,6	0
32	MG	A	3363	1/1	0.25	-	44,44,44,44	0
32	MG	A	2967	1/1	0.09	-	21,21,21,21	0
32	MG	A	555	1/1	0.07	-	10,10,10,10	0
32	MG	A	3688	1/1	0.13	-	38,38,38,38	0
32	MG	A	3434	1/1	0.13	-	17,17,17,17	0
32	MG	A	3393	1/1	0.15	-	29,29,29,29	0
32	MG	2	634	1/1	0.11	-	31,31,31,31	0
32	MG	A	3191	1/1	0.26	-	20,20,20,20	0
32	MG	B	350	1/1	0.17	-	62,62,62,62	0
32	MG	A	3634	1/1	0.49	-	21,21,21,21	0
32	MG	A	3228	1/1	0.13	-	19,19,19,19	0
32	MG	A	3420	1/1	0.20	-	16,16,16,16	0
32	MG	A	3511	1/1	0.09	-	43,43,43,43	0
32	MG	A	3067	1/1	0.25	-	28,28,28,28	0
32	MG	A	3429	1/1	0.10	-	1,1,1,1	0
32	MG	A	3472	1/1	0.49	-	46,46,46,46	0
32	MG	A	3165	1/1	0.12	-	8,8,8,8	0
32	MG	A	3300	1/1	0.18	-	12,12,12,12	0
32	MG	A	3501	1/1	0.09	-	45,45,45,45	0
32	MG	A	3320	1/1	0.12	-	5,5,5,5	0
32	MG	H	643	1/1	0.10	-	15,15,15,15	0
32	MG	A	3081	1/1	0.12	-	3,3,3,3	0
32	MG	A	3095	1/1	0.32	-	22,22,22,22	0
32	MG	A	3241	1/1	0.14	-	18,18,18,18	0
32	MG	A	3170	1/1	0.06	-	12,12,12,12	0
32	MG	A	3222	1/1	0.10	-	43,43,43,43	0
32	MG	A	2942	1/1	0.16	-	33,33,33,33	0
32	MG	A	2984	1/1	0.05	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3159	1/1	0.07	-	11,11,11,11	0
32	MG	A	3576	1/1	0.12	-	38,38,38,38	0
32	MG	A	170	1/1	0.08	-	4,4,4,4	0
32	MG	A	3493	1/1	0.08	-	41,41,41,41	0
32	MG	A	3174	1/1	0.15	-	39,39,39,39	0
32	MG	A	2928	1/1	0.11	-	13,13,13,13	0
32	MG	A	3009	1/1	0.34	-	21,21,21,21	0
32	MG	A	3059	1/1	0.10	-	41,41,41,41	0
32	MG	F	834	1/1	0.36	-	27,27,27,27	0
32	MG	A	3570	1/1	0.32	-	25,25,25,25	0
32	MG	A	3111	1/1	0.25	-	33,33,33,33	0
32	MG	A	3405	1/1	0.09	-	9,9,9,9	0
32	MG	A	3348	1/1	0.09	-	24,24,24,24	0
32	MG	A	3104	1/1	0.31	-	31,31,31,31	0
32	MG	A	3457	1/1	0.12	-	0,0,0,0	0
32	MG	A	3201	1/1	0.21	-	36,36,36,36	0
32	MG	A	3350	1/1	0.41	-	40,40,40,40	0
32	MG	A	3580	1/1	0.14	-	24,24,24,24	0
32	MG	7	736	1/1	0.23	-	47,47,47,47	0
32	MG	A	3459	1/1	0.09	-	40,40,40,40	0
32	MG	A	2995	1/1	0.09	-	40,40,40,40	0
32	MG	A	3308	1/1	0.31	-	15,15,15,15	0
32	MG	A	3366	1/1	0.41	-	39,39,39,39	0
32	MG	A	3328	1/1	0.16	-	26,26,26,26	0
32	MG	A	2908	1/1	0.08	-	2,2,2,2	0
32	MG	A	3069	1/1	0.12	-	3,3,3,3	0
32	MG	A	3020	1/1	0.10	-	20,20,20,20	0
32	MG	A	2951	1/1	0.11	-	17,17,17,17	0
32	MG	A	3618	1/1	0.11	-	28,28,28,28	0
32	MG	A	2916	1/1	0.08	-	0,0,0,0	0
32	MG	A	3141	1/1	0.27	-	41,41,41,41	0
32	MG	A	3517	1/1	0.11	-	53,53,53,53	0
32	MG	A	3118	1/1	0.10	-	9,9,9,9	0
32	MG	A	3181	1/1	0.15	-	1,1,1,1	0
32	MG	A	3232	1/1	0.19	-	28,28,28,28	0
32	MG	A	3637	1/1	0.17	-	63,63,63,63	0
32	MG	A	3229	1/1	0.13	-	23,23,23,23	0
32	MG	W	829	1/1	0.43	-	33,33,33,33	0
32	MG	A	3581	1/1	0.28	-	41,41,41,41	0
32	MG	J	779	1/1	0.14	-	59,59,59,59	0
32	MG	A	3049	1/1	0.10	-	53,53,53,53	0
32	MG	A	3436	1/1	0.30	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	367	1/1	0.10	-	29,29,29,29	0
32	MG	A	3689	1/1	0.12	-	34,34,34,34	0
32	MG	A	3540	1/1	0.23	-	33,33,33,33	0
32	MG	A	2913	1/1	0.08	-	2,2,2,2	0
32	MG	B	166	1/1	0.28	-	46,46,46,46	0
32	MG	A	3051	1/1	0.32	-	38,38,38,38	0
32	MG	R	697	1/1	0.10	-	24,24,24,24	0
32	MG	A	3082	1/1	0.35	-	48,48,48,48	0
32	MG	A	3148	1/1	0.18	-	44,44,44,44	0
32	MG	A	3076	1/1	0.20	-	15,15,15,15	0
32	MG	A	3519	1/1	0.22	-	34,34,34,34	0
32	MG	A	3115	1/1	0.32	-	55,55,55,55	0
32	MG	A	3482	1/1	0.34	-	46,46,46,46	0
32	MG	A	3442	1/1	0.29	-	19,19,19,19	0
32	MG	A	3477	1/1	0.14	-	62,62,62,62	0
32	MG	A	3498	1/1	0.26	-	34,34,34,34	0
32	MG	A	3527	1/1	0.17	-	54,54,54,54	0
32	MG	A	3113	1/1	0.10	-	20,20,20,20	0
32	MG	7	464	1/1	0.12	-	13,13,13,13	0
32	MG	A	3645	1/1	0.08	-	64,64,64,64	0
32	MG	A	3279	1/1	0.30	-	49,49,49,49	0
32	MG	B	123	1/1	0.17	-	34,34,34,34	0
32	MG	A	3532	1/1	0.28	-	32,32,32,32	0
32	MG	A	3319	1/1	0.17	-	17,17,17,17	0
32	MG	A	3253	1/1	0.12	-	33,33,33,33	0
32	MG	A	3443	1/1	0.28	-	54,54,54,54	0
32	MG	A	3216	1/1	0.28	-	51,51,51,51	0
32	MG	A	3690	1/1	0.09	-	32,32,32,32	0
32	MG	F	639	1/1	0.26	-	37,37,37,37	0
32	MG	A	2932	1/1	0.13	-	1,1,1,1	0
32	MG	A	169	1/1	0.20	-	34,34,34,34	0
32	MG	A	167	1/1	0.08	-	8,8,8,8	0
32	MG	A	3251	1/1	0.18	-	21,21,21,21	0
32	MG	A	3597	1/1	0.18	-	60,60,60,60	0
32	MG	A	3263	1/1	0.18	-	29,29,29,29	0
32	MG	A	3220	1/1	0.09	-	5,5,5,5	0
32	MG	2	633	1/1	0.07	-	32,32,32,32	0
32	MG	A	3194	1/1	0.12	-	44,44,44,44	0
32	MG	A	3410	1/1	0.11	-	7,7,7,7	0
32	MG	A	2960	1/1	0.09	-	39,39,39,39	0
32	MG	A	3508	1/1	0.11	-	49,49,49,49	0
32	MG	A	3591	1/1	0.18	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3248	1/1	0.11	-	40,40,40,40	0
32	MG	A	3048	1/1	0.09	-	22,22,22,22	0
32	MG	A	3296	1/1	0.24	-	43,43,43,43	0
32	MG	Q	654	1/1	0.42	-	43,43,43,43	0
32	MG	A	3214	1/1	0.26	-	35,35,35,35	0
32	MG	A	3545	1/1	0.15	-	27,27,27,27	0
32	MG	A	3203	1/1	0.16	-	9,9,9,9	0
32	MG	A	3073	1/1	0.08	-	8,8,8,8	0
32	MG	A	3488	1/1	0.11	-	13,13,13,13	0
32	MG	A	3169	1/1	0.21	-	6,6,6,6	0
32	MG	A	2909	1/1	0.06	-	9,9,9,9	0
32	MG	A	3462	1/1	0.16	-	35,35,35,35	0
32	MG	A	3696	1/1	0.13	-	54,54,54,54	0
32	MG	I	637	1/1	0.60	-	29,29,29,29	0
32	MG	A	2939	1/1	0.19	-	32,32,32,32	0
32	MG	A	3659	1/1	0.10	-	65,65,65,65	0
32	MG	A	3610	1/1	0.11	-	34,34,34,34	0
32	MG	A	3042	1/1	0.08	-	22,22,22,22	0
32	MG	A	3422	1/1	0.14	-	37,37,37,37	0
32	MG	A	3142	1/1	0.29	-	39,39,39,39	0
32	MG	A	3347	1/1	0.09	-	35,35,35,35	0
32	MG	A	3155	1/1	0.30	-	35,35,35,35	0
32	MG	A	3233	1/1	0.24	-	27,27,27,27	0
32	MG	A	3604	1/1	0.16	-	42,42,42,42	0
32	MG	A	3375	1/1	0.13	-	12,12,12,12	0
32	MG	A	2973	1/1	0.15	-	32,32,32,32	0
32	MG	T	776	1/1	0.17	-	42,42,42,42	0
32	MG	A	3015	1/1	0.10	-	10,10,10,10	0
32	MG	A	3667	1/1	0.18	-	40,40,40,40	0
32	MG	A	2918	1/1	0.09	-	16,16,16,16	0
32	MG	A	3129	1/1	0.18	-	25,25,25,25	0
32	MG	A	3638	1/1	0.22	-	45,45,45,45	0
32	MG	A	3260	1/1	0.10	-	22,22,22,22	0
32	MG	A	3054	1/1	0.11	-	7,7,7,7	0
32	MG	A	3199	1/1	0.17	-	42,42,42,42	0
32	MG	Q	570	1/1	0.23	-	38,38,38,38	0
32	MG	O	642	1/1	0.24	-	29,29,29,29	0
32	MG	N	854	1/1	0.26	-	49,49,49,49	0
32	MG	A	490	1/1	0.37	-	48,48,48,48	0
32	MG	A	3109	1/1	0.15	-	62,62,62,62	0
32	MG	A	3135	1/1	0.08	-	10,10,10,10	0
32	MG	A	3239	1/1	0.37	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3469	1/1	0.17	-	39,39,39,39	0
32	MG	A	2983	1/1	0.09	-	19,19,19,19	0
32	MG	A	3564	1/1	0.35	-	20,20,20,20	0
32	MG	A	3485	1/1	0.29	-	40,40,40,40	0
32	MG	A	42	1/1	0.15	-	20,20,20,20	0
32	MG	A	3672	1/1	0.08	-	19,19,19,19	0
32	MG	A	3184	1/1	0.60	-	46,46,46,46	0
32	MG	A	3345	1/1	0.10	-	26,26,26,26	0
32	MG	A	3074	1/1	0.29	-	51,51,51,51	0
32	MG	A	3547	1/1	0.15	-	37,37,37,37	0
32	MG	A	3062	1/1	0.08	-	26,26,26,26	0
32	MG	A	3396	1/1	0.10	-	10,10,10,10	0
32	MG	A	3557	1/1	0.70	-	33,33,33,33	0
32	MG	A	3386	1/1	0.21	-	39,39,39,39	0
32	MG	G	701	1/1	0.10	-	26,26,26,26	0
32	MG	A	3384	1/1	0.10	-	25,25,25,25	0
32	MG	A	3463	1/1	0.15	-	52,52,52,52	0
32	MG	A	3316	1/1	0.17	-	48,48,48,48	0
32	MG	A	3150	1/1	0.10	-	43,43,43,43	0
32	MG	A	3147	1/1	0.13	-	7,7,7,7	0
32	MG	A	3510	1/1	0.25	-	32,32,32,32	0
32	MG	A	3037	1/1	0.09	-	13,13,13,13	0
32	MG	Z	646	1/1	0.27	-	21,21,21,21	0
32	MG	A	2926	1/1	0.08	-	2,2,2,2	0
32	MG	A	3034	1/1	0.10	-	21,21,21,21	0
32	MG	A	2917	1/1	0.07	-	11,11,11,11	0
32	MG	A	3440	1/1	0.14	-	12,12,12,12	0
32	MG	A	3160	1/1	0.08	-	0,0,0,0	0
32	MG	A	3682	1/1	0.16	-	42,42,42,42	0
32	MG	A	3695	1/1	0.21	-	39,39,39,39	0
32	MG	A	3539	1/1	0.13	-	34,34,34,34	0
32	MG	A	3335	1/1	0.09	-	33,33,33,33	0
32	MG	A	3453	1/1	0.20	-	24,24,24,24	0
32	MG	A	3188	1/1	0.11	-	34,34,34,34	0
32	MG	A	3502	1/1	0.08	-	32,32,32,32	0
32	MG	A	3329	1/1	0.13	-	52,52,52,52	0
32	MG	A	3490	1/1	0.17	-	42,42,42,42	0
32	MG	B	377	1/1	0.37	-	50,50,50,50	0
32	MG	A	3616	1/1	0.33	-	66,66,66,66	0
32	MG	A	3400	1/1	0.39	-	39,39,39,39	0
32	MG	A	3504	1/1	0.13	-	2,2,2,2	0
32	MG	A	3235	1/1	0.44	-	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3285	1/1	0.11	-	32,32,32,32	0
32	MG	I	793	1/1	0.32	-	40,40,40,40	0
32	MG	Y	852	1/1	0.22	-	36,36,36,36	0
32	MG	A	2940	1/1	0.16	-	8,8,8,8	0
32	MG	A	2950	1/1	0.24	-	64,64,64,64	0
32	MG	F	651	1/1	0.17	-	40,40,40,40	0
32	MG	A	3177	1/1	0.16	-	6,6,6,6	0
32	MG	A	3369	1/1	0.12	-	45,45,45,45	0
32	MG	A	3425	1/1	0.20	-	34,34,34,34	0
32	MG	A	3385	1/1	0.10	-	10,10,10,10	0
32	MG	A	3128	1/1	0.11	-	35,35,35,35	0
32	MG	A	3250	1/1	0.13	-	35,35,35,35	0
32	MG	A	3590	1/1	0.10	-	24,24,24,24	0
32	MG	A	3542	1/1	0.19	-	40,40,40,40	0
32	MG	A	3499	1/1	0.17	-	11,11,11,11	0
32	MG	A	3178	1/1	0.10	-	4,4,4,4	0
32	MG	A	3365	1/1	0.08	-	15,15,15,15	0
32	MG	A	3505	1/1	0.08	-	32,32,32,32	0
32	MG	B	198	1/1	0.05	-	28,28,28,28	0
32	MG	A	3238	1/1	0.36	-	32,32,32,32	0
32	MG	A	3056	1/1	0.22	-	26,26,26,26	0
32	MG	A	3586	1/1	0.49	-	40,40,40,40	0
32	MG	A	2949	1/1	0.14	-	17,17,17,17	0
32	MG	A	3100	1/1	0.19	-	37,37,37,37	0
32	MG	H	692	1/1	0.13	-	34,34,34,34	0
32	MG	1	672	1/1	0.10	-	28,28,28,28	0
32	MG	A	3566	1/1	0.14	-	42,42,42,42	0
32	MG	A	3402	1/1	0.08	-	16,16,16,16	0
32	MG	A	3602	1/1	0.07	-	28,28,28,28	0
32	MG	A	3283	1/1	0.41	-	46,46,46,46	0
32	MG	A	3327	1/1	0.08	-	1,1,1,1	0
32	MG	A	3140	1/1	0.09	-	29,29,29,29	0
32	MG	A	3114	1/1	0.08	-	14,14,14,14	0
32	MG	A	3124	1/1	0.15	-	27,27,27,27	0
32	MG	A	3225	1/1	0.06	-	45,45,45,45	0
32	MG	A	3583	1/1	0.36	-	50,50,50,50	0

6.5 Other polymers

There are no such residues in this entry.