



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:29 AM GMT

PDB ID : 3F1H
Title : Crystal structure of a translation termination complex formed with release factor RF2. This file contains the 50S subunit of the second 70S ribosome. The entire crystal structure contains two 70S ribosomes as described in remark 400.
Authors : Korostelev, A.; Asahara, H.; Lancaster, L.; Laurberg, M.; Hirschi, A.; Noller, H.F.
Deposited on : 2008-10-27
Resolution : 3.00 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>

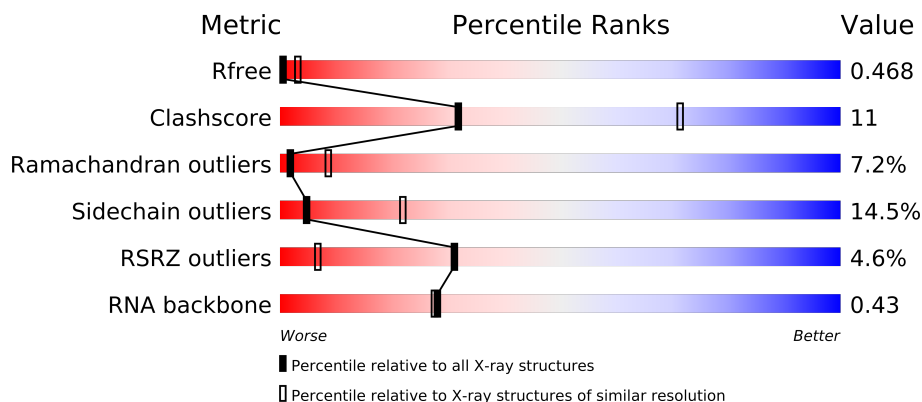
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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	K	147	
10	N	163	
11	O	122	
12	P	150	

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Mol	Chain	Length	Quality of chain
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	5	60	
28	6	54	
29	7	49	
30	8	65	
31	4	97	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 92164 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			

- 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	147	Total	C	N	O	S	0	0	0
			1088	692	191	199	6			

- 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 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	1	MET	-	INSERTION	UNP Q72IN1
N	2	VAL	-	INSERTION	UNP Q72IN1
N	3	LYS	-	INSERTION	UNP Q72IN1
N	4	SER	-	INSERTION	UNP Q72IN1

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Chain	Residue	Modelled	Actual	Comment	Reference
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	134	Total	C	N	O	S	0	0	0
			1064	680	201	178	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	187	Total	C	N	O	S	0	0	0
			1482	945	264	271	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	62	Total	C	N	O	S	0	0	0
			520	325	102	91	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	5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	MET	-	INSERTION	UNP Q72JR0
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

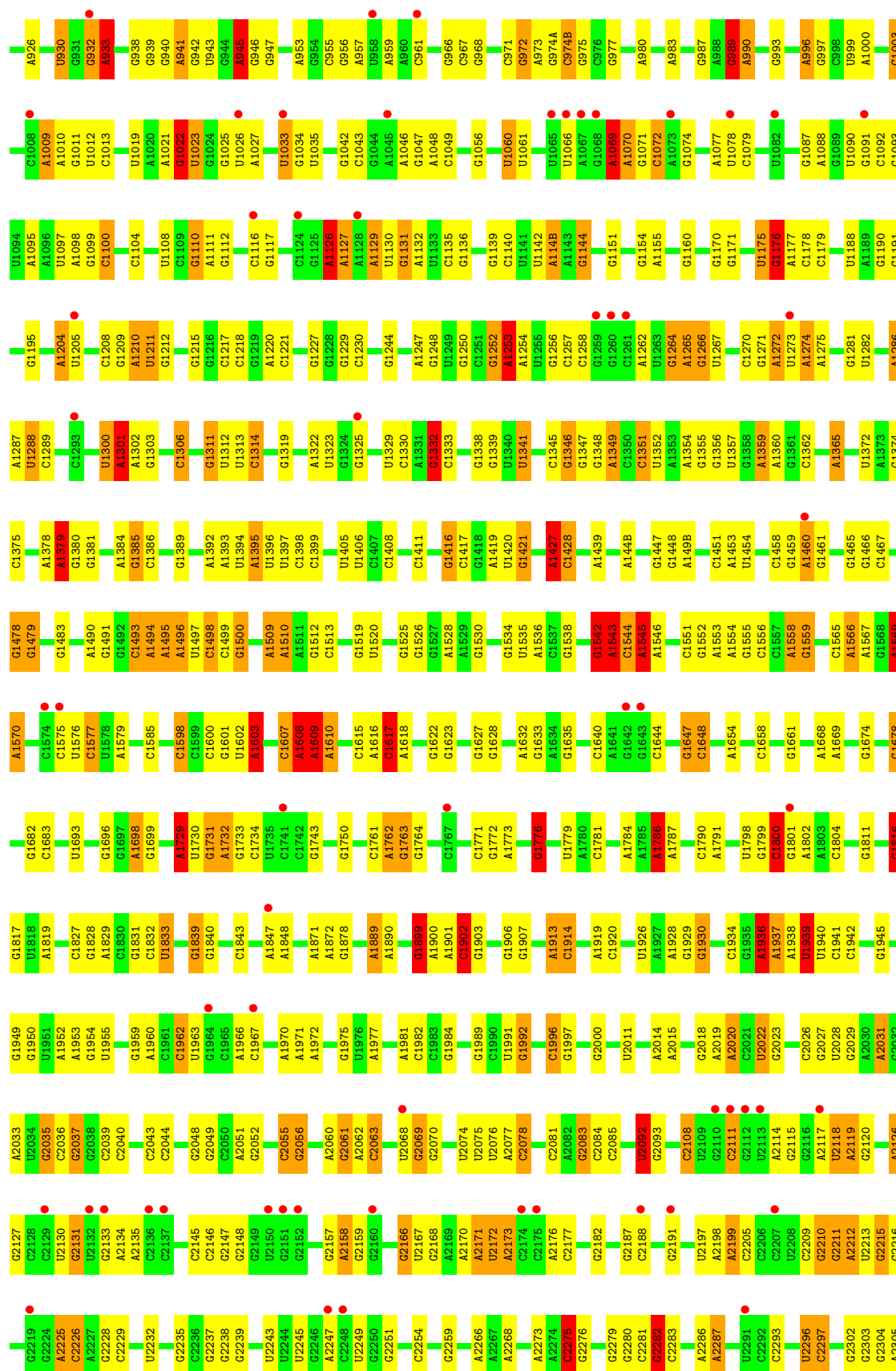
- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

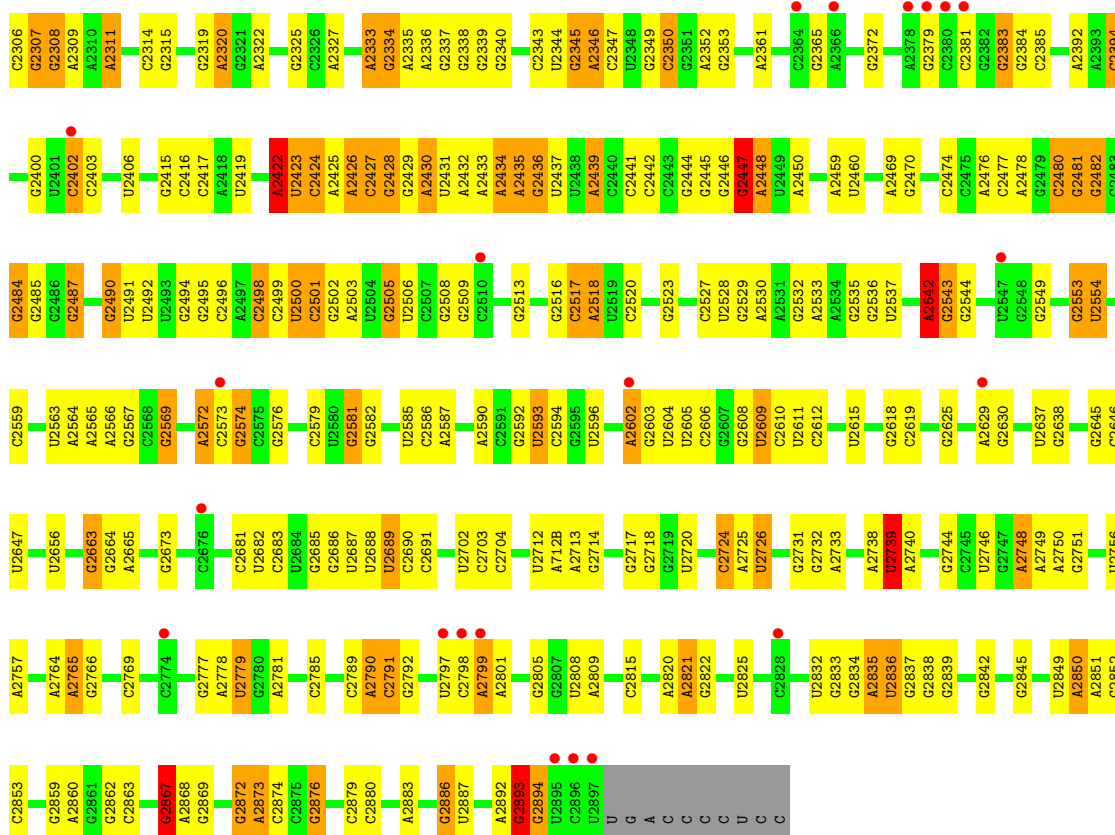
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	P	1	Total Mg 1 1	0	0
32	G	3	Total Mg 3 3	0	0
32	Q	2	Total Mg 2 2	0	0
32	D	12	Total Mg 12 12	0	0
32	K	1	Total Mg 1 1	0	0
32	E	1	Total Mg 1 1	0	0
32	B	10	Total Mg 10 10	0	0
32	I	1	Total Mg 1 1	0	0
32	6	1	Total Mg 1 1	0	0
32	1	2	Total Mg 2 2	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	486	Total Mg 486 486	0	0
32	T	1	Total Mg 1 1	0	0
32	V	1	Total Mg 1 1	0	0
32	N	1	Total Mg 1 1	0	0

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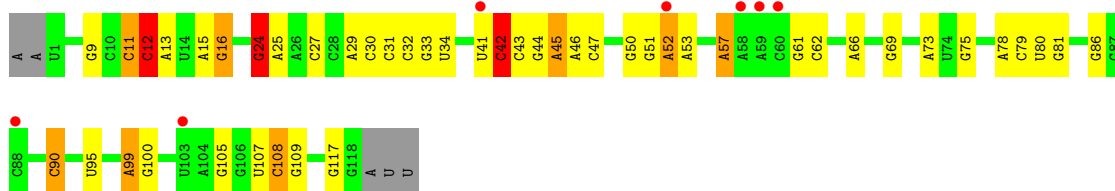
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	U	2	Total 2	Mg 2	0	0
32	8	1	Total 1	Mg 1	0	0
32	O	2	Total 2	Mg 2	0	0
32	R	1	Total 1	Mg 1	0	0
32	Y	1	Total 1	Mg 1	0	0
32	F	1	Total 1	Mg 1	0	0





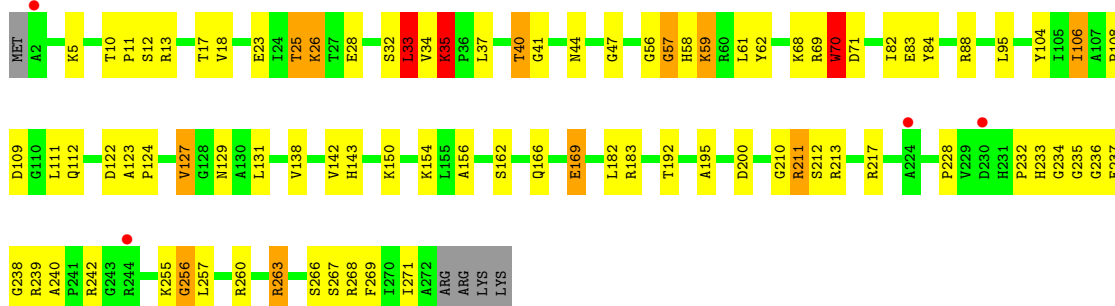
• Molecule 2: 5S rRNA

Chain B:



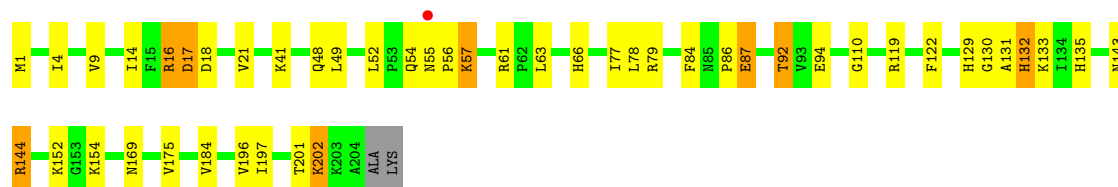
• Molecule 3: 50S ribosomal protein L2

Chain D:



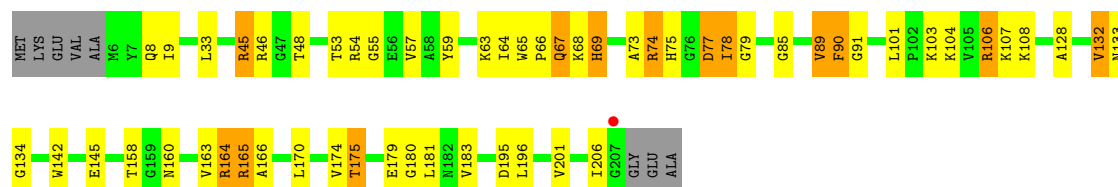
• Molecule 4: 50S ribosomal protein L3

Chain E:



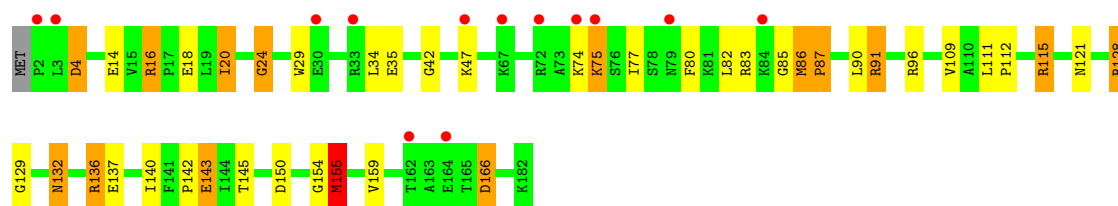
- Molecule 5: 50S ribosomal protein L4

Chain F:



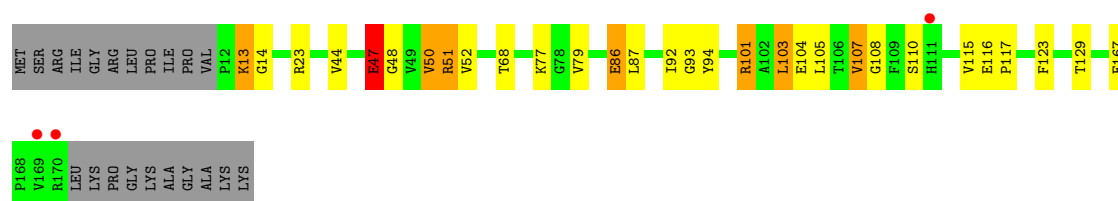
- Molecule 6: 50S ribosomal protein L5

Chain G:



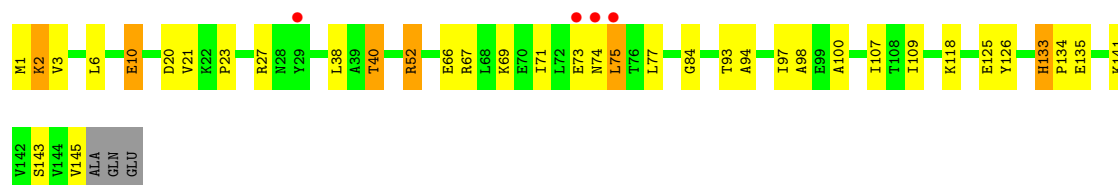
- Molecule 7: 50S ribosomal protein L6

Chain H:



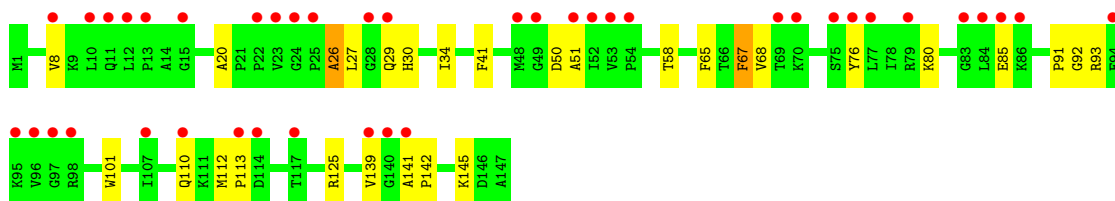
- Molecule 8: 50S ribosomal protein L9

Chain I:



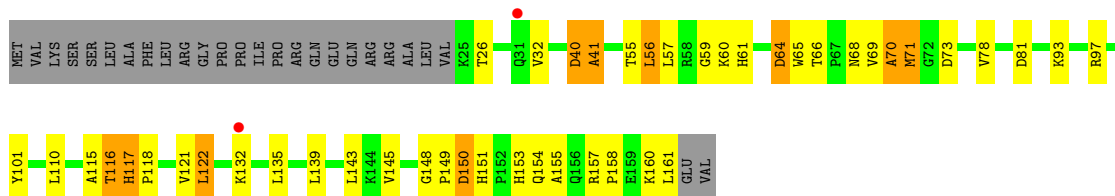
- Molecule 9: 50S ribosomal protein L11

Chain K:



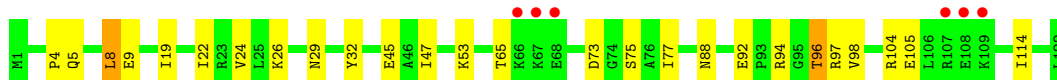
• Molecule 10: 50S ribosomal protein L13

Chain N:



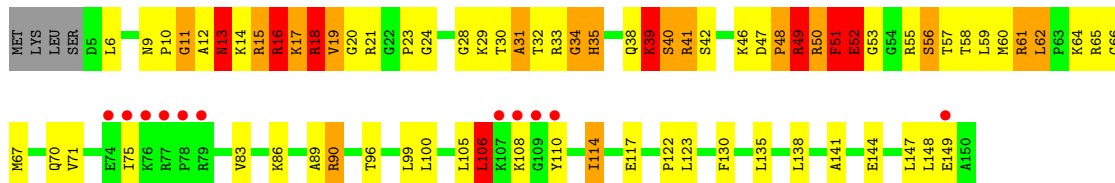
• Molecule 11: 50S ribosomal protein L14

Chain O:



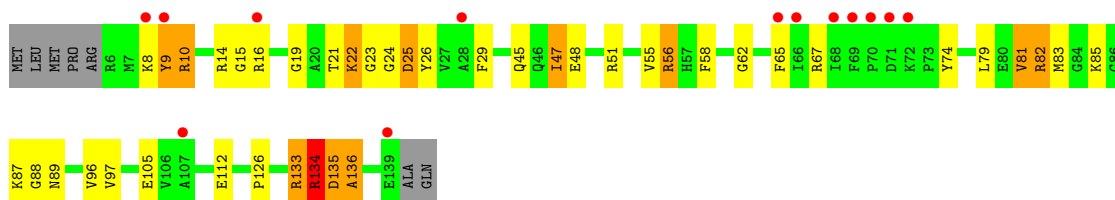
• Molecule 12: 50S ribosomal protein L15

Chain P:



• Molecule 13: 50S ribosomal protein L16

Chain Q:



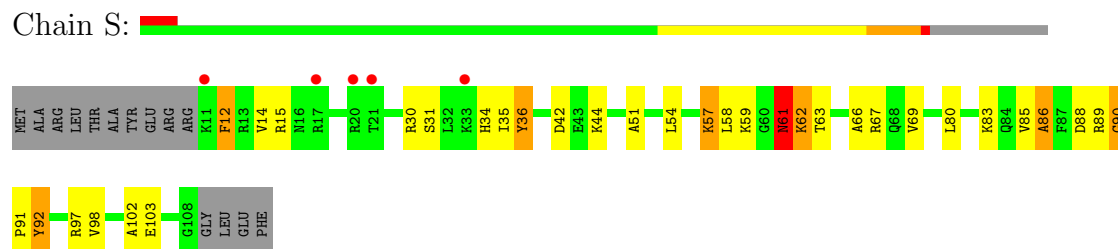
• Molecule 14: 50S ribosomal protein L17

Chain R:



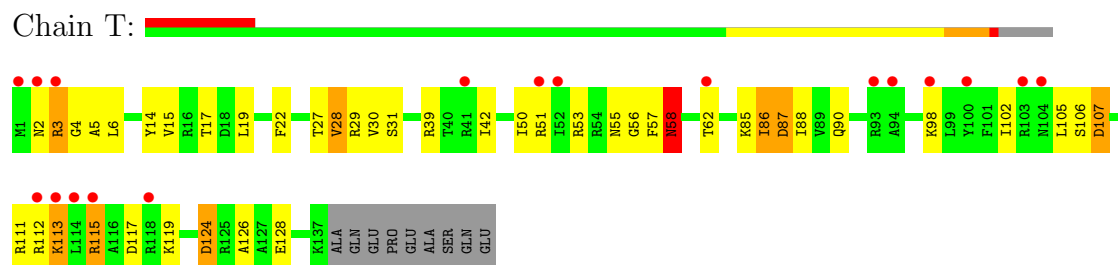
• Molecule 15: 50S ribosomal protein L18

Chain S:



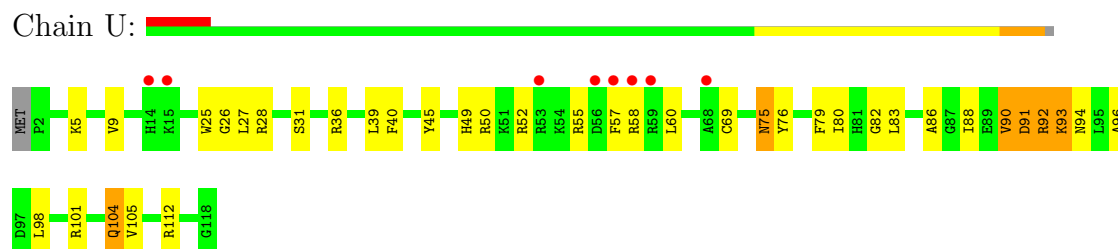
- Molecule 16: 50S ribosomal protein L19

Chain T:



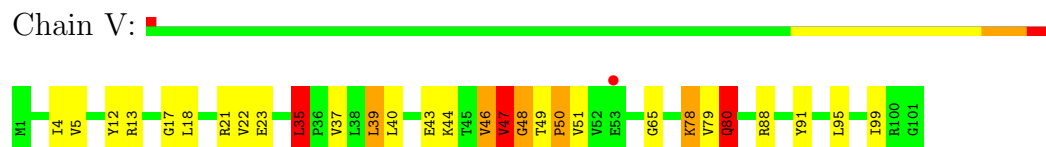
- Molecule 17: 50S ribosomal protein L20

Chain U:



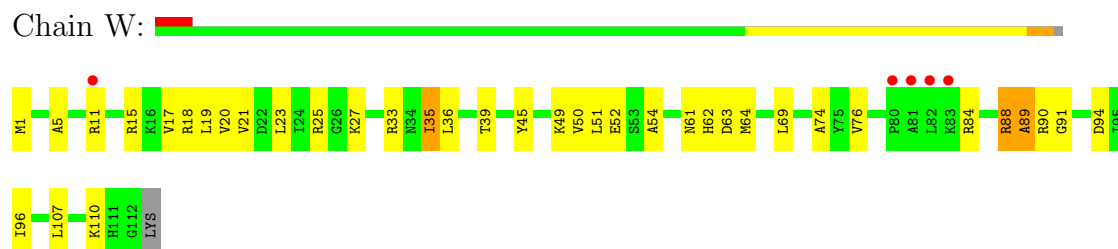
- Molecule 18: 50S ribosomal protein L21

Chain V:



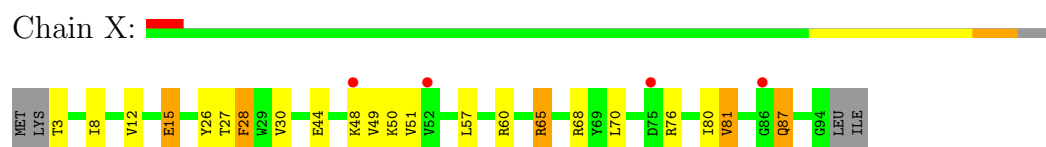
- Molecule 19: 50S ribosomal protein L22

Chain W:



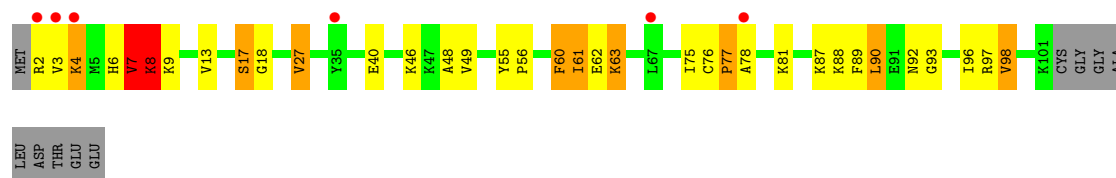
- Molecule 20: 50S ribosomal protein L23

Chain X:



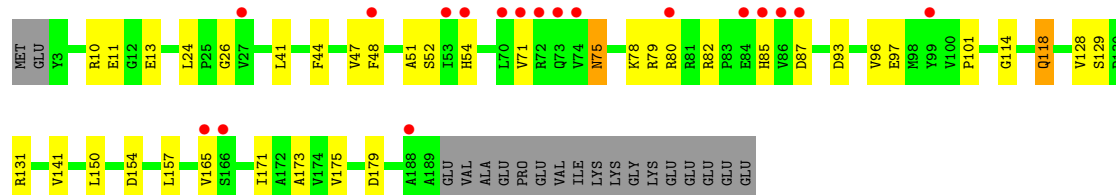
- Molecule 21: 50S ribosomal protein L24

Chain Y: 



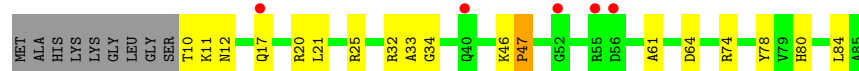
- Molecule 22: 50S ribosomal protein L25

Chain Z: 



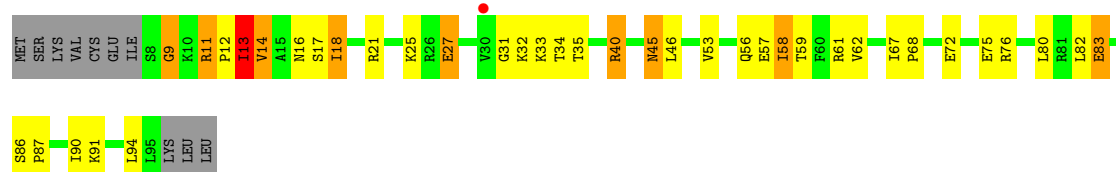
- Molecule 23: 50S ribosomal protein L27

Chain 0: 



- Molecule 24: 50S ribosomal protein L28

Chain 1: 



- Molecule 25: 50S ribosomal protein L29

Chain 2: 



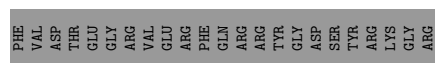
- Molecule 26: 50S ribosomal protein L30

Chain 3: 



- Molecule 27: 50S ribosomal protein L31

Chain 5: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.24Å 456.78Å 618.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 3.00 50.99 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.95-3.00) 97.2 (50.99-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.280 , 0.316 0.463 , 0.468	Depositor DCC
R_{free} test set	10573 reflections (0.92%)	DCC
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 1158087 reflections	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	92164	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.24% 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	0.66	2/69437 (0.0%)	1.22	323/108401 (0.3%)
2	B	0.52	0/2853	1.11	8/4451 (0.2%)
3	D	0.47	0/2154	0.67	1/2905 (0.0%)
4	E	0.34	0/1596	0.57	0/2153
5	F	0.38	0/1621	0.57	0/2194
6	G	0.27	0/1500	0.49	0/2017
7	H	0.28	0/1245	0.49	0/1682
8	I	0.32	0/1147	0.55	0/1552
9	K	0.24	0/1108	0.45	0/1500
10	N	0.33	0/1123	0.55	0/1515
11	O	0.35	0/942	0.55	0/1268
12	P	0.40	0/1131	0.72	2/1504 (0.1%)
13	Q	0.36	0/1084	0.59	0/1449
14	R	0.36	0/974	0.57	0/1302
15	S	0.26	0/778	0.48	0/1036
16	T	0.32	0/1157	0.51	0/1544
17	U	0.42	0/982	0.54	0/1306
18	V	0.37	0/790	0.59	0/1057
19	W	0.37	0/901	0.56	0/1209
20	X	0.42	0/739	0.56	0/993
21	Y	0.39	0/788	0.59	0/1051
22	Z	0.28	0/1514	0.49	0/2056
23	0	0.32	0/613	0.54	0/816
24	1	0.42	0/701	0.70	1/932 (0.1%)
25	2	0.40	0/522	0.63	0/690
26	3	0.31	0/472	0.49	0/634
27	5	0.33	0/418	0.58	0/567
28	6	0.29	0/387	0.50	0/518
29	7	0.44	0/426	0.64	0/561
30	8	0.42	0/515	0.65	0/679
31	4	0.26	0/228	0.52	0/309
All	All	0.59	2/99846 (0.0%)	1.09	335/149851 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
12	P	0	3
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	A	C3'-O3'	5.67	1.50	1.42
1	A	2447	G	C3'-O3'	5.48	1.49	1.42

The worst 5 of 335 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1559	G	C1'-O4'-C4'	-12.85	99.62	109.90
1	A	945	A	C1'-O4'-C4'	-12.85	99.62	109.90
1	A	1786	A	C1'-O4'-C4'	-12.74	99.70	109.90
1	A	1913	A	C1'-O4'-C4'	-11.53	100.68	109.90
1	A	1379	A	C3'-C2'-C1'	-11.08	92.64	101.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	40	THR	Peptide
12	P	51	PHE	Peptide
12	P	52	GLU	Peptide
12	P	9	ASN	Peptide

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	564	1
2	B	2551	0	0	27	1
3	D	2104	0	0	44	0
4	E	1563	0	0	23	0
5	F	1586	0	0	25	0
6	G	1475	0	0	17	0
7	H	1222	0	0	9	0
8	I	1132	0	0	13	0
9	K	1088	0	0	4	0
10	N	1096	0	0	15	0
11	O	932	0	0	7	0
12	P	1114	0	0	53	0
13	Q	1064	0	0	23	0
14	R	960	0	0	17	0
15	S	770	0	0	19	0
16	T	1143	0	0	16	0
17	U	964	0	0	23	0
18	V	779	0	0	13	0
19	W	890	0	0	15	0
20	X	725	0	0	9	0
21	Y	775	0	0	12	0
22	Z	1482	0	0	15	0
23	0	605	0	0	6	0
24	1	694	0	0	14	0
25	2	520	0	0	18	0
26	3	467	0	0	3	0
27	5	404	0	0	13	0
28	6	380	0	0	8	0
29	7	418	0	0	10	0
30	8	507	0	0	17	0
31	4	225	0	0	1	0
32	1	2	0	0	0	0
32	6	1	0	0	0	0
32	8	1	0	0	0	0
32	A	486	0	0	0	0
32	B	10	0	0	0	0
32	D	12	0	0	0	0
32	E	1	0	0	0	0
32	F	1	0	0	0	0
32	G	3	0	0	0	0
32	I	1	0	0	0	0
32	K	1	0	0	0	0
32	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	O	2	0	0	0	0
32	P	1	0	0	0	0
32	Q	2	0	0	0	0
32	R	1	0	0	0	0
32	T	1	0	0	0	0
32	U	2	0	0	0	0
32	V	1	0	0	0	0
32	Y	1	0	0	0	0
32	Z	1	0	0	0	0
All	All	92164	0	0	967	1

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 11.

The worst 5 of 967 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1899:G:N2	1:A:1902:C:N4	2.21	0.87
1:A:1658:C:OP1	4:E:132:HIS:ND1	2.11	0.82
3:D:33:LEU:O	3:D:35:LYS:N	2.18	0.77
1:A:603:A:C2	1:A:655:A:C6	2.74	0.75
25:2:47:ASN:O	25:2:49:LYS:N	2.21	0.74

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1411:C:O3'	2:B:53:A:O2'[1_655]	2.14	0.06

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%)	204 (76%)	46 (17%)	19 (7%)	2 9
4	E	202/206 (98%)	157 (78%)	37 (18%)	8 (4%)	5 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	200/210 (95%)	162 (81%)	26 (13%)	12 (6%)	2	14
6	G	179/182 (98%)	127 (71%)	39 (22%)	13 (7%)	2	8
7	H	157/180 (87%)	121 (77%)	28 (18%)	8 (5%)	3	18
8	I	143/148 (97%)	121 (85%)	19 (13%)	3 (2%)	11	47
9	K	145/147 (99%)	101 (70%)	35 (24%)	9 (6%)	2	13
10	N	135/163 (83%)	101 (75%)	19 (14%)	15 (11%)	1	3
11	O	120/122 (98%)	101 (84%)	15 (12%)	4 (3%)	6	32
12	P	144/150 (96%)	88 (61%)	34 (24%)	22 (15%)	0	1
13	Q	132/141 (94%)	93 (70%)	24 (18%)	15 (11%)	1	3
14	R	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	4	23
15	S	96/112 (86%)	56 (58%)	29 (30%)	11 (12%)	1	3
16	T	135/146 (92%)	91 (67%)	31 (23%)	13 (10%)	1	4
17	U	115/118 (98%)	91 (79%)	19 (16%)	5 (4%)	4	23
18	V	99/101 (98%)	74 (75%)	15 (15%)	10 (10%)	1	4
19	W	110/113 (97%)	87 (79%)	18 (16%)	5 (4%)	4	22
20	X	90/96 (94%)	73 (81%)	15 (17%)	2 (2%)	10	45
21	Y	98/110 (89%)	65 (66%)	17 (17%)	16 (16%)	0	1
22	Z	185/206 (90%)	145 (78%)	32 (17%)	8 (4%)	4	23
23	0	74/85 (87%)	61 (82%)	10 (14%)	3 (4%)	4	24
24	1	86/98 (88%)	59 (69%)	16 (19%)	11 (13%)	0	2
25	2	60/72 (83%)	44 (73%)	11 (18%)	5 (8%)	1	6
26	3	57/60 (95%)	50 (88%)	5 (9%)	2 (4%)	6	30
27	5	50/60 (83%)	40 (80%)	7 (14%)	3 (6%)	2	14
28	6	42/54 (78%)	27 (64%)	10 (24%)	5 (12%)	1	2
29	7	46/49 (94%)	42 (91%)	4 (9%)	0	100	100
30	8	61/65 (94%)	42 (69%)	12 (20%)	7 (12%)	1	3
31	4	28/97 (29%)	18 (64%)	6 (21%)	4 (14%)	0	1
All	All	3373/3685 (92%)	2532 (75%)	598 (18%)	243 (7%)	2	8

5 of 243 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	13	ARG

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Mol	Chain	Res	Type
3	D	33	LEU
3	D	34	VAL
3	D	57	GLY
3	D	59	LYS

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%)	181 (85%)	32 (15%)	4	20
4	E	165/166 (99%)	144 (87%)	21 (13%)	6	27
5	F	161/166 (97%)	140 (87%)	21 (13%)	6	26
6	G	155/156 (99%)	135 (87%)	20 (13%)	6	26
7	H	132/148 (89%)	115 (87%)	17 (13%)	6	26
8	I	122/124 (98%)	103 (84%)	19 (16%)	4	18
9	K	111/111 (100%)	95 (86%)	16 (14%)	5	22
10	N	116/139 (84%)	98 (84%)	18 (16%)	4	19
11	O	100/100 (100%)	85 (85%)	15 (15%)	4	20
12	P	112/116 (97%)	79 (70%)	33 (30%)	0	2
13	Q	105/111 (95%)	91 (87%)	14 (13%)	6	25
14	R	100/101 (99%)	91 (91%)	9 (9%)	14	47
15	S	77/88 (88%)	66 (86%)	11 (14%)	5	22
16	T	121/128 (94%)	101 (84%)	20 (16%)	3	16
17	U	93/94 (99%)	83 (89%)	10 (11%)	9	35
18	V	82/82 (100%)	69 (84%)	13 (16%)	4	17
19	W	91/92 (99%)	80 (88%)	11 (12%)	7	29
20	X	74/78 (95%)	59 (80%)	15 (20%)	2	9
21	Y	84/91 (92%)	70 (83%)	14 (17%)	3	16
22	Z	162/179 (90%)	150 (93%)	12 (7%)	20	58
23	0	61/67 (91%)	53 (87%)	8 (13%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	1	73/83 (88%)	57 (78%)	16 (22%)	1	7
25	2	58/67 (87%)	45 (78%)	13 (22%)	1	7
26	3	51/52 (98%)	49 (96%)	2 (4%)	43	85
27	5	45/52 (86%)	42 (93%)	3 (7%)	23	64
28	6	43/52 (83%)	34 (79%)	9 (21%)	1	8
29	7	41/42 (98%)	35 (85%)	6 (15%)	5	21
30	8	53/55 (96%)	47 (89%)	6 (11%)	9	33
31	4	27/84 (32%)	22 (82%)	5 (18%)	2	13
All	All	2828/3042 (93%)	2419 (86%)	409 (14%)	5	22

5 of 409 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	P	35	HIS
14	R	67	LEU
26	3	37	LEU
12	P	49	ARG
12	P	135	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%)	594 (20%)	173 (6%)
2	B	118/124 (95%)	18 (15%)	6 (5%)
All	All	2996/3018 (99%)	612 (20%)	179 (5%)

5 of 612 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	13	A
1	A	17	G
1	A	27	G
1	A	28	A

5 of 179 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1253	A
1	A	1542	G
1	A	2756	U
1	A	1286	A
1	A	1384	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 532 ligands modelled in this entry, 532 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%)	0.09	117 (4%) 35 7	10, 67, 204, 287	0
2	B	119/124 (95%)	0.43	7 (5%) 22 5	87, 147, 205, 258	0
3	D	271/276 (98%)	-0.05	4 (1%) 70 16	26, 51, 92, 146	0
4	E	204/206 (99%)	-0.07	1 (0%) 88 36	45, 85, 137, 186	0
5	F	202/210 (96%)	-0.12	1 (0%) 88 36	34, 66, 124, 190	0
6	G	181/182 (99%)	0.26	13 (7%) 15 4	113, 153, 182, 206	0
7	H	159/180 (88%)	-0.08	3 (1%) 64 13	79, 111, 154, 174	0
8	I	145/148 (97%)	-0.04	4 (2%) 50 10	58, 94, 129, 147	0
9	K	147/147 (100%)	1.28	41 (27%) 1 0	207, 236, 257, 274	0
10	N	137/163 (84%)	0.08	2 (1%) 70 16	59, 80, 130, 164	0
11	O	122/122 (100%)	-0.00	6 (4%) 28 6	47, 72, 108, 129	0
12	P	146/150 (97%)	0.19	11 (7%) 14 3	21, 93, 146, 183	0
13	Q	134/141 (95%)	0.46	13 (9%) 8 2	56, 91, 148, 192	0
14	R	117/118 (99%)	0.23	7 (5%) 21 5	48, 73, 130, 148	0
15	S	98/112 (87%)	0.32	5 (5%) 27 6	106, 144, 177, 218	0
16	T	137/146 (93%)	0.50	18 (13%) 4 1	66, 100, 155, 189	0
17	U	117/118 (99%)	0.33	8 (6%) 17 4	39, 68, 120, 194	0
18	V	101/101 (100%)	-0.08	1 (0%) 79 22	46, 91, 143, 206	0
19	W	112/113 (99%)	0.11	5 (4%) 32 7	31, 61, 119, 155	0
20	X	92/96 (95%)	0.12	4 (4%) 34 7	38, 65, 114, 150	0
21	Y	100/110 (90%)	0.29	6 (6%) 21 5	53, 86, 160, 186	0
22	Z	187/206 (90%)	0.33	18 (9%) 8 2	107, 139, 176, 201	0
23	0	76/85 (89%)	0.29	5 (6%) 18 4	73, 99, 139, 160	0
24	1	88/98 (89%)	-0.04	1 (1%) 77 21	34, 68, 143, 172	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	2	62/72 (86%)	-0.33	0 100 100	37, 75, 147, 177	0
26	3	59/60 (98%)	-0.31	0 100 100	57, 83, 129, 170	0
27	5	52/60 (86%)	0.05	2 (3%) 38 7	42, 80, 147, 167	0
28	6	44/54 (81%)	-0.06	1 (2%) 57 12	111, 140, 175, 192	0
29	7	48/49 (97%)	0.55	5 (10%) 7 2	31, 44, 96, 161	0
30	8	63/65 (96%)	0.37	5 (7%) 13 3	48, 72, 133, 168	0
31	4	30/97 (30%)	-0.26	0 100 100	115, 149, 178, 183	0
All	All	6429/6703 (95%)	0.13	314 (4%) 31 6	10, 79, 198, 287	0

The worst 5 of 314 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	K	85	GLU	10.5
9	K	54	PRO	9.3
9	K	52	ILE	9.1
5	F	207	GLY	8.6
1	A	615	G	8.4

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	5463	1/1	0.27	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5064	1/1	0.26	-	4,4,4,4	0
32	MG	A	5176	1/1	0.40	-	4,4,4,4	0
32	MG	A	5516	1/1	0.31	-	3,3,3,3	0
32	MG	A	5349	1/1	0.55	-	3,3,3,3	0
32	MG	A	5264	1/1	0.14	-	62,62,62,62	0
32	MG	R	5024	1/1	0.15	-	3,3,3,3	0
32	MG	A	5373	1/1	0.34	-	56,56,56,56	0
32	MG	D	5229	1/1	0.48	-	43,43,43,43	0
32	MG	A	5109	1/1	0.14	-	3,3,3,3	0
32	MG	A	5257	1/1	0.24	-	72,72,72,72	0
32	MG	A	5089	1/1	0.12	-	4,4,4,4	0
32	MG	A	5365	1/1	0.43	-	3,3,3,3	0
32	MG	A	5287	1/1	0.22	-	3,3,3,3	0
32	MG	Y	5028	1/1	0.11	-	3,3,3,3	0
32	MG	A	5234	1/1	0.21	-	4,4,4,4	0
32	MG	A	5206	1/1	0.33	-	3,3,3,3	0
32	MG	A	5484	1/1	0.17	-	27,27,27,27	0
32	MG	A	5072	1/1	0.23	-	3,3,3,3	0
32	MG	A	5401	1/1	0.18	-	92,92,92,92	0
32	MG	A	5133	1/1	0.32	-	59,59,59,59	0
32	MG	Z	5529	1/1	0.13	-	3,3,3,3	0
32	MG	A	5085	1/1	0.18	-	4,4,4,4	0
32	MG	A	5470	1/1	0.30	-	4,4,4,4	0
32	MG	A	5239	1/1	0.29	-	4,4,4,4	0
32	MG	A	5504	1/1	0.21	-	3,3,3,3	0
32	MG	A	5341	1/1	0.18	-	70,70,70,70	0
32	MG	A	5163	1/1	0.21	-	3,3,3,3	0
32	MG	A	5038	1/1	0.23	-	3,3,3,3	0
32	MG	A	5310	1/1	0.24	-	8,8,8,8	0
32	MG	A	5069	1/1	0.14	-	3,3,3,3	0
32	MG	A	5160	1/1	0.20	-	3,3,3,3	0
32	MG	A	5080	1/1	0.20	-	3,3,3,3	0
32	MG	A	5434	1/1	0.16	-	5,5,5,5	0
32	MG	A	5472	1/1	0.23	-	3,3,3,3	0
32	MG	A	5351	1/1	0.31	-	3,3,3,3	0
32	MG	A	5043	1/1	0.24	-	3,3,3,3	0
32	MG	A	5178	1/1	0.25	-	5,5,5,5	0
32	MG	E	5009	1/1	0.19	-	5,5,5,5	0
32	MG	A	5042	1/1	0.37	-	3,3,3,3	0
32	MG	P	5020	1/1	0.26	-	3,3,3,3	0
32	MG	A	5346	1/1	0.43	-	43,43,43,43	0
32	MG	A	5294	1/1	0.31	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5507	1/1	0.24	-	3,3,3,3	0
32	MG	A	5158	1/1	0.19	-	19,19,19,19	0
32	MG	A	5454	1/1	0.27	-	5,5,5,5	0
32	MG	A	5219	1/1	0.19	-	3,3,3,3	0
32	MG	A	5095	1/1	0.20	-	4,4,4,4	0
32	MG	A	5342	1/1	0.18	-	62,62,62,62	0
32	MG	A	5394	1/1	0.64	-	59,59,59,59	0
32	MG	A	5452	1/1	0.19	-	28,28,28,28	0
32	MG	A	5225	1/1	0.22	-	3,3,3,3	0
32	MG	A	5296	1/1	0.12	-	4,4,4,4	0
32	MG	A	5356	1/1	0.19	-	10,10,10,10	0
32	MG	A	5285	1/1	0.23	-	4,4,4,4	0
32	MG	A	5244	1/1	0.12	-	4,4,4,4	0
32	MG	A	5068	1/1	0.23	-	3,3,3,3	0
32	MG	A	5309	1/1	0.45	-	70,70,70,70	0
32	MG	A	5440	1/1	0.51	-	3,3,3,3	0
32	MG	A	5213	1/1	0.35	-	3,3,3,3	0
32	MG	A	5189	1/1	0.10	-	4,4,4,4	0
32	MG	A	5195	1/1	0.21	-	3,3,3,3	0
32	MG	A	5509	1/1	0.59	-	3,3,3,3	0
32	MG	A	5134	1/1	0.11	-	3,3,3,3	0
32	MG	A	5498	1/1	0.24	-	3,3,3,3	0
32	MG	A	5105	1/1	0.23	-	3,3,3,3	0
32	MG	A	5228	1/1	0.15	-	15,15,15,15	0
32	MG	A	5272	1/1	0.14	-	3,3,3,3	0
32	MG	A	5302	1/1	0.56	-	4,4,4,4	0
32	MG	A	5164	1/1	0.54	-	3,3,3,3	0
32	MG	A	5375	1/1	0.30	-	60,60,60,60	0
32	MG	A	5326	1/1	0.35	-	50,50,50,50	0
32	MG	A	5131	1/1	0.54	-	46,46,46,46	0
32	MG	A	5312	1/1	0.47	-	33,33,33,33	0
32	MG	A	5360	1/1	0.40	-	4,4,4,4	0
32	MG	A	5161	1/1	0.10	-	8,8,8,8	0
32	MG	A	5063	1/1	0.43	-	4,4,4,4	0
32	MG	A	5464	1/1	0.43	-	4,4,4,4	0
32	MG	A	5439	1/1	0.48	-	3,3,3,3	0
32	MG	A	5495	1/1	0.25	-	3,3,3,3	0
32	MG	A	5249	1/1	0.15	-	4,4,4,4	0
32	MG	A	5425	1/1	0.21	-	24,24,24,24	0
32	MG	A	5501	1/1	0.41	-	4,4,4,4	0
32	MG	A	5391	1/1	0.30	-	3,3,3,3	0
32	MG	A	5431	1/1	0.20	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5098	1/1	0.20	-	6,6,6,6	0
32	MG	A	5445	1/1	0.25	-	4,4,4,4	0
32	MG	A	5503	1/1	0.38	-	3,3,3,3	0
32	MG	B	5523	1/1	0.23	-	3,3,3,3	0
32	MG	A	5142	1/1	0.14	-	28,28,28,28	0
32	MG	A	5416	1/1	0.22	-	19,19,19,19	0
32	MG	A	5410	1/1	0.28	-	42,42,42,42	0
32	MG	A	5084	1/1	0.24	-	3,3,3,3	0
32	MG	A	5057	1/1	0.14	-	6,6,6,6	0
32	MG	A	5067	1/1	0.09	-	69,69,69,69	0
32	MG	A	5240	1/1	0.29	-	4,4,4,4	0
32	MG	A	5254	1/1	0.11	-	4,4,4,4	0
32	MG	A	5483	1/1	0.20	-	45,45,45,45	0
32	MG	A	5247	1/1	0.67	-	52,52,52,52	0
32	MG	A	5193	1/1	0.23	-	4,4,4,4	0
32	MG	A	5061	1/1	0.30	-	5,5,5,5	0
32	MG	A	5482	1/1	0.53	-	3,3,3,3	0
32	MG	A	5126	1/1	0.39	-	64,64,64,64	0
32	MG	A	5265	1/1	0.11	-	78,78,78,78	0
32	MG	A	5343	1/1	0.27	-	4,4,4,4	0
32	MG	A	5323	1/1	0.26	-	46,46,46,46	0
32	MG	A	5159	1/1	0.15	-	21,21,21,21	0
32	MG	A	5453	1/1	0.20	-	14,14,14,14	0
32	MG	A	5136	1/1	0.13	-	3,3,3,3	0
32	MG	A	5340	1/1	0.67	-	69,69,69,69	0
32	MG	A	5314	1/1	0.23	-	33,33,33,33	0
32	MG	D	5315	1/1	0.42	-	29,29,29,29	0
32	MG	A	5060	1/1	0.39	-	3,3,3,3	0
32	MG	A	5299	1/1	0.58	-	3,3,3,3	0
32	MG	A	5281	1/1	0.38	-	12,12,12,12	0
32	MG	G	5012	1/1	0.22	-	59,59,59,59	0
32	MG	A	5436	1/1	0.21	-	4,4,4,4	0
32	MG	A	5422	1/1	0.89	-	53,53,53,53	0
32	MG	A	5379	1/1	0.55	-	3,3,3,3	0
32	MG	A	5370	1/1	0.78	-	3,3,3,3	0
32	MG	A	5071	1/1	0.20	-	4,4,4,4	0
32	MG	A	5212	1/1	0.49	-	3,3,3,3	0
32	MG	A	5268	1/1	0.27	-	3,3,3,3	0
32	MG	A	5226	1/1	0.16	-	6,6,6,6	0
32	MG	A	5362	1/1	0.66	-	3,3,3,3	0
32	MG	A	5107	1/1	0.70	-	3,3,3,3	0
32	MG	B	5530	1/1	0.30	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5100	1/1	0.22	-	4,4,4,4	0
32	MG	A	5201	1/1	0.57	-	4,4,4,4	0
32	MG	A	5074	1/1	0.17	-	5,5,5,5	0
32	MG	B	5526	1/1	0.45	-	4,4,4,4	0
32	MG	B	5528	1/1	0.44	-	3,3,3,3	0
32	MG	A	5421	1/1	0.10	-	47,47,47,47	0
32	MG	D	5005	1/1	0.35	-	51,51,51,51	0
32	MG	A	5078	1/1	0.22	-	4,4,4,4	0
32	MG	A	5300	1/1	0.34	-	3,3,3,3	0
32	MG	A	5048	1/1	0.11	-	3,3,3,3	0
32	MG	A	5127	1/1	0.57	-	74,74,74,74	0
32	MG	A	5169	1/1	0.11	-	4,4,4,4	0
32	MG	A	5130	1/1	0.42	-	55,55,55,55	0
32	MG	A	5117	1/1	0.18	-	4,4,4,4	0
32	MG	D	5003	1/1	0.64	-	65,65,65,65	0
32	MG	A	5506	1/1	0.42	-	3,3,3,3	0
32	MG	A	5438	1/1	0.22	-	3,3,3,3	0
32	MG	A	5145	1/1	0.12	-	28,28,28,28	0
32	MG	A	5036	1/1	0.30	-	3,3,3,3	0
32	MG	A	5079	1/1	0.13	-	5,5,5,5	0
32	MG	A	5187	1/1	0.64	-	3,3,3,3	0
32	MG	A	5041	1/1	0.17	-	3,3,3,3	0
32	MG	A	5301	1/1	0.17	-	4,4,4,4	0
32	MG	D	5236	1/1	0.18	-	3,3,3,3	0
32	MG	A	5255	1/1	0.18	-	3,3,3,3	0
32	MG	A	5353	1/1	0.22	-	4,4,4,4	0
32	MG	A	5211	1/1	0.14	-	4,4,4,4	0
32	MG	A	5429	1/1	0.49	-	39,39,39,39	0
32	MG	A	5428	1/1	0.18	-	52,52,52,52	0
32	MG	A	5209	1/1	0.20	-	3,3,3,3	0
32	MG	A	5088	1/1	0.18	-	3,3,3,3	0
32	MG	A	5096	1/1	0.10	-	3,3,3,3	0
32	MG	A	5202	1/1	0.48	-	3,3,3,3	0
32	MG	A	5320	1/1	0.29	-	61,61,61,61	0
32	MG	A	5406	1/1	0.23	-	3,3,3,3	0
32	MG	A	5437	1/1	0.19	-	3,3,3,3	0
32	MG	A	5461	1/1	0.20	-	3,3,3,3	0
32	MG	A	5180	1/1	0.21	-	4,4,4,4	0
32	MG	A	5260	1/1	0.21	-	3,3,3,3	0
32	MG	A	5204	1/1	0.20	-	3,3,3,3	0
32	MG	A	5259	1/1	0.59	-	43,43,43,43	0
32	MG	A	5245	1/1	0.55	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	N	5016	1/1	0.37	-	3,3,3,3	0
32	MG	A	5191	1/1	0.23	-	3,3,3,3	0
32	MG	B	5531	1/1	0.14	-	3,3,3,3	0
32	MG	A	5053	1/1	0.35	-	4,4,4,4	0
32	MG	A	5171	1/1	0.23	-	3,3,3,3	0
32	MG	A	5417	1/1	0.58	-	70,70,70,70	0
32	MG	A	5184	1/1	0.24	-	3,3,3,3	0
32	MG	A	5050	1/1	0.58	-	3,3,3,3	0
32	MG	A	5197	1/1	0.23	-	3,3,3,3	0
32	MG	A	5274	1/1	0.09	-	3,3,3,3	0
32	MG	I	5013	1/1	0.13	-	38,38,38,38	0
32	MG	A	5177	1/1	0.43	-	5,5,5,5	0
32	MG	A	5413	1/1	0.09	-	51,51,51,51	0
32	MG	G	5011	1/1	0.28	-	3,3,3,3	0
32	MG	A	5082	1/1	0.25	-	3,3,3,3	0
32	MG	A	5289	1/1	0.21	-	4,4,4,4	0
32	MG	A	5066	1/1	0.10	-	52,52,52,52	0
32	MG	A	5144	1/1	0.25	-	58,58,58,58	0
32	MG	A	5059	1/1	0.18	-	6,6,6,6	0
32	MG	A	5270	1/1	0.10	-	5,5,5,5	0
32	MG	A	5108	1/1	0.26	-	3,3,3,3	0
32	MG	A	5348	1/1	0.19	-	4,4,4,4	0
32	MG	A	5471	1/1	0.21	-	3,3,3,3	0
32	MG	A	5037	1/1	0.26	-	3,3,3,3	0
32	MG	A	5162	1/1	0.46	-	3,3,3,3	0
32	MG	A	5511	1/1	0.30	-	4,4,4,4	0
32	MG	A	5515	1/1	0.39	-	3,3,3,3	0
32	MG	A	5387	1/1	1.21	-	56,56,56,56	0
32	MG	A	5398	1/1	0.59	-	71,71,71,71	0
32	MG	A	5156	1/1	0.72	-	31,31,31,31	0
32	MG	A	5311	1/1	0.26	-	4,4,4,4	0
32	MG	A	5352	1/1	0.32	-	3,3,3,3	0
32	MG	A	5091	1/1	0.41	-	43,43,43,43	0
32	MG	A	5400	1/1	0.29	-	3,3,3,3	0
32	MG	B	5521	1/1	0.16	-	3,3,3,3	0
32	MG	A	5333	1/1	0.29	-	3,3,3,3	0
32	MG	A	5223	1/1	0.24	-	4,4,4,4	0
32	MG	A	5278	1/1	0.38	-	23,23,23,23	0
32	MG	A	5465	1/1	0.56	-	4,4,4,4	0
32	MG	A	5479	1/1	0.29	-	12,12,12,12	0
32	MG	D	5004	1/1	0.13	-	42,42,42,42	0
32	MG	A	5022	1/1	0.12	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5332	1/1	0.31	-	23,23,23,23	0
32	MG	A	5328	1/1	0.16	-	42,42,42,42	0
32	MG	A	5319	1/1	0.19	-	74,74,74,74	0
32	MG	A	5175	1/1	0.21	-	4,4,4,4	0
32	MG	A	5290	1/1	0.20	-	4,4,4,4	0
32	MG	A	5510	1/1	0.30	-	4,4,4,4	0
32	MG	A	5256	1/1	0.07	-	58,58,58,58	0
32	MG	A	5203	1/1	0.31	-	4,4,4,4	0
32	MG	A	5447	1/1	0.23	-	3,3,3,3	0
32	MG	A	5086	1/1	0.30	-	4,4,4,4	0
32	MG	A	5120	1/1	0.32	-	3,3,3,3	0
32	MG	A	5081	1/1	0.37	-	63,63,63,63	0
32	MG	A	5344	1/1	0.19	-	43,43,43,43	0
32	MG	A	5121	1/1	0.45	-	3,3,3,3	0
32	MG	A	5207	1/1	0.16	-	3,3,3,3	0
32	MG	A	5441	1/1	0.28	-	3,3,3,3	0
32	MG	B	5527	1/1	0.10	-	3,3,3,3	0
32	MG	A	5293	1/1	0.38	-	3,3,3,3	0
32	MG	A	5532	1/1	0.47	-	3,3,3,3	0
32	MG	A	5185	1/1	0.64	-	3,3,3,3	0
32	MG	A	5399	1/1	0.24	-	56,56,56,56	0
32	MG	D	5002	1/1	0.63	-	33,33,33,33	0
32	MG	A	5196	1/1	0.08	-	3,3,3,3	0
32	MG	A	5186	1/1	0.45	-	3,3,3,3	0
32	MG	A	5097	1/1	0.15	-	3,3,3,3	0
32	MG	A	5114	1/1	0.29	-	4,4,4,4	0
32	MG	A	5418	1/1	0.65	-	73,73,73,73	0
32	MG	A	5371	1/1	0.27	-	25,25,25,25	0
32	MG	A	5322	1/1	0.92	-	33,33,33,33	0
32	MG	B	5524	1/1	0.13	-	3,3,3,3	0
32	MG	A	5354	1/1	0.30	-	4,4,4,4	0
32	MG	A	5282	1/1	0.23	-	6,6,6,6	0
32	MG	A	5306	1/1	0.27	-	34,34,34,34	0
32	MG	A	5491	1/1	0.63	-	3,3,3,3	0
32	MG	A	5415	1/1	0.18	-	77,77,77,77	0
32	MG	A	5056	1/1	0.42	-	3,3,3,3	0
32	MG	A	5402	1/1	0.26	-	3,3,3,3	0
32	MG	A	5395	1/1	0.20	-	3,3,3,3	0
32	MG	A	5499	1/1	0.36	-	4,4,4,4	0
32	MG	A	5303	1/1	0.52	-	3,3,3,3	0
32	MG	A	5486	1/1	0.23	-	4,4,4,4	0
32	MG	A	5224	1/1	0.33	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5313	1/1	0.18	-	10,10,10,10	0
32	MG	A	5304	1/1	0.24	-	60,60,60,60	0
32	MG	A	5336	1/1	0.27	-	4,4,4,4	0
32	MG	A	5505	1/1	0.22	-	3,3,3,3	0
32	MG	A	5058	1/1	0.27	-	4,4,4,4	0
32	MG	A	5519	1/1	0.25	-	3,3,3,3	0
32	MG	A	5102	1/1	0.13	-	5,5,5,5	0
32	MG	T	5025	1/1	0.28	-	3,3,3,3	0
32	MG	A	5106	1/1	0.32	-	4,4,4,4	0
32	MG	A	5427	1/1	0.49	-	58,58,58,58	0
32	MG	A	5295	1/1	0.10	-	3,3,3,3	0
32	MG	A	5388	1/1	0.34	-	78,78,78,78	0
32	MG	A	5374	1/1	1.02	-	35,35,35,35	0
32	MG	A	5467	1/1	0.14	-	6,6,6,6	0
32	MG	A	5266	1/1	0.26	-	3,3,3,3	0
32	MG	A	5345	1/1	0.12	-	45,45,45,45	0
32	MG	A	5500	1/1	0.33	-	4,4,4,4	0
32	MG	A	5451	1/1	0.25	-	39,39,39,39	0
32	MG	F	5010	1/1	0.53	-	3,3,3,3	0
32	MG	A	5405	1/1	0.90	-	43,43,43,43	0
32	MG	6	5031	1/1	0.14	-	43,43,43,43	0
32	MG	A	5518	1/1	0.42	-	4,4,4,4	0
32	MG	A	5034	1/1	0.35	-	3,3,3,3	0
32	MG	A	5055	1/1	0.17	-	4,4,4,4	0
32	MG	A	5366	1/1	0.20	-	6,6,6,6	0
32	MG	A	5488	1/1	0.35	-	4,4,4,4	0
32	MG	1	5233	1/1	0.30	-	53,53,53,53	0
32	MG	A	5174	1/1	0.22	-	3,3,3,3	0
32	MG	A	5232	1/1	0.38	-	50,50,50,50	0
32	MG	A	5409	1/1	0.34	-	3,3,3,3	0
32	MG	A	5377	1/1	0.30	-	63,63,63,63	0
32	MG	A	5216	1/1	0.22	-	4,4,4,4	0
32	MG	A	5284	1/1	0.14	-	6,6,6,6	0
32	MG	A	5477	1/1	0.56	-	21,21,21,21	0
32	MG	A	5283	1/1	0.71	-	3,3,3,3	0
32	MG	A	5157	1/1	0.49	-	65,65,65,65	0
32	MG	A	5103	1/1	0.21	-	4,4,4,4	0
32	MG	A	5199	1/1	0.12	-	3,3,3,3	0
32	MG	A	5241	1/1	0.18	-	4,4,4,4	0
32	MG	A	5489	1/1	0.17	-	6,6,6,6	0
32	MG	A	5396	1/1	0.28	-	43,43,43,43	0
32	MG	A	5019	1/1	0.34	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5329	1/1	0.62	-	44,44,44,44	0
32	MG	A	5446	1/1	0.29	-	3,3,3,3	0
32	MG	A	5047	1/1	0.12	-	3,3,3,3	0
32	MG	G	5525	1/1	0.12	-	4,4,4,4	0
32	MG	A	5368	1/1	0.30	-	3,3,3,3	0
32	MG	A	5267	1/1	0.16	-	73,73,73,73	0
32	MG	B	5520	1/1	0.39	-	3,3,3,3	0
32	MG	A	5481	1/1	0.21	-	38,38,38,38	0
32	MG	A	5221	1/1	0.24	-	4,4,4,4	0
32	MG	Q	5023	1/1	0.45	-	3,3,3,3	0
32	MG	A	5492	1/1	0.28	-	4,4,4,4	0
32	MG	D	5007	1/1	0.17	-	11,11,11,11	0
32	MG	A	5154	1/1	0.26	-	57,57,57,57	0
32	MG	A	5250	1/1	0.12	-	5,5,5,5	0
32	MG	A	5115	1/1	0.33	-	3,3,3,3	0
32	MG	A	5093	1/1	0.17	-	4,4,4,4	0
32	MG	A	5358	1/1	0.18	-	23,23,23,23	0
32	MG	A	5083	1/1	0.30	-	3,3,3,3	0
32	MG	A	5389	1/1	0.15	-	82,82,82,82	0
32	MG	A	5205	1/1	0.52	-	3,3,3,3	0
32	MG	A	5419	1/1	0.69	-	35,35,35,35	0
32	MG	A	5494	1/1	0.14	-	3,3,3,3	0
32	MG	A	5251	1/1	0.30	-	4,4,4,4	0
32	MG	A	5286	1/1	0.28	-	3,3,3,3	0
32	MG	A	5496	1/1	0.26	-	3,3,3,3	0
32	MG	A	5367	1/1	0.22	-	5,5,5,5	0
32	MG	A	5517	1/1	0.29	-	3,3,3,3	0
32	MG	A	5298	1/1	0.29	-	3,3,3,3	0
32	MG	A	5380	1/1	0.16	-	61,61,61,61	0
32	MG	A	5030	1/1	0.08	-	25,25,25,25	0
32	MG	A	5208	1/1	0.21	-	3,3,3,3	0
32	MG	O	5018	1/1	0.64	-	4,4,4,4	0
32	MG	A	5227	1/1	0.15	-	3,3,3,3	0
32	MG	A	5318	1/1	1.03	-	44,44,44,44	0
32	MG	1	5029	1/1	0.36	-	3,3,3,3	0
32	MG	A	5305	1/1	0.40	-	30,30,30,30	0
32	MG	A	5469	1/1	0.17	-	4,4,4,4	0
32	MG	A	5149	1/1	0.13	-	14,14,14,14	0
32	MG	A	5407	1/1	0.13	-	3,3,3,3	0
32	MG	A	5152	1/1	0.65	-	3,3,3,3	0
32	MG	A	5514	1/1	0.10	-	4,4,4,4	0
32	MG	A	5462	1/1	0.24	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5183	1/1	0.48	-	3,3,3,3	0
32	MG	A	5119	1/1	0.39	-	3,3,3,3	0
32	MG	A	5513	1/1	0.38	-	3,3,3,3	0
32	MG	A	5198	1/1	0.11	-	3,3,3,3	0
32	MG	A	5173	1/1	0.17	-	4,4,4,4	0
32	MG	D	5001	1/1	0.63	-	33,33,33,33	0
32	MG	A	5339	1/1	0.20	-	46,46,46,46	0
32	MG	A	5364	1/1	0.38	-	4,4,4,4	0
32	MG	A	5076	1/1	0.37	-	3,3,3,3	0
32	MG	A	5039	1/1	0.42	-	3,3,3,3	0
32	MG	A	5414	1/1	0.19	-	3,3,3,3	0
32	MG	A	5397	1/1	0.37	-	65,65,65,65	0
32	MG	A	5141	1/1	0.15	-	3,3,3,3	0
32	MG	A	5337	1/1	0.19	-	57,57,57,57	0
32	MG	A	5135	1/1	0.09	-	48,48,48,48	0
32	MG	A	5262	1/1	0.60	-	53,53,53,53	0
32	MG	A	5308	1/1	0.66	-	72,72,72,72	0
32	MG	A	5122	1/1	0.28	-	4,4,4,4	0
32	MG	A	5424	1/1	0.44	-	66,66,66,66	0
32	MG	K	5015	1/1	0.52	-	4,4,4,4	0
32	MG	A	5459	1/1	0.17	-	6,6,6,6	0
32	MG	A	5330	1/1	0.13	-	10,10,10,10	0
32	MG	A	5350	1/1	0.56	-	3,3,3,3	0
32	MG	A	5473	1/1	0.29	-	3,3,3,3	0
32	MG	A	5369	1/1	0.17	-	7,7,7,7	0
32	MG	A	5468	1/1	0.13	-	4,4,4,4	0
32	MG	A	5408	1/1	0.43	-	64,64,64,64	0
32	MG	D	5006	1/1	0.19	-	47,47,47,47	0
32	MG	A	5457	1/1	0.28	-	3,3,3,3	0
32	MG	A	5288	1/1	0.32	-	3,3,3,3	0
32	MG	A	5448	1/1	0.51	-	4,4,4,4	0
32	MG	A	5110	1/1	0.28	-	3,3,3,3	0
32	MG	A	5335	1/1	0.39	-	46,46,46,46	0
32	MG	A	5487	1/1	0.36	-	6,6,6,6	0
32	MG	A	5182	1/1	0.32	-	3,3,3,3	0
32	MG	A	5035	1/1	0.18	-	3,3,3,3	0
32	MG	A	5168	1/1	0.55	-	3,3,3,3	0
32	MG	A	5325	1/1	0.23	-	9,9,9,9	0
32	MG	A	5049	1/1	0.12	-	3,3,3,3	0
32	MG	A	5218	1/1	0.15	-	7,7,7,7	0
32	MG	A	5231	1/1	0.17	-	5,5,5,5	0
32	MG	A	5376	1/1	0.45	-	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5153	1/1	0.10	-	12,12,12,12	0
32	MG	A	5143	1/1	0.24	-	6,6,6,6	0
32	MG	A	5456	1/1	0.16	-	3,3,3,3	0
32	MG	A	5214	1/1	0.22	-	5,5,5,5	0
32	MG	A	5443	1/1	0.26	-	4,4,4,4	0
32	MG	A	5317	1/1	0.45	-	64,64,64,64	0
32	MG	A	5383	1/1	0.14	-	56,56,56,56	0
32	MG	A	5512	1/1	0.21	-	4,4,4,4	0
32	MG	A	5128	1/1	0.55	-	62,62,62,62	0
32	MG	A	5455	1/1	0.20	-	5,5,5,5	0
32	MG	A	5261	1/1	0.11	-	24,24,24,24	0
32	MG	A	5258	1/1	0.09	-	37,37,37,37	0
32	MG	A	5432	1/1	0.51	-	5,5,5,5	0
32	MG	A	5151	1/1	0.23	-	66,66,66,66	0
32	MG	A	5280	1/1	0.22	-	42,42,42,42	0
32	MG	A	5253	1/1	0.38	-	3,3,3,3	0
32	MG	A	5248	1/1	0.32	-	41,41,41,41	0
32	MG	A	5104	1/1	0.75	-	3,3,3,3	0
32	MG	A	5430	1/1	0.64	-	32,32,32,32	0
32	MG	A	5217	1/1	0.27	-	3,3,3,3	0
32	MG	A	5220	1/1	0.26	-	3,3,3,3	0
32	MG	A	5279	1/1	0.17	-	3,3,3,3	0
32	MG	A	5125	1/1	0.18	-	4,4,4,4	0
32	MG	A	5090	1/1	0.30	-	45,45,45,45	0
32	MG	A	5381	1/1	0.15	-	43,43,43,43	0
32	MG	A	5138	1/1	0.19	-	85,85,85,85	0
32	MG	A	5378	1/1	0.24	-	40,40,40,40	0
32	MG	B	5522	1/1	0.12	-	3,3,3,3	0
32	MG	A	5188	1/1	0.23	-	3,3,3,3	0
32	MG	A	5291	1/1	0.19	-	3,3,3,3	0
32	MG	A	5146	1/1	0.26	-	41,41,41,41	0
32	MG	A	5155	1/1	0.26	-	3,3,3,3	0
32	MG	A	5411	1/1	0.12	-	71,71,71,71	0
32	MG	A	5478	1/1	0.24	-	53,53,53,53	0
32	MG	A	5194	1/1	0.22	-	3,3,3,3	0
32	MG	A	5458	1/1	0.38	-	3,3,3,3	0
32	MG	A	5170	1/1	0.13	-	4,4,4,4	0
32	MG	A	5460	1/1	0.15	-	3,3,3,3	0
32	MG	A	5112	1/1	0.73	-	3,3,3,3	0
32	MG	A	5118	1/1	0.43	-	3,3,3,3	0
32	MG	A	5237	1/1	0.21	-	4,4,4,4	0
32	MG	A	5474	1/1	0.09	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5172	1/1	0.64	-	3,3,3,3	0
32	MG	A	5277	1/1	0.35	-	51,51,51,51	0
32	MG	A	5357	1/1	0.12	-	5,5,5,5	0
32	MG	A	5243	1/1	0.14	-	58,58,58,58	0
32	MG	A	5026	1/1	0.61	-	3,3,3,3	0
32	MG	A	5132	1/1	0.06	-	30,30,30,30	0
32	MG	A	5475	1/1	0.15	-	3,3,3,3	0
32	MG	A	5150	1/1	0.18	-	28,28,28,28	0
32	MG	A	5433	1/1	0.59	-	4,4,4,4	0
32	MG	A	5070	1/1	0.31	-	3,3,3,3	0
32	MG	A	5129	1/1	0.77	-	21,21,21,21	0
32	MG	A	5508	1/1	0.34	-	3,3,3,3	0
32	MG	A	5355	1/1	0.16	-	23,23,23,23	0
32	MG	A	5334	1/1	0.59	-	39,39,39,39	0
32	MG	A	5246	1/1	0.12	-	21,21,21,21	0
32	MG	A	5444	1/1	0.58	-	3,3,3,3	0
32	MG	A	5324	1/1	1.38	-	89,89,89,89	0
32	MG	A	5230	1/1	0.19	-	38,38,38,38	0
32	MG	A	5087	1/1	0.25	-	4,4,4,4	0
32	MG	A	5181	1/1	0.27	-	3,3,3,3	0
32	MG	U	5027	1/1	0.23	-	3,3,3,3	0
32	MG	D	5008	1/1	0.19	-	13,13,13,13	0
32	MG	A	5123	1/1	0.24	-	3,3,3,3	0
32	MG	A	5404	1/1	0.28	-	75,75,75,75	0
32	MG	A	5167	1/1	0.16	-	3,3,3,3	0
32	MG	A	5062	1/1	0.30	-	4,4,4,4	0
32	MG	A	5045	1/1	0.30	-	3,3,3,3	0
32	MG	A	5390	1/1	0.24	-	3,3,3,3	0
32	MG	A	5166	1/1	0.42	-	4,4,4,4	0
32	MG	A	5327	1/1	0.88	-	78,78,78,78	0
32	MG	A	5140	1/1	0.20	-	62,62,62,62	0
32	MG	A	5073	1/1	0.23	-	4,4,4,4	0
32	MG	A	5263	1/1	0.15	-	51,51,51,51	0
32	MG	A	5192	1/1	0.23	-	6,6,6,6	0
32	MG	A	5392	1/1	0.15	-	3,3,3,3	0
32	MG	A	5466	1/1	0.29	-	3,3,3,3	0
32	MG	A	5101	1/1	0.20	-	3,3,3,3	0
32	MG	A	5147	1/1	0.20	-	4,4,4,4	0
32	MG	A	5316	1/1	1.45	-	59,59,59,59	0
32	MG	8	5032	1/1	0.50	-	3,3,3,3	0
32	MG	A	5423	1/1	0.16	-	41,41,41,41	0
32	MG	A	5051	1/1	0.22	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5476	1/1	0.12	-	15,15,15,15	0
32	MG	A	5276	1/1	0.30	-	3,3,3,3	0
32	MG	A	5435	1/1	0.37	-	3,3,3,3	0
32	MG	A	5292	1/1	0.32	-	3,3,3,3	0
32	MG	A	5065	1/1	0.25	-	3,3,3,3	0
32	MG	A	5426	1/1	0.41	-	55,55,55,55	0
32	MG	A	5046	1/1	0.15	-	4,4,4,4	0
32	MG	A	5307	1/1	0.40	-	63,63,63,63	0
32	MG	A	5450	1/1	0.08	-	2,2,2,2	0
32	MG	A	5372	1/1	0.35	-	3,3,3,3	0
32	MG	A	5347	1/1	0.84	-	82,82,82,82	0
32	MG	U	5113	1/1	0.33	-	4,4,4,4	0
32	MG	A	5033	1/1	0.67	-	4,4,4,4	0
32	MG	A	5386	1/1	0.48	-	42,42,42,42	0
32	MG	A	5449	1/1	0.15	-	35,35,35,35	0
32	MG	V	5111	1/1	0.22	-	3,3,3,3	0
32	MG	A	5179	1/1	0.11	-	3,3,3,3	0
32	MG	A	5269	1/1	0.19	-	4,4,4,4	0
32	MG	A	5403	1/1	0.43	-	88,88,88,88	0
32	MG	A	5321	1/1	1.07	-	63,63,63,63	0
32	MG	A	5165	1/1	0.25	-	3,3,3,3	0
32	MG	A	5044	1/1	0.23	-	3,3,3,3	0
32	MG	A	5148	1/1	0.19	-	5,5,5,5	0
32	MG	A	5075	1/1	0.22	-	3,3,3,3	0
32	MG	A	5235	1/1	0.27	-	3,3,3,3	0
32	MG	A	5137	1/1	0.11	-	26,26,26,26	0
32	MG	A	5502	1/1	0.17	-	3,3,3,3	0
32	MG	A	5497	1/1	0.27	-	3,3,3,3	0
32	MG	A	5252	1/1	0.07	-	4,4,4,4	0
32	MG	O	5017	1/1	0.43	-	3,3,3,3	0
32	MG	A	5014	1/1	0.14	-	3,3,3,3	0
32	MG	D	5480	1/1	0.13	-	23,23,23,23	0
32	MG	A	5077	1/1	0.18	-	3,3,3,3	0
32	MG	A	5139	1/1	0.19	-	83,83,83,83	0
32	MG	A	5275	1/1	0.16	-	6,6,6,6	0
32	MG	A	5222	1/1	0.72	-	3,3,3,3	0
32	MG	A	5242	1/1	0.33	-	3,3,3,3	0
32	MG	Q	5021	1/1	0.22	-	4,4,4,4	0
32	MG	A	5297	1/1	0.12	-	3,3,3,3	0
32	MG	A	5040	1/1	0.26	-	6,6,6,6	0
32	MG	A	5382	1/1	0.24	-	56,56,56,56	0
32	MG	A	5124	1/1	0.32	-	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	5361	1/1	0.59	-	3,3,3,3	0
32	MG	A	5412	1/1	0.24	-	3,3,3,3	0
32	MG	A	5359	1/1	0.40	-	33,33,33,33	0
32	MG	A	5384	1/1	0.29	-	3,3,3,3	0
32	MG	A	5363	1/1	0.29	-	25,25,25,25	0
32	MG	A	5485	1/1	0.19	-	5,5,5,5	0
32	MG	A	5271	1/1	0.20	-	41,41,41,41	0
32	MG	A	5052	1/1	0.28	-	6,6,6,6	0
32	MG	A	5116	1/1	0.17	-	3,3,3,3	0
32	MG	A	5200	1/1	0.58	-	3,3,3,3	0
32	MG	A	5420	1/1	0.43	-	38,38,38,38	0
32	MG	A	5393	1/1	0.56	-	86,86,86,86	0
32	MG	A	5338	1/1	0.46	-	72,72,72,72	0
32	MG	A	5094	1/1	0.14	-	3,3,3,3	0
32	MG	A	5385	1/1	0.40	-	54,54,54,54	0
32	MG	A	5493	1/1	0.12	-	3,3,3,3	0
32	MG	A	5190	1/1	0.21	-	4,4,4,4	0
32	MG	A	5054	1/1	0.25	-	4,4,4,4	0
32	MG	A	5490	1/1	0.23	-	4,4,4,4	0
32	MG	A	5092	1/1	0.13	-	17,17,17,17	0
32	MG	A	5238	1/1	0.23	-	5,5,5,5	0
32	MG	A	5215	1/1	0.36	-	4,4,4,4	0
32	MG	A	5210	1/1	0.23	-	4,4,4,4	0
32	MG	A	5099	1/1	0.39	-	3,3,3,3	0
32	MG	A	5331	1/1	0.42	-	76,76,76,76	0
32	MG	A	5442	1/1	0.10	-	5,5,5,5	0
32	MG	A	5273	1/1	0.10	-	3,3,3,3	0

6.5 Other polymers ⓘ

There are no such residues in this entry.