



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:17 PM GMT

PDB ID : 3D5D
Title : Structural basis for translation termination on the 70S ribosome. 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 : 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 full wwPDB validation 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>

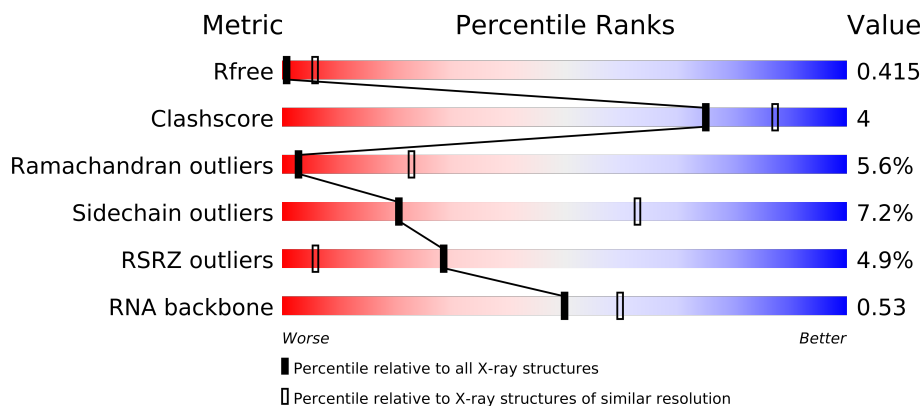
The following versions of software and data (see [references](#)) were used in the production of this report:

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.












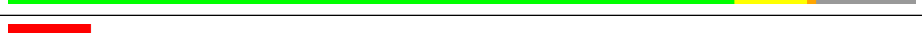

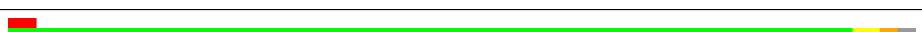


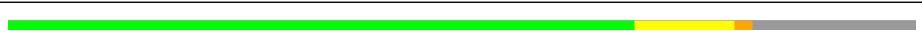





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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	D	276	
2	E	206	
3	F	210	
4	G	182	
5	H	180	
6	I	148	
7	J	173	
8	N	163	
9	O	122	
10	P	150	
11	Q	141	

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Mol	Chain	Length	Quality of chain
12	R	118	
13	S	112	
14	T	146	
15	U	118	
16	V	101	
17	W	113	
18	X	96	
19	Y	110	
20	Z	206	
21	0	85	
22	1	98	
23	2	72	
24	3	60	
25	4	97	
26	5	60	
27	6	54	
28	7	49	
29	8	65	
30	A	2894	
31	B	124	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 91732 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 protein called 50S ribosomal protein L2.

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

^ Molecule 2 is a protein called 50S ribosomal protein L3.

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

^ Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	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 4 is a protein called 50S ribosomal protein L5.

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

^ Molecule 5 is a protein called 50S ribosomal protein L6.

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

^ Molecule 6 is a protein called 50S ribosomal protein L9.

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

^ Molecule 7 is a protein called 50S ribosomal protein L10.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 9 is a protein called 50S ribosomal protein L14.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	76	Total	C	N	O	S	0	0	0
			605	376	126	102	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	1	88	Total	C	N	O	0	0	0
			694	435	141	118			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2	72	Total	C	N	O	S	0	0	0
			605	375	122	106	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

^ Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	5	52	Total	C	N	O	S	0	0	0
			404	255	79	65	5			

^ Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

^ Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

^ Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

^ Molecule 30 is a RNA chain called 23S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

^ Molecule 31 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	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 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	7	Total	Mg	0	0
			7	7		
32	B	28	Total	Mg	0	0
			28	28		
32	W	3	Total	Mg	0	0
			3	3		
32	N	1	Total	Mg	0	0
			1	1		
32	X	1	Total	Mg	0	0
			1	1		
32	2	2	Total	Mg	0	0
			2	2		
32	E	2	Total	Mg	0	0
			2	2		
32	V	1	Total	Mg	0	0
			1	1		
32	A	752	Total	Mg	0	0
			752	752		
32	5	1	Total	Mg	0	0
			1	1		
32	R	2	Total	Mg	0	0
			2	2		
32	D	1	Total	Mg	0	0
			1	1		
32	I	2	Total	Mg	0	0
			2	2		
32	Z	4	Total	Mg	0	0
			4	4		
32	4	3	Total	Mg	0	0
			3	3		

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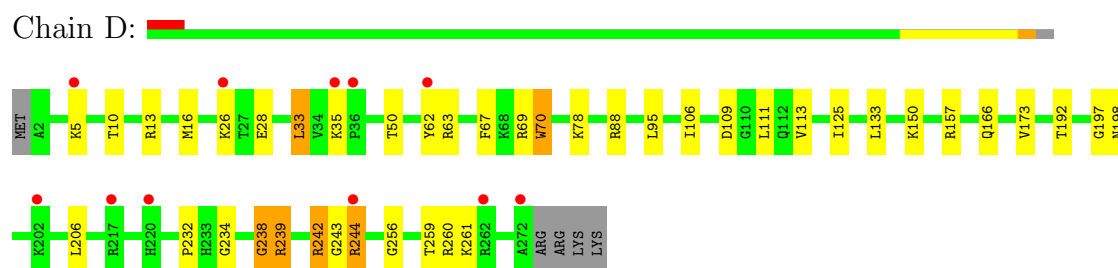
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	U	2	Total 2	Mg 2	0	0
32	G	1	Total 1	Mg 1	0	0
32	Q	1	Total 1	Mg 1	0	0
32	H	4	Total 4	Mg 4	0	0
32	7	2	Total 2	Mg 2	0	0
32	T	1	Total 1	Mg 1	0	0
32	8	1	Total 1	Mg 1	0	0
32	O	2	Total 2	Mg 2	0	0
32	3	1	Total 1	Mg 1	0	0
32	F	1	Total 1	Mg 1	0	0

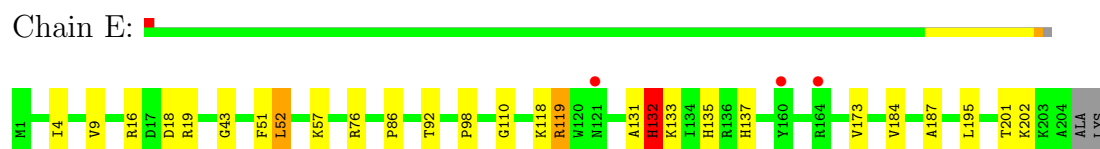
3 Residue-property plots

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

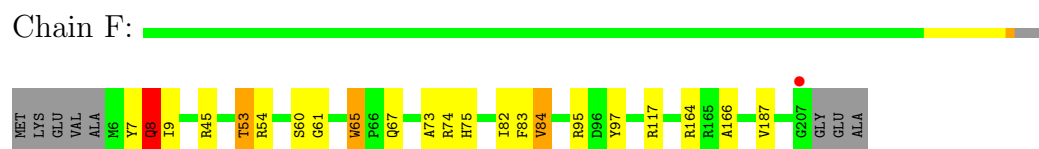
- Molecule 1: 50S ribosomal protein L2



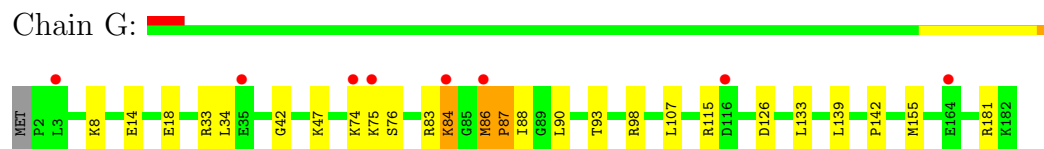
- Molecule 2: 50S ribosomal protein L3



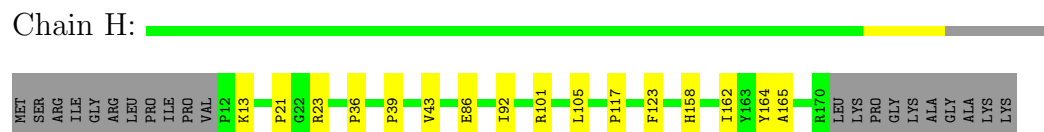
- Molecule 3: 50S ribosomal protein L4



- Molecule 4: 50S ribosomal protein L5

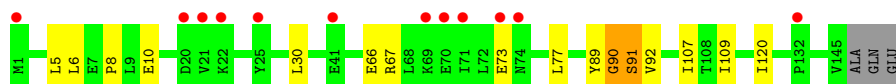


- Molecule 5: 50S ribosomal protein L6



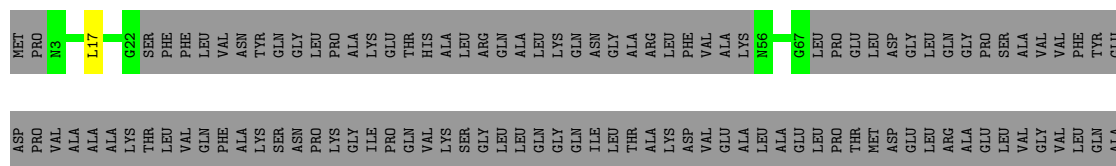
- Molecule 6: 50S ribosomal protein L9





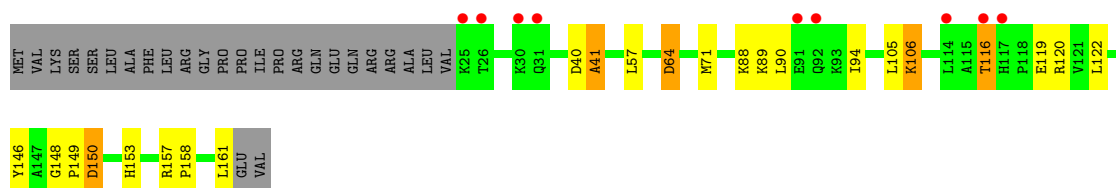
- Molecule 7: 50S ribosomal protein L10

Chain J:



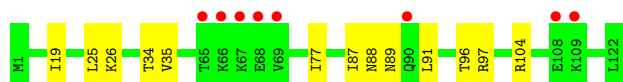
- Molecule 8: 50S ribosomal protein L13

Chain N:



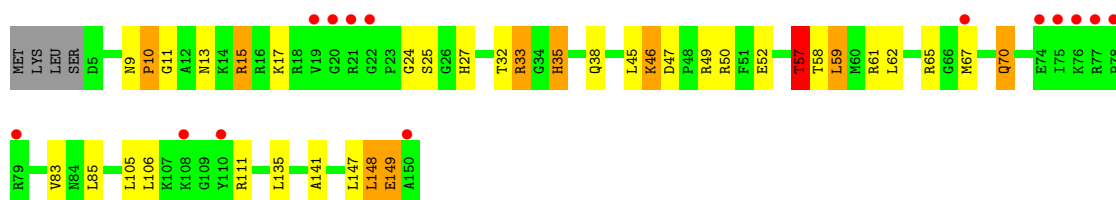
- Molecule 9: 50S ribosomal protein L14

Chain O:



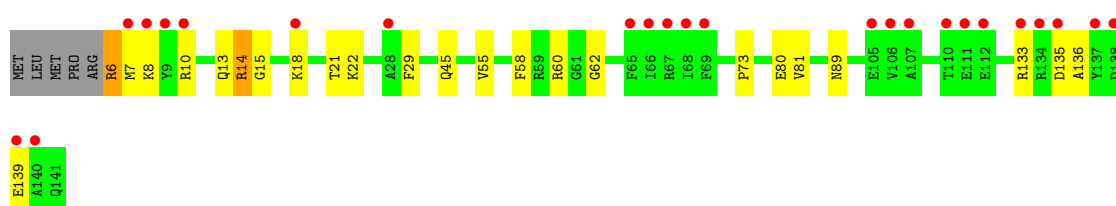
- Molecule 10: 50S ribosomal protein L15

Chain P:



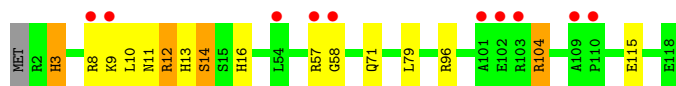
- Molecule 11: 50S ribosomal protein L16

Chain Q:



- Molecule 12: 50S ribosomal protein L17

Chain R: 



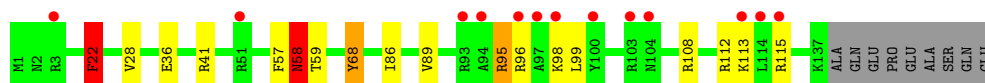
- Molecule 13: 50S ribosomal protein L18

Chain S: 



- Molecule 14: 50S ribosomal protein L19

Chain T: 



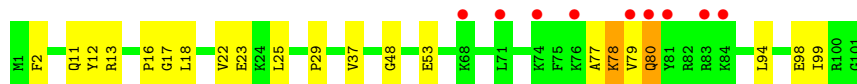
- Molecule 15: 50S ribosomal protein L20

Chain U: 



- Molecule 16: 50S ribosomal protein L21

Chain V: 



- Molecule 17: 50S ribosomal protein L22

Chain W: 



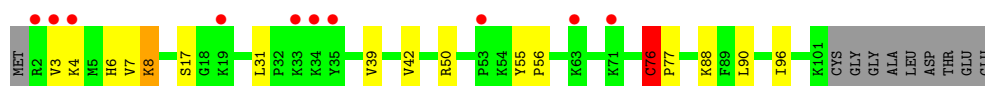
- Molecule 18: 50S ribosomal protein L23

Chain X: 



- Molecule 19: 50S ribosomal protein L24

Chain Y: 



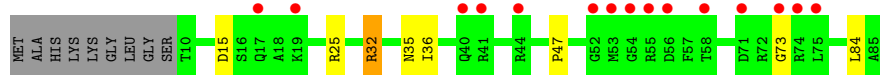
- Molecule 20: 50S ribosomal protein L25

Chain Z:



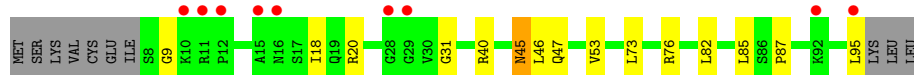
- Molecule 21: 50S ribosomal protein L27

Chain 0:



- Molecule 22: 50S ribosomal protein L28

Chain 1:



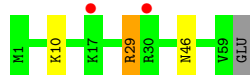
- Molecule 23: 50S ribosomal protein L29

Chain 2:



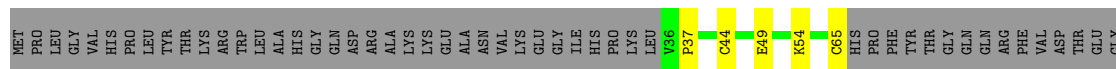
- Molecule 24: 50S ribosomal protein L30

Chain 3:



- Molecule 25: 50S ribosomal protein L31

Chain 4:



- Molecule 26: 50S ribosomal protein L32

Chain 5:



- Molecule 27: 50S ribosomal protein L33

Chain 6:



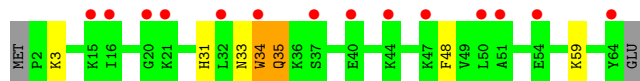
- Molecule 28: 50S ribosomal protein L34

Chain 7:



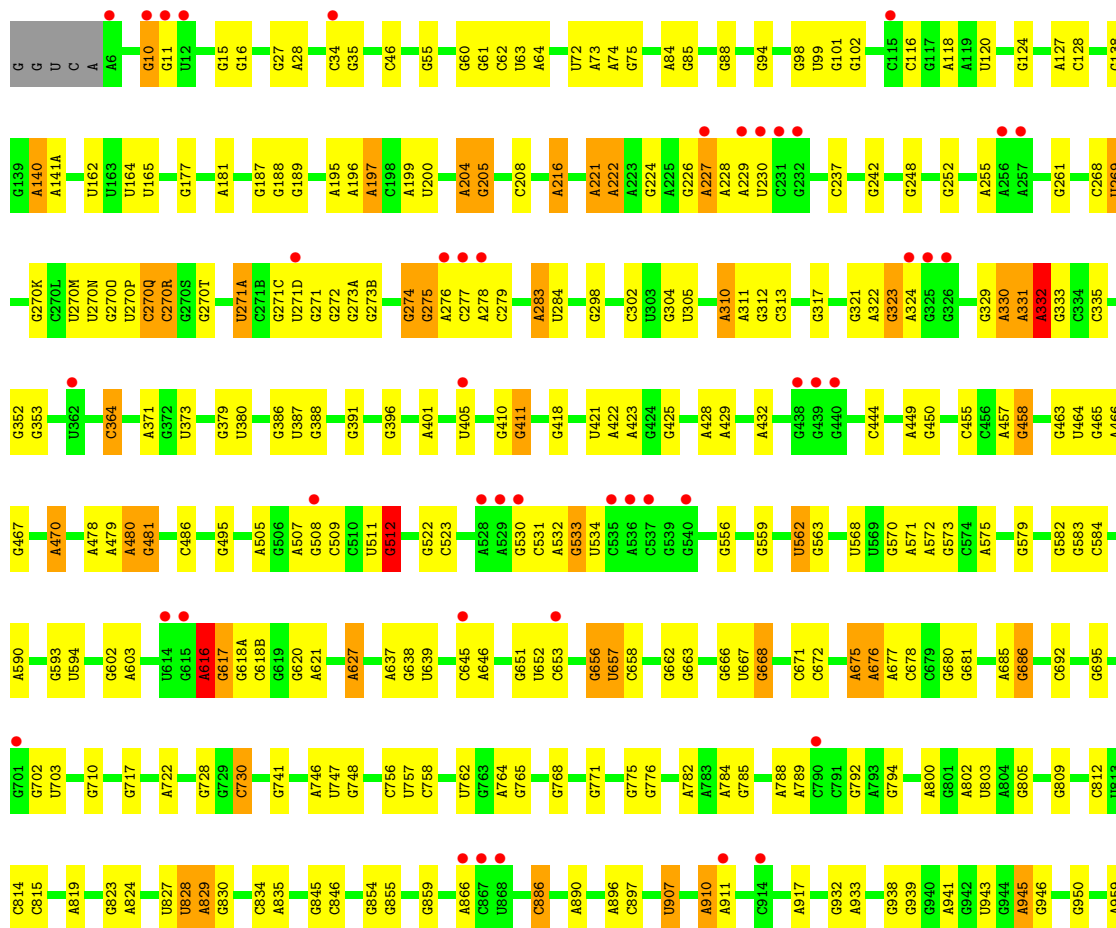
- Molecule 29: 50S ribosomal protein L35

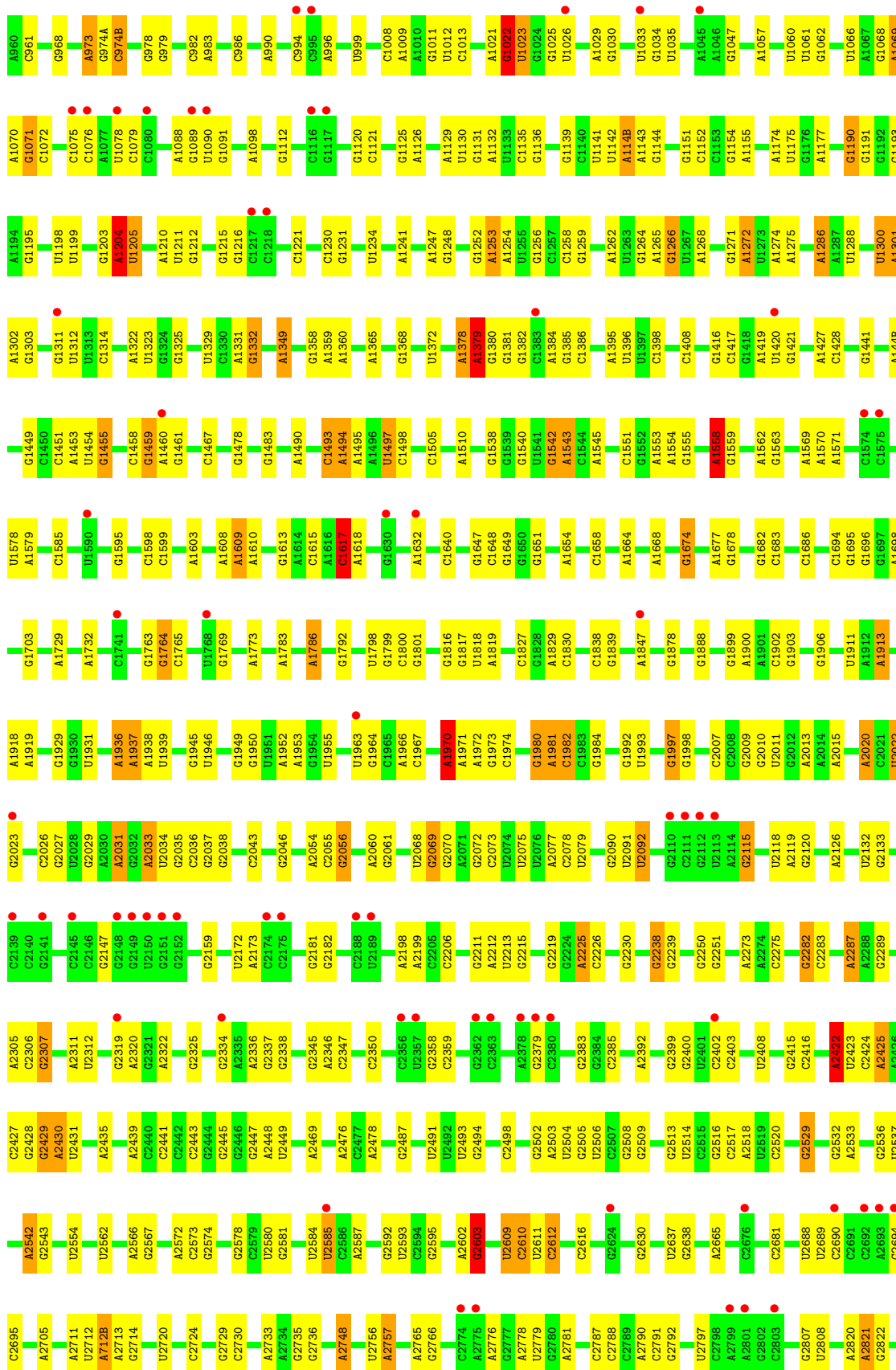
Chain 8:

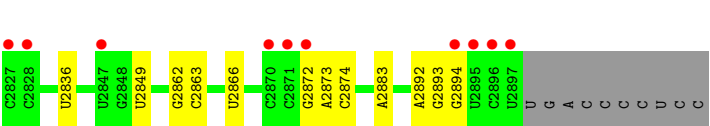


- Molecule 30: 23S rRNA

Chain A:







● Molecule 31: 5S rRNA

Chain B:



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 0.412 , 0.415	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)	0.11 , -2.7	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	91732	wwPDB-VP
Average B, all atoms (Å ²)	130.0	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	D	0.26	0/2154	0.44	0/2905
2	E	0.23	0/1596	0.44	0/2153
3	F	0.23	0/1621	0.40	0/2194
4	G	0.21	0/1500	0.40	0/2017
5	H	0.20	0/1245	0.40	0/1682
6	I	0.21	0/1147	0.41	0/1552
7	J	0.21	0/251	0.38	0/333
8	N	0.22	0/1123	0.44	0/1515
9	O	0.24	0/942	0.42	0/1268
10	P	0.24	0/1131	0.46	0/1504
11	Q	0.24	0/1099	0.44	0/1468
12	R	0.22	0/974	0.41	0/1302
13	S	0.21	0/778	0.38	0/1036
14	T	0.22	0/1157	0.39	0/1544
15	U	0.28	0/982	0.42	0/1306
16	V	0.23	0/790	0.40	0/1057
17	W	0.24	0/901	0.39	0/1209
18	X	0.24	0/739	0.41	0/993
19	Y	0.24	0/788	0.43	0/1051
20	Z	0.22	0/1523	0.42	0/2068
21	0	0.22	0/613	0.39	0/816
22	1	0.25	0/701	0.47	0/932
23	2	0.24	0/607	0.48	0/803
24	3	0.22	0/472	0.40	0/634
25	4	0.21	0/228	0.41	0/309
26	5	0.22	0/418	0.43	0/567
27	6	0.23	0/387	0.43	0/518
28	7	0.25	0/426	0.41	0/561
29	8	0.24	0/515	0.41	0/679
30	A	0.44	0/69437	0.89	55/108401 (0.1%)
31	B	0.41	0/2853	0.84	1/4451 (0.0%)
All	All	0.39	0/99098	0.80	56/148828 (0.0%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	1379	A	C1'-O4'-C4'	-11.90	100.38	109.90
30	A	1091	G	P-O3'-C3'	10.71	132.56	119.70
30	A	1786	A	C1'-O4'-C4'	-9.82	102.04	109.90
30	A	1786	A	C3'-C2'-C1'	-8.49	94.70	101.50
30	A	1071	G	P-O3'-C3'	-8.41	109.61	119.70
30	A	1069	A	P-O3'-C3'	8.08	129.39	119.70
30	A	1786	A	O4'-C1'-N9	7.79	114.43	108.20
30	A	1098	A	P-O3'-C3'	-7.72	110.43	119.70
30	A	1913	A	C1'-O4'-C4'	-7.67	103.76	109.90
30	A	1022	G	P-O3'-C3'	7.57	128.79	119.70
30	A	2603	G	C4'-C3'-C2'	-7.50	95.10	102.60
30	A	1558	A	P-O3'-C3'	7.35	128.52	119.70
30	A	1266	G	C3'-C2'-C1'	-7.02	95.89	101.50
30	A	2603	G	C1'-O4'-C4'	-6.85	104.42	109.90
30	A	1069	A	O4'-C1'-N9	6.70	113.56	108.20
30	A	512	G	C1'-O4'-C4'	-6.57	104.64	109.90
30	A	221	A	P-O3'-C3'	6.55	127.56	119.70
30	A	945	A	C1'-O4'-C4'	-6.51	104.69	109.90
30	A	1300	U	P-O3'-C3'	6.50	127.50	119.70
30	A	676	A	C1'-O4'-C4'	-6.49	104.71	109.90
30	A	1937	A	P-O3'-C3'	6.33	127.29	119.70
30	A	2603	G	O4'-C1'-N9	6.27	113.22	108.20
30	A	1786	A	O4'-C1'-C2'	-6.16	99.64	105.80
30	A	2422	A	P-O3'-C3'	6.03	126.94	119.70
30	A	1365	A	C4'-C3'-C2'	-5.97	96.62	102.60
30	A	2346	A	C1'-O4'-C4'	-5.84	105.23	109.90
30	A	1698	A	C3'-C2'-C1'	-5.71	96.93	101.50
30	A	205	G	C3'-C2'-C1'	-5.67	96.96	101.50
30	A	616	A	P-O3'-C3'	5.62	126.45	119.70
30	A	1913	A	O4'-C1'-N9	5.62	112.69	108.20
30	A	2225	A	P-O3'-C3'	5.47	126.26	119.70
30	A	387	U	C3'-C2'-C1'	-5.44	97.15	101.50
30	A	283	A	P-O3'-C3'	5.43	126.22	119.70
30	A	1195	G	C4'-C3'-C2'	-5.42	97.18	102.60
30	A	1241	A	C1'-O4'-C4'	-5.41	105.57	109.90
30	A	1204	A	C3'-C2'-C1'	-5.33	97.24	101.50
30	A	332	A	P-O3'-C3'	5.30	126.07	119.70
30	A	401	A	C1'-O4'-C4'	-5.28	105.68	109.90
30	A	128	C	P-O3'-C3'	-5.27	113.38	119.70
30	A	1970	A	C1'-O4'-C4'	-5.23	105.72	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	907	U	C4'-C3'-C2'	-5.20	97.40	102.60
30	A	317	G	C4'-C3'-C2'	-5.18	97.42	102.60
30	A	562	U	C3'-C2'-C1'	5.17	105.64	101.50
30	A	2609	U	C3'-C2'-C1'	-5.17	97.36	101.50
30	A	627	A	C3'-C2'-C1'	-5.16	97.37	101.50
30	A	1098	A	OP1-P-O3'	5.15	116.53	105.20
30	A	1494	A	P-O3'-C3'	5.12	125.85	119.70
30	A	1378	A	P-O3'-C3'	5.10	125.82	119.70
30	A	974(B)	C	C3'-C2'-C1'	-5.09	97.42	101.50
30	A	1071	G	N9-C1'-C2'	-5.09	106.40	112.00
30	A	2595	G	C4'-C3'-C2'	-5.08	97.52	102.60
31	B	84	C	C4'-C3'-C2'	-5.08	97.53	102.60
30	A	2092	U	P-O3'-C3'	5.07	125.79	119.70
30	A	2035	G	C1'-O4'-C4'	-5.07	105.85	109.90
30	A	2346	A	C3'-C2'-C1'	-5.03	97.47	101.50
30	A	1617	C	C4'-C3'-C2'	-5.02	97.58	102.60

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	D	2104	0	0	9	0
2	E	1563	0	0	8	0
3	F	1586	0	0	7	0
4	G	1475	0	0	4	0
5	H	1222	0	0	0	0
6	I	1132	0	0	1	0
7	J	253	0	0	0	0
8	N	1096	0	0	6	0
9	O	932	0	0	4	0
10	P	1114	0	0	8	0
11	Q	1079	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	R	960	0	0	7	0
13	S	770	0	0	3	0
14	T	1143	0	0	4	0
15	U	964	0	0	10	0
16	V	779	0	0	4	0
17	W	890	0	0	0	0
18	X	725	0	0	2	0
19	Y	775	0	0	2	0
20	Z	1491	0	0	3	0
21	0	605	0	0	1	0
22	1	694	0	0	2	0
23	2	605	0	0	8	0
24	3	467	0	0	0	0
25	4	225	0	0	0	0
26	5	404	0	0	3	0
27	6	380	0	0	1	0
28	7	418	0	0	2	0
29	8	507	0	0	2	0
30	A	61997	0	0	265	0
31	B	2551	0	0	8	0
32	2	2	0	0	0	0
32	3	1	0	0	0	0
32	4	3	0	0	0	0
32	5	1	0	0	0	0
32	7	2	0	0	0	0
32	8	1	0	0	0	0
32	A	752	0	0	0	0
32	B	28	0	0	0	0
32	D	1	0	0	0	0
32	E	2	0	0	0	0
32	F	1	0	0	0	0
32	G	1	0	0	0	0
32	H	4	0	0	0	0
32	I	2	0	0	0	0
32	N	1	0	0	0	0
32	O	2	0	0	0	0
32	P	7	0	0	0	0
32	Q	1	0	0	0	0
32	R	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	W	3	0	0	0	0
32	X	1	0	0	0	0
32	Z	4	0	0	0	0
All	All	91732	0	0	351	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.

All (351) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:83:PHE:O	3:F:84:VAL:C	2.39	0.61
19:Y:8:LYS:N	19:Y:8:LYS:NZ	2.49	0.59
19:Y:76:CYS:CB	19:Y:77:PRO:CD	2.81	0.59
11:Q:14:ARG:NH1	11:Q:14:ARG:CG	2.65	0.58
12:R:104:ARG:NH1	12:R:104:ARG:CG	2.66	0.57
15:U:31:SER:O	15:U:32:PHE:C	2.42	0.57
30:A:1899:G:N2	30:A:1902:C:N4	2.51	0.57
27:6:30:THR:O	27:6:32:ASN:N	2.38	0.57
30:A:910:A:C6	30:A:911:A:C6	2.93	0.57
20:Z:166:SER:O	20:Z:168:GLU:N	2.38	0.56
30:A:2637:U:C4	30:A:2638:G:C6	2.94	0.56
12:R:3:HIS:CE1	30:A:1654:A:OP2	2.59	0.56
4:G:86:MET:N	4:G:87:PRO:CD	2.69	0.55
30:A:216:A:C8	30:A:432:A:C6	2.94	0.55
30:A:332:A:C6	30:A:335:C:C2	2.94	0.55
1:D:238:GLY:O	1:D:239:ARG:C	2.45	0.55
30:A:140:A:C6	30:A:141(A):A:N6	2.76	0.54
2:E:110:GLY:N	30:A:2821:A:OP1	2.41	0.54
30:A:2580:U:C5	30:A:2581:G:C6	2.95	0.54
12:R:11:ASN:OD1	12:R:12:ARG:N	2.41	0.54
30:A:2513:G:C2	30:A:2514:U:C2	2.97	0.53
30:A:702:G:C6	30:A:703:U:C4	2.97	0.53
23:2:17:SER:CB	23:2:18:PRO:CD	2.86	0.53
1:D:242:ARG:CD	1:D:242:ARG:N	2.71	0.53
23:2:58:ALA:O	23:2:62:THR:N	2.41	0.53
30:A:1952:A:C6	30:A:1953:A:C6	2.97	0.53
30:A:1034:G:C5	30:A:1035:U:C4	2.97	0.53
30:A:756:C:C4	30:A:757:U:C5	2.97	0.52
16:V:78:LYS:NZ	30:A:973:A:OP2	2.42	0.52
2:E:132:HIS:ND1	30:A:1658:C:OP1	2.43	0.52
31:B:67:G:N2	31:B:68:C:C2	2.78	0.52
23:2:47:ASN:ND2	30:A:61:G:C5	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:A:1332:G:N2	30:A:1609:A:O2'	2.43	0.52
30:A:2807:G:N1	30:A:2893:G:O6	2.43	0.52
23:2:47:ASN:ND2	30:A:94:G:N2	2.58	0.51
30:A:2592:G:C2	30:A:2603:G:C2	2.98	0.51
30:A:204:A:OP1	30:A:204:A:C8	2.64	0.51
30:A:1570:A:C6	30:A:1571:A:C6	2.98	0.51
16:V:22:VAL:CG1	16:V:23:GLU:N	2.74	0.51
2:E:119:ARG:CG	2:E:119:ARG:NH1	2.74	0.51
30:A:481:G:O2'	30:A:507:A:N6	2.44	0.51
14:T:22:PHE:CD2	14:T:22:PHE:N	2.79	0.51
9:O:88:ASN:OD1	9:O:89:ASN:N	2.43	0.51
28:7:19:ARG:NH2	30:A:124:G:C6	2.79	0.51
30:A:10:G:C8	30:A:11:G:C8	3.00	0.50
23:2:17:SER:O	23:2:21:LEU:N	2.44	0.50
30:A:1203:G:O6	30:A:1204:A:N6	2.45	0.50
30:A:371:A:C8	30:A:373:U:C2	3.00	0.50
30:A:1952:A:C6	30:A:1953:A:N1	2.79	0.50
4:G:86:MET:O	4:G:87:PRO:O	2.30	0.50
30:A:27:G:O2'	30:A:28:A:C8	2.65	0.50
3:F:53:THR:OG1	3:F:54:ARG:N	2.45	0.49
30:A:2392:A:C6	30:A:2429:G:C8	2.99	0.49
31:B:46:A:C5	31:B:47:C:C4	3.01	0.49
30:A:1252:G:C2	30:A:1253:A:C2	3.01	0.49
30:A:656:G:C6	30:A:657:U:C4	3.01	0.49
6:I:90:GLY:O	6:I:91:SER:CB	2.60	0.49
30:A:1286:A:O2'	30:A:1288:U:OP2	2.30	0.49
1:D:67:PHE:CE1	1:D:157:ARG:NH1	2.80	0.49
30:A:686:G:N2	30:A:788:A:N6	2.60	0.49
10:P:57:THR:C	10:P:59:LEU:N	2.66	0.49
30:A:464:U:C2	30:A:788:A:C6	3.01	0.49
30:A:330:A:O2'	30:A:331:A:C8	2.65	0.49
30:A:1799:G:N1	30:A:1819:A:OP2	2.46	0.49
30:A:1331:A:O2'	30:A:1332:G:C8	2.66	0.49
30:A:2688:U:C5	30:A:2720:U:OP2	2.65	0.49
30:A:1900:A:N1	30:A:1970:A:C6	2.81	0.48
14:T:95:ARG:CG	14:T:95:ARG:NH1	2.74	0.48
30:A:1322:A:C5	30:A:1323:U:C5	3.01	0.48
30:A:410:G:C2	30:A:418:G:C2	3.01	0.48
30:A:1125:G:C6	30:A:1126:A:N6	2.81	0.48
30:A:463:G:N1	30:A:467:G:C6	2.81	0.48
23:2:61:LEU:O	23:2:65:ASN:N	2.46	0.48
30:A:583:G:C5	30:A:584:C:C5	3.02	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:A:680:G:C6	30:A:681:G:C6	3.01	0.48
30:A:1301:A:C8	30:A:1303:G:C8	3.02	0.48
1:D:243:GLY:O	1:D:244:ARG:CB	2.61	0.48
30:A:2282:G:C2	30:A:2425:A:C5	3.02	0.48
30:A:1997:G:C2	30:A:1998:G:C5	3.02	0.48
30:A:2026:C:C4	30:A:2027:G:N7	2.82	0.48
14:T:57:PHE:CG	14:T:58:ASN:N	2.81	0.48
13:S:90:GLY:O	13:S:92:TYR:N	2.47	0.48
2:E:131:ALA:O	2:E:133:LYS:N	2.47	0.47
30:A:768:G:O2'	30:A:1379:A:N6	2.48	0.47
30:A:1497:U:N3	30:A:1578:U:OP1	2.48	0.47
30:A:728:G:C2	30:A:730:C:C2	3.02	0.47
30:A:1936:A:C8	30:A:1945:G:C8	3.01	0.47
30:A:269:U:C4	30:A:271(A):U:C2	3.03	0.47
30:A:2069:G:N2	30:A:2443:C:C2	2.82	0.47
30:A:2592:G:C6	30:A:2593:U:C2	3.03	0.47
10:P:35:HIS:CD2	30:A:1191:G:OP1	2.68	0.47
12:R:13:HIS:O	12:R:14:SER:C	2.53	0.47
3:F:65:TRP:CZ3	3:F:75:HIS:CD2	3.03	0.47
14:T:68:TYR:N	14:T:68:TYR:CD2	2.83	0.47
3:F:45:ARG:NH2	3:F:97:TYR:CZ	2.83	0.47
30:A:938:G:C2	30:A:939:G:N7	2.83	0.47
29:8:31:HIS:CE1	30:A:2422:A:N7	2.83	0.47
30:A:1022:G:O2'	30:A:1023:U:P	2.73	0.46
30:A:1198:U:C2	30:A:1199:U:C5	3.03	0.46
30:A:2711:A:OP1	30:A:712(B):A:P	2.72	0.46
15:U:53:ARG:NH2	30:A:994:C:OP1	2.49	0.46
30:A:391:G:C5	30:A:411:G:C2	3.03	0.46
30:A:222:A:N6	30:A:224:G:C2	2.84	0.46
30:A:1408:C:C2	30:A:1595:G:N2	2.83	0.46
30:A:579:G:C2	30:A:1262:A:C4	3.04	0.46
2:E:135:HIS:CD2	30:A:1658:C:OP1	2.69	0.46
30:A:2069:G:C6	30:A:2070:G:N7	2.83	0.46
8:N:119:GLU:OE1	8:N:119:GLU:N	2.49	0.46
30:A:422:A:C6	30:A:423:A:C6	3.04	0.46
30:A:1651:G:C2	30:A:2007:C:N3	2.84	0.46
30:A:312:G:C6	30:A:313:C:C4	3.04	0.46
30:A:1349:A:N6	30:A:1598:C:N4	2.64	0.45
30:A:828:U:C5	30:A:829:A:N6	2.84	0.45
30:A:1190:G:C5'	30:A:1190:G:C8	2.99	0.45
30:A:2069:G:C2	30:A:2070:G:C8	3.04	0.45
30:A:2862:G:C6	30:A:2863:C:C4	3.04	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:A:1022:G:C6	30:A:1141:U:C5	3.04	0.45
8:N:105:LEU:O	8:N:106:LYS:C	2.54	0.45
13:S:34:HIS:N	13:S:34:HIS:CD2	2.85	0.45
29:8:34:TRP:CG	29:8:35:GLN:N	2.84	0.45
30:A:710:G:C6	30:A:722:A:C6	3.05	0.45
30:A:55:G:O2'	30:A:127:A:N1	2.48	0.45
18:X:55:ASN:ND2	18:X:55:ASN:N	2.65	0.45
22:1:45:ASN:ND2	22:1:47:GLN:NE2	2.65	0.45
15:U:90:VAL:O	15:U:92:ARG:N	2.50	0.45
21:0:32:ARG:N	21:0:35:ASN:ND2	2.65	0.45
30:A:1677:A:C5	30:A:1678:G:C5	3.05	0.45
9:O:88:ASN:O	9:O:91:LEU:N	2.49	0.45
30:A:304:G:C6	30:A:305:U:C4	3.05	0.45
30:A:823:G:C6	30:A:824:A:C6	3.05	0.45
30:A:2090:G:C6	30:A:2230:G:C6	3.05	0.45
30:A:2821:A:OP2	30:A:2822:G:OP2	2.34	0.45
30:A:583:G:C6	30:A:584:C:C5	3.04	0.45
31:B:9:G:C6	31:B:112:G:C6	3.05	0.45
30:A:2516:G:C6	30:A:2517:C:N4	2.84	0.45
30:A:1817:G:C6	30:A:1818:U:C5	3.05	0.44
30:A:449:A:C6	30:A:450:G:C5	3.05	0.44
30:A:272:G:C2	30:A:273(A):G:C4	3.05	0.44
26:5:4:HIS:O	30:A:2056:G:N2	2.50	0.44
3:F:67:GLN:NE2	30:A:675:A:C4'	2.81	0.44
30:A:449:A:N6	30:A:450:G:C6	2.85	0.44
30:A:478:A:C6	30:A:480:A:C6	3.05	0.44
30:A:1668:A:C5	30:A:1674:G:C5	3.06	0.44
31:B:82:G:C2	31:B:95:U:C2	3.05	0.44
30:A:1381:G:C6	30:A:1382:G:C6	3.06	0.44
30:A:950:G:C2	30:A:968:G:C2	3.05	0.44
31:B:89(A):G:C6	31:B:89(B):A:C6	3.06	0.44
30:A:2735:G:C2	30:A:2736:G:C5	3.05	0.44
30:A:618(A):G:C2	30:A:618(B):C:C2	3.05	0.44
30:A:1945:G:C6	30:A:1946:U:C4	3.06	0.44
22:1:45:ASN:ND2	22:1:45:ASN:C	2.70	0.44
30:A:2517:C:C2	30:A:2542:A:N1	2.85	0.44
30:A:1268:A:C2	30:A:2013:A:C4	3.06	0.44
30:A:2206:C:N3	30:A:2219:G:C2	2.86	0.44
30:A:1769:G:C6	30:A:1984:G:C6	3.06	0.44
30:A:2077:A:C5	30:A:2435:A:C5	3.05	0.44
15:U:14:HIS:CE1	15:U:32:PHE:CD2	3.06	0.44
30:A:1668:A:C4	30:A:1674:G:N7	2.86	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:A:2307:G:N2	30:A:2312:U:C4	2.86	0.44
30:A:2029:G:C4	30:A:2031:A:OP2	2.71	0.44
30:A:1066:U:O2'	30:A:1068:G:N7	2.51	0.44
30:A:1615:C:C5	30:A:1617:C:C4	3.06	0.44
30:A:590:A:C4	30:A:668:G:N2	2.85	0.44
30:A:854:G:C2	30:A:855:G:C5	3.05	0.44
15:U:79:PHE:CD1	15:U:79:PHE:C	2.90	0.44
30:A:1980:G:C6	30:A:1982:C:N4	2.86	0.44
31:B:16:G:C6	31:B:69:G:C2	3.06	0.44
30:A:2020:A:C5	30:A:2022:U:C5	3.06	0.44
30:A:1792:G:N2	30:A:1827:C:O2	2.51	0.44
8:N:40:ASP:CG	8:N:41:ALA:N	2.71	0.44
1:D:13:ARG:NH1	1:D:16:MET:SD	2.91	0.44
30:A:242:G:N2	30:A:255:A:OP2	2.50	0.44
12:R:3:HIS:NE2	30:A:1654:A:OP2	2.51	0.44
30:A:274:G:C6	30:A:275:G:N2	2.86	0.44
30:A:195:A:N7	30:A:197:A:OP1	2.51	0.44
30:A:666:G:C5	30:A:667:U:C4	3.06	0.44
30:A:226:G:O2'	30:A:227:A:C8	2.71	0.44
2:E:135:HIS:NE2	30:A:1658:C:OP1	2.51	0.43
30:A:1651:G:N2	30:A:2007:C:C2	2.86	0.43
20:Z:182:LYS:O	20:Z:186:GLU:N	2.50	0.43
10:P:9:ASN:N	10:P:10:PRO:CD	2.81	0.43
30:A:2748:A:C6	30:A:2757:A:N7	2.87	0.43
30:A:2181:G:C2	30:A:2182:G:C8	3.07	0.43
30:A:140:A:N6	30:A:141(A):A:N6	2.66	0.43
30:A:1075:C:C2'	30:A:1076:C:C6	3.01	0.43
30:A:950:G:C6	30:A:968:G:N1	2.86	0.43
30:A:2287:A:C6	30:A:2289:G:C4	3.07	0.43
30:A:2250:G:O4'	30:A:2250:G:N3	2.51	0.43
4:G:93:THR:N	31:B:42:C:O2	2.51	0.43
30:A:579:G:N2	30:A:1262:A:C4	2.87	0.43
30:A:616:A:O2'	30:A:617:G:P	2.76	0.43
30:A:638:G:C5	30:A:651:G:C2	3.07	0.43
30:A:1562:A:C2	30:A:1563:G:C4	3.07	0.43
30:A:273(B):G:C6	30:A:364:C:N4	2.87	0.43
30:A:616:A:O2'	30:A:617:G:O4'	2.36	0.43
26:5:2:ALA:N	30:A:2015:A:N3	2.67	0.43
4:G:83:ARG:CG	4:G:84:LYS:N	2.82	0.43
30:A:2090:G:C6	30:A:2091:U:C4	3.07	0.43
30:A:197:A:C6	30:A:2430:A:C8	3.07	0.43
30:A:2115:G:N1	30:A:2118:U:OP2	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:A:114(B):A:C4	30:A:1144:G:N7	2.87	0.43
30:A:2581:G:C6	30:A:2610:C:N3	2.86	0.43
9:O:96:THR:O	9:O:97:ARG:C	2.57	0.43
15:U:25:TRP:O	15:U:26:GLY:C	2.57	0.43
30:A:775:G:C4	30:A:794:G:C8	3.06	0.43
10:P:38:GLN:CD	30:A:943:U:OP2	2.57	0.43
15:U:45:TYR:O	15:U:49:HIS:CD2	2.72	0.43
30:A:511:U:C5	30:A:512:G:C5	3.06	0.43
28:7:12:ARG:CG	30:A:686:G:O6	2.67	0.43
30:A:1022:G:O2'	30:A:1023:U:OP2	2.37	0.43
30:A:15:G:C4	30:A:16:G:C8	3.07	0.43
30:A:802:A:C5	30:A:803:U:C4	3.07	0.43
10:P:45:LEU:CD2	10:P:46:LYS:N	2.82	0.43
16:V:78:LYS:NZ	30:A:568:U:O4	2.52	0.42
30:A:2037:G:C6	30:A:2038:G:C6	3.06	0.42
30:A:1478:G:O2'	30:A:1558:A:C2	2.72	0.42
8:N:88:LYS:O	8:N:90:LEU:N	2.52	0.42
16:V:77:ALA:O	16:V:79:VAL:N	2.52	0.42
30:A:1764:G:C2	30:A:1765:C:C2	3.07	0.42
10:P:24:GLY:CA	10:P:33:ARG:NH1	2.81	0.42
23:2:1:MET:SD	23:2:1:MET:O	2.77	0.42
1:D:62:TYR:CG	1:D:63:ARG:N	2.88	0.42
10:P:57:THR:O	10:P:59:LEU:N	2.52	0.42
30:A:310:A:O2'	30:A:311:A:O5'	2.37	0.42
30:A:187:G:C6	30:A:188:G:C5	3.07	0.42
30:A:1029:A:C8	30:A:1030:G:C8	3.07	0.42
30:A:2529:G:C8	30:A:2529:G:O5'	2.71	0.42
30:A:2072:G:C6	30:A:2073:C:C4	3.07	0.42
30:A:140:A:C8	30:A:1408:C:O2'	2.72	0.42
30:A:1952:A:C5	30:A:1953:A:C6	3.07	0.42
30:A:463:G:C2	30:A:467:G:C6	3.07	0.42
30:A:533:G:C6	30:A:534:U:C4	3.07	0.42
3:F:7:TYR:O	3:F:8:GLN:C	2.57	0.42
30:A:216:A:N7	30:A:432:A:C6	2.87	0.42
1:D:88:ARG:NH2	30:A:1817:G:OP1	2.52	0.42
30:A:1798:U:C4	30:A:1819:A:C2	3.08	0.42
30:A:273(B):G:C2	30:A:364:C:C4	3.08	0.42
30:A:2694:G:C6	30:A:2695:C:C4	3.08	0.42
30:A:886:C:C6	30:A:886:C:C3'	3.02	0.42
30:A:61:G:C6	30:A:62:C:C4	3.08	0.42
30:A:458:G:N2	30:A:470:A:OP2	2.52	0.42
30:A:486:C:C2	30:A:495:G:C2	3.07	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:N:157:ARG:N	8:N:158:PRO:CD	2.83	0.42
30:A:268:C:C2	30:A:425:G:C2	3.07	0.42
30:A:1682:G:C6	30:A:1683:C:C4	3.08	0.42
11:Q:58:PHE:CD1	11:Q:58:PHE:O	2.73	0.42
30:A:1919:A:O5'	30:A:1919:A:C8	2.72	0.42
30:A:2078:C:C4	30:A:2079:U:C4	3.07	0.42
30:A:602:G:N2	30:A:656:G:C4	2.88	0.42
10:P:27:HIS:CD2	30:A:814:C:N4	2.88	0.42
30:A:692:C:C2	30:A:771:G:C2	3.07	0.42
1:D:232:PRO:O	1:D:234:GLY:N	2.53	0.42
30:A:1632:A:C8	30:A:1632:A:O5'	2.73	0.42
30:A:1151:G:C6	30:A:1152:C:C4	3.07	0.42
30:A:216:A:C8	30:A:432:A:N6	2.88	0.42
30:A:1252:G:O2'	30:A:1253:A:C8	2.73	0.42
30:A:638:G:C6	30:A:639:U:C4	3.07	0.42
30:A:1441:G:N2	30:A:1551:C:C2	2.88	0.42
30:A:1215:G:C5	30:A:1216:G:N7	2.88	0.42
30:A:1542:G:C4'	30:A:1543:A:O5'	2.68	0.42
12:R:16:HIS:CD2	30:A:1275:A:C4	3.08	0.42
2:E:52:LEU:O	2:E:76:ARG:N	2.53	0.42
30:A:662:G:C2	30:A:663:G:C5	3.08	0.42
30:A:1216:G:N1	30:A:1234:U:C2	2.88	0.42
30:A:1911:U:C2	30:A:1918:A:C2	3.08	0.42
12:R:96:ARG:N	12:R:115:GLU:O	2.53	0.42
30:A:164:U:C4	30:A:165:U:C4	3.07	0.41
30:A:1455:G:C6	30:A:2705:A:C2	3.08	0.41
30:A:1272:A:OP2	30:A:1647:G:OP1	2.38	0.41
30:A:1120:G:C5	30:A:1121:C:C4	3.07	0.41
30:A:1817:G:C6	30:A:1818:U:C4	3.09	0.41
13:S:90:GLY:O	13:S:91:PRO:C	2.59	0.41
30:A:273(A):G:C4	30:A:273(B):G:C8	3.08	0.41
30:A:1980:G:C8	30:A:1980:G:C5'	3.04	0.41
30:A:1783:A:C2	30:A:2587:A:C5	3.08	0.41
15:U:33:ARG:O	15:U:34:LYS:C	2.58	0.41
30:A:2508:G:C4	30:A:2509:G:C8	3.08	0.41
30:A:593:G:C6	30:A:594:U:C4	3.08	0.41
30:A:2729:G:C2	30:A:2730:C:C2	3.08	0.41
30:A:741:G:N2	30:A:756:C:O2	2.53	0.41
30:A:582:G:C2	30:A:1259:G:C2	3.07	0.41
30:A:2054:A:C2	30:A:2616:C:C2	3.08	0.41
30:A:2536:G:C5	30:A:2537:U:C4	3.08	0.41
30:A:1945:G:C4	30:A:1946:U:C5	3.08	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:Q:6:ARG:NE	11:Q:6:ARG:N	2.68	0.41
30:A:617:G:C2	30:A:618(A):G:C4	3.09	0.41
15:U:49:HIS:ND1	30:A:559:G:N2	2.68	0.41
30:A:2337:G:C2	30:A:2338:G:C8	3.08	0.41
30:A:978:G:C2	30:A:986:C:C2	3.08	0.41
30:A:2010:G:C5	30:A:2011:U:C5	3.08	0.41
3:F:60:SER:OG	3:F:61:GLY:N	2.54	0.41
30:A:298:G:O2'	30:A:322:A:N1	2.53	0.41
30:A:758:C:O2'	30:A:1981:A:N3	2.53	0.41
30:A:672:C:C2	30:A:809:G:N2	2.89	0.41
8:N:64:ASP:N	8:N:64:ASP:OD1	2.54	0.41
30:A:1493:C:C2'	30:A:1493:C:O2	2.69	0.41
30:A:2681:C:C5	30:A:2724:C:N4	2.89	0.41
30:A:1649:G:N1	30:A:2009:G:C6	2.89	0.41
30:A:226:G:C2	30:A:227:A:C6	3.08	0.41
30:A:187:G:C6	30:A:188:G:N7	2.88	0.41
26:5:19:ARG:NH2	30:A:1264:G:OP1	2.54	0.41
30:A:270(Q):C:C2	30:A:270(R):C:C5	3.09	0.41
30:A:323:G:O2'	30:A:1205:U:N3	2.54	0.41
30:A:748:G:OP1	30:A:2612:C:N4	2.53	0.41
30:A:1949:G:C6	30:A:1950:G:C6	3.08	0.41
30:A:979:G:C4	30:A:982:C:N4	2.89	0.41
23:2:47:ASN:ND2	30:A:61:G:C6	2.89	0.41
30:A:1459:G:C6	30:A:1461:G:C5	3.09	0.41
30:A:2415:G:C6	30:A:2416:C:C4	3.08	0.41
1:D:70:TRP:C	1:D:70:TRP:CD1	2.94	0.41
30:A:2532:G:C6	30:A:2533:A:C5	3.08	0.41
30:A:237:C:N3	30:A:261:G:C2	2.88	0.41
30:A:815:C:C2	30:A:1193:G:C2	3.08	0.41
30:A:2493:U:C4	30:A:2494:G:C8	3.09	0.41
9:O:34:THR:O	9:O:35:VAL:C	2.59	0.41
30:A:1973:G:C6	30:A:1974:C:N4	2.89	0.41
30:A:522:G:C6	30:A:523:C:C4	3.09	0.41
30:A:568:U:O2'	30:A:570:G:N7	2.54	0.41
30:A:583:G:N2	30:A:1258:C:C2	2.89	0.41
30:A:1553:A:C6	30:A:1555:G:C4	3.09	0.41
30:A:1358:G:N1	30:A:1372:U:OP2	2.54	0.41
30:A:677:A:C6	30:A:678:C:C4	3.09	0.41
15:U:94:ASN:C	15:U:94:ASN:OD1	2.60	0.41
30:A:1230:C:C2	30:A:1231:G:N7	2.88	0.41
30:A:271(C):G:C2	30:A:421:U:C4	3.08	0.41
30:A:1686:C:N3	30:A:1703:G:C2	2.89	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:A:27:G:O5'	30:A:27:G:C8	2.74	0.40
30:A:657:U:C4	30:A:658:C:N4	2.89	0.40
2:E:201:THR:CG2	2:E:202:LYS:N	2.84	0.40
30:A:465:G:C6	30:A:466:A:N6	2.89	0.40
30:A:2787:C:N4	30:A:2788:C:N4	2.68	0.40
30:A:310:A:C6	30:A:330:A:N1	2.89	0.40
30:A:2029:G:O6	30:A:2033:A:OP1	2.39	0.40
30:A:2403:C:N3	30:A:2415:G:C2	2.90	0.40
30:A:2358:G:C5	30:A:2359:C:C5	3.09	0.40
30:A:656:G:C5	30:A:657:U:C4	3.10	0.40
30:A:677:A:C5	30:A:678:C:C5	3.10	0.40
30:A:2836:U:C4	30:A:2883:A:N6	2.90	0.40
20:Z:178:GLU:O	20:Z:179:ASP:O	2.39	0.40
30:A:834:C:C2	30:A:835:A:C8	3.09	0.40
30:A:428:A:N6	30:A:429:A:C6	2.90	0.40
30:A:756:C:C2	30:A:757:U:C6	3.09	0.40
30:A:55:G:C2	30:A:116:C:C2	3.09	0.40
30:A:2584:U:O2	30:A:2585:U:C4	2.74	0.40
30:A:379:G:C5	30:A:380:U:C5	3.10	0.40
30:A:2075:U:C4	30:A:2238:G:C6	3.10	0.40
18:X:15:GLU:N	18:X:15:GLU:CD	2.74	0.40
30:A:1021:A:C3'	30:A:1021:A:C8	3.04	0.40
31:B:81:G:N1	31:B:96:G:C2	2.90	0.40
30:A:2399:G:C6	30:A:2400:G:C5	3.09	0.40
30:A:189:G:N2	30:A:208:C:N4	2.69	0.40

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	
1	D	269/276 (98%)	213 (79%)	40 (15%)	16 (6%)	2	20
2	E	202/206 (98%)	151 (75%)	42 (21%)	9 (4%)	4	29
3	F	200/210 (95%)	158 (79%)	35 (18%)	7 (4%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	179/182 (98%)	124 (69%)	44 (25%)	11 (6%)	2	19
5	H	157/180 (87%)	126 (80%)	24 (15%)	7 (4%)	4	29
6	I	143/148 (97%)	112 (78%)	24 (17%)	7 (5%)	3	26
7	J	28/173 (16%)	27 (96%)	1 (4%)	0	100	100
8	N	135/163 (83%)	100 (74%)	27 (20%)	8 (6%)	2	20
9	O	120/122 (98%)	101 (84%)	18 (15%)	1 (1%)	27	77
10	P	144/150 (96%)	82 (57%)	45 (31%)	17 (12%)	1	4
11	Q	134/141 (95%)	87 (65%)	35 (26%)	12 (9%)	1	8
12	R	115/118 (98%)	91 (79%)	18 (16%)	6 (5%)	3	25
13	S	96/112 (86%)	61 (64%)	25 (26%)	10 (10%)	1	5
14	T	135/146 (92%)	103 (76%)	28 (21%)	4 (3%)	7	42
15	U	115/118 (98%)	89 (77%)	22 (19%)	4 (4%)	6	37
16	V	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	8
17	W	110/113 (97%)	91 (83%)	17 (16%)	2 (2%)	13	60
18	X	90/96 (94%)	69 (77%)	20 (22%)	1 (1%)	21	72
19	Y	98/110 (89%)	65 (66%)	21 (21%)	12 (12%)	1	3
20	Z	186/206 (90%)	142 (76%)	34 (18%)	10 (5%)	3	24
21	0	74/85 (87%)	55 (74%)	14 (19%)	5 (7%)	2	15
22	1	86/98 (88%)	53 (62%)	28 (33%)	5 (6%)	3	21
23	2	70/72 (97%)	48 (69%)	16 (23%)	6 (9%)	1	8
24	3	57/60 (95%)	44 (77%)	12 (21%)	1 (2%)	13	60
25	4	28/97 (29%)	14 (50%)	11 (39%)	3 (11%)	1	5
26	5	50/60 (83%)	36 (72%)	12 (24%)	2 (4%)	5	32
27	6	42/54 (78%)	31 (74%)	8 (19%)	3 (7%)	2	13
28	7	46/49 (94%)	39 (85%)	7 (15%)	0	100	100
29	8	61/65 (94%)	42 (69%)	15 (25%)	4 (7%)	2	16
All	All	3269/3711 (88%)	2423 (74%)	664 (20%)	182 (6%)	3	23

All (182) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	33	LEU
1	D	35	LYS

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Mol	Chain	Res	Type
1	D	244	ARG
2	E	16	ARG
2	E	86	PRO
3	F	73	ALA
3	F	84	VAL
4	G	75	LYS
4	G	87	PRO
5	H	92	ILE
6	I	89	TYR
6	I	91	SER
8	N	89	LYS
8	N	116	THR
8	N	149	PRO
8	N	153	HIS
10	P	15	ARG
11	Q	10	ARG
11	Q	21	THR
11	Q	133	ARG
11	Q	139	GLU
13	S	12	PHE
13	S	91	PRO
15	U	90	VAL
16	V	53	GLU
17	W	110	LYS
18	X	93	GLU
19	Y	3	VAL
19	Y	7	VAL
19	Y	88	LYS
20	Z	168	GLU
20	Z	179	ASP
21	0	32	ARG
21	0	47	PRO
23	2	17	SER
27	6	31	PRO
1	D	26	LYS
1	D	69	ARG
1	D	106	ILE
1	D	197	GLY
1	D	206	LEU
1	D	239	ARG
3	F	166	ALA
4	G	14	GLU

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Mol	Chain	Res	Type
5	H	165	ALA
6	I	90	GLY
8	N	148	GLY
10	P	57	THR
10	P	65	ARG
10	P	141	ALA
10	P	148	LEU
10	P	149	GLU
11	Q	7	MET
11	Q	15	GLY
11	Q	18	LYS
12	R	3	HIS
12	R	14	SER
12	R	57	ARG
12	R	58	GLY
13	S	44	LYS
13	S	59	LYS
13	S	90	GLY
13	S	101	LEU
14	T	58	ASN
14	T	115	ARG
15	U	24	TYR
15	U	26	GLY
16	V	78	LYS
17	W	11	ARG
19	Y	42	VAL
20	Z	167	PRO
21	0	73	GLY
23	2	47	ASN
23	2	58	ALA
27	6	28	ARG
27	6	51	GLU
29	8	35	GLN
1	D	70	TRP
1	D	198	ASN
1	D	260	ARG
2	E	43	GLY
2	E	51	PHE
2	E	132	HIS
2	E	187	ALA
3	F	8	GLN
3	F	74	ARG

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Mol	Chain	Res	Type
3	F	82	ILE
4	G	8	LYS
4	G	142	PRO
4	G	181	ARG
5	H	21	PRO
6	I	10	GLU
10	P	10	PRO
10	P	17	LYS
10	P	25	SER
10	P	46	LYS
10	P	58	THR
11	Q	62	GLY
11	Q	81	VAL
12	R	8	ARG
13	S	94	TYR
16	V	29	PRO
19	Y	39	VAL
19	Y	50	ARG
19	Y	56	PRO
20	Z	11	GLU
22	1	31	GLY
22	1	85	LEU
22	1	87	PRO
23	2	44	LEU
26	5	35	GLU
29	8	34	TRP
1	D	256	GLY
2	E	18	ASP
2	E	173	VAL
4	G	84	LYS
4	G	126	ASP
8	N	41	ALA
9	O	26	LYS
10	P	11	GLY
10	P	47	ASP
10	P	52	GLU
10	P	70	GLN
13	S	57	LYS
13	S	62	LYS
14	T	36	GLU
16	V	2	PHE
19	Y	17	SER

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Mol	Chain	Res	Type
19	Y	76	CYS
19	Y	96	ILE
20	Z	78	LYS
20	Z	165	VAL
20	Z	177	PRO
20	Z	180	VAL
22	1	9	GLY
23	2	21	LEU
25	4	44	CYS
29	8	3	LYS
1	D	125	ILE
3	F	187	VAL
4	G	76	SER
5	H	39	PRO
5	H	164	TYR
6	I	30	LEU
10	P	59	LEU
13	S	85	VAL
14	T	22	PHE
15	U	9	VAL
16	V	16	PRO
16	V	80	GLN
16	V	94	LEU
19	Y	55	TYR
19	Y	90	LEU
20	Z	80	ARG
21	0	15	ASP
22	1	53	VAL
24	3	29	ARG
25	4	37	PRO
25	4	54	LYS
26	5	45	VAL
29	8	59	LYS
2	E	98	PRO
4	G	88	ILE
8	N	106	LYS
8	N	150	ASP
10	P	33	ARG
11	Q	8	LYS
11	Q	136	ALA
12	R	12	ARG
23	2	50	ILE

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Mol	Chain	Res	Type
1	D	238	GLY
5	H	117	PRO
6	I	8	PRO
11	Q	73	PRO
20	Z	71	VAL
21	0	36	ILE
1	D	113	VAL
6	I	120	ILE
16	V	48	GLY
16	V	17	GLY
4	G	42	GLY
5	H	36	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	
1	D	213/218 (98%)	196 (92%)	17 (8%)	17	57
2	E	165/166 (99%)	153 (93%)	12 (7%)	20	62
3	F	161/166 (97%)	154 (96%)	7 (4%)	40	81
4	G	155/156 (99%)	142 (92%)	13 (8%)	16	53
5	H	132/148 (89%)	123 (93%)	9 (7%)	22	65
6	I	122/124 (98%)	113 (93%)	9 (7%)	20	62
7	J	27/135 (20%)	26 (96%)	1 (4%)	45	85
8	N	116/139 (84%)	106 (91%)	10 (9%)	15	52
9	O	100/100 (100%)	95 (95%)	5 (5%)	34	78
10	P	112/116 (97%)	92 (82%)	20 (18%)	2	12
11	Q	106/111 (96%)	95 (90%)	11 (10%)	10	39
12	R	100/101 (99%)	95 (95%)	5 (5%)	34	78
13	S	77/88 (88%)	70 (91%)	7 (9%)	14	47
14	T	121/128 (94%)	106 (88%)	15 (12%)	7	30
15	U	93/94 (99%)	89 (96%)	4 (4%)	40	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	82/82 (100%)	73 (89%)	9 (11%)	9	36
17	W	91/92 (99%)	89 (98%)	2 (2%)	64	91
18	X	74/78 (95%)	68 (92%)	6 (8%)	17	56
19	Y	84/91 (92%)	79 (94%)	5 (6%)	27	72
20	Z	163/179 (91%)	160 (98%)	3 (2%)	71	93
21	0	61/67 (91%)	59 (97%)	2 (3%)	50	87
22	1	73/83 (88%)	64 (88%)	9 (12%)	7	31
23	2	67/67 (100%)	64 (96%)	3 (4%)	38	81
24	3	51/52 (98%)	48 (94%)	3 (6%)	28	72
25	4	27/84 (32%)	25 (93%)	2 (7%)	20	62
26	5	45/52 (86%)	43 (96%)	2 (4%)	39	81
27	6	43/52 (83%)	40 (93%)	3 (7%)	21	64
28	7	41/42 (98%)	38 (93%)	3 (7%)	20	62
29	8	53/55 (96%)	51 (96%)	2 (4%)	44	84
All	All	2755/3066 (90%)	2556 (93%)	199 (7%)	21	63

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	5	LYS
1	D	10	THR
1	D	28	GLU
1	D	33	LEU
1	D	50	THR
1	D	78	LYS
1	D	95	LEU
1	D	109	ASP
1	D	111	LEU
1	D	133	LEU
1	D	150	LYS
1	D	166	GLN
1	D	173	VAL
1	D	192	THR
1	D	242	ARG
1	D	259	THR
1	D	261	LYS
2	E	4	ILE

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Mol	Chain	Res	Type
2	E	9	VAL
2	E	19	ARG
2	E	52	LEU
2	E	57	LYS
2	E	92	THR
2	E	118	LYS
2	E	119	ARG
2	E	132	HIS
2	E	137	HIS
2	E	184	VAL
2	E	195	LEU
3	F	8	GLN
3	F	9	ILE
3	F	53	THR
3	F	65	TRP
3	F	95	ARG
3	F	117	ARG
3	F	164	ARG
4	G	18	GLU
4	G	33	ARG
4	G	34	LEU
4	G	47	LYS
4	G	74	LYS
4	G	86	MET
4	G	90	LEU
4	G	98	ARG
4	G	107	LEU
4	G	115	ARG
4	G	133	LEU
4	G	139	LEU
4	G	155	MET
5	H	13	LYS
5	H	23	ARG
5	H	43	VAL
5	H	86	GLU
5	H	101	ARG
5	H	105	LEU
5	H	123	PHE
5	H	158	HIS
5	H	162	ILE
6	I	5	LEU
6	I	6	LEU

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Mol	Chain	Res	Type
6	I	66	GLU
6	I	67	ARG
6	I	73	GLU
6	I	77	LEU
6	I	92	VAL
6	I	107	ILE
6	I	109	ILE
7	J	17	LEU
8	N	57	LEU
8	N	64	ASP
8	N	71	MET
8	N	94	ILE
8	N	116	THR
8	N	120	ARG
8	N	122	LEU
8	N	146	TYR
8	N	150	ASP
8	N	161	LEU
9	O	19	ILE
9	O	25	LEU
9	O	77	ILE
9	O	87	ILE
9	O	104	ARG
10	P	13	ASN
10	P	15	ARG
10	P	32	THR
10	P	35	HIS
10	P	49	ARG
10	P	50	ARG
10	P	57	THR
10	P	61	ARG
10	P	62	LEU
10	P	67	MET
10	P	70	GLN
10	P	83	VAL
10	P	85	LEU
10	P	105	LEU
10	P	106	LEU
10	P	111	ARG
10	P	135	LEU
10	P	147	LEU
10	P	148	LEU

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Mol	Chain	Res	Type
10	P	149	GLU
11	Q	6	ARG
11	Q	13	GLN
11	Q	14	ARG
11	Q	22	LYS
11	Q	29	PHE
11	Q	45	GLN
11	Q	55	VAL
11	Q	60	ARG
11	Q	80	GLU
11	Q	89	ASN
11	Q	135	ASP
12	R	9	LYS
12	R	10	LEU
12	R	71	GLN
12	R	79	LEU
12	R	104	ARG
13	S	18	ILE
13	S	26	LEU
13	S	30	ARG
13	S	42	ASP
13	S	44	LYS
13	S	61	ASN
13	S	93	LYS
14	T	22	PHE
14	T	28	VAL
14	T	41	ARG
14	T	58	ASN
14	T	59	THR
14	T	68	TYR
14	T	86	ILE
14	T	89	VAL
14	T	95	ARG
14	T	96	ARG
14	T	98	LYS
14	T	99	LEU
14	T	108	ARG
14	T	112	ARG
14	T	113	LYS
15	U	31	SER
15	U	32	PHE
15	U	79	PHE

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Mol	Chain	Res	Type
15	U	92	ARG
16	V	11	GLN
16	V	12	TYR
16	V	13	ARG
16	V	18	LEU
16	V	25	LEU
16	V	37	VAL
16	V	80	GLN
16	V	98	GLU
16	V	99	ILE
17	W	11	ARG
17	W	95	ILE
18	X	28	PHE
18	X	55	ASN
18	X	65	ARG
18	X	68	ARG
18	X	75	ASP
18	X	81	VAL
19	Y	4	LYS
19	Y	6	HIS
19	Y	8	LYS
19	Y	31	LEU
19	Y	76	CYS
20	Z	70	LEU
20	Z	72	ARG
20	Z	76	LEU
21	0	25	ARG
21	0	84	LEU
22	1	18	ILE
22	1	20	ARG
22	1	40	ARG
22	1	45	ASN
22	1	46	LEU
22	1	73	LEU
22	1	76	ARG
22	1	82	LEU
22	1	95	LEU
23	2	2	LYS
23	2	37	PHE
23	2	56	GLN
24	3	10	LYS
24	3	29	ARG

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Mol	Chain	Res	Type
24	3	46	ASN
25	4	49	GLU
25	4	65	CYS
26	5	3	LYS
26	5	51	TYR
27	6	11	LEU
27	6	30	THR
27	6	34	LEU
28	7	4	THR
28	7	8	ASN
28	7	24	THR
29	8	33	ASN
29	8	48	PHE

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
30	A	2878/2894 (99%)	445 (15%)	102 (3%)
31	B	118/124 (95%)	12 (10%)	1 (0%)
All	All	2996/3018 (99%)	457 (15%)	103 (3%)

All (457) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	A	10	G
30	A	34	C
30	A	35	G
30	A	46	C
30	A	63	U
30	A	64	A
30	A	72	U
30	A	73	A
30	A	74	A
30	A	75	G
30	A	84	A
30	A	85	G
30	A	88	G
30	A	98	G

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Mol	Chain	Res	Type
30	A	99	U
30	A	101	G
30	A	102	G
30	A	118	A
30	A	120	U
30	A	138	G
30	A	140	A
30	A	162	U
30	A	181	A
30	A	196	A
30	A	197	A
30	A	199	A
30	A	200	U
30	A	204	A
30	A	205	G
30	A	216	A
30	A	221	A
30	A	222	A
30	A	227	A
30	A	228	A
30	A	229	A
30	A	230	U
30	A	248	G
30	A	252	G
30	A	269	U
30	A	270(K)	G
30	A	270(M)	U
30	A	270(N)	U
30	A	270(O)	G
30	A	270(P)	U
30	A	270(Q)	C
30	A	270(R)	C
30	A	270(T)	G
30	A	271(D)	U
30	A	271	G
30	A	274	G
30	A	275	G
30	A	276	A
30	A	277	C
30	A	278	A
30	A	279	C
30	A	283	A

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Mol	Chain	Res	Type
30	A	284	U
30	A	302	C
30	A	323	G
30	A	324	A
30	A	329	G
30	A	330	A
30	A	331	A
30	A	332	A
30	A	333	G
30	A	352	G
30	A	353	G
30	A	364	C
30	A	386	G
30	A	388	G
30	A	396	G
30	A	405	U
30	A	411	G
30	A	444	C
30	A	457	A
30	A	458	G
30	A	470	A
30	A	480	A
30	A	481	G
30	A	505	A
30	A	508	G
30	A	509	C
30	A	512	G
30	A	530	G
30	A	531	C
30	A	532	A
30	A	533	G
30	A	556	G
30	A	562	U
30	A	563	G
30	A	572	A
30	A	573	G
30	A	575	A
30	A	603	A
30	A	616	A
30	A	617	G
30	A	620	G
30	A	621	A

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Mol	Chain	Res	Type
30	A	627	A
30	A	637	A
30	A	645	C
30	A	646	A
30	A	652	U
30	A	653	C
30	A	656	G
30	A	657	U
30	A	668	G
30	A	671	C
30	A	676	A
30	A	686	G
30	A	695	G
30	A	717	G
30	A	730	C
30	A	746	A
30	A	747	U
30	A	765	G
30	A	776	G
30	A	782	A
30	A	784	A
30	A	785	G
30	A	789	A
30	A	792	G
30	A	800	A
30	A	805	G
30	A	812	C
30	A	819	A
30	A	827	U
30	A	828	U
30	A	830	G
30	A	845	G
30	A	846	C
30	A	859	G
30	A	866	A
30	A	886	C
30	A	890	A
30	A	896	A
30	A	897	C
30	A	907	U
30	A	910	A
30	A	917	A

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Mol	Chain	Res	Type
30	A	932	G
30	A	933	A
30	A	941	A
30	A	945	A
30	A	946	G
30	A	959	A
30	A	961	C
30	A	973	A
30	A	974(A)	G
30	A	974(B)	C
30	A	983	A
30	A	990	A
30	A	996	A
30	A	999	U
30	A	1008	C
30	A	1009	A
30	A	1011	G
30	A	1012	U
30	A	1013	C
30	A	1022	G
30	A	1023	U
30	A	1025	G
30	A	1026	U
30	A	1033	U
30	A	1047	G
30	A	1057	A
30	A	1060	U
30	A	1061	U
30	A	1062	G
30	A	1069	A
30	A	1070	A
30	A	1071	G
30	A	1072	C
30	A	1078	U
30	A	1079	C
30	A	1088	A
30	A	1090	U
30	A	1112	G
30	A	1129	A
30	A	1130	U
30	A	1131	G
30	A	1132	A

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Mol	Chain	Res	Type
30	A	1135	C
30	A	1136	G
30	A	1139	G
30	A	1142	U
30	A	114(B)	A
30	A	1143	A
30	A	1155	A
30	A	1174	A
30	A	1175	U
30	A	1177	A
30	A	1190	G
30	A	1204	A
30	A	1205	U
30	A	1210	A
30	A	1211	U
30	A	1212	G
30	A	1221	C
30	A	1247	A
30	A	1248	G
30	A	1253	A
30	A	1254	A
30	A	1256	G
30	A	1265	A
30	A	1271	G
30	A	1272	A
30	A	1274	A
30	A	1286	A
30	A	1300	U
30	A	1301	A
30	A	1302	A
30	A	1311	G
30	A	1312	U
30	A	1314	C
30	A	1325	G
30	A	1329	U
30	A	1332	G
30	A	1349	A
30	A	1359	A
30	A	1360	A
30	A	1368	G
30	A	1379	A
30	A	1380	G

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Mol	Chain	Res	Type
30	A	1384	A
30	A	1385	G
30	A	1386	C
30	A	1395	A
30	A	1396	U
30	A	1398	C
30	A	1416	G
30	A	1417	C
30	A	1420	U
30	A	1421	G
30	A	1428	C
30	A	144(B)	A
30	A	1449	G
30	A	1451	C
30	A	1453	A
30	A	1454	U
30	A	1455	G
30	A	1458	C
30	A	1459	G
30	A	1460	A
30	A	1467	C
30	A	1483	G
30	A	1490	A
30	A	1493	C
30	A	1494	A
30	A	1495	A
30	A	1497	U
30	A	1498	C
30	A	1505	C
30	A	1510	A
30	A	1538	G
30	A	1540	G
30	A	1542	G
30	A	1543	A
30	A	1545	A
30	A	1554	A
30	A	1558	A
30	A	1559	G
30	A	1569	A
30	A	1579	A
30	A	1585	C
30	A	1599	C

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Mol	Chain	Res	Type
30	A	1603	A
30	A	1608	A
30	A	1609	A
30	A	1610	A
30	A	1613	G
30	A	1617	C
30	A	1618	A
30	A	1640	C
30	A	1648	C
30	A	1664	A
30	A	1674	G
30	A	1694	C
30	A	1695	G
30	A	1696	G
30	A	1729	A
30	A	1732	A
30	A	1763	G
30	A	1764	G
30	A	1773	A
30	A	1786	A
30	A	1800	C
30	A	1801	G
30	A	1816	G
30	A	1830	C
30	A	1838	C
30	A	1839	G
30	A	1847	A
30	A	1878	G
30	A	1888	G
30	A	1903	G
30	A	1906	G
30	A	1913	A
30	A	1929	G
30	A	1931	U
30	A	1936	A
30	A	1938	A
30	A	1939	U
30	A	1955	U
30	A	1963	U
30	A	1964	G
30	A	1966	A
30	A	1967	C

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Mol	Chain	Res	Type
30	A	1971	A
30	A	1972	A
30	A	1980	G
30	A	1981	A
30	A	1982	C
30	A	1992	G
30	A	1993	U
30	A	1997	G
30	A	2020	A
30	A	2023	G
30	A	2031	A
30	A	2033	A
30	A	2034	U
30	A	2036	C
30	A	2043	C
30	A	2046	G
30	A	2055	C
30	A	2056	G
30	A	2060	A
30	A	2061	G
30	A	2068	U
30	A	2069	G
30	A	2092	U
30	A	2115	G
30	A	2119	A
30	A	2120	G
30	A	2126	A
30	A	2132	U
30	A	2133	G
30	A	2147	G
30	A	2159	G
30	A	2173	A
30	A	2198	A
30	A	2199	A
30	A	2211	G
30	A	2212	A
30	A	2213	U
30	A	2215	G
30	A	2225	A
30	A	2226	C
30	A	2238	G
30	A	2239	G

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Mol	Chain	Res	Type
30	A	2251	G
30	A	2273	A
30	A	2275	C
30	A	2283	C
30	A	2287	A
30	A	2305	A
30	A	2306	C
30	A	2307	G
30	A	2319	G
30	A	2320	A
30	A	2322	A
30	A	2325	G
30	A	2334	G
30	A	2336	A
30	A	2345	G
30	A	2347	C
30	A	2350	C
30	A	2379	G
30	A	2383	G
30	A	2385	C
30	A	2402	C
30	A	2408	U
30	A	2423	U
30	A	2424	C
30	A	2425	A
30	A	2427	C
30	A	2428	G
30	A	2429	G
30	A	2430	A
30	A	2431	U
30	A	2439	A
30	A	2441	C
30	A	2445	G
30	A	2447	G
30	A	2448	A
30	A	2449	U
30	A	2469	A
30	A	2476	A
30	A	2478	A
30	A	2487	G
30	A	2491	U
30	A	2498	C

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Mol	Chain	Res	Type
30	A	2502	G
30	A	2503	A
30	A	2504	U
30	A	2505	G
30	A	2506	U
30	A	2518	A
30	A	2520	C
30	A	2529	G
30	A	2542	A
30	A	2543	G
30	A	2554	U
30	A	2562	U
30	A	2566	A
30	A	2567	G
30	A	2572	A
30	A	2573	C
30	A	2574	G
30	A	2578	G
30	A	2585	U
30	A	2602	A
30	A	2603	G
30	A	2609	U
30	A	2610	C
30	A	2611	U
30	A	2612	C
30	A	2630	G
30	A	2665	A
30	A	2690	C
30	A	2712	U
30	A	712(B)	A
30	A	2713	A
30	A	2714	G
30	A	2733	A
30	A	2748	A
30	A	2757	A
30	A	2765	A
30	A	2766	G
30	A	2778	A
30	A	2779	U
30	A	2781	A
30	A	2790	A
30	A	2791	C

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Mol	Chain	Res	Type
30	A	2792	G
30	A	2797	U
30	A	2808	U
30	A	2820	A
30	A	2821	A
30	A	2849	U
30	A	2872	G
30	A	2873	A
30	A	2874	C
30	A	2892	A
30	A	2894	G
31	B	15	A
31	B	16	G
31	B	25	A
31	B	35	U
31	B	42	C
31	B	45	A
31	B	52	A
31	B	67	G
31	B	73	A
31	B	88	C
31	B	90	C
31	B	109	G

All (103) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	A	34	C
30	A	60	G
30	A	63	U
30	A	74	A
30	A	101	G
30	A	120	U
30	A	177	G
30	A	196	A
30	A	199	A
30	A	221	A
30	A	270(N)	U
30	A	271(A)	U
30	A	278	A
30	A	283	A
30	A	310	A

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Mol	Chain	Res	Type
30	A	321	G
30	A	331	A
30	A	332	A
30	A	455	C
30	A	457	A
30	A	479	A
30	A	531	C
30	A	532	A
30	A	571	A
30	A	616	A
30	A	652	U
30	A	675	A
30	A	685	A
30	A	746	A
30	A	762	U
30	A	764	A
30	A	776	G
30	A	829	A
30	A	945	A
30	A	974(A)	G
30	A	1008	C
30	A	1022	G
30	A	1047	G
30	A	1069	A
30	A	1071	G
30	A	1089	G
30	A	1131	G
30	A	1154	G
30	A	1190	G
30	A	1210	A
30	A	1211	U
30	A	1253	A
30	A	1266	G
30	A	1300	U
30	A	1301	A
30	A	1378	A
30	A	1379	A
30	A	1419	A
30	A	1427	A
30	A	1451	C
30	A	1453	A
30	A	1458	C

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Mol	Chain	Res	Type
30	A	1494	A
30	A	1495	A
30	A	1542	G
30	A	1558	A
30	A	1608	A
30	A	1617	C
30	A	1800	C
30	A	1816	G
30	A	1829	A
30	A	1838	C
30	A	1847	A
30	A	1937	A
30	A	1938	A
30	A	1939	U
30	A	1970	A
30	A	1980	G
30	A	1992	G
30	A	2022	U
30	A	2033	A
30	A	2060	A
30	A	2092	U
30	A	2172	U
30	A	2225	A
30	A	2282	G
30	A	2311	A
30	A	2319	G
30	A	2320	A
30	A	2345	G
30	A	2422	A
30	A	2427	C
30	A	2428	G
30	A	2448	A
30	A	2502	G
30	A	2529	G
30	A	2542	A
30	A	2572	A
30	A	2603	G
30	A	2610	C
30	A	2689	U
30	A	2713	A
30	A	2756	U
30	A	2776	A

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Mol	Chain	Res	Type
30	A	2791	C
30	A	2866	U
30	A	2873	A
31	B	56	G

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 826 ligands modelled in this entry, 826 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	D	271/276 (98%)	0.17	11 (4%) 35 7	93, 115, 140, 163	0
2	E	204/206 (99%)	-0.05	3 (1%) 70 21	99, 141, 171, 194	0
3	F	202/210 (96%)	-0.22	1 (0%) 88 46	92, 132, 163, 183	0
4	G	181/182 (99%)	-0.06	8 (4%) 33 7	146, 197, 233, 251	0
5	H	159/180 (88%)	-0.11	0 100 100	148, 172, 202, 215	0
6	I	145/148 (97%)	0.19	12 (8%) 11 3	125, 203, 254, 286	0
7	J	32/173 (18%)	-0.37	0 100 100	188, 222, 247, 258	0
8	N	137/163 (84%)	0.19	9 (6%) 18 4	112, 140, 165, 184	0
9	O	122/122 (100%)	0.14	8 (6%) 18 4	111, 128, 146, 175	0
10	P	146/150 (97%)	0.36	14 (9%) 8 2	100, 143, 178, 198	0
11	Q	136/141 (96%)	0.83	24 (17%) 2 1	105, 140, 174, 226	0
12	R	117/118 (99%)	0.41	10 (8%) 11 3	108, 129, 167, 183	0
13	S	98/112 (87%)	0.20	8 (8%) 12 3	164, 197, 225, 240	0
14	T	137/146 (93%)	0.34	13 (9%) 8 2	121, 145, 189, 205	0
15	U	117/118 (99%)	0.47	15 (12%) 4 1	102, 136, 170, 183	0
16	V	101/101 (100%)	0.19	9 (8%) 10 2	104, 150, 183, 202	0
17	W	112/113 (99%)	-0.04	0 100 100	92, 116, 145, 172	0
18	X	92/96 (95%)	0.11	4 (4%) 34 7	101, 120, 145, 174	0
19	Y	100/110 (90%)	0.40	10 (10%) 8 2	115, 135, 172, 199	0
20	Z	188/206 (91%)	-0.01	10 (5%) 25 5	134, 173, 200, 215	0
21	0	76/85 (89%)	0.76	15 (19%) 2 1	115, 148, 175, 193	0
22	1	88/98 (89%)	0.31	9 (10%) 7 2	102, 121, 165, 187	0
23	2	72/72 (100%)	-0.34	1 (1%) 72 22	115, 129, 183, 197	0
24	3	59/60 (98%)	0.06	2 (3%) 43 9	121, 143, 172, 212	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	4	30/97 (30%)	-0.19	0 100 100	208, 226, 243, 245	0
26	5	52/60 (86%)	0.05	1 (1%) 64 18	96, 126, 177, 192	0
27	6	44/54 (81%)	-0.24	0 100 100	134, 165, 193, 200	0
28	7	48/49 (97%)	0.13	2 (4%) 35 7	92, 97, 120, 175	0
29	8	63/65 (96%)	1.18	14 (22%) 1 1	109, 124, 151, 190	0
30	A	2879/2894 (99%)	-0.05	121 (4%) 35 7	59, 110, 238, 321	0
31	B	119/124 (95%)	0.49	11 (9%) 9 2	132, 181, 215, 265	0
All	All	6327/6729 (94%)	0.07	345 (5%) 28 5	59, 130, 222, 321	0

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	A	10	G	9.6
30	A	2895	U	9.2
30	A	1090	U	8.9
11	Q	139	GLU	8.9
30	A	11	G	7.8
30	A	12	U	7.6
14	T	115	ARG	7.3
6	I	70	GLU	7.2
30	A	2774	C	6.1
21	0	53	MET	6.1
31	B	52	A	6.1
30	A	529	A	6.0
30	A	2334	G	6.0
10	P	110	TYR	5.8
11	Q	140	ALA	5.7
21	0	74	ARG	5.6
12	R	8	ARG	5.5
13	S	11	LYS	5.4
30	A	2188	C	5.4
29	8	64	TYR	5.4
30	A	34	C	5.2
19	Y	2	ARG	5.2
31	B	13	A	5.2
14	T	96	ARG	5.1
31	B	60	C	5.1
30	A	2151	G	5.1
19	Y	34	LYS	5.0
30	A	508	G	5.0

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Mol	Chain	Res	Type	RSRZ
30	A	2801	A	5.0
10	P	150	ALA	4.9
30	A	2113	U	4.9
11	Q	9	TYR	4.9
9	O	68	GLU	4.7
9	O	108	GLU	4.6
30	A	1045	A	4.6
21	0	17	GLN	4.5
30	A	1026	U	4.5
30	A	2356	C	4.5
20	Z	76	LEU	4.4
11	Q	106	VAL	4.4
30	A	2174	C	4.3
30	A	2112	G	4.3
6	I	41	GLU	4.3
12	R	102	GLU	4.3
29	8	15	LYS	4.2
30	A	1741	C	4.2
31	B	58	A	4.2
10	P	76	LYS	4.2
20	Z	81	ARG	4.1
10	P	20	GLY	4.1
15	U	52	ARG	4.1
14	T	94	ALA	4.1
14	T	114	LEU	4.1
11	Q	65	PHE	4.1
30	A	2693	A	4.1
10	P	77	ARG	4.0
11	Q	112	GLU	4.0
11	Q	137	TYR	4.0
29	8	20	GLY	4.0
12	R	57	ARG	4.0
9	O	67	LYS	3.9
14	T	51	ARG	3.9
21	0	55	ARG	3.9
30	A	2149	G	3.9
30	A	2150	U	3.9
8	N	31	GLN	3.8
15	U	56	ASP	3.8
30	A	2362	G	3.8
20	Z	80	ARG	3.8
30	A	2152	G	3.8

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Mol	Chain	Res	Type	RSRZ
4	G	74	LYS	3.8
14	T	97	ALA	3.8
16	V	81	TYR	3.8
11	Q	67	ARG	3.7
30	A	1460	A	3.7
30	A	867	C	3.7
10	P	108	LYS	3.7
16	V	74	LYS	3.7
28	7	47	ARG	3.7
30	A	614	U	3.7
31	B	41	U	3.7
30	A	2110	G	3.7
22	1	95	LEU	3.6
29	8	21	LYS	3.6
13	S	20	ARG	3.6
30	A	362	U	3.6
1	D	262	ARG	3.6
30	A	227	A	3.6
20	Z	77	ASP	3.5
30	A	2379	G	3.5
15	U	58	ARG	3.5
30	A	528	A	3.5
30	A	2145	C	3.5
15	U	53	ARG	3.4
30	A	271(D)	U	3.4
30	A	1963	U	3.4
31	B	12	C	3.4
6	I	71	ILE	3.4
30	A	440	G	3.4
6	I	69	LYS	3.4
20	Z	83	PRO	3.4
31	B	16	G	3.4
19	Y	3	VAL	3.4
30	A	405	U	3.3
15	U	57	PHE	3.3
30	A	2624	G	3.3
30	A	2139	C	3.3
30	A	2896	C	3.3
30	A	2870	C	3.3
10	P	21	ARG	3.2
30	A	2319	G	3.2
15	U	54	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
13	S	21	THR	3.2
13	S	92	TYR	3.2
15	U	19	LYS	3.2
12	R	9	LYS	3.2
30	A	6	A	3.2
14	T	100	TYR	3.2
29	8	44	LYS	3.2
6	I	73	GLU	3.1
30	A	276	A	3.1
1	D	5	LYS	3.1
30	A	2799	A	3.1
30	A	232	G	3.1
18	X	76	ARG	3.1
21	0	41	ARG	3.1
30	A	536	A	3.1
30	A	1847	A	3.1
1	D	36	PRO	3.1
4	G	84	LYS	3.1
22	1	10	LYS	3.1
20	Z	84	GLU	3.1
30	A	2803	C	3.0
31	B	59	A	3.0
11	Q	69	PHE	3.0
21	0	54	GLY	3.0
10	P	79	ARG	3.0
22	1	92	LYS	3.0
29	8	16	ILE	3.0
8	N	25	LYS	3.0
8	N	91	GLU	3.0
14	T	98	LYS	3.0
29	8	54	GLU	3.0
30	A	1575	C	3.0
21	0	44	ARG	3.0
19	Y	33	LYS	3.0
30	A	257	A	3.0
30	A	866	A	3.0
11	Q	111	GLU	3.0
30	A	1117	G	3.0
12	R	58	GLY	2.9
30	A	1078	U	2.9
19	Y	19	LYS	2.9
29	8	40	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
15	U	22	LYS	2.9
30	A	2828	C	2.9
15	U	18	LEU	2.9
8	N	117	HIS	2.9
30	A	2897	U	2.9
10	P	19	VAL	2.9
16	V	84	LYS	2.8
30	A	2894	G	2.8
15	U	17	ILE	2.8
16	V	71	LEU	2.8
30	A	1076	C	2.8
30	A	1383	C	2.8
29	8	50	LEU	2.8
13	S	17	ARG	2.8
30	A	1116	C	2.8
21	0	52	GLY	2.8
11	Q	7	MET	2.8
15	U	48	ALA	2.8
1	D	35	LYS	2.8
30	A	2363	C	2.8
30	A	2690	C	2.8
30	A	2871	C	2.8
15	U	51	LYS	2.8
18	X	75	ASP	2.7
29	8	34	TRP	2.7
11	Q	66	ILE	2.7
30	A	2775	A	2.7
8	N	114	LEU	2.7
1	D	202	LYS	2.7
23	2	72	ALA	2.7
2	E	121	ASN	2.7
11	Q	8	LYS	2.7
30	A	701	G	2.7
30	A	868	U	2.7
19	Y	63	LYS	2.7
30	A	615	G	2.7
11	Q	28	ALA	2.7
31	B	91	C	2.7
30	A	2189	U	2.7
14	T	113	LYS	2.6
30	A	1089	G	2.6
20	Z	82	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
11	Q	68	ILE	2.6
20	Z	74	VAL	2.6
10	P	78	PRO	2.6
30	A	2692	C	2.6
9	O	69	VAL	2.6
16	V	76	LYS	2.6
30	A	914	C	2.6
31	B	11	C	2.6
11	Q	133	ARG	2.6
9	O	66	LYS	2.6
13	S	13	ARG	2.6
14	T	104	ASN	2.6
30	A	2585	U	2.6
30	A	995	C	2.6
14	T	93	ARG	2.6
1	D	220	HIS	2.6
20	Z	75	ASN	2.6
20	Z	78	LYS	2.5
8	N	116	THR	2.5
8	N	30	LYS	2.5
13	S	12	PHE	2.5
11	Q	107	ALA	2.5
30	A	324	A	2.5
10	P	67	MET	2.5
30	A	1632	A	2.5
30	A	2676	C	2.5
11	Q	105	GLU	2.5
30	A	2175	C	2.5
4	G	35	GLU	2.5
14	T	3	ARG	2.5
30	A	1033	U	2.5
22	1	15	ALA	2.5
24	3	17	LYS	2.5
4	G	75	LYS	2.4
6	I	20	ASP	2.4
29	8	32	LEU	2.4
21	0	40	GLN	2.4
30	A	2402	C	2.4
30	A	2694	G	2.4
30	A	229	A	2.4
11	Q	135	ASP	2.4
19	Y	71	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
21	0	56	ASP	2.4
22	1	29	GLY	2.4
29	8	37	SER	2.4
21	0	19	LYS	2.4
16	V	83	ARG	2.4
22	1	28	GLY	2.4
16	V	68	LYS	2.4
6	I	21	VAL	2.4
30	A	645	C	2.4
18	X	33	LYS	2.4
30	A	1590	U	2.4
30	A	1217	C	2.4
30	A	2872	G	2.4
4	G	86	MET	2.4
29	8	47	LYS	2.4
12	R	101	ALA	2.4
30	A	2378	A	2.4
2	E	164	ARG	2.3
30	A	530	G	2.3
30	A	535	C	2.3
16	V	80	GLN	2.3
30	A	325	G	2.3
30	A	326	G	2.3
12	R	103	ARG	2.3
30	A	230	U	2.3
30	A	1420	U	2.3
6	I	74	ASN	2.3
10	P	74	GLU	2.3
30	A	438	G	2.3
10	P	75	ILE	2.3
21	0	75	LEU	2.3
30	A	537	C	2.3
12	R	109	ALA	2.3
4	G	164	GLU	2.3
12	R	110	PRO	2.3
1	D	26	LYS	2.2
30	A	277	C	2.2
30	A	1574	C	2.2
26	5	37	LYS	2.2
1	D	244	ARG	2.2
19	Y	35	TYR	2.2
30	A	790	C	2.2

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Mol	Chain	Res	Type	RSRZ
12	R	54	LEU	2.2
30	A	2148	G	2.2
9	O	109	LYS	2.2
30	A	2357	U	2.2
1	D	62	TYR	2.2
4	G	116	ASP	2.2
1	D	217	ARG	2.2
8	N	92	GLN	2.2
16	V	79	VAL	2.2
15	U	49	HIS	2.2
30	A	115	C	2.2
30	A	2023	G	2.2
11	Q	18	LYS	2.2
1	D	272	ALA	2.2
19	Y	4	LYS	2.2
21	0	58	THR	2.2
29	8	51	ALA	2.2
15	U	20	LEU	2.1
19	Y	53	PRO	2.1
30	A	540	G	2.1
30	A	1630	G	2.1
30	A	1080	C	2.1
21	0	71	ASP	2.1
2	E	160	TYR	2.1
30	A	1768	U	2.1
30	A	439	G	2.1
3	F	207	GLY	2.1
11	Q	134	ARG	2.1
24	3	30	ARG	2.1
30	A	1075	C	2.1
30	A	2380	C	2.1
6	I	1	MET	2.1
8	N	26	THR	2.1
15	U	15	LYS	2.1
22	1	11	ARG	2.1
21	0	73	GLY	2.1
10	P	22	GLY	2.1
11	Q	110	THR	2.1
28	7	48	LYS	2.1
30	A	278	A	2.1
30	A	2141	G	2.1
4	G	3	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
30	A	653	C	2.1
22	1	16	ASN	2.1
11	Q	138	ASP	2.1
30	A	1311	G	2.1
30	A	1218	C	2.1
30	A	2847	U	2.1
9	O	65	THR	2.1
6	I	25	TYR	2.0
30	A	994	C	2.0
30	A	2827	C	2.0
30	A	2111	C	2.0
11	Q	10	ARG	2.0
30	A	256	A	2.0
30	A	911	A	2.0
30	A	231	C	2.0
13	S	30	ARG	2.0
18	X	52	VAL	2.0
31	B	30	C	2.0
9	O	90	GLN	2.0
22	1	12	PRO	2.0
6	I	22	LYS	2.0
6	I	132	PRO	2.0
14	T	103	ARG	2.0

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(\AA^2)	Q<0.9
32	MG	A	3103	1/1	0.11	-	27,27,27,27	0
32	MG	A	3403	1/1	0.31	-	44,44,44,44	0
32	MG	A	3210	1/1	0.09	-	1,1,1,1	0
32	MG	A	3603	1/1	0.09	-	24,24,24,24	0
32	MG	A	2987	1/1	0.09	-	26,26,26,26	0
32	MG	B	161	1/1	0.47	-	60,60,60,60	0
32	MG	A	3372	1/1	0.17	-	42,42,42,42	0
32	MG	A	3496	1/1	0.54	-	62,62,62,62	0
32	MG	A	3465	1/1	0.05	-	42,42,42,42	0
32	MG	A	3329	1/1	0.15	-	24,24,24,24	0
32	MG	A	3256	1/1	0.22	-	43,43,43,43	0
32	MG	A	3252	1/1	0.34	-	29,29,29,29	0
32	MG	A	2913	1/1	0.06	-	8,8,8,8	0
32	MG	A	3491	1/1	0.10	-	32,32,32,32	0
32	MG	A	437	1/1	0.24	-	27,27,27,27	0
32	MG	H	673	1/1	0.08	-	64,64,64,64	0
32	MG	A	2953	1/1	0.07	-	11,11,11,11	0
32	MG	A	2950	1/1	0.03	-	10,10,10,10	0
32	MG	A	3585	1/1	0.30	-	38,38,38,38	0
32	MG	A	3472	1/1	0.29	-	35,35,35,35	0
32	MG	A	3624	1/1	0.21	-	20,20,20,20	0
32	MG	A	3377	1/1	0.12	-	48,48,48,48	0
32	MG	Z	819	1/1	0.17	-	31,31,31,31	0
32	MG	A	3067	1/1	0.14	-	33,33,33,33	0
32	MG	A	3353	1/1	0.10	-	24,24,24,24	0
32	MG	A	3277	1/1	0.47	-	56,56,56,56	0
32	MG	A	3554	1/1	0.23	-	38,38,38,38	0
32	MG	A	3282	1/1	0.06	-	36,36,36,36	0
32	MG	A	3468	1/1	0.26	-	21,21,21,21	0
32	MG	A	3142	1/1	0.14	-	32,32,32,32	0
32	MG	A	3292	1/1	0.12	-	19,19,19,19	0
32	MG	A	3339	1/1	0.08	-	36,36,36,36	0
32	MG	A	3284	1/1	0.06	-	4,4,4,4	0
32	MG	A	2959	1/1	0.10	-	25,25,25,25	0
32	MG	A	3531	1/1	0.13	-	5,5,5,5	0
32	MG	A	3036	1/1	0.16	-	61,61,61,61	0
32	MG	A	2947	1/1	0.07	-	25,25,25,25	0
32	MG	A	3090	1/1	0.12	-	31,31,31,31	0
32	MG	Q	194	1/1	0.24	-	53,53,53,53	0
32	MG	P	811	1/1	0.11	-	33,33,33,33	0
32	MG	A	3207	1/1	0.11	-	25,25,25,25	0
32	MG	A	3334	1/1	0.11	-	25,25,25,25	0
32	MG	A	3441	1/1	0.10	-	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	A	3393	1/1	0.08	-	24,24,24,24	0
32	MG	A	3293	1/1	0.10	-	1,1,1,1	0
32	MG	A	3591	1/1	0.25	-	39,39,39,39	0
32	MG	W	589	1/1	0.35	-	54,54,54,54	0
32	MG	B	125	1/1	0.15	-	48,48,48,48	0
32	MG	A	3521	1/1	0.10	-	58,58,58,58	0
32	MG	A	2942	1/1	0.12	-	14,14,14,14	0
32	MG	A	3257	1/1	0.13	-	8,8,8,8	0
32	MG	A	3307	1/1	0.11	-	26,26,26,26	0
32	MG	A	3559	1/1	0.10	-	29,29,29,29	0
32	MG	A	3641	1/1	0.55	-	39,39,39,39	0
32	MG	A	3183	1/1	0.10	-	25,25,25,25	0
32	MG	A	3466	1/1	0.26	-	11,11,11,11	0
32	MG	A	3194	1/1	0.12	-	31,31,31,31	0
32	MG	A	3426	1/1	0.21	-	34,34,34,34	0
32	MG	A	3205	1/1	0.10	-	24,24,24,24	0
32	MG	A	3105	1/1	0.30	-	34,34,34,34	0
32	MG	A	3573	1/1	0.10	-	21,21,21,21	0
32	MG	A	3604	1/1	0.59	-	60,60,60,60	0
32	MG	A	3261	1/1	0.06	-	7,7,7,7	0
32	MG	A	2981	1/1	0.06	-	15,15,15,15	0
32	MG	A	3430	1/1	0.19	-	48,48,48,48	0
32	MG	A	3557	1/1	0.36	-	59,59,59,59	0
32	MG	A	2980	1/1	0.07	-	7,7,7,7	0
32	MG	A	3471	1/1	0.10	-	43,43,43,43	0
32	MG	A	3438	1/1	0.11	-	35,35,35,35	0
32	MG	A	3402	1/1	0.12	-	15,15,15,15	0
32	MG	A	3454	1/1	0.07	-	15,15,15,15	0
32	MG	A	3117	1/1	0.07	-	9,9,9,9	0
32	MG	A	3477	1/1	0.14	-	19,19,19,19	0
32	MG	A	3442	1/1	0.13	-	71,71,71,71	0
32	MG	A	3007	1/1	0.12	-	21,21,21,21	0
32	MG	A	3571	1/1	0.08	-	20,20,20,20	0
32	MG	A	3229	1/1	0.12	-	38,38,38,38	0
32	MG	A	3638	1/1	0.08	-	55,55,55,55	0
32	MG	R	729	1/1	0.23	-	6,6,6,6	0
32	MG	A	3055	1/1	0.21	-	15,15,15,15	0
32	MG	A	3111	1/1	0.16	-	46,46,46,46	0
32	MG	A	3289	1/1	0.16	-	19,19,19,19	0
32	MG	B	748	1/1	0.63	-	41,41,41,41	0
32	MG	A	3041	1/1	0.09	-	47,47,47,47	0
32	MG	B	124	1/1	0.10	-	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	P	151	1/1	0.13	-	46,46,46,46	0
32	MG	A	3584	1/1	0.35	-	73,73,73,73	0
32	MG	A	3508	1/1	0.40	-	51,51,51,51	0
32	MG	A	3266	1/1	0.05	-	24,24,24,24	0
32	MG	A	3113	1/1	0.16	-	22,22,22,22	0
32	MG	A	3143	1/1	0.08	-	32,32,32,32	0
32	MG	A	3379	1/1	0.14	-	24,24,24,24	0
32	MG	A	3364	1/1	0.22	-	34,34,34,34	0
32	MG	A	2937	1/1	0.10	-	10,10,10,10	0
32	MG	A	2958	1/1	0.14	-	26,26,26,26	0
32	MG	A	3086	1/1	0.27	-	17,17,17,17	0
32	MG	A	3487	1/1	0.19	-	39,39,39,39	0
32	MG	A	3543	1/1	0.11	-	35,35,35,35	0
32	MG	A	3609	1/1	0.10	-	28,28,28,28	0
32	MG	A	3332	1/1	0.29	-	41,41,41,41	0
32	MG	A	3044	1/1	0.15	-	24,24,24,24	0
32	MG	U	549	1/1	0.15	-	27,27,27,27	0
32	MG	A	3524	1/1	0.49	-	66,66,66,66	0
32	MG	A	3167	1/1	0.04	-	6,6,6,6	0
32	MG	A	3317	1/1	0.14	-	34,34,34,34	0
32	MG	A	3489	1/1	0.20	-	45,45,45,45	0
32	MG	A	3357	1/1	0.20	-	58,58,58,58	0
32	MG	A	3031	1/1	0.17	-	32,32,32,32	0
32	MG	A	2921	1/1	0.08	-	4,4,4,4	0
32	MG	A	3320	1/1	0.12	-	48,48,48,48	0
32	MG	A	3546	1/1	0.46	-	66,66,66,66	0
32	MG	A	3123	1/1	0.11	-	19,19,19,19	0
32	MG	A	3380	1/1	0.06	-	5,5,5,5	0
32	MG	A	3325	1/1	0.16	-	29,29,29,29	0
32	MG	B	303	1/1	0.07	-	15,15,15,15	0
32	MG	A	2994	1/1	0.08	-	12,12,12,12	0
32	MG	P	667	1/1	0.09	-	43,43,43,43	0
32	MG	A	3065	1/1	0.34	-	31,31,31,31	0
32	MG	A	2961	1/1	0.07	-	15,15,15,15	0
32	MG	A	3367	1/1	0.18	-	32,32,32,32	0
32	MG	A	3411	1/1	0.30	-	33,33,33,33	0
32	MG	R	672	1/1	0.17	-	32,32,32,32	0
32	MG	A	3360	1/1	0.10	-	47,47,47,47	0
32	MG	A	3234	1/1	0.17	-	31,31,31,31	0
32	MG	A	2990	1/1	0.12	-	27,27,27,27	0
32	MG	E	793	1/1	0.10	-	29,29,29,29	0
32	MG	A	3272	1/1	0.20	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2952	1/1	0.13	-	11,11,11,11	0
32	MG	A	3550	1/1	0.09	-	19,19,19,19	0
32	MG	A	3152	1/1	0.13	-	24,24,24,24	0
32	MG	A	3217	1/1	0.11	-	11,11,11,11	0
32	MG	A	3222	1/1	0.07	-	42,42,42,42	0
32	MG	A	3022	1/1	0.16	-	10,10,10,10	0
32	MG	A	3566	1/1	0.13	-	62,62,62,62	0
32	MG	G	820	1/1	0.04	-	34,34,34,34	0
32	MG	A	3285	1/1	0.18	-	37,37,37,37	0
32	MG	A	3450	1/1	0.07	-	17,17,17,17	0
32	MG	A	3444	1/1	0.09	-	20,20,20,20	0
32	MG	A	3644	1/1	1.79	-	63,63,63,63	0
32	MG	A	3140	1/1	0.10	-	21,21,21,21	0
32	MG	A	156	1/1	0.06	-	1,1,1,1	0
32	MG	A	3283	1/1	0.19	-	17,17,17,17	0
32	MG	A	3058	1/1	0.10	-	8,8,8,8	0
32	MG	4	792	1/1	0.38	-	40,40,40,40	0
32	MG	A	3636	1/1	0.25	-	47,47,47,47	0
32	MG	A	3195	1/1	0.12	-	31,31,31,31	0
32	MG	A	3446	1/1	0.06	-	30,30,30,30	0
32	MG	A	3567	1/1	0.09	-	28,28,28,28	0
32	MG	A	3077	1/1	0.15	-	22,22,22,22	0
32	MG	A	3087	1/1	0.07	-	42,42,42,42	0
32	MG	B	377	1/1	0.06	-	47,47,47,47	0
32	MG	A	3247	1/1	0.09	-	39,39,39,39	0
32	MG	A	2924	1/1	0.10	-	9,9,9,9	0
32	MG	B	404	1/1	0.22	-	35,35,35,35	0
32	MG	A	3174	1/1	0.07	-	4,4,4,4	0
32	MG	A	2946	1/1	0.14	-	7,7,7,7	0
32	MG	A	3470	1/1	0.11	-	27,27,27,27	0
32	MG	A	3507	1/1	0.16	-	49,49,49,49	0
32	MG	A	369	1/1	0.14	-	15,15,15,15	0
32	MG	A	3017	1/1	0.53	-	27,27,27,27	0
32	MG	A	3594	1/1	0.88	-	60,60,60,60	0
32	MG	A	3089	1/1	0.10	-	12,12,12,12	0
32	MG	A	3102	1/1	0.25	-	55,55,55,55	0
32	MG	A	3238	1/1	0.08	-	24,24,24,24	0
32	MG	A	3185	1/1	0.13	-	8,8,8,8	0
32	MG	7	393	1/1	0.15	-	22,22,22,22	0
32	MG	A	3311	1/1	0.42	-	45,45,45,45	0
32	MG	A	3570	1/1	0.16	-	50,50,50,50	0
32	MG	A	3239	1/1	0.10	-	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	3109	1/1	0.07	-	24,24,24,24	0
32	MG	A	3474	1/1	0.46	-	55,55,55,55	0
32	MG	A	3309	1/1	0.10	-	54,54,54,54	0
32	MG	A	2911	1/1	0.15	-	24,24,24,24	0
32	MG	A	3346	1/1	0.08	-	35,35,35,35	0
32	MG	A	3073	1/1	0.08	-	22,22,22,22	0
32	MG	A	3551	1/1	0.59	-	39,39,39,39	0
32	MG	A	158	1/1	0.26	-	28,28,28,28	0
32	MG	A	3410	1/1	0.09	-	7,7,7,7	0
32	MG	A	3490	1/1	0.09	-	32,32,32,32	0
32	MG	A	3097	1/1	0.12	-	28,28,28,28	0
32	MG	A	3028	1/1	0.12	-	37,37,37,37	0
32	MG	A	3231	1/1	0.20	-	25,25,25,25	0
32	MG	A	3388	1/1	0.07	-	59,59,59,59	0
32	MG	A	3033	1/1	0.09	-	16,16,16,16	0
32	MG	A	2929	1/1	0.09	-	24,24,24,24	0
32	MG	A	3259	1/1	0.29	-	60,60,60,60	0
32	MG	B	172	1/1	0.26	-	37,37,37,37	0
32	MG	A	3361	1/1	0.10	-	18,18,18,18	0
32	MG	A	3158	1/1	0.05	-	25,25,25,25	0
32	MG	A	3133	1/1	0.07	-	21,21,21,21	0
32	MG	A	3294	1/1	0.10	-	19,19,19,19	0
32	MG	A	3420	1/1	0.15	-	65,65,65,65	0
32	MG	A	3394	1/1	0.15	-	39,39,39,39	0
32	MG	A	3391	1/1	0.19	-	47,47,47,47	0
32	MG	A	3392	1/1	0.07	-	13,13,13,13	0
32	MG	A	3250	1/1	0.28	-	17,17,17,17	0
32	MG	A	3301	1/1	0.09	-	24,24,24,24	0
32	MG	B	122	1/1	0.04	-	14,14,14,14	0
32	MG	A	3131	1/1	0.09	-	2,2,2,2	0
32	MG	A	3483	1/1	0.32	-	17,17,17,17	0
32	MG	A	3178	1/1	0.06	-	15,15,15,15	0
32	MG	A	3428	1/1	0.14	-	0,0,0,0	0
32	MG	A	3172	1/1	0.06	-	20,20,20,20	0
32	MG	A	3437	1/1	0.04	-	13,13,13,13	0
32	MG	A	3368	1/1	0.25	-	18,18,18,18	0
32	MG	A	2984	1/1	0.18	-	47,47,47,47	0
32	MG	A	3296	1/1	0.44	-	32,32,32,32	0
32	MG	A	3075	1/1	0.15	-	23,23,23,23	0
32	MG	A	3586	1/1	0.06	-	10,10,10,10	0
32	MG	B	761	1/1	0.36	-	51,51,51,51	0
32	MG	A	3180	1/1	0.21	-	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3042	1/1	0.23	-	18,18,18,18	0
32	MG	A	3000	1/1	0.19	-	22,22,22,22	0
32	MG	A	3333	1/1	0.08	-	32,32,32,32	0
32	MG	A	490	1/1	0.43	-	47,47,47,47	0
32	MG	A	2992	1/1	0.07	-	19,19,19,19	0
32	MG	A	3270	1/1	0.09	-	17,17,17,17	0
32	MG	A	2954	1/1	0.06	-	11,11,11,11	0
32	MG	8	702	1/1	0.33	-	20,20,20,20	0
32	MG	A	3614	1/1	0.30	-	33,33,33,33	0
32	MG	A	3121	1/1	0.10	-	12,12,12,12	0
32	MG	A	3452	1/1	0.12	-	7,7,7,7	0
32	MG	A	3126	1/1	0.06	-	5,5,5,5	0
32	MG	A	2979	1/1	0.17	-	51,51,51,51	0
32	MG	A	3497	1/1	0.37	-	29,29,29,29	0
32	MG	A	3291	1/1	0.12	-	36,36,36,36	0
32	MG	A	3408	1/1	0.06	-	6,6,6,6	0
32	MG	A	3495	1/1	0.18	-	36,36,36,36	0
32	MG	B	594	1/1	0.10	-	23,23,23,23	0
32	MG	A	3387	1/1	0.08	-	47,47,47,47	0
32	MG	A	3347	1/1	0.12	-	37,37,37,37	0
32	MG	B	246	1/1	0.53	-	44,44,44,44	0
32	MG	A	3128	1/1	0.04	-	0,0,0,0	0
32	MG	A	2991	1/1	0.07	-	7,7,7,7	0
32	MG	A	3443	1/1	0.28	-	24,24,24,24	0
32	MG	A	169	1/1	0.23	-	1,1,1,1	0
32	MG	B	480	1/1	0.21	-	46,46,46,46	0
32	MG	A	3155	1/1	0.12	-	20,20,20,20	0
32	MG	A	3080	1/1	0.11	-	14,14,14,14	0
32	MG	A	3240	1/1	0.18	-	10,10,10,10	0
32	MG	A	3132	1/1	0.14	-	12,12,12,12	0
32	MG	A	3323	1/1	0.40	-	51,51,51,51	0
32	MG	A	3461	1/1	0.11	-	25,25,25,25	0
32	MG	A	2968	1/1	0.06	-	0,0,0,0	0
32	MG	A	2983	1/1	0.16	-	23,23,23,23	0
32	MG	A	2919	1/1	0.07	-	11,11,11,11	0
32	MG	A	3157	1/1	0.33	-	29,29,29,29	0
32	MG	A	3263	1/1	0.07	-	33,33,33,33	0
32	MG	A	3149	1/1	0.12	-	37,37,37,37	0
32	MG	A	3108	1/1	0.08	-	41,41,41,41	0
32	MG	A	3510	1/1	0.09	-	39,39,39,39	0
32	MG	A	2997	1/1	0.14	-	23,23,23,23	0
32	MG	A	2932	1/1	0.16	-	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	3605	1/1	0.14	-	47,47,47,47	0
32	MG	A	3220	1/1	0.12	-	13,13,13,13	0
32	MG	A	3070	1/1	0.12	-	3,3,3,3	0
32	MG	A	3431	1/1	0.12	-	20,20,20,20	0
32	MG	A	3066	1/1	0.15	-	31,31,31,31	0
32	MG	A	3319	1/1	0.31	-	61,61,61,61	0
32	MG	A	3493	1/1	0.15	-	54,54,54,54	0
32	MG	A	3511	1/1	0.13	-	39,39,39,39	0
32	MG	A	2972	1/1	0.08	-	15,15,15,15	0
32	MG	A	3232	1/1	0.19	-	47,47,47,47	0
32	MG	A	3009	1/1	0.21	-	34,34,34,34	0
32	MG	A	3478	1/1	0.10	-	37,37,37,37	0
32	MG	A	3212	1/1	0.07	-	18,18,18,18	0
32	MG	A	3423	1/1	0.12	-	42,42,42,42	0
32	MG	A	3280	1/1	0.09	-	3,3,3,3	0
32	MG	A	3324	1/1	0.18	-	21,21,21,21	0
32	MG	A	3192	1/1	0.13	-	1,1,1,1	0
32	MG	X	685	1/1	0.11	-	50,50,50,50	0
32	MG	A	3208	1/1	0.24	-	39,39,39,39	0
32	MG	A	3556	1/1	0.05	-	7,7,7,7	0
32	MG	A	2908	1/1	0.31	-	42,42,42,42	0
32	MG	A	3190	1/1	0.17	-	34,34,34,34	0
32	MG	A	3313	1/1	0.11	-	22,22,22,22	0
32	MG	A	157	1/1	0.16	-	58,58,58,58	0
32	MG	A	3255	1/1	0.14	-	36,36,36,36	0
32	MG	A	3476	1/1	0.07	-	14,14,14,14	0
32	MG	A	3013	1/1	0.18	-	43,43,43,43	0
32	MG	A	3509	1/1	0.06	-	34,34,34,34	0
32	MG	A	3425	1/1	0.11	-	19,19,19,19	0
32	MG	A	3049	1/1	0.10	-	18,18,18,18	0
32	MG	I	149	1/1	0.06	-	18,18,18,18	0
32	MG	A	3010	1/1	0.18	-	16,16,16,16	0
32	MG	A	3315	1/1	0.23	-	22,22,22,22	0
32	MG	A	3189	1/1	0.22	-	4,4,4,4	0
32	MG	A	3354	1/1	0.17	-	37,37,37,37	0
32	MG	A	3503	1/1	0.13	-	10,10,10,10	0
32	MG	A	3228	1/1	0.07	-	7,7,7,7	0
32	MG	A	3457	1/1	0.17	-	39,39,39,39	0
32	MG	A	3427	1/1	0.09	-	3,3,3,3	0
32	MG	A	3561	1/1	0.06	-	4,4,4,4	0
32	MG	A	2940	1/1	0.12	-	13,13,13,13	0
32	MG	B	495	1/1	0.12	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	168	1/1	0.06	-	35,35,35,35	0
32	MG	A	3088	1/1	0.11	-	28,28,28,28	0
32	MG	A	3134	1/1	0.06	-	12,12,12,12	0
32	MG	A	3081	1/1	0.07	-	9,9,9,9	0
32	MG	A	3019	1/1	0.10	-	41,41,41,41	0
32	MG	A	3572	1/1	0.13	-	30,30,30,30	0
32	MG	A	3628	1/1	0.22	-	43,43,43,43	0
32	MG	A	3622	1/1	0.21	-	56,56,56,56	0
32	MG	A	3558	1/1	0.06	-	6,6,6,6	0
32	MG	E	638	1/1	0.68	-	36,36,36,36	0
32	MG	A	3206	1/1	0.21	-	42,42,42,42	0
32	MG	A	3618	1/1	0.11	-	19,19,19,19	0
32	MG	A	3297	1/1	0.18	-	57,57,57,57	0
32	MG	A	3515	1/1	0.10	-	38,38,38,38	0
32	MG	A	3179	1/1	0.07	-	6,6,6,6	0
32	MG	A	2917	1/1	0.18	-	23,23,23,23	0
32	MG	A	3458	1/1	0.08	-	36,36,36,36	0
32	MG	A	3162	1/1	0.07	-	31,31,31,31	0
32	MG	A	3608	1/1	0.59	-	54,54,54,54	0
32	MG	A	2975	1/1	0.09	-	29,29,29,29	0
32	MG	A	3258	1/1	0.15	-	21,21,21,21	0
32	MG	Z	780	1/1	0.15	-	32,32,32,32	0
32	MG	A	3606	1/1	0.16	-	45,45,45,45	0
32	MG	A	3262	1/1	0.12	-	23,23,23,23	0
32	MG	A	3051	1/1	0.24	-	37,37,37,37	0
32	MG	A	2920	1/1	0.07	-	3,3,3,3	0
32	MG	A	3630	1/1	0.18	-	62,62,62,62	0
32	MG	A	3530	1/1	0.28	-	28,28,28,28	0
32	MG	A	3061	1/1	0.24	-	49,49,49,49	0
32	MG	A	3286	1/1	0.13	-	38,38,38,38	0
32	MG	A	3598	1/1	0.14	-	61,61,61,61	0
32	MG	A	3047	1/1	0.22	-	30,30,30,30	0
32	MG	A	2963	1/1	0.13	-	19,19,19,19	0
32	MG	A	3479	1/1	0.15	-	26,26,26,26	0
32	MG	A	2918	1/1	0.12	-	9,9,9,9	0
32	MG	A	3216	1/1	0.06	-	8,8,8,8	0
32	MG	A	3245	1/1	0.08	-	0,0,0,0	0
32	MG	A	3336	1/1	0.14	-	31,31,31,31	0
32	MG	A	3518	1/1	0.08	-	26,26,26,26	0
32	MG	A	3375	1/1	0.18	-	10,10,10,10	0
32	MG	A	3306	1/1	0.07	-	43,43,43,43	0
32	MG	A	3486	1/1	0.05	-	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	B	795	1/1	0.40	-	46,46,46,46	0
32	MG	A	3562	1/1	0.71	-	55,55,55,55	0
32	MG	A	3592	1/1	0.12	-	42,42,42,42	0
32	MG	A	3119	1/1	0.08	-	21,21,21,21	0
32	MG	A	3451	1/1	0.09	-	8,8,8,8	0
32	MG	A	3419	1/1	0.08	-	39,39,39,39	0
32	MG	A	3390	1/1	0.04	-	13,13,13,13	0
32	MG	A	2930	1/1	0.08	-	16,16,16,16	0
32	MG	A	3565	1/1	0.13	-	20,20,20,20	0
32	MG	A	3512	1/1	0.10	-	28,28,28,28	0
32	MG	A	3514	1/1	0.17	-	24,24,24,24	0
32	MG	A	3021	1/1	0.04	-	26,26,26,26	0
32	MG	A	3281	1/1	0.09	-	55,55,55,55	0
32	MG	B	167	1/1	0.18	-	39,39,39,39	0
32	MG	4	807	1/1	0.36	-	40,40,40,40	0
32	MG	O	631	1/1	0.35	-	23,23,23,23	0
32	MG	A	3328	1/1	0.25	-	41,41,41,41	0
32	MG	A	3620	1/1	0.17	-	51,51,51,51	0
32	MG	A	159	1/1	0.13	-	10,10,10,10	0
32	MG	A	3249	1/1	0.15	-	14,14,14,14	0
32	MG	A	3170	1/1	0.12	-	0,0,0,0	0
32	MG	A	3068	1/1	0.20	-	32,32,32,32	0
32	MG	A	3436	1/1	0.11	-	26,26,26,26	0
32	MG	A	3145	1/1	0.04	-	16,16,16,16	0
32	MG	A	3355	1/1	0.08	-	26,26,26,26	0
32	MG	A	2939	1/1	0.06	-	6,6,6,6	0
32	MG	A	3340	1/1	0.16	-	16,16,16,16	0
32	MG	A	2943	1/1	0.08	-	17,17,17,17	0
32	MG	A	3025	1/1	0.10	-	1,1,1,1	0
32	MG	B	633	1/1	0.12	-	59,59,59,59	0
32	MG	A	3341	1/1	0.17	-	29,29,29,29	0
32	MG	A	3147	1/1	0.07	-	35,35,35,35	0
32	MG	A	3488	1/1	0.12	-	17,17,17,17	0
32	MG	A	3100	1/1	0.16	-	20,20,20,20	0
32	MG	A	3500	1/1	0.21	-	26,26,26,26	0
32	MG	P	429	1/1	0.26	-	44,44,44,44	0
32	MG	A	3001	1/1	0.08	-	1,1,1,1	0
32	MG	H	744	1/1	0.12	-	19,19,19,19	0
32	MG	A	3599	1/1	0.10	-	27,27,27,27	0
32	MG	A	3048	1/1	0.13	-	20,20,20,20	0
32	MG	A	3349	1/1	0.10	-	44,44,44,44	0
32	MG	A	3191	1/1	0.06	-	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	3314	1/1	0.12	-	39,39,39,39	0
32	MG	A	3322	1/1	0.53	-	29,29,29,29	0
32	MG	A	3057	1/1	0.12	-	13,13,13,13	0
32	MG	A	3463	1/1	0.23	-	53,53,53,53	0
32	MG	A	3610	1/1	0.65	-	62,62,62,62	0
32	MG	B	368	1/1	0.18	-	20,20,20,20	0
32	MG	A	2936	1/1	0.15	-	0,0,0,0	0
32	MG	A	3230	1/1	0.07	-	23,23,23,23	0
32	MG	A	3116	1/1	0.06	-	26,26,26,26	0
32	MG	A	3469	1/1	0.08	-	16,16,16,16	0
32	MG	A	3264	1/1	0.19	-	30,30,30,30	0
32	MG	A	3115	1/1	0.04	-	2,2,2,2	0
32	MG	A	3093	1/1	0.07	-	12,12,12,12	0
32	MG	A	2966	1/1	0.07	-	0,0,0,0	0
32	MG	A	3407	1/1	0.18	-	13,13,13,13	0
32	MG	A	3024	1/1	0.18	-	24,24,24,24	0
32	MG	A	2931	1/1	0.09	-	22,22,22,22	0
32	MG	A	3071	1/1	0.09	-	47,47,47,47	0
32	MG	A	3226	1/1	0.08	-	4,4,4,4	0
32	MG	A	3578	1/1	0.17	-	46,46,46,46	0
32	MG	A	3016	1/1	0.26	-	13,13,13,13	0
32	MG	A	3532	1/1	0.06	-	20,20,20,20	0
32	MG	A	3405	1/1	0.18	-	62,62,62,62	0
32	MG	A	3460	1/1	0.07	-	36,36,36,36	0
32	MG	A	3008	1/1	0.07	-	12,12,12,12	0
32	MG	A	3547	1/1	0.15	-	44,44,44,44	0
32	MG	A	3331	1/1	0.18	-	71,71,71,71	0
32	MG	A	3040	1/1	0.16	-	52,52,52,52	0
32	MG	A	2996	1/1	0.23	-	32,32,32,32	0
32	MG	W	675	1/1	0.20	-	36,36,36,36	0
32	MG	A	3485	1/1	0.23	-	40,40,40,40	0
32	MG	A	3440	1/1	0.06	-	16,16,16,16	0
32	MG	A	3018	1/1	0.06	-	5,5,5,5	0
32	MG	A	3365	1/1	0.12	-	34,34,34,34	0
32	MG	A	3124	1/1	0.06	-	3,3,3,3	0
32	MG	A	3135	1/1	0.20	-	24,24,24,24	0
32	MG	2	660	1/1	0.09	-	58,58,58,58	0
32	MG	A	3120	1/1	0.10	-	37,37,37,37	0
32	MG	A	3574	1/1	0.29	-	63,63,63,63	0
32	MG	A	3308	1/1	0.12	-	53,53,53,53	0
32	MG	A	3186	1/1	0.10	-	10,10,10,10	0
32	MG	A	3597	1/1	0.08	-	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	3050	1/1	0.10	-	50,50,50,50	0
32	MG	A	3552	1/1	0.10	-	35,35,35,35	0
32	MG	A	3214	1/1	0.10	-	28,28,28,28	0
32	MG	A	3029	1/1	0.08	-	71,71,71,71	0
32	MG	A	3445	1/1	0.09	-	13,13,13,13	0
32	MG	A	3582	1/1	0.15	-	76,76,76,76	0
32	MG	A	3535	1/1	0.14	-	42,42,42,42	0
32	MG	A	3455	1/1	0.28	-	74,74,74,74	0
32	MG	A	3634	1/1	0.87	-	50,50,50,50	0
32	MG	A	3141	1/1	0.20	-	19,19,19,19	0
32	MG	A	3129	1/1	0.31	-	14,14,14,14	0
32	MG	Z	709	1/1	0.18	-	27,27,27,27	0
32	MG	A	2951	1/1	0.08	-	20,20,20,20	0
32	MG	A	3015	1/1	0.11	-	21,21,21,21	0
32	MG	A	3274	1/1	0.07	-	39,39,39,39	0
32	MG	A	3563	1/1	0.39	-	25,25,25,25	0
32	MG	A	3449	1/1	0.27	-	19,19,19,19	0
32	MG	A	3160	1/1	0.36	-	40,40,40,40	0
32	MG	A	2960	1/1	0.10	-	31,31,31,31	0
32	MG	A	3359	1/1	0.15	-	19,19,19,19	0
32	MG	A	3616	1/1	0.20	-	33,33,33,33	0
32	MG	A	3101	1/1	0.13	-	42,42,42,42	0
32	MG	A	3096	1/1	0.24	-	32,32,32,32	0
32	MG	A	2957	1/1	0.13	-	2,2,2,2	0
32	MG	A	3209	1/1	0.09	-	31,31,31,31	0
32	MG	A	3523	1/1	0.29	-	46,46,46,46	0
32	MG	A	3063	1/1	0.13	-	8,8,8,8	0
32	MG	A	3241	1/1	0.11	-	40,40,40,40	0
32	MG	A	3539	1/1	0.14	-	45,45,45,45	0
32	MG	F	781	1/1	0.35	-	45,45,45,45	0
32	MG	A	2914	1/1	0.11	-	2,2,2,2	0
32	MG	A	3448	1/1	0.10	-	8,8,8,8	0
32	MG	A	3406	1/1	0.10	-	48,48,48,48	0
32	MG	A	2964	1/1	0.09	-	4,4,4,4	0
32	MG	A	3373	1/1	0.10	-	19,19,19,19	0
32	MG	A	3385	1/1	0.08	-	13,13,13,13	0
32	MG	A	3161	1/1	0.08	-	48,48,48,48	0
32	MG	A	3480	1/1	0.34	-	47,47,47,47	0
32	MG	A	3200	1/1	0.15	-	47,47,47,47	0
32	MG	A	2977	1/1	0.17	-	19,19,19,19	0
32	MG	A	3248	1/1	0.16	-	38,38,38,38	0
32	MG	A	3125	1/1	0.07	-	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	A	3370	1/1	0.11	-	46,46,46,46	0
32	MG	A	3299	1/1	0.29	-	32,32,32,32	0
32	MG	A	3352	1/1	0.37	-	8,8,8,8	0
32	MG	A	3542	1/1	0.22	-	41,41,41,41	0
32	MG	A	2985	1/1	0.09	-	19,19,19,19	0
32	MG	A	3153	1/1	0.15	-	15,15,15,15	0
32	MG	A	3540	1/1	0.08	-	55,55,55,55	0
32	MG	A	3577	1/1	0.11	-	50,50,50,50	0
32	MG	A	3576	1/1	0.15	-	41,41,41,41	0
32	MG	A	3383	1/1	0.06	-	30,30,30,30	0
32	MG	D	277	1/1	0.08	-	0,0,0,0	0
32	MG	A	3330	1/1	0.19	-	17,17,17,17	0
32	MG	A	3225	1/1	0.09	-	50,50,50,50	0
32	MG	A	3601	1/1	0.20	-	50,50,50,50	0
32	MG	A	3004	1/1	0.29	-	33,33,33,33	0
32	MG	A	2988	1/1	0.27	-	35,35,35,35	0
32	MG	A	3053	1/1	0.09	-	14,14,14,14	0
32	MG	A	3171	1/1	0.08	-	11,11,11,11	0
32	MG	A	3268	1/1	0.10	-	35,35,35,35	0
32	MG	A	2941	1/1	0.11	-	57,57,57,57	0
32	MG	A	3159	1/1	0.04	-	31,31,31,31	0
32	MG	A	3453	1/1	0.12	-	36,36,36,36	0
32	MG	A	2925	1/1	0.07	-	2,2,2,2	0
32	MG	B	123	1/1	0.21	-	59,59,59,59	0
32	MG	I	693	1/1	0.06	-	18,18,18,18	0
32	MG	A	3223	1/1	0.12	-	36,36,36,36	0
32	MG	A	3529	1/1	0.23	-	26,26,26,26	0
32	MG	A	3196	1/1	0.09	-	12,12,12,12	0
32	MG	A	3613	1/1	0.08	-	27,27,27,27	0
32	MG	A	3076	1/1	0.19	-	12,12,12,12	0
32	MG	A	3621	1/1	0.10	-	64,64,64,64	0
32	MG	A	3154	1/1	0.08	-	33,33,33,33	0
32	MG	P	152	1/1	0.08	-	45,45,45,45	0
32	MG	A	3221	1/1	0.27	-	10,10,10,10	0
32	MG	A	3275	1/1	0.04	-	10,10,10,10	0
32	MG	A	3513	1/1	0.08	-	46,46,46,46	0
32	MG	A	3589	1/1	0.66	-	38,38,38,38	0
32	MG	A	3522	1/1	0.76	-	47,47,47,47	0
32	MG	A	3169	1/1	0.10	-	29,29,29,29	0
32	MG	A	3398	1/1	0.10	-	16,16,16,16	0
32	MG	A	3118	1/1	0.11	-	27,27,27,27	0
32	MG	A	3400	1/1	0.12	-	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	H	671	1/1	0.09	-	46,46,46,46	0
32	MG	A	2971	1/1	0.09	-	0,0,0,0	0
32	MG	A	3072	1/1	0.12	-	50,50,50,50	0
32	MG	A	3295	1/1	0.35	-	42,42,42,42	0
32	MG	A	3043	1/1	0.08	-	9,9,9,9	0
32	MG	A	3246	1/1	0.23	-	43,43,43,43	0
32	MG	A	3251	1/1	0.07	-	19,19,19,19	0
32	MG	A	3528	1/1	0.27	-	13,13,13,13	0
32	MG	A	3413	1/1	0.10	-	31,31,31,31	0
32	MG	3	555	1/1	0.10	-	43,43,43,43	0
32	MG	A	3611	1/1	0.34	-	44,44,44,44	0
32	MG	A	3600	1/1	0.13	-	28,28,28,28	0
32	MG	A	3537	1/1	0.10	-	63,63,63,63	0
32	MG	A	3409	1/1	0.29	-	63,63,63,63	0
32	MG	A	2926	1/1	0.12	-	19,19,19,19	0
32	MG	5	85	1/1	0.08	-	2,2,2,2	0
32	MG	A	3211	1/1	0.07	-	21,21,21,21	0
32	MG	A	3327	1/1	0.20	-	7,7,7,7	0
32	MG	A	3517	1/1	0.06	-	21,21,21,21	0
32	MG	A	3243	1/1	0.12	-	24,24,24,24	0
32	MG	A	3619	1/1	0.07	-	60,60,60,60	0
32	MG	A	3144	1/1	0.07	-	16,16,16,16	0
32	MG	A	3520	1/1	0.22	-	19,19,19,19	0
32	MG	O	661	1/1	0.05	-	14,14,14,14	0
32	MG	A	3626	1/1	0.08	-	25,25,25,25	0
32	MG	A	3138	1/1	0.15	-	5,5,5,5	0
32	MG	A	3110	1/1	0.12	-	20,20,20,20	0
32	MG	A	3038	1/1	0.11	-	11,11,11,11	0
32	MG	A	3615	1/1	0.22	-	50,50,50,50	0
32	MG	A	3536	1/1	0.12	-	19,19,19,19	0
32	MG	A	2956	1/1	0.13	-	46,46,46,46	0
32	MG	A	3439	1/1	0.34	-	17,17,17,17	0
32	MG	A	3498	1/1	0.09	-	21,21,21,21	0
32	MG	A	3481	1/1	0.19	-	28,28,28,28	0
32	MG	N	689	1/1	0.08	-	29,29,29,29	0
32	MG	T	817	1/1	0.08	-	25,25,25,25	0
32	MG	A	3376	1/1	0.16	-	35,35,35,35	0
32	MG	A	3193	1/1	0.18	-	16,16,16,16	0
32	MG	A	3130	1/1	0.27	-	31,31,31,31	0
32	MG	A	3276	1/1	0.14	-	20,20,20,20	0
32	MG	A	3175	1/1	0.09	-	20,20,20,20	0
32	MG	A	3148	1/1	0.12	-	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3084	1/1	0.05	-	48,48,48,48	0
32	MG	A	3607	1/1	0.08	-	11,11,11,11	0
32	MG	A	3374	1/1	0.15	-	6,6,6,6	0
32	MG	A	3039	1/1	0.08	-	20,20,20,20	0
32	MG	A	3288	1/1	0.09	-	21,21,21,21	0
32	MG	A	3030	1/1	0.10	-	46,46,46,46	0
32	MG	A	3560	1/1	0.73	-	65,65,65,65	0
32	MG	A	3541	1/1	0.07	-	41,41,41,41	0
32	MG	A	3342	1/1	0.12	-	5,5,5,5	0
32	MG	A	2967	1/1	0.24	-	11,11,11,11	0
32	MG	A	2982	1/1	0.18	-	12,12,12,12	0
32	MG	A	3351	1/1	0.21	-	41,41,41,41	0
32	MG	B	461	1/1	0.21	-	24,24,24,24	0
32	MG	A	3260	1/1	0.20	-	29,29,29,29	0
32	MG	A	3204	1/1	0.15	-	15,15,15,15	0
32	MG	A	2944	1/1	0.06	-	10,10,10,10	0
32	MG	A	2978	1/1	0.08	-	8,8,8,8	0
32	MG	A	3538	1/1	0.20	-	21,21,21,21	0
32	MG	A	3382	1/1	0.10	-	37,37,37,37	0
32	MG	A	3482	1/1	0.20	-	83,83,83,83	0
32	MG	A	3580	1/1	0.18	-	46,46,46,46	0
32	MG	A	3548	1/1	1.66	-	80,80,80,80	0
32	MG	A	3304	1/1	0.19	-	50,50,50,50	0
32	MG	A	3545	1/1	0.26	-	61,61,61,61	0
32	MG	A	2916	1/1	0.09	-	16,16,16,16	0
32	MG	A	3505	1/1	0.25	-	47,47,47,47	0
32	MG	A	3106	1/1	0.23	-	18,18,18,18	0
32	MG	A	3432	1/1	0.11	-	31,31,31,31	0
32	MG	A	3326	1/1	0.35	-	41,41,41,41	0
32	MG	A	3631	1/1	0.12	-	39,39,39,39	0
32	MG	A	3107	1/1	0.28	-	46,46,46,46	0
32	MG	A	3237	1/1	0.10	-	32,32,32,32	0
32	MG	A	3386	1/1	0.08	-	18,18,18,18	0
32	MG	A	3434	1/1	0.08	-	82,82,82,82	0
32	MG	A	3525	1/1	0.09	-	37,37,37,37	0
32	MG	A	3099	1/1	0.08	-	20,20,20,20	0
32	MG	A	3184	1/1	0.07	-	6,6,6,6	0
32	MG	A	3074	1/1	0.07	-	26,26,26,26	0
32	MG	B	636	1/1	0.12	-	53,53,53,53	0
32	MG	A	3643	1/1	0.52	-	43,43,43,43	0
32	MG	A	3244	1/1	0.09	-	38,38,38,38	0
32	MG	A	3278	1/1	0.09	-	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	3593	1/1	0.10	-	45,45,45,45	0
32	MG	A	3095	1/1	0.10	-	45,45,45,45	0
32	MG	A	2969	1/1	0.20	-	47,47,47,47	0
32	MG	A	3516	1/1	0.07	-	22,22,22,22	0
32	MG	A	3348	1/1	0.12	-	23,23,23,23	0
32	MG	A	3422	1/1	0.20	-	26,26,26,26	0
32	MG	B	196	1/1	0.05	-	39,39,39,39	0
32	MG	A	2962	1/1	0.12	-	27,27,27,27	0
32	MG	A	3421	1/1	0.42	-	12,12,12,12	0
32	MG	A	3166	1/1	0.07	-	0,0,0,0	0
32	MG	A	3462	1/1	0.08	-	45,45,45,45	0
32	MG	A	3467	1/1	0.23	-	24,24,24,24	0
32	MG	A	3389	1/1	0.10	-	25,25,25,25	0
32	MG	A	3564	1/1	0.31	-	27,27,27,27	0
32	MG	A	3633	1/1	0.06	-	23,23,23,23	0
32	MG	A	3122	1/1	0.08	-	1,1,1,1	0
32	MG	A	3035	1/1	0.12	-	21,21,21,21	0
32	MG	A	3271	1/1	0.76	-	51,51,51,51	0
32	MG	A	3527	1/1	0.06	-	40,40,40,40	0
32	MG	A	3163	1/1	0.10	-	35,35,35,35	0
32	MG	A	3345	1/1	0.16	-	12,12,12,12	0
32	MG	A	3137	1/1	0.42	-	57,57,57,57	0
32	MG	A	3456	1/1	0.11	-	44,44,44,44	0
32	MG	A	2935	1/1	0.07	-	21,21,21,21	0
32	MG	A	2974	1/1	0.40	-	31,31,31,31	0
32	MG	A	42	1/1	0.11	-	5,5,5,5	0
32	MG	A	3164	1/1	0.08	-	17,17,17,17	0
32	MG	A	2999	1/1	0.15	-	24,24,24,24	0
32	MG	A	2938	1/1	0.14	-	9,9,9,9	0
32	MG	A	3078	1/1	0.20	-	44,44,44,44	0
32	MG	A	3401	1/1	0.15	-	7,7,7,7	0
32	MG	A	3045	1/1	0.08	-	31,31,31,31	0
32	MG	A	3146	1/1	0.24	-	48,48,48,48	0
32	MG	A	3287	1/1	0.17	-	34,34,34,34	0
32	MG	A	3399	1/1	0.27	-	33,33,33,33	0
32	MG	Z	752	1/1	0.08	-	24,24,24,24	0
32	MG	A	3253	1/1	0.38	-	19,19,19,19	0
32	MG	A	3083	1/1	0.17	-	32,32,32,32	0
32	MG	2	664	1/1	0.28	-	49,49,49,49	0
32	MG	A	3002	1/1	0.09	-	23,23,23,23	0
32	MG	A	3581	1/1	0.37	-	52,52,52,52	0
32	MG	A	3254	1/1	0.13	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3316	1/1	0.57	-	43,43,43,43	0
32	MG	4	662	1/1	0.17	-	23,23,23,23	0
32	MG	A	3213	1/1	0.19	-	19,19,19,19	0
32	MG	A	3203	1/1	0.26	-	34,34,34,34	0
32	MG	A	3568	1/1	0.06	-	10,10,10,10	0
32	MG	A	3475	1/1	0.26	-	42,42,42,42	0
32	MG	A	3187	1/1	0.13	-	29,29,29,29	0
32	MG	A	3595	1/1	0.39	-	24,24,24,24	0
32	MG	A	3435	1/1	0.28	-	48,48,48,48	0
32	MG	A	3555	1/1	0.26	-	42,42,42,42	0
32	MG	A	3242	1/1	0.33	-	44,44,44,44	0
32	MG	A	3371	1/1	0.09	-	31,31,31,31	0
32	MG	A	2995	1/1	0.08	-	8,8,8,8	0
32	MG	A	3139	1/1	0.07	-	15,15,15,15	0
32	MG	A	3267	1/1	0.22	-	42,42,42,42	0
32	MG	A	2993	1/1	0.09	-	30,30,30,30	0
32	MG	A	3321	1/1	0.13	-	56,56,56,56	0
32	MG	A	3037	1/1	0.28	-	25,25,25,25	0
32	MG	A	3069	1/1	0.17	-	46,46,46,46	0
32	MG	A	3202	1/1	0.08	-	30,30,30,30	0
32	MG	A	3415	1/1	0.11	-	49,49,49,49	0
32	MG	A	3397	1/1	0.05	-	0,0,0,0	0
32	MG	A	3575	1/1	0.10	-	45,45,45,45	0
32	MG	A	170	1/1	0.20	-	33,33,33,33	0
32	MG	A	3612	1/1	0.13	-	34,34,34,34	0
32	MG	A	3265	1/1	0.09	-	41,41,41,41	0
32	MG	A	3378	1/1	0.07	-	10,10,10,10	0
32	MG	A	2934	1/1	0.27	-	17,17,17,17	0
32	MG	A	3381	1/1	0.08	-	44,44,44,44	0
32	MG	A	3151	1/1	0.08	-	39,39,39,39	0
32	MG	A	3236	1/1	0.24	-	35,35,35,35	0
32	MG	W	694	1/1	0.07	-	7,7,7,7	0
32	MG	A	2945	1/1	0.05	-	12,12,12,12	0
32	MG	A	3112	1/1	0.16	-	12,12,12,12	0
32	MG	A	3198	1/1	0.09	-	29,29,29,29	0
32	MG	A	2973	1/1	0.22	-	20,20,20,20	0
32	MG	A	3305	1/1	0.09	-	28,28,28,28	0
32	MG	A	3534	1/1	0.15	-	19,19,19,19	0
32	MG	A	3302	1/1	0.10	-	17,17,17,17	0
32	MG	A	3003	1/1	0.05	-	3,3,3,3	0
32	MG	P	785	1/1	0.35	-	42,42,42,42	0
32	MG	A	3027	1/1	0.09	-	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	A	2948	1/1	0.06	-	7,7,7,7	0
32	MG	A	3602	1/1	0.27	-	54,54,54,54	0
32	MG	A	3023	1/1	0.28	-	23,23,23,23	0
32	MG	A	3136	1/1	0.11	-	41,41,41,41	0
32	MG	A	3484	1/1	0.06	-	41,41,41,41	0
32	MG	V	747	1/1	0.14	-	61,61,61,61	0
32	MG	A	3176	1/1	0.42	-	36,36,36,36	0
32	MG	A	3412	1/1	0.20	-	44,44,44,44	0
32	MG	A	2949	1/1	0.07	-	10,10,10,10	0
32	MG	A	2927	1/1	0.09	-	7,7,7,7	0
32	MG	A	3235	1/1	0.17	-	12,12,12,12	0
32	MG	A	3494	1/1	0.23	-	44,44,44,44	0
32	MG	A	2970	1/1	0.13	-	17,17,17,17	0
32	MG	A	3094	1/1	0.16	-	43,43,43,43	0
32	MG	A	3085	1/1	0.14	-	67,67,67,67	0
32	MG	B	776	1/1	0.81	-	53,53,53,53	0
32	MG	A	3310	1/1	0.20	-	33,33,33,33	0
32	MG	A	2965	1/1	0.09	-	31,31,31,31	0
32	MG	A	100	1/1	0.10	-	5,5,5,5	0
32	MG	A	3215	1/1	0.41	-	46,46,46,46	0
32	MG	A	3358	1/1	0.08	-	30,30,30,30	0
32	MG	A	3127	1/1	0.06	-	8,8,8,8	0
32	MG	A	3082	1/1	0.12	-	40,40,40,40	0
32	MG	A	2989	1/1	0.18	-	42,42,42,42	0
32	MG	A	3501	1/1	0.12	-	55,55,55,55	0
32	MG	A	3350	1/1	0.07	-	22,22,22,22	0
32	MG	A	3416	1/1	0.12	-	14,14,14,14	0
32	MG	A	3502	1/1	0.22	-	40,40,40,40	0
32	MG	B	754	1/1	0.04	-	34,34,34,34	0
32	MG	A	3590	1/1	0.12	-	34,34,34,34	0
32	MG	A	3459	1/1	0.10	-	26,26,26,26	0
32	MG	H	769	1/1	0.07	-	11,11,11,11	0
32	MG	A	3011	1/1	0.08	-	1,1,1,1	0
32	MG	A	3544	1/1	0.33	-	38,38,38,38	0
32	MG	A	3201	1/1	0.11	-	36,36,36,36	0
32	MG	A	3569	1/1	0.12	-	89,89,89,89	0
32	MG	A	3092	1/1	0.16	-	0,0,0,0	0
32	MG	A	3464	1/1	0.08	-	18,18,18,18	0
32	MG	A	3020	1/1	0.15	-	24,24,24,24	0
32	MG	A	3553	1/1	0.10	-	23,23,23,23	0
32	MG	A	3506	1/1	0.36	-	23,23,23,23	0
32	MG	A	2910	1/1	0.13	-	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	3579	1/1	0.27	-	30,30,30,30	0
32	MG	A	538	1/1	0.44	-	41,41,41,41	0
32	MG	A	3642	1/1	0.12	-	53,53,53,53	0
32	MG	A	3429	1/1	0.23	-	53,53,53,53	0
32	MG	A	3165	1/1	0.12	-	0,0,0,0	0
32	MG	A	3362	1/1	0.36	-	39,39,39,39	0
32	MG	A	3526	1/1	0.38	-	13,13,13,13	0
32	MG	A	3366	1/1	0.10	-	37,37,37,37	0
32	MG	A	3290	1/1	0.10	-	26,26,26,26	0
32	MG	A	3627	1/1	0.21	-	2,2,2,2	0
32	MG	A	3034	1/1	0.10	-	11,11,11,11	0
32	MG	A	3369	1/1	0.19	-	44,44,44,44	0
32	MG	A	2976	1/1	0.08	-	34,34,34,34	0
32	MG	A	3098	1/1	0.17	-	24,24,24,24	0
32	MG	7	619	1/1	0.09	-	28,28,28,28	0
32	MG	A	3218	1/1	0.05	-	34,34,34,34	0
32	MG	A	3150	1/1	0.16	-	32,32,32,32	0
32	MG	A	2933	1/1	0.21	-	25,25,25,25	0
32	MG	A	3629	1/1	0.41	-	52,52,52,52	0
32	MG	A	2909	1/1	0.06	-	1,1,1,1	0
32	MG	A	3062	1/1	0.10	-	42,42,42,42	0
32	MG	B	217	1/1	0.06	-	43,43,43,43	0
32	MG	P	710	1/1	0.21	-	3,3,3,3	0
32	MG	A	3424	1/1	0.11	-	35,35,35,35	0
32	MG	A	3533	1/1	0.18	-	55,55,55,55	0
32	MG	A	3079	1/1	0.11	-	47,47,47,47	0
32	MG	A	2922	1/1	0.18	-	3,3,3,3	0
32	MG	A	3418	1/1	0.23	-	51,51,51,51	0
32	MG	A	3596	1/1	0.14	-	21,21,21,21	0
32	MG	A	166	1/1	0.18	-	52,52,52,52	0
32	MG	A	3233	1/1	0.20	-	33,33,33,33	0
32	MG	A	3632	1/1	0.18	-	43,43,43,43	0
32	MG	A	2986	1/1	0.15	-	24,24,24,24	0
32	MG	B	367	1/1	0.46	-	45,45,45,45	0
32	MG	A	3338	1/1	0.21	-	36,36,36,36	0
32	MG	A	3032	1/1	0.05	-	20,20,20,20	0
32	MG	A	3404	1/1	0.10	-	5,5,5,5	0
32	MG	A	3639	1/1	0.31	-	32,32,32,32	0
32	MG	A	3447	1/1	0.20	-	44,44,44,44	0
32	MG	A	3549	1/1	0.15	-	24,24,24,24	0
32	MG	A	160	1/1	0.18	-	38,38,38,38	0
32	MG	A	3473	1/1	0.07	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2998	1/1	0.11	-	13,13,13,13	0
32	MG	A	2928	1/1	0.22	-	12,12,12,12	0
32	MG	A	3006	1/1	0.09	-	16,16,16,16	0
32	MG	B	374	1/1	0.34	-	34,34,34,34	0
32	MG	A	3104	1/1	0.09	-	23,23,23,23	0
32	MG	A	3046	1/1	0.10	-	11,11,11,11	0
32	MG	A	3343	1/1	0.17	-	25,25,25,25	0
32	MG	A	3181	1/1	0.17	-	12,12,12,12	0
32	MG	A	3623	1/1	0.32	-	58,58,58,58	0
32	MG	A	3318	1/1	0.07	-	7,7,7,7	0
32	MG	A	3188	1/1	0.16	-	37,37,37,37	0
32	MG	A	3182	1/1	0.44	-	31,31,31,31	0
32	MG	A	3303	1/1	0.11	-	26,26,26,26	0
32	MG	A	3363	1/1	0.12	-	55,55,55,55	0
32	MG	A	3177	1/1	0.10	-	7,7,7,7	0
32	MG	A	2915	1/1	0.20	-	17,17,17,17	0
32	MG	A	3625	1/1	0.23	-	27,27,27,27	0
32	MG	A	3091	1/1	0.14	-	51,51,51,51	0
32	MG	A	3026	1/1	0.14	-	27,27,27,27	0
32	MG	A	3344	1/1	0.09	-	23,23,23,23	0
32	MG	A	3273	1/1	0.21	-	36,36,36,36	0
32	MG	A	3384	1/1	0.12	-	5,5,5,5	0
32	MG	A	3587	1/1	0.18	-	27,27,27,27	0
32	MG	A	2955	1/1	0.20	-	38,38,38,38	0
32	MG	A	3356	1/1	0.11	-	20,20,20,20	0
32	MG	A	3269	1/1	0.06	-	21,21,21,21	0
32	MG	A	3433	1/1	0.05	-	50,50,50,50	0
32	MG	B	627	1/1	0.20	-	49,49,49,49	0
32	MG	U	215	1/1	0.45	-	38,38,38,38	0
32	MG	A	3519	1/1	0.14	-	32,32,32,32	0
32	MG	A	3583	1/1	0.11	-	36,36,36,36	0
32	MG	A	3012	1/1	0.14	-	19,19,19,19	0
32	MG	A	3640	1/1	0.19	-	59,59,59,59	0
32	MG	A	2912	1/1	0.04	-	9,9,9,9	0
32	MG	A	3637	1/1	0.81	-	48,48,48,48	0
32	MG	A	3298	1/1	0.23	-	33,33,33,33	0
32	MG	A	3168	1/1	0.13	-	2,2,2,2	0
32	MG	A	2923	1/1	0.07	-	5,5,5,5	0
32	MG	A	3417	1/1	0.12	-	7,7,7,7	0
32	MG	A	3173	1/1	0.09	-	3,3,3,3	0
32	MG	A	3056	1/1	0.04	-	21,21,21,21	0
32	MG	A	3414	1/1	0.09	-	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3395	1/1	0.10	-	30,30,30,30	0
32	MG	A	3635	1/1	0.20	-	34,34,34,34	0
32	MG	A	3300	1/1	0.12	-	31,31,31,31	0
32	MG	A	3054	1/1	0.15	-	30,30,30,30	0
32	MG	A	3492	1/1	0.09	-	43,43,43,43	0
32	MG	A	3219	1/1	0.08	-	27,27,27,27	0
32	MG	A	3588	1/1	0.29	-	42,42,42,42	0
32	MG	A	3224	1/1	0.18	-	0,0,0,0	0
32	MG	A	3312	1/1	0.07	-	26,26,26,26	0
32	MG	A	3014	1/1	0.06	-	6,6,6,6	0
32	MG	A	3156	1/1	0.13	-	22,22,22,22	0
32	MG	A	3005	1/1	0.10	-	5,5,5,5	0
32	MG	A	3499	1/1	0.25	-	41,41,41,41	0
32	MG	A	3227	1/1	0.08	-	8,8,8,8	0
32	MG	A	3052	1/1	0.23	-	35,35,35,35	0
32	MG	A	3617	1/1	0.09	-	60,60,60,60	0
32	MG	A	3335	1/1	0.09	-	11,11,11,11	0
32	MG	A	3114	1/1	0.10	-	11,11,11,11	0
32	MG	A	3199	1/1	0.08	-	15,15,15,15	0
32	MG	A	3059	1/1	0.21	-	44,44,44,44	0
32	MG	A	3504	1/1	0.15	-	47,47,47,47	0
32	MG	A	3060	1/1	0.20	-	23,23,23,23	0
32	MG	A	3279	1/1	0.07	-	13,13,13,13	0
32	MG	A	3337	1/1	0.26	-	20,20,20,20	0
32	MG	A	3064	1/1	0.09	-	52,52,52,52	0
32	MG	A	3197	1/1	0.07	-	10,10,10,10	0
32	MG	A	3396	1/1	0.14	-	6,6,6,6	0

6.5 Other polymers

There are no such residues in this entry.