



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 06:27 PM BST

PDB ID : 4V90
Title : THERMUS THERMOPHILUS RIBOSOME
Authors : CHEN, Y.; FENG, S.; KUMAR, V.; ERO, R.; GAO, Y.G.
Deposited on : 2014-02-22
Resolution : 2.95 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

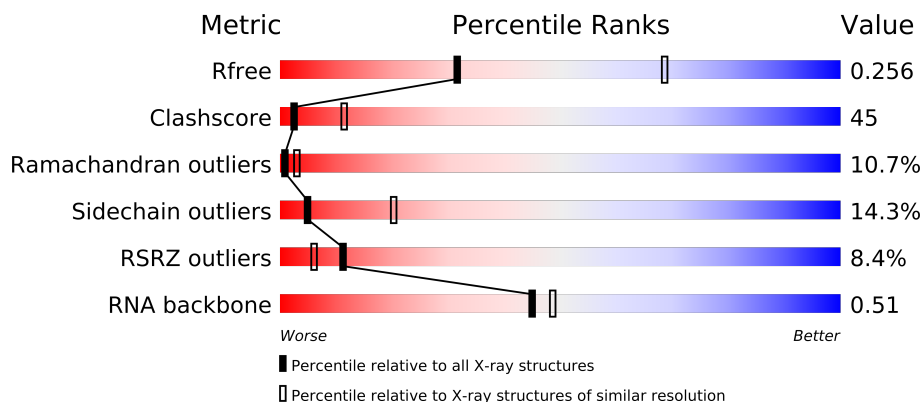
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
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) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)
RNA backbone	1838	1019 (3.46-2.46)

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	AA	1519	
2	AB	256	
3	AC	239	
4	AD	209	
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	132	


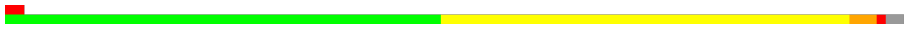


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Mol	Chain	Length	Quality of chain
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	76	
23	AX	9	
24	AY	691	
25	B0	84	
26	B1	97	
27	B2	71	
28	B3	60	
29	B4	71	
30	B5	59	
31	B6	53	
32	B7	48	
33	B8	64	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	228	
38	BD	275	
39	BE	206	
40	BF	210	
41	BG	181	
42	BH	180	
43	BJ	130	
44	BK	140	
45	BL	71	
46	BN	140	
47	BO	122	
48	BP	149	
49	BQ	141	
50	BR	117	
51	BS	111	
52	BT	146	
53	BU	117	
54	BV	101	

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Mol	Chain	Length	Quality of chain
55	BW	113	
56	BX	95	
57	BY	109	
58	BZ	205	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 153829 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1507	Total	C	N	O	P	0	0	0
			32391	14418	6002	10465	1506			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	1030	C	-	INSERTION	GB 48256
AA	1034	G	-	INSERTION	GB 48256
AA	1245	A	-	INSERTION	GB 48256
AA	1246	C	-	INSERTION	GB 48256

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O		0	0	0
			574	367	112	95				

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	88	Total	C	N	O	S	0	0	1
			692	440	128	122	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O		0	0	1
			209	128	51	30				

- Molecule 22 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	291	530	75			

- Molecule 23 is a RNA chain called 5'-R(*UP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			188	86	34	60	8			

- Molecule 24 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	687	Total	C	N	O	S	0	0	1
			5376	3412	922	1022	20			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2901	Total	C	N	O	P	0	0	0
			62476	27807	11683	20086	2900			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	2155	G	A	CONFLICT	GB 55771382

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BC	227	Total	C	N	O	S	0	0	0
			1735	1096	318	318	3			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BG	179	Total	C	N	O	S	0	0	0
			1459	931	266	258	4			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BH	176	Total	C	N	O	S	0	0	1
			1345	853	253	237	2			

- Molecule 43 is a protein called CHAIN J.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BJ	130	Total	C	N	O	0	0	0
			654	393	130	131			

- Molecule 44 is a protein called CHAIN K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BK	140	Total	C	N	O	0	0	0
			701	420	140	141			

- Molecule 45 is a protein called CHAIN L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BL	71	Total	C	N	O	0	0	0
			356	213	71	72			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	S	0	0	1
			726	471	132	123				

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B5	1	Total	Mg	0	0
			1	1		
59	BU	1	Total	Mg	0	0
			1	1		
59	BA	320	Total	Mg	0	0
			320	320		

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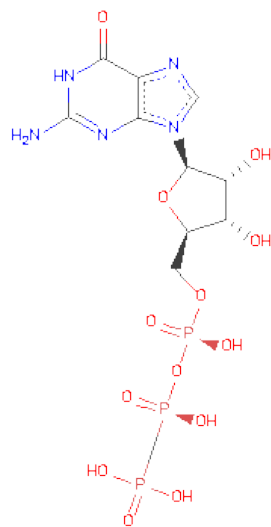
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	198	Total	Mg	0	0
			198	198		
59	B0	1	Total	Mg	0	0
			1	1		
59	AY	1	Total	Mg	0	0
			1	1		
59	BC	1	Total	Mg	0	0
			1	1		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B9	1	Total	Zn	0	0
			1	1		
60	AD	1	Total	Zn	0	0
			1	1		
60	AN	1	Total	Zn	0	0
			1	1		

- Molecule 61 is PHOSPHOMETHYLPHOSPHONICACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

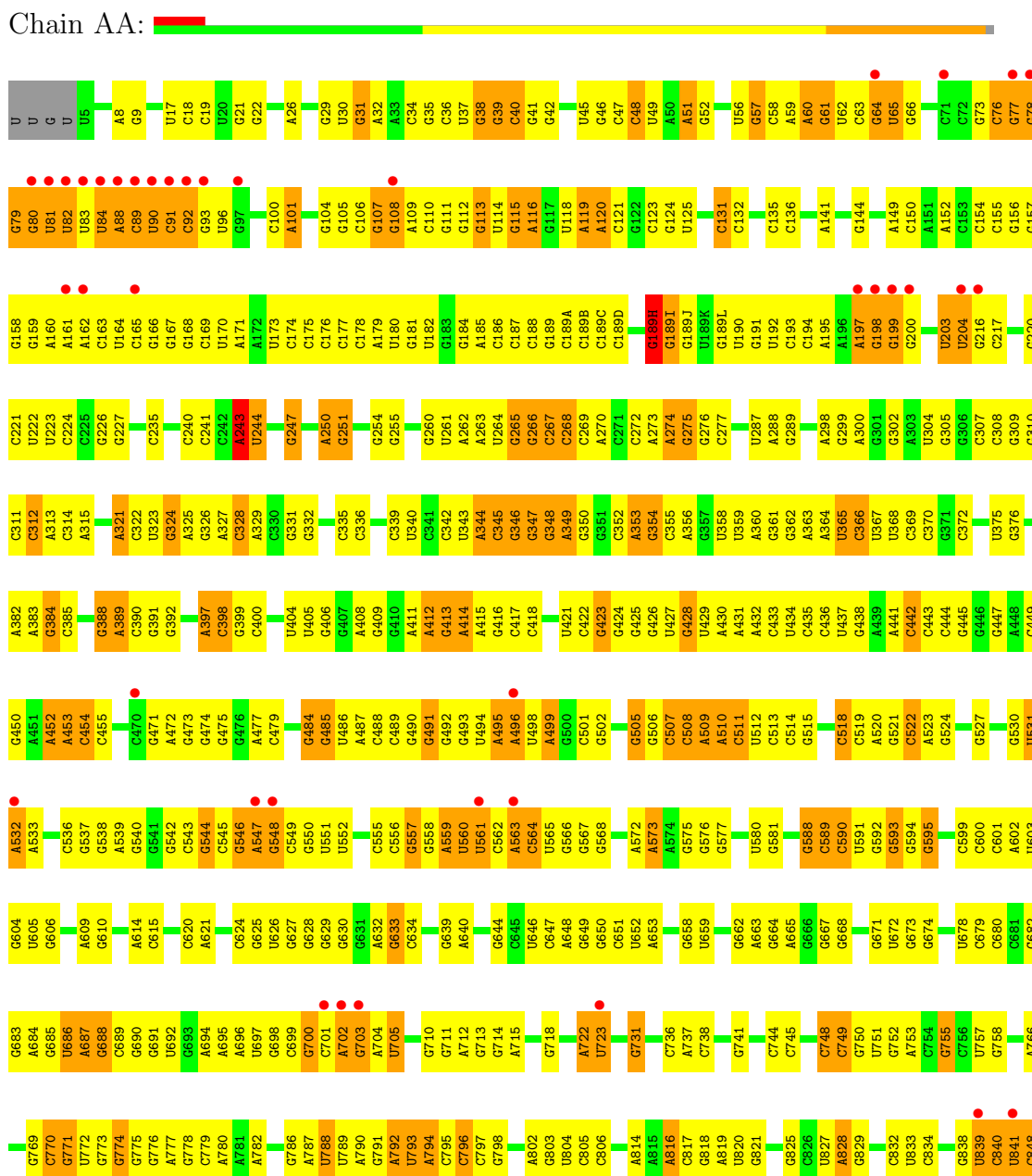
- Molecule 62 is water.

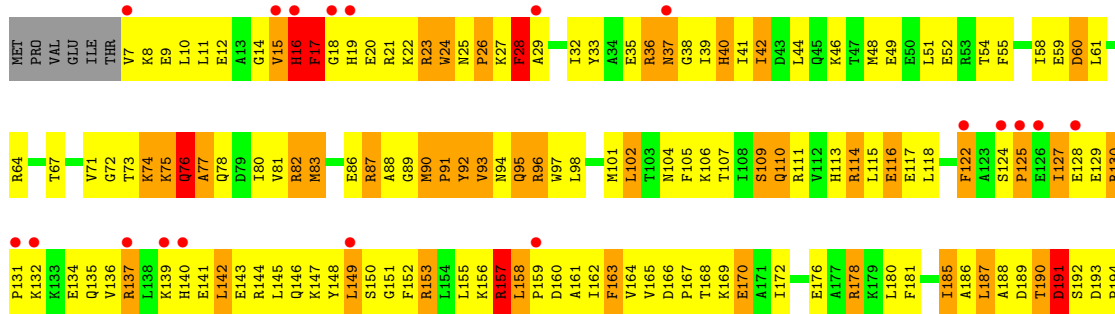
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	AY	2	Total	O	0	0
			2	2		

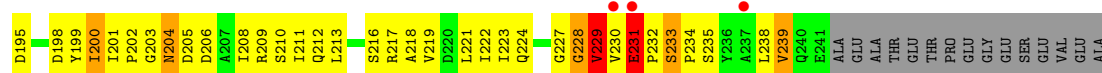
3 Residue-property plots

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: 16S RIBOSOMAL RNA

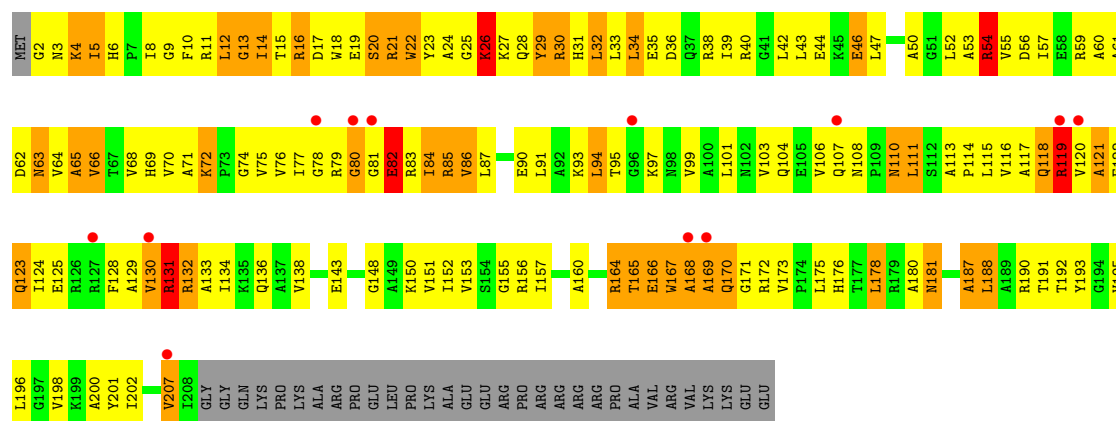






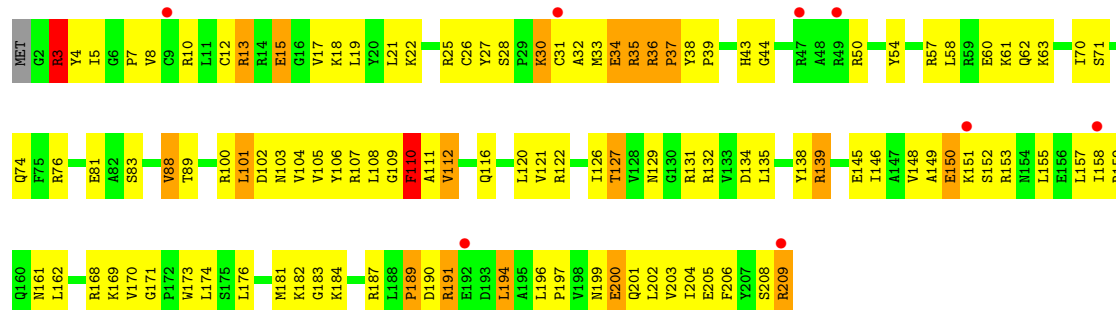
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



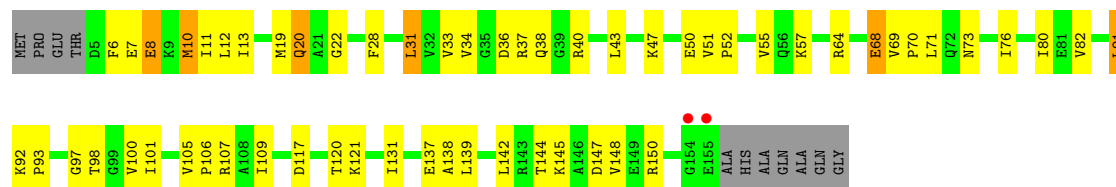
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:



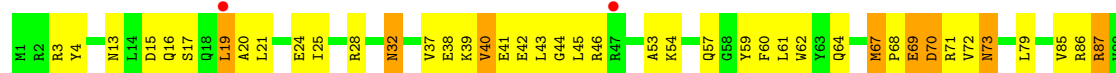
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

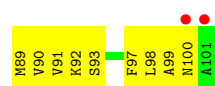
Chain AE:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

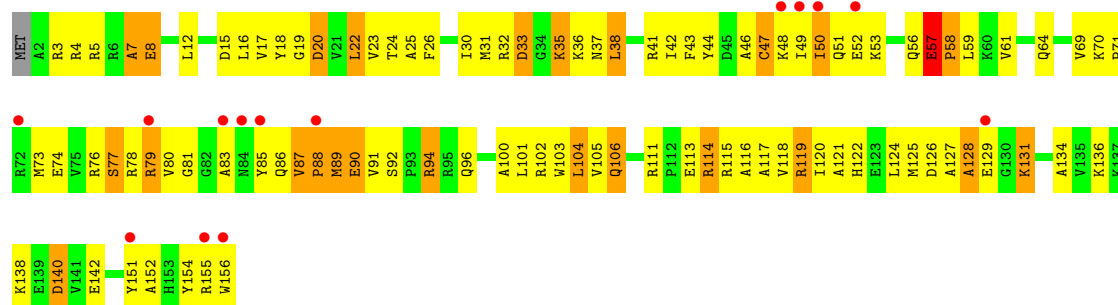
Chain AF:





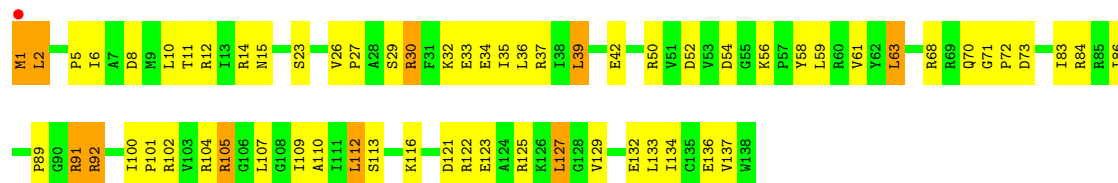
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



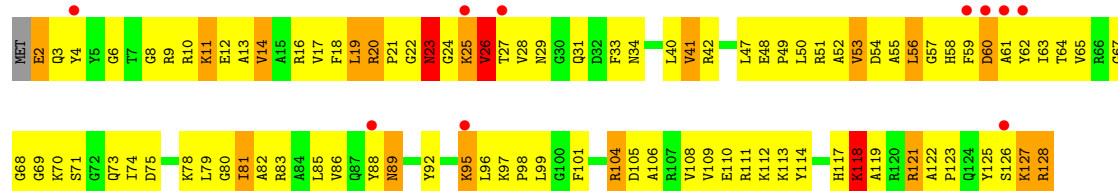
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



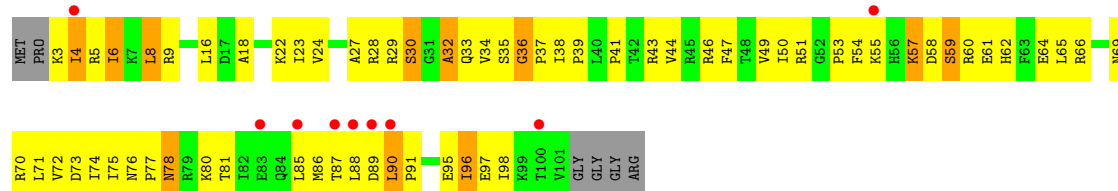
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



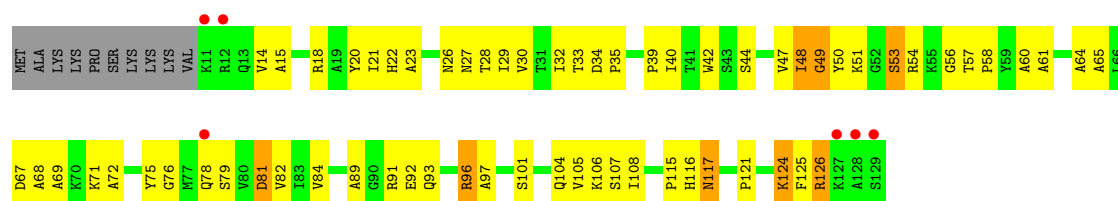
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



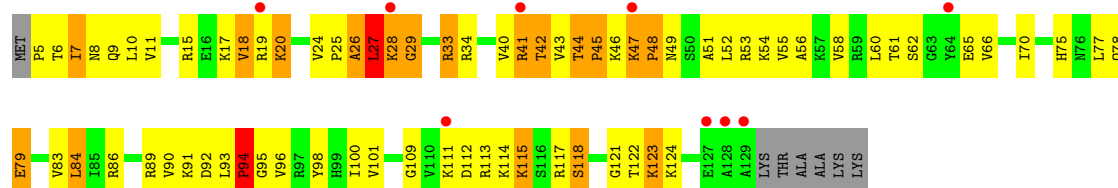
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



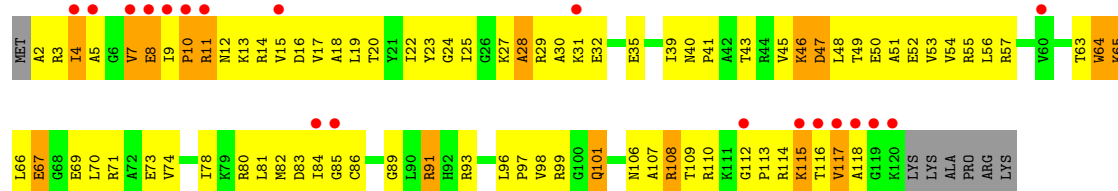
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

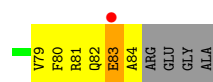
Chain AO:



• Molecule 16: 30S RIBOSOMAL PROTEIN S16

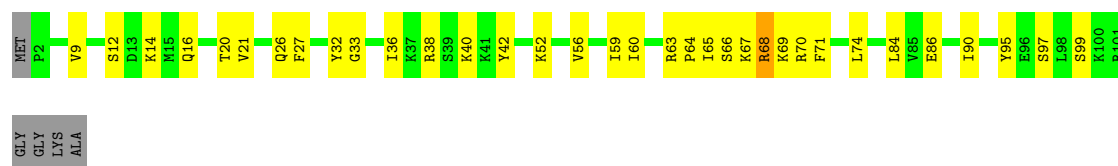
Chain AP:





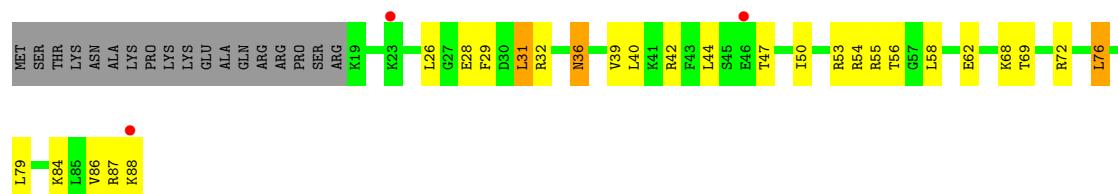
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



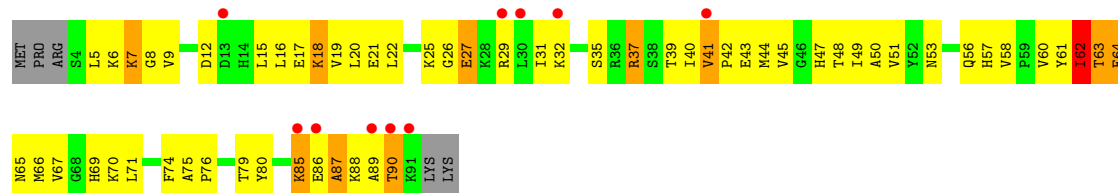
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



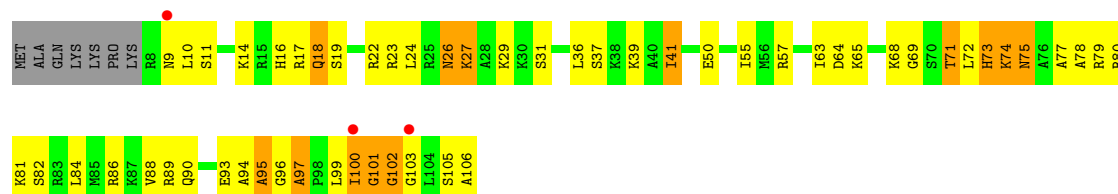
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



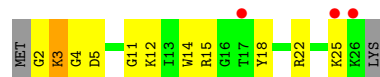
• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



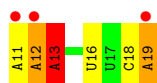
• Molecule 22: RNA (77-MER)

Chain AV:



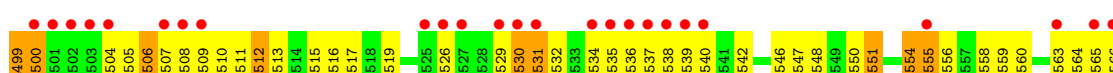
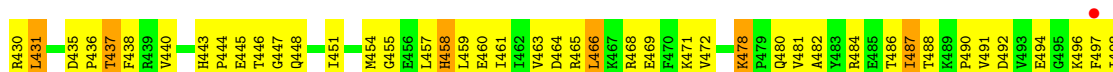
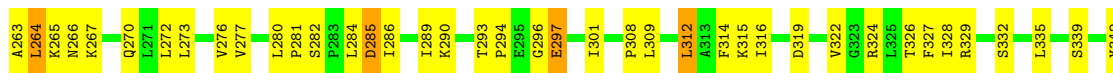
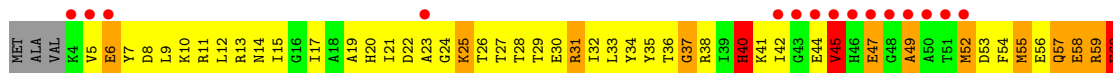
- Molecule 23: 5'-R(*UP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

Chain AX:



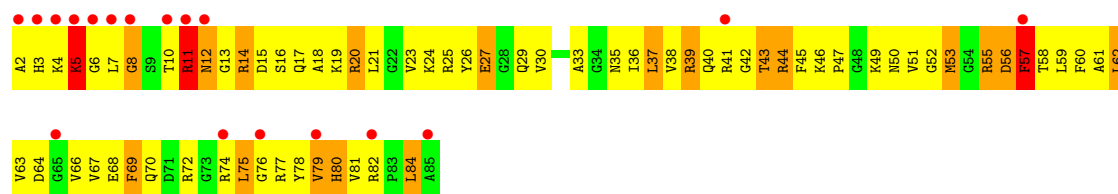
- Molecule 24: ELONGATION FACTOR G

Chain AY:



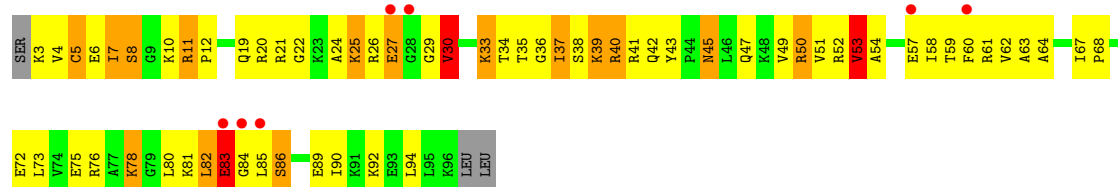
- Molecule 25: 50S RIBOSOMAL PROTEIN L27

Chain B0:



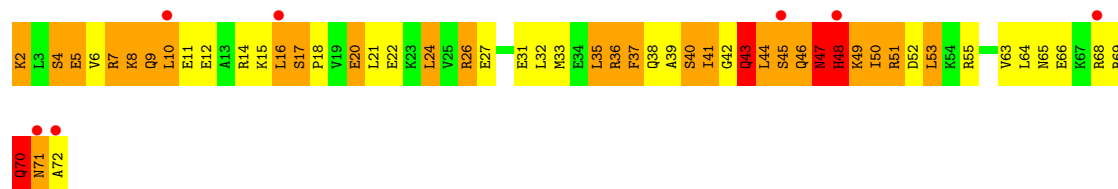
• Molecule 26: 50S RIBOSOMAL PROTEIN L28

Chain B1:



• Molecule 27: 50S RIBOSOMAL PROTEIN L29

Chain B2:



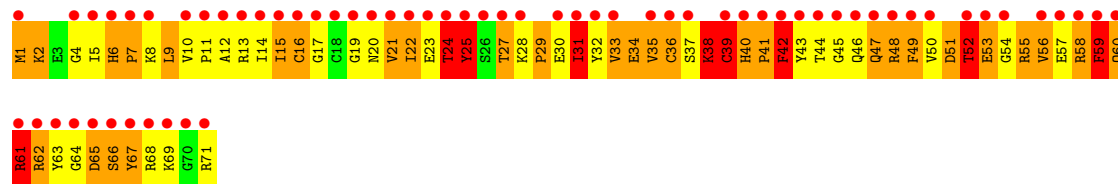
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

Chain B3:



• Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



• Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



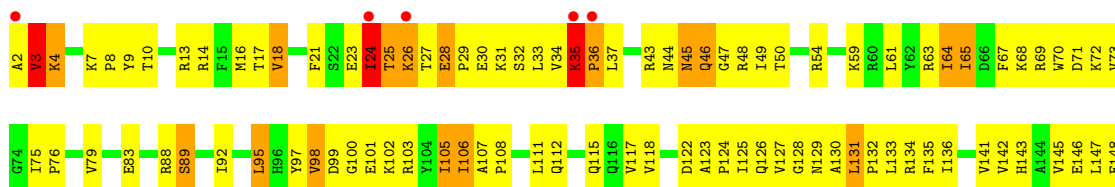
• Molecule 31: 50S RIBOSOMAL PROTEIN L33

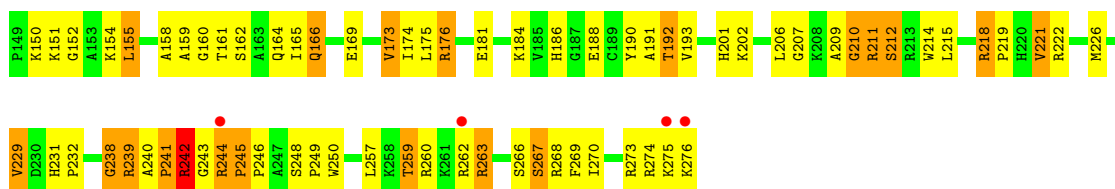
Chain B6:





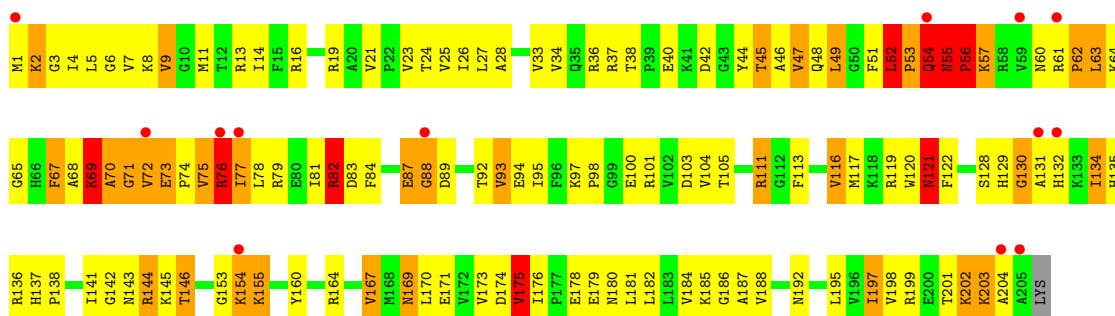
U2563	G2484	U2408	G2343	G2271	G2194	G2127	C2043	A1981	G1901	G1817	G1748	G1568
A2564	G2485	G2409	U2344	U2272	C2195	C2128	C2043	C1982	C1902	U1818	A1749	A1569
A2565	G2410	G2410	G2345	A2273	C2196	C2129	A2051	C1983	G1903	A1819	A1750	A1570
G2566	A2346	A2411	A2346	A2274	U2197	U2130	G2052	G1984	G1906	A1821	C1751	A1571
G2567	U2492	G2414	C2347	G2275	A2198	U2132	C2055	G1985	G1907	G1822	C1754	A1572
G2568	U2493	G2415	C2350	G2277	C2200	A2133	G2056	G1987	G1908	G1823	G1681	C1577
G2569	G2494	G2415	G2351	A2278	C2201	A2134	G2056	G1988	A1912	G1824	A1762	U1578
G2570	C2498	U2419	A2352	G2282	C2202	A2135	A2060	G1989	A1913	G1825	G1763	U1579
G2571	C2499	G2420	G2353	G2283	C2203	C2136	A2061	G1990	A1914	G1826	G1764	A1580
C2572	G2502	G2421	G2354	G2284	C2205	C2137	A2062	U1991	U1915	G1828	G1765	G1581
G2576	A2503	A2422	C2355	C2285	G2206	C2138	C2065	U1992	U1916	G1829	U1766	G1674
A2577	U2504	G2424	G2356	A2286	A2207	U1993	C2066	U1993	U1917	C1835	C1767	C1584
G2578	G2505	A2425	G2357	A2287	U2218	G2141	C2067	C1994	A1918	U1768	A1676	A1586
C2579	G2506	A2426	G2358	A2288	G2219	C2142	G2068	U1995	A1919	G1769	A1677	A1587
U2580	G2508	C2427	G2359	A2289	G2220	G2143	G2069	G1997	G1921	C1838	C1770	C1588
G2581	G2512	G2428	A2360	U2291	G2221	U2144	G2070	G1998	G1922	G1839	G1772	C1589
G2584	G2513	G2429	A2361	C2292	G2222	C2145	A2071	C1999	U1923	A1773	G1682	G1591
U2585	G2514	A2430	C2362	C2293	G2223	G2146	U2074	G2000	G1924	C1774	C1683	C1592
C2586	C2515	U2431	C2363	C2297	G2224	C2147	U2075	G2002	C1925	U1776	C1684	G1593
A2587	G2516	A2432	G2364	A2298	A2225	G2148	U2076	G2006	U1926	G1777	C1678	G1594
G2588	C2517	G2439	G2365	G2299	C2226	G2149	U2078	C2007	A1927	G1778	U1688	G1595
G2591	U2518	C2440	A2369	G2300	G2230	U2150	C2078	C2008	G1930	U1779	A1596	A1597
C2592	G2523	C2441	G2373	A2305	C2231	G2151	U2079	C2008	U1931	A1780	C1598	C1598
U2593	C2442	G2442	C2374	G2306	U2232	G2152	U2086	G2009	U1932	C1781	C1599	C1599
C2594	G2443	C2443	G2375	G2307	G2233	G2154	G2087	G2010	G1933	C1782	C1600	C1600
G2595	G2444	G2444	A2376	G2308	G2234	G2155	G2090	U2011	A1936	A1783	U1693	G1601
U2596	G2445	G2445	A2377	G2309	G2235	G2156	U2091	A2013	A1937	A1785	C1694	U1602
G2597	G2446	G2446	A2378	A2309	G2236	A2158	U2092	A2014	A1938	G1856	G1695	G1695
G2600	G2447	G2447	G2379	A2310	G2237	G2159	U2092	A2015	G1857	A1786	G1696	C1607
A2601	A2448	A2448	C2380	A2311	G2238	G2160	C2095	U2016	G1858	A1787	G1697	A1608
A2602	U2449	U2449	C2381	A2312	G2239	G2161	U2096	U2017	A1941	A1609	A1698	A1609
G2603	G2454	G2454	G2382	C2313	C2240	C2163	U2097	U2018	C1942	C1788	G1699	A1610
C2606	G2457	G2457	G2383	C2314	A2241	A2169	C2097	A2019	G1945	A1790	A1700	A1616
G2607	G2458	G2458	G2384	G2315	G2242	A2170	U2098	G2020	U1946	G1702	A1701	C1617
G2608	U2462	U2462	G2385	C2316	U2243	A2171	U2099	C2021	C1947	G1703	G1703	A1618
U2609	C2461	C2461	C2386	C2317	U2244	U2172	G2100	U2022	G1865	U1794	C1625	C1625
C2610	U2462	U2462	A2387	G2318	U2245	A2173	G2101	G1954	C1876	U1796	C1710	G1709
U2611	G2463	G2463	A2388	G2319	G2246	C2174	C2102	U1955	G1878	C1797	C1711	C1711
C2612	C2464	C2464	G2389	A2320	A2247	C2175	C2103	U1956	C1881	G1798	G1712	C1836
U2613	G2465	G2465	G2390	G2321	C2248	A2176	G2104	C2026	C1882	C1800	U1713	A1637
G2616	C2466	C2466	G2391	A2327	U2249	C2178	G2106	G2027	G1883	G1801	G1714	C1638
C2617	C2467	C2467	A2392	A2328	G2252	C2179	U2109	U2028	A1884	A1802	G1717	U1639
G2620	G2468	G2468	G2393	G2329	G2253	U2180	G2110	G2029	A1885	A1803	G1718	C1640
C2626	U2475	A2476	C2394	G2330	C2261	G2181	C2111	A2031	A1886	C1804	G1719	A1641
G2629	G2477	G2477	G2395	G2331	G2262	G2182	G2112	G2032	C1887	U1806	U1720	G1642
U2630	A2478	A2478	C2396	G2332	C2263	C2183	G2112	C2033	C1888	C1806	G1721	G1643
G2631	G2479	G2479	G2397	A2333	G2264	G2184	G2115	C2034	A1889	C1807	A1722	C1644
A2632	C2480	C2480	G2399	G2334	C2265	C2185	G2116	U2034	A1890	U1808	G1740	C1645
G2633	G2481	G2481	G2400	A2335	C2266	G2186	U2117	G2035	G1967	U1809	A1741	G1646
G2634	U2482	U2482	C2401	A2336	G2267	G2187	U2118	C2036	A1968	A1809	C1745	G1647
G2635	G2483	G2483	G2402	G2337	C2268	G2188	U2119	G2037	A1971	C1892	G1740	C1648
G2636	C2484	C2484	C2403	G2338	U2269	U2189	G2123	G2038	A1972	C1893	G1649	G1649
G2637	G2485	G2485	G2404	G2339	A2267	G2190	G2124	C2039	G1973	A1812	C1746	G1650
G2638	U2486	U2486	G2405	G2340	A2268	G2191	G2125	C2040	C1974	G1813	G1747	A1652
G2639	G2487	G2487	G2406	G2341	A2269	G2192	A2126	U2041	G1980	G1816	G1747	G1747
G2640	G2488	G2488	G2407	G2342	G2270	G2193		A2042				





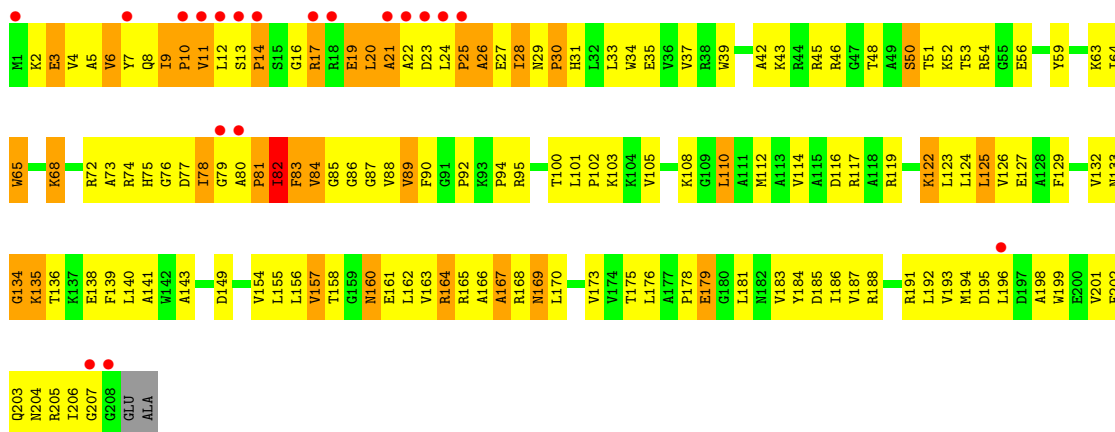
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



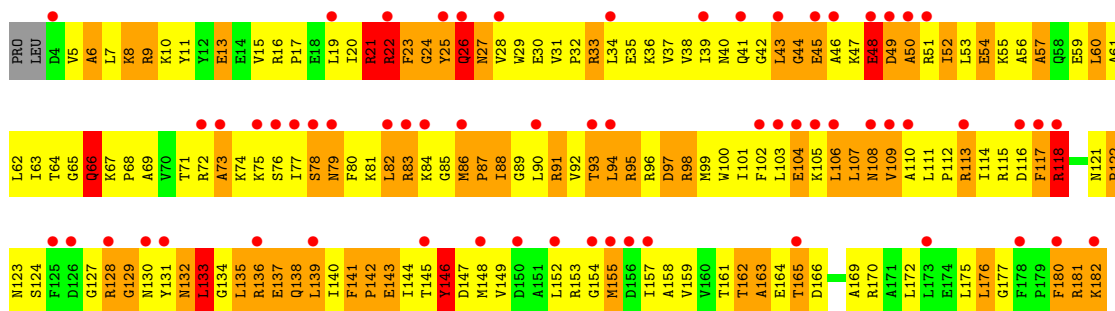
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

Chain BF:



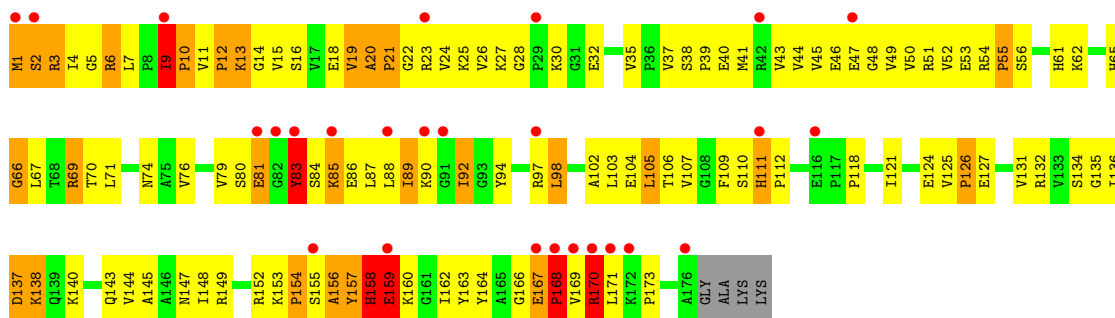
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

Chain BG:



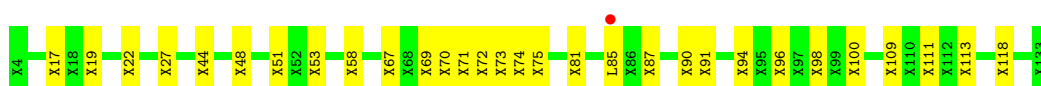
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



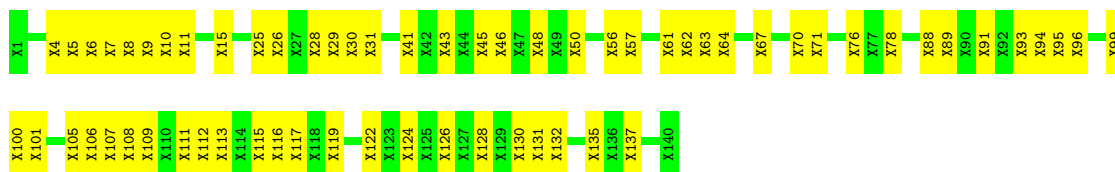
• Molecule 43: CHAIN J

Chain BJ:



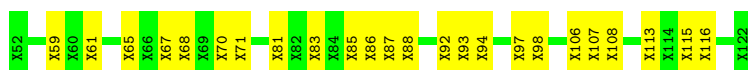
• Molecule 44: CHAIN K

Chain BK:



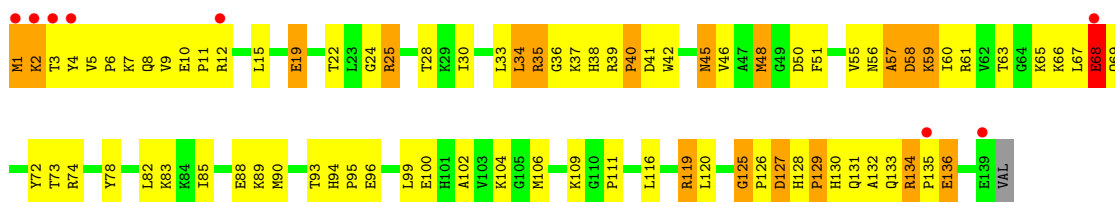
• Molecule 45: CHAIN L

Chain BL:



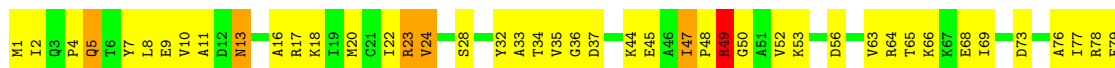
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



• Molecule 47: 50S RIBOSOMAL PROTEIN L14

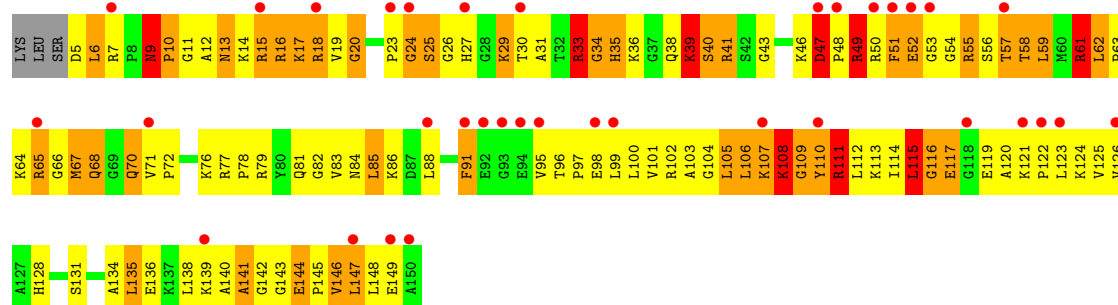
Chain BO:





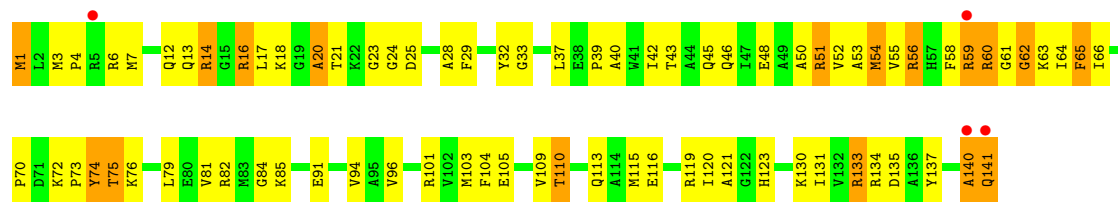
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

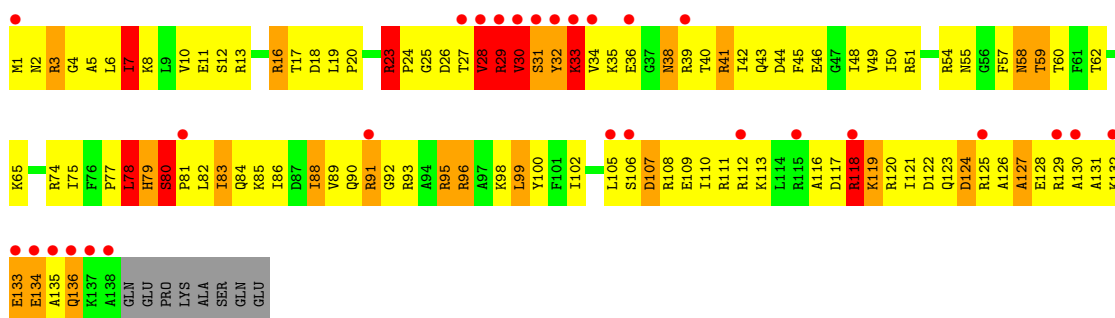
Chain BP:



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

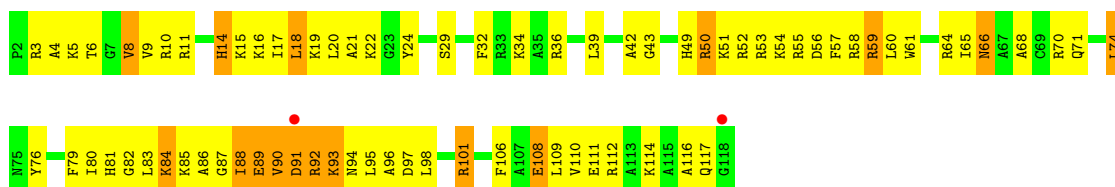
Chain BQ:





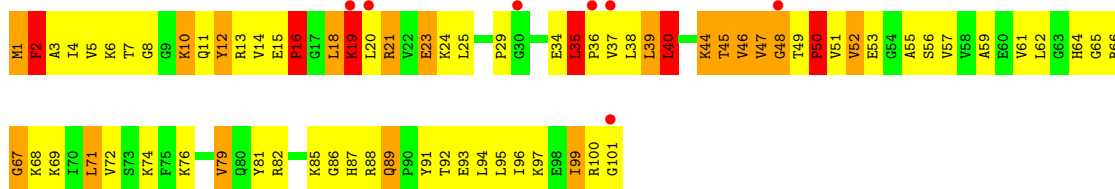
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



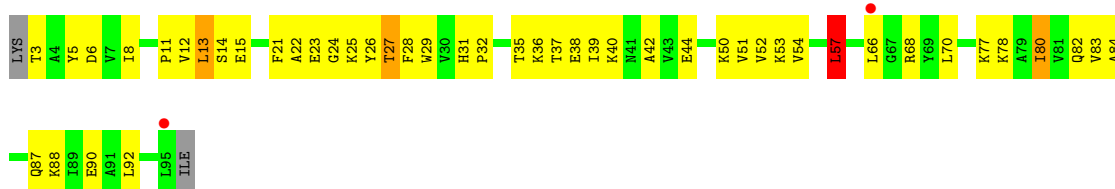
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



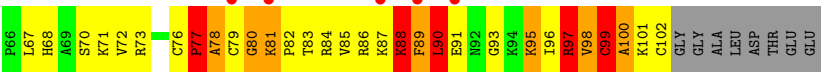
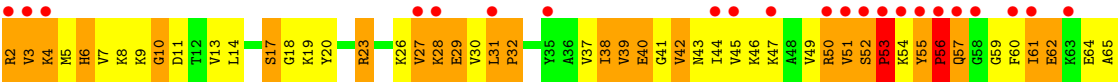
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



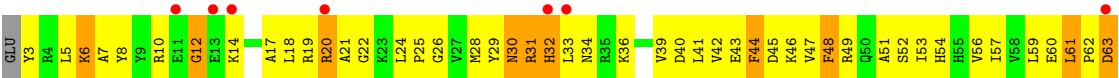
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY: 



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	202.90Å 242.63Å 309.32Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	49.75 – 2.95 49.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-2.95) 100.0 (49.75-2.95)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.244 0.226 , 0.256	Depositor DCC
R_{free} test set	30895 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 28.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 617901 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	153829	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: GCP, ZN, 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	AA	0.41	0/36258	0.70	5/56589 (0.0%)
2	AB	0.26	0/1936	0.46	0/2611
3	AC	0.36	0/1637	0.58	0/2207
4	AD	0.36	0/1733	0.61	0/2318
5	AE	0.46	0/1163	0.67	0/1566
6	AF	0.36	0/856	0.63	0/1154
7	AG	0.36	0/1276	0.62	0/1709
8	AH	0.39	0/1136	0.69	0/1527
9	AI	0.36	0/1029	0.69	0/1379
10	AJ	0.40	0/808	0.69	0/1087
11	AK	0.39	0/900	0.68	0/1213
12	AL	0.42	0/987	0.73	1/1322 (0.1%)
13	AM	0.32	0/948	0.60	0/1272
14	AN	0.41	0/501	0.77	0/664
15	AO	0.37	0/745	0.62	0/992
16	AP	0.40	0/717	0.71	0/965
17	AQ	0.40	0/837	0.69	0/1119
18	AR	0.38	0/579	0.60	0/768
19	AS	0.37	0/706	0.64	0/950
20	AT	0.39	0/765	0.76	0/1007
21	AU	0.43	0/213	0.62	0/279
22	AV	0.84	2/1809 (0.1%)	1.27	7/2819 (0.2%)
23	AX	1.26	2/210 (1.0%)	1.37	2/325 (0.6%)
24	AY	0.33	0/5477	0.61	3/7415 (0.0%)
25	B0	0.29	0/671	0.43	0/892
26	B1	0.37	0/739	0.58	0/983
27	B2	10.54	1/600 (0.2%)	0.42	0/793
28	B3	0.32	0/473	0.50	0/636
29	B4	0.29	0/594	0.45	0/795
30	B5	0.40	0/473	0.70	0/639
31	B6	0.48	0/440	0.80	0/586
32	B7	0.44	0/427	0.71	0/561

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.56	0/516	0.87	1/681 (0.1%)
34	B9	0.45	0/310	0.72	0/407
35	BA	0.46	1/69972 (0.0%)	0.72	25/109230 (0.0%)
36	BB	0.37	0/2853	0.72	1/4451 (0.0%)
37	BC	0.32	0/1766	0.62	0/2380
38	BD	0.47	0/2195	0.82	1/2955 (0.0%)
39	BE	0.42	0/1597	0.71	0/2155
40	BF	0.39	0/1659	0.66	0/2246
41	BG	0.45	0/1483	0.80	1/1994 (0.1%)
42	BH	0.40	0/1371	0.67	0/1853
43	BJ	0.20	0/7	0.87	0/8
46	BN	0.46	0/1132	0.76	0/1527
47	BO	0.44	0/943	0.71	0/1269
48	BP	0.45	0/1131	0.86	4/1504 (0.3%)
49	BQ	0.41	0/1143	0.65	0/1527
50	BR	0.43	0/974	0.75	0/1302
51	BS	0.39	0/779	0.66	0/1038
52	BT	0.42	0/1156	0.66	0/1544
53	BU	0.48	0/975	0.70	0/1297
54	BV	0.40	0/790	0.72	0/1057
55	BW	0.42	0/907	0.71	0/1216
56	BX	0.47	0/740	0.69	1/995 (0.1%)
57	BY	0.52	0/789	0.87	0/1053
58	BZ	0.34	0/1500	0.63	0/2037
All	All	0.77	6/164331 (0.0%)	0.71	52/244868 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	1
24	AY	0	1
35	BA	0	19
36	BB	0	2
All	All	0	23

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B2	72	ALA	C-OXT	258.07	6.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BA	1453	U	O3'-P	-17.05	1.40	1.61
22	AV	37	A	N3-C4	7.56	1.39	1.34
22	AV	37	A	C6-N1	7.26	1.40	1.35
23	AX	11	A	N9-C4	5.43	1.41	1.37

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BA	2208	A	P-O3'-C3'	9.92	131.60	119.70
22	AV	37	A	N1-C2-N3	-9.87	124.36	129.30
22	AV	74	C	O4'-C1'-N1	8.40	114.92	108.20
22	AV	37	A	N9-C4-C5	-7.54	102.79	105.80
22	AV	37	A	N1-C6-N6	6.87	122.72	118.60

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	189(H)	G	Sidechain
24	AY	499	ARG	Sidechain
35	BA	271(H)	G	Sidechain
35	BA	271(Q)	G	Sidechain
35	BA	271(Y)	U	Sidechain

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	AA	32391	0	16349	1995	0
2	AB	1901	0	1947	322	1
3	AC	1613	0	1677	223	28
4	AD	1703	0	1765	125	0
5	AE	1147	0	1207	56	0
6	AF	843	0	857	53	0
7	AG	1257	0	1296	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	AH	1116	0	1177	63	0
9	AI	1010	0	1037	150	0
10	AJ	795	0	840	114	0
11	AK	885	0	904	56	0
12	AL	971	0	1057	112	0
13	AM	938	0	995	124	0
14	AN	492	0	529	68	0
15	AO	734	0	771	49	0
16	AP	701	0	720	58	0
17	AQ	824	0	891	47	0
18	AR	574	0	644	26	0
19	AS	692	0	714	109	0
20	AT	763	0	861	71	11
21	AU	209	0	221	12	0
22	AV	1619	0	823	60	0
23	AX	188	0	98	7	0
24	AY	5376	0	5433	565	0
25	B0	662	0	688	160	0
26	B1	732	0	808	114	0
27	B2	598	0	651	125	11
28	B3	468	0	523	66	0
29	B4	581	0	577	214	0
30	B5	459	0	478	75	0
31	B6	433	0	461	128	0
32	B7	419	0	467	29	0
33	B8	508	0	576	112	0
34	B9	307	0	335	31	0
35	BA	62476	0	31499	3287	28
36	BB	2551	0	1295	107	0
37	BC	1735	0	1790	277	1
38	BD	2145	0	2234	255	0
39	BE	1564	0	1629	233	0
40	BF	1624	0	1677	220	0
41	BG	1459	0	1516	395	0
42	BH	1345	0	1430	187	0
43	BJ	654	0	156	22	0
44	BK	701	0	168	46	0
45	BL	356	0	86	20	0
46	BN	1105	0	1180	111	0
47	BO	933	0	996	67	0
48	BP	1114	0	1186	302	0
49	BQ	1122	0	1179	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	BR	960	0	1021	104	0
51	BS	771	0	832	158	0
52	BT	1142	0	1200	229	0
53	BU	958	0	1015	122	0
54	BV	779	0	852	147	0
55	BW	896	0	953	56	0
56	BX	726	0	778	47	0
57	BY	776	0	870	164	0
58	BZ	1468	0	1492	216	0
59	AA	198	0	0	0	0
59	AY	1	0	0	0	0
59	B0	1	0	0	0	0
59	B5	1	0	0	0	0
59	BA	320	0	0	0	0
59	BC	1	0	0	0	0
59	BU	1	0	0	0	0
60	AD	1	0	0	0	0
60	AN	1	0	0	0	0
60	B9	1	0	0	0	0
61	AY	32	0	14	11	0
62	AY	2	0	0	2	0
All	All	153829	0	105425	11647	40

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 45.

The worst 5 of 11647 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
30:B5:46:CYS:SG	30:B5:47:PRO:HD2	1.41	1.57
29:B4:12:ALA:H	29:B4:24:THR:CG2	1.16	1.56
9:AI:19:LEU:HA	9:AI:61:ALA:CB	1.39	1.53
52:BT:80:SER:HB3	52:BT:81:PRO:CD	1.40	1.51
9:AI:18:PHE:C	9:AI:61:ALA:HB1	1.27	1.50

The worst 5 of 40 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:AT:100:ILE:CG1	27:B2:43:GLN:CD[2_554]	0.34	1.86
20:AT:100:ILE:CD1	27:B2:43:GLN:NE2[2_554]	0.69	1.51
3:AC:79:ARG:CD	35:BA:2139:C:C4[2_555]	0.83	1.37
3:AC:79:ARG:CD	35:BA:2139:C:C5[2_555]	0.87	1.33

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:AC:79:ARG:CG	35:BA:2139:C:C6[2_555]	0.96	1.24

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	
2	AB	233/256 (91%)	163 (70%)	44 (19%)	26 (11%)	1	2
3	AC	205/239 (86%)	145 (71%)	32 (16%)	28 (14%)	0	1
4	AD	206/209 (99%)	160 (78%)	35 (17%)	11 (5%)	3	15
5	AE	149/162 (92%)	134 (90%)	12 (8%)	3 (2%)	11	47
6	AF	99/101 (98%)	80 (81%)	13 (13%)	6 (6%)	2	12
7	AG	153/156 (98%)	113 (74%)	26 (17%)	14 (9%)	1	4
8	AH	136/138 (99%)	122 (90%)	13 (10%)	1 (1%)	30	76
9	AI	125/128 (98%)	93 (74%)	21 (17%)	11 (9%)	1	5
10	AJ	97/105 (92%)	73 (75%)	15 (16%)	9 (9%)	1	4
11	AK	117/129 (91%)	95 (81%)	19 (16%)	3 (3%)	8	37
12	AL	123/132 (93%)	101 (82%)	11 (9%)	11 (9%)	1	5
13	AM	117/126 (93%)	74 (63%)	32 (27%)	11 (9%)	1	4
14	AN	58/61 (95%)	44 (76%)	7 (12%)	7 (12%)	1	2
15	AO	86/89 (97%)	78 (91%)	7 (8%)	1 (1%)	19	63
16	AP	82/88 (93%)	73 (89%)	7 (8%)	2 (2%)	9	40
17	AQ	98/105 (93%)	86 (88%)	10 (10%)	2 (2%)	11	47
18	AR	68/88 (77%)	58 (85%)	8 (12%)	2 (3%)	7	33
19	AS	86/93 (92%)	53 (62%)	21 (24%)	12 (14%)	0	1
20	AT	97/106 (92%)	79 (81%)	10 (10%)	8 (8%)	1	5
21	AU	23/27 (85%)	17 (74%)	4 (17%)	2 (9%)	1	5
24	AY	685/691 (99%)	537 (78%)	99 (14%)	49 (7%)	2	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	B0	82/84 (98%)	56 (68%)	19 (23%)	7 (8%)	1	5
26	B1	92/97 (95%)	73 (79%)	14 (15%)	5 (5%)	3	15
27	B2	69/71 (97%)	45 (65%)	11 (16%)	13 (19%)	0	0
28	B3	58/60 (97%)	50 (86%)	7 (12%)	1 (2%)	14	52
29	B4	69/71 (97%)	16 (23%)	17 (25%)	36 (52%)	0	0
30	B5	57/59 (97%)	45 (79%)	3 (5%)	9 (16%)	0	1
31	B6	48/53 (91%)	22 (46%)	11 (23%)	15 (31%)	0	0
32	B7	46/48 (96%)	43 (94%)	3 (6%)	0	100	100
33	B8	62/64 (97%)	42 (68%)	8 (13%)	12 (19%)	0	0
34	B9	35/37 (95%)	23 (66%)	9 (26%)	3 (9%)	1	5
37	BC	225/228 (99%)	121 (54%)	56 (25%)	48 (21%)	0	0
38	BD	273/275 (99%)	222 (81%)	33 (12%)	18 (7%)	2	9
39	BE	203/206 (98%)	145 (71%)	34 (17%)	24 (12%)	1	2
40	BF	206/210 (98%)	165 (80%)	19 (9%)	22 (11%)	1	3
41	BG	177/181 (98%)	78 (44%)	49 (28%)	50 (28%)	0	0
42	BH	174/180 (97%)	112 (64%)	31 (18%)	31 (18%)	0	1
43	BJ	1/130 (1%)	0	1 (100%)	0	100	100
46	BN	137/140 (98%)	110 (80%)	15 (11%)	12 (9%)	1	5
47	BO	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	9	38
48	BP	144/149 (97%)	84 (58%)	23 (16%)	37 (26%)	0	0
49	BQ	139/141 (99%)	115 (83%)	18 (13%)	6 (4%)	4	21
50	BR	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	2	8
51	BS	97/111 (87%)	52 (54%)	25 (26%)	20 (21%)	0	0
52	BT	136/146 (93%)	90 (66%)	25 (18%)	21 (15%)	0	1
53	BU	115/117 (98%)	87 (76%)	22 (19%)	6 (5%)	3	16
54	BV	99/101 (98%)	73 (74%)	11 (11%)	15 (15%)	0	1
55	BW	111/113 (98%)	93 (84%)	14 (13%)	4 (4%)	5	26
56	BX	91/95 (96%)	79 (87%)	11 (12%)	1 (1%)	21	66
57	BY	99/109 (91%)	54 (54%)	17 (17%)	28 (28%)	0	0
58	BZ	183/205 (89%)	131 (72%)	30 (16%)	22 (12%)	1	2
All	All	6506/6949 (94%)	4803 (74%)	1007 (16%)	696 (11%)	1	3

5 of 696 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	26	PRO
2	AB	37	ASN
2	AB	76	GLN
2	AB	77	ALA

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	
2	AB	202/220 (92%)	157 (78%)	45 (22%)	1	6
3	AC	160/188 (85%)	129 (81%)	31 (19%)	2	10
4	AD	180/181 (99%)	155 (86%)	25 (14%)	5	21
5	AE	115/123 (94%)	109 (95%)	6 (5%)	32	74
6	AF	90/90 (100%)	83 (92%)	7 (8%)	18	53
7	AG	126/127 (99%)	108 (86%)	18 (14%)	5	20
8	AH	119/119 (100%)	103 (87%)	16 (13%)	6	22
9	AI	98/99 (99%)	85 (87%)	13 (13%)	6	23
10	AJ	88/92 (96%)	82 (93%)	6 (7%)	22	61
11	AK	90/99 (91%)	84 (93%)	6 (7%)	23	62
12	AL	104/109 (95%)	90 (86%)	14 (14%)	6	22
13	AM	94/101 (93%)	84 (89%)	10 (11%)	10	34
14	AN	49/50 (98%)	43 (88%)	6 (12%)	7	27
15	AO	79/80 (99%)	71 (90%)	8 (10%)	11	37
16	AP	72/74 (97%)	68 (94%)	4 (6%)	30	71
17	AQ	94/97 (97%)	92 (98%)	2 (2%)	66	93
18	AR	61/77 (79%)	55 (90%)	6 (10%)	12	39
19	AS	74/80 (92%)	68 (92%)	6 (8%)	17	51
20	AT	76/82 (93%)	68 (90%)	8 (10%)	10	35
21	AU	19/22 (86%)	18 (95%)	1 (5%)	32	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	AY	579/582 (100%)	516 (89%)	63 (11%)	9	33
25	B0	66/66 (100%)	45 (68%)	21 (32%)	0	2
26	B1	78/82 (95%)	60 (77%)	18 (23%)	1	5
27	B2	66/66 (100%)	42 (64%)	24 (36%)	0	1
28	B3	51/52 (98%)	44 (86%)	7 (14%)	5	22
29	B4	63/63 (100%)	48 (76%)	15 (24%)	1	4
30	B5	51/51 (100%)	42 (82%)	9 (18%)	3	12
31	B6	49/51 (96%)	37 (76%)	12 (24%)	1	4
32	B7	41/41 (100%)	39 (95%)	2 (5%)	35	76
33	B8	53/54 (98%)	42 (79%)	11 (21%)	2	7
34	B9	34/34 (100%)	31 (91%)	3 (9%)	14	46
37	BC	179/180 (99%)	160 (89%)	19 (11%)	10	34
38	BD	217/217 (100%)	185 (85%)	32 (15%)	4	19
39	BE	165/166 (99%)	133 (81%)	32 (19%)	2	10
40	BF	165/166 (99%)	146 (88%)	19 (12%)	8	30
41	BG	153/155 (99%)	123 (80%)	30 (20%)	2	9
42	BH	146/148 (99%)	131 (90%)	15 (10%)	10	36
43	BJ	1/1 (100%)	1 (100%)	0	100	100
46	BN	117/119 (98%)	103 (88%)	14 (12%)	7	28
47	BO	100/100 (100%)	93 (93%)	7 (7%)	21	60
48	BP	112/115 (97%)	84 (75%)	28 (25%)	1	3
49	BQ	111/111 (100%)	96 (86%)	15 (14%)	6	22
50	BR	100/100 (100%)	82 (82%)	18 (18%)	2	12
51	BS	77/87 (88%)	62 (80%)	15 (20%)	2	9
52	BT	120/127 (94%)	94 (78%)	26 (22%)	1	6
53	BU	92/93 (99%)	80 (87%)	12 (13%)	6	24
54	BV	82/82 (100%)	65 (79%)	17 (21%)	2	7
55	BW	91/92 (99%)	79 (87%)	12 (13%)	6	23
56	BX	74/77 (96%)	68 (92%)	6 (8%)	17	51
57	BY	84/90 (93%)	65 (77%)	19 (23%)	1	5
58	BZ	162/178 (91%)	138 (85%)	24 (15%)	4	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5469/5656 (97%)	4686 (86%)	783 (14%)	5 20

5 of 783 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	B2	44	LEU
37	BC	138	LEU
55	BW	21	VAL
28	B3	8	LEU
31	B6	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 168 such sidechains are listed below:

Mol	Chain	Res	Type
25	B0	17	GLN
37	BC	189	ASN
53	BU	94	ASN
25	B0	70	GLN
28	B3	46	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1505/1519 (99%)	320 (21%)	51 (3%)
22	AV	75/76 (98%)	24 (32%)	2 (2%)
23	AX	8/9 (88%)	3 (37%)	0
35	BA	2897/2915 (99%)	665 (22%)	60 (2%)
36	BB	118/122 (96%)	26 (22%)	2 (1%)
All	All	4603/4641 (99%)	1038 (22%)	115 (2%)

5 of 1038 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	38	G
1	AA	39	G

5 of 115 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	AV	16	C
35	BA	627	A
35	BA	2439	A
35	BA	49	A
35	BA	331	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 527 ligands modelled in this entry, 526 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	GCP	AY	701	59	34,34,34	1.88	13 (38%)	52,54,54	3.66	14 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	GCP	AY	701	59	-	0/20/38/38	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GCP	PG-O3G	-3.82	1.47	1.54
61	AY	701	GCP	C5-N7	-3.79	1.33	1.38
61	AY	701	GCP	PG-O2G	-3.23	1.48	1.54
61	AY	701	GCP	PB-O2B	-3.14	1.48	1.56
61	AY	701	GCP	PG-C3B	-3.10	1.76	1.79

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	AY	701	GCP	C6-C5-N7	-22.09	131.16	134.14
61	AY	701	GCP	C4'-O4'-C1'	-5.24	103.96	109.72
61	AY	701	GCP	PB-C3B-PG	-4.95	109.50	118.95
61	AY	701	GCP	C2-N3-C4	4.48	120.68	115.30
61	AY	701	GCP	C5-C4-N3	-4.30	121.11	126.07

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	BA	3
1	AA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	496:A	O3'	498:U	P	3.07
1	BA	45:C	O3'	47:C	P	2.97
1	BA	1133:U	O3'	1135:C	P	2.48
1	BA	2203:U	O3'	2205:C	P	2.42

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	AA	1507/1519 (99%)	0.49	90 (5%) 21 11	24, 47, 125, 239	0
2	AB	235/256 (91%)	0.53	22 (9%) 9 4	34, 61, 112, 122	0
3	AC	207/239 (86%)	0.40	12 (5%) 22 12	30, 54, 84, 102	0
4	AD	208/209 (99%)	0.21	8 (3%) 38 18	36, 57, 80, 89	0
5	AE	151/162 (93%)	-0.07	2 (1%) 74 35	29, 40, 59, 81	0
6	AF	101/101 (100%)	0.31	4 (3%) 36 17	41, 68, 86, 99	0
7	AG	155/156 (99%)	0.61	14 (9%) 10 5	44, 67, 112, 126	0
8	AH	138/138 (100%)	-0.11	1 (0%) 84 44	32, 45, 63, 74	0
9	AI	127/128 (99%)	0.49	10 (7%) 13 7	33, 61, 81, 90	0
10	AJ	99/105 (94%)	0.53	9 (9%) 9 5	38, 58, 100, 104	0
11	AK	119/129 (92%)	0.33	6 (5%) 28 14	26, 53, 76, 94	0
12	AL	125/132 (94%)	0.36	9 (7%) 15 8	27, 45, 64, 96	0
13	AM	119/126 (94%)	1.15	19 (15%) 3 2	46, 83, 107, 117	0
14	AN	60/61 (98%)	0.55	8 (13%) 4 2	35, 48, 83, 91	0
15	AO	88/89 (98%)	0.25	2 (2%) 57 26	33, 51, 75, 85	0
16	AP	84/88 (95%)	0.17	1 (1%) 75 36	37, 47, 70, 95	0
17	AQ	100/105 (95%)	-0.04	0 100 100	27, 44, 62, 65	0
18	AR	70/88 (79%)	0.31	3 (4%) 34 16	36, 57, 94, 95	0
19	AS	88/93 (94%)	0.90	10 (11%) 6 3	59, 82, 103, 109	0
20	AT	99/106 (93%)	0.18	3 (3%) 48 21	33, 45, 68, 73	0
21	AU	25/27 (92%)	1.08	3 (12%) 5 3	43, 59, 79, 81	0
22	AV	76/76 (100%)	0.77	7 (9%) 9 4	33, 74, 111, 145	0
23	AX	9/9 (100%)	1.66	3 (33%) 1 0	28, 51, 122, 134	0
24	AY	687/691 (99%)	0.59	64 (9%) 9 4	39, 67, 119, 141	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B0	84/84 (100%)	1.93	18 (21%) 1 1	43, 56, 121, 140	0
26	B1	94/97 (96%)	0.55	7 (7%) 14 8	26, 47, 76, 88	0
27	B2	71/71 (100%)	0.73	7 (9%) 8 4	41, 57, 88, 112	0
28	B3	60/60 (100%)	0.74	4 (6%) 17 10	35, 56, 75, 100	0
29	B4	71/71 (100%)	4.17	63 (88%) 0 0	129, 151, 159, 159	0
30	B5	59/59 (100%)	0.76	10 (16%) 2 2	20, 42, 109, 122	0
31	B6	50/53 (94%)	1.63	12 (24%) 1 1	41, 72, 91, 98	0
32	B7	48/48 (100%)	0.02	1 (2%) 60 27	18, 30, 60, 86	0
33	B8	64/64 (100%)	0.73	9 (14%) 3 2	32, 49, 70, 87	0
34	B9	37/37 (100%)	0.78	2 (5%) 25 12	40, 52, 62, 76	0
35	BA	2901/2915 (99%)	0.50	158 (5%) 25 12	18, 42, 116, 244	0
36	BB	119/122 (97%)	0.53	2 (1%) 67 31	42, 88, 115, 130	0
37	BC	227/228 (99%)	0.92	44 (19%) 2 1	25, 78, 124, 135	0
38	BD	275/275 (100%)	0.03	9 (3%) 44 20	18, 32, 58, 93	0
39	BE	205/206 (99%)	0.38	13 (6%) 19 10	23, 42, 78, 86	0
40	BF	208/210 (99%)	0.48	19 (9%) 9 5	17, 52, 104, 121	0
41	BG	179/181 (98%)	1.64	62 (34%) 1 0	94, 122, 138, 144	0
42	BH	176/180 (97%)	0.97	26 (14%) 3 2	52, 75, 97, 108	0
43	BJ	1/130 (0%)	2.96	1 (100%) 0 0	121, 121, 121, 121	0
44	BK	0/140	-	-	-	-
45	BL	0/71	-	-	-	-
46	BN	139/140 (99%)	0.19	8 (5%) 22 12	31, 45, 72, 93	0
47	BO	122/122 (100%)	-0.25	0 100 100	25, 39, 54, 63	0
48	BP	146/149 (97%)	1.42	35 (23%) 1 1	34, 67, 96, 118	0
49	BQ	141/141 (100%)	0.30	4 (2%) 50 22	33, 49, 75, 115	0
50	BR	117/117 (100%)	0.16	4 (3%) 43 19	23, 40, 59, 67	0
51	BS	99/111 (89%)	1.17	19 (19%) 2 1	68, 91, 113, 122	0
52	BT	138/146 (94%)	1.07	28 (20%) 1 1	32, 53, 122, 144	0
53	BU	117/117 (100%)	-0.02	2 (1%) 67 31	28, 42, 69, 85	0
54	BV	101/101 (100%)	0.45	7 (6%) 17 9	25, 62, 83, 87	0
55	BW	113/113 (100%)	0.18	5 (4%) 33 16	26, 38, 69, 104	0
56	BX	93/95 (97%)	-0.12	2 (2%) 59 26	30, 41, 58, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
57	BY	101/109 (92%)	1.47	27 (26%) 1 1	37, 61, 118, 127	0
58	BZ	185/205 (90%)	0.93	28 (15%) 3 2	25, 81, 96, 109	0
All	All	11218/11801 (95%)	0.55	946 (8%) 11 6	17, 52, 116, 244	0

The worst 5 of 946 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
35	BA	654(E)	G	18.7
39	BE	205	ALA	16.5
35	BA	654(V)	A	15.7
24	AY	48	GLY	15.5
49	BQ	140	ALA	15.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
59	MG	AA	1740	1/1	0.77	-	79,79,79,79	0
59	MG	BA	3132	1/1	0.29	-	59,59,59,59	0
59	MG	BA	3074	1/1	0.34	-	3,3,3,3	0
59	MG	BA	3257	1/1	0.22	-	43,43,43,43	0
59	MG	BA	3317	1/1	0.26	-	29,29,29,29	0
59	MG	BA	3284	1/1	0.40	-	61,61,61,61	0
59	MG	BA	3047	1/1	0.36	-	42,42,42,42	0
59	MG	AA	1647	1/1	0.38	-	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3003	1/1	0.31	-	20,20,20,20	0
59	MG	AA	1622	1/1	0.45	-	49,49,49,49	0
59	MG	AA	1682	1/1	0.28	-	53,53,53,53	0
59	MG	BA	3079	1/1	0.33	-	34,34,34,34	0
59	MG	AA	1639	1/1	0.31	-	55,55,55,55	0
59	MG	BA	3249	1/1	0.30	-	22,22,22,22	0
59	MG	AA	1616	1/1	0.37	-	30,30,30,30	0
59	MG	AA	1618	1/1	0.37	-	47,47,47,47	0
60	ZN	AD	301	1/1	0.35	-	54,54,54,54	0
59	MG	AA	1716	1/1	0.33	-	71,71,71,71	0
59	MG	AA	1638	1/1	0.17	-	38,38,38,38	0
59	MG	AA	1670	1/1	0.22	-	57,57,57,57	0
59	MG	BA	3315	1/1	0.33	-	52,52,52,52	0
59	MG	AA	1631	1/1	0.20	-	40,40,40,40	0
59	MG	BA	3247	1/1	0.36	-	49,49,49,49	0
59	MG	BC	301	1/1	0.20	-	115,115,115,115	0
59	MG	BA	3148	1/1	0.24	-	53,53,53,53	0
59	MG	AA	1607	1/1	0.36	-	97,97,97,97	0
59	MG	AA	1695	1/1	0.32	-	50,50,50,50	0
59	MG	AA	1727	1/1	0.12	-	55,55,55,55	0
59	MG	BA	3216	1/1	0.17	-	54,54,54,54	0
59	MG	BA	3097	1/1	0.38	-	37,37,37,37	0
59	MG	AA	1706	1/1	0.15	-	43,43,43,43	0
59	MG	BA	3090	1/1	0.31	-	56,56,56,56	0
59	MG	AA	1705	1/1	0.07	-	23,23,23,23	0
59	MG	BA	3266	1/1	0.32	-	71,71,71,71	0
59	MG	BA	3227	1/1	0.28	-	27,27,27,27	0
59	MG	AA	1630	1/1	0.51	-	56,56,56,56	0
59	MG	BA	3231	1/1	0.31	-	13,13,13,13	0
59	MG	AA	1697	1/1	0.12	-	61,61,61,61	0
59	MG	AA	1746	1/1	0.34	-	47,47,47,47	0
59	MG	AA	1793	1/1	0.24	-	50,50,50,50	0
59	MG	BA	3300	1/1	0.17	-	65,65,65,65	0
59	MG	AA	1666	1/1	0.52	-	83,83,83,83	0
59	MG	AA	1794	1/1	0.23	-	53,53,53,53	0
59	MG	BA	3078	1/1	0.18	-	26,26,26,26	0
59	MG	BA	3065	1/1	0.28	-	21,21,21,21	0
59	MG	AA	1667	1/1	0.33	-	33,33,33,33	0
59	MG	BA	3111	1/1	0.30	-	30,30,30,30	0
59	MG	BA	3057	1/1	0.29	-	29,29,29,29	0
59	MG	BA	3018	1/1	0.52	-	43,43,43,43	0
61	GCP	AY	701	32/32	0.20	-	41,53,61,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3224	1/1	0.43	-	32,32,32,32	0
59	MG	AA	1770	1/1	0.28	-	41,41,41,41	0
59	MG	BA	3168	1/1	0.12	-	58,58,58,58	0
59	MG	AA	1683	1/1	0.22	-	25,25,25,25	0
59	MG	AA	1781	1/1	0.28	-	54,54,54,54	0
59	MG	BA	3208	1/1	0.21	-	34,34,34,34	0
59	MG	AA	1645	1/1	0.25	-	22,22,22,22	0
59	MG	BA	3016	1/1	0.55	-	77,77,77,77	0
59	MG	BA	3028	1/1	0.40	-	60,60,60,60	0
59	MG	BA	3087	1/1	0.32	-	41,41,41,41	0
59	MG	AA	1787	1/1	0.21	-	55,55,55,55	0
59	MG	BA	3081	1/1	0.28	-	23,23,23,23	0
59	MG	BA	3095	1/1	0.34	-	47,47,47,47	0
59	MG	BA	3239	1/1	0.27	-	87,87,87,87	0
59	MG	BA	3102	1/1	0.24	-	30,30,30,30	0
59	MG	BA	3307	1/1	0.16	-	40,40,40,40	0
59	MG	AA	1709	1/1	0.22	-	41,41,41,41	0
59	MG	BA	3314	1/1	0.09	-	49,49,49,49	0
59	MG	BA	3201	1/1	0.41	-	64,64,64,64	0
59	MG	AA	1769	1/1	0.34	-	33,33,33,33	0
59	MG	BA	3170	1/1	0.50	-	41,41,41,41	0
59	MG	AA	1776	1/1	0.28	-	25,25,25,25	0
59	MG	AA	1606	1/1	0.48	-	60,60,60,60	0
59	MG	AA	1730	1/1	0.10	-	62,62,62,62	0
59	MG	BA	3241	1/1	0.14	-	65,65,65,65	0
59	MG	BA	3140	1/1	0.12	-	45,45,45,45	0
59	MG	BA	3131	1/1	0.41	-	33,33,33,33	0
59	MG	BA	3075	1/1	0.23	-	31,31,31,31	0
59	MG	AA	1767	1/1	0.33	-	60,60,60,60	0
59	MG	BA	3160	1/1	0.18	-	55,55,55,55	0
59	MG	AA	1763	1/1	0.31	-	51,51,51,51	0
59	MG	AA	1701	1/1	0.14	-	30,30,30,30	0
59	MG	BA	3202	1/1	0.38	-	43,43,43,43	0
59	MG	AA	1687	1/1	0.20	-	30,30,30,30	0
59	MG	BA	3032	1/1	0.22	-	73,73,73,73	0
59	MG	BA	3205	1/1	0.11	-	35,35,35,35	0
59	MG	BA	3062	1/1	0.13	-	13,13,13,13	0
59	MG	BA	3178	1/1	0.25	-	43,43,43,43	0
59	MG	BA	3051	1/1	0.35	-	31,31,31,31	0
59	MG	AA	1611	1/1	0.32	-	75,75,75,75	0
59	MG	BA	3222	1/1	0.29	-	44,44,44,44	0
59	MG	BA	3019	1/1	0.59	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3213	1/1	0.36	-	31,31,31,31	0
59	MG	BA	3258	1/1	0.30	-	51,51,51,51	0
59	MG	BA	3042	1/1	0.34	-	45,45,45,45	0
59	MG	AA	1798	1/1	0.07	-	39,39,39,39	0
59	MG	AA	1756	1/1	0.37	-	54,54,54,54	0
59	MG	AA	1720	1/1	0.45	-	37,37,37,37	0
59	MG	AA	1738	1/1	0.17	-	53,53,53,53	0
59	MG	BA	3211	1/1	0.62	-	58,58,58,58	0
59	MG	BA	3256	1/1	0.37	-	52,52,52,52	0
59	MG	AA	1655	1/1	0.38	-	30,30,30,30	0
59	MG	BA	3174	1/1	0.64	-	97,97,97,97	0
59	MG	BA	3104	1/1	0.30	-	30,30,30,30	0
59	MG	BA	3119	1/1	0.25	-	24,24,24,24	0
59	MG	BA	3083	1/1	0.40	-	23,23,23,23	0
59	MG	BA	3251	1/1	0.27	-	44,44,44,44	0
59	MG	BA	3195	1/1	0.22	-	32,32,32,32	0
59	MG	AA	1795	1/1	0.14	-	46,46,46,46	0
59	MG	AA	1766	1/1	0.28	-	58,58,58,58	0
59	MG	BA	3157	1/1	0.17	-	17,17,17,17	0
59	MG	AA	1775	1/1	0.13	-	45,45,45,45	0
59	MG	BA	3254	1/1	0.24	-	18,18,18,18	0
59	MG	AA	1741	1/1	0.47	-	58,58,58,58	0
59	MG	BA	3146	1/1	0.21	-	29,29,29,29	0
59	MG	BA	3092	1/1	0.57	-	37,37,37,37	0
59	MG	BA	3268	1/1	0.36	-	85,85,85,85	0
59	MG	AA	1617	1/1	0.46	-	49,49,49,49	0
59	MG	BA	3285	1/1	0.29	-	40,40,40,40	0
59	MG	AA	1620	1/1	0.41	-	75,75,75,75	0
59	MG	AA	1786	1/1	0.15	-	35,35,35,35	0
59	MG	AA	1725	1/1	0.25	-	35,35,35,35	0
59	MG	BA	3064	1/1	0.13	-	62,62,62,62	0
59	MG	AA	1796	1/1	0.26	-	44,44,44,44	0
59	MG	BA	3204	1/1	0.38	-	60,60,60,60	0
59	MG	AA	1722	1/1	0.21	-	32,32,32,32	0
59	MG	BA	3113	1/1	0.50	-	32,32,32,32	0
59	MG	BA	3177	1/1	0.39	-	31,31,31,31	0
59	MG	BA	3108	1/1	0.23	-	34,34,34,34	0
60	ZN	AN	101	1/1	0.13	-	45,45,45,45	0
59	MG	AA	1712	1/1	0.20	-	66,66,66,66	0
59	MG	BA	3190	1/1	0.37	-	81,81,81,81	0
59	MG	BA	3237	1/1	0.21	-	94,94,94,94	0
59	MG	BA	3053	1/1	0.31	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3260	1/1	0.42	-	72,72,72,72	0
59	MG	BU	201	1/1	0.16	-	28,28,28,28	0
59	MG	AA	1640	1/1	0.25	-	74,74,74,74	0
59	MG	AA	1615	1/1	0.72	-	51,51,51,51	0
59	MG	BA	3045	1/1	0.64	-	54,54,54,54	0
59	MG	AA	1658	1/1	0.19	-	25,25,25,25	0
59	MG	BA	3162	1/1	0.27	-	45,45,45,45	0
59	MG	BA	3023	1/1	0.12	-	87,87,87,87	0
59	MG	BA	3302	1/1	0.37	-	52,52,52,52	0
59	MG	BA	3137	1/1	0.16	-	49,49,49,49	0
59	MG	BA	3320	1/1	0.15	-	39,39,39,39	0
59	MG	BA	3037	1/1	0.39	-	49,49,49,49	0
59	MG	BA	3277	1/1	0.35	-	57,57,57,57	0
59	MG	BA	3054	1/1	0.26	-	31,31,31,31	0
59	MG	AA	1685	1/1	0.40	-	40,40,40,40	0
59	MG	BA	3246	1/1	0.28	-	34,34,34,34	0
59	MG	BA	3006	1/1	0.40	-	30,30,30,30	0
59	MG	AA	1623	1/1	0.51	-	33,33,33,33	0
59	MG	BA	3214	1/1	0.27	-	39,39,39,39	0
59	MG	BA	3297	1/1	0.17	-	39,39,39,39	0
59	MG	BA	3082	1/1	0.46	-	23,23,23,23	0
59	MG	BA	3058	1/1	0.30	-	31,31,31,31	0
59	MG	AA	1774	1/1	0.57	-	51,51,51,51	0
59	MG	AA	1652	1/1	0.43	-	41,41,41,41	0
59	MG	BA	3186	1/1	0.12	-	50,50,50,50	0
59	MG	AA	1699	1/1	0.24	-	33,33,33,33	0
59	MG	AA	1679	1/1	0.55	-	32,32,32,32	0
59	MG	AA	1664	1/1	0.37	-	29,29,29,29	0
59	MG	AA	1710	1/1	0.06	-	35,35,35,35	0
59	MG	BA	3255	1/1	0.24	-	35,35,35,35	0
59	MG	AA	1789	1/1	0.29	-	61,61,61,61	0
59	MG	AA	1791	1/1	0.08	-	57,57,57,57	0
59	MG	BA	3020	1/1	0.20	-	63,63,63,63	0
59	MG	BA	3118	1/1	0.28	-	29,29,29,29	0
59	MG	BA	3156	1/1	0.18	-	25,25,25,25	0
59	MG	BA	3151	1/1	0.13	-	33,33,33,33	0
59	MG	AA	1610	1/1	0.61	-	46,46,46,46	0
59	MG	BA	3319	1/1	0.11	-	35,35,35,35	0
59	MG	BA	3197	1/1	0.56	-	58,58,58,58	0
59	MG	BA	3044	1/1	0.38	-	21,21,21,21	0
59	MG	BA	3234	1/1	0.21	-	63,63,63,63	0
59	MG	AA	1636	1/1	0.51	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1748	1/1	0.33	-	56,56,56,56	0
59	MG	BA	3280	1/1	0.23	-	87,87,87,87	0
59	MG	BA	3060	1/1	0.35	-	31,31,31,31	0
59	MG	AA	1753	1/1	0.49	-	89,89,89,89	0
59	MG	BA	3175	1/1	0.20	-	62,62,62,62	0
59	MG	BA	3271	1/1	0.32	-	28,28,28,28	0
59	MG	BA	3106	1/1	0.22	-	47,47,47,47	0
59	MG	AA	1634	1/1	0.22	-	43,43,43,43	0
59	MG	BA	3144	1/1	0.21	-	28,28,28,28	0
59	MG	AA	1768	1/1	0.44	-	34,34,34,34	0
59	MG	BA	3232	1/1	0.21	-	33,33,33,33	0
59	MG	BA	3142	1/1	0.19	-	48,48,48,48	0
59	MG	BA	3166	1/1	0.28	-	68,68,68,68	0
59	MG	AA	1689	1/1	0.41	-	79,79,79,79	0
59	MG	AA	1674	1/1	0.42	-	74,74,74,74	0
59	MG	AA	1649	1/1	0.38	-	23,23,23,23	0
59	MG	BA	3149	1/1	0.47	-	29,29,29,29	0
59	MG	BA	3230	1/1	0.32	-	40,40,40,40	0
59	MG	AA	1761	1/1	0.17	-	30,30,30,30	0
59	MG	BA	3296	1/1	0.35	-	38,38,38,38	0
59	MG	BA	3105	1/1	0.20	-	69,69,69,69	0
59	MG	BA	3009	1/1	0.72	-	77,77,77,77	0
59	MG	BA	3077	1/1	0.31	-	31,31,31,31	0
59	MG	AA	1694	1/1	0.14	-	19,19,19,19	0
59	MG	BA	3303	1/1	0.10	-	42,42,42,42	0
59	MG	BA	3100	1/1	0.09	-	24,24,24,24	0
59	MG	AA	1707	1/1	0.20	-	60,60,60,60	0
59	MG	BA	3056	1/1	0.36	-	38,38,38,38	0
59	MG	BA	3183	1/1	0.15	-	58,58,58,58	0
59	MG	AA	1762	1/1	0.44	-	100,100,100,100	0
59	MG	AA	1765	1/1	0.54	-	63,63,63,63	0
59	MG	AA	1788	1/1	0.26	-	73,73,73,73	0
59	MG	BA	3225	1/1	0.14	-	44,44,44,44	0
60	ZN	B9	101	1/1	0.07	-	49,49,49,49	0
59	MG	BA	3242	1/1	0.41	-	78,78,78,78	0
59	MG	BA	3085	1/1	0.20	-	25,25,25,25	0
59	MG	BA	3120	1/1	0.35	-	43,43,43,43	0
59	MG	BA	3001	1/1	0.11	-	35,35,35,35	0
59	MG	AA	1739	1/1	0.40	-	28,28,28,28	0
59	MG	BA	3196	1/1	0.35	-	53,53,53,53	0
59	MG	AA	1755	1/1	0.34	-	60,60,60,60	0
59	MG	AA	1657	1/1	0.10	-	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3007	1/1	0.41	-	26,26,26,26	0
59	MG	BA	3267	1/1	0.31	-	62,62,62,62	0
59	MG	AA	1603	1/1	0.37	-	38,38,38,38	0
59	MG	AA	1757	1/1	0.27	-	57,57,57,57	0
59	MG	BA	3121	1/1	0.34	-	33,33,33,33	0
59	MG	AA	1659	1/1	0.37	-	34,34,34,34	0
59	MG	BA	3295	1/1	0.30	-	32,32,32,32	0
59	MG	BA	3128	1/1	0.25	-	38,38,38,38	0
59	MG	BA	3134	1/1	0.29	-	65,65,65,65	0
59	MG	BA	3069	1/1	0.32	-	18,18,18,18	0
59	MG	AA	1625	1/1	0.34	-	17,17,17,17	0
59	MG	AA	1729	1/1	0.47	-	45,45,45,45	0
59	MG	BA	3279	1/1	0.40	-	63,63,63,63	0
59	MG	BA	3219	1/1	0.17	-	44,44,44,44	0
59	MG	AA	1626	1/1	0.39	-	59,59,59,59	0
59	MG	BA	3150	1/1	0.13	-	15,15,15,15	0
59	MG	BA	3059	1/1	0.42	-	45,45,45,45	0
59	MG	AA	1779	1/1	0.54	-	81,81,81,81	0
59	MG	BA	3312	1/1	0.51	-	44,44,44,44	0
59	MG	BA	3229	1/1	0.12	-	5,5,5,5	0
59	MG	BA	3198	1/1	0.15	-	63,63,63,63	0
59	MG	BA	3228	1/1	0.32	-	23,23,23,23	0
59	MG	BA	3114	1/1	0.19	-	29,29,29,29	0
59	MG	BA	3310	1/1	0.28	-	20,20,20,20	0
59	MG	AA	1743	1/1	0.37	-	38,38,38,38	0
59	MG	BA	3291	1/1	0.29	-	27,27,27,27	0
59	MG	BA	3243	1/1	0.22	-	32,32,32,32	0
59	MG	AA	1677	1/1	0.38	-	77,77,77,77	0
59	MG	BA	3048	1/1	0.37	-	28,28,28,28	0
59	MG	BA	3171	1/1	0.21	-	19,19,19,19	0
59	MG	AA	1773	1/1	0.52	-	60,60,60,60	0
59	MG	BA	3013	1/1	0.44	-	37,37,37,37	0
59	MG	BA	3220	1/1	0.18	-	56,56,56,56	0
59	MG	AA	1635	1/1	0.21	-	65,65,65,65	0
59	MG	BA	3143	1/1	0.22	-	57,57,57,57	0
59	MG	BA	3259	1/1	0.11	-	39,39,39,39	0
59	MG	BA	3153	1/1	0.23	-	54,54,54,54	0
59	MG	AA	1643	1/1	0.21	-	38,38,38,38	0
59	MG	AA	1764	1/1	0.26	-	61,61,61,61	0
59	MG	BA	3273	1/1	0.60	-	72,72,72,72	0
59	MG	AA	1671	1/1	0.61	-	43,43,43,43	0
59	MG	BA	3305	1/1	0.10	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3163	1/1	0.26	-	55,55,55,55	0
59	MG	BA	3289	1/1	0.21	-	51,51,51,51	0
59	MG	AA	1629	1/1	0.27	-	44,44,44,44	0
59	MG	BA	3179	1/1	0.45	-	87,87,87,87	0
59	MG	BA	3250	1/1	0.20	-	53,53,53,53	0
59	MG	AA	1797	1/1	0.17	-	58,58,58,58	0
59	MG	AA	1678	1/1	0.33	-	29,29,29,29	0
59	MG	BA	3293	1/1	0.42	-	76,76,76,76	0
59	MG	AA	1686	1/1	0.25	-	34,34,34,34	0
59	MG	BA	3063	1/1	0.13	-	22,22,22,22	0
59	MG	BA	3169	1/1	0.34	-	43,43,43,43	0
59	MG	BA	3125	1/1	0.35	-	122,122,122,122	0
59	MG	BA	3217	1/1	0.15	-	35,35,35,35	0
59	MG	AA	1612	1/1	0.44	-	47,47,47,47	0
59	MG	BA	3200	1/1	0.27	-	71,71,71,71	0
59	MG	BA	3172	1/1	0.43	-	31,31,31,31	0
59	MG	BA	3269	1/1	0.16	-	48,48,48,48	0
59	MG	BA	3039	1/1	0.37	-	38,38,38,38	0
59	MG	AA	1604	1/1	0.38	-	59,59,59,59	0
59	MG	BA	3286	1/1	0.32	-	42,42,42,42	0
59	MG	BA	3212	1/1	0.26	-	46,46,46,46	0
59	MG	AA	1784	1/1	0.17	-	37,37,37,37	0
59	MG	BA	3088	1/1	0.22	-	27,27,27,27	0
59	MG	BA	3086	1/1	0.24	-	46,46,46,46	0
59	MG	AA	1646	1/1	0.37	-	34,34,34,34	0
59	MG	BA	3316	1/1	0.36	-	34,34,34,34	0
59	MG	BA	3094	1/1	0.30	-	25,25,25,25	0
59	MG	BA	3084	1/1	0.53	-	38,38,38,38	0
59	MG	BA	3015	1/1	0.52	-	63,63,63,63	0
59	MG	AA	1742	1/1	0.22	-	45,45,45,45	0
59	MG	BA	3030	1/1	1.17	-	86,86,86,86	0
59	MG	AA	1752	1/1	0.21	-	59,59,59,59	0
59	MG	AA	1653	1/1	0.31	-	19,19,19,19	0
59	MG	AA	1751	1/1	0.12	-	46,46,46,46	0
59	MG	AA	1724	1/1	0.40	-	48,48,48,48	0
59	MG	B5	101	1/1	0.24	-	47,47,47,47	0
59	MG	BA	3027	1/1	0.26	-	71,71,71,71	0
59	MG	AA	1708	1/1	0.27	-	57,57,57,57	0
59	MG	BA	3099	1/1	0.20	-	19,19,19,19	0
59	MG	AA	1692	1/1	0.22	-	48,48,48,48	0
59	MG	BA	3182	1/1	0.23	-	73,73,73,73	0
59	MG	BA	3154	1/1	0.57	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3115	1/1	0.29	-	52,52,52,52	0
59	MG	BA	3049	1/1	0.43	-	47,47,47,47	0
59	MG	BA	3215	1/1	0.59	-	81,81,81,81	0
59	MG	AA	1627	1/1	0.22	-	74,74,74,74	0
59	MG	BA	3185	1/1	0.41	-	36,36,36,36	0
59	MG	BA	3309	1/1	0.16	-	50,50,50,50	0
59	MG	AA	1642	1/1	0.24	-	61,61,61,61	0
59	MG	AA	1662	1/1	0.30	-	34,34,34,34	0
59	MG	BA	3055	1/1	0.17	-	33,33,33,33	0
59	MG	BA	3287	1/1	0.16	-	41,41,41,41	0
59	MG	AA	1644	1/1	0.19	-	60,60,60,60	0
59	MG	AA	1614	1/1	0.39	-	26,26,26,26	0
59	MG	AA	1669	1/1	0.20	-	40,40,40,40	0
59	MG	BA	3223	1/1	0.32	-	32,32,32,32	0
59	MG	BA	3004	1/1	0.36	-	24,24,24,24	0
59	MG	BA	3181	1/1	0.18	-	32,32,32,32	0
59	MG	BA	3116	1/1	0.25	-	78,78,78,78	0
59	MG	AA	1602	1/1	0.45	-	42,42,42,42	0
59	MG	AA	1782	1/1	0.08	-	39,39,39,39	0
59	MG	BA	3248	1/1	0.48	-	58,58,58,58	0
59	MG	AA	1605	1/1	0.37	-	40,40,40,40	0
59	MG	AA	1619	1/1	0.34	-	37,37,37,37	0
59	MG	BA	3068	1/1	0.19	-	33,33,33,33	0
59	MG	AA	1632	1/1	0.25	-	56,56,56,56	0
59	MG	BA	3194	1/1	0.35	-	74,74,74,74	0
59	MG	BA	3133	1/1	0.30	-	39,39,39,39	0
59	MG	AA	1778	1/1	0.11	-	6,6,6,6	0
59	MG	BA	3107	1/1	0.27	-	44,44,44,44	0
59	MG	BA	3096	1/1	0.18	-	23,23,23,23	0
59	MG	BA	3136	1/1	0.29	-	90,90,90,90	0
59	MG	BA	3036	1/1	0.26	-	47,47,47,47	0
59	MG	BA	3276	1/1	0.50	-	46,46,46,46	0
59	MG	AA	1654	1/1	0.22	-	24,24,24,24	0
59	MG	BA	3292	1/1	0.46	-	64,64,64,64	0
59	MG	BA	3072	1/1	0.60	-	70,70,70,70	0
59	MG	BA	3187	1/1	0.84	-	68,68,68,68	0
59	MG	AA	1733	1/1	0.35	-	67,67,67,67	0
59	MG	AA	1723	1/1	0.12	-	10,10,10,10	0
59	MG	BA	3245	1/1	0.22	-	25,25,25,25	0
59	MG	AA	1749	1/1	0.12	-	38,38,38,38	0
59	MG	AA	1651	1/1	0.20	-	68,68,68,68	0
59	MG	BA	3313	1/1	0.25	-	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	AA	1715	1/1	0.25	-	42,42,42,42	0
59	MG	AA	1681	1/1	0.42	-	34,34,34,34	0
59	MG	BA	3191	1/1	0.39	-	72,72,72,72	0
59	MG	BA	3052	1/1	0.29	-	32,32,32,32	0
59	MG	BA	3002	1/1	0.15	-	39,39,39,39	0
59	MG	AA	1717	1/1	0.41	-	41,41,41,41	0
59	MG	BA	3110	1/1	0.45	-	31,31,31,31	0
59	MG	AA	1637	1/1	0.52	-	65,65,65,65	0
59	MG	AA	1790	1/1	0.25	-	57,57,57,57	0
59	MG	BA	3124	1/1	0.26	-	15,15,15,15	0
59	MG	BA	3282	1/1	0.28	-	67,67,67,67	0
59	MG	BA	3192	1/1	0.32	-	51,51,51,51	0
59	MG	BA	3123	1/1	0.43	-	32,32,32,32	0
59	MG	BA	3301	1/1	0.38	-	45,45,45,45	0
59	MG	AA	1696	1/1	0.34	-	35,35,35,35	0
59	MG	AA	1668	1/1	0.16	-	34,34,34,34	0
59	MG	BA	3005	1/1	0.47	-	16,16,16,16	0
59	MG	AA	1704	1/1	0.35	-	25,25,25,25	0
59	MG	BA	3265	1/1	0.57	-	65,65,65,65	0
59	MG	AA	1672	1/1	0.16	-	42,42,42,42	0
59	MG	BA	3126	1/1	0.39	-	55,55,55,55	0
59	MG	BA	3158	1/1	0.29	-	27,27,27,27	0
59	MG	AA	1758	1/1	0.40	-	75,75,75,75	0
59	MG	AA	1745	1/1	0.41	-	66,66,66,66	0
59	MG	AA	1621	1/1	0.38	-	68,68,68,68	0
59	MG	BA	3270	1/1	0.32	-	70,70,70,70	0
59	MG	AA	1719	1/1	0.15	-	32,32,32,32	0
59	MG	AA	1744	1/1	0.19	-	90,90,90,90	0
59	MG	BA	3089	1/1	0.23	-	18,18,18,18	0
59	MG	BA	3029	1/1	0.25	-	73,73,73,73	0
59	MG	BA	3173	1/1	0.25	-	20,20,20,20	0
59	MG	B0	101	1/1	0.69	-	72,72,72,72	0
59	MG	AA	1656	1/1	0.15	-	46,46,46,46	0
59	MG	BA	3025	1/1	0.30	-	42,42,42,42	0
59	MG	BA	3067	1/1	0.26	-	71,71,71,71	0
59	MG	BA	3221	1/1	0.10	-	43,43,43,43	0
59	MG	BA	3235	1/1	0.19	-	29,29,29,29	0
59	MG	AA	1714	1/1	0.50	-	44,44,44,44	0
59	MG	AA	1780	1/1	0.18	-	54,54,54,54	0
59	MG	BA	3281	1/1	0.46	-	79,79,79,79	0
59	MG	BA	3236	1/1	0.25	-	52,52,52,52	0
59	MG	AA	1777	1/1	0.29	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3061	1/1	0.05	-	37,37,37,37	0
59	MG	BA	3041	1/1	0.22	-	75,75,75,75	0
59	MG	BA	3109	1/1	0.43	-	20,20,20,20	0
59	MG	BA	3184	1/1	0.21	-	40,40,40,40	0
59	MG	BA	3193	1/1	0.49	-	64,64,64,64	0
59	MG	BA	3022	1/1	0.50	-	65,65,65,65	0
59	MG	BA	3152	1/1	0.40	-	64,64,64,64	0
59	MG	BA	3043	1/1	0.19	-	28,28,28,28	0
59	MG	AA	1728	1/1	0.30	-	47,47,47,47	0
59	MG	BA	3026	1/1	0.34	-	67,67,67,67	0
59	MG	AA	1721	1/1	0.11	-	17,17,17,17	0
59	MG	BA	3101	1/1	0.33	-	29,29,29,29	0
59	MG	BA	3080	1/1	0.38	-	38,38,38,38	0
59	MG	AA	1698	1/1	0.29	-	58,58,58,58	0
59	MG	AA	1760	1/1	0.60	-	70,70,70,70	0
59	MG	AA	1624	1/1	0.78	-	61,61,61,61	0
59	MG	BA	3130	1/1	0.54	-	56,56,56,56	0
59	MG	BA	3038	1/1	0.31	-	40,40,40,40	0
59	MG	BA	3311	1/1	0.32	-	22,22,22,22	0
59	MG	BA	3240	1/1	0.34	-	60,60,60,60	0
59	MG	BA	3209	1/1	0.61	-	81,81,81,81	0
59	MG	BA	3180	1/1	0.30	-	47,47,47,47	0
59	MG	BA	3012	1/1	0.40	-	79,79,79,79	0
59	MG	AA	1754	1/1	0.37	-	75,75,75,75	0
59	MG	BA	3141	1/1	0.21	-	29,29,29,29	0
59	MG	AY	702	1/1	0.08	-	23,23,23,23	0
59	MG	BA	3031	1/1	0.33	-	35,35,35,35	0
59	MG	AA	1691	1/1	0.10	-	65,65,65,65	0
59	MG	BA	3070	1/1	0.41	-	25,25,25,25	0
59	MG	BA	3093	1/1	0.38	-	69,69,69,69	0
59	MG	AA	1650	1/1	0.26	-	36,36,36,36	0
59	MG	AA	1772	1/1	0.55	-	79,79,79,79	0
59	MG	BA	3299	1/1	0.35	-	53,53,53,53	0
59	MG	BA	3165	1/1	0.43	-	29,29,29,29	0
59	MG	BA	3050	1/1	0.12	-	23,23,23,23	0
59	MG	BA	3306	1/1	0.20	-	39,39,39,39	0
59	MG	AA	1690	1/1	0.46	-	35,35,35,35	0
59	MG	BA	3040	1/1	0.41	-	71,71,71,71	0
59	MG	AA	1759	1/1	0.31	-	37,37,37,37	0
59	MG	BA	3138	1/1	0.43	-	57,57,57,57	0
59	MG	BA	3244	1/1	0.21	-	41,41,41,41	0
59	MG	BA	3071	1/1	0.34	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3304	1/1	0.37	-	32,32,32,32	0
59	MG	BA	3127	1/1	0.19	-	38,38,38,38	0
59	MG	AA	1732	1/1	0.22	-	20,20,20,20	0
59	MG	AA	1750	1/1	0.28	-	42,42,42,42	0
59	MG	BA	3189	1/1	0.15	-	26,26,26,26	0
59	MG	AA	1735	1/1	0.34	-	62,62,62,62	0
59	MG	BA	3218	1/1	0.23	-	58,58,58,58	0
59	MG	BA	3264	1/1	0.50	-	77,77,77,77	0
59	MG	BA	3278	1/1	0.19	-	91,91,91,91	0
59	MG	AA	1702	1/1	0.51	-	44,44,44,44	0
59	MG	BA	3263	1/1	0.31	-	63,63,63,63	0
59	MG	AA	1688	1/1	0.24	-	30,30,30,30	0
59	MG	BA	3011	1/1	0.27	-	46,46,46,46	0
59	MG	AA	1660	1/1	0.08	-	19,19,19,19	0
59	MG	AA	1684	1/1	0.80	-	61,61,61,61	0
59	MG	AA	1731	1/1	0.10	-	48,48,48,48	0
59	MG	AA	1703	1/1	0.45	-	81,81,81,81	0
59	MG	BA	3176	1/1	0.43	-	23,23,23,23	0
59	MG	BA	3017	1/1	0.30	-	37,37,37,37	0
59	MG	BA	3283	1/1	0.20	-	73,73,73,73	0
59	MG	BA	3147	1/1	0.51	-	119,119,119,119	0
59	MG	BA	3238	1/1	0.29	-	42,42,42,42	0
59	MG	BA	3272	1/1	0.42	-	52,52,52,52	0
59	MG	AA	1676	1/1	0.24	-	62,62,62,62	0
59	MG	BA	3066	1/1	0.15	-	27,27,27,27	0
59	MG	AA	1675	1/1	0.26	-	45,45,45,45	0
59	MG	BA	3274	1/1	0.15	-	79,79,79,79	0
59	MG	BA	3294	1/1	0.19	-	42,42,42,42	0
59	MG	AA	1648	1/1	0.35	-	29,29,29,29	0
59	MG	AA	1693	1/1	0.17	-	30,30,30,30	0
59	MG	BA	3164	1/1	0.32	-	49,49,49,49	0
59	MG	AA	1601	1/1	0.23	-	97,97,97,97	0
59	MG	BA	3046	1/1	0.27	-	27,27,27,27	0
59	MG	AA	1718	1/1	0.47	-	35,35,35,35	0
59	MG	AA	1663	1/1	0.43	-	37,37,37,37	0
59	MG	BA	3290	1/1	0.41	-	43,43,43,43	0
59	MG	BA	3288	1/1	0.17	-	24,24,24,24	0
59	MG	AA	1785	1/1	0.08	-	47,47,47,47	0
59	MG	AA	1641	1/1	0.16	-	17,17,17,17	0
59	MG	AA	1713	1/1	0.14	-	40,40,40,40	0
59	MG	BA	3129	1/1	0.28	-	51,51,51,51	0
59	MG	BA	3098	1/1	0.21	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3207	1/1	0.28	-	30,30,30,30	0
59	MG	BA	3203	1/1	0.25	-	30,30,30,30	0
59	MG	AA	1737	1/1	0.16	-	61,61,61,61	0
59	MG	BA	3117	1/1	0.18	-	26,26,26,26	0
59	MG	BA	3159	1/1	0.22	-	36,36,36,36	0
59	MG	BA	3035	1/1	0.47	-	31,31,31,31	0
59	MG	AA	1628	1/1	0.38	-	64,64,64,64	0
59	MG	BA	3233	1/1	0.20	-	42,42,42,42	0
59	MG	BA	3252	1/1	0.58	-	50,50,50,50	0
59	MG	BA	3135	1/1	0.23	-	58,58,58,58	0
59	MG	BA	3298	1/1	0.17	-	20,20,20,20	0
59	MG	AA	1700	1/1	0.31	-	27,27,27,27	0
59	MG	AA	1661	1/1	0.25	-	40,40,40,40	0
59	MG	AA	1680	1/1	0.18	-	37,37,37,37	0
59	MG	BA	3210	1/1	0.27	-	23,23,23,23	0
59	MG	AA	1711	1/1	0.18	-	34,34,34,34	0
59	MG	BA	3155	1/1	0.26	-	60,60,60,60	0
59	MG	BA	3188	1/1	0.40	-	34,34,34,34	0
59	MG	AA	1613	1/1	0.17	-	65,65,65,65	0
59	MG	BA	3253	1/1	0.30	-	98,98,98,98	0
59	MG	BA	3167	1/1	0.17	-	61,61,61,61	0
59	MG	AA	1747	1/1	0.08	-	23,23,23,23	0
59	MG	BA	3308	1/1	0.12	-	58,58,58,58	0
59	MG	BA	3262	1/1	0.14	-	68,68,68,68	0
59	MG	BA	3206	1/1	0.24	-	65,65,65,65	0
59	MG	BA	3010	1/1	0.40	-	33,33,33,33	0
59	MG	AA	1792	1/1	0.12	-	37,37,37,37	0
59	MG	BA	3103	1/1	0.20	-	35,35,35,35	0
59	MG	AA	1665	1/1	0.40	-	28,28,28,28	0
59	MG	AA	1783	1/1	0.13	-	43,43,43,43	0
59	MG	AA	1608	1/1	0.34	-	48,48,48,48	0
59	MG	BA	3226	1/1	0.32	-	56,56,56,56	0
59	MG	BA	3014	1/1	0.33	-	53,53,53,53	0
59	MG	BA	3008	1/1	0.46	-	45,45,45,45	0
59	MG	BA	3034	1/1	0.20	-	36,36,36,36	0
59	MG	BA	3199	1/1	0.27	-	26,26,26,26	0
59	MG	AA	1736	1/1	0.17	-	29,29,29,29	0
59	MG	BA	3112	1/1	0.65	-	51,51,51,51	0
59	MG	BA	3275	1/1	0.38	-	52,52,52,52	0
59	MG	BA	3139	1/1	0.27	-	35,35,35,35	0
59	MG	BA	3261	1/1	0.14	-	67,67,67,67	0
59	MG	AA	1771	1/1	0.22	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
59	MG	BA	3033	1/1	0.16	-	41,41,41,41	0
59	MG	AA	1609	1/1	0.40	-	40,40,40,40	0
59	MG	BA	3145	1/1	0.22	-	32,32,32,32	0
59	MG	BA	3091	1/1	0.21	-	21,21,21,21	0
59	MG	BA	3076	1/1	0.26	-	18,18,18,18	0
59	MG	AA	1734	1/1	0.11	-	41,41,41,41	0
59	MG	BA	3024	1/1	0.28	-	44,44,44,44	0
59	MG	BA	3021	1/1	0.31	-	37,37,37,37	0
59	MG	BA	3318	1/1	0.08	-	46,46,46,46	0
59	MG	AA	1673	1/1	0.20	-	35,35,35,35	0
59	MG	BA	3122	1/1	0.15	-	26,26,26,26	0
59	MG	AA	1726	1/1	0.19	-	45,45,45,45	0
59	MG	AA	1633	1/1	0.48	-	52,52,52,52	0
59	MG	BA	3161	1/1	0.39	-	30,30,30,30	0
59	MG	BA	3073	1/1	0.32	-	83,83,83,83	0

6.5 Other polymers

There are no such residues in this entry.