



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:38 PM UTC

PDB ID : 4V8X / pdb_00004v8x
Title : Structure of Thermus thermophilus ribosome
Authors : Feng, S.; Chen, Y.; Kamada, K.; Wang, H.; Tang, K.; Wang, M.; Gao, Y.G.
Deposited on : 2013-07-19
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

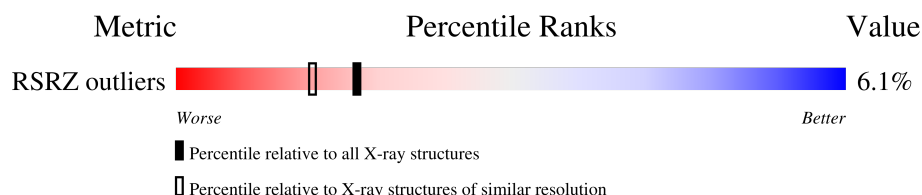
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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))
RSRZ outliers	180081	1099 (3.40-3.32)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	AA	1602	-	-	-	X
60	MG	AA	1613	-	-	-	X
60	MG	AA	1634	-	-	-	X
60	MG	AA	1638	-	-	-	X
60	MG	AA	1641	-	-	-	X
60	MG	AA	1643	-	-	-	X
60	MG	AA	1646	-	-	-	X
60	MG	AA	1649	-	-	-	X
60	MG	AA	1662	-	-	-	X
60	MG	AA	1665	-	-	-	X
60	MG	AA	1667	-	-	-	X
60	MG	AA	1672	-	-	-	X
60	MG	AA	1688	-	-	-	X
60	MG	AA	1700	-	-	-	X
60	MG	AA	1703	-	-	-	X
60	MG	AX	101	-	-	-	X
60	MG	BA	2901	-	-	-	X
60	MG	BA	2920	-	-	-	X
60	MG	BA	2930	-	-	-	X
60	MG	BA	2937	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	BA	2942	-	-	-	X
60	MG	BA	2945	-	-	-	X
60	MG	BA	2953	-	-	-	X
60	MG	BA	2955	-	-	-	X
60	MG	BA	2970	-	-	-	X
60	MG	BA	2972	-	-	-	X
60	MG	BA	2974	-	-	-	X
60	MG	BA	2987	-	-	-	X
60	MG	BA	2988	-	-	-	X
60	MG	BA	3002	-	-	-	X
60	MG	BA	3009	-	-	-	X
60	MG	BA	3011	-	-	-	X
60	MG	BA	3022	-	-	-	X
60	MG	BA	3030	-	-	-	X
60	MG	BA	3070	-	-	-	X
60	MG	BA	3072	-	-	-	X
60	MG	BA	3076	-	-	-	X
60	MG	BA	3080	-	-	-	X
60	MG	BA	3090	-	-	-	X
60	MG	BA	3114	-	-	-	X
60	MG	BA	3126	-	-	-	X
60	MG	BB	202	-	-	-	X
60	MG	BX	101	-	-	-	X
60	MG	CA	1604	-	-	-	X
60	MG	CA	1615	-	-	-	X
60	MG	CA	1620	-	-	-	X
60	MG	CA	1624	-	-	-	X
60	MG	CA	1650	-	-	-	X
60	MG	CA	1653	-	-	-	X
60	MG	CA	1660	-	-	-	X
60	MG	CA	1662	-	-	-	X
60	MG	CA	1666	-	-	-	X
60	MG	CA	1667	-	-	-	X
60	MG	CA	1698	-	-	-	X
60	MG	CV	102	-	-	-	X
60	MG	D1	101	-	-	-	X
60	MG	DA	2901	-	-	-	X
60	MG	DA	2942	-	-	-	X
60	MG	DA	2951	-	-	-	X
60	MG	DA	2964	-	-	-	X
60	MG	DA	2965	-	-	-	X
60	MG	DA	2969	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	MG	DA	2980	-	-	-	X
60	MG	DA	2990	-	-	-	X
60	MG	DA	3003	-	-	-	X
60	MG	DA	3013	-	-	-	X
60	MG	DA	3029	-	-	-	X
60	MG	DA	3041	-	-	-	X
60	MG	DA	3047	-	-	-	X
60	MG	DA	3048	-	-	-	X
60	MG	DA	3050	-	-	-	X
60	MG	DA	3068	-	-	-	X
60	MG	DA	3071	-	-	-	X
60	MG	DA	3078	-	-	-	X
60	MG	DA	3080	-	-	-	X
60	MG	DA	3088	-	-	-	X
60	MG	DA	3096	-	-	-	X
60	MG	DA	3104	-	-	-	X
60	MG	DA	3106	-	-	-	X
60	MG	DA	3122	-	-	-	X
60	MG	DA	3127	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298206 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- 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			
2	CB	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			
3	CC	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			
4	CD	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			
5	CE	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			
6	CF	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			
7	CG	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			
8	CH	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				
9	CI	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	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			
11	CK	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			
12	CL	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			
13	CM	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			
14	CN	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			
15	CO	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			
16	CP	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			
17	CQ	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			
18	CR	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	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			
20	CT	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			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 23 is a RNA chain called transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 24 is a RNA chain called 5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*AP*AP*AP *AP*AP*UP*G U2M A2M A2MP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			239	111	49	69	10			

- Molecule 25 is a protein called TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	AZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
25	CY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	CZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
27	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
28	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
29	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
30	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			
33	D7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
34	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
36	DA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

- Molecule 37 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
38	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
39	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
42	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
43	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
44	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			
45	DJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- 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			
46	DN	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DO	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			
48	DP	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	1
			1113	710	211	185	7			
49	DQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	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				
50	DR	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				
51	DS	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	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			
52	DT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	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			
53	DU	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			
54	DV	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			
55	DW	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	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	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			
57	DY	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			
58	DZ	185	Total	C	N	O	S	0	0	1
			1468	936	262	268	2			

- Molecule 59 is a RNA chain called BACTERIAL TOXIN YOEB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	10	Total	C	N	O	P	0	0	0
			217	101	44	63	9			

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	103	Total	Mg	0	0
			103	103		
60	AL	1	Total	Mg	0	0
			1	1		
60	AV	1	Total	Mg	0	0
			1	1		
60	AX	1	Total	Mg	0	0
			1	1		
60	B0	1	Total	Mg	0	0
			1	1		
60	B1	2	Total	Mg	0	0
			2	2		
60	B5	2	Total	Mg	0	0
			2	2		
60	BA	236	Total	Mg	0	0
			236	236		
60	BB	2	Total	Mg	0	0
			2	2		
60	BF	1	Total	Mg	0	0
			1	1		
60	BP	1	Total	Mg	0	0
			1	1		
60	BX	1	Total	Mg	0	0
			1	1		
60	CA	103	Total	Mg	0	0
			103	103		
60	CG	1	Total	Mg	0	0
			1	1		
60	CL	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CV	2	Total 2	Mg 2	0	0
60	D1	1	Total 1	Mg 1	0	0
60	D5	1	Total 1	Mg 1	0	0
60	DA	242	Total 242	Mg 242	0	0
60	DB	1	Total 1	Mg 1	0	0
60	DF	1	Total 1	Mg 1	0	0
60	DR	1	Total 1	Mg 1	0	0
60	DX	1	Total 1	Mg 1	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AD	1	Total 1	Zn 1	0	0
61	AN	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	CN	1	Total 1	Zn 1	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.59Å 455.43Å 616.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.35 49.79 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.79-3.35) 99.7 (49.79-3.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.261 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	96.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	298206	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
24	OMU	AX	19	24	19,22,23	0.60	1 (5%)	25,31,34	0.96	1 (4%)
24	A2M	AX	21	24	22,25,26	0.18	0	30,36,39	1.28	1 (3%)
24	A2M	AX	20	24,60	22,25,26	0.18	0	30,36,39	0.94	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OMU	CX	19	59	19,22,23	0.55	0	25,31,34	0.78	1 (4%)
22	5MU	AV	54	22	19,22,23	0.30	0	27,32,35	0.37	0
59	A2M	CX	20	59	22,25,26	0.18	0	30,36,39	0.86	1 (3%)
59	A2M	CX	21	59	22,25,26	0.19	0	30,36,39	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	OMU	AX	19	24	-	3/9/27/28	0/2/2/2
24	A2M	AX	21	24	-	4/9/27/28	0/3/3/3
24	A2M	AX	20	24,60	-	6/9/27/28	0/3/3/3
59	OMU	CX	19	59	-	2/9/27/28	0/2/2/2
22	5MU	AV	54	22	-	0/7/25/26	0/2/2/2
59	A2M	CX	20	59	-	4/9/27/28	0/3/3/3
59	A2M	CX	21	59	-	6/9/27/28	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	19	OMU	O2'-CM2	-2.26	1.34	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	21	A2M	CM'-O2'-C2'	-6.88	96.81	114.47
24	AX	20	A2M	CM'-O2'-C2'	-4.96	101.75	114.47
59	CX	20	A2M	CM'-O2'-C2'	-4.51	102.89	114.47
24	AX	19	OMU	CM2-O2'-C2'	-4.41	103.14	114.47
59	CX	19	OMU	CM2-O2'-C2'	3.42	123.24	114.47

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AX	19	OMU	C1'-C2'-O2'-CM2
24	AX	20	A2M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
24	AX	21	A2M	C4'-C5'-O5'-P
59	CX	21	A2M	C4'-C5'-O5'-P
59	CX	21	A2M	C3'-C4'-C5'-O5'
59	CX	20	A2M	O4'-C1'-N9-C8
59	CX	20	A2M	O4'-C1'-N9-C4
24	AX	20	A2M	C3'-C4'-C5'-O5'
59	CX	20	A2M	O4'-C4'-C5'-O5'
59	CX	21	A2M	O4'-C4'-C5'-O5'
59	CX	19	OMU	C2'-C1'-N1-C2
59	CX	20	A2M	C3'-C4'-C5'-O5'
59	CX	21	A2M	C2'-C1'-N9-C8
24	AX	21	A2M	C3'-C4'-C5'-O5'
24	AX	20	A2M	C2'-C1'-N9-C8
59	CX	19	OMU	C2'-C1'-N1-C6
24	AX	21	A2M	C2'-C1'-N9-C8
24	AX	20	A2M	C2'-C1'-N9-C4
59	CX	21	A2M	C2'-C1'-N9-C4
24	AX	19	OMU	C2'-C1'-N1-C2
24	AX	19	OMU	C2'-C1'-N1-C6
24	AX	20	A2M	O4'-C1'-N9-C8
59	CX	21	A2M	O4'-C1'-N9-C8
24	AX	20	A2M	O4'-C1'-N9-C4
24	AX	21	A2M	O4'-C1'-N9-C8

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 711 ligands modelled in this entry, 711 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.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
42	DG	1
42	BG	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DG	112:PRO	C	113:ARG	N	5.57
1	CM	69:GLU	C	70:LEU	N	4.17
1	AM	69:GLU	C	70:LEU	N	4.16
1	CM	112:GLY	C	113:PRO	N	3.94
1	AM	112:GLY	C	113:PRO	N	3.93
1	BG	112:PRO	C	113:ARG	N	3.73
1	AI	53:VAL	C	54:ASP	N	3.05
1	CI	53:VAL	C	54:ASP	N	3.05
1	CM	65:LYS	C	66:LEU	N	2.83
1	AM	118:ALA	C	119:GLY	N	2.81
1	CM	118:ALA	C	119:GLY	N	2.80
1	AM	65:LYS	C	66:LEU	N	2.79
1	CI	104:ARG	C	105:ASP	N	2.67
1	AI	104:ARG	C	105:ASP	N	2.66
1	CM	97:PRO	C	98:VAL	N	2.63
1	AM	97:PRO	C	98:VAL	N	2.61

5 Fit of model and data ⓘ

5.1 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	1504/1504 (100%)	0.02	42 (2%) 55 40	63, 109, 201, 216	0
1	CA	1504/1504 (100%)	0.39	43 (2%) 53 39	65, 139, 211, 216	0
2	AB	235/256 (91%)	0.55	14 (5%) 27 20	87, 146, 195, 216	0
2	CB	235/256 (91%)	0.68	19 (8%) 18 15	86, 165, 206, 216	0
3	AC	207/239 (86%)	0.42	10 (4%) 35 25	83, 143, 188, 216	0
3	CC	207/239 (86%)	0.57	10 (4%) 35 25	100, 164, 200, 216	0
4	AD	208/209 (99%)	0.42	9 (4%) 40 28	70, 104, 147, 167	0
4	CD	208/209 (99%)	1.16	33 (15%) 5 5	95, 151, 199, 216	0
5	AE	151/162 (93%)	0.09	0 100 100	62, 102, 142, 216	0
5	CE	151/162 (93%)	0.47	7 (4%) 37 27	60, 125, 168, 210	0
6	AF	101/101 (100%)	0.41	5 (4%) 34 24	73, 128, 164, 183	0
6	CF	101/101 (100%)	0.21	5 (4%) 34 24	63, 112, 156, 181	0
7	AG	155/156 (99%)	0.47	7 (4%) 38 27	91, 136, 181, 210	0
7	CG	155/156 (99%)	0.59	12 (7%) 19 15	91, 153, 194, 216	0
8	AH	138/138 (100%)	0.24	3 (2%) 62 46	73, 108, 147, 193	0
8	CH	138/138 (100%)	0.68	8 (5%) 29 21	89, 132, 183, 213	0
9	AI	127/128 (99%)	1.13	23 (18%) 3 4	95, 155, 190, 216	0
9	CI	127/128 (99%)	1.24	26 (20%) 2 4	113, 170, 211, 216	0
10	AJ	99/105 (94%)	1.13	17 (17%) 4 5	88, 159, 208, 216	0
10	CJ	99/105 (94%)	1.36	22 (22%) 2 3	122, 174, 215, 216	0
11	AK	119/129 (92%)	0.37	7 (5%) 28 20	70, 120, 170, 212	0
11	CK	119/129 (92%)	0.53	8 (6%) 24 18	70, 120, 167, 195	0
12	AL	125/132 (94%)	0.41	11 (8%) 15 14	60, 89, 139, 216	0
12	CL	125/132 (94%)	0.86	15 (12%) 9 9	77, 113, 157, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	119/126 (94%)	0.83	9 (7%) 20 16	80, 143, 183, 216	0
13	CM	119/126 (94%)	0.97	16 (13%) 7 7	97, 167, 210, 216	0
14	AN	60/61 (98%)	1.02	7 (11%) 9 9	84, 136, 187, 204	0
14	CN	60/61 (98%)	1.33	15 (25%) 2 3	92, 154, 192, 206	0
15	AO	88/89 (98%)	0.11	0 100 100	66, 108, 148, 176	0
15	CO	88/89 (98%)	0.43	3 (3%) 48 34	70, 114, 149, 174	0
16	AP	84/88 (95%)	0.54	6 (7%) 22 17	70, 94, 143, 199	0
16	CP	84/88 (95%)	0.88	10 (11%) 9 9	99, 138, 175, 208	0
17	AQ	100/105 (95%)	0.21	2 (2%) 65 48	70, 99, 129, 161	0
17	CQ	100/105 (95%)	0.87	12 (12%) 9 9	90, 125, 158, 179	0
18	AR	70/88 (79%)	0.57	3 (4%) 40 28	87, 128, 170, 181	0
18	CR	70/88 (79%)	0.42	2 (2%) 53 39	77, 118, 168, 186	0
19	AS	79/93 (84%)	0.83	10 (12%) 8 8	111, 163, 209, 216	0
19	CS	79/93 (84%)	1.05	11 (13%) 6 7	122, 169, 213, 216	0
20	AT	99/106 (93%)	0.76	11 (11%) 10 10	71, 107, 163, 187	0
20	CT	99/106 (93%)	1.22	24 (24%) 2 3	93, 143, 181, 216	0
21	AU	25/27 (92%)	1.87	11 (44%) 0 0	99, 143, 176, 193	0
21	CU	25/27 (92%)	2.58	15 (60%) 0 0	102, 155, 182, 191	0
22	AV	76/77 (98%)	-0.16	1 (1%) 75 61	71, 108, 162, 206	0
23	AW	77/77 (100%)	0.99	8 (10%) 11 11	151, 218, 220, 221	0
23	CV	77/77 (100%)	0.18	3 (3%) 43 30	76, 126, 184, 211	0
23	CW	77/77 (100%)	0.66	7 (9%) 15 13	151, 218, 220, 221	0
24	AX	8/25 (32%)	3.07	6 (75%) 0 0	52, 100, 165, 180	0
25	AY	84/84 (100%)	0.74	6 (7%) 22 17	105, 142, 171, 199	0
25	AZ	84/84 (100%)	0.19	0 100 100	121, 166, 197, 200	0
25	CY	84/84 (100%)	1.03	12 (14%) 6 7	103, 160, 194, 200	0
25	CZ	84/84 (100%)	0.64	6 (7%) 22 17	132, 182, 200, 200	0
26	B0	84/85 (98%)	0.67	12 (14%) 6 7	69, 103, 160, 207	0
26	D0	84/85 (98%)	0.72	8 (9%) 14 13	76, 107, 163, 198	0
27	B1	94/98 (95%)	0.25	2 (2%) 63 47	55, 87, 144, 208	0
27	D1	94/98 (95%)	0.35	4 (4%) 40 28	53, 83, 132, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	B2	71/72 (98%)	0.32	4 (5%)	30	22	81, 122, 156, 205	0
28	D2	71/72 (98%)	0.05	3 (4%)	40	28	51, 84, 123, 188	0
29	B3	60/60 (100%)	0.44	3 (5%)	34	24	66, 97, 144, 212	0
29	D3	60/60 (100%)	0.09	0	100	100	61, 92, 159, 199	0
30	B4	58/71 (81%)	0.44	2 (3%)	48	34	104, 171, 212, 216	0
30	D4	58/71 (81%)	0.73	4 (6%)	23	18	145, 180, 214, 216	0
31	B5	56/60 (93%)	0.54	3 (5%)	31	23	49, 92, 147, 216	0
31	D5	56/60 (93%)	0.24	1 (1%)	67	51	49, 83, 151, 216	0
32	B6	50/54 (92%)	1.22	12 (24%)	2	3	89, 132, 180, 182	0
32	D6	50/54 (92%)	0.90	7 (14%)	6	7	97, 140, 188, 210	0
33	B7	48/49 (97%)	0.41	5 (10%)	11	11	50, 73, 123, 163	0
33	D7	48/49 (97%)	0.04	4 (8%)	17	14	42, 57, 101, 161	0
34	B8	64/65 (98%)	1.04	12 (18%)	3	4	57, 85, 144, 170	0
34	D8	64/65 (98%)	1.20	16 (25%)	2	3	48, 85, 142, 210	0
35	B9	37/37 (100%)	1.61	11 (29%)	1	2	94, 118, 162, 186	0
35	D9	37/37 (100%)	1.64	11 (29%)	1	2	93, 119, 162, 173	0
36	BA	2848/2848 (100%)	-0.20	49 (1%)	69	53	46, 88, 203, 216	0
36	DA	2848/2848 (100%)	-0.24	45 (1%)	70	55	43, 82, 203, 216	0
37	BB	119/119 (100%)	0.27	4 (3%)	48	34	88, 144, 195, 212	0
37	DB	119/119 (100%)	0.76	9 (7%)	20	16	90, 173, 210, 216	0
38	BC	120/229 (52%)	1.18	20 (16%)	4	5	139, 202, 216, 216	0
38	DC	120/229 (52%)	1.06	19 (15%)	5	6	145, 202, 216, 216	0
39	BD	272/276 (98%)	0.24	11 (4%)	42	29	45, 83, 120, 188	0
39	DD	272/276 (98%)	0.34	14 (5%)	33	24	45, 77, 113, 185	0
40	BE	205/206 (99%)	0.34	13 (6%)	26	19	50, 89, 166, 201	0
40	DE	205/206 (99%)	0.31	15 (7%)	21	17	37, 89, 146, 194	0
41	BF	208/210 (99%)	0.19	3 (1%)	73	59	49, 88, 164, 216	0
41	DF	208/210 (99%)	0.06	5 (2%)	59	44	36, 82, 164, 211	0
42	BG	181/182 (99%)	0.47	7 (3%)	43	30	100, 143, 188, 212	0
42	DG	181/182 (99%)	1.19	39 (21%)	2	4	109, 171, 215, 216	0
43	BH	165/180 (91%)	1.16	31 (18%)	3	4	98, 166, 214, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	DH	165/180 (91%)	0.94	26 (15%) 5 6	67, 127, 186, 216	0
44	BI	146/148 (98%)	1.66	43 (29%) 1 2	84, 172, 216, 216	0
44	DI	146/148 (98%)	1.05	25 (17%) 4 5	69, 144, 211, 216	0
45	BJ	0/130	-	-	-	-
45	DJ	0/130	-	-	-	-
46	BN	139/140 (99%)	0.43	7 (5%) 34 24	63, 97, 149, 192	0
46	DN	139/140 (99%)	0.39	8 (5%) 29 21	54, 90, 144, 175	0
47	BO	122/122 (100%)	-0.04	1 (0%) 82 71	48, 78, 111, 141	0
47	DO	122/122 (100%)	0.05	0 100 100	60, 89, 121, 138	0
48	BP	146/150 (97%)	0.94	19 (13%) 7 8	51, 103, 161, 216	0
48	DP	146/150 (97%)	0.92	18 (12%) 8 8	51, 105, 162, 210	0
49	BQ	141/141 (100%)	0.31	7 (4%) 34 24	65, 96, 134, 209	0
49	DQ	141/141 (100%)	0.53	9 (6%) 25 19	67, 103, 149, 208	0
50	BR	117/118 (99%)	0.34	7 (5%) 27 20	55, 89, 123, 137	0
50	DR	117/118 (99%)	0.36	7 (5%) 27 20	51, 84, 121, 145	0
51	BS	99/112 (88%)	1.30	24 (24%) 2 3	93, 141, 189, 208	0
51	DS	99/112 (88%)	1.26	24 (24%) 2 3	91, 154, 199, 216	0
52	BT	136/146 (93%)	0.45	4 (2%) 53 39	64, 97, 176, 216	0
52	DT	136/146 (93%)	0.66	14 (10%) 12 11	68, 110, 189, 215	0
53	BU	117/118 (99%)	0.38	7 (5%) 27 20	53, 86, 139, 210	0
53	DU	117/118 (99%)	0.19	4 (3%) 48 34	45, 75, 122, 215	0
54	BV	101/101 (100%)	0.29	3 (2%) 52 38	53, 109, 158, 206	0
54	DV	101/101 (100%)	0.14	1 (0%) 79 66	38, 93, 133, 216	0
55	BW	113/113 (100%)	0.07	2 (1%) 67 51	55, 80, 132, 199	0
55	DW	113/113 (100%)	-0.06	1 (0%) 81 69	40, 72, 121, 209	0
56	BX	93/96 (96%)	0.72	5 (5%) 31 23	63, 106, 136, 155	0
56	DX	93/96 (96%)	0.15	3 (3%) 50 36	55, 79, 117, 164	0
57	BY	101/110 (91%)	1.33	25 (24%) 2 3	62, 114, 180, 206	0
57	DY	101/110 (91%)	0.86	16 (15%) 5 6	56, 102, 168, 211	0
58	BZ	185/206 (89%)	0.38	8 (4%) 40 28	85, 131, 186, 216	0
58	DZ	185/206 (89%)	0.65	8 (4%) 40 28	88, 144, 202, 215	0
59	CX	7/10 (70%)	2.55	6 (85%) 0 0	110, 144, 193, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21436/22467 (95%)	0.33	1312 (6%) 27 20	36, 111, 202, 221	0

All (1312) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
44	DI	88	ILE	12.6
11	AK	129	SER	12.1
44	BI	100	ALA	11.0
31	B5	2	ALA	10.1
42	BG	2	PRO	10.0
13	AM	99	ARG	7.8
51	DS	12	PHE	7.8
44	BI	68	LEU	7.5
1	CA	89	C	7.5
38	BC	193	PHE	7.5
44	BI	72	LEU	7.0
51	BS	12	PHE	6.9
11	CK	129	SER	6.9
57	BY	44	ILE	6.4
35	D9	1	MET	6.3
21	CU	14	TRP	6.3
9	CI	106	ALA	6.2
44	BI	119	PRO	6.2
2	CB	101	MET	6.1
57	BY	4	LYS	6.1
19	AS	82	GLY	6.0
26	B0	2	ALA	6.0
42	DG	11	TYR	5.9
36	DA	508	G	5.9
35	B9	28	GLU	5.9
36	DA	654(N)	G	5.8
20	CT	22	ARG	5.8
43	DH	171	LEU	5.7
25	AY	60	ILE	5.6
21	AU	6	ARG	5.5
24	AX	23	A	5.5
44	BI	97	ILE	5.4
17	CQ	37	LYS	5.4
20	CT	23	ARG	5.4
46	DN	68	GLU	5.3
10	CJ	57	LYS	5.3
4	CD	139	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
19	CS	81	ARG	5.3
39	DD	36	PRO	5.2
9	CI	41	VAL	5.2
33	B7	47	ARG	5.2
35	D9	28	GLU	5.2
14	CN	2	ALA	5.2
10	CJ	58	ASP	5.2
34	D8	48	PHE	5.1
48	BP	62	LEU	5.1
48	BP	65	ARG	5.1
4	CD	67	ILE	5.1
57	BY	28	LYS	5.1
19	CS	80	TYR	5.1
44	BI	120	ILE	5.0
42	DG	165	THR	5.0
48	BP	27	HIS	5.0
58	DZ	28	MET	5.0
26	B0	5	LYS	5.0
36	DA	654(L)	G	5.0
59	CX	22	A	5.0
44	DI	130	TYR	5.0
17	CQ	24	GLU	4.9
16	AP	25	ARG	4.9
44	BI	63	ALA	4.9
36	DA	277	C	4.8
42	DG	99	MET	4.8
9	AI	106	ALA	4.8
8	AH	1	MET	4.8
1	AA	1030(B)	C	4.8
24	AX	13	A	4.7
25	AY	84	TYR	4.7
34	D8	2	PRO	4.7
1	AA	89	C	4.7
10	CJ	72	VAL	4.7
21	CU	17	THR	4.7
52	DT	25	GLY	4.7
42	DG	106	LEU	4.7
56	BX	92	LEU	4.7
13	CM	31	LYS	4.6
3	AC	158	GLY	4.6
43	DH	115	VAL	4.6
57	BY	43	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
36	BA	654(H)	G	4.6
11	CK	127	LYS	4.6
6	AF	90	VAL	4.6
11	CK	128	ALA	4.6
7	AG	8	GLU	4.6
9	CI	127	LYS	4.6
21	CU	10	ARG	4.6
57	BY	39	VAL	4.6
57	BY	61	ILE	4.5
20	CT	29	LYS	4.5
43	BH	9	ILE	4.5
8	AH	2	LEU	4.5
49	DQ	141	GLN	4.5
20	CT	14	LYS	4.5
12	AL	19	ARG	4.5
48	DP	68	GLN	4.5
36	DA	654(O)	G	4.5
13	CM	96	LEU	4.4
2	CB	81	VAL	4.4
9	AI	105	ASP	4.4
36	DA	654(J)	A	4.4
8	CH	1	MET	4.4
51	BS	60	GLY	4.4
33	D7	47	ARG	4.4
36	BA	275	G	4.4
44	BI	101	LEU	4.4
4	CD	157	LEU	4.3
36	BA	654(E)	G	4.3
38	BC	44	VAL	4.3
34	B8	65	GLU	4.3
9	CI	13	ALA	4.3
13	CM	112	GLY	4.3
11	CK	126	ARG	4.3
44	BI	111	PRO	4.3
33	B7	48	LYS	4.3
2	AB	155	LEU	4.3
42	DG	34	LEU	4.3
21	CU	16	GLY	4.3
13	AM	102	ARG	4.2
42	DG	93	THR	4.2
44	DI	118	LYS	4.2
1	CA	1036	G	4.2

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Mol	Chain	Res	Type	RSRZ
14	AN	46	GLU	4.2
4	AD	32	ALA	4.2
26	D0	2	ALA	4.2
39	DD	35	LYS	4.2
1	CA	88	A	4.2
13	CM	90	LEU	4.2
10	AJ	54	PHE	4.2
49	DQ	140	ALA	4.2
48	BP	64	LYS	4.2
57	BY	67	LEU	4.2
1	AA	80	G	4.1
13	CM	94	ARG	4.1
12	AL	28	LYS	4.1
43	DH	167	GLU	4.1
43	BH	10	PRO	4.1
13	AM	117	VAL	4.1
13	CM	117	VAL	4.1
11	CK	25	TYR	4.1
48	BP	28	GLY	4.1
34	D8	65	GLU	4.0
4	AD	9	CYS	4.0
48	DP	65	ARG	4.0
10	AJ	73	ASP	4.0
9	AI	81	ILE	4.0
52	BT	105	LEU	4.0
44	DI	92	VAL	3.9
21	AU	14	TRP	3.9
42	DG	64	THR	3.9
19	AS	67	VAL	3.9
43	BH	52	VAL	3.9
7	AG	5	ARG	3.9
14	CN	35	ARG	3.9
4	CD	125	HIS	3.9
26	D0	3	HIS	3.9
44	BI	59	ALA	3.9
38	DC	170	GLY	3.9
36	BA	654(K)	C	3.9
19	CS	71	LEU	3.9
38	DC	172	ILE	3.9
35	B9	20	HIS	3.9
20	AT	22	ARG	3.9
36	BA	654(L)	G	3.9

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Mol	Chain	Res	Type	RSRZ
1	CA	81	U	3.9
32	B6	54	ILE	3.9
48	DP	76	LYS	3.9
8	CH	2	LEU	3.9
44	DI	94	ALA	3.9
21	CU	6	ARG	3.8
51	DS	13	ARG	3.8
9	CI	115	GLY	3.8
3	AC	157	ILE	3.8
38	BC	174	ALA	3.8
46	BN	2	LYS	3.8
34	B8	35	GLN	3.8
50	BR	6	SER	3.8
36	BA	654(F)	C	3.8
2	AB	99	GLY	3.8
12	AL	29	GLY	3.8
3	CC	91	LEU	3.8
44	DI	116	LEU	3.8
52	DT	105	LEU	3.8
40	BE	127	ASP	3.8
43	BH	144	VAL	3.8
34	B8	32	LEU	3.8
41	DF	24	LEU	3.8
14	AN	2	ALA	3.8
44	BI	66	GLU	3.8
49	DQ	9	TYR	3.8
1	AA	83	U	3.8
36	BA	1026	U	3.8
38	DC	46	ALA	3.7
20	AT	74	LYS	3.7
13	AM	88	ARG	3.7
48	DP	33	ARG	3.7
52	DT	91	ARG	3.7
25	AY	19	THR	3.7
44	BI	94	ALA	3.7
42	DG	29	TRP	3.7
10	AJ	59	SER	3.7
57	BY	3	VAL	3.7
58	DZ	88	PHE	3.7
13	CM	97	PRO	3.7
20	CT	12	ALA	3.7
40	BE	131	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
42	DG	103	LEU	3.7
51	BS	11	LYS	3.7
19	AS	4	SER	3.7
57	BY	82	PRO	3.7
36	BA	654(I)	C	3.7
36	DA	654(T)	C	3.7
46	DN	1	MET	3.7
51	DS	11	LYS	3.7
34	B8	45	GLY	3.7
39	BD	36	PRO	3.6
36	DA	2319	G	3.6
10	CJ	38	ILE	3.6
17	CQ	26	GLN	3.6
48	DP	62	LEU	3.6
43	DH	65	HIS	3.6
48	DP	64	LYS	3.6
3	AC	10	PHE	3.6
13	AM	100	GLY	3.6
14	CN	57	ARG	3.6
20	CT	19	SER	3.6
25	CY	84	TYR	3.6
42	DG	7	LEU	3.6
35	D9	9	ARG	3.6
19	CS	41	VAL	3.6
44	BI	65	ALA	3.6
13	CM	87	TYR	3.6
20	CT	10	LEU	3.6
39	BD	35	LYS	3.6
35	D9	20	HIS	3.6
23	CV	33	U	3.6
44	DI	98	ALA	3.6
4	CD	108	LEU	3.6
51	BS	35	ILE	3.6
37	DB	88	C	3.6
51	BS	30	ARG	3.6
32	D6	42	TRP	3.6
35	D9	18	ARG	3.5
51	BS	13	ARG	3.5
2	CB	98	LEU	3.5
10	AJ	43	ARG	3.5
17	AQ	101	ARG	3.5
48	BP	33	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
10	AJ	72	VAL	3.5
18	CR	68	LYS	3.5
44	BI	92	VAL	3.5
17	CQ	28	PRO	3.5
36	BA	2751	G	3.5
7	CG	85	TYR	3.5
19	AS	80	TYR	3.5
39	DD	262	ARG	3.5
43	BH	158	HIS	3.5
43	BH	17	VAL	3.5
10	CJ	40	LEU	3.5
9	AI	9	ARG	3.5
43	BH	167	GLU	3.5
36	DA	2178	C	3.5
43	DH	24	VAL	3.5
42	DG	46	ALA	3.5
43	DH	117	PRO	3.5
36	BA	2117	A	3.5
50	DR	3	HIS	3.5
38	DC	56	ASP	3.5
20	CT	15	ARG	3.5
40	BE	76	ARG	3.5
1	AA	81	U	3.5
49	BQ	140	ALA	3.4
1	CA	1030(B)	C	3.4
11	AK	127	LYS	3.4
42	DG	102	PHE	3.4
27	D1	95	LEU	3.4
42	DG	111	LEU	3.4
48	DP	27	HIS	3.4
10	CJ	6	ILE	3.4
51	BS	14	VAL	3.4
1	CA	307	C	3.4
36	DA	975	C	3.4
10	CJ	39	PRO	3.4
4	AD	26	CYS	3.4
2	CB	187	LEU	3.4
53	DU	58	ARG	3.4
7	AG	81	GLY	3.4
9	CI	119	ALA	3.4
41	DF	69	HIS	3.4
42	DG	142	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
36	BA	975	C	3.4
34	B8	48	PHE	3.4
10	AJ	85	LEU	3.4
53	BU	97	ASP	3.4
58	BZ	80	ARG	3.4
24	AX	22	A	3.3
6	CF	90	VAL	3.3
14	AN	18	VAL	3.3
20	AT	12	ALA	3.3
46	DN	109	LYS	3.3
57	DY	43	ASN	3.3
10	CJ	47	PHE	3.3
20	AT	11	SER	3.3
1	AA	723	U	3.3
36	DA	654(K)	C	3.3
10	CJ	71	LEU	3.3
36	DA	654(C)	G	3.3
9	CI	123	PRO	3.3
36	DA	1535	A	3.3
39	BD	233	HIS	3.3
51	BS	106	ARG	3.3
58	DZ	80	ARG	3.3
51	DS	87	PHE	3.3
9	CI	116	LYS	3.3
4	CD	70	ILE	3.3
19	CS	82	GLY	3.3
40	BE	130	GLY	3.3
42	DG	68	PRO	3.3
38	BC	210	LEU	3.3
57	BY	45	VAL	3.3
24	AX	14	A	3.3
1	AA	1397	C	3.3
38	DC	174	ALA	3.3
53	BU	37	GLU	3.3
43	BH	7	LEU	3.2
44	BI	58	LEU	3.2
26	B0	3	HIS	3.2
9	AI	41	VAL	3.2
38	DC	30	VAL	3.2
40	DE	121	ASN	3.2
50	DR	11	ASN	3.2
4	CD	2	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
9	AI	12	GLU	3.2
36	BA	508	G	3.2
1	AA	1503	A	3.2
36	DA	654(I)	C	3.2
44	BI	143	SER	3.2
20	CT	73	HIS	3.2
51	DS	28	VAL	3.2
36	DA	654(H)	G	3.2
36	BA	654(G)	C	3.2
53	DU	97	ASP	3.2
9	CI	66	ARG	3.2
6	CF	92	LYS	3.2
12	CL	21	LYS	3.2
20	CT	75	ASN	3.2
42	DG	67	LYS	3.2
38	BC	176	VAL	3.2
32	B6	23	THR	3.2
35	B9	22	ARG	3.2
1	AA	1493	A	3.2
32	B6	42	TRP	3.2
28	B2	5	GLU	3.2
50	BR	4	LEU	3.2
7	AG	85	TYR	3.2
34	B8	64	TYR	3.2
48	DP	71	VAL	3.2
44	BI	88	ILE	3.2
44	DI	138	ILE	3.2
8	CH	97	VAL	3.1
22	AV	1	C	3.1
24	AX	18	G	3.1
34	D8	46	ARG	3.1
39	DD	41	GLY	3.1
51	BS	73	LEU	3.1
25	CY	62	GLU	3.1
34	D8	56	GLU	3.1
48	DP	51	PHE	3.1
40	DE	76	ARG	3.1
9	AI	11	LYS	3.1
9	AI	127	LYS	3.1
9	CI	113	LYS	3.1
20	AT	14	LYS	3.1
34	D8	26	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
38	DC	27	ALA	3.1
23	CV	1	C	3.1
21	CU	11	GLY	3.1
43	BH	82	GLY	3.1
13	AM	10	PRO	3.1
44	BI	69	LYS	3.1
44	BI	109	ILE	3.1
1	AA	88	A	3.1
44	BI	93	THR	3.1
21	CU	22	ARG	3.1
48	BP	51	PHE	3.1
58	BZ	97	GLU	3.1
58	DZ	81	ARG	3.1
52	BT	32	TYR	3.1
49	BQ	28	ALA	3.1
42	DG	66	GLN	3.1
51	DS	30	ARG	3.1
33	D7	46	VAL	3.1
28	B2	11	GLU	3.1
1	AA	1357	A	3.1
7	CG	36	LYS	3.1
36	BA	654(J)	A	3.1
17	CQ	30	PRO	3.1
35	B9	1	MET	3.1
1	AA	79	G	3.0
1	CA	1356	G	3.0
20	AT	25	ARG	3.0
36	BA	2115	G	3.0
56	BX	45	THR	3.0
1	CA	84	U	3.0
51	BS	85	VAL	3.0
43	BH	159	GLU	3.0
43	BH	8	PRO	3.0
43	BH	64	LEU	3.0
2	CB	144	ARG	3.0
32	B6	37	ARG	3.0
1	CA	1366	C	3.0
2	CB	8	LYS	3.0
35	B9	15	LYS	3.0
25	CY	60	ILE	3.0
36	DA	1026	U	3.0
36	DA	1534	U	3.0

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Mol	Chain	Res	Type	RSRZ
35	B9	12	ASP	3.0
50	BR	8	ARG	3.0
2	CB	133	LYS	3.0
12	CL	28	LYS	3.0
16	CP	65	GLN	3.0
21	CU	3	LYS	3.0
44	DI	87	LYS	3.0
36	BA	2170	A	3.0
23	CW	34	C	3.0
44	DI	79	ILE	3.0
4	CD	208	SER	3.0
50	DR	6	SER	3.0
9	AI	66	ARG	3.0
13	CM	99	ARG	3.0
34	D8	64	TYR	3.0
51	BS	33	LYS	3.0
7	AG	82	GLY	3.0
1	CA	1117	G	3.0
43	BH	68	THR	3.0
20	CT	72	LEU	3.0
4	CD	65	ARG	3.0
11	AK	128	ALA	3.0
48	BP	107	LYS	3.0
43	DH	158	HIS	3.0
48	BP	68	GLN	3.0
32	B6	13	CYS	3.0
16	AP	6	LEU	2.9
10	CJ	66	ARG	2.9
1	CA	944	G	2.9
12	CL	31	PRO	2.9
33	B7	23	ARG	2.9
48	DP	15	ARG	2.9
36	BA	2131	G	2.9
35	B9	13	LYS	2.9
49	DQ	8	LYS	2.9
57	BY	19	LYS	2.9
26	D0	73	GLY	2.9
43	BH	43	VAL	2.9
4	CD	75	PHE	2.9
2	AB	214	ILE	2.9
1	CA	90	U	2.9
4	CD	21	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
5	CE	139	LEU	2.9
19	AS	81	ARG	2.9
50	BR	10	LEU	2.9
9	AI	70	LYS	2.9
44	DI	111	PRO	2.9
32	B6	22	ALA	2.9
38	BC	46	ALA	2.9
39	DD	42	GLY	2.9
36	DA	654(S)	G	2.9
42	DG	141	PHE	2.9
51	BS	87	PHE	2.9
58	DZ	33	LEU	2.9
59	CX	13	A	2.9
6	AF	7	ASN	2.9
12	CL	49	ASN	2.9
1	CA	824	C	2.9
3	CC	168	ALA	2.9
42	BG	13	GLU	2.9
4	CD	133	VAL	2.9
2	CB	152	PHE	2.9
12	AL	89	ARG	2.9
58	DZ	124	ILE	2.9
44	BI	128	LEU	2.9
51	BS	54	LEU	2.9
17	CQ	100	LYS	2.9
1	CA	1030(C)	G	2.9
4	AD	31	CYS	2.9
38	DC	215	VAL	2.9
21	AU	10	ARG	2.9
57	DY	44	ILE	2.9
46	BN	73	THR	2.9
48	BP	57	THR	2.9
57	DY	66	PRO	2.9
4	CD	104	VAL	2.9
11	AK	126	ARG	2.9
13	CM	100	GLY	2.9
36	BA	2155	G	2.9
57	DY	19	LYS	2.9
10	CJ	68	HIS	2.8
14	CN	32	SER	2.8
57	BY	77	PRO	2.8
43	DH	37	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
16	CP	25	ARG	2.8
32	B6	36	LEU	2.8
44	BI	106	GLY	2.8
29	B3	1	MET	2.8
35	B9	26	ILE	2.8
38	DC	50	ILE	2.8
40	DE	131	ALA	2.8
1	AA	1190	G	2.8
23	AW	19	G	2.8
36	BA	654(N)	G	2.8
2	CB	165	VAL	2.8
10	AJ	49	VAL	2.8
21	AU	9	ARG	2.8
40	BE	59	VAL	2.8
48	DP	7	ARG	2.8
44	DI	95	LYS	2.8
12	CL	32	PHE	2.8
17	CQ	33	GLY	2.8
21	CU	18	TYR	2.8
43	DH	156	ALA	2.8
42	DG	2	PRO	2.8
57	DY	47	LYS	2.8
3	CC	43	LEU	2.8
5	CE	136	MET	2.8
20	CT	9	ASN	2.8
36	BA	2125	G	2.8
36	DA	654(D)	G	2.8
10	CJ	56	HIS	2.8
44	BI	105	HIS	2.8
6	AF	6	VAL	2.8
9	AI	116	LYS	2.8
10	CJ	59	SER	2.8
26	B0	4	LYS	2.8
32	B6	35	GLU	2.8
42	BG	35	GLU	2.8
44	BI	135	GLU	2.8
44	BI	71	ILE	2.8
48	BP	53	GLY	2.8
49	BQ	103	MET	2.8
32	B6	26	ASN	2.8
1	AA	82	U	2.8
36	BA	2173	A	2.8

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Mol	Chain	Res	Type	RSRZ
1	CA	1037	C	2.8
31	D5	2	ALA	2.8
39	BD	272	ALA	2.8
4	AD	7	PRO	2.8
51	DS	91	PRO	2.8
44	DI	91	SER	2.8
51	DS	27	SER	2.8
10	AJ	38	ILE	2.8
44	BI	79	ILE	2.8
50	BR	68	ARG	2.7
57	BY	2	ARG	2.7
1	CA	1364	U	2.7
9	AI	14	VAL	2.7
24	AX	15	A	2.7
36	BA	2801	A	2.7
38	BC	42	VAL	2.7
59	CX	14	A	2.7
44	BI	80	PRO	2.7
57	BY	53	PRO	2.7
4	CD	58	LEU	2.7
38	BC	197	LEU	2.7
40	DE	52	LEU	2.7
50	DR	4	LEU	2.7
3	CC	192	THR	2.7
6	AF	89	MET	2.7
1	CA	1365	G	2.7
51	DS	15	ARG	2.7
14	CN	58	LYS	2.7
39	BD	39	LYS	2.7
51	BS	61	ASN	2.7
56	BX	32	PRO	2.7
36	BA	1033	U	2.7
42	DG	104	GLU	2.7
4	CD	69	GLY	2.7
25	CY	16	TRP	2.7
50	DR	64	ARG	2.7
51	DS	89	ARG	2.7
35	B9	2	LYS	2.7
23	CW	1	C	2.7
9	CI	114	TYR	2.7
44	DI	89	TYR	2.7
12	AL	27	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
36	BA	11	G	2.7
36	BA	272(B)	G	2.7
3	AC	2	GLY	2.7
9	CI	110	GLU	2.7
9	AI	128	ARG	2.7
38	BC	170	GLY	2.7
14	CN	17	LYS	2.7
26	D0	4	LYS	2.7
38	BC	41	THR	2.7
40	DE	57	LYS	2.7
44	DI	143	SER	2.7
23	CW	17(A)	U	2.7
1	CA	968	A	2.7
40	DE	127	ASP	2.7
4	CD	64	LEU	2.7
9	AI	117	HIS	2.7
20	AT	73	HIS	2.7
38	BC	12	LEU	2.7
43	DH	33	LEU	2.7
43	DH	169	VAL	2.7
16	AP	1	MET	2.7
42	DG	178	PHE	2.7
57	DY	89	PHE	2.7
15	CO	20	GLY	2.7
20	CT	21	LYS	2.7
25	CY	80	CYS	2.7
36	BA	2147	G	2.7
14	CN	34	TYR	2.7
25	CY	82	TYR	2.7
58	DZ	163	LEU	2.7
41	DF	23	ASP	2.7
40	BE	121	ASN	2.7
2	CB	163	PHE	2.6
4	CD	74	GLN	2.6
6	AF	94	GLN	2.6
38	BC	2	PRO	2.6
51	DS	35	ILE	2.6
20	CT	56	MET	2.6
4	CD	3	ARG	2.6
53	BU	58	ARG	2.6
11	CK	124	LYS	2.6
14	CN	15	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
21	CU	12	LYS	2.6
30	D4	2	LYS	2.6
3	AC	159	GLY	2.6
34	D8	40	GLU	2.6
36	DA	654(M)	C	2.6
43	DH	46	GLU	2.6
2	AB	112	VAL	2.6
14	AN	10	ALA	2.6
27	B1	95	LEU	2.6
3	CC	193	TYR	2.6
19	CS	47	HIS	2.6
35	D9	12	ASP	2.6
20	AT	21	LYS	2.6
21	CU	23	PRO	2.6
34	D8	35	GLN	2.6
39	BD	15	PHE	2.6
39	DD	5	LYS	2.6
52	DT	90	GLN	2.6
52	BT	4	GLY	2.6
7	CG	8	GLU	2.6
39	DD	28	GLU	2.6
36	DA	34	C	2.6
43	BH	38	SER	2.6
9	AI	114	TYR	2.6
42	DG	75	LYS	2.6
43	DH	60	ARG	2.6
44	BI	118	LYS	2.6
19	AS	10	PHE	2.6
38	DC	2	PRO	2.6
21	CU	5	ASP	2.6
57	DY	41	GLY	2.6
32	D6	35	GLU	2.6
9	AI	61	ALA	2.6
13	AM	7	VAL	2.6
19	CS	39	THR	2.6
43	DH	7	LEU	2.6
4	CD	22	LYS	2.6
16	CP	3	LYS	2.6
21	AU	25	LYS	2.6
23	AW	76	A	2.6
43	BH	85	LYS	2.6
52	DT	85	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
4	CD	152	SER	2.6
54	BV	36	PRO	2.6
1	AA	1030	C	2.6
37	DB	31	C	2.6
49	BQ	141	GLN	2.6
51	DS	104	GLY	2.6
9	CI	82	ALA	2.6
20	CT	80	ARG	2.6
8	CH	80	ILE	2.6
1	AA	1030(A)	G	2.6
57	BY	55	TYR	2.6
23	CW	37	A	2.6
23	CW	38	A	2.6
36	DA	2310	A	2.6
3	AC	13	GLY	2.6
38	DC	166	ASN	2.6
57	DY	31	LEU	2.6
10	AJ	44	VAL	2.6
23	AW	75	C	2.6
37	DB	6	C	2.6
2	AB	133	LYS	2.6
40	DE	187	ALA	2.6
44	DI	115	ALA	2.6
51	BS	89	ARG	2.6
53	BU	96	ALA	2.6
40	BE	77	ILE	2.5
43	DH	8	PRO	2.5
10	CJ	35	SER	2.5
43	BH	155	SER	2.5
14	CN	39	LEU	2.5
31	B5	30	LEU	2.5
42	BG	82	LEU	2.5
1	AA	1186	G	2.5
1	CA	527	G	2.5
2	AB	137	ARG	2.5
8	AH	32	LYS	2.5
12	CL	13	LYS	2.5
36	BA	2112	G	2.5
43	BH	90	LYS	2.5
49	DQ	130	LYS	2.5
4	CD	32	ALA	2.5
37	BB	52	A	2.5

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Mol	Chain	Res	Type	RSRZ
51	BS	86	ALA	2.5
3	CC	167	TRP	2.5
41	BF	65	TRP	2.5
5	CE	28	PHE	2.5
23	CW	74	C	2.5
2	AB	131	PRO	2.5
2	AB	118	LEU	2.5
34	D8	45	GLY	2.5
42	DG	127	GLY	2.5
44	DI	114	LEU	2.5
51	DS	58	LEU	2.5
21	CU	25	LYS	2.5
42	DG	16	ARG	2.5
2	CB	112	VAL	2.5
10	AJ	61	GLU	2.5
11	CK	117	ASN	2.5
12	CL	68	ALA	2.5
9	CI	81	ILE	2.5
44	BI	138	ILE	2.5
58	BZ	124	ILE	2.5
2	AB	97	TRP	2.5
1	AA	1492	A	2.5
36	BA	2116	G	2.5
36	BA	2319	G	2.5
37	DB	86	G	2.5
14	CN	21	TYR	2.5
25	CZ	38	PRO	2.5
42	DG	87	PRO	2.5
1	CA	999	C	2.5
2	CB	137	ARG	2.5
16	AP	12	LYS	2.5
21	CU	24	ARG	2.5
39	BD	38	LYS	2.5
42	BG	34	LEU	2.5
39	DD	167	GLY	2.5
49	BQ	10	ARG	2.5
49	DQ	107	ALA	2.5
39	BD	30	GLU	2.5
51	DS	43	GLU	2.5
52	DT	21	GLU	2.5
57	BY	38	ILE	2.5
3	AC	167	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
9	CI	33	PHE	2.5
44	DI	86	THR	2.5
9	CI	117	HIS	2.5
13	CM	102	ARG	2.5
14	CN	12	ARG	2.5
35	B9	35	ARG	2.5
4	CD	124	GLY	2.5
52	DT	92	GLY	2.5
38	DC	44	VAL	2.5
43	DH	43	VAL	2.5
48	DP	70	GLN	2.5
49	DQ	12	GLN	2.5
53	BU	100	VAL	2.5
36	DA	2334	G	2.5
37	DB	87	G	2.5
43	BH	80	SER	2.5
1	AA	1249	C	2.5
8	CH	132	GLU	2.5
36	BA	654(M)	C	2.5
46	BN	68	GLU	2.5
57	BY	5	MET	2.5
10	AJ	47	PHE	2.5
1	AA	1364	U	2.5
14	CN	61	TRP	2.5
18	CR	44	LEU	2.5
20	CT	25	ARG	2.5
21	AU	3	LYS	2.5
28	B2	24	LEU	2.5
48	DP	50	ARG	2.5
49	BQ	16	ARG	2.5
57	DY	2	ARG	2.5
39	DD	166	GLN	2.5
42	DG	69	ALA	2.4
19	CS	40	ILE	2.4
40	DE	77	ILE	2.4
25	CZ	29	GLU	2.4
36	DA	276	A	2.4
39	DD	237	GLU	2.4
2	CB	96	ARG	2.4
38	DC	211	ARG	2.4
43	DH	42	ARG	2.4
49	DQ	18	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
34	B8	34	TRP	2.4
10	CJ	8	LEU	2.4
34	D8	32	LEU	2.4
36	DA	2168	G	2.4
36	DA	2794	C	2.4
40	BE	52	LEU	2.4
38	BC	175	PRO	2.4
43	BH	168	PRO	2.4
1	CA	5	U	2.4
20	CT	16	HIS	2.4
36	DA	2113	U	2.4
48	BP	110	TYR	2.4
8	CH	130	GLY	2.4
42	DG	157	ILE	2.4
51	DS	18	ILE	2.4
19	CS	44	MET	2.4
10	AJ	63	PHE	2.4
7	AG	79	ARG	2.4
29	B3	29	ARG	2.4
44	BI	121	LYS	2.4
51	DS	17	ARG	2.4
26	B0	58	THR	2.4
44	BI	134	PRO	2.4
59	CX	15	A	2.4
9	AI	125	TYR	2.4
14	CN	33	VAL	2.4
19	AS	69	HIS	2.4
40	DE	186	GLY	2.4
44	DI	133	HIS	2.4
1	CA	1359	C	2.4
23	AW	1	C	2.4
1	CA	743	U	2.4
1	CA	1026	G	2.4
1	CA	1224	G	2.4
2	CB	200	ILE	2.4
36	BA	2137	C	2.4
36	DA	1052	C	2.4
17	AQ	93	GLN	2.4
36	BA	654(D)	G	2.4
36	DA	2802	G	2.4
38	DC	190	ILE	2.4
43	BH	72	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
51	BS	40	ILE	2.4
4	CD	118	ARG	2.4
10	CJ	7	LYS	2.4
57	DY	4	LYS	2.4
58	BZ	186	GLU	2.4
43	DH	155	SER	2.4
2	CB	155	LEU	2.4
43	BH	171	LEU	2.4
30	D4	27	THR	2.4
34	D8	63	PRO	2.4
10	AJ	58	ASP	2.4
12	CL	18	VAL	2.4
38	DC	176	VAL	2.4
21	AU	13	ILE	2.4
33	B7	45	ALA	2.4
35	D9	17	ILE	2.4
42	BG	46	ALA	2.4
9	CI	120	ARG	2.4
15	CO	48	LYS	2.4
16	CP	31	LYS	2.4
41	BF	1	MET	2.4
1	AA	1189	C	2.4
2	CB	196	LEU	2.4
44	BI	102	SER	2.4
4	CD	121	VAL	2.4
5	CE	77	PRO	2.4
42	DG	28	VAL	2.4
43	BH	35	VAL	2.4
43	DH	66	GLY	2.4
44	BI	110	ASP	2.4
47	BO	110	GLY	2.4
7	CG	154	TYR	2.4
17	CQ	32	TYR	2.4
27	D1	7	ILE	2.4
10	AJ	46	ARG	2.4
10	AJ	66	ARG	2.4
17	CQ	101	ARG	2.4
32	B6	6	ARG	2.4
52	DT	1	MET	2.4
20	CT	20	LEU	2.4
43	DH	40	GLU	2.4
44	BI	64	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
9	CI	71	SER	2.4
38	BC	55	SER	2.4
9	CI	109	VAL	2.4
23	AW	17(A)	U	2.4
40	DE	75	VAL	2.4
51	DS	14	VAL	2.4
36	DA	654(P)	C	2.3
19	AS	37	ARG	2.3
20	CT	77	ALA	2.3
34	D8	59	LYS	2.3
40	DE	132	HIS	2.3
30	D4	25	TYR	2.3
55	DW	9	TYR	2.3
36	BA	2120	G	2.3
37	BB	89	G	2.3
5	CE	31	LEU	2.3
9	CI	101	PHE	2.3
26	D0	57	PHE	2.3
13	AM	8	GLU	2.3
2	AB	165	VAL	2.3
19	CS	67	VAL	2.3
1	CA	975	A	2.3
25	CY	57	SER	2.3
7	CG	81	GLY	2.3
12	CL	46	LYS	2.3
14	AN	4	LYS	2.3
25	CY	54	GLY	2.3
26	D0	13	GLY	2.3
39	DD	258	LYS	2.3
57	DY	33	LYS	2.3
35	D9	35	ARG	2.3
9	CI	43	ALA	2.3
42	DG	39	ILE	2.3
42	DG	101	ILE	2.3
26	B0	12	ASN	2.3
36	BA	1534	U	2.3
36	DA	2796	U	2.3
43	BH	164	TYR	2.3
59	CX	17	U	2.3
1	AA	1317	C	2.3
23	CV	32	C	2.3
6	CF	95	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
14	AN	8	GLU	2.3
1	CA	306	G	2.3
31	B5	31	VAL	2.3
59	CX	18	G	2.3
11	AK	124	LYS	2.3
20	CT	34	LYS	2.3
27	D1	81	LYS	2.3
34	B8	11	LYS	2.3
39	BD	26	LYS	2.3
39	DD	38	LYS	2.3
9	AI	10	ARG	2.3
10	CJ	70	ARG	2.3
40	BE	61	ARG	2.3
52	DT	24	PRO	2.3
12	AL	128	ALA	2.3
41	DF	22	ALA	2.3
52	DT	27	THR	2.3
16	CP	1	MET	2.3
42	DG	131	TYR	2.3
7	CG	101	LEU	2.3
20	CT	104	LEU	2.3
48	BP	106	LEU	2.3
16	CP	9	PHE	2.3
36	BA	1535	A	2.3
2	AB	12	GLU	2.3
1	CA	744	C	2.3
1	CA	967	C	2.3
2	AB	7	VAL	2.3
7	CG	9	VAL	2.3
11	AK	11	LYS	2.3
23	AW	34	C	2.3
21	CU	7	ARG	2.3
49	DQ	6	ARG	2.3
12	AL	129	ALA	2.3
57	BY	78	ALA	2.3
4	CD	91	SER	2.3
4	CD	137	SER	2.3
2	CB	215	LEU	2.3
7	CG	38	LEU	2.3
28	D2	61	LEU	2.3
58	BZ	163	LEU	2.3
1	CA	823	G	2.3

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Mol	Chain	Res	Type	RSRZ
1	CA	1253	G	2.3
8	CH	62	TYR	2.3
25	AY	82	TYR	2.3
2	AB	152	PHE	2.3
36	DA	2795	G	2.3
37	DB	89	G	2.3
25	CY	51	ASN	2.3
40	DE	55	ASN	2.3
50	BR	11	ASN	2.3
38	DC	57	GLN	2.3
8	CH	32	LYS	2.3
44	DI	121	LYS	2.3
57	BY	34	LYS	2.3
1	AA	1111	A	2.3
9	AI	26	VAL	2.3
26	B0	11	ARG	2.3
34	B8	56	GLU	2.3
44	DI	81	VAL	2.3
51	DS	106	ARG	2.3
48	BP	114	ILE	2.3
25	CY	41	GLY	2.3
39	BD	41	GLY	2.3
53	BU	25	TRP	2.3
4	CD	78	LEU	2.3
34	B8	60	LEU	2.3
51	BS	48	LEU	2.3
54	DV	20	LEU	2.3
53	DU	15	LYS	2.3
26	B0	72	ARG	2.3
33	B7	46	VAL	2.3
44	BI	70	GLU	2.2
44	BI	122	GLU	2.2
48	BP	149	GLU	2.2
36	DA	2159	G	2.2
10	AJ	50	ILE	2.2
43	BH	75	ALA	2.2
48	BP	43	GLY	2.2
57	DY	77	PRO	2.2
25	CZ	1	MET	2.2
51	BS	100	ALA	2.2
1	AA	1041	A	2.2
1	AA	1183	A	2.2

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Mol	Chain	Res	Type	RSRZ
4	CD	120	LEU	2.2
10	CJ	90	LEU	2.2
26	B0	7	LEU	2.2
11	CK	123	LYS	2.2
12	CL	20	LYS	2.2
44	BI	91	SER	2.2
26	B0	74	ARG	2.2
37	DB	32	C	2.2
49	BQ	5	ARG	2.2
56	DX	60	ARG	2.2
19	AS	9	VAL	2.2
43	DH	52	VAL	2.2
38	DC	51	ASP	2.2
48	DP	47	ASP	2.2
13	CM	84	ILE	2.2
2	CB	51	LEU	2.2
4	CD	135	LEU	2.2
28	D2	72	ALA	2.2
36	BA	2334	G	2.2
36	DA	272(B)	G	2.2
3	AC	190	ARG	2.2
11	AK	25	TYR	2.2
32	D6	19	ARG	2.2
40	DE	149	ARG	2.2
43	DH	157	TYR	2.2
46	BN	75	TYR	2.2
1	CA	621	A	2.2
37	DB	53	A	2.2
2	CB	136	VAL	2.2
44	DI	136	VAL	2.2
57	DY	45	VAL	2.2
53	DU	117	GLN	2.2
9	CI	77	ILE	2.2
1	CA	1354	C	2.2
16	AP	23	ASP	2.2
18	AR	33	ASP	2.2
7	CG	82	GLY	2.2
46	BN	1	MET	2.2
50	DR	10	LEU	2.2
51	BS	58	LEU	2.2
57	DY	10	GLY	2.2
57	DY	22	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
4	AD	22	LYS	2.2
14	CN	50	LYS	2.2
16	CP	35	LYS	2.2
25	AY	21	LYS	2.2
27	D1	48	LYS	2.2
29	B3	17	LYS	2.2
34	D8	34	TRP	2.2
43	BH	69	ARG	2.2
44	BI	108	THR	2.2
3	AC	193	TYR	2.2
34	B8	49	VAL	2.2
1	AA	90	U	2.2
1	AA	1000	U	2.2
36	BA	12	U	2.2
4	CD	158	ILE	2.2
10	CJ	98	ILE	2.2
35	D9	26	ILE	2.2
12	CL	8	ASN	2.2
1	AA	1001	A	2.2
1	AA	1531	A	2.2
1	CA	1285	A	2.2
36	BA	1847	A	2.2
36	BA	2158	A	2.2
36	DA	654(E)	G	2.2
6	CF	98	LEU	2.2
32	D6	36	LEU	2.2
57	BY	62	GLU	2.2
57	DY	5	MET	2.2
9	AI	123	PRO	2.2
10	CJ	53	PRO	2.2
48	BP	118	GLY	2.2
51	DS	109	GLY	2.2
46	BN	109	LYS	2.2
51	BS	99	LYS	2.2
53	BU	15	LYS	2.2
52	DT	51	ARG	2.2
56	BX	65	ARG	2.2
1	AA	1029	C	2.2
4	CD	112	VAL	2.2
32	D6	39	TYR	2.2
40	BE	75	VAL	2.2
4	AD	208	SER	2.2

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Mol	Chain	Res	Type	RSRZ
16	CP	33	ILE	2.2
4	AD	157	LEU	2.2
17	CQ	43	LEU	2.2
32	B6	10	LEU	2.2
4	CD	81	GLU	2.2
7	CG	73	MET	2.2
42	DG	164	GLU	2.2
3	AC	155	GLY	2.2
10	CJ	37	PRO	2.2
12	AL	23	LYS	2.2
12	AL	88	GLY	2.2
38	DC	49	GLY	2.2
40	BE	62	PRO	2.2
46	DN	70	LYS	2.2
56	BX	72	LYS	2.2
17	CQ	75	ARG	2.2
43	BH	101	ARG	2.2
56	DX	68	ARG	2.2
12	AL	92	ASP	2.2
21	AU	5	ASP	2.2
46	BN	51	PHE	2.2
51	DS	29	PHE	2.2
55	BW	94	ASP	2.2
36	DA	2790	A	2.2
1	AA	1001(A)	G	2.2
1	AA	1124	G	2.2
36	BA	274	G	2.2
9	CI	44	VAL	2.1
30	B4	50	VAL	2.1
34	B8	23	VAL	2.1
43	BH	49	VAL	2.1
36	DA	654(Q)	C	2.1
36	DA	1536	C	2.1
58	BZ	133	ILE	2.1
2	AB	98	LEU	2.1
20	AT	18	GLN	2.1
9	CI	118	LYS	2.1
12	CL	114	LYS	2.1
16	AP	27	LYS	2.1
57	BY	47	LYS	2.1
46	DN	18	ALA	2.1
28	B2	55	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
42	DG	32	PRO	2.1
52	DT	58	ASN	2.1
30	D4	49	PHE	2.1
4	CD	31	CYS	2.1
48	BP	47	ASP	2.1
9	AI	65	VAL	2.1
1	CA	1357	A	2.1
1	CA	1503	A	2.1
35	B9	24	TYR	2.1
44	BI	51	ILE	2.1
51	BS	36	TYR	2.1
44	BI	38	LEU	2.1
52	BT	6	LEU	2.1
1	AA	1312	G	2.1
25	CY	79	ALA	2.1
44	BI	67	ARG	2.1
13	CM	95	GLY	2.1
1	CA	135	C	2.1
19	CS	76	PRO	2.1
39	BD	28	GLU	2.1
58	DZ	169	GLU	2.1
23	AW	74	C	2.1
36	DA	2139	C	2.1
42	BG	70	VAL	2.1
43	BH	44	VAL	2.1
43	BH	50	VAL	2.1
43	DH	44	VAL	2.1
46	DN	50	ASP	2.1
3	CC	204	LEU	2.1
4	AD	19	LEU	2.1
20	CT	27	LYS	2.1
38	BC	190	ILE	2.1
39	DD	27	THR	2.1
42	DG	173	LEU	2.1
51	DS	21	THR	2.1
54	BV	35	LEU	2.1
57	BY	33	LYS	2.1
13	AM	11	ARG	2.1
50	DR	2	ARG	2.1
28	D2	70	GLN	2.1
51	DS	105	ALA	2.1
1	AA	1286	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	CA	1030(D)	A	2.1
3	CC	205	GLY	2.1
19	AS	68	GLY	2.1
36	BA	2119	A	2.1
44	DI	90	GLY	2.1
57	BY	64	GLU	2.1
25	CZ	39	PHE	2.1
38	DC	209	PHE	2.1
48	DP	91	PHE	2.1
1	CA	998	G	2.1
13	CM	17	VAL	2.1
13	CM	98	VAL	2.1
36	BA	2157	G	2.1
38	BC	15	VAL	2.1
44	BI	145	VAL	2.1
23	CW	16	C	2.1
36	DA	2143	C	2.1
37	BB	12	C	2.1
5	CE	78	HIS	2.1
12	AL	91	LYS	2.1
15	CO	51	HIS	2.1
42	DG	8	LYS	2.1
32	D6	54	ILE	2.1
51	BS	34	HIS	2.1
16	CP	69	THR	2.1
26	D0	74	ARG	2.1
33	D7	23	ARG	2.1
38	BC	208	THR	2.1
43	DH	69	ARG	2.1
46	DN	36	GLY	2.1
12	CL	5	PRO	2.1
18	AR	81	PHE	2.1
38	BC	227	PRO	2.1
58	BZ	68	PRO	2.1
20	CT	70	SER	2.1
39	DD	12	SER	2.1
52	DT	70	VAL	2.1
1	AA	722	A	2.1
1	CA	872	A	2.1
12	CL	47	LYS	2.1
34	D8	3	LYS	2.1
35	D9	2	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
36	DA	2892	A	2.1
37	DB	90	A	2.1
38	BC	3	LYS	2.1
44	DI	22	LYS	2.1
48	DP	108	LYS	2.1
56	DX	72	LYS	2.1
58	BZ	78	LYS	2.1
14	AN	3	ARG	2.1
16	CP	6	LEU	2.1
20	AT	84	LEU	2.1
21	AU	24	ARG	2.1
25	CZ	31	ILE	2.1
32	D6	37	ARG	2.1
52	DT	6	LEU	2.1
50	BR	3	HIS	2.1
9	CI	36	TYR	2.1
51	DS	92	TYR	2.1
1	CA	631	G	2.1
7	CG	39	ALA	2.1
36	BA	654(P)	C	2.1
36	BA	2146	C	2.1
36	DA	2108	C	2.1
12	CL	121	GLY	2.1
21	AU	16	GLY	2.1
35	D9	21	GLY	2.1
41	DF	131	GLY	2.1
6	CF	96	PRO	2.1
32	B6	24	GLU	2.1
43	DH	123	PHE	2.1
51	DS	107	GLU	2.1
18	AR	71	LYS	2.0
27	B1	96	LYS	2.0
36	DA	1033	U	2.0
57	BY	37	VAL	2.0
7	CG	42	ILE	2.0
20	AT	72	LEU	2.0
25	CZ	23	ILE	2.0
26	B0	75	LEU	2.0
26	D0	75	LEU	2.0
33	D7	41	ARG	2.0
38	BC	172	ILE	2.0
41	BF	46	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
42	DG	95	ARG	2.0
44	DI	120	ILE	2.0
48	BP	147	LEU	2.0
1	AA	975	A	2.0
1	AA	1287	A	2.0
9	AI	119	ALA	2.0
36	BA	2892	A	2.0
36	DA	2320	A	2.0
42	DG	171	ALA	2.0
48	DP	110	TYR	2.0
10	AJ	33	GLN	2.0
14	CN	14	PRO	2.0
40	DE	62	PRO	2.0
1	CA	1363	C	2.0
36	DA	654(B)	C	2.0
42	DG	15	VAL	2.0
57	BY	98	VAL	2.0
1	AA	1224	G	2.0
1	AA	1530	G	2.0
1	CA	80	G	2.0
36	BA	2154	G	2.0
36	BA	2156	G	2.0
37	BB	87	G	2.0
42	DG	96	ARG	2.0
20	CT	11	SER	2.0
23	AW	55	U	2.0
43	BH	74	ASN	2.0
25	CY	64	HIS	2.0
40	BE	66	HIS	2.0
40	DE	205	ALA	2.0
44	BI	98	ALA	2.0
3	CC	201	TYR	2.0
46	DN	3	THR	2.0
55	BW	9	TYR	2.0
25	AY	20	ASP	2.0
7	AG	133	GLY	2.0
10	CJ	10	GLY	2.0
26	B0	6	GLY	2.0
51	BS	22	GLY	2.0
17	CQ	87	LYS	2.0
48	DP	17	LYS	2.0
1	AA	1248	A	2.0

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Mol	Chain	Res	Type	RSRZ
9	AI	111	ARG	2.0
9	CI	28	VAL	2.0
13	CM	7	VAL	2.0
34	D8	54	GLU	2.0
36	BA	71	A	2.0
21	AU	15	ARG	2.0
40	BE	72	VAL	2.0
43	DH	114	VAL	2.0
3	CC	14	ILE	2.0
5	CE	11	ILE	2.0
30	B4	31	ILE	2.0
54	BV	99	ILE	2.0
1	AA	980	C	2.0
1	AA	1115	C	2.0
36	BA	2138	C	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	A2M	CX	20	23/24	0.49	0.23	168,174,200,200	0
24	A2M	AX	20	23/24	0.58	0.26	158,164,194,194	0
24	OMU	AX	19	21/22	0.73	0.22	99,130,198,198	0
24	A2M	AX	21	23/24	0.80	0.17	140,147,161,184	0
59	OMU	CX	19	21/22	0.83	0.19	117,161,200,200	0
59	A2M	CX	21	23/24	0.86	0.18	177,179,187,190	0
22	5MU	AV	54	21/22	0.91	0.11	114,133,152,153	0

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3009	1/1	-0.04	0.27	168,168,168,168	0
60	MG	CA	1667	1/1	0.01	0.62	83,83,83,83	1
60	MG	CA	1680	1/1	0.02	0.36	148,148,148,148	0
60	MG	CA	1696	1/1	0.03	0.36	162,162,162,162	0
60	MG	AA	1652	1/1	0.06	0.32	103,103,103,103	1
60	MG	CV	102	1/1	0.07	0.55	132,132,132,132	1
60	MG	CA	1678	1/1	0.07	0.25	86,86,86,86	1
60	MG	DA	2965	1/1	0.13	0.42	96,96,96,96	0
60	MG	CA	1698	1/1	0.14	0.88	145,145,145,145	0
60	MG	AA	1665	1/1	0.15	0.58	121,121,121,121	0
60	MG	AA	1636	1/1	0.16	0.39	142,142,142,142	0
60	MG	BA	3101	1/1	0.17	0.39	123,123,123,123	0
60	MG	CA	1627	1/1	0.17	0.16	162,162,162,162	0
60	MG	AA	1646	1/1	0.18	0.49	125,125,125,125	0
60	MG	BA	3089	1/1	0.18	0.34	155,155,155,155	0
60	MG	DA	3096	1/1	0.20	0.50	124,124,124,124	0
60	MG	AA	1654	1/1	0.22	0.34	139,139,139,139	0
60	MG	CA	1606	1/1	0.22	0.17	118,118,118,118	0
60	MG	BA	3030	1/1	0.23	0.55	96,96,96,96	0
60	MG	CA	1653	1/1	0.25	0.42	127,127,127,127	0
60	MG	AA	1662	1/1	0.25	0.55	127,127,127,127	0
60	MG	AA	1612	1/1	0.26	0.32	102,102,102,102	0
60	MG	BA	3053	1/1	0.28	0.38	122,122,122,122	0
60	MG	CA	1699	1/1	0.30	0.32	134,134,134,134	0
60	MG	CA	1650	1/1	0.31	0.51	127,127,127,127	0
60	MG	BA	2995	1/1	0.33	0.34	105,105,105,105	0
60	MG	CA	1665	1/1	0.33	0.21	111,111,111,111	1
60	MG	AA	1620	1/1	0.33	0.30	134,134,134,134	0
60	MG	DA	3097	1/1	0.33	0.34	112,112,112,112	0
60	MG	DA	3078	1/1	0.34	0.42	122,122,122,122	0
60	MG	CA	1670	1/1	0.35	0.19	153,153,153,153	0
60	MG	BB	202	1/1	0.35	0.43	117,117,117,117	0
60	MG	CA	1637	1/1	0.35	0.28	141,141,141,141	0
60	MG	AA	1651	1/1	0.35	0.22	113,113,113,113	0
60	MG	AA	1634	1/1	0.36	0.49	120,120,120,120	0
60	MG	CA	1647	1/1	0.37	0.12	97,97,97,97	0
60	MG	DA	3098	1/1	0.37	0.25	107,107,107,107	0
60	MG	BB	201	1/1	0.38	0.26	84,84,84,84	0
60	MG	CA	1603	1/1	0.39	0.33	113,113,113,113	0
60	MG	BA	3017	1/1	0.39	0.12	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1623	1/1	0.41	0.19	100,100,100,100	0
60	MG	BA	3107	1/1	0.41	0.32	87,87,87,87	0
60	MG	DA	3041	1/1	0.42	0.54	154,154,154,154	0
60	MG	BA	3078	1/1	0.43	0.28	104,104,104,104	0
60	MG	DA	3048	1/1	0.43	0.42	129,129,129,129	0
60	MG	CA	1651	1/1	0.44	0.16	144,144,144,144	0
60	MG	DA	3018	1/1	0.44	0.23	114,114,114,114	0
60	MG	BA	2942	1/1	0.44	0.48	107,107,107,107	0
60	MG	BA	3094	1/1	0.44	0.23	100,100,100,100	0
60	MG	BA	3114	1/1	0.45	0.60	130,130,130,130	0
60	MG	AA	1672	1/1	0.46	0.48	136,136,136,136	0
60	MG	AA	1674	1/1	0.47	0.33	87,87,87,87	1
60	MG	DA	3029	1/1	0.47	0.59	99,99,99,99	0
60	MG	CA	1691	1/1	0.48	0.34	105,105,105,105	0
60	MG	BA	3031	1/1	0.48	0.36	108,108,108,108	0
60	MG	AA	1604	1/1	0.48	0.23	132,132,132,132	0
60	MG	CA	1662	1/1	0.48	0.43	113,113,113,113	0
60	MG	BA	3090	1/1	0.48	0.72	123,123,123,123	0
60	MG	CA	1640	1/1	0.49	0.20	102,102,102,102	0
60	MG	BA	3100	1/1	0.49	0.19	117,117,117,117	0
60	MG	AA	1657	1/1	0.49	0.33	121,121,121,121	0
60	MG	CA	1664	1/1	0.49	0.27	112,112,112,112	0
60	MG	DA	3115	1/1	0.50	0.18	162,162,162,162	0
60	MG	CA	1692	1/1	0.51	0.25	117,117,117,117	0
60	MG	CA	1607	1/1	0.51	0.19	101,101,101,101	0
60	MG	DA	3075	1/1	0.51	0.38	75,75,75,75	0
60	MG	DA	3004	1/1	0.51	0.34	113,113,113,113	0
60	MG	BA	2920	1/1	0.52	0.57	98,98,98,98	0
60	MG	DA	2980	1/1	0.52	0.40	111,111,111,111	0
60	MG	AA	1618	1/1	0.53	0.13	121,121,121,121	0
60	MG	BA	3080	1/1	0.53	0.41	115,115,115,115	0
60	MG	AA	1637	1/1	0.53	0.34	99,99,99,99	0
60	MG	BA	2978	1/1	0.54	0.22	134,134,134,134	0
60	MG	BA	3047	1/1	0.54	0.27	105,105,105,105	0
60	MG	BA	3007	1/1	0.54	0.16	125,125,125,125	0
60	MG	DA	3106	1/1	0.54	0.54	143,143,143,143	0
60	MG	DA	3003	1/1	0.54	0.45	69,69,69,69	1
60	MG	DA	3068	1/1	0.55	0.47	102,102,102,102	0
60	MG	DA	3099	1/1	0.55	0.30	108,108,108,108	0
60	MG	DA	3071	1/1	0.55	0.53	123,123,123,123	0
60	MG	CA	1688	1/1	0.55	0.37	103,103,103,103	0
60	MG	AA	1633	1/1	0.56	0.17	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1697	1/1	0.56	0.28	126,126,126,126	0
60	MG	CA	1687	1/1	0.56	0.24	119,119,119,119	0
60	MG	CA	1655	1/1	0.56	0.30	111,111,111,111	0
60	MG	BA	2983	1/1	0.56	0.29	108,108,108,108	0
60	MG	BA	2987	1/1	0.56	0.40	100,100,100,100	0
60	MG	CA	1612	1/1	0.57	0.21	102,102,102,102	0
60	MG	DA	3055	1/1	0.57	0.21	106,106,106,106	0
60	MG	CA	1663	1/1	0.57	0.18	121,121,121,121	0
60	MG	BA	3084	1/1	0.57	0.29	126,126,126,126	0
60	MG	DA	3100	1/1	0.57	0.36	113,113,113,113	0
60	MG	DA	3103	1/1	0.57	0.12	82,82,82,82	0
60	MG	CA	1611	1/1	0.57	0.26	97,97,97,97	0
60	MG	CA	1659	1/1	0.57	0.23	104,104,104,104	1
60	MG	AA	1677	1/1	0.58	0.22	114,114,114,114	0
60	MG	AA	1691	1/1	0.58	0.21	96,96,96,96	0
60	MG	CA	1604	1/1	0.58	0.46	115,115,115,115	0
60	MG	AA	1613	1/1	0.58	0.48	114,114,114,114	0
60	MG	CA	1685	1/1	0.58	0.16	115,115,115,115	0
60	MG	BA	3009	1/1	0.58	0.43	117,117,117,117	0
60	MG	DA	3010	1/1	0.59	0.28	92,92,92,92	0
60	MG	CA	1624	1/1	0.59	0.45	119,119,119,119	0
60	MG	AA	1675	1/1	0.59	0.23	93,93,93,93	0
60	MG	AA	1699	1/1	0.59	0.21	109,109,109,109	0
60	MG	AA	1650	1/1	0.59	0.27	111,111,111,111	0
60	MG	DA	2901	1/1	0.59	0.41	136,136,136,136	0
60	MG	DA	3094	1/1	0.60	0.16	87,87,87,87	0
60	MG	BA	2921	1/1	0.60	0.26	98,98,98,98	0
60	MG	BA	3001	1/1	0.60	0.32	157,157,157,157	0
60	MG	DA	3058	1/1	0.60	0.28	104,104,104,104	0
60	MG	DA	2963	1/1	0.60	0.29	70,70,70,70	0
60	MG	BA	3006	1/1	0.60	0.37	91,91,91,91	0
60	MG	AA	1671	1/1	0.60	0.39	96,96,96,96	0
60	MG	BA	2977	1/1	0.60	0.38	107,107,107,107	0
60	MG	DA	3083	1/1	0.60	0.36	112,112,112,112	0
60	MG	CA	1700	1/1	0.61	0.35	113,113,113,113	0
60	MG	CA	1643	1/1	0.61	0.21	105,105,105,105	0
60	MG	BA	2901	1/1	0.61	0.50	145,145,145,145	0
60	MG	AA	1700	1/1	0.61	0.48	111,111,111,111	0
60	MG	BA	2952	1/1	0.61	0.33	87,87,87,87	0
60	MG	AA	1660	1/1	0.62	0.22	105,105,105,105	0
60	MG	BA	2949	1/1	0.62	0.37	77,77,77,77	0
60	MG	BA	3088	1/1	0.62	0.18	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1641	1/1	0.62	0.40	93,93,93,93	0
60	MG	BA	3077	1/1	0.63	0.28	84,84,84,84	0
60	MG	DA	3019	1/1	0.63	0.36	112,112,112,112	0
60	MG	DA	2985	1/1	0.63	0.25	85,85,85,85	0
60	MG	AA	1667	1/1	0.63	0.41	118,118,118,118	0
60	MG	AA	1676	1/1	0.63	0.28	104,104,104,104	0
60	MG	BA	3128	1/1	0.63	0.19	117,117,117,117	0
60	MG	CA	1652	1/1	0.63	0.38	148,148,148,148	0
60	MG	BA	2902	1/1	0.64	0.16	155,155,155,155	0
60	MG	BA	3091	1/1	0.64	0.39	79,79,79,79	0
60	MG	BA	3018	1/1	0.64	0.33	109,109,109,109	0
60	MG	CA	1681	1/1	0.64	0.21	113,113,113,113	1
60	MG	AA	1655	1/1	0.64	0.27	94,94,94,94	1
60	MG	CA	1609	1/1	0.64	0.17	84,84,84,84	0
60	MG	AA	1670	1/1	0.64	0.24	130,130,130,130	0
60	MG	DA	3081	1/1	0.64	0.29	104,104,104,104	0
60	MG	DA	3045	1/1	0.64	0.38	104,104,104,104	0
60	MG	BA	3126	1/1	0.65	0.57	131,131,131,131	0
60	MG	AA	1603	1/1	0.65	0.39	94,94,94,94	0
60	MG	CA	1703	1/1	0.65	0.27	107,107,107,107	0
60	MG	AA	1622	1/1	0.65	0.21	128,128,128,128	0
60	MG	BA	3065	1/1	0.65	0.35	122,122,122,122	0
60	MG	BA	2990	1/1	0.65	0.29	81,81,81,81	0
60	MG	BA	3106	1/1	0.66	0.30	97,97,97,97	0
60	MG	DA	3057	1/1	0.66	0.40	92,92,92,92	0
60	MG	BA	2991	1/1	0.66	0.38	122,122,122,122	0
60	MG	AA	1627	1/1	0.66	0.30	101,101,101,101	0
60	MG	DA	2984	1/1	0.66	0.37	120,120,120,120	0
60	MG	DA	2953	1/1	0.66	0.28	65,65,65,65	0
60	MG	DA	3137	1/1	0.66	0.26	121,121,121,121	0
60	MG	BA	2988	1/1	0.67	0.44	117,117,117,117	0
60	MG	BA	3050	1/1	0.67	0.30	116,116,116,116	0
60	MG	DA	2964	1/1	0.67	0.48	109,109,109,109	0
60	MG	AA	1643	1/1	0.67	0.53	106,106,106,106	0
60	MG	BA	2960	1/1	0.67	0.33	105,105,105,105	0
60	MG	CA	1644	1/1	0.67	0.29	94,94,94,94	0
60	MG	CA	1668	1/1	0.67	0.18	93,93,93,93	0
60	MG	BA	3045	1/1	0.67	0.20	88,88,88,88	0
60	MG	CA	1676	1/1	0.67	0.17	119,119,119,119	0
60	MG	AX	101	1/1	0.68	0.43	96,96,96,96	0
60	MG	CA	1634	1/1	0.68	0.14	122,122,122,122	0
60	MG	AA	1642	1/1	0.68	0.25	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	2989	1/1	0.68	0.38	87,87,87,87	0
60	MG	BA	2930	1/1	0.68	0.53	117,117,117,117	0
60	MG	BA	3051	1/1	0.68	0.39	72,72,72,72	0
60	MG	CA	1666	1/1	0.68	0.51	137,137,137,137	1
60	MG	BA	3115	1/1	0.68	0.37	85,85,85,85	0
60	MG	AV	101	1/1	0.68	0.40	83,83,83,83	1
60	MG	DA	3056	1/1	0.68	0.25	126,126,126,126	0
60	MG	BA	2912	1/1	0.68	0.38	71,71,71,71	0
60	MG	BA	2999	1/1	0.68	0.33	121,121,121,121	0
60	MG	CA	1626	1/1	0.68	0.39	102,102,102,102	0
60	MG	DA	3008	1/1	0.68	0.24	92,92,92,92	0
60	MG	CA	1674	1/1	0.69	0.29	137,137,137,137	0
60	MG	AA	1695	1/1	0.69	0.29	105,105,105,105	0
60	MG	BA	2985	1/1	0.69	0.18	87,87,87,87	0
60	MG	BA	2954	1/1	0.69	0.31	66,66,66,66	0
60	MG	AA	1703	1/1	0.69	0.53	102,102,102,102	0
60	MG	AA	1697	1/1	0.69	0.40	127,127,127,127	0
60	MG	DA	2969	1/1	0.69	0.43	84,84,84,84	0
60	MG	AA	1635	1/1	0.69	0.15	111,111,111,111	0
60	MG	DA	3104	1/1	0.69	0.41	118,118,118,118	0
60	MG	DA	2981	1/1	0.69	0.23	105,105,105,105	0
60	MG	CA	1672	1/1	0.69	0.38	109,109,109,109	0
60	MG	DA	3117	1/1	0.69	0.39	123,123,123,123	0
60	MG	DA	3044	1/1	0.69	0.26	79,79,79,79	0
60	MG	DA	3047	1/1	0.70	0.43	112,112,112,112	0
60	MG	BA	2994	1/1	0.70	0.15	77,77,77,77	0
60	MG	BA	3073	1/1	0.70	0.26	100,100,100,100	0
60	MG	B0	101	1/1	0.70	0.36	98,98,98,98	0
60	MG	DA	3017	1/1	0.70	0.07	97,97,97,97	0
60	MG	BA	2955	1/1	0.70	0.60	109,109,109,109	0
60	MG	DA	3059	1/1	0.70	0.38	110,110,110,110	0
60	MG	DA	3063	1/1	0.70	0.39	94,94,94,94	0
60	MG	AA	1668	1/1	0.70	0.33	109,109,109,109	0
60	MG	BA	3025	1/1	0.70	0.36	95,95,95,95	0
60	MG	DA	2929	1/1	0.70	0.39	94,94,94,94	0
60	MG	BA	2953	1/1	0.70	0.42	113,113,113,113	0
60	MG	DA	3122	1/1	0.70	0.55	79,79,79,79	0
60	MG	DA	3124	1/1	0.70	0.33	98,98,98,98	0
60	MG	BA	3064	1/1	0.70	0.33	86,86,86,86	0
60	MG	BA	3011	1/1	0.71	0.45	106,106,106,106	0
60	MG	AA	1629	1/1	0.71	0.16	65,65,65,65	1
60	MG	BA	3062	1/1	0.71	0.16	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3023	1/1	0.71	0.38	103,103,103,103	0
60	MG	BA	3098	1/1	0.71	0.36	89,89,89,89	0
60	MG	BA	3044	1/1	0.71	0.22	108,108,108,108	0
60	MG	CA	1615	1/1	0.71	0.42	127,127,127,127	0
60	MG	CA	1620	1/1	0.71	0.40	115,115,115,115	0
60	MG	BA	3120	1/1	0.71	0.30	111,111,111,111	0
60	MG	BA	3066	1/1	0.72	0.28	113,113,113,113	0
60	MG	CA	1630	1/1	0.72	0.13	105,105,105,105	0
60	MG	BA	3072	1/1	0.72	0.41	89,89,89,89	0
60	MG	AA	1678	1/1	0.72	0.26	121,121,121,121	0
60	MG	AA	1685	1/1	0.72	0.22	66,66,66,66	0
60	MG	AA	1601	1/1	0.72	0.33	100,100,100,100	0
60	MG	AA	1639	1/1	0.72	0.17	98,98,98,98	1
60	MG	DA	2991	1/1	0.72	0.31	126,126,126,126	0
60	MG	BA	2976	1/1	0.72	0.31	66,66,66,66	0
60	MG	DA	3080	1/1	0.72	0.44	130,130,130,130	0
60	MG	BA	3102	1/1	0.72	0.30	108,108,108,108	0
60	MG	BX	101	1/1	0.72	0.42	110,110,110,110	1
60	MG	AA	1615	1/1	0.72	0.30	84,84,84,84	0
60	MG	DA	3141	1/1	0.72	0.26	92,92,92,92	0
60	MG	DX	101	1/1	0.72	0.34	72,72,72,72	1
60	MG	DA	2990	1/1	0.73	0.41	88,88,88,88	0
60	MG	CG	201	1/1	0.73	0.19	83,83,83,83	1
60	MG	DA	3050	1/1	0.73	0.62	105,105,105,105	0
60	MG	BA	3070	1/1	0.73	0.43	118,118,118,118	0
60	MG	BA	2937	1/1	0.73	0.44	70,70,70,70	0
60	MG	AA	1649	1/1	0.73	0.42	124,124,124,124	0
60	MG	DA	2951	1/1	0.73	0.47	91,91,91,91	0
60	MG	CA	1625	1/1	0.73	0.25	96,96,96,96	0
60	MG	BA	2956	1/1	0.73	0.31	64,64,64,64	0
60	MG	BA	3033	1/1	0.73	0.24	92,92,92,92	0
60	MG	CA	1671	1/1	0.73	0.12	95,95,95,95	0
60	MG	BA	2908	1/1	0.73	0.35	103,103,103,103	0
60	MG	CA	1632	1/1	0.73	0.15	79,79,79,79	0
60	MG	BA	2923	1/1	0.73	0.26	78,78,78,78	0
60	MG	BA	3130	1/1	0.73	0.25	111,111,111,111	0
60	MG	AA	1689	1/1	0.73	0.13	98,98,98,98	0
60	MG	BA	3022	1/1	0.74	0.43	125,125,125,125	0
60	MG	BA	3058	1/1	0.74	0.33	88,88,88,88	0
60	MG	BA	2974	1/1	0.74	0.48	68,68,68,68	0
60	MG	BA	2906	1/1	0.74	0.23	100,100,100,100	0
60	MG	CA	1608	1/1	0.74	0.11	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3022	1/1	0.74	0.25	81,81,81,81	0
60	MG	AA	1602	1/1	0.74	0.47	131,131,131,131	0
60	MG	AA	1659	1/1	0.74	0.39	113,113,113,113	0
60	MG	AA	1688	1/1	0.74	0.50	113,113,113,113	0
60	MG	BA	3015	1/1	0.74	0.38	94,94,94,94	0
60	MG	BA	2970	1/1	0.74	0.52	86,86,86,86	0
60	MG	DA	2942	1/1	0.74	0.42	90,90,90,90	0
60	MG	BA	2972	1/1	0.74	0.44	76,76,76,76	0
60	MG	DA	3090	1/1	0.74	0.21	106,106,106,106	0
60	MG	BA	3020	1/1	0.74	0.31	103,103,103,103	0
60	MG	BA	2982	1/1	0.75	0.28	100,100,100,100	0
60	MG	AA	1626	1/1	0.75	0.22	99,99,99,99	0
60	MG	AA	1608	1/1	0.75	0.27	81,81,81,81	0
60	MG	DA	3030	1/1	0.75	0.22	101,101,101,101	0
60	MG	BA	3103	1/1	0.75	0.35	107,107,107,107	0
60	MG	DA	3006	1/1	0.75	0.30	65,65,65,65	0
60	MG	DA	3007	1/1	0.75	0.21	82,82,82,82	0
60	MG	CA	1686	1/1	0.75	0.26	94,94,94,94	0
60	MG	BA	3005	1/1	0.75	0.37	85,85,85,85	0
60	MG	CA	1623	1/1	0.75	0.21	82,82,82,82	0
60	MG	DA	3088	1/1	0.75	0.41	110,110,110,110	0
60	MG	DA	3127	1/1	0.75	0.46	112,112,112,112	0
60	MG	DA	3128	1/1	0.75	0.39	92,92,92,92	0
60	MG	BA	3032	1/1	0.75	0.37	98,98,98,98	0
60	MG	BA	3134	1/1	0.75	0.35	75,75,75,75	0
60	MG	DR	201	1/1	0.75	0.35	117,117,117,117	0
60	MG	BA	3135	1/1	0.75	0.20	83,83,83,83	0
60	MG	CA	1677	1/1	0.76	0.30	88,88,88,88	0
60	MG	BA	2940	1/1	0.76	0.39	64,64,64,64	0
60	MG	D1	101	1/1	0.76	0.41	92,92,92,92	0
60	MG	CA	1660	1/1	0.76	0.41	95,95,95,95	0
60	MG	CA	1661	1/1	0.76	0.19	81,81,81,81	0
60	MG	BA	3002	1/1	0.76	0.46	97,97,97,97	0
60	MG	AA	1638	1/1	0.76	0.54	139,139,139,139	1
60	MG	CA	1638	1/1	0.76	0.27	81,81,81,81	0
60	MG	BA	3054	1/1	0.76	0.37	94,94,94,94	0
60	MG	CA	1617	1/1	0.76	0.10	93,93,93,93	0
60	MG	BA	2945	1/1	0.76	0.41	73,73,73,73	0
60	MG	AA	1653	1/1	0.76	0.19	94,94,94,94	0
60	MG	AA	1645	1/1	0.76	0.29	99,99,99,99	0
60	MG	DA	3028	1/1	0.76	0.28	123,123,123,123	0
60	MG	AA	1679	1/1	0.76	0.34	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1682	1/1	0.76	0.27	98,98,98,98	0
60	MG	DA	3031	1/1	0.76	0.40	92,92,92,92	0
60	MG	DA	3142	1/1	0.76	0.25	81,81,81,81	0
60	MG	AA	1624	1/1	0.76	0.22	111,111,111,111	0
60	MG	AA	1686	1/1	0.76	0.36	99,99,99,99	0
60	MG	AA	1690	1/1	0.77	0.34	96,96,96,96	0
60	MG	BA	3052	1/1	0.77	0.27	99,99,99,99	0
60	MG	AA	1611	1/1	0.77	0.26	82,82,82,82	0
60	MG	AA	1607	1/1	0.77	0.16	107,107,107,107	0
60	MG	BP	201	1/1	0.77	0.22	71,71,71,71	0
60	MG	BA	2946	1/1	0.77	0.20	66,66,66,66	0
60	MG	AA	1681	1/1	0.77	0.32	99,99,99,99	0
60	MG	BA	3109	1/1	0.77	0.30	101,101,101,101	0
60	MG	BA	3037	1/1	0.77	0.39	79,79,79,79	0
60	MG	BA	2962	1/1	0.77	0.35	64,64,64,64	0
60	MG	CA	1702	1/1	0.77	0.27	96,96,96,96	0
60	MG	BA	2965	1/1	0.77	0.32	111,111,111,111	0
60	MG	BA	2950	1/1	0.77	0.33	81,81,81,81	0
60	MG	DA	2989	1/1	0.77	0.35	79,79,79,79	0
60	MG	BA	3096	1/1	0.77	0.16	84,84,84,84	0
60	MG	AA	1609	1/1	0.77	0.24	106,106,106,106	0
60	MG	DA	3037	1/1	0.77	0.25	74,74,74,74	0
60	MG	DA	2993	1/1	0.77	0.30	79,79,79,79	0
60	MG	DA	2999	1/1	0.77	0.12	94,94,94,94	0
60	MG	DA	3093	1/1	0.77	0.32	86,86,86,86	0
60	MG	CA	1682	1/1	0.78	0.12	151,151,151,151	0
60	MG	CA	1633	1/1	0.78	0.20	93,93,93,93	0
60	MG	DA	3042	1/1	0.78	0.15	81,81,81,81	0
60	MG	DA	3043	1/1	0.78	0.19	96,96,96,96	0
60	MG	BA	2914	1/1	0.78	0.31	83,83,83,83	0
60	MG	BA	3069	1/1	0.78	0.14	87,87,87,87	0
60	MG	BA	3046	1/1	0.78	0.33	112,112,112,112	0
60	MG	BA	2931	1/1	0.78	0.37	72,72,72,72	0
60	MG	CA	1642	1/1	0.78	0.25	97,97,97,97	0
60	MG	CA	1694	1/1	0.78	0.33	112,112,112,112	0
60	MG	BA	3026	1/1	0.78	0.15	85,85,85,85	0
60	MG	BA	3076	1/1	0.78	0.53	108,108,108,108	0
60	MG	BA	3063	1/1	0.78	0.12	136,136,136,136	0
60	MG	BA	3028	1/1	0.78	0.25	89,89,89,89	0
60	MG	AA	1647	1/1	0.78	0.27	104,104,104,104	0
60	MG	DA	2903	1/1	0.79	0.39	85,85,85,85	0
60	MG	AA	1666	1/1	0.79	0.23	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	BA	3016	1/1	0.79	0.12	102,102,102,102	0
60	MG	DA	3027	1/1	0.79	0.34	92,92,92,92	0
60	MG	CA	1631	1/1	0.79	0.34	111,111,111,111	0
60	MG	BF	301	1/1	0.79	0.25	100,100,100,100	0
60	MG	DA	2956	1/1	0.79	0.31	63,63,63,63	0
60	MG	BA	3124	1/1	0.79	0.18	120,120,120,120	0
60	MG	DA	3034	1/1	0.79	0.23	72,72,72,72	0
60	MG	DA	3072	1/1	0.79	0.23	102,102,102,102	0
60	MG	CA	1684	1/1	0.79	0.20	101,101,101,101	0
60	MG	AA	1640	1/1	0.79	0.14	64,64,64,64	1
60	MG	BA	3035	1/1	0.79	0.14	86,86,86,86	0
60	MG	BA	3129	1/1	0.79	0.24	84,84,84,84	0
60	MG	BA	3082	1/1	0.79	0.30	101,101,101,101	0
60	MG	DA	3013	1/1	0.79	0.41	89,89,89,89	0
60	MG	DA	3046	1/1	0.79	0.39	76,76,76,76	0
60	MG	BA	2966	1/1	0.79	0.16	92,92,92,92	0
60	MG	BA	2968	1/1	0.79	0.36	72,72,72,72	0
60	MG	DA	2952	1/1	0.80	0.22	56,56,56,56	0
60	MG	AA	1658	1/1	0.80	0.42	92,92,92,92	0
60	MG	CA	1629	1/1	0.80	0.45	95,95,95,95	0
60	MG	DA	2957	1/1	0.80	0.20	66,66,66,66	0
60	MG	DA	2960	1/1	0.80	0.31	59,59,59,59	0
60	MG	AA	1616	1/1	0.80	0.28	84,84,84,84	0
60	MG	CA	1622	1/1	0.80	0.15	93,93,93,93	0
60	MG	BA	3023	1/1	0.80	0.45	79,79,79,79	0
60	MG	BA	2986	1/1	0.80	0.30	81,81,81,81	0
60	MG	CA	1613	1/1	0.80	0.19	89,89,89,89	0
60	MG	CA	1636	1/1	0.80	0.26	90,90,90,90	0
60	MG	BA	3014	1/1	0.80	0.27	74,74,74,74	0
60	MG	DA	2949	1/1	0.81	0.42	102,102,102,102	0
60	MG	AA	1621	1/1	0.81	0.21	95,95,95,95	0
60	MG	BA	2963	1/1	0.81	0.38	103,103,103,103	0
60	MG	BA	3085	1/1	0.81	0.40	118,118,118,118	0
60	MG	CA	1675	1/1	0.81	0.10	122,122,122,122	0
60	MG	BA	3086	1/1	0.81	0.23	114,114,114,114	0
60	MG	BA	3008	1/1	0.81	0.35	96,96,96,96	0
60	MG	DA	3049	1/1	0.81	0.43	85,85,85,85	0
60	MG	BA	2975	1/1	0.81	0.28	92,92,92,92	0
60	MG	BA	2996	1/1	0.81	0.78	106,106,106,106	0
60	MG	BA	3110	1/1	0.81	0.72	101,101,101,101	0
60	MG	DA	3105	1/1	0.81	0.22	93,93,93,93	0
60	MG	AA	1684	1/1	0.81	0.40	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	2972	1/1	0.81	0.21	100,100,100,100	0
60	MG	AA	1632	1/1	0.81	0.37	75,75,75,75	0
60	MG	BA	2957	1/1	0.81	0.24	63,63,63,63	0
60	MG	BA	3123	1/1	0.81	0.19	80,80,80,80	0
60	MG	BA	3097	1/1	0.81	0.21	88,88,88,88	0
60	MG	DA	2926	1/1	0.81	0.26	47,47,47,47	0
60	MG	DA	3135	1/1	0.81	0.23	103,103,103,103	0
60	MG	AA	1628	1/1	0.81	0.25	87,87,87,87	0
60	MG	DA	3033	1/1	0.81	0.18	100,100,100,100	0
60	MG	DA	2932	1/1	0.81	0.34	64,64,64,64	0
60	MG	DA	2940	1/1	0.81	0.34	72,72,72,72	0
60	MG	CA	1628	1/1	0.81	0.29	66,66,66,66	0
60	MG	DA	2998	1/1	0.82	0.25	91,91,91,91	0
60	MG	BA	3024	1/1	0.82	0.26	96,96,96,96	0
60	MG	DA	2975	1/1	0.82	0.60	138,138,138,138	0
60	MG	BA	3095	1/1	0.82	0.12	97,97,97,97	0
60	MG	BA	3104	1/1	0.82	0.13	115,115,115,115	0
60	MG	AA	1694	1/1	0.82	0.29	102,102,102,102	0
60	MG	BA	3004	1/1	0.82	0.24	63,63,63,63	0
60	MG	CA	1658	1/1	0.82	0.16	93,93,93,93	0
60	MG	BA	2905	1/1	0.82	0.27	58,58,58,58	0
60	MG	DA	3011	1/1	0.82	0.10	88,88,88,88	0
60	MG	DA	3038	1/1	0.82	0.46	77,77,77,77	0
60	MG	BA	3083	1/1	0.82	0.19	87,87,87,87	0
60	MG	AA	1656	1/1	0.82	0.11	140,140,140,140	0
60	MG	DA	2994	1/1	0.82	0.36	52,52,52,52	0
60	MG	DA	2996	1/1	0.82	0.15	63,63,63,63	0
60	MG	BA	3059	1/1	0.83	0.23	95,95,95,95	0
60	MG	DA	3024	1/1	0.83	0.40	106,106,106,106	0
60	MG	DA	3114	1/1	0.83	0.41	96,96,96,96	0
60	MG	CA	1654	1/1	0.83	0.14	107,107,107,107	0
60	MG	CA	1690	1/1	0.83	0.25	100,100,100,100	0
60	MG	DA	3060	1/1	0.83	0.44	107,107,107,107	0
60	MG	BA	3121	1/1	0.83	0.25	112,112,112,112	0
60	MG	BA	3079	1/1	0.83	0.23	72,72,72,72	0
60	MG	CA	1639	1/1	0.83	0.21	99,99,99,99	0
60	MG	DA	3132	1/1	0.83	0.26	120,120,120,120	0
60	MG	DA	3000	1/1	0.83	0.27	77,77,77,77	0
60	MG	DA	3136	1/1	0.83	0.11	94,94,94,94	0
60	MG	BA	2935	1/1	0.83	0.31	110,110,110,110	0
60	MG	DA	3076	1/1	0.83	0.21	119,119,119,119	0
60	MG	DA	3102	1/1	0.83	0.22	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DF	301	1/1	0.83	0.12	100,100,100,100	0
60	MG	DA	2944	1/1	0.83	0.25	74,74,74,74	0
60	MG	BA	3038	1/1	0.83	0.25	90,90,90,90	0
60	MG	BA	3108	1/1	0.84	0.28	102,102,102,102	0
60	MG	DA	3092	1/1	0.84	0.18	86,86,86,86	0
60	MG	BA	3136	1/1	0.84	0.40	106,106,106,106	0
60	MG	DA	2992	1/1	0.84	0.20	75,75,75,75	0
60	MG	BA	2948	1/1	0.84	0.25	67,67,67,67	0
60	MG	BA	2973	1/1	0.84	0.26	92,92,92,92	0
60	MG	BA	2944	1/1	0.84	0.26	58,58,58,58	0
60	MG	DA	2909	1/1	0.84	0.43	55,55,55,55	0
60	MG	DA	3077	1/1	0.84	0.15	96,96,96,96	0
60	MG	CA	1641	1/1	0.84	0.52	94,94,94,94	0
60	MG	BA	3075	1/1	0.84	0.31	100,100,100,100	0
60	MG	BA	2916	1/1	0.84	0.26	71,71,71,71	0
60	MG	DA	3082	1/1	0.84	0.18	77,77,77,77	0
60	MG	DA	2986	1/1	0.84	0.27	87,87,87,87	0
60	MG	BA	2925	1/1	0.84	0.22	97,97,97,97	0
60	MG	BA	2993	1/1	0.85	0.54	92,92,92,92	0
60	MG	AA	1617	1/1	0.85	0.40	104,104,104,104	0
60	MG	DA	2954	1/1	0.85	0.16	57,57,57,57	0
60	MG	AA	1631	1/1	0.85	0.44	87,87,87,87	0
60	MG	BA	3132	1/1	0.85	0.28	116,116,116,116	0
60	MG	DA	3032	1/1	0.85	0.18	67,67,67,67	0
60	MG	DA	3123	1/1	0.85	0.38	82,82,82,82	0
60	MG	AA	1663	1/1	0.85	0.32	83,83,83,83	0
60	MG	DA	3125	1/1	0.85	0.28	72,72,72,72	0
60	MG	CA	1683	1/1	0.85	0.08	93,93,93,93	0
60	MG	DA	3035	1/1	0.85	0.42	105,105,105,105	0
60	MG	BA	2919	1/1	0.85	0.34	75,75,75,75	0
60	MG	DA	3134	1/1	0.85	0.40	89,89,89,89	0
60	MG	DA	3061	1/1	0.85	0.33	94,94,94,94	0
60	MG	DA	3015	1/1	0.85	0.19	76,76,76,76	0
60	MG	DA	2935	1/1	0.85	0.42	68,68,68,68	0
60	MG	BA	3057	1/1	0.85	0.28	73,73,73,73	0
60	MG	CA	1673	1/1	0.85	0.20	116,116,116,116	0
60	MG	BA	3019	1/1	0.85	0.23	74,74,74,74	0
60	MG	BA	2938	1/1	0.85	0.24	67,67,67,67	0
60	MG	BA	2927	1/1	0.85	0.34	59,59,59,59	0
60	MG	BA	2932	1/1	0.86	0.31	61,61,61,61	0
60	MG	AA	1614	1/1	0.86	0.35	98,98,98,98	0
60	MG	DA	2961	1/1	0.86	0.29	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1693	1/1	0.86	0.34	119,119,119,119	0
60	MG	DA	3016	1/1	0.86	0.18	83,83,83,83	0
60	MG	DA	3091	1/1	0.86	0.35	107,107,107,107	0
60	MG	AA	1605	1/1	0.86	0.24	66,66,66,66	0
60	MG	BA	2939	1/1	0.86	0.29	50,50,50,50	0
60	MG	CA	1614	1/1	0.86	0.12	87,87,87,87	0
60	MG	DA	3067	1/1	0.86	0.25	52,52,52,52	0
60	MG	BA	3093	1/1	0.86	0.40	99,99,99,99	0
60	MG	DA	3069	1/1	0.86	0.29	73,73,73,73	0
60	MG	BA	3068	1/1	0.86	0.46	103,103,103,103	0
60	MG	DA	2950	1/1	0.86	0.26	55,55,55,55	0
60	MG	DA	3140	1/1	0.86	0.40	77,77,77,77	0
60	MG	BA	3055	1/1	0.86	0.43	87,87,87,87	0
60	MG	BA	2929	1/1	0.86	0.29	65,65,65,65	0
60	MG	B1	101	1/1	0.86	0.26	113,113,113,113	0
60	MG	AA	1687	1/1	0.86	0.20	74,74,74,74	0
60	MG	DA	2921	1/1	0.86	0.45	49,49,49,49	0
60	MG	DA	2918	1/1	0.87	0.31	59,59,59,59	0
60	MG	DA	2979	1/1	0.87	0.11	57,57,57,57	0
60	MG	CA	1616	1/1	0.87	0.14	105,105,105,105	0
60	MG	BA	2933	1/1	0.87	0.28	77,77,77,77	0
60	MG	BA	3049	1/1	0.87	0.28	65,65,65,65	0
60	MG	BA	3010	1/1	0.87	0.24	88,88,88,88	0
60	MG	BA	2984	1/1	0.87	0.34	95,95,95,95	0
60	MG	BA	3071	1/1	0.87	0.22	61,61,61,61	0
60	MG	DA	3066	1/1	0.87	0.38	102,102,102,102	0
60	MG	CA	1646	1/1	0.87	0.26	119,119,119,119	0
60	MG	BA	3113	1/1	0.87	0.29	126,126,126,126	0
60	MG	BA	2913	1/1	0.87	0.30	59,59,59,59	0
60	MG	BA	2947	1/1	0.87	0.31	88,88,88,88	0
60	MG	BA	3074	1/1	0.87	0.24	104,104,104,104	0
60	MG	BA	3000	1/1	0.87	0.20	52,52,52,52	1
60	MG	AA	1661	1/1	0.87	0.39	94,94,94,94	0
60	MG	AA	1664	1/1	0.87	0.26	90,90,90,90	0
60	MG	AA	1698	1/1	0.87	0.50	80,80,80,80	0
60	MG	DA	3002	1/1	0.87	0.12	95,95,95,95	0
60	MG	BA	2909	1/1	0.87	0.34	64,64,64,64	0
60	MG	BA	3039	1/1	0.87	0.34	67,67,67,67	0
60	MG	AA	1669	1/1	0.87	0.17	96,96,96,96	0
60	MG	DA	2962	1/1	0.87	0.35	89,89,89,89	0
60	MG	BA	2992	1/1	0.87	0.30	61,61,61,61	0
60	MG	DA	2907	1/1	0.87	0.35	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	2922	1/1	0.87	0.51	53,53,53,53	0
60	MG	DA	2911	1/1	0.87	0.22	62,62,62,62	0
60	MG	DA	2970	1/1	0.87	0.08	47,47,47,47	0
60	MG	DA	2913	1/1	0.87	0.38	70,70,70,70	0
60	MG	BA	3040	1/1	0.88	0.36	99,99,99,99	0
60	MG	DA	3118	1/1	0.88	0.13	73,73,73,73	0
60	MG	DA	3119	1/1	0.88	0.33	75,75,75,75	0
60	MG	BA	2903	1/1	0.88	0.31	97,97,97,97	0
60	MG	DA	2971	1/1	0.88	0.32	66,66,66,66	0
60	MG	CA	1601	1/1	0.88	0.26	86,86,86,86	0
60	MG	DA	2973	1/1	0.88	0.32	51,51,51,51	0
60	MG	BA	3029	1/1	0.88	0.17	139,139,139,139	0
60	MG	CA	1689	1/1	0.88	0.24	75,75,75,75	0
60	MG	DA	2910	1/1	0.88	0.21	57,57,57,57	0
60	MG	AA	1683	1/1	0.88	0.15	89,89,89,89	0
60	MG	DA	2983	1/1	0.88	0.26	93,93,93,93	0
60	MG	DA	3040	1/1	0.88	0.24	64,64,64,64	0
60	MG	DA	2948	1/1	0.88	0.23	60,60,60,60	0
60	MG	B5	101	1/1	0.88	0.36	76,76,76,76	0
60	MG	DA	3086	1/1	0.88	0.42	78,78,78,78	0
60	MG	DA	3108	1/1	0.88	0.30	61,61,61,61	0
60	MG	DB	201	1/1	0.88	0.27	69,69,69,69	0
60	MG	DA	3112	1/1	0.88	0.25	83,83,83,83	0
60	MG	BA	3048	1/1	0.88	0.17	87,87,87,87	0
60	MG	BA	2997	1/1	0.88	0.13	79,79,79,79	0
60	MG	DA	2915	1/1	0.89	0.23	64,64,64,64	0
60	MG	CA	1669	1/1	0.89	0.12	113,113,113,113	0
60	MG	DA	3111	1/1	0.89	0.56	62,62,62,62	0
60	MG	DA	2919	1/1	0.89	0.45	73,73,73,73	0
60	MG	DA	2987	1/1	0.89	0.18	86,86,86,86	0
60	MG	BA	3060	1/1	0.89	0.48	83,83,83,83	0
60	MG	DA	3116	1/1	0.89	0.42	104,104,104,104	0
60	MG	DA	2922	1/1	0.89	0.26	59,59,59,59	0
60	MG	BA	3061	1/1	0.89	0.23	71,71,71,71	0
60	MG	BA	2967	1/1	0.89	0.25	57,57,57,57	0
60	MG	DA	3085	1/1	0.89	0.31	86,86,86,86	0
60	MG	AA	1692	1/1	0.89	0.40	101,101,101,101	0
60	MG	DA	2934	1/1	0.89	0.23	86,86,86,86	0
60	MG	B1	102	1/1	0.89	0.34	83,83,83,83	0
60	MG	BA	3021	1/1	0.89	0.14	79,79,79,79	0
60	MG	CA	1621	1/1	0.89	0.16	96,96,96,96	0
60	MG	DA	2902	1/1	0.89	0.10	152,152,152,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3133	1/1	0.89	0.45	87,87,87,87	0
60	MG	DA	3001	1/1	0.89	0.22	69,69,69,69	0
60	MG	DA	3095	1/1	0.89	0.15	98,98,98,98	0
60	MG	BA	2907	1/1	0.89	0.40	55,55,55,55	0
60	MG	AA	1644	1/1	0.89	0.09	141,141,141,141	0
60	MG	DA	2978	1/1	0.89	0.45	85,85,85,85	0
60	MG	CA	1679	1/1	0.89	0.08	79,79,79,79	0
60	MG	CA	1610	1/1	0.89	0.07	116,116,116,116	0
60	MG	BA	3127	1/1	0.89	0.22	84,84,84,84	0
60	MG	DA	3070	1/1	0.89	0.27	79,79,79,79	0
60	MG	DA	2982	1/1	0.89	0.39	75,75,75,75	0
60	MG	BA	2958	1/1	0.89	0.09	76,76,76,76	0
60	MG	BA	2941	1/1	0.90	0.26	49,49,49,49	0
60	MG	DA	3087	1/1	0.90	0.30	68,68,68,68	0
60	MG	DA	3014	1/1	0.90	0.36	77,77,77,77	0
60	MG	DA	3089	1/1	0.90	0.41	92,92,92,92	0
60	MG	CA	1656	1/1	0.90	0.21	90,90,90,90	0
60	MG	DA	3120	1/1	0.90	0.21	71,71,71,71	0
60	MG	DA	2930	1/1	0.90	0.35	55,55,55,55	0
60	MG	DA	2997	1/1	0.90	0.10	79,79,79,79	0
60	MG	DA	2931	1/1	0.90	0.28	52,52,52,52	0
60	MG	AA	1680	1/1	0.90	0.14	75,75,75,75	0
60	MG	AA	1630	1/1	0.90	0.09	109,109,109,109	1
60	MG	AA	1610	1/1	0.90	0.14	84,84,84,84	0
60	MG	CA	1618	1/1	0.90	0.26	83,83,83,83	0
60	MG	DA	2914	1/1	0.90	0.20	49,49,49,49	0
60	MG	DA	3073	1/1	0.90	0.32	87,87,87,87	0
60	MG	DA	3074	1/1	0.90	0.48	96,96,96,96	0
60	MG	CV	101	1/1	0.90	0.20	67,67,67,67	0
60	MG	BA	3012	1/1	0.90	0.48	91,91,91,91	0
60	MG	DA	2988	1/1	0.90	0.19	111,111,111,111	0
60	MG	DA	3052	1/1	0.90	0.13	57,57,57,57	0
60	MG	DA	3054	1/1	0.90	0.30	80,80,80,80	0
60	MG	BA	3013	1/1	0.90	0.12	72,72,72,72	0
60	MG	AA	1606	1/1	0.90	0.40	98,98,98,98	0
60	MG	BA	3056	1/1	0.90	0.16	55,55,55,55	0
60	MG	DA	2924	1/1	0.90	0.15	87,87,87,87	0
60	MG	BA	2981	1/1	0.91	0.10	88,88,88,88	0
60	MG	BA	3043	1/1	0.91	0.10	83,83,83,83	0
60	MG	BA	2964	1/1	0.91	0.25	80,80,80,80	0
60	MG	CA	1695	1/1	0.91	0.29	80,80,80,80	0
60	MG	DA	2958	1/1	0.91	0.11	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	2905	1/1	0.91	0.23	59,59,59,59	0
60	MG	BA	3087	1/1	0.91	0.55	112,112,112,112	0
60	MG	DA	2908	1/1	0.91	0.33	83,83,83,83	0
60	MG	DA	2933	1/1	0.91	0.21	53,53,53,53	0
60	MG	AA	1702	1/1	0.91	0.37	74,74,74,74	0
60	MG	BA	2911	1/1	0.91	0.39	74,74,74,74	0
60	MG	AA	1625	1/1	0.91	0.20	85,85,85,85	0
60	MG	DA	2912	1/1	0.91	0.21	45,45,45,45	0
60	MG	DA	3129	1/1	0.91	0.37	113,113,113,113	0
60	MG	DA	2943	1/1	0.91	0.12	59,59,59,59	0
60	MG	BA	3125	1/1	0.91	0.24	91,91,91,91	0
60	MG	DA	2945	1/1	0.91	0.14	57,57,57,57	0
60	MG	AA	1648	1/1	0.91	0.37	92,92,92,92	0
60	MG	DA	3026	1/1	0.91	0.17	78,78,78,78	0
60	MG	DA	3051	1/1	0.91	0.15	56,56,56,56	0
60	MG	BA	2926	1/1	0.91	0.18	58,58,58,58	0
60	MG	BA	3081	1/1	0.91	0.43	103,103,103,103	0
60	MG	DA	3107	1/1	0.91	0.32	59,59,59,59	0
60	MG	BA	2971	1/1	0.91	0.09	52,52,52,52	0
60	MG	DA	3110	1/1	0.91	0.32	63,63,63,63	0
60	MG	BA	2980	1/1	0.91	0.36	82,82,82,82	0
60	MG	DA	3084	1/1	0.91	0.18	103,103,103,103	0
60	MG	DA	3121	1/1	0.92	0.37	104,104,104,104	0
60	MG	BA	3119	1/1	0.92	0.43	99,99,99,99	0
60	MG	CA	1701	1/1	0.92	0.37	58,58,58,58	0
60	MG	B5	102	1/1	0.92	0.26	79,79,79,79	0
60	MG	DA	3036	1/1	0.92	0.26	59,59,59,59	0
60	MG	BA	2951	1/1	0.92	0.11	63,63,63,63	0
60	MG	BA	3027	1/1	0.92	0.35	51,51,51,51	0
60	MG	DA	3039	1/1	0.92	0.29	85,85,85,85	0
60	MG	CL	201	1/1	0.92	0.26	87,87,87,87	1
60	MG	CA	1693	1/1	0.92	0.26	65,65,65,65	0
60	MG	BA	3133	1/1	0.92	0.74	73,73,73,73	0
60	MG	BA	2998	1/1	0.92	0.37	88,88,88,88	0
60	MG	BA	3042	1/1	0.92	0.22	78,78,78,78	0
60	MG	DA	3025	1/1	0.92	0.32	51,51,51,51	0
60	MG	BA	2918	1/1	0.92	0.42	64,64,64,64	0
60	MG	CA	1657	1/1	0.92	0.07	56,56,56,56	1
60	MG	BA	3117	1/1	0.92	0.30	72,72,72,72	0
60	MG	DA	2946	1/1	0.92	0.21	57,57,57,57	0
60	MG	DA	2923	1/1	0.92	0.15	52,52,52,52	0
60	MG	DA	2906	1/1	0.92	0.13	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	2925	1/1	0.92	0.23	58,58,58,58	0
60	MG	DA	3012	1/1	0.93	0.10	53,53,53,53	0
60	MG	CA	1649	1/1	0.93	0.06	82,82,82,82	0
60	MG	BA	3036	1/1	0.93	0.18	97,97,97,97	0
60	MG	BA	2961	1/1	0.93	0.30	78,78,78,78	0
60	MG	BA	2979	1/1	0.93	0.07	103,103,103,103	0
60	MG	DA	3130	1/1	0.93	0.31	115,115,115,115	0
60	MG	BA	2915	1/1	0.93	0.18	51,51,51,51	0
60	MG	AA	1696	1/1	0.93	0.24	90,90,90,90	0
60	MG	BA	3116	1/1	0.93	0.24	91,91,91,91	0
60	MG	BA	2969	1/1	0.93	0.23	61,61,61,61	0
60	MG	BA	3118	1/1	0.93	0.36	110,110,110,110	0
60	MG	BA	3067	1/1	0.93	0.13	93,93,93,93	0
60	MG	BA	2959	1/1	0.93	0.28	59,59,59,59	0
60	MG	DA	2974	1/1	0.93	0.60	92,92,92,92	0
60	MG	DA	2938	1/1	0.93	0.26	45,45,45,45	0
60	MG	AA	1619	1/1	0.93	0.08	72,72,72,72	0
60	MG	DA	3062	1/1	0.93	0.42	49,49,49,49	0
60	MG	BA	3122	1/1	0.93	0.28	84,84,84,84	0
60	MG	DA	3065	1/1	0.93	0.43	75,75,75,75	0
60	MG	DA	3101	1/1	0.94	0.13	88,88,88,88	0
60	MG	DA	2917	1/1	0.94	0.39	58,58,58,58	0
60	MG	BA	2910	1/1	0.94	0.23	75,75,75,75	0
60	MG	D5	101	1/1	0.94	0.24	56,56,56,56	0
60	MG	AL	201	1/1	0.94	0.44	125,125,125,125	1
60	MG	AA	1701	1/1	0.94	0.27	71,71,71,71	0
60	MG	DA	2995	1/1	0.94	0.34	75,75,75,75	0
60	MG	DA	3131	1/1	0.94	0.36	102,102,102,102	0
60	MG	DA	2947	1/1	0.94	0.09	51,51,51,51	0
60	MG	BA	3003	1/1	0.94	0.52	68,68,68,68	0
60	MG	CA	1602	1/1	0.94	0.10	92,92,92,92	0
60	MG	DA	2936	1/1	0.94	0.15	59,59,59,59	0
60	MG	DA	2966	1/1	0.94	0.26	48,48,48,48	0
60	MG	DA	2967	1/1	0.94	0.23	51,51,51,51	0
60	MG	DA	2937	1/1	0.94	0.13	45,45,45,45	0
60	MG	DA	3020	1/1	0.94	0.12	50,50,50,50	0
60	MG	DA	3021	1/1	0.94	0.09	81,81,81,81	0
60	MG	BA	3099	1/1	0.94	0.16	117,117,117,117	0
60	MG	DA	3079	1/1	0.94	0.20	131,131,131,131	0
60	MG	DA	2939	1/1	0.94	0.19	41,41,41,41	0
60	MG	BA	3105	1/1	0.94	0.05	68,68,68,68	0
60	MG	BA	2928	1/1	0.95	0.46	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1673	1/1	0.95	0.06	79,79,79,79	0
60	MG	BA	2934	1/1	0.95	0.22	55,55,55,55	0
60	MG	BA	2904	1/1	0.95	0.49	56,56,56,56	0
60	MG	DA	3139	1/1	0.95	0.33	69,69,69,69	0
60	MG	DA	2928	1/1	0.95	0.21	42,42,42,42	0
60	MG	DA	2977	1/1	0.95	0.22	104,104,104,104	0
60	MG	DA	2959	1/1	0.95	0.28	61,61,61,61	0
60	MG	DA	2968	1/1	0.95	0.13	43,43,43,43	0
60	MG	BA	3112	1/1	0.95	0.33	47,47,47,47	0
60	MG	BA	2917	1/1	0.95	0.33	58,58,58,58	0
60	MG	DA	3064	1/1	0.95	0.20	66,66,66,66	0
60	MG	DA	3138	1/1	0.96	0.28	113,113,113,113	0
60	MG	DA	2955	1/1	0.96	0.19	54,54,54,54	0
60	MG	DA	3109	1/1	0.96	0.31	45,45,45,45	0
60	MG	BA	3041	1/1	0.96	0.36	71,71,71,71	0
60	MG	BA	3131	1/1	0.96	0.33	79,79,79,79	0
60	MG	DA	3126	1/1	0.96	0.39	76,76,76,76	0
60	MG	CA	1635	1/1	0.96	0.05	98,98,98,98	0
60	MG	DA	3113	1/1	0.96	0.27	96,96,96,96	0
60	MG	BA	3092	1/1	0.96	0.18	82,82,82,82	0
60	MG	BA	2943	1/1	0.97	0.46	56,56,56,56	0
60	MG	DA	2904	1/1	0.97	0.44	49,49,49,49	0
60	MG	BA	3034	1/1	0.97	0.07	82,82,82,82	0
60	MG	BA	2936	1/1	0.97	0.34	58,58,58,58	0
60	MG	DA	2941	1/1	0.97	0.12	45,45,45,45	0
60	MG	DA	2927	1/1	0.97	0.38	52,52,52,52	0
60	MG	BA	3111	1/1	0.97	0.44	103,103,103,103	0
60	MG	DA	2976	1/1	0.97	0.36	53,53,53,53	0
60	MG	CA	1645	1/1	0.97	0.07	68,68,68,68	0
60	MG	DA	3005	1/1	0.97	0.40	53,53,53,53	0
61	ZN	AN	101	1/1	0.97	0.12	153,153,153,153	0
61	ZN	CN	101	1/1	0.97	0.12	153,153,153,153	0
60	MG	DA	3053	1/1	0.98	0.07	71,71,71,71	0
60	MG	CA	1619	1/1	0.98	0.04	67,67,67,67	0
60	MG	CA	1605	1/1	0.98	0.04	104,104,104,104	0
60	MG	DA	2920	1/1	0.98	0.05	75,75,75,75	0
61	ZN	AD	301	1/1	0.98	0.07	106,106,106,106	0
60	MG	CA	1648	1/1	0.98	0.12	71,71,71,71	0
61	ZN	CD	301	1/1	0.98	0.05	106,106,106,106	0
60	MG	BA	2924	1/1	0.98	0.09	52,52,52,52	0
60	MG	DA	2916	1/1	0.99	0.33	53,53,53,53	0

5.5 Other polymers [i](#)

There are no such residues in this entry.