Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2023 – 10:57 AM JST

PDB ID	:	6LKQ
Title	:	The Structural Basis for Inhibition of Ribosomal Translocation by Viomycin
Authors	:	Zhang, L.; Wang, Y.H.; Lancaster, L.; Zhou, J.; Noller, H.F.
Deposited on	:	2019-12-20
Resolution	:	3.10 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 (i) 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 (i)) were used in the production of this report:

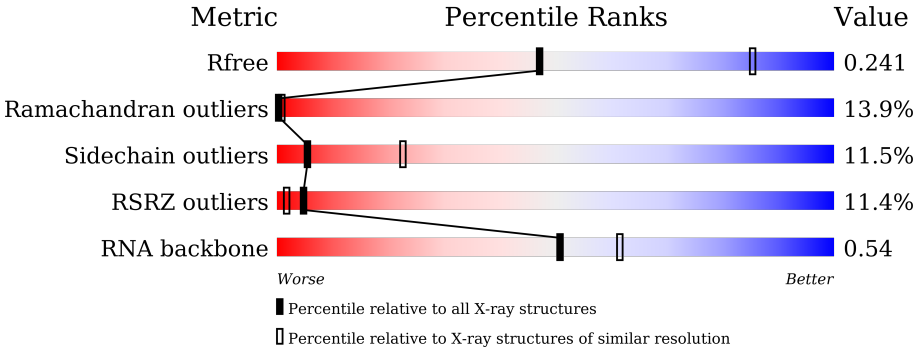
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	218	26%, 74%, 22%, •
2	B	206	7%, 80%, 18%, •
3	C	205	22%, 68%, 29%, •
4	D	150	2%, 79%, 20%, •
5	E	100	14%, 74%, 21%, 5%
6	F	151	42%, 85%, 15%

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Mol	Chain	Length	Quality of chain
7	G	129	6% 91% 9%
8	H	127	29% 76% 22%
9	I	98	13% 73% 24%
10	J	117	7% 79% 18%
11	K	123	4% 78% 19%
12	L	114	55% 80% 20%
13	M	100	39% 79% 14%
14	N	88	8% 82% 18%
15	O	82	24% 73% 26%
16	P	80	34% 69% 29%
17	Q	55	11% 80% 18%
18	R	79	65% 81% 18%
19	S	85	8% 85% 14%
20	T	51	39% 78% 22%
21	U	271	3% 80% 19%
22	V	209	78% 19%
23	W	201	3% 82% 16%
24	X	177	23% 79% 20%
25	Y	176	2% 74% 23%
26	Z	141	70% 82% 18%
27	0	142	4% 75% 23%
28	1	122	% 80% 19%
29	2	143	6% 75% 25%
30	3	136	% 79% 21%
31	4	120	2% 81% 18%

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Mol	Chain	Length	Quality of chain
32	5	116	31% 86% 13%
33	6	114	3% 76% 22%
34	8	117	3% 81% 18%
35	9	103	3% 88% 10%
36	a	110	% 82% 17%
37	b	93	14% 75% 22%
38	c	102	21% 74% 25%
39	d	94	9% 84% 16%
40	e	79	6% 58% 35% 6%
41	f	77	4% 82% 16%
42	g	63	5% 76% 22%
43	h	58	17% 74% 22%
44	i	56	5% 79% 21%
45	j	50	70% 90% 10%
46	k	46	4% 83% 17%
47	l	64	88% 12%
48	m	38	3% 74% 26%
49	n	163	69% 77% 20%
50	o	30	17% 70% 27%
50	p	30	27% 83% 17%
50	q	30	57% 93% 7%
50	r	30	37% 80% 20%
51	s	1532	6% 79% 19%
52	t	2903	3% 73% 21%
53	u	118	84% 16%

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Mol	Chain	Length	Quality of chain
54	v	525	11% 78% 18%
55	w	6	83% 67% 33%
56	7	6	17% 33% 67%
56	AA	6	33% 33% 67%
56	BA	6	17% 50% 50%
56	y	6	50% 50%
56	z	6	17% 33% 67%

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
56	UAL	7	5	-	-	-	X
56	5OH	7	6	-	-	-	X
56	KBE	AA	1	-	-	-	X
56	DPP	AA	2	-	-	-	X
56	5OH	AA	6	-	-	-	X
56	KBE	BA	1	-	-	-	X
56	DPP	BA	2	-	-	-	X
56	UAL	BA	5	-	-	-	X
56	KBE	y	1	-	-	-	X
56	KBE	z	1	-	-	-	X
56	5OH	z	6	-	-	-	X

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 146817 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1702	1079	305	312	6	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	206	1625	1028	305	289	3	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	205	1643	1026	315	298	4	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	150	1106	687	211	202	6	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	100	818	515	148	149	6	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	151	1182	735	227	216	4	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	G	129	979	616	173	184	6	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	127	1022	634	206	179	3	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	98	787	493	150	143	1	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	117	877	540	174	160	3	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	123	955	590	196	165	4	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	114	884	546	178	157	3	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	96	774	483	160	128	3	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	N	88	714	439	144	130	1	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	O	82	649	406	128	114	1	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	P	80	649	411	121	114	3	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	Q	55	456	288	86	82	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	R	79	638	408	120	108	2	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	S	85	665	411	137	114	3	0	0	0

- Molecule 20 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	T	51	426	265	86	74	1	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	U	271	2083	1288	423	365	7	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	V	209	1565	979	288	294	4	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	W	201	1552	974	283	290	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	X	177	1411	899	249	257	6	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	Y	176	1323	832	243	246	2	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	Z	141	1032	651	179	196	6	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	0	142	1129	714	212	199	4	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	1	122	939	587	180	166	6	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	2	143	1045	649	206	189	1	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	3	136	1074	686	205	177	6	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	4	120	961	593	196	167	5	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
32	5	116	892	552	178	162	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	6	114	917	574	179	163	1	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
34	8	117	947	604	192	151	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	9	103	816	516	153	145	2	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	a	110	857	532	166	156	3	0	0	0

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	b	93	739	466	139	132	2	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
38	c	102	780	492	146	142	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	d	94	753	479	137	134	3	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	e	79	596	367	120	108	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	f	77	625	388	129	106	2	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	g	63	509	313	99	95	2	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	h	58	449	281	87	79	2	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	i	56	444	269	94	80	1	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
45	j	50	410	263	75	72	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	k	46	377	228	90	57	2	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	l	64	504	323	105	74	2	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	m	38	302	185	65	48	4	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	n	163	1234	779	219	229	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	85	LEU	SER	conflict	UNP A0A1X3LA41
n	160	GLU	ASP	conflict	UNP A0A1X3LA41

- Molecule 50 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	o	30	228	144	33	48	3	0	0	0
50	p	30	228	144	33	48	3	0	0	0
50	q	30	228	144	33	48	3	0	0	0
50	r	30	228	144	33	48	3	0	0	0

- Molecule 51 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
51	s	1532	32870	14661	6031	10647	1531	0	0	0

- Molecule 52 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
52	t	2850	61183	27295	11261	19778	2849	0	0	0

- Molecule 53 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
53	u	118	2526	1126	464	819	117	0	0	0

- Molecule 54 is a protein called Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	v	525	4144	2617	722	783	22	0	0	0

- Molecule 55 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
55	w	6	126	58	24	39	5	0	0	0

- Molecule 56 is a protein called Viomycin.

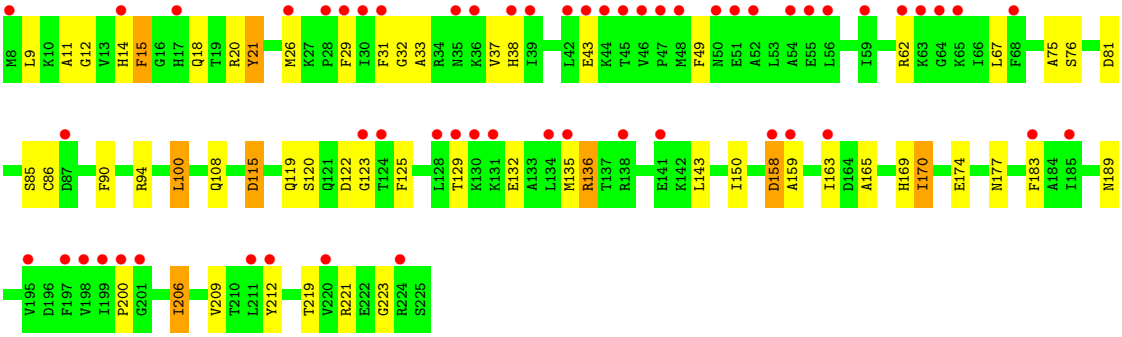
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	y	6	48	25	13	10	0	0	0
56	z	6	48	25	13	10	0	0	0
56	7	6	48	25	13	10	0	0	0
56	AA	6	48	25	13	10	0	0	0
56	BA	6	48	25	13	10	0	0	0

3 Residue-property plots (i)

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

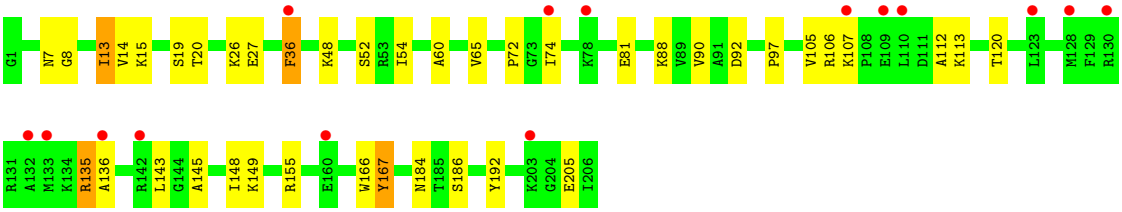
• Molecule 1: 30S ribosomal protein S2

Chain A:



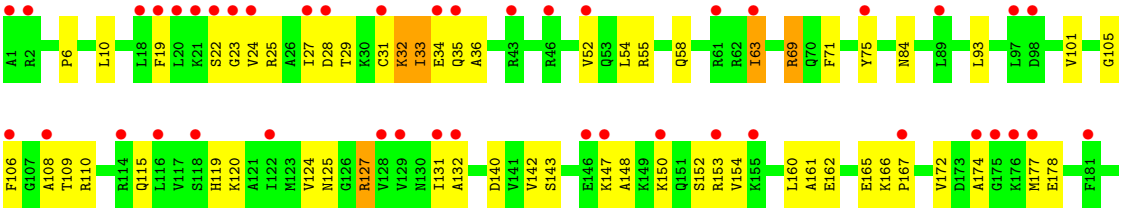
• Molecule 2: 30S ribosomal protein S3

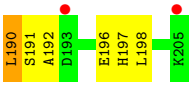
Chain B:



• Molecule 3: 30S ribosomal protein S4

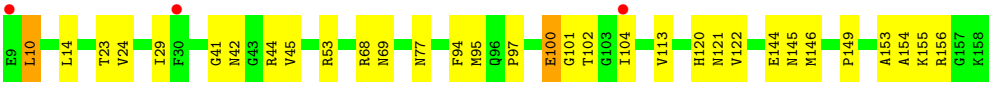
Chain C:





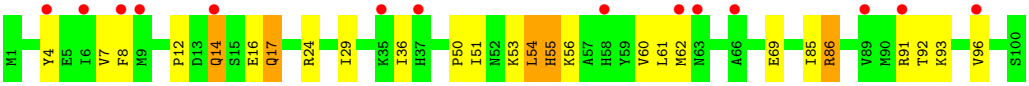
• Molecule 4: 30S ribosomal protein S5

Chain D:



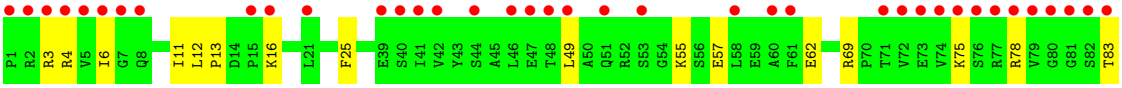
• Molecule 5: 30S ribosomal protein S6

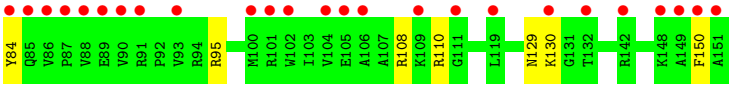
Chain E:



• Molecule 6: 30S ribosomal protein S7

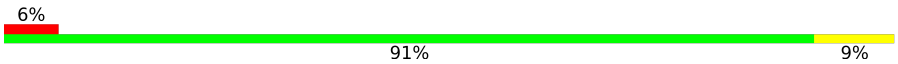
Chain F:

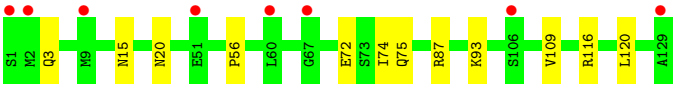




• Molecule 7: 30S ribosomal protein S8

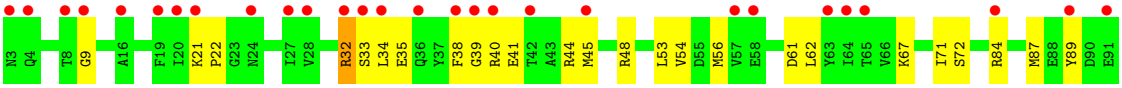
Chain G:

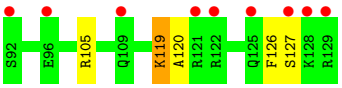




• Molecule 8: 30S ribosomal protein S9

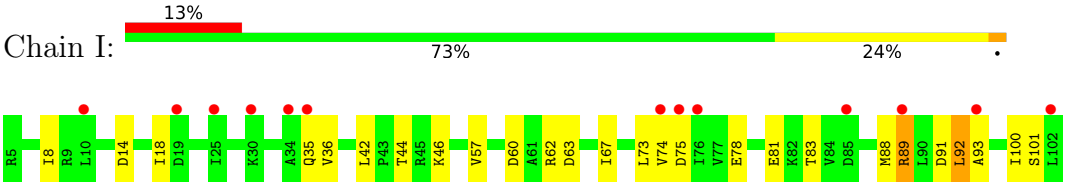
Chain H:





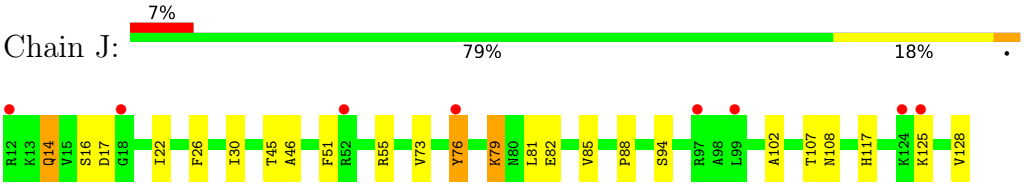
• Molecule 9: 30S ribosomal protein S10

Chain I:



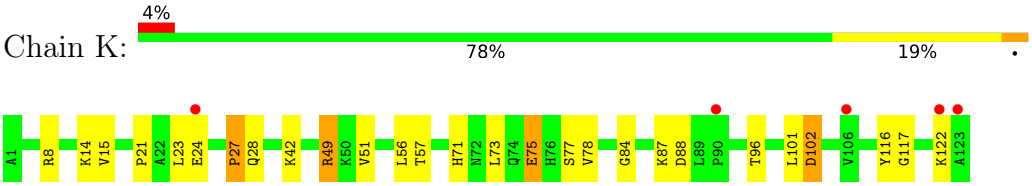
- Molecule 10: 30S ribosomal protein S11

Chain J:



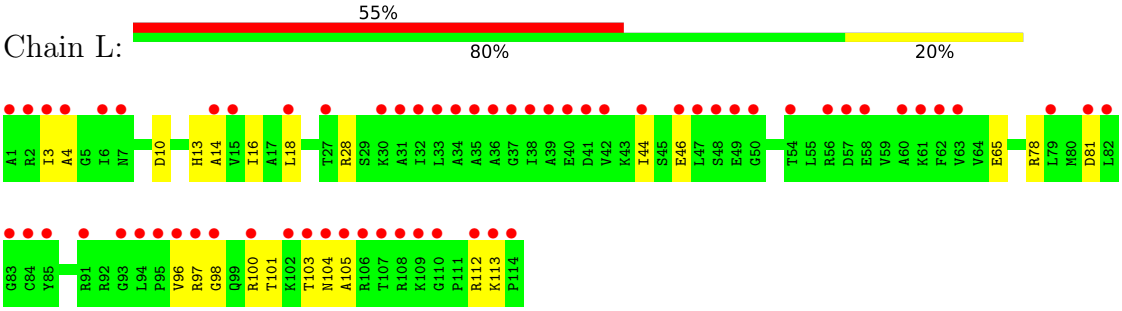
- Molecule 11: 30S ribosomal protein S12

Chain K:



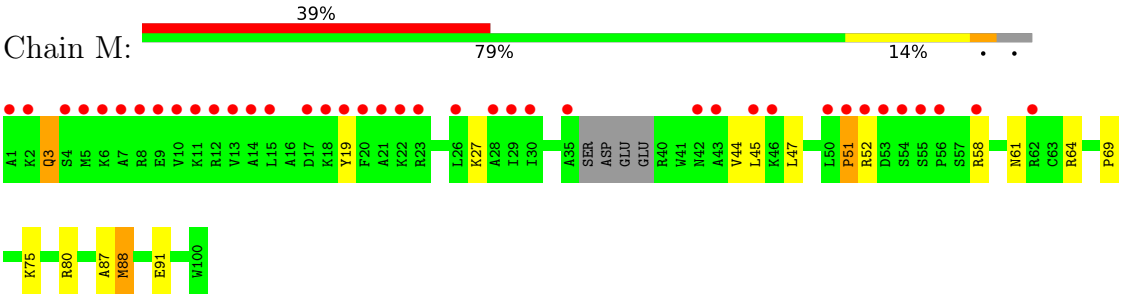
- Molecule 12: 30S ribosomal protein S13

Chain L:



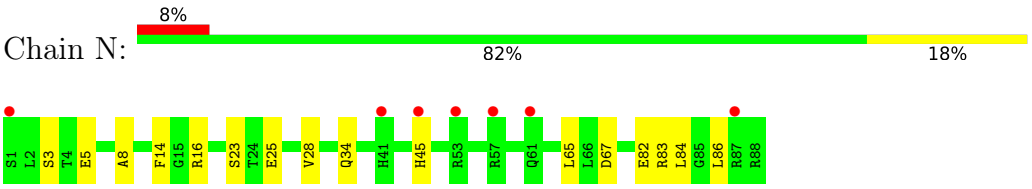
- Molecule 13: 30S ribosomal protein S14

Chain M:



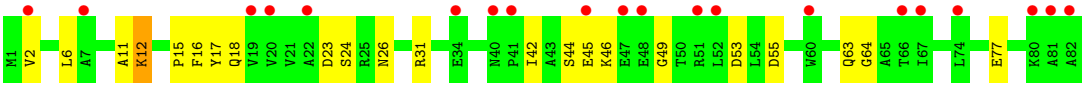
- Molecule 14: 30S ribosomal protein S15

Chain N:



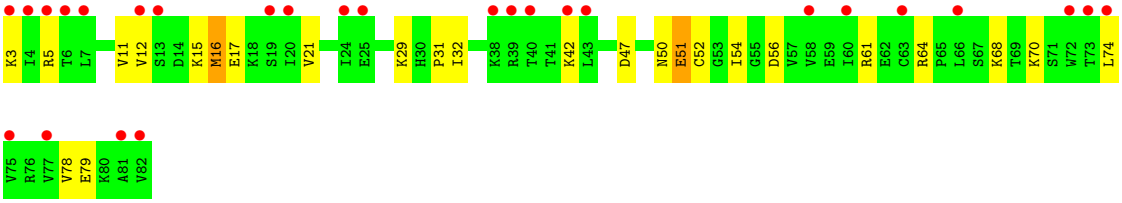
- Molecule 15: 30S ribosomal protein S16

Chain O:



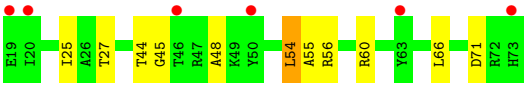
- Molecule 16: 30S ribosomal protein S17

Chain P:



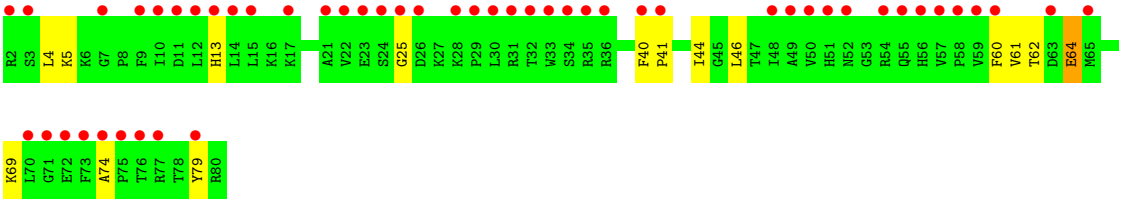
- Molecule 17: 30S ribosomal protein S18

Chain Q:



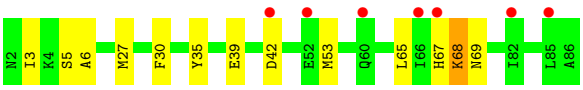
- Molecule 18: 30S ribosomal protein S19

Chain R:



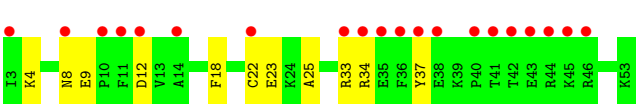
- Molecule 19: 30S ribosomal protein S20

Chain S:



- Molecule 20: 30S ribosomal protein S21

Chain T:



- Molecule 21: 50S ribosomal protein L2

Chain U: 3% 80% 19%

A1 S9 P10 G11 R12 P21 E22 L23 F29 L32 L33 E34 S37 R51 H52 K58 Q59 A60 V64 R68 N69 K70 I73 P74 A75 V76 V77 E78 R79 V93 L109 K110 Q114 I123 T128 R132 V140 H141 N142 R155 Y160

A165 L173 R176 E184 A185 R188 L191 N196 L204 W212 M224 N225 P226 V227 D228 H231 G232 G233 G234 F239 T251 K254 K255 T256 R257 S258 N259 K260 K264 F265 R268 R269 R270 S271

- Molecule 22: 50S ribosomal protein L3

Chain V: 78% 19%

M1 L4 E17 L40 D43 V50 K55 A69 K70 A71 G72 V73 E86 T91 V92 G93 Q94 S95 K106 V107 D108 V109 K114 F118 A119 G120 T121 V122 K123 R124 R128 T129 T133 G144 S145 Q150 T151 K159 M165 R169 V170

Q173 S174 L175 D176 V177 V178 R179 K190 G191 P194 L201 I202 V203 A209

- Molecule 23: 50S ribosomal protein L4

Chain W: 3% 82% 16%

M1 K6 D7 A8 Q9 S10 A11 L12 T13 V28 A45 Q46 R49 A50 E51 R61 R69 S70 I73 W78 R79 S80 V83 V96 N97 R102 I108 L109 L118 I119 K123 F124 E127 I148 I149 T150 G151 E152 L153 L157 N163 L164

H165 K166 R170 I175 D176 A201

- Molecule 24: 50S ribosomal protein L5

Chain X: 23% 79% 20%

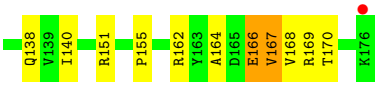
A1 Y7 K8 K13 K14 L15 M16 F19 N20 Y21 V24 V30 E31 T34 L35 I43 A44 D45 K46 G61 L65 I66 T67 K68 S72 V73 A74 G75 F76 K77 I78 R79 Q80 G81 Y82 C86 R91 G92 E93 R94 M95 W96 I103 P108 R109 I110

R111 D112 F113 R114 G115 L116 S117 A118 F121 R124 G125 M129 R132 E133 Q134 I135 I136 D146 R147 V148 L151 T157 T158 A159 K160 S161 D162 E163 A167 L168 F172 D173 F174 P175 F176 R177

- Molecule 25: 50S ribosomal protein L6

Chain Y: 2% 74% 23%

S1 V8 V9 V10 P11 V14 D15 V16 K17 I18 K28 W29 G30 E31 L32 T33 R34 D38 H44 A45 P53 R54 D55 D59 G60 R68 N72 V75 I76 T79 T83 K84 K85 V97 K98 H110 D113 P117 A118 G119 I120 V131 L132

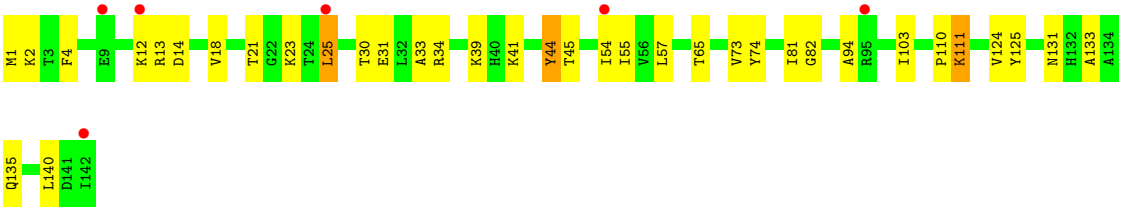


• Molecule 26: 50S ribosomal protein L11

Chain Z:

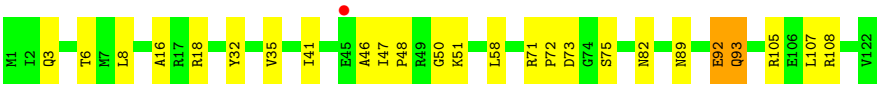
• Molecule 27: 50S ribosomal protein L13

Chain 0:



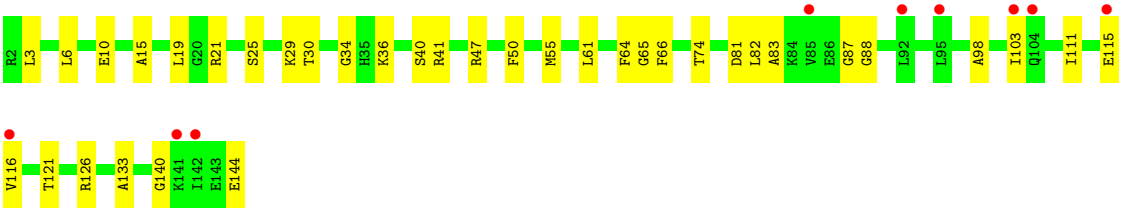
• Molecule 28: 50S ribosomal protein L14

Chain 1:



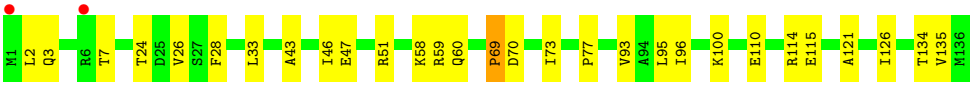
• Molecule 29: 50S ribosomal protein L15

Chain 2:



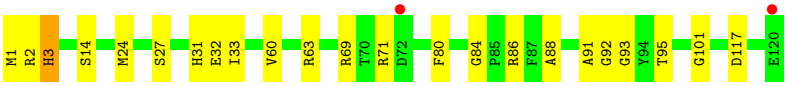
• Molecule 30: 50S ribosomal protein L16

Chain 3:



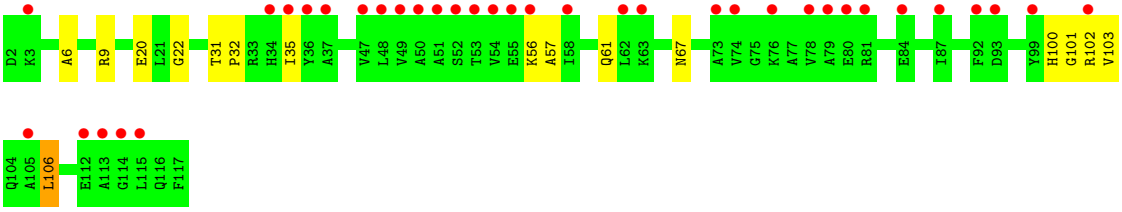
• Molecule 31: 50S ribosomal protein L17

Chain 4:



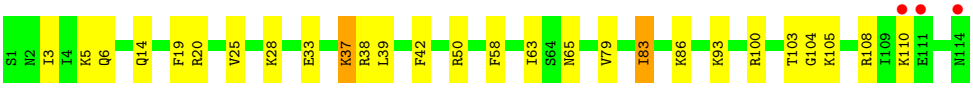
• Molecule 32: 50S ribosomal protein L18

Chain 5:



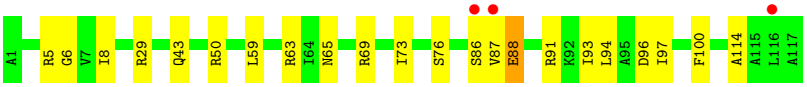
• Molecule 33: 50S ribosomal protein L19

Chain 6:



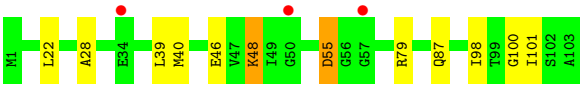
• Molecule 34: 50S ribosomal protein L20

Chain 8:



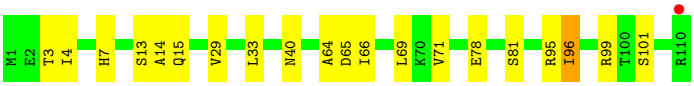
• Molecule 35: 50S ribosomal protein L21

Chain 9:



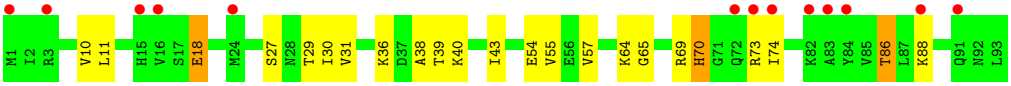
• Molecule 36: 50S ribosomal protein L22

Chain a:



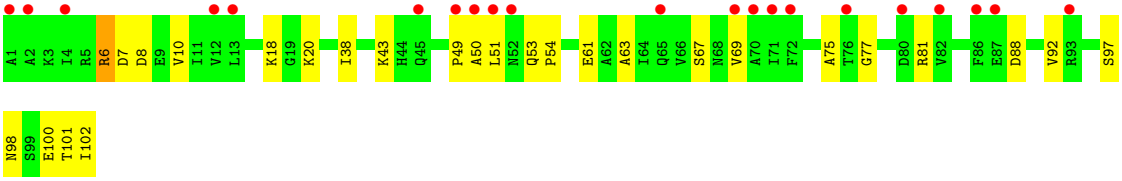
• Molecule 37: 50S ribosomal protein L23

Chain b:



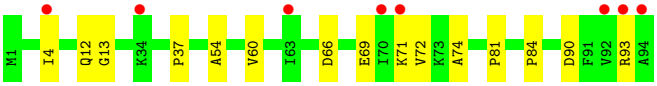
• Molecule 38: 50S ribosomal protein L24

Chain c:



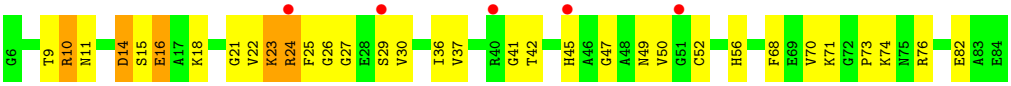
• Molecule 39: 50S ribosomal protein L25

Chain d:



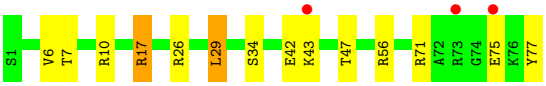
• Molecule 40: 50S ribosomal protein L27

Chain e:



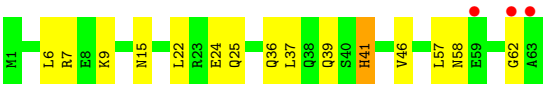
• Molecule 41: 50S ribosomal protein L28

Chain f:



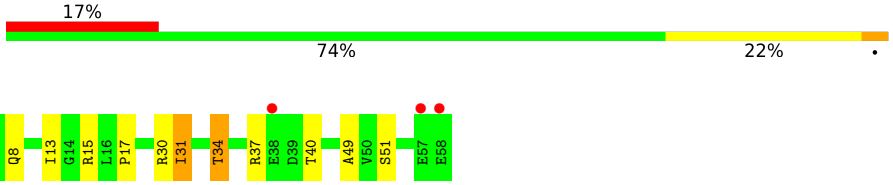
• Molecule 42: 50S ribosomal protein L29

Chain g:



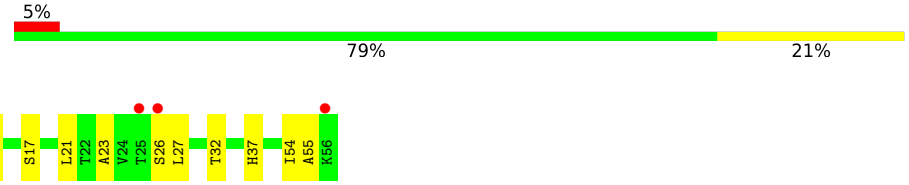
• Molecule 43: 50S ribosomal protein L30

Chain h:



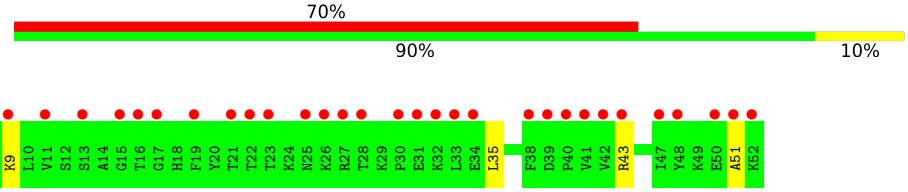
• Molecule 44: 50S ribosomal protein L32

Chain i:



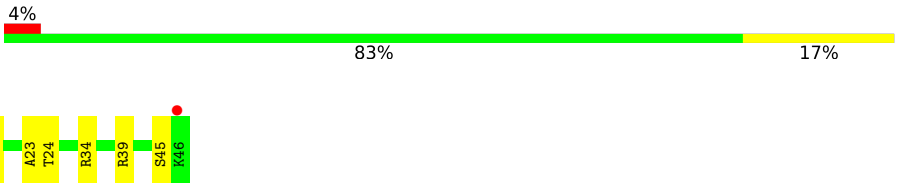
• Molecule 45: 50S ribosomal protein L33

Chain j:



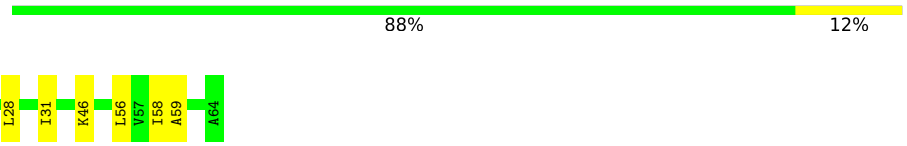
• Molecule 46: 50S ribosomal protein L34

Chain k:



• Molecule 47: 50S ribosomal protein L35

Chain l:

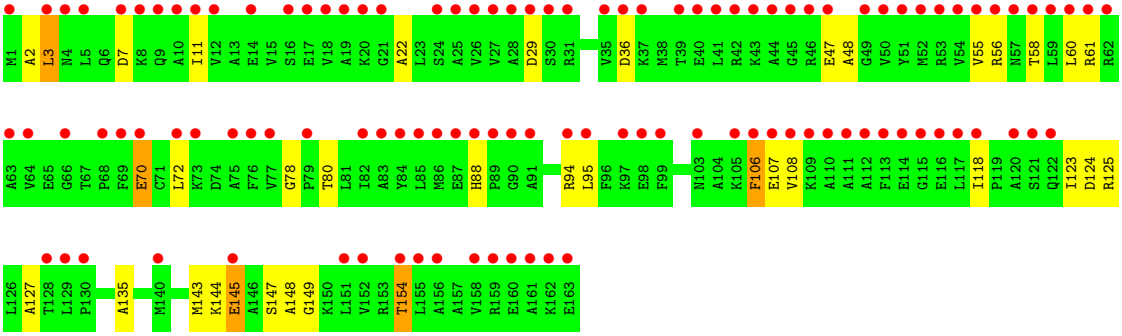


• Molecule 48: 50S ribosomal protein L36

Chain m:

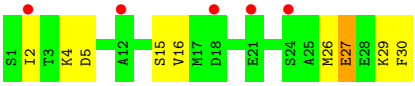
• Molecule 49: 50S ribosomal protein L10

Chain n:



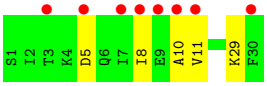
- Molecule 50: 50S ribosomal protein L7/L12

Chain o:



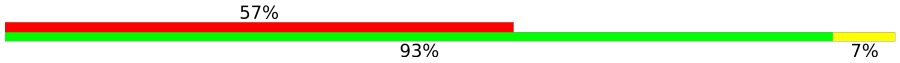
- Molecule 50: 50S ribosomal protein L7/L12

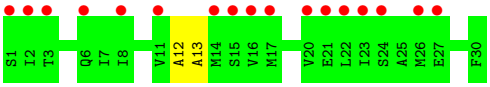
Chain p:



- Molecule 50: 50S ribosomal protein L7/L12

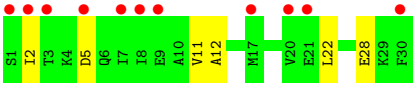
Chain q:





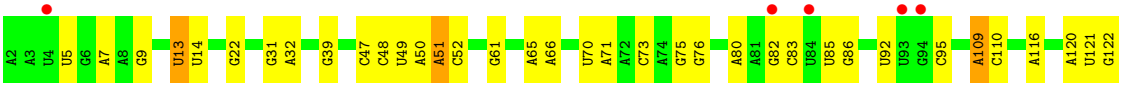
- Molecule 50: 50S ribosomal protein L7/L12

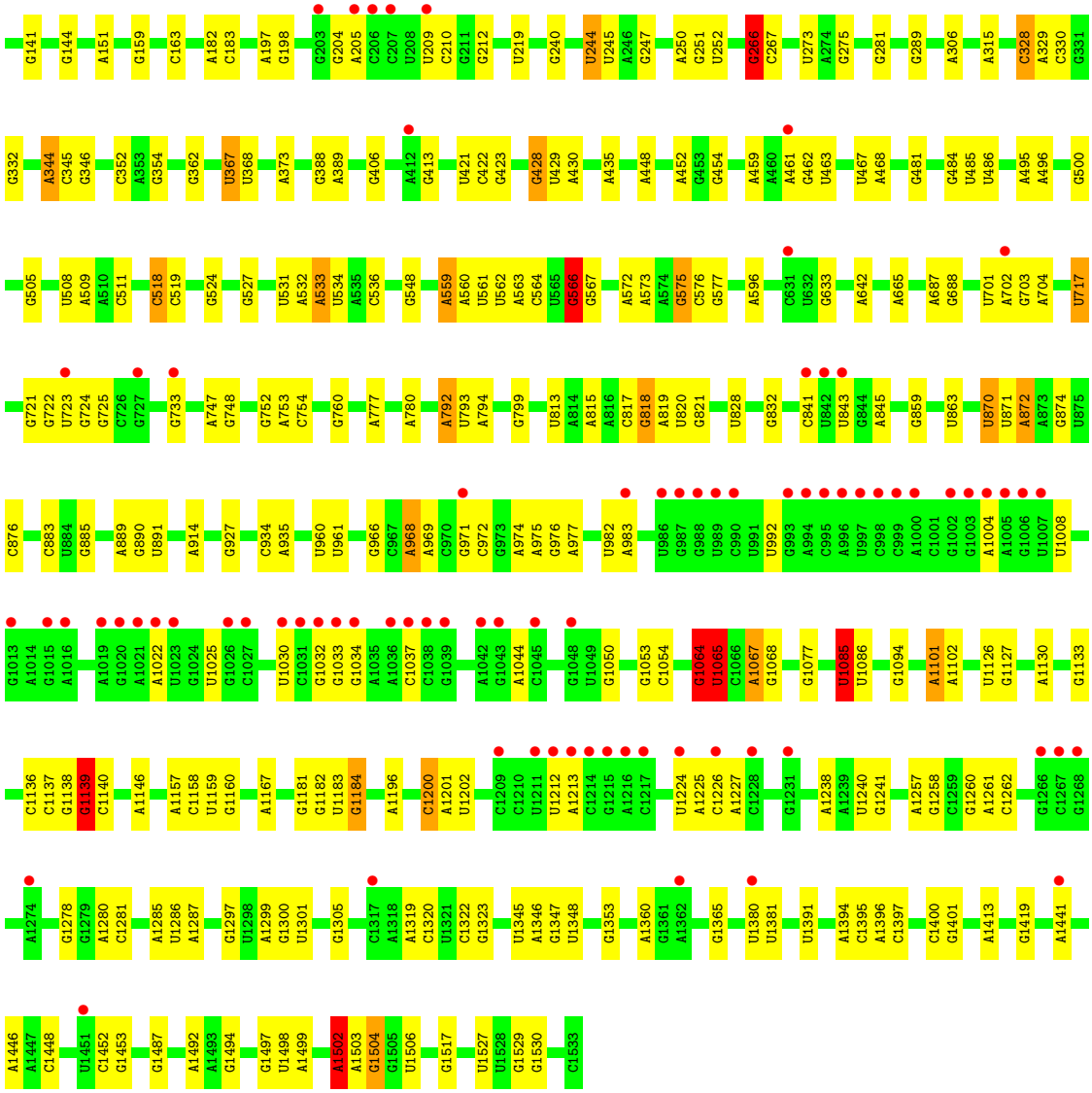
Chain r:



- Molecule 51: 16S ribosomal RNA

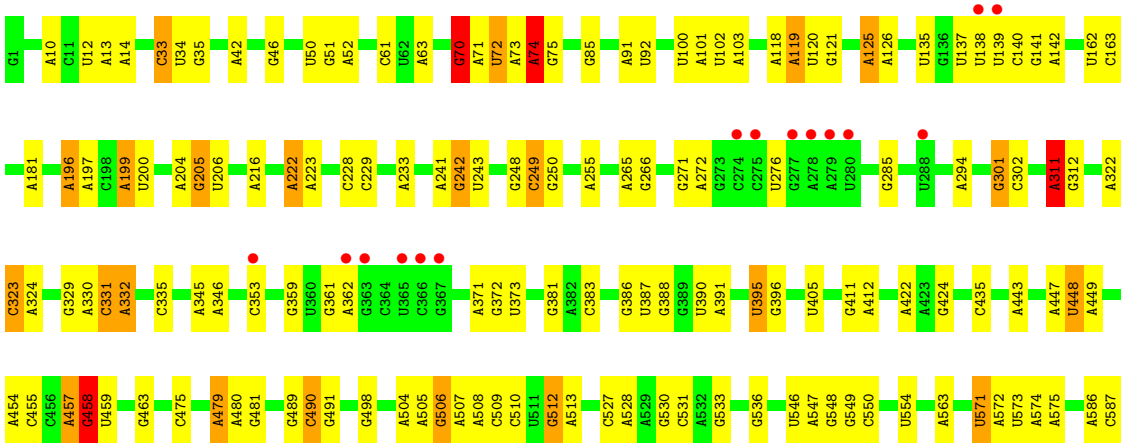
Chain s:

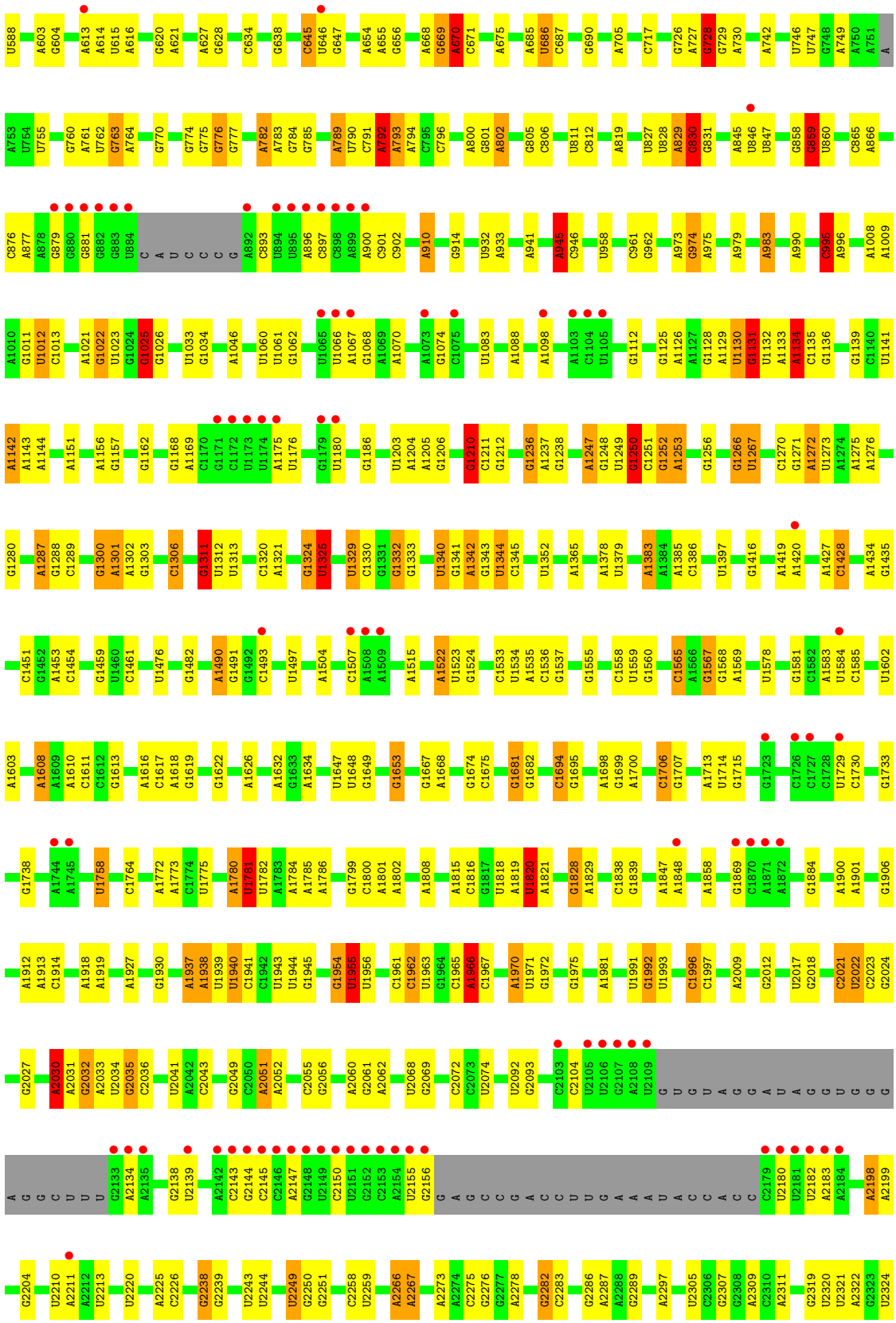


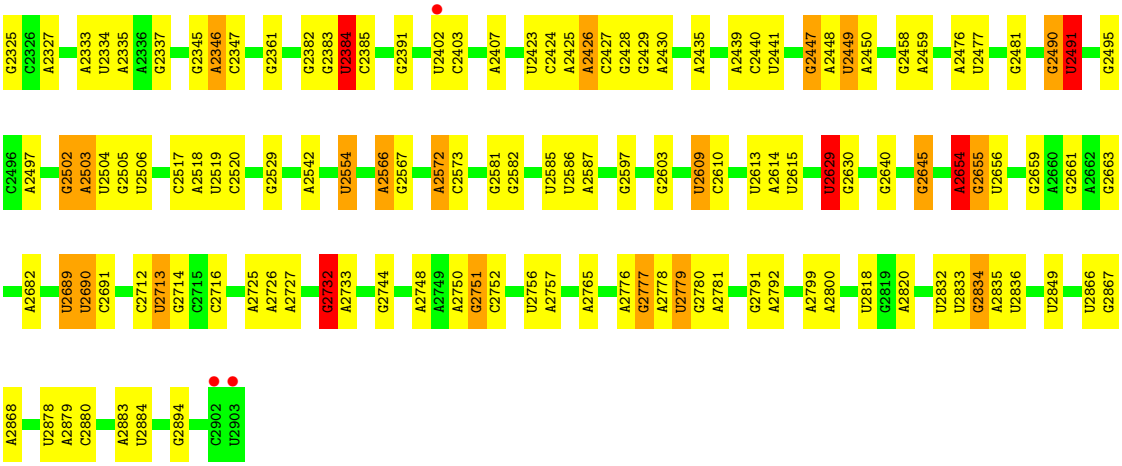


• Molecule 52: 23S ribosomal RNA

Chain t:




U588 A603 G604 A613 A614 U615 A616 G620 A621 A627 G628 C634 G638 C645 U646 G647 A654 A655 G656 A668 G669 A670 C671 A675 A685 U686 C687 G690 A705 C717 G726 A727 G728 G729 A730 A742 U746 U747 G748 A749 A750 A751 A
A753 U754 U755 G760 A761 U762 G763 A764 G770 G774 G775 G776 G777 A782 A783 G784 G785 A789 U790 C791 A792 A793 A794 C795 C796 A800 G801 A802 G805 C806 U811 C812 A819 U827 U828 A829 G830 G831 A845 U846 U847 G858 G859 U860 C865 A866
C876 A877 A878 G879 G880 G881 G882 G883 U884 C A U C C C G A892 C893 U894 U895 A896 C897 C898 A899 A900 C901 C902 A910 G914 U932 A933 A941 A945 C946 U958 C961 G962 A973 G974 A975 A979 A983 A990 C995 A996 A1008 A1009
A1010 G1011 U1012 C1013 A1021 G1022 U1023 G1024 G1025 G1026 U1033 G1034 A1046 U1060 U1061 G1062 U1065 U1066 A1067 G1068 A1069 A1070 A1073 G1074 C1075 U1083 A1088 A1098 A1103 C1104 U1105 G1112 G1125 A1126 A1127 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 G1136 G1139 C1140 U1141
A1142 A1143 A1144 A1151 A1156 G1157 G1162 G1168 A1169 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1179 U1180 G1186 U1203 A1204 A1205 G1206 G1210 C1211 G1212 G1236 A1237 G1238 A1247 G1248 U1249 G1250 C1251 G1252 A1253 G1256 G1266 U1267 C1270 G1271 A1272 U1273 A1274 A1275 A1276
G1280 A1287 G1288 C1289 G1300 A1301 A1302 G1303 C1306 G1311 U1312 U1313 C1320 A1321 G1324 U1325 U1329 C1330 G1331 G1332 G1333 U1340 G1341 A1342 G1343 U1344 C1345 U1352 A1365 A1378 U1379 A1383 A1384 A1385 C1386 U1397 G1416 A1419 A1420 A1427 C1428 A1434 G1435
C1451 G1452 A1453 C1454 G1459 U1460 C1461 U1476 G1482 A1490 G1491 G1492 C1493 U1497 A1504 C1507 A1508 A1509 A1515 A1522 U1523 G1524 C1533 U1534 A1535 C1536 G1537 G1555 C1558 U1559 G1560 C1565 A1566 G1567 G1568 A1569 U1578 G1581 C1582 A1583 U1584 C1585 U1602
A1603 A1608 A1609 A1610 C1611 C1612 G1613 A1616 C1617 A1618 G1619 G1622 A1626 A1632 G1633 A1634 U1647 U1648 G1649 G1653 G1667 A1668 G1674 C1675 G1681 G1682 C1694 G1695 A1698 G1699 A1700 C1706 G1707 A1713 U1714 G1715 G1723 C1726 C1727 C1728 U1729 C1730 G1733
G1738 A1744 A1745 U1758 C1764 A1772 A1773 C1774 U1775 A1780 U1781 U1782 A1783 A1784 A1785 A1786 G1799 C1800 A1801 A1802 A1808 A1815 C1816 G1817 U1818 A1819 U1820 A1821 G1828 A1829 C1838 G1839 A1847 A1848 A1858 G1869 C1870 A1871 A1872 G1884 A1900 A1901 G1906
A1912 A1913 C1914 A1918 A1919 A1927 G1930 A1937 A1938 U1939 U1940 C1941 C1942 U1943 U1944 G1945 G1954 U1955 U1956 C1961 C1962 U1963 G1964 C1965 A1966 C1967 A1970 U1971 G1972 G1975 A1981 U1991 G1992 U1993 C1996 C1997 A2009 G2012 U2017 G2018 C2021 U2022 C2023 G2024
G2027 A2030 A2031 G2032 A2033 U2034 G2035 C2036 U2041 A2042 C2043 G2049 C2050 A2051 A2052 C2055 G2056 A2060 G2061 A2062 U2068 G2069 C2072 C2073 U2074 U2092 G2093 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G U G U A G G A U A G G U G G G
A G G C U U U G2133 A2134 A2135 G2138 U2139 A2142 C2143 G2144 C2145 C2146 A2147 G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G A G C C G A C C U U G A A A U A C C A C C C2179 U2180 U2181 U2182 A2183 A2184 A2198 A2199
G2204 U2210 A2211 A2212 U2213 U2220 A2225 C2226 G2238 G2239 U2243 U2244 U2249 G2250 G2251 C2258 U2259 A2266 A2267 A2273 A2274 C2275 G2276 G2277 A2278 G2282 C2283 G2286 A2287 A2288 G2289 A2297 U2305 C2306 G2307 G2308 A2309 C2310 A2311 G2319 U2320 U2321 A2322 G2323 U2324

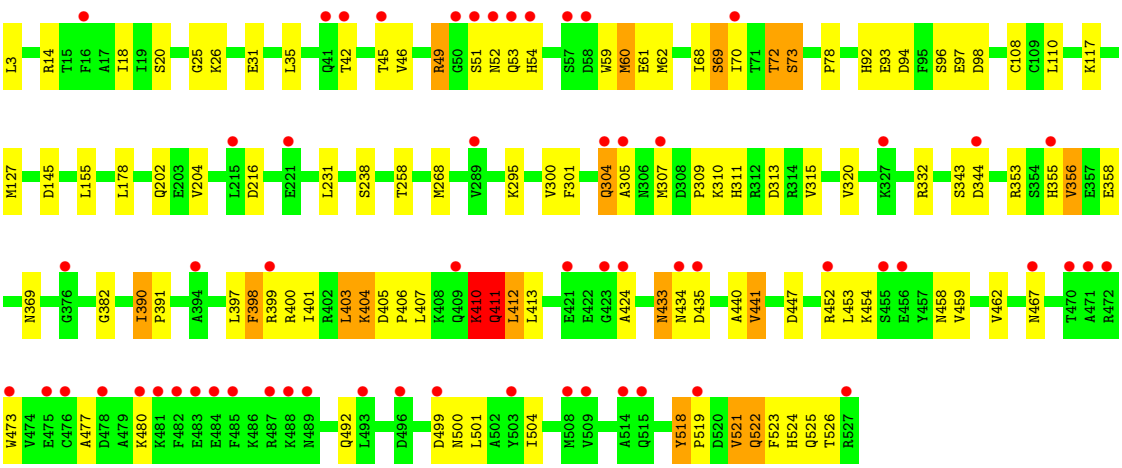


• Molecule 53: 5S ribosomal RNA

Chain u: 84% 16%

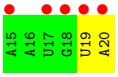
• Molecule 54: Peptide chain release factor 3

Chain v: 11% 78% 18%



• Molecule 55: messenger RNA

Chain w: 83% 67% 33%



• Molecule 56: Viomycin

Chain y: 50% 50%

• Molecule 56: Viomycin

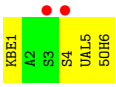
Chain z:

• Molecule 56: Viomycin

Chain 7:

• Molecule 56: Viomycin

Chain AA:



• Molecule 56: Viomycin

Chain BA:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	257.60Å 312.90Å 328.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.10 59.36 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (100.00-3.10) 99.9 (59.36-3.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6	Depositor
R, R_{free}	0.210 , 0.240 0.236 , 0.241	Depositor DCC
R_{free} test set	26311 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	64.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 86.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	146817	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UAL, DPP, KBE, 5OH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.33	0/1732	0.59	0/2333
2	B	0.34	0/1652	0.61	0/2225
3	C	0.34	0/1665	0.61	0/2227
4	D	0.38	0/1119	0.70	0/1504
5	E	0.34	0/836	0.57	0/1128
6	F	0.27	0/1196	0.54	0/1602
7	G	0.34	0/989	0.61	0/1326
8	H	0.31	0/1034	0.59	0/1375
9	I	0.33	0/797	0.63	0/1077
10	J	0.34	0/893	0.61	0/1205
11	K	0.44	0/969	0.79	0/1300
12	L	0.24	0/893	0.54	0/1193
13	M	0.32	0/785	0.56	0/1043
14	N	0.32	0/722	0.60	0/964
15	O	0.39	0/659	0.63	0/884
16	P	0.35	0/658	0.65	0/881
17	Q	0.39	0/463	0.59	0/621
18	R	0.28	0/653	0.54	0/877
19	S	0.37	0/671	0.58	0/888
20	T	0.38	0/431	0.58	0/570
21	U	0.47	0/2122	0.83	1/2852 (0.0%)
22	V	0.52	0/1586	0.82	1/2134 (0.0%)
23	W	0.41	0/1571	0.70	0/2113
24	X	0.32	0/1435	0.57	0/1926
25	Y	0.42	0/1343	0.71	0/1816
26	Z	0.26	0/1046	0.52	0/1410
27	0	0.47	0/1152	0.78	1/1551 (0.1%)
28	1	0.53	0/948	0.81	0/1268
29	2	0.39	0/1054	0.76	0/1403
30	3	0.46	0/1093	0.72	0/1460
31	4	0.45	0/974	0.76	0/1301
32	5	0.32	0/902	0.60	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	6	0.46	0/929	0.79	1/1242 (0.1%)
34	8	0.45	0/960	0.68	0/1278
35	9	0.39	0/829	0.71	0/1107
36	a	0.48	0/864	0.75	0/1156
37	b	0.43	0/745	0.76	0/994
38	c	0.41	0/788	0.73	0/1051
39	d	0.36	0/766	0.57	0/1025
40	e	0.49	0/603	0.79	1/797 (0.1%)
41	f	0.39	0/635	0.74	1/848 (0.1%)
42	g	0.36	0/510	0.71	0/677
43	h	0.37	0/453	0.67	0/605
44	i	0.47	0/450	0.78	0/599
45	j	0.33	0/417	0.55	0/554
46	k	0.50	0/380	0.79	0/498
47	l	0.41	0/513	0.70	0/676
48	m	0.46	0/303	0.83	1/397 (0.3%)
49	n	0.30	0/1248	0.60	0/1679
50	o	0.34	0/228	0.66	0/304
50	p	0.29	0/228	0.49	0/304
50	q	0.31	0/228	0.58	0/304
50	r	0.31	0/228	0.58	0/304
51	s	0.40	0/36806	0.74	26/57419 (0.0%)
52	t	0.53	0/68523	0.83	141/106893 (0.1%)
53	u	0.36	0/2825	0.69	0/4406
54	v	0.47	2/4221 (0.0%)	0.73	5/5702 (0.1%)
55	w	0.27	0/141	0.70	0/218
56	7	1.41	0/11	1.06	0/13
56	AA	1.56	0/11	0.97	0/13
56	BA	1.40	0/11	0.64	0/13
56	y	1.33	0/11	0.91	0/13
56	z	1.48	0/11	1.40	0/13
All	All	0.46	2/158919 (0.0%)	0.76	179/236768 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
51	s	0	29
52	t	0	109
53	u	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	v	0	2
All	All	0	141

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	v	72	THR	C-O	6.02	1.34	1.23
54	v	73	SER	CB-OG	5.44	1.49	1.42

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	t	1340	U	N1-C1'-C2'	10.45	127.59	114.00
52	t	974	G	N9-C1'-C2'	9.82	126.77	114.00
52	t	70	G	N9-C1'-C2'	9.73	126.65	114.00
52	t	2447	G	N9-C1'-C2'	9.40	126.22	114.00
52	t	2732	G	N9-C1'-C2'	9.32	126.12	114.00
52	t	686	U	N1-C1'-C2'	9.19	125.95	114.00
52	t	728	G	N9-C1'-C2'	9.03	125.74	114.00
52	t	1025	G	N9-C1'-C2'	8.91	125.59	114.00
52	t	249	C	N1-C1'-C2'	8.86	125.52	114.00
52	t	2030	A	N9-C1'-C2'	8.83	125.48	114.00
52	t	1250	G	N9-C1'-C2'	8.80	125.44	114.00
52	t	1237	A	N9-C1'-C2'	8.79	125.43	114.00
52	t	792	A	N9-C1'-C2'	8.56	125.12	114.00
52	t	2566	A	N9-C1'-C2'	8.33	124.83	114.00
52	t	1828	G	N9-C1'-C2'	8.32	124.81	114.00
52	t	746	U	N1-C1'-C2'	8.26	124.74	114.00
52	t	1820	U	N1-C1'-C2'	8.12	124.56	114.00
52	t	1252	G	N9-C1'-C2'	8.11	124.55	114.00
52	t	1955	U	N1-C1'-C2'	8.09	124.52	114.00
52	t	1210	G	N9-C1'-C2'	7.88	124.25	114.00
52	t	1311	G	N9-C1'-C2'	7.86	124.21	114.00
51	s	872	A	N9-C1'-C2'	7.69	124.00	114.00
52	t	1781	U	N1-C1'-C2'	7.64	123.93	114.00
52	t	1937	A	N9-C1'-C2'	7.61	123.89	114.00
52	t	1966	A	N9-C1'-C2'	7.57	123.84	114.00
52	t	2384	U	N1-C1'-C2'	7.49	123.73	114.00
51	s	1085	U	N1-C1'-C2'	7.47	123.71	114.00
52	t	332	A	N9-C1'-C2'	7.36	123.57	114.00
51	s	818	G	N9-C1'-C2'	7.28	123.47	114.00
52	t	1490	A	N9-C1'-C2'	7.25	123.43	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	t	1131	G	N9-C1'-C2'	7.22	123.39	114.00
52	t	2490	G	N9-C1'-C2'	7.15	123.30	114.00
51	s	1504	G	N9-C1'-C2'	7.13	123.26	114.00
52	t	1970	A	N9-C1'-C2'	7.11	123.24	114.00
52	t	1332	G	N9-C1'-C2'	7.07	123.19	114.00
52	t	506	G	N9-C1'-C2'	7.05	123.16	114.00
52	t	1428	C	N1-C1'-C2'	7.03	123.14	114.00
52	t	1653	G	N9-C1'-C2'	7.02	123.12	114.00
52	t	72	U	N1-C1'-C2'	6.99	123.09	114.00
52	t	2654	A	N9-C1'-C2'	6.99	123.08	114.00
52	t	2346	A	N9-C1'-C2'	6.87	122.93	114.00
52	t	119	A	N9-C1'-C2'	6.83	122.88	114.00
51	s	1065	U	N1-C1'-C2'	6.83	122.88	114.00
48	m	15	LYS	N-CA-C	6.80	129.37	111.00
51	s	266	G	N9-C1'-C2'	6.77	122.80	114.00
52	t	1634	A	N9-C1'-C2'	6.75	122.77	114.00
52	t	196	A	N9-C1'-C2'	6.74	122.77	114.00
52	t	1134	A	N9-C1'-C2'	6.71	122.72	114.00
52	t	1940	U	N1-C1'-C2'	6.67	122.68	114.00
51	s	328	C	N1-C1'-C2'	6.67	122.67	114.00
52	t	2249	U	N1-C1'-C2'	6.65	122.64	114.00
52	t	199	A	N9-C1'-C2'	6.63	122.62	114.00
52	t	995	C	N1-C1'-C2'	6.63	122.62	114.00
52	t	1128	G	N9-C1'-C2'	6.59	122.57	114.00
52	t	1253	A	N9-C1'-C2'	6.56	122.52	114.00
52	t	2491	U	N1-C1'-C2'	6.50	122.45	114.00
52	t	670	A	N9-C1'-C2'	6.44	122.37	114.00
51	s	47	C	N1-C1'-C2'	6.42	122.34	114.00
52	t	479	A	N9-C1'-C2'	6.42	122.34	114.00
52	t	323	C	N1-C1'-C2'	6.40	122.33	114.00
52	t	1938	A	N9-C1'-C2'	6.40	122.33	114.00
52	t	1247	A	N9-C1'-C2'	6.40	122.32	114.00
52	t	2022	U	C5'-C4'-C3'	-6.40	105.77	116.00
52	t	2751	G	N9-C1'-C2'	6.37	122.28	114.00
52	t	1786	A	N9-C1'-C2'	6.35	122.26	114.00
52	t	2689	U	N1-C1'-C2'	6.33	122.22	114.00
52	t	2654	A	C2'-C3'-O3'	6.31	123.79	113.70
51	s	1126	U	N1-C1'-C2'	6.30	122.19	114.00
52	t	774	G	N9-C1'-C2'	6.29	122.18	114.00
52	t	1758	U	N1-C1'-C2'	6.29	122.17	114.00
52	t	782	A	N9-C1'-C2'	6.27	122.15	114.00
52	t	1300	G	O4'-C1'-N9	6.20	113.16	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	t	2282	G	N9-C1'-C2'	6.17	122.03	114.00
54	v	26	LYS	CA-C-N	-6.17	103.63	117.20
52	t	685	A	N9-C1'-C2'	6.16	122.01	114.00
52	t	1301	A	N9-C1'-C2'	6.10	121.93	114.00
52	t	2035	G	N9-C1'-C2'	6.09	121.91	114.00
52	t	2713	U	N1-C1'-C2'	6.06	121.88	114.00
52	t	531	C	N1-C1'-C2'	6.04	121.86	114.00
51	s	367	U	N1-C1'-C2'	6.01	121.81	114.00
51	s	344	A	N9-C1'-C2'	5.98	121.78	114.00
52	t	1567	G	N9-C1'-C2'	5.96	121.74	114.00
51	s	870	U	N1-C1'-C2'	5.94	121.72	114.00
52	t	645	C	N1-C1'-C2'	5.92	121.69	114.00
51	s	109	A	N9-C1'-C2'	5.91	121.68	114.00
52	t	2051	A	N9-C1'-C2'	5.89	121.65	114.00
40	e	21	GLY	N-CA-C	-5.87	98.42	113.10
54	v	522	GLN	C-N-CA	5.87	136.37	121.70
52	t	829	A	N9-C1'-C2'	5.86	121.62	114.00
52	t	2198	A	N9-C1'-C2'	5.85	121.61	114.00
52	t	1667	G	N9-C1'-C2'	5.83	121.58	114.00
52	t	2021	C	OP1-P-O3'	5.83	118.02	105.20
51	s	1139	G	N9-C1'-C2'	5.81	121.56	114.00
51	s	244	U	N1-C1'-C2'	5.79	121.53	114.00
52	t	783	A	N9-C1'-C2'	-5.79	105.63	112.00
52	t	1324	G	N9-C1'-C2'	5.78	121.52	114.00
52	t	2572	A	N9-C1'-C2'	5.76	121.49	114.00
52	t	527	C	N1-C1'-C2'	5.75	121.48	114.00
52	t	331	C	N1-C1'-C2'	5.75	121.48	114.00
52	t	2572	A	OP1-P-O3'	5.72	117.79	105.20
52	t	458	G	N9-C1'-C2'	5.72	121.44	114.00
52	t	1329	U	N1-C1'-C2'	5.71	121.43	114.00
54	v	26	LYS	O-C-N	5.71	131.84	122.70
52	t	2629	U	N1-C1'-C2'	5.71	121.42	114.00
21	U	251	THR	N-CA-C	-5.70	95.62	111.00
52	t	776	G	N9-C1'-C2'	5.67	121.38	114.00
51	s	575	G	N9-C1'-C2'	5.65	121.34	114.00
52	t	512	G	N9-C1'-C2'	5.64	121.33	114.00
52	t	1522	A	N9-C1'-C2'	5.64	121.33	114.00
52	t	2266	A	N9-C1'-C2'	5.62	121.31	114.00
52	t	512	G	O4'-C1'-N9	5.61	112.69	108.20
51	s	717	U	N1-C1'-C2'	5.56	121.23	114.00
54	v	25	GLY	O-C-N	-5.55	113.82	122.70
52	t	457	A	N9-C1'-C2'	5.54	121.20	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	t	830	G	N9-C1'-C2'	5.54	121.20	114.00
52	t	1325	U	N1-C1'-C2'	5.54	121.20	114.00
52	t	119	A	C2'-C3'-O3'	5.52	122.53	113.70
52	t	301	G	N9-C1'-C2'	5.50	121.15	114.00
51	s	559	A	N9-C1'-C2'	5.50	121.14	114.00
52	t	2391	G	N9-C1'-C2'	5.49	121.14	114.00
52	t	1694	C	N1-C1'-C2'	5.46	121.10	114.00
52	t	1344	U	N1-C1'-C2'	5.46	121.09	114.00
52	t	1681	G	N9-C1'-C2'	5.44	121.07	114.00
52	t	2655	G	N9-C1'-C2'	5.43	121.06	114.00
51	s	1502	A	N9-C1'-C2'	5.43	121.06	114.00
52	t	125	A	N9-C1'-C2'	5.40	121.02	114.00
52	t	2503	A	N9-C1'-C2'	5.40	121.02	114.00
52	t	242	G	N9-C1'-C2'	5.39	121.01	114.00
52	t	1668	A	C2'-C3'-O3'	-5.39	97.65	109.50
51	s	1064	G	N9-C1'-C2'	5.37	120.98	114.00
52	t	2542	A	N9-C1'-C2'	5.37	120.98	114.00
22	V	191	GLY	N-CA-C	5.36	126.51	113.10
52	t	669	G	N9-C1'-C2'	5.36	120.97	114.00
52	t	1130	U	N1-C1'-C2'	5.33	120.93	114.00
51	s	518	C	O4'-C1'-N1	5.32	112.45	108.20
52	t	1022	G	N9-C1'-C2'	5.31	120.90	114.00
52	t	2502	G	N9-C1'-C2'	5.31	120.90	114.00
52	t	789	A	OP2-P-O3'	5.30	116.85	105.20
52	t	205	G	OP2-P-O3'	5.29	116.84	105.20
52	t	1565	C	N1-C1'-C2'	5.29	120.88	114.00
51	s	566	G	N9-C1'-C2'	5.29	120.88	114.00
41	f	29	LEU	CA-CB-CG	5.28	127.45	115.30
52	t	2725	A	N9-C1'-C2'	5.28	120.86	114.00
52	t	2032	G	N9-C1'-C2'	5.27	120.85	114.00
54	v	69	SER	N-CA-C	5.26	125.21	111.00
52	t	2238	G	N9-C1'-C2'	5.25	120.82	114.00
51	s	315	A	N9-C1'-C2'	5.24	120.81	114.00
51	s	13	U	N1-C1'-C2'	5.23	120.81	114.00
52	t	1236	G	N9-C1'-C2'	5.23	120.80	114.00
52	t	945	A	OP2-P-O3'	5.21	116.67	105.20
52	t	2287	A	N9-C1'-C2'	5.19	120.74	114.00
52	t	1250	G	O4'-C1'-N9	-5.18	104.06	108.20
51	s	792	A	O4'-C1'-N9	5.18	112.34	108.20
52	t	1012	U	N1-C1'-C2'	5.17	120.72	114.00
52	t	2024	G	OP2-P-O3'	5.17	116.57	105.20
52	t	1706	C	C2'-C3'-O3'	-5.16	98.15	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	t	395	U	N1-C1'-C2'	5.14	120.69	114.00
51	s	1101	A	N9-C1'-C2'	5.14	120.69	114.00
52	t	242	G	OP2-P-O3'	5.14	116.51	105.20
52	t	513	A	OP2-P-O3'	5.13	116.49	105.20
52	t	1954	G	N9-C1'-C2'	5.12	120.65	114.00
52	t	1780	A	N9-C1'-C2'	5.11	120.65	114.00
52	t	74	A	N9-C1'-C2'	5.11	120.64	114.00
52	t	311	A	N9-C1'-C2'	5.11	120.64	114.00
52	t	1342	A	N9-C1'-C2'	5.08	120.61	114.00
52	t	448	U	C5'-C4'-C3'	-5.08	107.87	116.00
52	t	793	A	N9-C1'-C2'	5.08	120.60	114.00
52	t	1247	A	C2'-C3'-O3'	5.08	121.82	113.70
52	t	859	G	N9-C1'-C2'	5.06	120.58	114.00
52	t	686	U	C1'-O4'-C4'	-5.05	105.86	109.90
52	t	571	U	N1-C1'-C2'	5.05	120.56	114.00
52	t	1962	C	C5'-C4'-O4'	-5.05	103.04	109.10
52	t	490	C	N1-C1'-C2'	5.04	120.55	114.00
27	0	82	GLY	N-CA-C	-5.02	100.55	113.10
33	6	6	GLN	N-CA-C	-5.02	97.44	111.00
52	t	2779	U	N1-C1'-C2'	5.02	120.53	114.00
52	t	2713	U	C1'-O4'-C4'	-5.01	105.89	109.90
52	t	222	A	N9-C1'-C2'	5.01	120.51	114.00
52	t	858	G	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	s	1064	G	Sidechain
51	s	1065	U	Sidechain
51	s	1067	A	Sidechain
51	s	1077	G	Sidechain
51	s	1085	U	Sidechain
51	s	1139	G	Sidechain
51	s	1181	G	Sidechain
51	s	1184	G	Sidechain
51	s	1200	C	Sidechain
51	s	1345	U	Sidechain
51	s	1391	U	Sidechain
51	s	1502	A	Sidechain
51	s	1527	U	Sidechain
51	s	266	G	Sidechain

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Mol	Chain	Res	Type	Group
51	s	362	G	Sidechain
51	s	388	G	Sidechain
51	s	428	G	Sidechain
51	s	51	A	Sidechain
51	s	527	G	Sidechain
51	s	533	A	Sidechain
51	s	566	G	Sidechain
51	s	7	A	Sidechain
51	s	717	U	Sidechain
51	s	760	G	Sidechain
51	s	780	A	Sidechain
51	s	863	U	Sidechain
51	s	870	U	Sidechain
51	s	883	C	Sidechain
51	s	968	A	Sidechain
52	t	100	U	Sidechain
52	t	1025	G	Sidechain
52	t	1125	G	Sidechain
52	t	1131	G	Sidechain
52	t	1134	A	Sidechain
52	t	1142	A	Sidechain
52	t	1156	A	Sidechain
52	t	1162	G	Sidechain
52	t	1203	U	Sidechain
52	t	1210	G	Sidechain
52	t	1247	A	Sidechain
52	t	1250	G	Sidechain
52	t	1266	G	Sidechain
52	t	1267	U	Sidechain
52	t	1270	C	Sidechain
52	t	1272	A	Sidechain
52	t	1280	G	Sidechain
52	t	1287	A	Sidechain
52	t	1306	C	Sidechain
52	t	1311	G	Sidechain
52	t	1325	U	Sidechain
52	t	1340	U	Sidechain
52	t	1383	A	Sidechain
52	t	1434	A	Sidechain
52	t	1567	G	Sidechain
52	t	1608	A	Sidechain
52	t	1613	G	Sidechain

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Mol	Chain	Res	Type	Group
52	t	1626	A	Sidechain
52	t	1632	A	Sidechain
52	t	1772	A	Sidechain
52	t	1775	U	Sidechain
52	t	1781	U	Sidechain
52	t	1818	U	Sidechain
52	t	1820	U	Sidechain
52	t	1828	G	Sidechain
52	t	1955	U	Sidechain
52	t	1966	A	Sidechain
52	t	1992	G	Sidechain
52	t	1996	C	Sidechain
52	t	2009	A	Sidechain
52	t	2012	G	Sidechain
52	t	2027	G	Sidechain
52	t	2030	A	Sidechain
52	t	2041	U	Sidechain
52	t	2074	U	Sidechain
52	t	2220	U	Sidechain
52	t	2243	U	Sidechain
52	t	2244	U	Sidechain
52	t	2267	A	Sidechain
52	t	2324	U	Sidechain
52	t	2384	U	Sidechain
52	t	2426	A	Sidechain
52	t	2449	U	Sidechain
52	t	2477	U	Sidechain
52	t	2481	G	Sidechain
52	t	2491	U	Sidechain
52	t	2495	G	Sidechain
52	t	2554	U	Sidechain
52	t	2572	A	Sidechain
52	t	2581	G	Sidechain
52	t	2587	A	Sidechain
52	t	2597	G	Sidechain
52	t	2609	U	Sidechain
52	t	2629	U	Sidechain
52	t	2645	G	Sidechain
52	t	2654	A	Sidechain
52	t	2659	G	Sidechain
52	t	2661	G	Sidechain
52	t	2690	U	Sidechain

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Mol	Chain	Res	Type	Group
52	t	2732	G	Sidechain
52	t	2777	G	Sidechain
52	t	2832	U	Sidechain
52	t	2834	G	Sidechain
52	t	2878	U	Sidechain
52	t	311	A	Sidechain
52	t	33	C	Sidechain
52	t	381	G	Sidechain
52	t	454	A	Sidechain
52	t	458	G	Sidechain
52	t	463	G	Sidechain
52	t	498	G	Sidechain
52	t	512	G	Sidechain
52	t	536	G	Sidechain
52	t	554	U	Sidechain
52	t	603	A	Sidechain
52	t	670	A	Sidechain
52	t	675	A	Sidechain
52	t	690	G	Sidechain
52	t	70	G	Sidechain
52	t	726	G	Sidechain
52	t	728	G	Sidechain
52	t	74	A	Sidechain
52	t	742	A	Sidechain
52	t	749	A	Sidechain
52	t	755	U	Sidechain
52	t	760	G	Sidechain
52	t	761	A	Sidechain
52	t	763	G	Sidechain
52	t	770	G	Sidechain
52	t	792	A	Sidechain
52	t	796	C	Sidechain
52	t	802	A	Sidechain
52	t	830	G	Sidechain
52	t	859	G	Sidechain
52	t	910	A	Sidechain
52	t	945	A	Sidechain
52	t	979	A	Sidechain
52	t	983	A	Sidechain
52	t	995	C	Sidechain
53	u	80	U	Sidechain
54	v	410	LYS	Peptide

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Mol	Chain	Res	Type	Group
54	v	411	GLN	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	216/218 (99%)	122 (56%)	56 (26%)	38 (18%)	0 0
2	B	204/206 (99%)	140 (69%)	36 (18%)	28 (14%)	0 1
3	C	203/205 (99%)	108 (53%)	46 (23%)	49 (24%)	0 0
4	D	148/150 (99%)	90 (61%)	36 (24%)	22 (15%)	0 0
5	E	98/100 (98%)	52 (53%)	26 (26%)	20 (20%)	0 0
6	F	149/151 (99%)	95 (64%)	41 (28%)	13 (9%)	1 4
7	G	127/129 (98%)	92 (72%)	29 (23%)	6 (5%)	2 14
8	H	125/127 (98%)	81 (65%)	26 (21%)	18 (14%)	0 1
9	I	96/98 (98%)	64 (67%)	17 (18%)	15 (16%)	0 0
10	J	115/117 (98%)	82 (71%)	21 (18%)	12 (10%)	0 3
11	K	121/123 (98%)	80 (66%)	20 (16%)	21 (17%)	0 0
12	L	112/114 (98%)	62 (55%)	33 (30%)	17 (15%)	0 0
13	M	92/100 (92%)	51 (55%)	27 (29%)	14 (15%)	0 0
14	N	86/88 (98%)	52 (60%)	28 (33%)	6 (7%)	1 7
15	O	80/82 (98%)	48 (60%)	18 (22%)	14 (18%)	0 0
16	P	78/80 (98%)	55 (70%)	10 (13%)	13 (17%)	0 0
17	Q	53/55 (96%)	30 (57%)	17 (32%)	6 (11%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	77/79 (98%)	45 (58%)	21 (27%)	11 (14%)	0	1
19	S	83/85 (98%)	51 (61%)	24 (29%)	8 (10%)	0	3
20	T	49/51 (96%)	25 (51%)	17 (35%)	7 (14%)	0	1
21	U	269/271 (99%)	204 (76%)	39 (14%)	26 (10%)	0	3
22	V	207/209 (99%)	138 (67%)	37 (18%)	32 (16%)	0	0
23	W	199/201 (99%)	135 (68%)	40 (20%)	24 (12%)	0	1
24	X	175/177 (99%)	114 (65%)	34 (19%)	27 (15%)	0	0
25	Y	174/176 (99%)	108 (62%)	36 (21%)	30 (17%)	0	0
26	Z	139/141 (99%)	66 (48%)	51 (37%)	22 (16%)	0	0
27	0	140/142 (99%)	94 (67%)	27 (19%)	19 (14%)	0	1
28	1	120/122 (98%)	82 (68%)	24 (20%)	14 (12%)	0	1
29	2	141/143 (99%)	94 (67%)	23 (16%)	24 (17%)	0	0
30	3	134/136 (98%)	95 (71%)	23 (17%)	16 (12%)	0	1
31	4	118/120 (98%)	83 (70%)	20 (17%)	15 (13%)	0	1
32	5	114/116 (98%)	79 (69%)	25 (22%)	10 (9%)	1	4
33	6	112/114 (98%)	71 (63%)	23 (20%)	18 (16%)	0	0
34	8	115/117 (98%)	73 (64%)	31 (27%)	11 (10%)	0	3
35	9	101/103 (98%)	73 (72%)	20 (20%)	8 (8%)	1	5
36	a	108/110 (98%)	80 (74%)	18 (17%)	10 (9%)	0	3
37	b	91/93 (98%)	54 (59%)	18 (20%)	19 (21%)	0	0
38	c	100/102 (98%)	63 (63%)	17 (17%)	20 (20%)	0	0
39	d	92/94 (98%)	62 (67%)	19 (21%)	11 (12%)	0	1
40	e	77/79 (98%)	29 (38%)	21 (27%)	27 (35%)	0	0
41	f	75/77 (97%)	54 (72%)	16 (21%)	5 (7%)	1	7
42	g	61/63 (97%)	34 (56%)	15 (25%)	12 (20%)	0	0
43	h	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	4
44	i	54/56 (96%)	44 (82%)	5 (9%)	5 (9%)	0	3
45	j	48/50 (96%)	32 (67%)	14 (29%)	2 (4%)	3	16
46	k	44/46 (96%)	36 (82%)	4 (9%)	4 (9%)	1	4
47	l	62/64 (97%)	45 (73%)	11 (18%)	6 (10%)	0	3
48	m	36/38 (95%)	30 (83%)	2 (6%)	4 (11%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	n	161/163 (99%)	77 (48%)	53 (33%)	31 (19%)	0	0
50	o	28/30 (93%)	12 (43%)	9 (32%)	7 (25%)	0	0
50	p	28/30 (93%)	16 (57%)	8 (29%)	4 (14%)	0	1
50	q	28/30 (93%)	14 (50%)	12 (43%)	2 (7%)	1	6
50	r	28/30 (93%)	19 (68%)	6 (21%)	3 (11%)	0	2
54	v	523/525 (100%)	381 (73%)	82 (16%)	60 (12%)	0	2
56	7	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
56	AA	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
56	BA	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
56	y	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
56	z	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
All	All	6280/6414 (98%)	4060 (65%)	1346 (21%)	874 (14%)	0	1

All (874) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ALA
1	A	67	LEU
1	A	75	ALA
1	A	94	ARG
1	A	120	SER
1	A	163	ILE
1	A	165	ALA
1	A	169	HIS
1	A	219	THR
2	B	14	VAL
2	B	112	ALA
2	B	186	SER
3	C	22	SER
3	C	24	VAL
3	C	28	ASP
3	C	31	CYS
3	C	33	ILE
3	C	34	GLU
3	C	36	ALA
3	C	52	VAL
3	C	108	ALA
3	C	143	SER

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Mol	Chain	Res	Type
3	C	147	LYS
3	C	150	LYS
3	C	152	SER
3	C	191	SER
3	C	192	ALA
4	D	100	GLU
4	D	122	VAL
4	D	144	GLU
4	D	153	ALA
5	E	7	VAL
5	E	56	LYS
5	E	61	LEU
5	E	69	GLU
5	E	91	ARG
6	F	95	ARG
6	F	110	ARG
6	F	129	ASN
7	G	3	GLN
8	H	22	PRO
8	H	34	LEU
8	H	44	ARG
8	H	71	ILE
9	I	36	VAL
9	I	57	VAL
9	I	62	ARG
9	I	88	MET
9	I	92	LEU
9	I	101	SER
10	J	26	PHE
10	J	76	TYR
10	J	107	THR
10	J	125	LYS
11	K	8	ARG
11	K	23	LEU
11	K	24	GLU
11	K	75	GLU
11	K	87	LYS
11	K	88	ASP
12	L	3	ILE
12	L	65	GLU
12	L	97	ARG
12	L	105	ALA

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Mol	Chain	Res	Type
13	M	44	VAL
13	M	45	LEU
13	M	51	PRO
13	M	52	ARG
13	M	87	ALA
13	M	91	GLU
14	N	3	SER
15	O	16	PHE
15	O	24	SER
15	O	45	GLU
16	P	11	VAL
16	P	12	VAL
16	P	16	MET
16	P	52	CYS
17	Q	54	LEU
18	R	62	THR
18	R	64	GLU
18	R	69	LYS
19	S	3	ILE
19	S	5	SER
19	S	67	HIS
20	T	8	ASN
20	T	23	GLU
20	T	25	ALA
20	T	34	ARG
21	U	9	SER
21	U	70	LYS
21	U	77	VAL
21	U	232	GLY
21	U	234	GLY
22	V	43	ASP
22	V	70	LYS
22	V	71	ALA
22	V	73	VAL
22	V	92	VAL
22	V	94	GLN
22	V	106	LYS
22	V	118	PHE
22	V	119	ALA
22	V	169	ARG
22	V	174	SER
22	V	175	LEU

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Mol	Chain	Res	Type
22	V	191	GLY
23	W	46	GLN
23	W	61	ARG
23	W	69	ARG
23	W	80	SER
23	W	165	HIS
23	W	166	LYS
23	W	175	ILE
24	X	160	LYS
24	X	175	PRO
25	Y	28	LYS
25	Y	31	GLU
25	Y	79	THR
25	Y	84	LYS
25	Y	118	ALA
25	Y	164	ALA
25	Y	167	VAL
25	Y	168	VAL
26	Z	3	LYS
26	Z	6	ALA
26	Z	22	PRO
26	Z	30	GLN
26	Z	85	ILE
26	Z	89	SER
26	Z	92	PRO
26	Z	97	VAL
27	0	13	ARG
27	0	25	LEU
27	0	41	LYS
27	0	44	TYR
27	0	73	VAL
27	0	81	ILE
28	1	3	GLN
28	1	16	ALA
28	1	75	SER
28	1	108	ARG
29	2	29	LYS
29	2	36	LYS
29	2	41	ARG
29	2	66	PHE
29	2	82	LEU
29	2	98	ALA

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Mol	Chain	Res	Type
29	2	111	ILE
29	2	116	VAL
30	3	2	LEU
30	3	60	GLN
30	3	69	PRO
30	3	77	PRO
30	3	134	THR
30	3	135	VAL
31	4	14	SER
31	4	80	PHE
31	4	93	GLY
31	4	101	GLY
31	4	117	ASP
33	6	19	PHE
33	6	33	GLU
33	6	37	LYS
33	6	50	ARG
33	6	83	ILE
33	6	103	THR
33	6	104	GLY
33	6	105	LYS
34	8	86	SER
34	8	91	ARG
34	8	114	ALA
35	9	40	MET
35	9	101	ILE
36	a	14	ALA
37	b	11	LEU
37	b	18	GLU
37	b	29	THR
37	b	73	ARG
37	b	74	ILE
37	b	86	THR
37	b	88	LYS
38	c	6	ARG
38	c	20	LYS
38	c	63	ALA
38	c	88	ASP
38	c	98	ASN
39	d	60	VAL
39	d	69	GLU
40	e	9	THR

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Mol	Chain	Res	Type
40	e	14	ASP
40	e	18	LYS
40	e	29	SER
40	e	30	VAL
40	e	36	ILE
40	e	47	GLY
40	e	50	VAL
40	e	70	VAL
40	e	82	GLU
42	g	24	GLU
42	g	25	GLN
42	g	46	VAL
43	h	13	ILE
44	i	23	ALA
45	j	51	ALA
47	l	22	LYS
48	m	37	GLN
49	n	11	ILE
49	n	47	GLU
49	n	48	ALA
49	n	55	VAL
49	n	60	LEU
49	n	70	GLU
49	n	94	ARG
49	n	95	LEU
49	n	108	VAL
49	n	118	ILE
49	n	124	ASP
49	n	145	GLU
49	n	147	SER
49	n	148	ALA
50	o	4	LYS
50	o	5	ASP
50	o	15	SER
50	o	26	MET
50	o	27	GLU
50	q	12	ALA
50	q	13	ALA
54	v	52	ASN
54	v	61	GLU
54	v	69	SER
54	v	98	ASP

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Mol	Chain	Res	Type
54	v	301	PHE
54	v	305	ALA
54	v	309	PRO
54	v	313	ASP
54	v	315	VAL
54	v	390	ILE
54	v	398	PHE
54	v	399	ARG
54	v	406	PRO
54	v	434	ASN
54	v	440	ALA
54	v	441	VAL
54	v	521	VAL
54	v	522	GLN
56	z	4	SER
56	AA	4	SER
1	A	9	LEU
1	A	15	PHE
1	A	21	TYR
1	A	32	GLY
1	A	37	VAL
1	A	38	HIS
1	A	86	CYS
1	A	100	LEU
1	A	123	GLY
1	A	136	ARG
1	A	150	ILE
1	A	170	ILE
1	A	206	ILE
2	B	8	GLY
2	B	36	PHE
2	B	60	ALA
2	B	88	LYS
2	B	113	LYS
2	B	155	ARG
3	C	6	PRO
3	C	29	THR
3	C	32	LYS
3	C	69	ARG
3	C	101	VAL
3	C	115	GLN
3	C	120	LYS

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Mol	Chain	Res	Type
3	C	125	ASN
3	C	127	ARG
3	C	148	ALA
3	C	165	GLU
3	C	197	HIS
4	D	23	THR
4	D	44	ARG
4	D	97	PRO
4	D	121	ASN
4	D	145	ASN
4	D	154	ALA
5	E	12	PRO
5	E	14	GLN
5	E	17	GLN
5	E	86	ARG
6	F	6	ILE
6	F	55	LYS
6	F	57	GLU
6	F	75	LYS
6	F	78	ARG
6	F	84	TYR
8	H	32	ARG
8	H	33	SER
8	H	40	ARG
8	H	53	LEU
8	H	119	LYS
8	H	127	SER
9	I	60	ASP
10	J	94	SER
10	J	102	ALA
11	K	117	GLY
12	L	13	HIS
12	L	18	LEU
12	L	44	ILE
12	L	46	GLU
12	L	98	GLY
13	M	61	ASN
15	O	44	SER
16	P	17	GLU
16	P	50	ASN
16	P	56	ASP
16	P	79	GLU

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Mol	Chain	Res	Type
17	Q	45	GLY
17	Q	48	ALA
18	R	5	LYS
18	R	44	ILE
18	R	46	LEU
19	S	6	ALA
19	S	68	LYS
20	T	12	ASP
21	U	140	VAL
21	U	142	ASN
21	U	185	ALA
21	U	239	PHE
21	U	260	LYS
21	U	264	LYS
22	V	72	GLY
22	V	91	THR
22	V	95	SER
22	V	121	THR
22	V	144	GLY
22	V	190	LYS
23	W	6	LYS
24	X	20	ASN
24	X	61	GLY
24	X	72	SER
24	X	95	MET
24	X	96	TRP
24	X	110	ILE
24	X	111	ARG
24	X	113	PHE
24	X	118	ALA
24	X	148	VAL
24	X	176	PHE
25	Y	9	VAL
25	Y	14	VAL
25	Y	30	GLY
25	Y	33	THR
25	Y	38	ASP
25	Y	44	HIS
25	Y	53	PRO
25	Y	60	GLY
25	Y	166	GLU
26	Z	62	ALA

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Mol	Chain	Res	Type
26	Z	83	ALA
26	Z	90	GLY
26	Z	96	LYS
27	0	4	PHE
27	0	12	LYS
27	0	45	THR
27	0	111	LYS
28	1	6	THR
28	1	50	GLY
28	1	93	GLN
29	2	3	LEU
29	2	10	GLU
29	2	15	ALA
29	2	30	THR
29	2	88	GLY
29	2	115	GLU
30	3	110	GLU
31	4	24	MET
31	4	32	GLU
31	4	86	ARG
32	5	22	GLY
32	5	57	ALA
32	5	67	ASN
32	5	100	HIS
32	5	101	GLY
32	5	106	LEU
33	6	65	ASN
33	6	79	VAL
33	6	100	ARG
34	8	5	ARG
35	9	55	ASP
35	9	79	ARG
35	9	100	GLY
36	a	13	SER
36	a	64	ALA
36	a	65	ASP
36	a	71	VAL
37	b	27	SER
37	b	38	ALA
37	b	39	THR
37	b	55	VAL
37	b	57	VAL

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Mol	Chain	Res	Type
37	b	65	GLY
38	c	50	ALA
38	c	75	ALA
38	c	92	VAL
38	c	97	SER
38	c	100	GLU
39	d	66	ASP
39	d	93	ARG
40	e	23	LYS
40	e	24	ARG
40	e	26	GLY
40	e	27	GLY
40	e	42	THR
41	f	34	SER
42	g	57	LEU
43	h	31	ILE
43	h	49	ALA
46	k	7	PRO
46	k	23	ALA
47	l	28	LEU
47	l	46	LYS
48	m	8	LYS
48	m	20	ASP
49	n	3	LEU
49	n	22	ALA
49	n	58	THR
49	n	80	THR
49	n	107	GLU
50	p	10	ALA
50	p	11	VAL
50	r	28	GLU
54	v	60	MET
54	v	68	ILE
54	v	96	SER
54	v	300	VAL
54	v	356	VAL
54	v	410	LYS
54	v	413	LEU
54	v	424	ALA
54	v	433	ASN
54	v	500	ASN
54	v	504	ILE

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Mol	Chain	Res	Type
54	v	524	HIS
54	v	526	THR
1	A	12	GLY
1	A	62	ARG
1	A	85	SER
1	A	115	ASP
1	A	132	GLU
1	A	158	ASP
2	B	26	LYS
2	B	72	PRO
2	B	81	GLU
2	B	145	ALA
3	C	35	GLN
3	C	84	ASN
3	C	106	PHE
3	C	132	ALA
3	C	161	ALA
3	C	167	PRO
3	C	172	VAL
3	C	174	ALA
3	C	177	MET
3	C	178	GLU
3	C	196	GLU
4	D	149	PRO
5	E	53	LYS
5	E	62	MET
6	F	16	LYS
7	G	87	ARG
7	G	116	ARG
8	H	56	MET
9	I	35	GLN
9	I	75	ASP
9	I	89	ARG
10	J	14	GLN
10	J	16	SER
10	J	88	PRO
11	K	27	PRO
11	K	42	LYS
11	K	77	SER
11	K	84	GLY
11	K	101	LEU
11	K	102	ASP

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Mol	Chain	Res	Type
11	K	122	LYS
12	L	4	ALA
12	L	104	ASN
13	M	75	LYS
13	M	88	MET
14	N	8	ALA
14	N	25	GLU
14	N	83	ARG
14	N	86	LEU
15	O	17	TYR
15	O	49	GLY
16	P	68	LYS
16	P	70	LYS
17	Q	55	ALA
18	R	4	LEU
21	U	11	GLY
21	U	23	LEU
21	U	34	GLU
21	U	58	LYS
21	U	109	LEU
21	U	184	GLU
21	U	196	ASN
21	U	256	THR
22	V	55	LYS
22	V	69	ALA
22	V	107	VAL
22	V	170	VAL
23	W	153	LEU
23	W	157	LEU
24	X	77	LYS
24	X	93	GLU
24	X	134	GLN
25	Y	45	ALA
25	Y	83	THR
25	Y	169	ARG
26	Z	49	GLU
26	Z	64	ARG
26	Z	129	GLU
27	0	94	ALA
28	1	35	VAL
28	1	46	ALA
28	1	71	ARG

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Mol	Chain	Res	Type
28	1	89	ASN
28	1	92	GLU
29	2	40	SER
29	2	65	GLY
29	2	81	ASP
29	2	83	ALA
30	3	58	LYS
30	3	121	ALA
31	4	2	ARG
31	4	3	HIS
31	4	60	VAL
31	4	88	ALA
32	5	32	PRO
32	5	61	GLN
33	6	20	ARG
33	6	42	PHE
33	6	110	LYS
34	8	87	VAL
35	9	48	LYS
37	b	10	VAL
37	b	40	LYS
37	b	54	GLU
37	b	69	ARG
38	c	7	ASP
38	c	77	GLY
38	c	81	ARG
39	d	54	ALA
39	d	74	ALA
40	e	41	GLY
41	f	43	LYS
42	g	22	LEU
43	h	34	THR
44	i	17	SER
44	i	32	THR
48	m	16	ILE
49	n	78	GLY
49	n	135	ALA
54	v	18	ILE
54	v	49	ARG
54	v	53	GLN
54	v	54	HIS
54	v	62	MET

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Mol	Chain	Res	Type
54	v	92	HIS
54	v	391	PRO
54	v	404	LYS
54	v	405	ASP
54	v	435	ASP
54	v	477	ALA
54	v	492	GLN
54	v	523	PHE
1	A	76	SER
1	A	159	ALA
1	A	177	ASN
2	B	7	ASN
2	B	135	ARG
2	B	136	ALA
2	B	205	GLU
3	C	27	ILE
3	C	166	LYS
3	C	190	LEU
4	D	42	ASN
4	D	102	THR
4	D	146	MET
5	E	54	LEU
5	E	55	HIS
6	F	83	THR
7	G	109	VAL
8	H	38	PHE
8	H	41	GLU
8	H	72	SER
8	H	120	ALA
9	I	91	ASP
11	K	49	ARG
11	K	116	TYR
12	L	113	LYS
13	M	3	GLN
13	M	47	LEU
13	M	58	ARG
13	M	69	PRO
13	M	80	ARG
14	N	45	HIS
15	O	31	ARG
15	O	64	GLY
16	P	5	ARG

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Mol	Chain	Res	Type
16	P	51	GLU
17	Q	66	LEU
18	R	61	VAL
19	S	27	MET
19	S	69	ASN
21	U	64	VAL
21	U	204	LEU
21	U	231	HIS
21	U	258	SER
22	V	86	GLU
22	V	109	VAL
22	V	179	ARG
22	V	194	PRO
23	W	123	LYS
23	W	124	PHE
23	W	148	ILE
24	X	86	CYS
24	X	94	ARG
24	X	103	ILE
24	X	151	LEU
25	Y	75	VAL
25	Y	113	ASP
26	Z	9	LYS
27	0	14	ASP
27	0	21	THR
27	0	133	ALA
30	3	43	ALA
30	3	59	ARG
30	3	73	ILE
30	3	100	LYS
31	4	91	ALA
31	4	92	GLY
32	5	6	ALA
33	6	86	LYS
33	6	93	LYS
34	8	73	ILE
34	8	76	SER
34	8	88	GLU
35	9	28	ALA
36	a	3	THR
36	a	66	ILE
36	a	96	ILE

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Mol	Chain	Res	Type
37	b	36	LYS
38	c	49	PRO
38	c	51	LEU
38	c	54	PRO
38	c	101	THR
39	d	13	GLY
39	d	37	PRO
39	d	71	LYS
40	e	10	ARG
40	e	15	SER
40	e	16	GLU
40	e	52	CYS
40	e	56	HIS
41	f	17	ARG
41	f	42	GLU
41	f	71	ARG
42	g	6	LEU
42	g	9	LYS
42	g	36	GLN
43	h	3	THR
46	k	17	GLY
49	n	56	ARG
49	n	88	HIS
49	n	106	PHE
49	n	125	ARG
49	n	144	LYS
49	n	154	THR
50	r	11	VAL
50	r	12	ALA
54	v	20	SER
54	v	295	LYS
54	v	403	LEU
54	v	412	LEU
54	v	480	LYS
56	7	4	SER
1	A	11	ALA
1	A	18	GLN
1	A	81	ASP
2	B	13	ILE
2	B	52	SER
2	B	65	VAL
2	B	167	TYR

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Mol	Chain	Res	Type
3	C	58	GLN
3	C	105	GLY
3	C	142	VAL
3	C	153	ARG
3	C	154	VAL
4	D	10	LEU
4	D	24	VAL
4	D	41	GLY
4	D	53	ARG
4	D	69	ASN
5	E	8	PHE
5	E	92	THR
6	F	130	LYS
7	G	20	ASN
9	I	93	ALA
10	J	46	ALA
10	J	73	VAL
11	K	56	LEU
11	K	73	LEU
11	K	78	VAL
12	L	78	ARG
15	O	11	ALA
15	O	12	LYS
15	O	23	ASP
15	O	26	ASN
16	P	31	PRO
17	Q	44	THR
19	S	39	GLU
20	T	22	CYS
21	U	21	PRO
21	U	37	SER
21	U	110	LYS
22	V	122	VAL
22	V	133	THR
22	V	173	GLN
23	W	9	GLN
23	W	13	THR
23	W	45	ALA
23	W	49	ARG
23	W	73	ILE
23	W	79	ARG
23	W	83	VAL

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Mol	Chain	Res	Type
23	W	96	VAL
23	W	151	GLY
24	X	8	LYS
24	X	108	PRO
24	X	132	ARG
24	X	133	GLU
25	Y	68	ARG
25	Y	85	LYS
25	Y	117	PRO
25	Y	170	THR
26	Z	131	THR
27	0	33	ALA
27	0	74	TYR
27	0	125	TYR
29	2	19	LEU
29	2	87	GLY
29	2	133	ALA
30	3	28	PHE
30	3	46	ILE
33	6	63	ILE
36	a	95	ARG
37	b	70	HIS
40	e	11	ASN
40	e	68	PHE
40	e	73	PRO
40	e	76	ARG
42	g	7	ARG
42	g	37	LEU
42	g	41	HIS
44	i	55	ALA
45	j	43	ARG
46	k	45	SER
47	l	59	ALA
49	n	2	ALA
49	n	72	LEU
49	n	127	ALA
50	o	16	VAL
54	v	93	GLU
54	v	304	GLN
54	v	467	ASN
54	v	473	TRP
1	A	43	GLU

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Mol	Chain	Res	Type
1	A	209	VAL
2	B	48	LYS
2	B	92	ASP
4	D	101	GLY
4	D	104	ILE
5	E	16	GLU
5	E	50	PRO
8	H	9	GLY
8	H	39	GLY
8	H	54	VAL
9	I	74	VAL
10	J	79	LYS
12	L	14	ALA
12	L	103	THR
22	V	145	SER
23	W	70	SER
23	W	163	ASN
24	X	125	GLY
25	Y	11	PRO
25	Y	16	VAL
25	Y	97	VAL
26	Z	119	ALA
29	2	103	ILE
30	3	3	GLN
31	4	84	GLY
32	5	56	LYS
33	6	5	LYS
34	8	100	PHE
35	9	98	ILE
39	d	84	PRO
40	e	74	LYS
47	l	31	ILE
47	l	58	ILE
50	p	29	LYS
54	v	320	VAL
54	v	407	LEU
54	v	411	GLN
2	B	97	PRO
2	B	107	LYS
3	C	63	ILE
3	C	124	VAL
7	G	56	PRO

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Mol	Chain	Res	Type
11	K	15	VAL
15	O	15	PRO
18	R	41	PRO
18	R	74	ALA
24	X	135	ILE
26	Z	18	ASN
34	8	6	GLY
36	a	29	VAL
38	c	53	GLN
44	i	54	ILE
50	o	2	ILE
4	D	113	VAL
5	E	60	VAL
20	T	9	GLU
25	Y	155	PRO
27	0	110	PRO
28	1	72	PRO
40	e	37	VAL
50	p	8	ILE
54	v	518	TYR
1	A	223	GLY
2	B	74	ILE
2	B	90	VAL
2	B	105	VAL
3	C	23	GLY
5	E	96	VAL
9	I	42	LEU
15	O	42	ILE
18	R	25	GLY
22	V	151	THR
24	X	136	ILE
26	Z	88	GLY
27	0	124	VAL
42	g	62	GLY
5	E	29	ILE
6	F	13	PRO
9	I	8	ILE
11	K	21	PRO
12	L	16	ILE
12	L	96	VAL
26	Z	8	VAL
26	Z	25	PRO

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Mol	Chain	Res	Type
29	2	34	GLY
29	2	140	GLY
34	8	97	ILE
38	c	38	ILE
38	c	69	VAL
54	v	78	PRO
54	v	382	GLY
1	A	200	PRO
28	1	48	PRO
39	d	72	VAL
49	n	149	GLY
54	v	519	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/180 (99%)	152 (85%)	27 (15%)	3	12
2	B	170/170 (100%)	153 (90%)	17 (10%)	7	28
3	C	172/172 (100%)	150 (87%)	22 (13%)	4	18
4	D	113/113 (100%)	101 (89%)	12 (11%)	6	26
5	E	87/87 (100%)	76 (87%)	11 (13%)	4	18
6	F	124/124 (100%)	114 (92%)	10 (8%)	11	39
7	G	104/104 (100%)	98 (94%)	6 (6%)	20	51
8	H	105/105 (100%)	91 (87%)	14 (13%)	4	16
9	I	86/86 (100%)	73 (85%)	13 (15%)	3	12
10	J	90/90 (100%)	75 (83%)	15 (17%)	2	9
11	K	103/103 (100%)	93 (90%)	10 (10%)	8	30
12	L	92/92 (100%)	86 (94%)	6 (6%)	17	47
13	M	79/83 (95%)	73 (92%)	6 (8%)	13	41
14	N	76/76 (100%)	66 (87%)	10 (13%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	65/65 (100%)	56 (86%)	9 (14%)	3	16
16	P	74/74 (100%)	60 (81%)	14 (19%)	1	6
17	Q	48/48 (100%)	42 (88%)	6 (12%)	4	18
18	R	70/70 (100%)	65 (93%)	5 (7%)	14	44
19	S	65/65 (100%)	59 (91%)	6 (9%)	9	33
20	T	44/44 (100%)	40 (91%)	4 (9%)	9	33
21	U	216/216 (100%)	188 (87%)	28 (13%)	4	18
22	V	164/164 (100%)	144 (88%)	20 (12%)	5	19
23	W	165/165 (100%)	148 (90%)	17 (10%)	7	27
24	X	148/148 (100%)	135 (91%)	13 (9%)	10	36
25	Y	137/137 (100%)	116 (85%)	21 (15%)	2	12
26	Z	109/109 (100%)	104 (95%)	5 (5%)	27	59
27	0	116/116 (100%)	97 (84%)	19 (16%)	2	10
28	1	103/103 (100%)	90 (87%)	13 (13%)	4	18
29	2	102/102 (100%)	90 (88%)	12 (12%)	5	21
30	3	109/109 (100%)	95 (87%)	14 (13%)	4	18
31	4	100/100 (100%)	91 (91%)	9 (9%)	9	34
32	5	86/86 (100%)	79 (92%)	7 (8%)	11	39
33	6	99/99 (100%)	89 (90%)	10 (10%)	7	28
34	8	89/89 (100%)	77 (86%)	12 (14%)	4	16
35	9	84/84 (100%)	78 (93%)	6 (7%)	14	44
36	a	93/93 (100%)	82 (88%)	11 (12%)	5	21
37	b	80/80 (100%)	73 (91%)	7 (9%)	10	36
38	c	83/83 (100%)	75 (90%)	8 (10%)	8	31
39	d	78/78 (100%)	74 (95%)	4 (5%)	24	56
40	e	59/59 (100%)	49 (83%)	10 (17%)	2	9
41	f	67/67 (100%)	57 (85%)	10 (15%)	3	13
42	g	55/55 (100%)	51 (93%)	4 (7%)	14	43
43	h	48/48 (100%)	36 (75%)	12 (25%)	0	2
44	i	47/47 (100%)	40 (85%)	7 (15%)	3	13
45	j	45/45 (100%)	42 (93%)	3 (7%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	k	38/38 (100%)	34 (90%)	4 (10%)	7	26
47	l	51/51 (100%)	49 (96%)	2 (4%)	32	65
48	m	34/34 (100%)	29 (85%)	5 (15%)	3	13
49	n	123/123 (100%)	112 (91%)	11 (9%)	9	34
50	o	26/26 (100%)	23 (88%)	3 (12%)	5	22
50	p	26/26 (100%)	25 (96%)	1 (4%)	33	66
50	q	26/26 (100%)	26 (100%)	0	100	100
50	r	26/26 (100%)	23 (88%)	3 (12%)	5	22
54	v	447/449 (100%)	381 (85%)	66 (15%)	3	13
56	7	2/2 (100%)	2 (100%)	0	100	100
56	AA	2/2 (100%)	2 (100%)	0	100	100
56	BA	2/2 (100%)	2 (100%)	0	100	100
56	y	2/2 (100%)	2 (100%)	0	100	100
56	z	2/2 (100%)	2 (100%)	0	100	100
All	All	5235/5242 (100%)	4635 (88%)	600 (12%)	5	22

All (600) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	15	PHE
1	A	20	ARG
1	A	21	TYR
1	A	26	MET
1	A	29	PHE
1	A	31	PHE
1	A	49	PHE
1	A	90	PHE
1	A	100	LEU
1	A	108	GLN
1	A	115	ASP
1	A	119	GLN
1	A	122	ASP
1	A	125	PHE
1	A	129	THR
1	A	135	MET
1	A	136	ARG

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Mol	Chain	Res	Type
1	A	143	LEU
1	A	158	ASP
1	A	170	ILE
1	A	174	GLU
1	A	183	PHE
1	A	189	ASN
1	A	206	ILE
1	A	212	TYR
1	A	221	ARG
2	B	13	ILE
2	B	15	LYS
2	B	19	SER
2	B	20	THR
2	B	27	GLU
2	B	36	PHE
2	B	54	ILE
2	B	106	ARG
2	B	120	THR
2	B	135	ARG
2	B	143	LEU
2	B	148	ILE
2	B	149	LYS
2	B	166	TRP
2	B	167	TYR
2	B	184	ASN
2	B	192	TYR
3	C	10	LEU
3	C	19	PHE
3	C	25	ARG
3	C	32	LYS
3	C	33	ILE
3	C	54	LEU
3	C	55	ARG
3	C	63	ILE
3	C	69	ARG
3	C	71	PHE
3	C	75	TYR
3	C	93	LEU
3	C	109	THR
3	C	110	ARG
3	C	119	HIS
3	C	127	ARG

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Mol	Chain	Res	Type
3	C	131	ILE
3	C	140	ASP
3	C	160	LEU
3	C	162	GLU
3	C	190	LEU
3	C	198	LEU
4	D	10	LEU
4	D	14	LEU
4	D	29	ILE
4	D	45	VAL
4	D	68	ARG
4	D	77	ASN
4	D	94	PHE
4	D	95	MET
4	D	100	GLU
4	D	120	HIS
4	D	155	LYS
4	D	156	ARG
5	E	4	TYR
5	E	14	GLN
5	E	17	GLN
5	E	24	ARG
5	E	36	ILE
5	E	51	ILE
5	E	54	LEU
5	E	55	HIS
5	E	85	ILE
5	E	86	ARG
5	E	93	LYS
6	F	3	ARG
6	F	4	ARG
6	F	11	ILE
6	F	12	LEU
6	F	25	PHE
6	F	49	LEU
6	F	62	GLU
6	F	69	ARG
6	F	108	ARG
6	F	150	PHE
7	G	15	ASN
7	G	72	GLU
7	G	74	ILE

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Mol	Chain	Res	Type
7	G	75	GLN
7	G	93	LYS
7	G	120	LEU
8	H	21	LYS
8	H	32	ARG
8	H	35	GLU
8	H	45	MET
8	H	48	ARG
8	H	61	ASP
8	H	62	LEU
8	H	67	LYS
8	H	84	ARG
8	H	87	MET
8	H	89	TYR
8	H	105	ARG
8	H	119	LYS
8	H	126	PHE
9	I	14	ASP
9	I	18	ILE
9	I	44	THR
9	I	46	LYS
9	I	63	ASP
9	I	67	ILE
9	I	73	LEU
9	I	78	GLU
9	I	81	GLU
9	I	83	THR
9	I	89	ARG
9	I	92	LEU
9	I	100	ILE
10	J	14	GLN
10	J	17	ASP
10	J	22	ILE
10	J	30	ILE
10	J	45	THR
10	J	51	PHE
10	J	55	ARG
10	J	76	TYR
10	J	79	LYS
10	J	81	LEU
10	J	82	GLU
10	J	85	VAL

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Mol	Chain	Res	Type
10	J	108	ASN
10	J	117	HIS
10	J	128	VAL
11	K	14	LYS
11	K	27	PRO
11	K	28	GLN
11	K	49	ARG
11	K	51	VAL
11	K	57	THR
11	K	71	HIS
11	K	75	GLU
11	K	96	THR
11	K	102	ASP
12	L	10	ASP
12	L	28	ARG
12	L	81	ASP
12	L	100	ARG
12	L	101	THR
12	L	112	ARG
13	M	3	GLN
13	M	19	TYR
13	M	27	LYS
13	M	51	PRO
13	M	64	ARG
13	M	88	MET
14	N	5	GLU
14	N	14	PHE
14	N	16	ARG
14	N	23	SER
14	N	28	VAL
14	N	34	GLN
14	N	65	LEU
14	N	67	ASP
14	N	82	GLU
14	N	84	LEU
15	O	2	VAL
15	O	6	LEU
15	O	12	LYS
15	O	18	GLN
15	O	46	LYS
15	O	53	ASP
15	O	55	ASP

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Mol	Chain	Res	Type
15	O	63	GLN
15	O	77	GLU
16	P	3	LYS
16	P	15	LYS
16	P	16	MET
16	P	21	VAL
16	P	29	LYS
16	P	32	ILE
16	P	42	LYS
16	P	47	ASP
16	P	51	GLU
16	P	54	ILE
16	P	61	ARG
16	P	64	ARG
16	P	74	LEU
16	P	78	VAL
17	Q	25	ILE
17	Q	27	THR
17	Q	54	LEU
17	Q	56	ARG
17	Q	60	ARG
17	Q	71	ASP
18	R	13	HIS
18	R	40	PHE
18	R	60	PHE
18	R	64	GLU
18	R	79	TYR
19	S	30	PHE
19	S	35	TYR
19	S	42	ASP
19	S	53	MET
19	S	65	LEU
19	S	68	LYS
20	T	4	LYS
20	T	18	PHE
20	T	33	ARG
20	T	37	TYR
21	U	12	ARG
21	U	23	LEU
21	U	51	ARG
21	U	52	HIS
21	U	68	ARG

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Mol	Chain	Res	Type
21	U	73	ILE
21	U	76	VAL
21	U	79	ARG
21	U	93	VAL
21	U	114	GLN
21	U	123	ILE
21	U	128	THR
21	U	132	ARG
21	U	142	ASN
21	U	155	ARG
21	U	160	TYR
21	U	173	LEU
21	U	176	ARG
21	U	188	ARG
21	U	191	LEU
21	U	212	TRP
21	U	224	MET
21	U	226	PRO
21	U	228	ASP
21	U	254	LYS
21	U	265	PHE
21	U	269	ARG
21	U	270	ARG
22	V	4	LEU
22	V	17	GLU
22	V	40	LEU
22	V	50	VAL
22	V	91	THR
22	V	92	VAL
22	V	114	LYS
22	V	118	PHE
22	V	124	ARG
22	V	128	ARG
22	V	129	THR
22	V	150	GLN
22	V	151	THR
22	V	159	LYS
22	V	165	MET
22	V	170	VAL
22	V	175	LEU
22	V	177	VAL
22	V	201	LEU

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Mol	Chain	Res	Type
22	V	203	VAL
23	W	12	LEU
23	W	28	VAL
23	W	51	GLU
23	W	70	SER
23	W	73	ILE
23	W	78	TRP
23	W	102	ARG
23	W	108	ILE
23	W	109	LEU
23	W	118	LEU
23	W	119	ILE
23	W	123	LYS
23	W	127	GLU
23	W	150	THR
23	W	153	LEU
23	W	170	ARG
23	W	176	ASP
24	X	16	MET
24	X	34	THR
24	X	35	LEU
24	X	46	LYS
24	X	76	PHE
24	X	82	TYR
24	X	109	ARG
24	X	114	ARG
24	X	129	MET
24	X	132	ARG
24	X	146	ASP
24	X	151	LEU
24	X	157	THR
25	Y	8	VAL
25	Y	15	ASP
25	Y	18	ILE
25	Y	34	ARG
25	Y	55	ASP
25	Y	59	ASP
25	Y	68	ARG
25	Y	72	ASN
25	Y	76	ILE
25	Y	83	THR
25	Y	84	LYS

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Mol	Chain	Res	Type
25	Y	110	HIS
25	Y	120	ILE
25	Y	131	VAL
25	Y	132	LEU
25	Y	138	GLN
25	Y	140	ILE
25	Y	151	ARG
25	Y	162	ARG
25	Y	166	GLU
25	Y	167	VAL
26	Z	7	TYR
26	Z	68	PHE
26	Z	71	LYS
26	Z	131	THR
26	Z	135	MET
27	0	1	MET
27	0	2	LYS
27	0	18	VAL
27	0	23	LYS
27	0	25	LEU
27	0	30	THR
27	0	31	GLU
27	0	34	ARG
27	0	39	LYS
27	0	44	TYR
27	0	54	ILE
27	0	55	ILE
27	0	57	LEU
27	0	65	THR
27	0	103	ILE
27	0	111	LYS
27	0	131	ASN
27	0	135	GLN
27	0	140	LEU
28	1	8	LEU
28	1	18	ARG
28	1	32	TYR
28	1	41	ILE
28	1	47	ILE
28	1	51	LYS
28	1	58	LEU
28	1	73	ASP

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Mol	Chain	Res	Type
28	1	82	ASN
28	1	92	GLU
28	1	93	GLN
28	1	105	ARG
28	1	107	LEU
29	2	6	LEU
29	2	21	ARG
29	2	25	SER
29	2	47	ARG
29	2	50	PHE
29	2	55	MET
29	2	61	LEU
29	2	64	PHE
29	2	74	THR
29	2	121	THR
29	2	126	ARG
29	2	144	GLU
30	3	7	THR
30	3	24	THR
30	3	26	VAL
30	3	33	LEU
30	3	47	GLU
30	3	51	ARG
30	3	69	PRO
30	3	70	ASP
30	3	93	VAL
30	3	95	LEU
30	3	96	ILE
30	3	114	ARG
30	3	115	GLU
30	3	126	ILE
31	4	1	MET
31	4	3	HIS
31	4	27	SER
31	4	31	HIS
31	4	33	ILE
31	4	63	ARG
31	4	69	ARG
31	4	71	ARG
31	4	95	THR
32	5	9	ARG
32	5	20	GLU

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Mol	Chain	Res	Type
32	5	31	THR
32	5	35	ILE
32	5	102	ARG
32	5	103	VAL
32	5	106	LEU
33	6	3	ILE
33	6	14	GLN
33	6	25	VAL
33	6	28	LYS
33	6	37	LYS
33	6	38	ARG
33	6	39	LEU
33	6	58	PHE
33	6	83	ILE
33	6	108	ARG
34	8	8	ILE
34	8	29	ARG
34	8	43	GLN
34	8	50	ARG
34	8	59	LEU
34	8	63	ARG
34	8	65	ASN
34	8	69	ARG
34	8	88	GLU
34	8	93	ILE
34	8	94	LEU
34	8	96	ASP
35	9	22	LEU
35	9	39	LEU
35	9	46	GLU
35	9	48	LYS
35	9	55	ASP
35	9	87	GLN
36	a	4	ILE
36	a	7	HIS
36	a	15	GLN
36	a	33	LEU
36	a	40	ASN
36	a	69	LEU
36	a	78	GLU
36	a	81	SER
36	a	96	ILE

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Mol	Chain	Res	Type
36	a	99	ARG
36	a	101	SER
37	b	18	GLU
37	b	30	ILE
37	b	31	VAL
37	b	43	ILE
37	b	64	LYS
37	b	70	HIS
37	b	86	THR
38	c	6	ARG
38	c	8	ASP
38	c	10	VAL
38	c	18	LYS
38	c	43	LYS
38	c	61	GLU
38	c	67	SER
38	c	102	ILE
39	d	4	ILE
39	d	12	GLN
39	d	81	PRO
39	d	90	ASP
40	e	10	ARG
40	e	14	ASP
40	e	16	GLU
40	e	22	VAL
40	e	23	LYS
40	e	24	ARG
40	e	25	PHE
40	e	45	HIS
40	e	49	ASN
40	e	71	LYS
41	f	6	VAL
41	f	7	THR
41	f	10	ARG
41	f	17	ARG
41	f	26	ARG
41	f	29	LEU
41	f	47	THR
41	f	56	ARG
41	f	75	GLU
41	f	77	TYR
42	g	15	ASN

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Mol	Chain	Res	Type
42	g	39	GLN
42	g	41	HIS
42	g	58	ASN
43	h	2	LYS
43	h	4	ILE
43	h	6	ILE
43	h	8	GLN
43	h	15	ARG
43	h	17	PRO
43	h	30	ARG
43	h	31	ILE
43	h	34	THR
43	h	37	ARG
43	h	40	THR
43	h	51	SER
44	i	2	VAL
44	i	9	ARG
44	i	14	MET
44	i	21	LEU
44	i	26	SER
44	i	27	LEU
44	i	37	HIS
45	j	4	ILE
45	j	9	LYS
45	j	35	LEU
46	k	3	ARG
46	k	24	THR
46	k	34	ARG
46	k	39	ARG
47	l	7	ARG
47	l	56	LEU
48	m	2	LYS
48	m	3	VAL
48	m	12	ARG
48	m	13	ASN
48	m	17	VAL
49	n	3	LEU
49	n	7	ASP
49	n	29	ASP
49	n	36	ASP
49	n	61	ARG
49	n	70	GLU

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Mol	Chain	Res	Type
49	n	106	PHE
49	n	123	ILE
49	n	143	MET
49	n	145	GLU
49	n	154	THR
50	o	27	GLU
50	o	29	LYS
50	o	30	PHE
50	p	5	ASP
50	r	2	ILE
50	r	5	ASP
50	r	22	LEU
54	v	3	LEU
54	v	14	ARG
54	v	31	GLU
54	v	35	LEU
54	v	42	THR
54	v	45	THR
54	v	46	VAL
54	v	49	ARG
54	v	51	SER
54	v	59	TRP
54	v	60	MET
54	v	70	ILE
54	v	72	THR
54	v	73	SER
54	v	94	ASP
54	v	97	GLU
54	v	108	CYS
54	v	110	LEU
54	v	117	LYS
54	v	127	MET
54	v	145	ASP
54	v	155	LEU
54	v	178	LEU
54	v	202	GLN
54	v	204	VAL
54	v	216	ASP
54	v	231	LEU
54	v	238	SER
54	v	258	THR
54	v	268	MET

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Mol	Chain	Res	Type
54	v	304	GLN
54	v	307	MET
54	v	310	LYS
54	v	311	HIS
54	v	332	ARG
54	v	343	SER
54	v	344	ASP
54	v	353	ARG
54	v	355	HIS
54	v	356	VAL
54	v	358	GLU
54	v	369	ASN
54	v	390	ILE
54	v	397	LEU
54	v	398	PHE
54	v	400	ARG
54	v	401	ILE
54	v	403	LEU
54	v	404	LYS
54	v	410	LYS
54	v	411	GLN
54	v	412	LEU
54	v	433	ASN
54	v	441	VAL
54	v	447	ASP
54	v	452	ARG
54	v	453	LEU
54	v	454	LYS
54	v	458	ASN
54	v	459	VAL
54	v	462	VAL
54	v	499	ASP
54	v	501	LEU
54	v	518	TYR
54	v	521	VAL
54	v	525	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	189	ASN
2	B	101	ASN
3	C	35	GLN
3	C	39	GLN
3	C	73	ASN
3	C	84	ASN
3	C	130	ASN
3	C	135	GLN
4	D	11	GLN
4	D	81	GLN
5	E	37	HIS
6	F	67	ASN
6	F	141	HIS
7	G	15	ASN
8	H	24	ASN
8	H	49	GLN
10	J	14	GLN
10	J	39	ASN
10	J	108	ASN
12	L	7	ASN
13	M	3	GLN
13	M	59	GLN
13	M	65	GLN
14	N	61	GLN
16	P	46	HIS
18	R	52	ASN
19	S	20	ASN
19	S	47	GLN
19	S	81	GLN
21	U	24	HIS
21	U	85	ASN
21	U	114	GLN
21	U	152	GLN
21	U	199	HIS
21	U	259	ASN
22	V	136	ASN
22	V	140	HIS
22	V	150	GLN
22	V	173	GLN
23	W	41	GLN
23	W	136	GLN
24	X	26	GLN

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Mol	Chain	Res	Type
25	Y	114	HIS
26	Z	18	ASN
27	0	128	ASN
28	1	5	GLN
29	2	4	ASN
29	2	99	ASN
31	4	9	GLN
31	4	107	ASN
32	5	61	GLN
33	6	11	GLN
34	8	65	ASN
35	9	18	GLN
36	a	40	ASN
36	a	57	ASN
36	a	61	ASN
37	b	70	HIS
38	c	68	ASN
39	d	12	GLN
39	d	78	GLN
39	d	80	HIS
39	d	87	GLN
40	e	39	GLN
41	f	15	ASN
41	f	16	ASN
42	g	36	GLN
42	g	41	HIS
43	h	8	GLN
43	h	33	HIS
44	i	3	GLN
44	i	18	HIS
48	m	35	GLN
49	n	4	ASN
49	n	9	GLN
49	n	57	ASN
54	v	21	HIS
54	v	76	GLN
54	v	306	ASN
54	v	369	ASN
54	v	525	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	s	1531/1532 (99%)	298 (19%)	0
52	t	2845/2903 (98%)	660 (23%)	0
53	u	117/118 (99%)	18 (15%)	0
55	w	5/6 (83%)	2 (40%)	0
All	All	4498/4559 (98%)	978 (21%)	0

All (978) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	s	5	U
51	s	9	G
51	s	13	U
51	s	14	U
51	s	22	G
51	s	31	G
51	s	32	A
51	s	39	G
51	s	48	C
51	s	49	U
51	s	50	A
51	s	51	A
51	s	52	C
51	s	61	G
51	s	65	A
51	s	66	A
51	s	70	U
51	s	71	A
51	s	73	C
51	s	75	G
51	s	76	G
51	s	80	A
51	s	82	G
51	s	83	C
51	s	85	U
51	s	86	G
51	s	92	U
51	s	95	C
51	s	109	A
51	s	110	C
51	s	116	A
51	s	120	A
51	s	121	U
51	s	122	G

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Mol	Chain	Res	Type
51	s	141	G
51	s	144	G
51	s	151	A
51	s	159	G
51	s	163	C
51	s	182	A
51	s	183	C
51	s	197	A
51	s	198	G
51	s	204	G
51	s	205	A
51	s	209	U
51	s	210	C
51	s	212	G
51	s	219	U
51	s	240	G
51	s	244	U
51	s	245	U
51	s	247	G
51	s	250	A
51	s	251	G
51	s	252	U
51	s	266	G
51	s	267	C
51	s	273	U
51	s	275	G
51	s	281	G
51	s	289	G
51	s	306	A
51	s	328	C
51	s	329	A
51	s	330	C
51	s	332	G
51	s	344	A
51	s	345	C
51	s	346	G
51	s	352	C
51	s	354	G
51	s	367	U
51	s	368	U
51	s	373	A
51	s	389	A

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Mol	Chain	Res	Type
51	s	406	G
51	s	413	G
51	s	421	U
51	s	422	C
51	s	423	G
51	s	428	G
51	s	429	U
51	s	430	A
51	s	435	A
51	s	448	A
51	s	452	A
51	s	454	G
51	s	459	A
51	s	461	A
51	s	462	G
51	s	463	U
51	s	467	U
51	s	468	A
51	s	481	G
51	s	484	G
51	s	485	U
51	s	486	U
51	s	495	A
51	s	496	A
51	s	500	G
51	s	505	G
51	s	508	U
51	s	509	A
51	s	511	C
51	s	518	C
51	s	519	C
51	s	524	G
51	s	531	U
51	s	532	A
51	s	533	A
51	s	534	U
51	s	536	C
51	s	548	G
51	s	559	A
51	s	560	A
51	s	561	U
51	s	562	U

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Mol	Chain	Res	Type
51	s	563	A
51	s	564	C
51	s	566	G
51	s	567	G
51	s	572	A
51	s	573	A
51	s	575	G
51	s	576	C
51	s	577	G
51	s	596	A
51	s	633	G
51	s	642	A
51	s	665	A
51	s	687	A
51	s	688	G
51	s	701	U
51	s	702	A
51	s	703	G
51	s	704	A
51	s	721	G
51	s	722	G
51	s	723	U
51	s	724	G
51	s	725	G
51	s	733	G
51	s	747	A
51	s	748	G
51	s	752	G
51	s	753	A
51	s	754	C
51	s	777	A
51	s	792	A
51	s	793	U
51	s	794	A
51	s	799	G
51	s	813	U
51	s	815	A
51	s	817	C
51	s	818	G
51	s	819	A
51	s	820	U
51	s	821	G

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Mol	Chain	Res	Type
51	s	828	U
51	s	832	G
51	s	841	C
51	s	843	U
51	s	845	A
51	s	859	G
51	s	871	U
51	s	872	A
51	s	874	G
51	s	876	C
51	s	885	G
51	s	889	A
51	s	890	G
51	s	891	U
51	s	914	A
51	s	927	G
51	s	934	C
51	s	935	A
51	s	960	U
51	s	961	U
51	s	966	G
51	s	968	A
51	s	969	A
51	s	971	G
51	s	972	C
51	s	974	A
51	s	975	A
51	s	976	G
51	s	977	A
51	s	982	U
51	s	983	A
51	s	992	U
51	s	1004	A
51	s	1008	U
51	s	1022	A
51	s	1025	U
51	s	1030	U
51	s	1032	G
51	s	1033	G
51	s	1034	G
51	s	1037	C
51	s	1044	A

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Mol	Chain	Res	Type
51	s	1050	G
51	s	1053	G
51	s	1054	C
51	s	1064	G
51	s	1065	U
51	s	1067	A
51	s	1068	G
51	s	1085	U
51	s	1086	U
51	s	1094	G
51	s	1101	A
51	s	1102	A
51	s	1127	G
51	s	1130	A
51	s	1133	G
51	s	1136	C
51	s	1137	C
51	s	1138	G
51	s	1139	G
51	s	1140	C
51	s	1146	A
51	s	1157	A
51	s	1158	C
51	s	1159	U
51	s	1160	G
51	s	1167	A
51	s	1182	G
51	s	1183	U
51	s	1184	G
51	s	1196	A
51	s	1200	C
51	s	1201	A
51	s	1202	U
51	s	1212	U
51	s	1213	A
51	s	1224	U
51	s	1225	A
51	s	1226	C
51	s	1227	A
51	s	1238	A
51	s	1240	U
51	s	1241	G

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Mol	Chain	Res	Type
51	s	1257	A
51	s	1258	G
51	s	1260	G
51	s	1261	A
51	s	1262	C
51	s	1278	G
51	s	1280	A
51	s	1281	C
51	s	1285	A
51	s	1286	U
51	s	1287	A
51	s	1297	G
51	s	1299	A
51	s	1300	G
51	s	1301	U
51	s	1305	G
51	s	1319	A
51	s	1320	C
51	s	1322	C
51	s	1323	G
51	s	1346	A
51	s	1347	G
51	s	1348	U
51	s	1353	G
51	s	1360	A
51	s	1365	G
51	s	1380	U
51	s	1381	U
51	s	1394	A
51	s	1395	C
51	s	1396	A
51	s	1397	C
51	s	1400	C
51	s	1401	G
51	s	1413	A
51	s	1419	G
51	s	1441	A
51	s	1446	A
51	s	1448	C
51	s	1452	C
51	s	1453	G
51	s	1487	G

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Mol	Chain	Res	Type
51	s	1492	A
51	s	1494	G
51	s	1497	G
51	s	1498	U
51	s	1499	A
51	s	1502	A
51	s	1503	A
51	s	1504	G
51	s	1506	U
51	s	1517	G
51	s	1529	G
51	s	1530	G
52	t	10	A
52	t	12	U
52	t	13	A
52	t	14	A
52	t	33	C
52	t	34	U
52	t	35	G
52	t	42	A
52	t	46	G
52	t	50	U
52	t	51	G
52	t	52	A
52	t	61	C
52	t	63	A
52	t	70	G
52	t	71	A
52	t	72	U
52	t	73	A
52	t	74	A
52	t	75	G
52	t	85	G
52	t	91	A
52	t	92	U
52	t	101	A
52	t	102	U
52	t	103	A
52	t	118	A
52	t	119	A
52	t	120	U
52	t	121	G

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Mol	Chain	Res	Type
52	t	125	A
52	t	126	A
52	t	135	U
52	t	137	U
52	t	138	U
52	t	139	U
52	t	140	C
52	t	141	G
52	t	142	A
52	t	162	U
52	t	163	C
52	t	181	A
52	t	196	A
52	t	197	A
52	t	199	A
52	t	200	U
52	t	204	A
52	t	205	G
52	t	206	U
52	t	216	A
52	t	222	A
52	t	223	A
52	t	228	C
52	t	229	C
52	t	233	A
52	t	241	A
52	t	242	G
52	t	243	U
52	t	248	G
52	t	249	C
52	t	250	G
52	t	255	A
52	t	265	A
52	t	266	G
52	t	271	G
52	t	272	A
52	t	276	U
52	t	285	G
52	t	294	A
52	t	301	G
52	t	302	C
52	t	311	A

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Mol	Chain	Res	Type
52	t	312	G
52	t	322	A
52	t	323	C
52	t	324	A
52	t	329	G
52	t	330	A
52	t	331	C
52	t	332	A
52	t	335	C
52	t	345	A
52	t	346	A
52	t	353	C
52	t	359	G
52	t	361	G
52	t	362	A
52	t	371	A
52	t	372	G
52	t	373	U
52	t	383	C
52	t	386	G
52	t	387	U
52	t	388	G
52	t	390	U
52	t	391	A
52	t	395	U
52	t	396	G
52	t	405	U
52	t	411	G
52	t	412	A
52	t	422	A
52	t	424	G
52	t	435	C
52	t	443	A
52	t	447	A
52	t	448	U
52	t	449	A
52	t	455	C
52	t	457	A
52	t	458	G
52	t	459	U
52	t	475	C
52	t	479	A

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Mol	Chain	Res	Type
52	t	480	A
52	t	481	G
52	t	489	G
52	t	490	C
52	t	491	G
52	t	504	A
52	t	505	A
52	t	506	G
52	t	507	A
52	t	508	A
52	t	509	C
52	t	510	C
52	t	528	A
52	t	530	G
52	t	533	G
52	t	546	U
52	t	547	A
52	t	548	G
52	t	549	G
52	t	550	C
52	t	563	A
52	t	571	U
52	t	572	A
52	t	573	U
52	t	574	A
52	t	575	A
52	t	586	A
52	t	587	C
52	t	588	U
52	t	604	G
52	t	613	A
52	t	614	A
52	t	615	U
52	t	616	A
52	t	620	G
52	t	621	A
52	t	627	A
52	t	628	G
52	t	634	C
52	t	638	G
52	t	645	C
52	t	646	U

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Mol	Chain	Res	Type
52	t	647	G
52	t	654	A
52	t	655	A
52	t	656	G
52	t	668	A
52	t	669	G
52	t	670	A
52	t	671	C
52	t	686	U
52	t	687	C
52	t	705	A
52	t	717	C
52	t	727	A
52	t	728	G
52	t	729	G
52	t	730	A
52	t	747	U
52	t	762	U
52	t	763	G
52	t	764	A
52	t	775	G
52	t	776	G
52	t	777	G
52	t	782	A
52	t	784	G
52	t	785	G
52	t	789	A
52	t	790	U
52	t	791	C
52	t	792	A
52	t	793	A
52	t	794	A
52	t	800	A
52	t	801	G
52	t	802	A
52	t	805	G
52	t	806	C
52	t	811	U
52	t	812	C
52	t	819	A
52	t	827	U
52	t	828	U

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Mol	Chain	Res	Type
52	t	829	A
52	t	830	G
52	t	831	G
52	t	845	A
52	t	846	U
52	t	847	U
52	t	859	G
52	t	860	U
52	t	865	C
52	t	866	A
52	t	876	C
52	t	877	A
52	t	879	G
52	t	881	G
52	t	893	C
52	t	896	A
52	t	897	C
52	t	900	A
52	t	901	C
52	t	902	C
52	t	910	A
52	t	914	G
52	t	932	U
52	t	933	A
52	t	941	A
52	t	945	A
52	t	946	C
52	t	958	U
52	t	961	C
52	t	962	G
52	t	973	A
52	t	974	G
52	t	975	A
52	t	983	A
52	t	990	A
52	t	995	C
52	t	996	A
52	t	1008	A
52	t	1009	A
52	t	1011	G
52	t	1012	U
52	t	1013	C

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Mol	Chain	Res	Type
52	t	1021	A
52	t	1022	G
52	t	1023	U
52	t	1025	G
52	t	1026	G
52	t	1033	U
52	t	1034	G
52	t	1046	A
52	t	1060	U
52	t	1061	U
52	t	1062	G
52	t	1066	U
52	t	1067	A
52	t	1068	G
52	t	1070	A
52	t	1074	G
52	t	1083	U
52	t	1088	A
52	t	1098	A
52	t	1112	G
52	t	1126	A
52	t	1129	A
52	t	1130	U
52	t	1131	G
52	t	1132	U
52	t	1133	A
52	t	1134	A
52	t	1135	C
52	t	1136	G
52	t	1139	G
52	t	1141	U
52	t	1142	A
52	t	1143	A
52	t	1144	A
52	t	1151	A
52	t	1157	G
52	t	1168	G
52	t	1169	A
52	t	1175	A
52	t	1176	U
52	t	1180	U
52	t	1186	G

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Mol	Chain	Res	Type
52	t	1204	A
52	t	1205	A
52	t	1206	G
52	t	1210	G
52	t	1211	C
52	t	1212	G
52	t	1236	G
52	t	1238	G
52	t	1248	G
52	t	1249	U
52	t	1250	G
52	t	1251	C
52	t	1252	G
52	t	1253	A
52	t	1256	G
52	t	1266	G
52	t	1267	U
52	t	1271	G
52	t	1272	A
52	t	1273	U
52	t	1275	A
52	t	1276	A
52	t	1287	A
52	t	1288	G
52	t	1289	C
52	t	1300	G
52	t	1301	A
52	t	1302	A
52	t	1303	G
52	t	1306	C
52	t	1311	G
52	t	1312	U
52	t	1313	U
52	t	1320	C
52	t	1321	A
52	t	1324	G
52	t	1325	U
52	t	1329	U
52	t	1330	C
52	t	1332	G
52	t	1333	G
52	t	1341	G

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Mol	Chain	Res	Type
52	t	1342	A
52	t	1343	G
52	t	1344	U
52	t	1345	C
52	t	1352	U
52	t	1365	A
52	t	1378	A
52	t	1379	U
52	t	1383	A
52	t	1385	A
52	t	1386	C
52	t	1397	U
52	t	1416	G
52	t	1419	A
52	t	1420	A
52	t	1427	A
52	t	1428	C
52	t	1435	G
52	t	1451	C
52	t	1453	A
52	t	1454	C
52	t	1459	G
52	t	1461	C
52	t	1476	U
52	t	1482	G
52	t	1490	A
52	t	1491	G
52	t	1493	C
52	t	1497	U
52	t	1504	A
52	t	1507	C
52	t	1515	A
52	t	1522	A
52	t	1523	U
52	t	1524	G
52	t	1533	C
52	t	1534	U
52	t	1535	A
52	t	1536	C
52	t	1537	G
52	t	1555	G
52	t	1558	C

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Mol	Chain	Res	Type
52	t	1559	U
52	t	1560	G
52	t	1565	C
52	t	1568	G
52	t	1569	A
52	t	1578	U
52	t	1581	G
52	t	1583	A
52	t	1584	U
52	t	1585	C
52	t	1602	U
52	t	1603	A
52	t	1608	A
52	t	1610	A
52	t	1611	C
52	t	1616	A
52	t	1617	C
52	t	1618	A
52	t	1619	G
52	t	1622	G
52	t	1647	U
52	t	1648	U
52	t	1649	G
52	t	1653	G
52	t	1674	G
52	t	1675	C
52	t	1681	G
52	t	1682	G
52	t	1694	C
52	t	1695	G
52	t	1698	A
52	t	1699	G
52	t	1700	A
52	t	1706	C
52	t	1707	G
52	t	1713	A
52	t	1714	U
52	t	1715	G
52	t	1729	U
52	t	1730	C
52	t	1733	G
52	t	1738	G

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Mol	Chain	Res	Type
52	t	1758	U
52	t	1764	C
52	t	1773	A
52	t	1780	A
52	t	1781	U
52	t	1782	U
52	t	1784	A
52	t	1785	A
52	t	1799	G
52	t	1800	C
52	t	1801	A
52	t	1802	A
52	t	1808	A
52	t	1815	A
52	t	1816	C
52	t	1819	A
52	t	1820	U
52	t	1821	A
52	t	1829	A
52	t	1838	C
52	t	1839	G
52	t	1847	A
52	t	1848	A
52	t	1858	A
52	t	1869	G
52	t	1884	G
52	t	1900	A
52	t	1901	A
52	t	1906	G
52	t	1912	A
52	t	1913	A
52	t	1914	C
52	t	1918	A
52	t	1919	A
52	t	1927	A
52	t	1930	G
52	t	1937	A
52	t	1938	A
52	t	1939	U
52	t	1940	U
52	t	1941	C
52	t	1943	U

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Mol	Chain	Res	Type
52	t	1944	U
52	t	1945	G
52	t	1954	G
52	t	1955	U
52	t	1956	U
52	t	1961	C
52	t	1962	C
52	t	1963	U
52	t	1965	C
52	t	1966	A
52	t	1967	C
52	t	1970	A
52	t	1971	U
52	t	1972	G
52	t	1975	G
52	t	1981	A
52	t	1991	U
52	t	1992	G
52	t	1993	U
52	t	1996	C
52	t	1997	C
52	t	2017	U
52	t	2018	G
52	t	2021	C
52	t	2022	U
52	t	2023	C
52	t	2030	A
52	t	2031	A
52	t	2032	G
52	t	2033	A
52	t	2034	U
52	t	2035	G
52	t	2036	C
52	t	2043	C
52	t	2049	G
52	t	2051	A
52	t	2052	A
52	t	2055	C
52	t	2056	G
52	t	2060	A
52	t	2061	G
52	t	2062	A

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Mol	Chain	Res	Type
52	t	2068	U
52	t	2069	G
52	t	2072	C
52	t	2092	U
52	t	2093	G
52	t	2104	C
52	t	2134	A
52	t	2138	G
52	t	2139	U
52	t	2143	C
52	t	2144	G
52	t	2145	C
52	t	2147	A
52	t	2150	C
52	t	2155	U
52	t	2156	G
52	t	2180	U
52	t	2182	U
52	t	2183	A
52	t	2198	A
52	t	2199	A
52	t	2204	G
52	t	2210	U
52	t	2211	A
52	t	2213	U
52	t	2225	A
52	t	2226	C
52	t	2238	G
52	t	2239	G
52	t	2249	U
52	t	2250	G
52	t	2251	G
52	t	2258	C
52	t	2259	U
52	t	2266	A
52	t	2267	A
52	t	2273	A
52	t	2275	C
52	t	2276	G
52	t	2278	A
52	t	2282	G
52	t	2283	C

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Mol	Chain	Res	Type
52	t	2286	G
52	t	2289	G
52	t	2297	A
52	t	2305	U
52	t	2307	G
52	t	2309	A
52	t	2311	A
52	t	2319	G
52	t	2320	U
52	t	2321	U
52	t	2322	A
52	t	2325	G
52	t	2327	A
52	t	2333	A
52	t	2334	U
52	t	2335	A
52	t	2337	G
52	t	2345	G
52	t	2346	A
52	t	2347	C
52	t	2361	G
52	t	2382	G
52	t	2383	G
52	t	2384	U
52	t	2385	C
52	t	2402	U
52	t	2403	C
52	t	2407	A
52	t	2423	U
52	t	2424	C
52	t	2425	A
52	t	2426	A
52	t	2427	C
52	t	2428	G
52	t	2429	G
52	t	2430	A
52	t	2435	A
52	t	2439	A
52	t	2440	C
52	t	2441	U
52	t	2447	G
52	t	2448	A

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Mol	Chain	Res	Type
52	t	2449	U
52	t	2450	A
52	t	2458	G
52	t	2459	A
52	t	2476	A
52	t	2490	G
52	t	2491	U
52	t	2497	A
52	t	2502	G
52	t	2503	A
52	t	2504	U
52	t	2505	G
52	t	2506	U
52	t	2517	C
52	t	2518	A
52	t	2519	U
52	t	2520	C
52	t	2529	G
52	t	2554	U
52	t	2566	A
52	t	2567	G
52	t	2573	C
52	t	2582	G
52	t	2585	U
52	t	2586	U
52	t	2603	G
52	t	2609	U
52	t	2610	C
52	t	2613	U
52	t	2614	A
52	t	2615	U
52	t	2629	U
52	t	2630	G
52	t	2640	G
52	t	2645	G
52	t	2654	A
52	t	2655	G
52	t	2656	U
52	t	2663	G
52	t	2682	A
52	t	2689	U
52	t	2690	U

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Mol	Chain	Res	Type
52	t	2691	C
52	t	2712	C
52	t	2713	U
52	t	2714	G
52	t	2716	C
52	t	2726	A
52	t	2727	A
52	t	2732	G
52	t	2733	A
52	t	2744	G
52	t	2748	A
52	t	2750	A
52	t	2751	G
52	t	2752	C
52	t	2756	U
52	t	2757	A
52	t	2765	A
52	t	2776	A
52	t	2777	G
52	t	2778	A
52	t	2779	U
52	t	2780	G
52	t	2781	A
52	t	2791	G
52	t	2792	A
52	t	2799	A
52	t	2800	A
52	t	2818	U
52	t	2820	A
52	t	2833	U
52	t	2834	G
52	t	2835	A
52	t	2836	U
52	t	2849	U
52	t	2866	U
52	t	2867	G
52	t	2868	A
52	t	2879	A
52	t	2880	C
52	t	2883	A
52	t	2884	U
52	t	2894	G

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Mol	Chain	Res	Type
53	u	13	G
53	u	15	A
53	u	16	G
53	u	25	U
53	u	30	C
53	u	35	C
53	u	41	G
53	u	44	G
53	u	45	A
53	u	53	A
53	u	57	A
53	u	67	G
53	u	87	U
53	u	88	C
53	u	89	U
53	u	90	C
53	u	99	A
53	u	109	A
55	w	19	U
55	w	20	A

There are no RNA pucker outliers to report.

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

20 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	$\#\|Z\| > 2$
56	UAL	7	5	56	7,8,9	2.72	1 (14%)	5,9,11	1.18	0
56	KBE	7	1	56	8,8,9	0.73	0	7,8,10	1.22	1 (14%)
56	5OH	BA	6	56	8,12,13	1.17	0	3,16,18	2.21	2 (66%)
56	DPP	z	2	56	3,5,6	0.78	0	1,5,7	0.36	0
56	UAL	z	5	56	7,8,9	1.82	3 (42%)	5,9,11	2.61	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
56	DPP	y	2	56	3,5,6	0.39	0	1,5,7	0.30	0
56	UAL	BA	5	56	7,8,9	2.69	1 (14%)	5,9,11	1.62	1 (20%)
56	KBE	BA	1	56	8,8,9	1.21	1 (12%)	7,8,10	1.32	1 (14%)
56	KBE	z	1	56	8,8,9	1.22	1 (12%)	7,8,10	2.16	1 (14%)
56	KBE	y	1	56	8,8,9	1.36	1 (12%)	7,8,10	2.04	1 (14%)
56	5OH	AA	6	56	8,12,13	1.33	1 (12%)	3,16,18	1.68	1 (33%)
56	5OH	z	6	56	8,12,13	1.13	1 (12%)	3,16,18	1.13	0
56	DPP	AA	2	56	3,5,6	1.13	0	1,5,7	1.21	0
56	DPP	BA	2	56	3,5,6	1.30	0	1,5,7	0.08	0
56	UAL	AA	5	56	7,8,9	2.53	1 (14%)	5,9,11	1.33	1 (20%)
56	5OH	y	6	56	8,12,13	0.92	0	3,16,18	2.40	2 (66%)
56	KBE	AA	1	56	8,8,9	1.66	2 (25%)	7,8,10	3.54	1 (14%)
56	5OH	7	6	56	8,12,13	1.77	2 (25%)	3,16,18	2.93	1 (33%)
56	DPP	7	2	56	3,5,6	0.50	0	1,5,7	0.90	0
56	UAL	y	5	56	7,8,9	2.26	2 (28%)	5,9,11	1.39	1 (20%)

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
56	UAL	7	5	56	-	0/3/7/9	-
56	KBE	7	1	56	-	3/7/7/8	-
56	5OH	BA	6	56	-	2/2/18/20	0/1/1/1
56	DPP	z	2	56	-	0/2/4/6	-
56	UAL	z	5	56	-	0/3/7/9	-
56	DPP	y	2	56	-	0/2/4/6	-
56	UAL	BA	5	56	-	0/3/7/9	-
56	KBE	BA	1	56	-	4/7/7/8	-
56	KBE	z	1	56	-	2/7/7/8	-
56	KBE	y	1	56	-	2/7/7/8	-
56	5OH	AA	6	56	-	0/2/18/20	0/1/1/1
56	5OH	z	6	56	-	1/2/18/20	0/1/1/1
56	DPP	AA	2	56	-	0/2/4/6	-
56	DPP	BA	2	56	-	0/2/4/6	-
56	UAL	AA	5	56	-	0/3/7/9	-
56	5OH	y	6	56	-	0/2/18/20	0/1/1/1
56	KBE	AA	1	56	-	0/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	5OH	7	6	56	-	0/2/18/20	0/1/1/1
56	DPP	7	2	56	-	0/2/4/6	-
56	UAL	y	5	56	-	0/3/7/9	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	7	5	UAL	C-CA	6.99	1.56	1.45
56	BA	5	UAL	C-CA	6.80	1.56	1.45
56	AA	5	UAL	C-CA	6.04	1.54	1.45
56	y	5	UAL	C-CA	5.10	1.53	1.45
56	AA	1	KBE	CA-CB	3.46	1.57	1.53
56	7	6	5OH	CA-CB	3.20	1.58	1.54
56	y	1	KBE	CA-CB	3.06	1.57	1.53
56	7	6	5OH	CR-CB	2.77	1.57	1.53
56	AA	1	KBE	CA-C	2.70	1.56	1.49
56	z	5	UAL	C-CA	2.68	1.49	1.45
56	z	1	KBE	CA-CB	2.68	1.56	1.53
56	z	5	UAL	C1-N1	-2.67	1.36	1.40
56	y	5	UAL	C1-N1	-2.44	1.36	1.40
56	z	5	UAL	CB-N1	-2.40	1.29	1.35
56	AA	6	5OH	CB-NP	2.27	1.51	1.47
56	BA	1	KBE	CA-CB	2.16	1.56	1.53
56	z	6	5OH	CB-NP	2.10	1.51	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	AA	1	KBE	CB-CA-C	9.12	125.67	112.25
56	z	5	UAL	O-C-CA	-5.34	118.61	125.39
56	z	1	KBE	CB-CA-C	5.23	119.95	112.25
56	y	1	KBE	CB-CA-C	5.05	119.68	112.25
56	7	6	5OH	CR-CB-CA	4.99	117.99	112.61
56	y	6	5OH	CR-CB-CA	3.63	116.52	112.61
56	BA	5	UAL	O-C-CA	-3.24	121.27	125.39
56	BA	6	5OH	CR-CB-CA	3.23	116.09	112.61
56	AA	6	5OH	CR-CB-CA	2.80	115.63	112.61
56	BA	1	KBE	CB-CA-C	2.60	116.08	112.25
56	AA	5	UAL	O-C-CA	-2.57	122.12	125.39
56	7	1	KBE	CB-CA-C	2.55	116.00	112.25
56	y	5	UAL	O-C-CA	-2.48	122.24	125.39
56	BA	6	5OH	O-C-CA	-2.04	119.44	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	y	6	5OH	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	y	1	KBE	CA-CB-CG-CD
56	z	1	KBE	C-CA-CB-N
56	z	1	KBE	C-CA-CB-CG
56	7	1	KBE	C-CA-CB-N
56	7	1	KBE	C-CA-CB-CG
56	7	1	KBE	CA-CB-CG-CD
56	BA	1	KBE	C-CA-CB-CG
56	BA	1	KBE	CA-CB-CG-CD
56	z	6	5OH	C-CA-CB-CR
56	BA	6	5OH	O-C-CA-CB
56	BA	6	5OH	C-CA-CB-CR
56	BA	1	KBE	C-CA-CB-N
56	y	1	KBE	N-CB-CG-CD
56	BA	1	KBE	N-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	218/218 (100%)	1.26	57 (26%)	0	0	96, 133, 180, 198	0
2	B	206/206 (100%)	0.40	15 (7%)	15	6	73, 120, 145, 151	0
3	C	205/205 (100%)	1.14	46 (22%)	0	0	88, 115, 150, 205	0
4	D	150/150 (100%)	0.02	3 (2%)	65	44	73, 94, 139, 171	0
5	E	100/100 (100%)	0.78	14 (14%)	2	1	101, 135, 155, 159	0
6	F	151/151 (100%)	2.06	63 (41%)	0	0	111, 187, 225, 236	0
7	G	129/129 (100%)	0.51	8 (6%)	20	9	77, 101, 133, 142	0
8	H	127/127 (100%)	1.45	37 (29%)	0	0	82, 134, 190, 220	0
9	I	98/98 (100%)	0.91	13 (13%)	3	1	90, 110, 193, 210	0
10	J	117/117 (100%)	0.52	8 (6%)	17	7	76, 111, 147, 165	0
11	K	123/123 (100%)	0.53	5 (4%)	37	18	53, 76, 115, 156	0
12	L	114/114 (100%)	2.96	63 (55%)	0	0	166, 207, 253, 272	0
13	M	96/100 (96%)	2.11	39 (40%)	0	0	79, 143, 196, 206	0
14	N	88/88 (100%)	0.49	7 (7%)	12	5	76, 104, 140, 149	0
15	O	82/82 (100%)	1.45	20 (24%)	0	0	78, 101, 164, 212	0
16	P	80/80 (100%)	1.59	27 (33%)	0	0	79, 119, 168, 183	0
17	Q	55/55 (100%)	1.06	6 (10%)	5	2	80, 100, 133, 190	0
18	R	79/79 (100%)	3.64	51 (64%)	0	0	156, 207, 226, 233	0
19	S	85/85 (100%)	0.70	7 (8%)	11	4	82, 111, 136, 153	0
20	T	51/51 (100%)	1.88	20 (39%)	0	0	119, 147, 188, 197	0
21	U	271/271 (100%)	0.17	9 (3%)	46	24	37, 65, 82, 107	0
22	V	209/209 (100%)	-0.06	1 (0%)	91	81	31, 58, 94, 119	0
23	W	201/201 (100%)	0.09	6 (2%)	50	27	38, 76, 115, 160	0
24	X	177/177 (100%)	1.10	40 (22%)	0	0	113, 142, 190, 256	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	176/176 (100%)	0.30	4 (2%) 60 39	58, 82, 124, 141	0
26	Z	141/141 (100%)	3.49	98 (69%) 0 0	185, 260, 305, 346	0
27	0	142/142 (100%)	0.42	6 (4%) 36 18	49, 64, 94, 128	0
28	1	122/122 (100%)	0.18	1 (0%) 86 72	46, 61, 88, 115	0
29	2	143/143 (100%)	0.54	9 (6%) 20 8	45, 85, 123, 154	0
30	3	136/136 (100%)	0.36	2 (1%) 73 54	44, 70, 103, 137	0
31	4	120/120 (100%)	0.21	2 (1%) 70 49	41, 57, 70, 171	0
32	5	116/116 (100%)	1.37	36 (31%) 0 0	85, 106, 130, 136	0
33	6	114/114 (100%)	0.19	3 (2%) 56 33	48, 72, 115, 141	0
34	8	117/117 (100%)	0.08	3 (2%) 56 33	34, 60, 98, 119	0
35	9	103/103 (100%)	0.26	3 (2%) 51 28	46, 88, 128, 139	0
36	a	110/110 (100%)	-0.12	1 (0%) 84 69	41, 55, 86, 138	0
37	b	93/93 (100%)	0.88	13 (13%) 2 1	49, 81, 143, 167	0
38	c	102/102 (100%)	1.14	21 (20%) 1 0	65, 84, 153, 167	0
39	d	94/94 (100%)	0.64	8 (8%) 10 4	69, 98, 120, 143	0
40	e	79/79 (100%)	0.77	5 (6%) 20 8	66, 90, 125, 136	0
41	f	77/77 (100%)	0.46	3 (3%) 39 20	57, 72, 124, 133	0
42	g	63/63 (100%)	-0.00	3 (4%) 30 14	73, 99, 138, 170	0
43	h	58/58 (100%)	0.73	10 (17%) 1 0	63, 76, 133, 144	0
44	i	56/56 (100%)	0.19	3 (5%) 25 12	38, 61, 105, 136	0
45	j	50/50 (100%)	2.98	35 (70%) 0 0	128, 148, 161, 206	0
46	k	46/46 (100%)	0.22	2 (4%) 35 17	43, 55, 74, 119	0
47	l	64/64 (100%)	0.31	0 100 100	55, 67, 82, 89	0
48	m	38/38 (100%)	0.50	1 (2%) 56 33	62, 77, 89, 107	0
49	n	163/163 (100%)	4.42	112 (68%) 0 0	136, 200, 265, 312	1 (0%)
50	o	30/30 (100%)	1.02	5 (16%) 1 1	148, 184, 209, 215	0
50	p	30/30 (100%)	1.39	8 (26%) 0 0	170, 194, 226, 233	0
50	q	30/30 (100%)	3.14	17 (56%) 0 0	160, 205, 254, 264	0
50	r	30/30 (100%)	2.33	11 (36%) 0 0	148, 191, 224, 232	0
51	s	1532/1532 (100%)	0.35	85 (5%) 25 11	50, 102, 211, 316	0
52	t	2850/2903 (98%)	0.18	100 (3%) 44 23	36, 66, 212, 419	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
53	u	118/118 (100%)	-0.04	0 100 100	60, 110, 147, 189	0
54	v	525/525 (100%)	0.70	60 (11%) 5 2	47, 99, 188, 267	0
55	w	6/6 (100%)	3.84	5 (83%) 0 0	186, 194, 202, 203	0
56	7	2/6 (33%)	2.01	1 (50%) 0 0	103, 103, 103, 112	0
56	AA	2/6 (33%)	3.05	2 (100%) 0 0	103, 103, 103, 108	0
56	BA	2/6 (33%)	2.80	1 (50%) 0 0	100, 100, 100, 101	0
56	y	2/6 (33%)	-0.21	0 100 100	99, 99, 99, 102	0
56	z	2/6 (33%)	1.90	1 (50%) 0 0	93, 93, 93, 103	0
All	All	10896/10973 (99%)	0.65	1245 (11%) 5 2	31, 90, 212, 419	1 (0%)

All (1245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	n	50	VAL	24.7
49	n	88	HIS	20.5
18	R	55	GLN	19.4
49	n	112	ALA	19.4
49	n	89	PRO	19.1
49	n	113	PHE	18.1
26	Z	66	PHE	15.8
13	M	51	PRO	15.8
49	n	49	GLY	14.9
12	L	36	ALA	13.6
12	L	39	ALA	13.4
49	n	84	TYR	13.2
6	F	79	VAL	13.1
26	Z	12	VAL	12.9
3	C	24	VAL	12.6
50	r	1	SER	12.2
18	R	32	THR	12.2
52	t	2151	U	11.8
52	t	2108	A	11.6
6	F	84	TYR	11.6
52	t	2152	G	11.4
49	n	114	GLU	11.4
12	L	34	ALA	11.3
49	n	31	ARG	11.2
18	R	49	ALA	11.2
52	t	2180	U	10.6

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Mol	Chain	Res	Type	RSRZ
52	t	2109	U	10.6
49	n	85	LEU	10.5
52	t	2133	G	10.4
52	t	2903	U	10.3
49	n	58	THR	10.2
52	t	881	G	10.2
13	M	56	PRO	10.2
49	n	56	ARG	10.1
18	R	54	ARG	10.1
52	t	1508	A	9.8
52	t	2179	C	9.8
12	L	37	GLY	9.8
49	n	43	LYS	9.7
13	M	53	ASP	9.7
26	Z	79	LEU	9.6
52	t	2107	G	9.6
39	d	94	ALA	9.6
18	R	31	ARG	9.5
17	Q	19	GLU	9.4
49	n	17	GLU	9.4
49	n	116	GLU	9.2
26	Z	111	THR	9.2
49	n	30	SER	9.1
12	L	113	LYS	9.0
45	j	52	LYS	9.0
49	n	115	GLY	9.0
49	n	57	ASN	8.9
26	Z	94	LYS	8.9
6	F	4	ARG	8.8
26	Z	4	VAL	8.8
18	R	12	LEU	8.8
50	q	16	VAL	8.8
52	t	880	G	8.7
50	q	23	ILE	8.6
49	n	99	PHE	8.6
1	A	51	GLU	8.6
26	Z	77	VAL	8.6
26	Z	67	THR	8.6
13	M	52	ARG	8.5
50	q	22	LEU	8.5
26	Z	86	LYS	8.5
26	Z	87	SER	8.4

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Mol	Chain	Res	Type	RSRZ
49	n	54	VAL	8.4
51	s	995	C	8.3
16	P	82	VAL	8.3
52	t	1174	U	8.3
13	M	11	LYS	8.3
45	j	8	ILE	8.3
52	t	2148	G	8.2
26	Z	58	ILE	8.2
49	n	69	PHE	8.2
18	R	75	PRO	8.1
12	L	33	LEU	8.0
52	t	2156	G	8.0
49	n	39	THR	8.0
49	n	26	VAL	8.0
26	Z	91	LYS	8.0
10	J	12	ARG	7.9
26	Z	137	LEU	7.9
52	t	2149	U	7.9
49	n	117	LEU	7.8
15	O	82	ALA	7.8
49	n	86	MET	7.8
26	Z	11	GLN	7.8
32	5	50	ALA	7.7
49	n	25	ALA	7.7
49	n	52	MET	7.6
50	r	9	GLU	7.6
12	L	62	PHE	7.6
49	n	20	LYS	7.6
52	t	2144	G	7.5
49	n	158	VAL	7.5
3	C	23	GLY	7.4
26	Z	7	TYR	7.4
12	L	107	THR	7.4
55	w	18	G	7.3
26	Z	65	SER	7.3
8	H	129	ARG	7.2
12	L	38	ILE	7.2
12	L	114	PRO	7.2
50	q	6	GLN	7.1
49	n	111	ALA	7.1
45	j	51	ALA	7.1
13	M	19	TYR	7.0

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Mol	Chain	Res	Type	RSRZ
11	K	123	ALA	7.0
49	n	37	LYS	7.0
49	n	14	GLU	6.9
26	Z	93	ASN	6.9
52	t	2153	C	6.9
54	v	54	HIS	6.9
26	Z	60	VAL	6.9
49	n	68	PRO	6.9
52	t	2150	C	6.8
45	j	22	THR	6.8
6	F	77	ARG	6.8
12	L	6	ILE	6.8
8	H	39	GLY	6.8
44	i	26	SER	6.7
49	n	62	ARG	6.7
12	L	35	ALA	6.7
52	t	1870	C	6.7
49	n	103	ASN	6.6
51	s	1032	G	6.6
49	n	10	ALA	6.6
12	L	4	ALA	6.6
49	n	95	LEU	6.6
54	v	305	ALA	6.5
52	t	899	A	6.5
8	H	9	GLY	6.4
6	F	5	VAL	6.4
52	t	1509	A	6.4
13	M	7	ALA	6.4
49	n	160	GLU	6.3
1	A	124	THR	6.2
18	R	36	ARG	6.2
18	R	56	HIS	6.2
49	n	4	ASN	6.2
32	5	80	GLU	6.2
51	s	1031	C	6.2
49	n	9	GLN	6.1
6	F	7	GLY	6.1
40	e	24	ARG	6.1
49	n	27	VAL	6.1
1	A	55	GLU	6.1
12	L	3	ILE	6.0
1	A	64	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
26	Z	132	ALA	6.0
54	v	509	VAL	6.0
50	r	8	ILE	6.0
49	n	98	GLU	6.0
38	c	1	ALA	5.9
6	F	86	VAL	5.9
54	v	493	LEU	5.9
12	L	112	ARG	5.9
50	q	11	VAL	5.8
26	Z	20	SER	5.8
52	t	1729	U	5.8
18	R	59	VAL	5.8
49	n	18	VAL	5.8
51	s	1033	G	5.8
51	s	996	A	5.8
50	p	9	GLU	5.7
54	v	519	PRO	5.7
18	R	40	PHE	5.7
26	Z	85	ILE	5.7
12	L	98	GLY	5.7
26	Z	95	ASP	5.6
52	t	1175	A	5.6
6	F	87	PRO	5.6
35	9	50	GLY	5.6
26	Z	136	GLY	5.5
55	w	20	A	5.5
12	L	32	ILE	5.5
12	L	31	ALA	5.5
45	j	21	THR	5.5
26	Z	78	LEU	5.5
1	A	43	GLU	5.5
12	L	15	VAL	5.5
49	n	45	GLY	5.5
6	F	83	THR	5.5
49	n	51	TYR	5.5
20	T	41	THR	5.5
6	F	82	SER	5.4
49	n	107	GLU	5.4
51	s	994	A	5.4
6	F	1	PRO	5.4
49	n	36	ASP	5.4
26	Z	116	MET	5.4

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Mol	Chain	Res	Type	RSRZ
20	T	37	TYR	5.4
26	Z	98	GLY	5.4
52	t	892	A	5.4
20	T	34	ARG	5.4
49	n	44	ALA	5.3
15	O	51	ARG	5.3
52	t	2134	A	5.3
12	L	84	CYS	5.3
45	j	25	ASN	5.3
13	M	28	ALA	5.3
18	R	24	SER	5.3
15	O	22	ALA	5.3
46	k	46	LYS	5.3
24	X	79	ARG	5.2
51	s	1038	C	5.2
18	R	50	VAL	5.2
52	t	1065	U	5.2
50	r	30	PHE	5.2
51	s	1030	U	5.2
18	R	65	MET	5.2
18	R	73	PHE	5.2
7	G	67	GLY	5.2
12	L	105	ALA	5.2
20	T	35	GLU	5.2
49	n	21	GLY	5.1
45	j	42	VAL	5.1
49	n	106	PHE	5.1
49	n	61	ARG	5.1
52	t	139	U	5.1
32	5	48	LEU	5.1
50	r	2	ILE	5.1
12	L	42	VAL	5.1
26	Z	53	PRO	5.1
13	M	1	ALA	5.1
26	Z	13	ALA	5.1
12	L	104	ASN	5.0
52	t	2154	A	5.0
6	F	51	GLN	5.0
6	F	72	VAL	5.0
52	t	1067	A	5.0
18	R	14	LEU	5.0
45	j	15	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
52	t	884	U	5.0
27	0	142	ILE	5.0
6	F	78	ARG	5.0
16	P	73	THR	4.9
20	T	42	THR	4.9
52	t	2145	C	4.9
1	A	8	MET	4.9
51	s	1016	A	4.9
54	v	456	GLU	4.9
24	X	44	ALA	4.9
49	n	90	GLY	4.9
49	n	46	ARG	4.9
18	R	9	PHE	4.9
26	Z	2	LYS	4.9
18	R	79	TYR	4.9
18	R	77	ARG	4.9
8	H	57	VAL	4.9
26	Z	3	LYS	4.8
52	t	883	G	4.8
51	s	461	A	4.8
49	n	55	VAL	4.8
18	R	23	GLU	4.8
18	R	60	PHE	4.8
43	h	58	GLU	4.8
2	B	74	ILE	4.8
26	Z	54	ILE	4.8
13	M	6	LYS	4.8
11	K	24	GLU	4.8
49	n	24	SER	4.7
12	L	100	ARG	4.7
51	s	1267	C	4.7
3	C	18	LEU	4.7
54	v	423	GLY	4.7
1	A	50	ASN	4.7
54	v	455	SER	4.7
52	t	2135	A	4.7
26	Z	37	PHE	4.7
20	T	36	PHE	4.7
26	Z	38	CYS	4.6
32	5	55	GLU	4.6
13	M	8	ARG	4.6
12	L	63	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
34	8	87	VAL	4.6
26	Z	10	LEU	4.6
49	n	82	ILE	4.6
45	j	40	PRO	4.6
12	L	58	GLU	4.6
24	X	163	GLU	4.6
35	9	57	GLY	4.6
9	I	35	GLN	4.6
50	o	24	SER	4.6
6	F	61	PHE	4.6
49	n	53	ARG	4.6
38	c	51	LEU	4.6
52	t	897	C	4.5
49	n	122	GLN	4.5
51	s	841	C	4.5
1	A	185	ILE	4.5
18	R	10	ILE	4.5
6	F	88	VAL	4.5
6	F	76	SER	4.5
6	F	6	ILE	4.5
34	8	86	SER	4.5
8	H	33	SER	4.5
1	A	48	MET	4.5
5	E	37	HIS	4.5
3	C	177	MET	4.5
6	F	149	ALA	4.5
26	Z	83	ALA	4.5
12	L	30	LYS	4.5
52	t	1172	C	4.5
32	5	114	GLY	4.4
49	n	11	ILE	4.4
50	q	21	GLU	4.4
26	Z	21	PRO	4.4
12	L	57	ASP	4.4
11	K	122	LYS	4.4
49	n	91	ALA	4.4
49	n	130	PRO	4.4
18	R	11	ASP	4.4
45	j	16	THR	4.4
13	M	14	ALA	4.4
49	n	154	THR	4.4
49	n	163	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
24	X	78	ILE	4.4
51	s	1214	C	4.4
52	t	879	G	4.3
50	r	5	ASP	4.3
18	R	17	LYS	4.3
12	L	108	ARG	4.3
13	M	55	SER	4.3
26	Z	119	ALA	4.3
13	M	13	VAL	4.3
51	s	1215	G	4.3
16	P	43	LEU	4.3
26	Z	105	LEU	4.3
1	A	199	ILE	4.3
8	H	89	TYR	4.3
1	A	200	PRO	4.3
26	Z	90	GLY	4.3
9	I	30	LYS	4.3
13	M	9	GLU	4.3
54	v	304	GLN	4.3
52	t	2147	A	4.2
13	M	30	ILE	4.2
32	5	62	LEU	4.2
12	L	1	ALA	4.2
54	v	527	ARG	4.2
12	L	46	GLU	4.2
12	L	91	ARG	4.2
50	q	20	VAL	4.2
12	L	14	ALA	4.2
13	M	22	LYS	4.2
49	n	41	LEU	4.2
26	Z	81	LYS	4.2
52	t	2143	C	4.2
12	L	44	ILE	4.2
26	Z	40	ALA	4.1
6	F	48	THR	4.1
51	s	993	G	4.1
18	R	2	ARG	4.1
26	Z	24	GLY	4.1
52	t	898	C	4.1
37	b	24	MET	4.1
1	A	158	ASP	4.1
13	M	10	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
19	S	52	GLU	4.1
42	g	63	ALA	4.1
50	q	26	MET	4.1
1	A	62	ARG	4.1
32	5	115	LEU	4.1
52	t	1869	G	4.1
18	R	22	VAL	4.1
20	T	40	PRO	4.0
43	h	1	ALA	4.0
18	R	76	THR	4.0
54	v	307	MET	4.0
1	A	128	LEU	4.0
13	M	29	ILE	4.0
1	A	198	VAL	4.0
51	s	82	G	4.0
51	s	205	A	4.0
33	6	114	ASN	4.0
26	Z	68	PHE	4.0
51	s	412	A	4.0
26	Z	32	VAL	4.0
43	h	57	GLU	4.0
5	E	66	ALA	4.0
13	M	20	PHE	4.0
49	n	97	LYS	4.0
45	j	6	GLU	4.0
51	s	998	C	4.0
24	X	43	ILE	4.0
8	H	127	SER	4.0
29	2	142	ILE	4.0
10	J	125	LYS	4.0
49	n	161	ALA	4.0
18	R	7	GLY	4.0
56	BA	4	SER	4.0
26	Z	122	GLU	3.9
37	b	74	ILE	3.9
18	R	51	HIS	3.9
12	L	97	ARG	3.9
54	v	515	GLN	3.9
54	v	508	MET	3.9
45	j	28	THR	3.9
51	s	987	G	3.9
31	4	120	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
51	s	1004	A	3.9
50	q	3	THR	3.9
56	AA	4	SER	3.9
18	R	30	LEU	3.9
49	n	70	GLU	3.9
12	L	110	GLY	3.9
26	Z	27	LEU	3.9
8	H	128	LYS	3.9
26	Z	92	PRO	3.9
45	j	30	PRO	3.9
16	P	19	SER	3.9
9	I	102	LEU	3.9
3	C	150	LYS	3.9
26	Z	130	GLY	3.9
26	Z	131	THR	3.9
49	n	63	ALA	3.9
49	n	145	GLU	3.9
22	V	209	ALA	3.9
52	t	2106	U	3.9
49	n	152	VAL	3.9
51	s	1006	G	3.9
51	s	1045	C	3.8
12	L	94	LEU	3.8
17	Q	73	HIS	3.8
40	e	45	HIS	3.8
18	R	33	TRP	3.8
1	A	59	ILE	3.8
16	P	42	LYS	3.8
52	t	882	G	3.8
12	L	41	ASP	3.8
50	r	7	ILE	3.8
24	X	16	MET	3.8
50	o	21	GLU	3.8
16	P	39	ARG	3.8
26	Z	6	ALA	3.8
54	v	482	PHE	3.8
36	a	110	ARG	3.8
52	t	2139	U	3.8
3	C	28	ASP	3.8
54	v	514	ALA	3.8
6	F	81	GLY	3.8
26	Z	97	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
52	t	280	U	3.7
8	H	125	GLN	3.7
51	s	1216	A	3.7
49	n	108	VAL	3.7
12	L	93	GLY	3.7
16	P	6	THR	3.7
49	n	42	ARG	3.7
26	Z	96	LYS	3.7
52	t	138	U	3.7
54	v	221	GLU	3.7
1	A	212	TYR	3.7
51	s	94	G	3.7
51	s	990	C	3.7
45	j	50	GLU	3.7
9	I	75	ASP	3.7
50	p	11	VAL	3.7
18	R	13	HIS	3.7
26	Z	104	GLN	3.7
8	H	20	ILE	3.7
51	s	1212	U	3.7
52	t	1171	G	3.7
26	Z	52	LEU	3.7
26	Z	107	GLU	3.7
45	j	23	THR	3.7
1	A	87	ASP	3.7
26	Z	123	ALA	3.7
12	L	7	ASN	3.7
49	n	59	LEU	3.7
26	Z	63	ASP	3.7
3	C	19	PHE	3.7
18	R	71	GLY	3.6
54	v	52	ASN	3.7
13	M	50	LEU	3.6
26	Z	39	LYS	3.6
12	L	79	LEU	3.6
52	t	2181	U	3.6
38	c	70	ALA	3.6
54	v	424	ALA	3.6
13	M	4	SER	3.6
18	R	3	SER	3.6
50	r	3	THR	3.6
1	A	47	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
6	F	2	ARG	3.6
26	Z	74	PRO	3.6
21	U	271	SER	3.6
8	H	91	GLU	3.6
52	t	2142	A	3.6
1	A	63	LYS	3.6
39	d	34	LYS	3.6
6	F	3	ARG	3.6
49	n	47	GLU	3.6
16	P	81	ALA	3.6
49	n	75	ALA	3.6
13	M	35	ALA	3.6
49	n	121	SER	3.6
27	0	9	GLU	3.6
49	n	105	LYS	3.6
18	R	21	ALA	3.5
54	v	435	ASP	3.5
30	3	1	MET	3.5
54	v	50	GLY	3.5
54	v	16	PHE	3.5
1	A	224	ARG	3.5
8	H	32	ARG	3.5
18	R	34	SER	3.5
20	T	46	ARG	3.5
13	M	15	LEU	3.5
49	n	3	LEU	3.5
49	n	8	LYS	3.5
49	n	129	LEU	3.5
51	s	1037	C	3.5
15	O	81	ALA	3.5
13	M	12	ARG	3.5
1	A	42	LEU	3.5
52	t	2103	C	3.5
8	H	58	GLU	3.5
7	G	2	MET	3.5
10	J	52	ARG	3.5
18	R	72	GLU	3.5
52	t	1075	C	3.5
49	n	72	LEU	3.5
6	F	8	GLN	3.5
24	X	21	TYR	3.5
24	X	1	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
5	E	96	VAL	3.4
18	R	26	ASP	3.4
1	A	163	ILE	3.4
6	F	80	GLY	3.4
14	N	61	GLN	3.4
1	A	29	PHE	3.4
25	Y	31	GLU	3.4
26	Z	75	ALA	3.4
1	A	138	ARG	3.4
40	e	40	ARG	3.4
18	R	41	PRO	3.4
26	Z	46	ASP	3.4
1	A	183	PHE	3.4
26	Z	128	ILE	3.4
52	t	900	A	3.4
45	j	26	LYS	3.4
3	C	35	GLN	3.4
52	t	2184	A	3.4
43	h	5	LYS	3.4
49	n	66	GLY	3.4
18	R	48	ILE	3.4
54	v	472	ARG	3.3
52	t	1507	C	3.3
9	I	76	ILE	3.3
37	b	88	LYS	3.3
29	2	95	LEU	3.3
26	Z	82	ALA	3.3
12	L	56	ARG	3.3
49	n	5	LEU	3.3
12	L	102	LYS	3.3
6	F	71	THR	3.3
32	5	112	GLU	3.3
39	d	71	LYS	3.3
41	f	43	LYS	3.3
49	n	109	LYS	3.3
52	t	1871	A	3.3
26	Z	80	LYS	3.3
16	P	13	SER	3.3
54	v	57	SER	3.3
18	R	28	LYS	3.3
52	t	1179	G	3.3
18	R	70	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
6	F	90	VAL	3.3
56	z	4	SER	3.3
38	c	82	VAL	3.3
13	M	18	LYS	3.3
8	H	40	ARG	3.3
13	M	21	ALA	3.3
1	A	130	LYS	3.3
1	A	131	LYS	3.3
5	E	9	MET	3.2
7	G	1	SER	3.2
9	I	85	ASP	3.2
49	n	40	GLU	3.2
32	5	79	ALA	3.2
50	q	24	SER	3.2
54	v	478	ASP	3.2
52	t	367	G	3.2
13	M	2	LYS	3.2
24	X	168	LEU	3.2
52	t	2402	U	3.2
1	A	30	ILE	3.2
8	H	3	ASN	3.2
12	L	106	ARG	3.2
49	n	29	ASP	3.2
50	p	10	ALA	3.2
51	s	1019	A	3.2
18	R	57	VAL	3.2
51	s	1226	C	3.2
2	B	133	MET	3.2
50	p	8	ILE	3.2
51	s	1000	A	3.2
1	A	56	LEU	3.2
29	2	92	LEU	3.2
26	Z	76	ALA	3.2
17	Q	63	TYR	3.2
51	s	988	G	3.2
26	Z	139	VAL	3.2
33	6	111	GLU	3.2
45	j	19	PHE	3.2
25	Y	14	VAL	3.2
20	T	10	PRO	3.2
6	F	109	LYS	3.2
15	O	74	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
26	Z	135	MET	3.2
6	F	46	LEU	3.1
18	R	63	ASP	3.1
24	X	67	THR	3.1
54	v	42	THR	3.1
54	v	496	ASP	3.1
26	Z	138	VAL	3.1
15	O	80	LYS	3.1
29	2	115	GLU	3.1
54	v	51	SER	3.1
52	t	646	U	3.1
20	T	3	ILE	3.1
6	F	75	LYS	3.1
26	Z	16	MET	3.1
50	r	21	GLU	3.1
49	n	128	THR	3.1
49	n	159	ARG	3.1
51	s	842	U	3.1
54	v	70	ILE	3.1
51	s	1042	A	3.1
8	H	28	VAL	3.1
9	I	74	VAL	3.1
5	E	14	GLN	3.1
26	Z	121	ILE	3.1
5	E	63	ASN	3.1
52	t	366	C	3.1
45	j	33	LEU	3.1
8	H	38	PHE	3.1
38	c	52	ASN	3.1
26	Z	120	ASP	3.1
13	M	58	ARG	3.1
16	P	60	ILE	3.1
26	Z	34	ILE	3.1
6	F	60	ALA	3.1
24	X	80	GLN	3.1
1	A	46	VAL	3.1
45	j	31	GLU	3.1
12	L	95	PRO	3.1
39	d	93	ARG	3.1
54	v	476	CYS	3.1
3	C	193	ASP	3.0
14	N	1	SER	3.0

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Mol	Chain	Res	Type	RSRZ
26	Z	115	ASP	3.0
54	v	376	GLY	3.0
52	t	1066	U	3.0
54	v	452	ARG	3.0
54	v	327	LYS	3.0
54	v	399	ARG	3.0
18	R	15	LEU	3.0
3	C	174	ALA	3.0
1	A	35	ASN	3.0
13	M	23	ARG	3.0
45	j	27	ARG	3.0
18	R	58	PRO	3.0
12	L	47	LEU	3.0
18	R	74	ALA	3.0
49	n	28	ALA	3.0
52	t	895	U	3.0
3	C	63	ILE	3.0
12	L	40	GLU	3.0
49	n	155	LEU	3.0
3	C	114	ARG	3.0
8	H	16	ALA	3.0
54	v	475	GLU	3.0
24	X	116	LEU	3.0
50	q	15	SER	3.0
1	A	54	ALA	3.0
15	O	47	GLU	3.0
20	T	38	GLU	3.0
32	5	58	ILE	3.0
6	F	42	VAL	3.0
52	t	288	U	3.0
52	t	2211	A	3.0
54	v	473	TRP	3.0
8	H	27	ILE	3.0
19	S	82	ILE	3.0
1	A	14	HIS	3.0
24	X	65	LEU	3.0
51	s	1020	G	3.0
26	Z	42	ASN	3.0
24	X	68	LYS	3.0
6	F	47	GLU	3.0
49	n	120	ALA	3.0
9	I	89	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
26	Z	57	VAL	3.0
50	q	27	GLU	3.0
9	I	93	ALA	3.0
12	L	82	LEU	3.0
45	j	5	ARG	2.9
24	X	124	ARG	2.9
54	v	355	HIS	2.9
51	s	203	G	2.9
29	2	104	GLN	2.9
54	v	489	ASN	2.9
50	p	5	ASP	2.9
1	A	31	PHE	2.9
20	T	11	PHE	2.9
5	E	89	VAL	2.9
12	L	18	LEU	2.9
27	0	54	ILE	2.9
26	Z	41	PHE	2.9
10	J	18	GLY	2.9
32	5	49	VAL	2.9
49	n	64	VAL	2.9
51	s	1015	G	2.9
6	F	93	VAL	2.9
10	J	76	TYR	2.9
51	s	1005	A	2.9
13	M	42	ASN	2.9
55	w	17	U	2.9
8	H	8	THR	2.9
50	r	17	MET	2.9
29	2	141	LYS	2.9
37	b	83	ALA	2.9
52	t	275	C	2.9
51	s	1036	A	2.9
51	s	1362	A	2.9
54	v	421	GLU	2.9
49	n	83	ALA	2.9
51	s	1209	C	2.9
17	Q	46	THR	2.9
20	T	45	LYS	2.9
51	s	4	U	2.9
51	s	1268	G	2.9
8	H	64	ILE	2.9
49	n	77	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
51	s	702	A	2.9
51	s	1213	A	2.9
24	X	172	PHE	2.9
51	s	1007	U	2.9
3	C	153	ARG	2.9
7	G	60	LEU	2.9
13	M	26	LEU	2.9
24	X	75	GLY	2.9
38	c	71	ILE	2.8
13	M	45	LEU	2.8
52	t	1848	A	2.8
3	C	2	ARG	2.8
6	F	58	LEU	2.8
15	O	20	VAL	2.8
45	j	7	LYS	2.8
55	w	15	A	2.8
6	F	53	SER	2.8
15	O	67	ILE	2.8
38	c	72	PHE	2.8
38	c	86	PHE	2.8
49	n	1	MET	2.8
4	D	9	GLU	2.8
12	L	83	GLY	2.8
54	v	45	THR	2.8
50	o	2	ILE	2.8
54	v	488	LYS	2.8
6	F	150	PHE	2.8
13	M	17	ASP	2.8
51	s	1266	G	2.8
49	n	35	VAL	2.8
32	5	56	LYS	2.8
38	c	50	ALA	2.8
51	s	1380	U	2.8
52	t	1173	U	2.8
1	A	201	GLY	2.8
43	h	6	ILE	2.8
37	b	1	MET	2.8
21	U	165	ALA	2.8
54	v	471	ALA	2.8
50	q	8	ILE	2.8
20	T	8	ASN	2.8
45	j	34	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
51	s	1043	G	2.8
6	F	119	LEU	2.8
38	c	2	ALA	2.8
42	g	62	GLY	2.8
32	5	35	ILE	2.8
32	5	92	PHE	2.8
45	j	43	ARG	2.8
6	F	151	ALA	2.8
24	X	15	LEU	2.8
26	Z	26	ALA	2.8
51	s	1217	C	2.8
51	s	1317	C	2.8
8	H	122	ARG	2.8
23	W	96	VAL	2.8
52	t	279	A	2.8
6	F	49	LEU	2.8
26	Z	117	THR	2.8
3	C	27	ILE	2.7
41	f	75	GLU	2.7
52	t	2183	A	2.7
26	Z	22	PRO	2.7
49	n	87	GLU	2.7
51	s	93	U	2.7
9	I	34	ALA	2.7
50	r	20	VAL	2.7
3	C	106	PHE	2.7
8	H	63	TYR	2.7
26	Z	8	VAL	2.7
51	s	1211	U	2.7
52	t	2155	U	2.7
3	C	34	GLU	2.7
39	d	70	ILE	2.7
18	R	29	PRO	2.7
43	h	38	GLU	2.7
49	n	79	PRO	2.7
2	B	78	LYS	2.7
32	5	93	ASP	2.7
45	j	4	ILE	2.7
51	s	207	C	2.7
6	F	130	LYS	2.7
54	v	480	LYS	2.7
24	X	76	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
20	T	22	CYS	2.7
24	X	167	ALA	2.7
20	T	44	ARG	2.7
45	j	13	SER	2.7
51	s	209	U	2.7
6	F	104	VAL	2.7
45	j	41	VAL	2.7
1	A	38	HIS	2.7
49	n	162	LYS	2.7
54	v	58	ASP	2.7
2	B	109	GLU	2.7
26	Z	134	SER	2.7
32	5	52	SER	2.7
51	s	723	U	2.7
52	t	363	G	2.7
46	k	1	MET	2.7
38	c	87	GLU	2.7
18	R	52	ASN	2.7
55	w	19	U	2.7
3	C	20	LEU	2.7
44	i	56	LYS	2.7
51	s	1003	G	2.7
8	H	45	MET	2.7
5	E	6	ILE	2.7
6	F	73	GLU	2.7
16	P	58	VAL	2.7
51	s	1026	G	2.7
5	E	35	LYS	2.6
20	T	14	ALA	2.7
50	p	3	THR	2.6
1	A	135	MET	2.6
3	C	155	LYS	2.6
3	C	108	ALA	2.6
8	H	121	ARG	2.6
37	b	73	ARG	2.6
3	C	118	SER	2.6
51	s	1002	G	2.6
19	S	42	ASP	2.6
6	F	15	PRO	2.6
52	t	1420	A	2.6
54	v	503	TYR	2.6
18	R	35	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
38	c	45	GLN	2.6
3	C	131	ILE	2.6
21	U	268	ARG	2.6
38	c	65	GLN	2.6
17	Q	20	ILE	2.6
3	C	43	ARG	2.6
13	M	54	SER	2.6
52	t	1872	A	2.6
3	C	98	ASP	2.6
16	P	25	GLU	2.6
18	R	25	GLY	2.6
5	E	62	MET	2.6
1	A	195	VAL	2.6
3	C	52	VAL	2.6
51	s	1451	U	2.6
8	H	42	THR	2.6
12	L	27	THR	2.6
49	n	12	VAL	2.6
6	F	100	MET	2.6
51	s	989	U	2.6
50	q	1	SER	2.6
19	S	66	ILE	2.6
50	p	30	PHE	2.6
12	L	109	LYS	2.6
32	5	54	VAL	2.6
49	n	73	LYS	2.6
15	O	40	ASN	2.6
2	B	123	LEU	2.6
7	G	9	MET	2.6
16	P	20	ILE	2.6
51	s	1022	A	2.6
24	X	159	ALA	2.6
52	t	2105	U	2.6
7	G	129	ALA	2.5
52	t	1073	A	2.5
40	e	29	SER	2.5
3	C	21	LYS	2.5
6	F	85	GLN	2.5
38	c	49	PRO	2.5
51	s	999	C	2.5
5	E	58	HIS	2.5
15	O	66	THR	2.5

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Mol	Chain	Res	Type	RSRZ
38	c	13	LEU	2.5
54	v	344	ASP	2.5
21	U	75	ALA	2.5
32	5	47	VAL	2.5
16	P	38	LYS	2.5
50	q	17	MET	2.5
51	s	843	U	2.5
12	L	61	LYS	2.5
24	X	46	LYS	2.5
26	Z	69	VAL	2.5
37	b	84	TYR	2.5
49	n	19	ALA	2.5
9	I	25	ILE	2.5
16	P	5	ARG	2.5
12	L	48	SER	2.5
54	v	53	GLN	2.5
13	M	5	MET	2.5
27	0	12	LYS	2.5
6	F	142	ARG	2.5
10	J	124	LYS	2.5
2	B	160	GLU	2.5
13	M	62	ARG	2.5
32	5	113	ALA	2.5
38	c	12	VAL	2.5
16	P	24	ILE	2.5
54	v	470	THR	2.5
51	s	1034	G	2.5
23	W	7	ASP	2.5
33	6	110	LYS	2.5
29	2	103	ILE	2.5
15	O	60	TRP	2.5
35	9	34	GLU	2.5
45	j	17	GLY	2.5
1	A	28	PRO	2.5
8	H	92	SER	2.5
14	N	53	ARG	2.5
50	p	7	ILE	2.5
51	s	1013	G	2.5
24	X	77	LYS	2.4
45	j	9	LYS	2.4
51	s	1027	C	2.4
51	s	1231	G	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	142	ARG	2.4
8	H	84	ARG	2.4
54	v	434	ASN	2.4
49	n	7	ASP	2.4
1	A	52	ALA	2.4
23	W	9	GLN	2.4
51	s	84	U	2.4
3	C	128	VAL	2.4
1	A	39	ILE	2.4
24	X	13	LYS	2.4
12	L	103	THR	2.4
2	B	128	MET	2.4
3	C	167	PRO	2.4
14	N	57	ARG	2.4
1	A	17	HIS	2.4
56	7	4	SER	2.4
43	h	4	ILE	2.4
14	N	87	ARG	2.4
34	8	116	LEU	2.4
45	j	39	ASP	2.4
13	M	43	ALA	2.4
28	1	45	GLU	2.4
45	j	47	ILE	2.4
6	F	74	VAL	2.4
12	L	96	VAL	2.4
43	h	3	THR	2.4
3	C	181	PHE	2.4
49	n	76	PHE	2.4
21	U	60	ALA	2.4
51	s	997	U	2.4
51	s	1023	U	2.4
8	H	21	LYS	2.4
25	Y	176	LYS	2.4
52	t	1493	C	2.4
27	0	95	ARG	2.4
49	n	110	ALA	2.4
3	C	97	LEU	2.4
16	P	3	LYS	2.4
2	B	36	PHE	2.4
8	H	109	GLN	2.4
16	P	12	VAL	2.4
32	5	84	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
38	c	76	THR	2.4
37	b	15	HIS	2.4
3	C	116	LEU	2.4
6	F	91	ARG	2.4
15	O	34	GLU	2.4
2	B	136	ALA	2.4
32	5	51	ALA	2.4
2	B	203	LYS	2.3
32	5	87	ILE	2.3
38	c	4	ILE	2.3
52	t	274	C	2.3
3	C	146	GLU	2.3
8	H	36	GLN	2.3
51	s	1021	A	2.3
5	E	91	ARG	2.3
5	E	8	PHE	2.3
45	j	38	PHE	2.3
52	t	277	G	2.3
6	F	105	GLU	2.3
52	t	2146	C	2.3
23	W	10	SER	2.3
52	t	362	A	2.3
8	H	19	PHE	2.3
38	c	69	VAL	2.3
54	v	481	LYS	2.3
15	O	45	GLU	2.3
24	X	20	ASN	2.3
43	h	7	THR	2.3
1	A	36	LYS	2.3
15	O	2	VAL	2.3
3	C	175	GLY	2.3
52	t	1180	U	2.3
26	Z	45	THR	2.3
52	t	2902	C	2.3
51	s	733	G	2.3
3	C	61	ARG	2.3
54	v	484	GLU	2.3
54	v	41	GLN	2.3
1	A	123	GLY	2.3
15	O	41	PRO	2.3
8	H	4	GLN	2.3
37	b	72	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
52	t	846	U	2.3
24	X	19	PHE	2.3
42	g	59	GLU	2.3
6	F	44	SER	2.3
52	t	1727	C	2.3
8	H	65	THR	2.3
15	O	48	GLU	2.3
1	A	211	LEU	2.3
8	H	34	LEU	2.3
21	U	114	GLN	2.3
39	d	63	ILE	2.3
24	X	121	PHE	2.3
16	P	40	THR	2.3
43	h	2	LYS	2.3
27	0	25	LEU	2.3
52	t	613	A	2.3
26	Z	5	GLN	2.3
3	C	1	ALA	2.3
45	j	32	LYS	2.3
6	F	111	GLY	2.3
24	X	31	GLU	2.3
54	v	499	ASP	2.3
6	F	21	LEU	2.3
26	Z	25	PRO	2.3
12	L	85	TYR	2.3
32	5	105	ALA	2.3
38	c	93	ARG	2.2
50	q	14	MET	2.2
52	t	1105	U	2.2
16	P	4	ILE	2.2
54	v	289	VAL	2.2
19	S	67	HIS	2.2
12	L	54	THR	2.2
52	t	1584	U	2.2
3	C	132	ALA	2.2
5	E	4	TYR	2.2
6	F	102	TRP	2.2
20	T	12	ASP	2.2
51	s	1274	A	2.2
3	C	31	CYS	2.2
37	b	16	VAL	2.2
39	d	92	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
54	v	467	ASN	2.2
15	O	7	ALA	2.2
32	5	36	TYR	2.2
51	s	986	U	2.2
51	s	1048	G	2.2
2	B	107	LYS	2.2
16	P	66	LEU	2.2
39	d	4	ILE	2.2
49	n	118	ILE	2.2
24	X	45	ASP	2.2
6	F	106	ALA	2.2
26	Z	1	ALA	2.2
32	5	53	THR	2.2
45	j	48	TYR	2.2
3	C	22	SER	2.2
16	P	72	TRP	2.2
54	v	485	PHE	2.2
16	P	75	VAL	2.2
3	C	147	LYS	2.2
12	L	49	GLU	2.2
49	n	151	LEU	2.2
52	t	896	A	2.2
1	A	220	VAL	2.2
6	F	41	ILE	2.2
56	AA	3	SER	2.2
1	A	141	GLU	2.2
38	c	80	ASP	2.2
51	s	727	G	2.2
51	s	1228	C	2.2
44	i	25	THR	2.2
24	X	160	LYS	2.2
26	Z	124	MET	2.2
1	A	68	PHE	2.2
1	A	129	THR	2.2
6	F	132	THR	2.2
8	H	96	GLU	2.2
24	X	30	VAL	2.2
49	n	140	MET	2.2
54	v	483	GLU	2.2
40	e	51	GLY	2.2
52	t	1098	A	2.2
2	B	110	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
11	K	90	PRO	2.2
50	o	18	ASP	2.2
4	D	30	PHE	2.2
6	F	40	SER	2.2
26	Z	29	GLN	2.2
3	C	129	VAL	2.2
3	C	46	ARG	2.2
24	X	7	TYR	2.2
11	K	106	VAL	2.2
20	T	43	GLU	2.2
48	m	22	VAL	2.2
8	H	24	ASN	2.2
14	N	45	HIS	2.2
26	Z	84	GLY	2.2
30	3	6	ARG	2.2
24	X	74	ALA	2.1
52	t	353	C	2.1
52	t	365	U	2.1
52	t	894	U	2.1
9	I	19	ASP	2.1
10	J	97	ARG	2.1
31	4	72	ASP	2.1
32	5	63	LYS	2.1
10	J	99	LEU	2.1
7	G	106	SER	2.1
21	U	93	VAL	2.1
24	X	72	SER	2.1
29	2	116	VAL	2.1
32	5	74	VAL	2.1
50	q	2	ILE	2.1
21	U	32	LEU	2.1
1	A	159	ALA	2.1
26	Z	61	TYR	2.1
32	5	37	ALA	2.1
6	F	148	LYS	2.1
20	T	33	ARG	2.1
4	D	104	ILE	2.1
51	s	206	C	2.1
32	5	78	VAL	2.1
37	b	91	GLN	2.1
12	L	50	GLY	2.1
51	s	1039	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	45	THR	2.1
3	C	122	ILE	2.1
26	Z	118	GLY	2.1
3	C	205	LYS	2.1
6	F	101	ARG	2.1
32	5	81	ARG	2.1
37	b	3	ARG	2.1
49	n	16	SER	2.1
12	L	60	ALA	2.1
52	t	278	A	2.1
7	G	51	GLU	2.1
32	5	34	HIS	2.1
51	s	1224	U	2.1
3	C	176	LYS	2.1
17	Q	50	TYR	2.1
21	U	29	PHE	2.1
2	B	132	ALA	2.1
6	F	89	GLU	2.1
52	t	2182	U	2.1
16	P	74	LEU	2.1
23	W	97	ASN	2.1
54	v	215	LEU	2.1
54	v	487	ARG	2.1
16	P	77	VAL	2.1
2	B	130	ARG	2.1
14	N	41	HIS	2.1
24	X	14	LYS	2.1
45	j	11	VAL	2.1
3	C	89	LEU	2.1
52	t	1103	A	2.1
24	X	24	VAL	2.1
1	A	134	LEU	2.1
26	Z	106	GLN	2.1
1	A	197	PHE	2.1
32	5	73	ALA	2.1
41	f	73	ARG	2.1
49	n	156	ALA	2.1
51	s	631	C	2.1
9	I	10	LEU	2.1
52	t	1723	G	2.1
54	v	409	GLN	2.1
24	X	91	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
51	s	1441	A	2.1
26	Z	127	SER	2.1
24	X	162	ASP	2.1
24	X	173	ASP	2.1
1	A	44	LYS	2.0
1	A	65	LYS	2.0
49	n	94	ARG	2.0
26	Z	31	GLY	2.0
1	A	26	MET	2.0
26	Z	9	LYS	2.0
19	S	60	GLN	2.0
32	5	102	ARG	2.0
6	F	39	GLU	2.0
52	t	1104	C	2.0
3	C	75	TYR	2.0
23	W	201	ALA	2.0
50	o	12	ALA	2.0
26	Z	55	PRO	2.0
49	n	60	LEU	2.0
6	F	16	LYS	2.0
12	L	81	ASP	2.0
26	Z	140	GLU	2.0
52	t	1744	A	2.0
54	v	394	ALA	2.0
13	M	46	LYS	2.0
25	Y	98	LYS	2.0
12	L	2	ARG	2.0
16	P	63	CYS	2.0
51	s	971	G	2.0
16	P	7	LEU	2.0
32	5	3	LYS	2.0
32	5	76	LYS	2.0
26	Z	35	MET	2.0
15	O	19	VAL	2.0
24	X	96	TRP	2.0
29	2	85	VAL	2.0
15	O	52	LEU	2.0
19	S	85	LEU	2.0
51	s	983	A	2.0
52	t	1745	A	2.0
37	b	82	LYS	2.0
52	t	1726	C	2.0

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Mol	Chain	Res	Type	RSRZ
32	5	99	TYR	2.0

6.2 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
56	DPP	BA	2	6/7	0.28	0.42	97,99,99,100	0
56	KBE	BA	1	9/10	0.37	0.52	73,86,98,100	0
56	UAL	7	5	9/10	0.50	0.87	117,119,122,122	0
56	KBE	AA	1	9/10	0.51	0.57	74,80,92,93	0
56	5OH	7	6	12/13	0.55	0.58	107,109,112,116	0
56	KBE	y	1	9/10	0.64	0.53	105,106,108,108	0
56	5OH	z	6	12/13	0.67	0.84	100,106,109,110	0
56	KBE	z	1	9/10	0.72	0.45	86,90,94,94	0
56	DPP	AA	2	6/7	0.74	0.51	95,100,101,102	0
56	5OH	AA	6	12/13	0.76	0.54	101,103,104,105	0
56	UAL	BA	5	9/10	0.79	0.61	96,100,100,101	0
56	DPP	z	2	6/7	0.80	0.38	94,95,98,101	0
56	KBE	7	1	9/10	0.83	0.60	86,89,93,95	0
56	UAL	AA	5	9/10	0.85	0.65	103,105,106,106	0
56	5OH	BA	6	12/13	0.85	0.38	99,102,103,103	0
56	UAL	y	5	9/10	0.87	0.21	102,103,109,109	0
56	UAL	z	5	9/10	0.87	0.39	99,100,101,102	0
56	DPP	7	2	6/7	0.87	0.42	98,103,106,109	0
56	DPP	y	2	6/7	0.92	0.23	98,99,100,104	0
56	5OH	y	6	12/13	0.94	0.32	99,102,105,109	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.