

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 06:08 PM EDT

PDB ID	:	6N1D
Title	:	X-ray Crystal complex showing Spontaneous Ribosomal Translocation of
		mRNA and tRNAs into a Chimeric Hybrid State
Authors	:	Noller, H.F.; Donohue, J.P.; Lancaster, L.; Zhou, J.
Deposited on	:	2018-11-08
Resolution	:	3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) 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	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.20 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

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	A16S	1518	77%	22%	
1	B16S	1518	78%	21%	
2	A23S	2881	% 77%	22%	•
2	B23S	2881	% 	22%	•



Mol

Chain Quality of chain Length 8% 3 A5S11948% 39% 13% 4% 3 B5S1198% • 63% 28% 30% AL01 2284 81% 18% 59% 4 **BL01** 22872% 28% 11% AL02276589% 9% • % 5BL0227687% 12% . 4% AL03 6 20689% 10% • 3% BL03• 6 20689% 10% % AL04720592% 6% • 2% 7 **BL04** 20589% 10% • 61% 8 AL05181 83% 17% . 52% BL058 181 86% 14% 4% 9 AL06 180• 7% 77% 16% 11% 9 **BL06** 18072% • 7% 20% 9% AL09 10 14889% 8% •• 7% 10 BL09148• 90% 8% 11 AL13 14086% 12% • BL1311 14084% 14% • • 12AL14122• 98% 2% 12BL1412295% 5% 6% 13AL15150• • 81% 13% 4% BL15. . 13 15079% 17% 4% AL16 1414182% 13% 5% 4% BL161414185% 5% 10% 2% AL171511892% 8% •

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Mol	Chain	Length	Quality of chain	
15	BL17	118	<u>6%</u> 86%	12% ••
16	AL18	111	78%	10% 12%
16	BL18	111	28%	14% · 12%
17	AL19	146	% • 84%	10% 6%
17	BL19	146	85%	9% 6%
18	AL20	118	5% 92%	6% ••
18	BL20	118	% • 88%	11% •
19	AL21	101	3% 87%	13%
19	BL21	101	92%	7% •
20	AL22	113	90%	9% •
20	BL22	113	93%	5% ••
21	AL23	96	7% 91%	5% •
21	BL23	96	89%	7% •
22	AL24	110	34%	13% • 9%
22	BL24	110	9%	14% <mark>•</mark> 9%
23	AL25	206	25%	7% 9%
23	BL25	206	% • 83%	8% 9%
24	AL27	84	61% 82%	14% ••
24	BL27	84	44% 81%	17% ·
25	AL28	98	83%	6% • 10%
25	BL28	98	10%	13% 10%
26	AL29	72	4% 78%	8% 14%
26	BL29	72	6% 81%	6% 14%
27	AL30	60	20% 92%	7%•
27	BL30	60	3% 93%	5%•

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Mol	Chain	Length	Quality of chain							
	A.T. o.d	_	30%							
28	AL31	71	32% 25% 6%	37%						
28	BL31	71	35% 25%	37%						
29	AL32	59	75%	22% •						
29	BL32	59	78%	17% ••						
30	AL33	54	59% 22%	19%						
30	BL33	54	57% 22%	• 19%						
31	AL34	49	86%	12% ·						
31	BL34	49	96%							
32	AL35	64	83%	16% •						
32	BL35	64	81%	17% •						
33	AL36	37	95%	5%						
33	BL36	37	81%	19%						
34	AMRN	17	29% 29%	41%						
34	BMRN	17	12% 71%	18%						
35	APTN	76	32% 57%	12%						
35	BPTN	76	11% 32% 58	%						
36	AS02	255	82%	9% 8%						
36	BS02	255	82%	9% 8%						
37	AS03	238	78%	8% • 13%						
37	BS03	238	77%	10% 13%						
38	AS04	208	90%	9%						
38	BS04	208	91%	7% •						
39	AS05	161	88%	6% • 6%						
39	BS05	161	86%	8% 6%						
40	AS06	101	6% 91%	8% •						

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Mol

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Length

Chain

Quality of chain

.% **BS06** 40 101 . . 95% 3% AS0741 15590% 8% • 14% 41 **BS07** 15590% 9% • AS084213888% 11% . 7% 42BS0813892% 8% 9% 43AS0912888% 12% 38% BS091284314% 85% 14% AS1044104• 6% 90% 5% **BS10** 10444 6% 81% 13% 27% AS11 4512882% 7% 11% 4% 45**BS11** 12883% 5%• 11% % AS1246 13188% 5% 7% 3% BS1246 1317% 82% 11% 14% AS134712578% 6% 15% 44% BS134712579% 14% • 6% 28% AS144860 77% 23% 12% BS144860 88% 12% 3% AS154988 11% 88% • % BS154988 90% 10% 8% AS165088 89% 6% 6% 22% 50BS16 88 5% 6% 90% AS17 51104•• 5% 93% 3% BS175110488% 8% 5% .% AS18875220% 72% 8% BS185287 8% 20% 72% Continued on next page...



Contr	nucu jiom	i previous j	Juye			
Mol	Chain	Length	Quality of cha	ain		
			51%			
53	AS19	92	70%	14%	• 15%	6
			38%			
53	BS19	92	73%	11%	• 15%	6
			17%			
54	AS20	105	88%		7%	6%
			3%			
54	BS20	105	83%		11%	6%
			62%	-		
55	ATHX	26	62%	23%	8%	8%
			81%			
55	BTHX	26	85%		8%	8%
			59%			
56	BATN	85	9% 39%	52%		

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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	5MU	BATN	54	-	-	-	Х
56	PSU	BATN	55	-	-	-	Х
57	MG	A23S	2911	-	-	-	Х
57	MG	AL02	302	-	-	-	Х
57	MG	AL34	100	-	-	-	Х
57	MG	BL23	101	-	-	-	Х



6N1D

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 295025 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A 169	1517	Total	С	Ν	Ο	Р	0	0	0
1 A105	1017	32600	14510	6031	10542	1517	0	0	0	
1	DICC	1517	Total	С	Ν	0	Р	0	0	0
1	1 B105	1917	32600	14510	6031	10542	1517	0	0	

• Molecule 1 is a RNA chain called 16S rRNA.

• Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues		Atoms					AltConf	Trace
2	A23S	2879	Total 61999	C 27595	N 11586	O 19940	Р 2878	0	0	0
2	B23S	2879	Total 62000	C 27595	N 11586	O 19941	Р 2878	0	0	0

• Molecule 3 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A5S	119	Total 2551	C 1136	N 471	O 826	Р 118	0	0	0
3	B5S	119	Total 2551	C 1136	N 471	O 826	Р 118	0	0	0

• Molecule 4 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4 AT 01	228	Total	С	Ν	0	S	0	0	0
4 AL01	ALUI	220	1742	1101	319	319	3	0	0	
4	4 DI 01	1 228	Total	С	Ν	0	S	0	0	0
4 1	DL01		1742	1101	319	319	3	0	0	

• Molecule 5 is a protein called 50S ribosomal protein L2.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
Б	AT 02	271	Total	С	Ν	0	\mathbf{S}	0	0	0
0	AL02	271	2104	1329	416	356	3	0	0	0
Б	BI 00	271	Total	С	Ν	0	S	0	0	0
0	DL02	271	2104	1329	416	356	3	0	0	0

• Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	AT 02	204	Total	С	Ν	0	S	0	0	0
0	AL05	204	1563	988	299	270	6	0	0	0
6	DI 09	204	Total	С	Ν	0	S	0	0	0
0	DL05	204	1563	988	299	270	6	0	0	0

• Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	AL04	202	Total 1586	C 1011	N 297	0 275	${ m S} { m 3}$	0	0	0
7	BL04	202	Total 1586	C 1011	N 297	0 275	${f S}\ 3$	0	0	0

• Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
8	AT 05	181	Total	С	Ν	0	S	0	0	0
0	AL05	101	1475	943	268	260	4	0	0	0
0	BI 05	191	Total	С	Ν	0	S	0	0	0
0	DL05	101	1475	943	268	260	4	0	0	0

• Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
0	AT 06	167	Total	С	Ν	0	S	0	0	0
9	AL00	107	1282	814	239	228	1	0	0	0
0	BI 06	167	Total	С	Ν	0	S	0	0	0
9	DL00	107	1282	814	239	228	1			U

• Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		Atoms					AltConf	Trace
10	AL09	145	Total 1131	С 724	N 199	O 207	S 1	0	0	0



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	BL09	145	Total 1132	С 724	N 200	O 207	S 1	0	0	0

• Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
11	AT 13	137	Total	С	Ν	0	S	0	0	0
11	ALIS	157	1096	707	205	181	3	0	0	0
11	DI 12	127	Total	С	Ν	0	S	0	0	0
	DL15	107	1096	707	205	181	3	0	0	0

• Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19	AT 14	199	Total	С	Ν	0	S	0	0	0
12	AL14	122	932	587	171	170	4	0	0	0
10	DI 14	199	Total	С	Ν	0	S	0	0	0
	DL14	122	932	587	171	170	4			U

• Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19	AT 15	146	Total	С	Ν	0	S	0	0	0
10	ALIJ	140	1114	692	227	193	2	0	0	0
19	DI 15	146	Total	С	Ν	0	S	0	0	0
15	DL10	140	1114	692	227	193	2	0	0	0

• Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
14	AL 16	134	Total	С	Ν	0	S	0	0	0
14	ALIO	104	1064	680	201	178	5	0	0	0
14	BI 16	134	Total	С	Ν	0	S	0	0	0
14	DLIO	104	1064	680	201	178	5			U

• Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		Ato	\mathbf{ms}		ZeroOcc	AltConf	Trace
15	AT 17	117	Total	С	Ν	Ο	0	0	0
10	ALI	117	960	599	202	159	0	0	0
15	DI 17	117	Total	С	Ν	Ο	0	0	0
10	DL1(117	960	599	202	159	0	0	0



• Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
16	AT 18	08	Total	С	Ν	Ο	0	0	0
10	ALIO	90	770	486	154	130	0	0	0
16	DI 19	08	Total	С	Ν	Ο	0	0	0
10	DLIO	90	770	486	154	130	0	0	0

• Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
17	AT 10	197	Total	С	Ν	0	S	0	0	0
11	AL19	107	1143	713	234	195	1	0	0	0
17	BI 10	127	Total	С	Ν	0	S	0	0	0
11	DL19	101	1143	713	234	195	1			U

• Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
18	AL20	117	Total 964	C 610	N 202	0 151	S 1	0	0	0
18	BL20	117	Total 964	C 610	N 202	0 151	1 S 1	0	0	0

• Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
10	AT 91	101	Total	С	Ν	0	S	0	0	0
19	ALZI	101	779	501	142	135	1	0	0	0
10	PI 91	101	Total	С	Ν	0	S	0	0	0
19	DL21	101	779	501	142	135	1	0	0	0

• Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	AT 99	119	Total	С	Ν	0	S	0	0	0
20	ALZZ	112	890	560	175	153	2	0	0	0
20	PI 99	119	Total	С	Ν	0	S	0	0	0
20	DL22	112	890	560	175	153	2	0	0	0

• Molecule 21 is a protein called 50S ribosomal protein L23.



Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
21	AL23	92	Total 725	C 471	N 131	0 123	0	0	0
			Total	$\frac{411}{C}$	N	0			
21	BL23	92	725	471	131	123	0	0	0

• Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
	AT 94	100	Total	С	Ν	0	S	0	0	0
	AL24	100	775	500	148	123	4	0	0	0
	DI 94	100	Total	С	Ν	0	S	0	0	0
	DL24	100	775	500	148	123	4			U

• Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
23	AL25	187	Total 1482	C 945	N 264	0 271	S 2	0	0	0
23	BL25	187	Total 1482	C 945	N 264	0 271	S 2	0	0	0

• Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
24	AT 27	80	Total	С	Ν	0	S	0	0	0
24	ALZI	02	647	401	136	109	1	0	0	0
24	BI 97	80	Total	С	Ν	0	S	0	0	0
24		02	647	401	136	109	1		U	U

• Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
25	AT 28	88	Total	С	Ν	Ο	0	0	0
2.0	AL ₂₀	00	694	435	141	118	0	0	0
25	BI 98	00	Total	С	Ν	Ο	0	0	0
20	DL20	00	694	435	141	118	0	0	0

• Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
26	AL29	62	Total 520	$\begin{array}{c} \mathrm{C} \\ \mathrm{325} \end{array}$	N 102	0 91	${ m S} { m 2}$	0	0	0



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Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
26	BL29	62	Total 520	C 325	N 102	O 91	${ m S} { m 2}$	0	0	0

• Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
97	AT 30	50	Total	С	Ν	0	S	0	0	0
21	AL50		467	298	90	78	1	0	0	0
97	BI 30	50	Total	С	Ν	0	S	0	0	0
	DL30		467	298	90	78	1	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
20	AT 21	45	Total	С	Ν	0	S	0	0	0
20	AL91	40	351	224	61	62	4	0	0	0
20	DI 21	45	Total	С	Ν	0	S	0	0	0
20	DT91	40	351	224	61	62	4		0	U

• Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
20	AT 20	50	Total	С	Ν	Ο	S	0	0	0
29	AL52		459	288	90	76	5	0	0	0
20	DI 20	50	Total	С	Ν	Ο	S	0	0	0
29	DL32		459	288	90	76	5	0	U	U

• Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
30	AT 33	4.4	Total	С	Ν	Ο	S	0	0	0
- 50	AL55	44	380	235	77	64	4	0	0	0
20	DI 33	4.4	Total	С	Ν	Ο	S	0	0	0
- 50	DL99	44	380	235	77	64	4	0	0	0

• Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
21	AT 34	18	Total	С	Ν	Ο	\mathbf{S}	0	0	0
51	AL54	40	418	257	104	55	2	0	0	0
21	DI 24	18	Total	С	Ν	0	S	0	0	0
51	DL04	40	418	257	104	55	2	0	0	0



• Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
30	ΔL35	63	Total	С	Ν	Ο	\mathbf{S}	0	0	0
52	AL55	05	507	326	101	78	2	0	0	0
20	DI 25	62	Total	С	Ν	0	S	0	0	0
32	DL99	05	507	326	101	78	2	0	0	0

• Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Atc	\mathbf{ms}			ZeroOcc	AltConf	Trace
22	AT 36	37	Total	С	Ν	Ο	S	0	0	0
00	AL50	51	307	188	68	47	4	0	0	0
22	BI 36	27	Total	С	Ν	Ο	\mathbf{S}	0	0	0
- 33	DL30	57	307	188	68	47	4	0	0	0

• Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
34	AMRN	10	Total	С	Ν	Ο	Р	0	0	0
- 54	AWITT	10	223	99	47	67	10	0	0	0
34	BMBN	17	Total	С	Ν	Ο	Р	0	0	0
- 54	DIVITUN	11	373	167	76	113	17	0	0	0

• Molecule 35 is a RNA chain called P-tRNA.

Mol	Chain	Residues		-	Atom	IS			ZeroOcc	AltConf	Trace
35	APTN	76	Total 1631	C 728	N 292	O 534	Р 76	S 1	0	0	0
35	BPTN	76	Total 1631	C 728	N 292	O 534	Р 76	S 1	0	0	0

• Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
36	AS02	234	Total 1900	C 1213	N 341	0 341	${f S}{5}$	0	0	0
36	BS02	234	Total 1900	C 1213	N 341	0 341	${f S}{5}$	0	0	0

• Molecule 37 is a protein called 30S ribosomal protein S3.



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
27	1503	206	Total	С	Ν	0	S	0	0	0
51	ASUS	200	1612	1016	314	281	1	0	0	0
27	BS03	206	Total	С	Ν	0	S	0	0	0
57	D202	200	1612	1016	314	281	1	0	0	0

• Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
20	4 504	208	Total	С	Ν	0	S	0	0	0
30	A504	208	1665	1043	329	286	7	0	0	0
20	DS04	208	Total	С	Ν	0	S	0	0	0
30	D504	208	1665	1043	329	286	7	0	0	0

• Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
30	4 \$05	151	Total	С	Ν	Ο	S	0	0	0
03	A909	101	1155	729	218	204	4	0	0	0
30	BS05	151	Total	С	Ν	Ο	S	0	0	0
- 39	D202	101	1155	729	218	204	4	0	0	0

• Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
40	1506	101	Total	С	Ν	0	S	0	0	0
40	ASUU	101	843	531	155	154	3	0	0	0
40	BS06	101	Total	С	Ν	0	S	0	0	0
40	0060	101	843	531	155	154	3			U

• Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
41	1807	155	Total	С	Ν	0	S	0	0	0
41	ASUT	100	1257	781	252	218	6	0	0	0
41	BS07	155	Total	С	Ν	0	S	0	0	0
41	D307	100	1257	781	252	218	6	0		U

• Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
42	AS08	138	Total 1116	C 705	N 215	O 193	${ m S} { m 3}$	0	0	0



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Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
42	BS08	138	Total 1116	$\begin{array}{c} \mathrm{C} \\ 705 \end{array}$	N 215	O 193	${ m S} { m 3}$	0	0	0

• Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
43	1500	197	Total	С	Ν	Ο	0	0	0
40	A509	121	1011	639	198	174	0	0	0
42	BS00	197	Total	С	Ν	Ο	0	0	0
40	D309	121	1011	639	198	174		U	U

• Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
4.4	AS10	08	Total	С	Ν	0	S	0	0	0
44	ASIU	90	794	499	156	138	1	0	0	0
4.4	PS10	08	Total	С	Ν	0	S	0	0	0
44	D310	90	794	499	156	138	1			U

• Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
45	AS11	114	Total	С	Ν	0	S	0	0	0
40	11011	114	842	522	159	158	3	0	0	0
45	DC11	11/	Total	С	Ν	0	\mathbf{S}	0	0	0
40	DSII	114	842	522	159	158	3			U

• Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
46	AS12	199	Total	С	Ν	0	S	0	0	Ο
-10	11012	122	956	603	193	159	1	0	0	0
46	BS19	199	Total	С	Ν	0	\mathbf{S}	0	0	0
40	D512	122	956	603	193	159	1	0	0	0

• Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
47	1812	117	Total	С	Ν	0	\mathbf{S}	0	0	0
41	ASIS	111	933	577	192	162	2	0	0	0
47	PS12	117	Total	С	Ν	0	S	0	0	0
41	DOLO	111	933	577	192	162	2	0	0	0



• Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
18	AS14	60	Total	С	Ν	Ο	\mathbf{S}	0	Ο	0
40	A314	00	492	312	104	72	4	0	0	0
19	PS14	60	Total	С	Ν	0	S	0	0	0
40	D514	00	492	312	104	72	4	0	0	0

• Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
40	A S 15	<u> </u>	Total	С	Ν	0	S	0	0	0
49	ASIS	00	734	459	147	126	2	0	0	0
40	PS15	<u> </u>	Total	С	Ν	0	S	0	0	0
49	D210	00	734	459	147	126	2			U

• Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	AS16	83	Total 700	C 443	N 139	0 117	S 1	0	0	0
50	BS16	83	Total 700	C 443	N 139	0 117	S 1	0	0	0

• Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	AS17	00	Total	С	Ν	0	S	0	0	0
51	ASIT	99	823	528	152	141	2	0	0	0
51	PS17	00	Total	С	Ν	0	S	0	0	0
101	DOLL	99	823	528	152	141	2	0		U

• Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace	
52	AS18	70	Total 574	C 367	N 112	0 95	0	0	0
52	BS18	70	Total 574	C 367	N 112	0 95	0	0	0

• Molecule 53 is a protein called 30S ribosomal protein S19.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	AS10	78	Total	С	Ν	0	S	0	0	0
55	ASI9	10	629	403	114	110	2	0	0	
52	PS10	79	Total	С	Ν	0	S	0	0	0
55	D319	10	629	403	114	110	2	0	0	0

• Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	1 5 2 0	00	Total	С	Ν	0	S	0	0	0
04	A520	99	762	469	162	129	2	0	0	0
54	DC00	00	Total	С	Ν	0	S	0	0	0
- 54	D520	99	762	469	162	129	2	0	0	0

• Molecule 55 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
55	ATHX	24	Total 208	C 128	N 50	O 30	0	0	0
55	BTHX	24	Total 208	C 128	N 50	O 30	0	0	0

• Molecule 56 is a RNA chain called A tRNA.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
56	BATN	85	Total 1824	C 821	N 323	O 594	Р 85	S 1	0	0	0

• Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	A16S	33	Total Mg 33 33	0	0
57	A23S	73	TotalMg7373	0	0
57	A5S	3	Total Mg 3 3	0	0
57	AL01	2	Total Mg 2 2	0	0
57	AL02	2	Total Mg 2 2	0	0
57	AL04	3	Total Mg 3 3	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AL06	1	Total Mg 1 1	0	0
57	AL14	1	Total Mg 1 1	0	0
57	AL15	2	Total Mg 2 2	0	0
57	AL17	2	Total Mg 2 2	0	0
57	AL20	1	Total Mg 1 1	0	0
57	AL21	3	Total Mg 3 3	0	0
57	AL23	2	Total Mg 2 2	0	0
57	AL24	1	Total Mg 1 1	0	0
57	AL27	1	Total Mg 1 1	0	0
57	AL28	2	Total Mg 2 2	0	0
57	AL33	3	Total Mg 3 3	0	0
57	AL34	1	Total Mg 1 1	0	0
57	AS02	1	Total Mg 1 1	0	0
57	AS03	1	Total Mg 1 1	0	0
57	AS06	2	Total Mg 2 2	0	0
57	AS08	1	Total Mg 1 1	0	0
57	B16S	32	Total Mg 32 32	0	0
57	B23S	133	Total Mg 133 133	0	0
57	B5S	5	Total Mg 5 5	0	0
57	BATN	1	TotalMg11	0	0
57	BL01	2	Total Mg 2 2	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BL02	5	Total Mg 5 5	0	0
57	BL03	1	Total Mg 1 1	0	0
57	BL04	1	Total Mg 1 1	0	0
57	BL15	3	Total Mg 3 3	0	0
57	BL16	3	Total Mg 3 3	0	0
57	BL18	3	Total Mg 3 3	0	0
57	BL19	2	Total Mg 2 2	0	0
57	BL20	1	Total Mg 1 1	0	0
57	BL21	1	Total Mg 1 1	0	0
57	BL22	1	Total Mg 1 1	0	0
57	BL23	1	Total Mg 1 1	0	0
57	BL24	2	Total Mg 2 2	0	0
57	BL25	1	Total Mg 1 1	0	0
57	BL28	2	Total Mg 2 2	0	0
57	BL29	5	Total Mg 5 5	0	0
57	BL30	1	Total Mg 1 1	0	0
57	BL31	1	$\begin{array}{c c} \hline \text{Total} & \text{Mg} \\ \hline 1 & 1 \end{array}$	0	0
57	BL32	1	Total Mg 1 1	0	0
57	BL33	3	Total Mg 3 3	0	0
57	BL34	2	Total Mg 2 2	0	0
57	BL35	1	Total Mg 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BL36	1	Total Mg 1 1	0	0
57	BS16	1	Total Mg 1 1	0	0
57	BS17	1	Total Mg 1 1	0	0
57	BTHX	1	Total Mg 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AS04	1	Total Fe S 8 4 4	0	0
58	BS04	1	TotalFeS844	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: 16S rRNA





 \bullet Molecule 1: 16S rRNA





AG	G10	G17	G27	C34	G35 636	000	C46	USO	G51	<mark>G61</mark>	C62 1163	A64	A 7 1		0.75	<u>675</u>	A84	104	TAN	<mark>695</mark>	<mark>698</mark>	66N	G101 G102		C105	A118	A119 U120	A126		G131	G137B	G137C	A137E		U155B	U155C U155D	U155E G171	C172
A181	A106	A197	C198 A199	G205		4215 A216	A001	A222 A222		A228 A228	A229 11230		A233	A241		G245 C246	G247	G248	G250 G250	A251	G252	C267	C268 U269		U270M G270N	U2700	C2700	LOZOT	G270Y	G971B	U271C	G271D	G271M	A0710	C271R	C284	G295	-
C302	U306	G308	A320	G323	A324	<mark>G329</mark>	A330	A345	A346	G352	G353	G357F	A3671	C357M	C357N	C35/U	G372	<u>1373</u>	G379	U380	U384	C385	G386	<mark>G396</mark>	G400	A401	C404	U405 C406	5	G411 A412		G418	A423	G424	C444	C451	G452	C455
C456 A457		N4 I O	G474	G481 A482	A483	C487		A505	CEO8	C509	CE 10	A513	AFOR	C527	2L 2L 2	C531 A532		G563	U569	G570	A571 A572	G573	C574 A575		G583	C587	G602	A603	G610	G61F	A611F	G611G	C618	A607		A637	G642	A646
G647	C650	C653	U654 A655	G656	A670		A676	G686	U230	0000	U740	U747	G748	G765	0177	6776 6776		A782	A784	<mark>G785</mark>	C791	G792	6798	6799	A 800	<mark>6805</mark>	C812	4810		U827 11828	A829	G 830	U833	C846	U847	<mark>G859</mark>	U860	G879
C884	C885	A887	C888 C886 C886	<u>A896</u>	C897	A910	C914	ET CO	A917	G919	1 030	A933	4041	TLOV	G946	A957		C961	G974	C974A	A983		A990	9996	G1003		C1 007 C1 008	A1009	G1011	U1012 C1013		G1017	A1020	A1021 G1022	U1023	G1024 G1025	U1026	<mark>G1034</mark>
C1041		A1045 A1046	G1047 A1048	U1066	A1067	A1069	A1070 G1071	C1072	A1073	A1077	U1078 C1079	C1080	U1081	20010	A1086	G1087 A1088	G1089		A1095 A1096	U1097	A1098	C1104	G1112	-	G1122	A1129	01130	C1135 C1136		A1155 A1156	G1157	U1171	G1172	A1173 111174	G1175		G1195	A1204
U1205	A1210	11710	C1217 C1218	C1220		41226 A1226	G1227	G1236	74744	11271	A1253	G1256	A1 765		G1271	A12/2	<mark>U1300</mark>	A1301		G1309	G1310 G1311	U1312	01313 C1314	-	A1321	U1 <mark>329</mark>	01341	C1 345		A1349 C1350	C1351	01352	A1359	A1360	G1 <mark>364</mark>	G1371	A1378	A1379
61385	C1386	A1392	A1395	01396	G1416		U1420 61421	17210	A1427	G1429	C1441		A1444A		A1453	01454 G1455		A1460	G1461 C1462	1	C1467 C1468	A1468A	G1468J		G1483	A1490	C1493	A1494 A1495	A1496	U1497 C1498				C1506K	G1526	G1527	C1533 G1534	<mark>U1535</mark>
A1536 C1537	G1538	G1540	01541 G1542	A1543 C1543A	A1544	C1547	A1554		A1558 C1550	G1560	A 1 5 66		A1569	C1584		61595	C1598	1 1 C / C / C	T TOUS	G1606	C1607 A1608		C1611	C1617	A1618	A1634	U1639	C1640	C1644	G1645 C1646	G1647	C1648	G1651	A1665		G1674	G1696 G1697	A1698
G1699	A1712H	A1712K	G1712Q	G1756	U1757	00 / 15	A1762 C1763	G1764	A1 77 3	C1774	A1 784	A1785	A1786	C1800	G1801	A1802 A1803	C1804		01809		A1815 G1816		C1827 G1828	A1829	A1847	A1848	A1853	A1 86 AC	A1864D	G1878	<mark>G1</mark> 883	11 22 6	C1887	G1888	<mark>C1893</mark>	G1899	G1903	
1 <u>906</u>	1913		1927 1928	1929 1930	1931	1936	1937 1938	1939	1013	0#0	1952 1953	1954	1955	1 <mark>962</mark>	1963 	1967		1971 1970	Tarr	1981	1982	1 <mark>991</mark>	1992 1993	1994	1995 1996		2000	2023	2030	2031 2032	2033			2046	2049	2052	2055	2056
A2057 A2058	A2059	62061	A2062 C2063	0 00068	G2069	G2093	G2094	C2111 0	G2112	G2116	A A A A A A A A	G2120	Coton U	G2125	A2126 U	U2132 C	G2133	A2134 A	A 21 35 C 21 36	C2137 A	G2141	C2142 U	C2145	C2146	G2149 C	U2150	G2152 G2152	G2153 C2154	G2155	G2156 G2157 G2157	A2158	G2159	C2161	A0171	U2172 G	A2173 C2174 G	C2177	C2178







 \bullet Molecule 3: 5s rRNA















• Molecule 10: 50S ribosomal protein L9 Chain BL09: 90% 8% • Molecule 11: 50S ribosomal protein L13 Chain AL13: 86% 12% • Molecule 11: 50S ribosomal protein L13 Chain BL13: 84% 14% E4 G4 • Molecule 12: 50S ribosomal protein L14 Chain AL14: 98% • Molecule 12: 50S ribosomal protein L14 Chain BL14: 95% 5% • Molecule 13: 50S ribosomal protein L15 Chain AL15: 81% 13% NE LEU SEI SEI SEI • Molecule 13: 50S ribosomal protein L15 Chain BL15: 79% 17%







• Molecule 17: 50S riboson	nal protein L19	
Chain AL19:	84%	10% 6%
M1 N2 R3 G4 R5 B5 B5 B5 B5 B5 B5 C5 B5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5	111 111 111 111 111 111 111 111 111 11	
• Molecule 17: 50S riboson	nal protein L19	
Chain BL19:	85%	9% 6%
M R23 R29 R39 R39 R39 R53 R53 R53 R53 R53 R53 R53 R53 R53 R55 R53 R55 R53 R55 R53 R55 R53 R55 R53 R55 R55	D107 122 1228 1228 1228 1228 1228 1228 1228	
• Molecule 18: 50S riboson	nal protein L20	
Chain AL20:	92%	6% ••
MET R3 R3 R4 R4 R5 R5 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3 R3	102 E1 02 01 17 01 17 01 18	
• Molecule 18: 50S riboson	nal protein L20	
Chain BL20:	88%	11% •
MET P 2 C 2 C 2 C 2 C 2 C 2 C 4 C 4 C 4 C 4 C 4 C 4 C 4 C 4	188 1991 118 118	
• Molecule 19: 50S riboson	nal protein L21	
Chain AL21:	87%	13%
M1 K10 G17 D26 K44 F50 F50 K44 K74 K75 K75	480 193 194 194 194 101 101	
• Molecule 19: 50S riboson	nal protein L21	
Chain BL21:	92%	7% •
M1 F2 K6 K24 664 K77 K78 K78 K78 K78 K78 K78 G101		

• Molecule 20: 50S ribosomal protein L22



Chain AL22:	90	0%	9% •
M1 R11 N40 D63 K72 A73 A74	E78 679 679 680 A81 L82 A81 B87 A82 H82 H82 B94 H102 H110 H111 H112 H111 CH112 H111 LYS		
• Molecule 20:	50S ribosomal protein L22		
Chain BL22:		93%	5% ••
M1 D63 D67 D67 P80 P87	ABO R90 G112 LYS		
• Molecule 21:	50S ribosomal protein L23		
Chain AL23:	9	1%	5% •
MET LYS D6 E15 K40 V51	R60 R65 L66 L66 R73 R78 R78 R78 R78 C86 C86 C86 C86 C86 C86 C86 C86 C86 C8		
• Molecule 21:	50S ribosomal protein L23		
Chain BL23:	% 89	%	7% •
MET LYS 13 13 113 113 113 113 113 113 113 113	V52 L57 L57 L57 R76 A84 A84 A84 E93 L92 L92 C94 L92 L92 L92 L92 L92 L92 L92 L92 L92 L92		
• Molecule 22:	50S ribosomal protein L24		
Chain AL24:	34%		13% • 9%
MET N2 K4 M5 K4 M5 K4 K3 K4 K3 K4 K3 K4 K3 K4 K3 K4 K3 K4 K4 K4 K4 K4 K4 K4 K4 K4 K4 K4 K4 K4	G18 G25 K26 K26 K28 K28 K28 K28 K28 K28 K28 K28 K28 K28	144 1445 1445 1447 1450 1451 1451 1452 1452 1451 1451 1451 1451	E652 E654 E654 E654 E656 E656 E656 E656 E656
C79 P82 L90 R97 V98 K101 CVS	GLY ALA LEU ASP ASP ASP CLU GLU GLU		
• Molecule 22:	50S ribosomal protein L24		
Chain BL24:	9% 76%		14% • 9%
MET R2 V3 V7 K8 K19 K19 K19	K21 K21 K47 K55 F55 F55 F55 G58 G58 G58 G59 G59 G59 G59 G59 G59 F74	A78 A78 CO CO CO CO CO K101 F82 F82 F82 F82 F82 CV CV CV CV CV CV CV CV CV CV CV CV CV	ALEO ARR GLU GLU GLU
• Molecule 23:	50S ribosomal protein L25		
Chain AL25:	25%		7% 9%





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PROTEIN DATA BANK




• Molecule 32:	50S ribosomal	protein L35		
Chain BL35:	%	81%		17% •
P2 K3 H7 K8 C20 G20 R30	H31 L32 N33 W34 K52 K52 K57	beg Aeta Acta		
• Molecule 33:	50S ribosomal	protein L36		
Chain AL36:	16%	959	%	5%
M1 K2 V3 Y24 Y24 C27 C37 C37 C37 C34 C34 C34 C34 C34 C34 C34 C34 C34 C34				
• Molecule 33:	50S ribosomal	protein L36		
Chain BL36:	22%	81%		19%
M1 K2 K2 K3 K3 K5 86 86 86 110 110 110 111 011	K13 C14 C14 V15 V15 Y24 Y24 R29 N29 N29	<mark>83</mark> 4		
• Molecule 34:	mRNA			
Chain AMRN:	12% 29%	29%		41%
A A G 6 0 10 C 10 C 10 A A A A A A A A A	A15 G16 U17 A18 A			
• Molecule 34:	mRNA			
Chain BMRN:	12%	7	71%	18%
A4 A5 G6 G7 G7 B8 G9 G10 U11 A13 A14	A15 G16 U17 A18 U19 A20			
• Molecule 35:	P-tRNA			
Chain APTN:	17% 32%		57%	12%
61 62 03 04 04 04 05 05 01 010 011	U12 C13 C13 C15 C16 C16 C16 C16 C16 C16 C16 C16 C19 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20	A23 624 725 726 726 726 728 728 728 728 730 732 733 733 733 733	A34 A37 A37 A37 A37 A37 A41 A41 C40 C43 C43 C43 C43 C43 C43 C43 C43 C43 C45 C46 C46 C46 C46 C46 C46 C46 C46 C46 C46	047 048 650 650 651 053 053 053 055 055 065 065
C71 C72 A73 C74 C75 C75 A76				
• Molecule 35:	P-tRNA			
Chain BPTN:	11%	32%	58%	5



• Molecule 36: 30S ribosomal protein S2



Chain AS04:

W O R L D W I D E POTEIN DATA BANK 9%

90%



 \bullet Molecule 38: 30S ribosomal protein S4

 \bullet Molecule 39: 30S ribosomal protein S5

Chain AS05:	88%	6% • 6%
PR0 CLU DB M10 M11 111 111 236 236 644 644 644	466 466 463 463 464 464 464 464 4110 4110 41110 41110 41110 41133 41133 4114	HIS ALA GLN GLN GLN
• Molecule 39: 30S ribosoma	al protein S5	
Chain BS05:	86%	8% 6%
PR0 GLU THR D5 D5 D5 D5 D5 D5 D5 D5 D5 D5 D5 D5 D5	E83 F84 F84 K88 K88 K88 K92 K11 K11 K115 K113 K133 K140 K140 K140 K140	L151 R152 R153 R153 R154 L154 L154 A154 A14 A14 A14 A14 A14 GLN GLN GLN
• Molecule 40: 30S ribosoma	al protein S6	
Chain AS06:	91%	8% •
M1 P12 R36 F42 F42 F51 F51 F51 F53 F53 F53 F53 F53 F53 F53 F53 F53 F53		
• Molecule 40: 30S ribosoma	al protein S6	
Chain BS06:	95%	•••



• Molecule 41: 30S ribosomal protein S7



Chain AS07:	90%	8% •
A2 R4 L12 V17 R41 D45	F62 P71 681 682 682 682 682 682 682 682 682 682 7156 7156 7156 7156 7156	
• Molecule 41:	30S ribosomal protein S7	
Chain BS07:	90%	9% •
A2 R5 A7 A7 E8 R10 Q11 Q11 C12 Q13	G19 P20 P21 P23 P23 P23 P23 P23 P23 P23 P31 P31 P31 P31 P31 P31 P31 P3	A121 H122 1154 R155 W156
• Molecule 42:	30S ribosomal protein S8	
Chain AS08:	88%	11% •
M1 R14 E42 E42 R50 R60	R68 180 180 180 84 84 84 84 84 8102 180 1112 1112 1112 1112 1112 1112	
• Molecule 42:	30S ribosomal protein S8	
Chain BS08:	92%	8%
M1 L2 T17 Y20 K46 R46	R80 P74 V79 V93 A110 A110 C112 C113 C135 C135 C135 C135 C135 C135 C135	
• Molecule 43:	30S ribosomal protein S9	
Chain AS09:	9%	12% •
MET 82 83 94 94 810 810 810 810	D32 Y956 R61 A61 A61 F65 F73 F66 K73 F73 F165 K13 F11 F11 F11 F11 F11 F11 F11 F11 F11 F	
• Molecule 43:	30S ribosomal protein S9	
Chain BS09:	38% 85% 1	.4% •
MET E2 RG RG RG RG RG RG RG RG RG RG RG RG RG	V17 119 127 127 127 127 127 128 129 129 129 129 129 129 129 129 129 129	ITT KT8 LT9 A82
A84 191 191 192 193 193 193 190 100 100	D105 K113 C114 C115 A119 A122 P122 P123 R128 R128 R128	
• Molecule 44:	30S ribosomal protein S10	
Chain AS10:	90%	• 6%















 \bullet Molecule 53: 30S ribosomal protein S19





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	207.45Å 442.87Å 613.00Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	100.00 - 3.20	Depositor
Resolution (A)	252.03 - 2.61	EDS
% Data completeness	95.5 (100.00-3.20)	Depositor
(in resolution range)	$78.2\ (252.03-2.61)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.28	Depositor
$< I/\sigma(I) > 1$	$0.95 (at 2.62 \text{\AA})$	Xtriage
Refinement program	PHENIX	Depositor
B B.	0.268 , 0.321	Depositor
Π, Π_{free}	0.269 , 0.322	DCC
R_{free} test set	65984 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	78.9	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.28 , 60.6	EDS
L-test for $twinning^2$	$ < L >=0.37, < L^2>=0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	295025	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: MIA, 6MZ, PSU, MG, 4SU, QUO, CM0, SF4, 5MU, G7M

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).

Mal	Chain	Bond lengths		Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A16S	0.71	33/36490~(0.1%)	0.99	80/56951~(0.1%)	
1	B16S	0.71	30/36490~(0.1%)	0.99	69/56951~(0.1%)	
2	A23S	0.74	3/69437~(0.0%)	0.95	75/108394~(0.1%)	
2	B23S	0.83	9/69438~(0.0%)	0.96	76/108396~(0.1%)	
3	A5S	0.69	3/2853~(0.1%)	0.98	10/4451~(0.2%)	
3	B5S	0.74	2/2853~(0.1%)	1.00	13/4451~(0.3%)	
4	AL01	0.28	0/1774	0.52	0/2391	
4	BL01	0.28	0/1774	0.51	0/2391	
5	AL02	0.48	1/2154~(0.0%)	0.55	0/2905	
5	BL02	0.49	0/2154	0.54	0/2905	
6	AL03	0.41	0/1596	0.52	0/2153	
6	BL03	0.45	0/1596	0.54	0/2153	
7	AL04	0.38	0/1621	0.49	0/2194	
7	BL04	0.43	0/1621	0.50	0/2194	
8	AL05	0.31	0/1500	0.52	0/2017	
8	BL05	0.32	0/1500	0.51	0/2017	
9	AL06	0.64	0/1307	0.79	0/1769	
9	BL06	0.58	0/1307	0.80	0/1769	
10	AL09	0.31	0/1146	0.47	0/1551	
10	BL09	0.32	0/1147	0.50	0/1552	
11	AL13	0.37	0/1123	0.48	0/1515	
11	BL13	0.41	0/1123	0.51	0/1515	
12	AL14	0.45	0/942	0.51	0/1268	
12	BL14	0.46	0/942	0.51	0/1268	
13	AL15	0.35	0/1131	0.59	0/1504	
13	BL15	0.37	0/1131	0.58	0/1504	
14	AL16	0.38	0/1084	0.50	0/1449	
14	BL16	0.42	0/1084	0.51	0/1449	
15	AL17	0.40	0/974	0.51	0/1302	
15	BL17	0.40	0/974	0.53	0/1302	
16	AL18	0.36	0/778	0.48	0/1036	
16	BL18	0.36	0/778	0.51	0/1036	



ЪД-1		Bond lengths		Bond angles		
NIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
17	AL19	0.39	0/1157	0.52	0/1544	
17	BL19	0.42	0/1157	0.48	0/1544	
18	AL20	0.36	0/982	0.44	0/1306	
18	BL20	0.45	0/982	0.46	0/1306	
19	AL21	0.37	0/790	0.55	0/1057	
19	BL21	0.41	0/790	0.56	0/1057	
20	AL22	0.39	0/901	0.47	0/1209	
20	BL22	0.43	0/901	0.51	0/1209	
21	AL23	0.40	0/739	0.48	0/993	
21	BL23	0.41	0/739	0.53	1/993~(0.1%)	
22	AL24	0.34	0/788	0.53	0/1051	
22	BL24	0.37	0/788	0.49	0/1051	
23	AL25	0.34	0/1514	0.47	0/2056	
23	BL25	0.37	0/1514	0.49	0/2056	
24	AL27	0.99	0/655	1.13	3/870~(0.3%)	
24	BL27	1.03	1/655~(0.2%)	1.31	2/870 (0.2%)	
25	AL28	0.37	0/701	0.53	0/932	
25	BL28	0.39	0/701	0.55	0/932	
26	AL29	0.30	0/522	0.47	0/690	
26	BL29	0.33	0/522	0.48	0/690	
27	AL30	0.33	0/472	0.48	0/634	
27	BL30	0.36	0/472	0.47	0/634	
28	AL31	0.85	1/360~(0.3%)	0.96	0/488	
28	BL31	0.98	3/360~(0.8%)	1.00	2/488~(0.4%)	
29	AL32	1.15	3/473~(0.6%)	1.13	1/639~(0.2%)	
29	BL32	1.74	6/473~(1.3%)	1.41	9/639~(1.4%)	
30	AL33	0.37	0/387	0.63	0/518	
30	BL33	0.38	0/387	0.57	0/518	
31	AL34	0.38	0/426	0.51	0/561	
31	BL34	0.47	0/426	0.48	0/561	
32	AL35	0.38	0/515	0.52	0/679	
32	BL35	0.39	0/515	0.59	0/679	
33	AL36	0.38	0/310	0.59	1/407~(0.2%)	
33	BL36	0.52	0/310	0.63	0/407	
34	AMRN	0.47	0/250	0.86	0/387	
34	BMRN	1.58	6/420~(1.4%)	3.17	57/654~(8.7%)	
35	APTN	0.68	2/1672~(0.1%)	1.30	17/2599~(0.7%)	
35	BPTN	1.57	$\overline{33/1672}~(2.0\%)$	2.69	$\overline{160/2599}~(6.2\%)$	
36	AS02	0.33	0/1935	0.47	0/2609	
36	BS02	0.31	0/1935	0.45	0/2609	
37	AS03	0.33	0/1636	0.47	0/2205	
37	BS03	0.32	0/1636	0.47	0/2205	
38	AS04	0.40	0/1695	0.47	0/2274	



Mal	Chain	E	Bond lengths	Bond angles	
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
38	BS04	0.37	0/1695	0.47	0/2274
39	AS05	0.38	0/1171	0.49	0/1576
39	BS05	0.36	0/1171	0.50	0/1576
40	AS06	0.38	0/856	0.50	0/1154
40	BS06	0.37	0/856	0.47	0/1154
41	AS07	0.30	0/1276	0.43	0/1709
41	BS07	0.29	0/1276	0.43	0/1709
42	AS08	0.40	0/1136	0.47	0/1527
42	BS08	0.39	0/1136	0.49	0/1527
43	AS09	0.31	0/1029	0.51	0/1378
43	BS09	0.31	0/1029	0.48	0/1378
44	AS10	0.29	0/807	0.46	0/1085
44	BS10	0.29	0/807	0.49	0/1085
45	AS11	0.34	0/856	0.48	0/1157
45	BS11	0.32	0/856	0.46	0/1157
46	AS12	0.40	0/972	0.50	0/1301
46	BS12	0.39	0/972	0.52	0/1301
47	AS13	0.29	0/943	0.49	0/1265
47	BS13	0.29	0/943	0.48	0/1265
48	AS14	0.34	0/501	0.51	0/664
48	BS14	0.34	0/501	0.46	0/664
49	AS15	0.35	0/745	0.45	0/992
49	BS15	0.34	0/745	0.46	0/992
50	AS16	0.35	0/716	0.48	0/963
50	BS16	0.38	0/716	0.54	0/963
51	AS17	0.42	0/836	0.48	0/1117
51	BS17	0.41	0/836	0.48	0/1117
52	AS18	0.35	0/579	0.52	0/768
52	BS18	0.32	0/579	0.52	0/768
53	AS19	0.29	0/642	0.49	0/865
53	BS19	0.30	0/642	0.47	0/865
54	AS20	0.29	0/764	0.47	0/1006
54	BS20	0.29	0/764	0.46	0/1006
55	ATHX	0.35	0/212	0.68	1/277~(0.4%)
55	BTHX	0.31	0/212	0.51	0/277
56	BATN	1.35	20/1899 (1.1%)	2.63	$197/2\overline{952}\ (\overline{6.7\%})$
All	All	0.69	156/319733~(0.0%)	0.92	774/477946~(0.2%)

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



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Mol	Chain	#Chirality outliers	#Planarity outliers
9	AL06	0	1
15	BL17	0	1
22	BL24	0	1
24	AL27	0	1
24	BL27	0	1
28	AL31	0	2
29	AL32	0	2
29	BL32	0	2
34	BMRN	0	3
43	BS09	0	1
All	All	0	15

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
29	BL32	60	VAL	CB-CG2	-19.93	1.10	1.52
29	BL32	59	GLU	CB-CG	17.61	1.85	1.52
1	B16S	4	U	C2-N3	15.46	1.48	1.37
1	B16S	3	G	C5-C6	14.63	1.56	1.42
1	B16S	3	G	N9-C4	13.83	1.49	1.38

The worst 5 of 774 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
34	BMRN	16	G	N9-C1'-C2'	-31.99	72.41	114.00
35	BPTN	32	С	O4'-C4'-C3'	-29.66	74.34	104.00
35	APTN	35	А	P-O3'-C3'	28.14	153.47	119.70
34	BMRN	12	А	N9-C1'-C2'	-27.96	77.65	114.00
1	A16S	1364	U	C5-C4-O4	-24.36	111.28	125.90

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	AL06	157	TYR	Peptide
24	AL27	8	GLY	Peptide
28	AL31	37	SER	Peptide
28	AL31	42	PHE	Peptide
29	AL32	3	LYS	Peptide



5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A16S	32600	0	0	0	0
1	B16S	32600	0	0	0	1
2	A23S	61999	0	0	0	1
2	B23S	62000	0	0	0	0
3	A5S	2551	0	1295	68	0
3	B5S	2551	0	1295	30	0
4	AL01	1742	0	0	0	0
4	BL01	1742	0	0	0	0
5	AL02	2104	0	0	0	0
5	BL02	2104	0	0	0	0
6	AL03	1563	0	0	0	0
6	BL03	1563	0	0	0	0
7	AL04	1586	0	0	0	0
7	BL04	1586	0	0	0	0
8	AL05	1475	0	0	0	0
8	BL05	1475	0	0	0	0
9	AL06	1282	0	0	0	0
9	BL06	1282	0	0	0	0
10	AL09	1131	0	0	0	0
10	BL09	1132	0	0	0	0
11	AL13	1096	0	0	0	0
11	BL13	1096	0	0	0	0
12	AL14	932	0	0	0	0
12	BL14	932	0	0	0	0
13	AL15	1114	0	0	0	0
13	BL15	1114	0	0	0	0
14	AL16	1064	0	0	0	0
14	BL16	1064	0	0	0	0
15	AL17	960	0	0	0	0
15	BL17	960	0	0	0	0
16	AL18	770	0	0	0	0
16	BL18	770	0	0	0	0
17	AL19	1143	0	0	0	0
17	BL19	1143	0	0	0	0
18	AL20	964	0	0	0	0
18	BL20	964	0	0	0	3
19	AL21	779	0	0	0	0



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	Choin	Non H	puye	U(addad)	Clashes	Summ Clashes
		<u>11011-П</u>		п(added)	Clashes	Symm-Clasnes
19	BL21	119	0	0	0	3
20	AL22	890	0	0	0	0
20	BL22	890	0	0	0	0
21	AL23	725	0	0	0	0
21	BL23	(25	0	0	0	0
22	AL24	(()	0	0	0	0
22	BL24	775	0	0	0	0
23	AL25	1482	0	0	0	0
23	BL25	1482	0	0	0	0
24	AL27	647	0	0	0	0
24	BL27	647	0	0	0	0
25	AL28	694	0	0	0	0
25	BL28	694	0	0	0	0
26	AL29	520	0	0	0	0
26	BL29	520	0	0	0	0
27	AL30	467	0	0	0	0
27	BL30	467	0	0	0	0
28	AL31	351	0	0	0	0
28	BL31	351	0	0	0	0
29	AL32	459	0	0	0	0
29	BL32	459	0	0	0	6
30	AL33	380	0	0	0	0
30	BL33	380	0	0	0	0
31	AL34	418	0	0	0	0
31	BL34	418	0	0	0	0
32	AL35	507	0	0	0	0
32	BL35	507	0	0	0	0
33	AL36	307	0	0	0	0
33	BL36	307	0	0	0	0
34	AMRN	223	0	0	0	0
34	BMRN	373	0	0	0	0
35	APTN	1631	0	0	0	0
35	BPTN	1631	0	0	0	0
36	AS02	1900	0	0	0	0
36	BS02	1900	0	0	0	0
37	AS03	1612	0	0	0	0
37	BS03	1612	0	0	0	0
38	AS04	1665	0	0	0	0
38	BS04	1665	0	0	0	0
39	AS05	1155	0	0	0	0
39	BS05	1155	0	0	0	0
40	AS06	843	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	BS06	843	0	0	0	0
41	AS07	1257	0	0	0	0
41	BS07	1257	0	0	0	0
42	AS08	1116	0	0	0	0
42	BS08	1116	0	0	0	0
43	AS09	1011	0	0	0	0
43	BS09	1011	0	0	0	0
44	AS10	794	0	0	0	0
44	BS10	794	0	0	0	0
45	AS11	842	0	0	0	0
45	BS11	842	0	0	0	0
46	AS12	956	0	0	0	0
46	BS12	956	0	0	0	0
47	AS13	933	0	0	0	0
47	BS13	933	0	0	0	0
48	AS14	492	0	0	0	0
48	BS14	492	0	0	0	0
49	AS15	734	0	0	0	0
49	BS15	734	0	0	0	0
50	AS16	700	0	0	0	0
50	BS16	700	0	0	0	0
51	AS17	823	0	0	0	0
51	BS17	823	0	0	0	0
52	AS18	574	0	0	0	0
52	BS18	574	0	0	0	0
53	AS19	629	0	0	0	0
53	BS19	629	0	0	0	0
54	AS20	762	0	0	0	0
54	BS20	762	0	0	0	0
55	ATHX	208	0	0	0	0
55	BTHX	208	0	0	0	0
56	BATN	1824	0	0	0	0
57	A16S	33	0	0	0	0
57	A23S	73	0	0	0	0
57	A5S	3	0	0	0	0
57	AL01	2	0	0	0	0
57	AL02	2	0	0	0	0
57	AL04	3	0	0	0	0
57	AL06	1	0	0	0	0
57	AL14	1	0	0	0	0
57	AL15	2	0	0	0	0
57	AL17	2	0	0	0	0

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	Chain	Non H	page	U(addad)	Clashes	Summe Clashes
IVIOI	Chain	INON-H	H(model)	H(added)	Clasnes	Symm-Clasnes
57	AL20	1	0	0	0	0
57	AL21	3	0	0	0	0
57	AL23	2	0	0	0	0
57	AL24	1	0	0	0	0
57	AL2/	1	0	0	0	0
57	AL28	2	0	0	0	0
57	AL33	3	0	0	0	0
57	AL34	1	0	0	0	0
57	AS02	1	0	0	0	0
57	AS03	1	0	0	0	0
57	AS06	2	0	0	0	0
57	AS08	1	0	0	0	0
57	B16S	32	0	0	0	0
57	B23S	133	0	0	0	0
57	B5S	5	0	0	0	0
57	BATN	1	0	0	0	0
57	BL01	2	0	0	0	0
57	BL02	5	0	0	0	0
57	BL03	1	0	0	0	0
57	BL04	1	0	0	0	0
57	BL15	3	0	0	0	0
57	BL16	3	0	0	0	0
57	BL18	3	0	0	0	0
57	BL19	2	0	0	0	0
57	BL20	1	0	0	0	0
57	BL21	1	0	0	0	0
57	BL22	1	0	0	0	0
57	BL23	1	0	0	0	0
57	BL24	2	0	0	0	0
57	BL25	1	0	0	0	0
57	BL28	2	0	0	0	0
57	BL29	5	0	0	0	0
57	BL30	1	0	0	0	0
57	BL31	1	0	0	0	0
57	BL32	1	0	0	0	0
57	BL33	3	0	0	0	0
57	BL34	2	0	0	0	0
57	BL35	1	0	0	0	0
57	BL36	1	0	0	0	0
57	BS16	1	0	0	0	0
57	BS17	1	0	0	0	0
57	BTHX	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes		
58	AS04	8	0	0	0	0		
58	BS04	8	0	0	0	0		
All	All	295025	0	2590	98	7		

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The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

The worst 5 of 98 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A5S:78:A:N6	3:A5S:98:G:H21	1.42	1.17
3:A5S:78:A:H62	3:A5S:98:G:N2	1.43	1.16
3:B5S:40:U:N3	3:B5S:44:G:OP2	1.97	0.97
3:B5S:13:A:O2'	3:B5S:15:A:OP2	1.90	0.88
3:B5S:14:U:OP2	3:B5S:70:C:O2'	2.02	0.76

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A23S:2154:G:N2	$1:B16S:999:U:OP2[4_545]$	1.96	0.24
18:BL20:89:GLU:N	29:BL32:60:VAL:O[4_455]	1.96	0.24
19:BL21:6:LYS:CE	29:BL32:59:GLU:OE2[4_455]	2.02	0.18
19:BL21:6:LYS:NZ	29:BL32:59:GLU:N[4_455]	2.04	0.16
18:BL20:89:GLU:OE2	29:BL32:59:GLU:O[4_455]	2.10	0.10

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
4	AL01	226/228~(99%)	116 (51%)	74(33%)	36 (16%)	0 0



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
4	BL01	226/228~(99%)	108 (48%)	67~(30%)	51 (23%)	0	0
5	AL02	269/276~(98%)	213 (79%)	39~(14%)	17~(6%)	1	10
5	BL02	269/276~(98%)	198 (74%)	47~(18%)	24 (9%)	1	4
6	AL03	202/206~(98%)	145 (72%)	39~(19%)	18 (9%)	1	4
6	BL03	202/206~(98%)	152 (75%)	36~(18%)	14 (7%)	1	8
7	AL04	200/205~(98%)	162 (81%)	28~(14%)	10 (5%)	2	16
7	BL04	200/205~(98%)	154 (77%)	32~(16%)	14~(7%)	1	8
8	AL05	179/181~(99%)	120 (67%)	40 (22%)	19 (11%)	0	2
8	BL05	179/181~(99%)	120 (67%)	45~(25%)	14 (8%)	1	6
9	AL06	165/180~(92%)	99 (60%)	41 (25%)	25~(15%)	0	1
9	BL06	165/180~(92%)	95 (58%)	37~(22%)	33 (20%)	0	0
10	AL09	143/148~(97%)	116 (81%)	19~(13%)	8~(6%)	2	14
10	BL09	143/148~(97%)	106 (74%)	31~(22%)	6 (4%)	3	20
11	AL13	135/140~(96%)	102 (76%)	19~(14%)	14 (10%)	0	3
11	BL13	135/140~(96%)	106 (78%)	15~(11%)	14 (10%)	0	3
12	AL14	120/122~(98%)	97 (81%)	20~(17%)	3(2%)	5	32
12	BL14	120/122~(98%)	99 (82%)	16~(13%)	5(4%)	3	20
13	AL15	144/150~(96%)	90 (62%)	37~(26%)	17 (12%)	0	2
13	BL15	144/150~(96%)	85 (59%)	42~(29%)	17 (12%)	0	2
14	AL16	132/141~(94%)	89 (67%)	28~(21%)	15 (11%)	0	2
14	BL16	132/141~(94%)	103 (78%)	19~(14%)	10 (8%)	1	7
15	AL17	115/118~(98%)	92 (80%)	18 (16%)	5(4%)	2	20
15	BL17	115/118 (98%)	89 (77%)	18~(16%)	8 (7%)	1	8
16	AL18	96/111~(86%)	68 (71%)	21 (22%)	7 (7%)	1	7
16	BL18	96/111~(86%)	67 (70%)	16~(17%)	13~(14%)	0	1
17	AL19	135/146~(92%)	97 (72%)	29~(22%)	9~(7%)	1	9
17	BL19	135/146~(92%)	107 (79%)	23~(17%)	5(4%)	3	22
18	AL20	115/118~(98%)	92 (80%)	17 (15%)	6 (5%)	2	15
18	BL20	115/118~(98%)	82 (71%)	25~(22%)	8 (7%)	1	8
19	AL21	99/101~(98%)	73 (74%)	18 (18%)	8 (8%)	1	5
19	BL21	99/101~(98%)	79 (80%)	16 (16%)	4 (4%)	3	21



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	entil	\mathbf{es}
20	AL22	110/113~(97%)	79 (72%)	25~(23%)	6 (6%)	2	14	
20	BL22	110/113~(97%)	81 (74%)	24~(22%)	5 (4%)	2	18	
21	AL23	90/96~(94%)	74 (82%)	14~(16%)	2(2%)	6	35	
21	BL23	90/96~(94%)	77 (86%)	10 (11%)	3 (3%)	4	25	
22	AL24	98/110~(89%)	54 (55%)	32~(33%)	12 (12%)	0	2	
22	BL24	98/110 (89%)	56 (57%)	29~(30%)	13 (13%)	0	1	
23	AL25	185/206~(90%)	143 (77%)	32~(17%)	10 (5%)	2	14	
23	BL25	185/206~(90%)	144 (78%)	32~(17%)	9(5%)	2	17	
24	AL27	80/84~(95%)	62 (78%)	11 (14%)	7 (9%)	1	4	-
24	BL27	80/84~(95%)	60 (75%)	11 (14%)	9 (11%)	0	2	
25	AL28	86/98~(88%)	59 (69%)	22~(26%)	5 (6%)	1	13	
25	BL28	86/98~(88%)	60 (70%)	18 (21%)	8 (9%)	0	3	
26	AL29	60/72~(83%)	48 (80%)	8 (13%)	4 (7%)	1	9	
26	BL29	60/72~(83%)	45 (75%)	12~(20%)	3~(5%)	2	16	
27	AL30	57/60~(95%)	49 (86%)	7~(12%)	1 (2%)	8	41	
27	BL30	57/60~(95%)	51 (90%)	4 (7%)	2 (4%)	3	24	
28	AL31	43/71~(61%)	16 (37%)	8 (19%)	19 (44%)	0	0	
28	BL31	43/71~(61%)	16 (37%)	15~(35%)	12 (28%)	0	0	
29	AL32	57/59~(97%)	36~(63%)	12~(21%)	9 (16%)	0	1	
29	BL32	57/59~(97%)	43 (75%)	8 (14%)	6 (10%)	0	3	
30	AL33	42/54~(78%)	27 (64%)	8 (19%)	7 (17%)	0	0	
30	BL33	42/54~(78%)	23~(55%)	11~(26%)	8 (19%)	0	0	
31	AL34	46/49~(94%)	39~(85%)	5(11%)	2(4%)	2	20	
31	BL34	46/49~(94%)	43 (94%)	2~(4%)	1 (2%)	6	35	
32	AL35	61/64~(95%)	44 (72%)	11 (18%)	6 (10%)	0	3	
32	BL35	61/64~(95%)	40 (66%)	13~(21%)	8 (13%)	0	1	
33	AL36	35/37~(95%)	30~(86%)	4 (11%)	1 (3%)	4	28	
33	BL36	35/37~(95%)	28 (80%)	2(6%)	5 (14%)	0	1	
36	AS02	232/255~(91%)	189 (82%)	27~(12%)	16 (7%)	1	8	
36	BS02	$232/255~(\overline{91\%})$	174 (75%)	42 (18%)	16(7%)	1	8	
37	AS03	204/238~(86%)	150 (74%)	39~(19%)	15 (7%)	1	7	



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perc	centil	\mathbf{les}
37	BS03	204/238~(86%)	144 (71%)	43~(21%)	17 (8%)	1	5	
38	AS04	206/208~(99%)	171 (83%)	24~(12%)	11 (5%)	2	15	
38	BS04	206/208~(99%)	159 (77%)	35~(17%)	12 (6%)	1	13	
39	AS05	149/161~(92%)	122 (82%)	19~(13%)	8 (5%)	2	14	
39	BS05	149/161~(92%)	122 (82%)	21~(14%)	6 (4%)	3	21	
40	AS06	99/101~(98%)	79 (80%)	15~(15%)	5 (5%)	2	15	
40	BS06	99/101~(98%)	79 (80%)	17~(17%)	3 (3%)	4	28	
41	AS07	153/155~(99%)	119 (78%)	25~(16%)	9 (6%)	1	12	
41	BS07	153/155~(99%)	110 (72%)	33~(22%)	10 (6%)	1	10	
42	AS08	136/138~(99%)	107 (79%)	22~(16%)	7 (5%)	2	15	
42	BS08	136/138~(99%)	115 (85%)	15 (11%)	6 (4%)	2	19	
43	AS09	125/128~(98%)	94 (75%)	28 (22%)	3 (2%)	6	34	
43	BS09	125/128~(98%)	92 (74%)	21~(17%)	12 (10%)	0	3	
44	AS10	96/104~(92%)	83 (86%)	11 (12%)	2(2%)	7	37	
44	BS10	96/104~(92%)	76 (79%)	12~(12%)	8 (8%)	1	5	
45	AS11	112/128~(88%)	87 (78%)	21~(19%)	4 (4%)	3	23	
45	BS11	112/128~(88%)	89 (80%)	18~(16%)	5 (4%)	2	18	
46	AS12	120/131~(92%)	86 (72%)	29~(24%)	5 (4%)	3	20	
46	BS12	120/131~(92%)	84 (70%)	28~(23%)	8 (7%)	1	9	
47	AS13	115/125~(92%)	72 (63%)	27~(24%)	16 (14%)	0	1	
47	BS13	115/125~(92%)	81 (70%)	20~(17%)	14 (12%)	0	2	
48	AS14	58/60~(97%)	37 (64%)	12~(21%)	9~(16%)	0	1	
48	BS14	58/60~(97%)	45 (78%)	8 (14%)	5 (9%)	1	4	
49	AS15	86/88~(98%)	74 (86%)	8 (9%)	4 (5%)	2	17	
49	BS15	86/88~(98%)	70 (81%)	9 (10%)	7 (8%)	1	5	
50	AS16	81/88~(92%)	63 (78%)	17~(21%)	1 (1%)	13	49	ł
50	BS16	81/88 (92%)	65~(80%)	13 (16%)	3 (4%)	3	22	
51	AS17	97/104~(93%)	79 (81%)	16 (16%)	2(2%)	7	37	
51	BS17	97/104~(93%)	75 (77%)	19 (20%)	3 (3%)	4	26	
52	AS18	68/87~(78%)	52 (76%)	12 (18%)	4 (6%)	1	12	
52	BS18	68/87~(78%)	55 (81%)	10 (15%)	3 (4%)	2	19	



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
53	AS19	76/92~(83%)	46 (60%)	20~(26%)	10 (13%)	0	1
53	BS19	76/92~(83%)	53 (70%)	15 (20%)	8 (10%)	0	3
54	AS20	97/105~(92%)	72 (74%)	20 (21%)	5 (5%)	2	15
54	BS20	97/105~(92%)	75 (77%)	14 (14%)	8 (8%)	1	5
55	ATHX	22/26~(85%)	5 (23%)	13~(59%)	4 (18%)	0	0
55	BTHX	22/26~(85%)	13 (59%)	7 (32%)	2(9%)	1	3
All	All	11714/12532~(94%)	8611 (74%)	2167 (18%)	936 (8%)	1	6

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5 of 936 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AL01	141	PRO
4	AL01	172	ILE
4	AL01	181	PHE
4	AL01	182	PRO
4	AL01	225	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
4	AL01	180/180~(100%)	170 (94%)	10~(6%)	21	57
4	BL01	180/180~(100%)	166~(92%)	14 (8%)	12	43
5	AL02	213/218~(98%)	204 (96%)	9~(4%)	30	65
5	BL02	213/218~(98%)	205~(96%)	8 (4%)	33	67
6	AL03	165/166~(99%)	163~(99%)	2(1%)	71	88
6	BL03	165/166~(99%)	159~(96%)	6 (4%)	35	69
7	AL04	161/162~(99%)	158 (98%)	3~(2%)	57	81
7	BL04	161/162~(99%)	155~(96%)	6 (4%)	34	68
8	AL05	155/155~(100%)	142 (92%)	13 (8%)	11	39
8	BL05	155/155~(100%)	143 (92%)	12 (8%)	13	44



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
9	AL06	139/148~(94%)	135~(97%)	4(3%)	42	74
9	BL06	139/148~(94%)	132~(95%)	7 (5%)	24	60
10	AL09	121/124 (98%)	115 (95%)	6~(5%)	24	60
10	BL09	122/124~(98%)	116 (95%)	6~(5%)	25	61
11	AL13	116/119~(98%)	113 (97%)	3(3%)	46	76
11	BL13	116/119~(98%)	109 (94%)	7 (6%)	19	54
12	AL14	100/100~(100%)	100 (100%)	0	100	100
12	BL14	100/100~(100%)	99~(99%)	1 (1%)	76	90
13	AL15	112/116~(97%)	101 (90%)	11 (10%)	8	31
13	BL15	112/116~(97%)	101 (90%)	11 (10%)	8	31
14	AL16	105/111~(95%)	101 (96%)	4 (4%)	33	67
14	BL16	105/111~(95%)	101 (96%)	4 (4%)	33	67
15	AL17	100/101~(99%)	96 (96%)	4 (4%)	31	66
15	BL17	100/101~(99%)	93~(93%)	7 (7%)	15	48
16	AL18	77/87~(88%)	73~(95%)	4 (5%)	23	59
16	BL18	77/87~(88%)	70 (91%)	7 (9%)	9	34
17	AL19	121/128 (94%)	115 (95%)	6(5%)	24	60
17	BL19	121/128 (94%)	113 (93%)	8 (7%)	16	51
18	AL20	93/94~(99%)	90~(97%)	3(3%)	39	71
18	BL20	93/94 (99%)	89 (96%)	4 (4%)	29	64
19	AL21	82/82~(100%)	77 (94%)	5~(6%)	18	54
19	BL21	82/82~(100%)	78~(95%)	4 (5%)	25	61
20	AL22	91/92~(99%)	87~(96%)	4 (4%)	28	64
20	BL22	91/92~(99%)	88 (97%)	3(3%)	38	71
21	AL23	74/78~(95%)	71 (96%)	3 (4%)	30	66
21	BL23	74/78~(95%)	71 (96%)	3 (4%)	30	66
22	AL24	84/91 (92%)	78~(93%)	6 (7%)	14	47
22	BL24	84/91~(92%)	81 (96%)	3 (4%)	35	69
23	AL25	162/179~(90%)	157 (97%)	5(3%)	40	72
23	BL25	162/179~(90%)	153 (94%)	9~(6%)	21	57
24	AL27	65/66~(98%)	62 (95%)	3~(5%)	27	63



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BL27	65/66~(98%)	64~(98%)	1 (2%)	65	85
25	AL28	73/83~(88%)	70~(96%)	3~(4%)	30	66
25	BL28	73/83~(88%)	68~(93%)	5(7%)	16	49
26	AL29	58/67~(87%)	56~(97%)	2(3%)	37	70
26	BL29	58/67~(87%)	57~(98%)	1 (2%)	60	83
27	AL30	51/52~(98%)	48 (94%)	3~(6%)	19	54
27	BL30	51/52~(98%)	50 (98%)	1 (2%)	55	80
28	AL31	40/63~(64%)	36~(90%)	4 (10%)	7	30
28	BL31	40/63~(64%)	39~(98%)	1 (2%)	47	77
29	AL32	51/51~(100%)	48 (94%)	3 (6%)	19	54
29	BL32	51/51~(100%)	48 (94%)	3 (6%)	19	54
30	AL33	43/52~(83%)	38~(88%)	5 (12%)	5	24
30	BL33	43/52~(83%)	37~(86%)	6 (14%)	3	16
31	AL34	41/42~(98%)	37~(90%)	4 (10%)	8	31
31	BL34	41/42 (98%)	41 (100%)	0	100	100
32	AL35	53/54~(98%)	49 (92%)	4 (8%)	13	45
32	BL35	53/54~(98%)	50 (94%)	3~(6%)	20	56
33	AL36	34/34~(100%)	34 (100%)	0	100	100
33	BL36	34/34~(100%)	32~(94%)	2~(6%)	19	54
36	AS02	202/219~(92%)	194 (96%)	8 (4%)	31	66
36	BS02	202/219~(92%)	192~(95%)	10 (5%)	24	60
37	AS03	160/187~(86%)	152 (95%)	8 (5%)	24	60
37	BS03	160/187~(86%)	154 (96%)	6 (4%)	33	67
38	AS04	171/180~(95%)	161 (94%)	10 (6%)	20	55
38	BS04	171/180~(95%)	162 (95%)	9(5%)	22	58
39	AS05	116/122~(95%)	113~(97%)	3 (3%)	46	76
39	BS05	116/122~(95%)	109 (94%)	7~(6%)	19	54
40	AS06	90/90~(100%)	85 (94%)	5 (6%)	21	57
40	BS06	90/90~(100%)	87~(97%)	3 (3%)	38	71
41	AS07	126/126~(100%)	118 (94%)	8 (6%)	18	52
41	BS07	126/126~(100%)	120~(95%)	6(5%)	25	61



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
42	AS08	119/119~(100%)	109~(92%)	10 (8%)	11	39
42	BS08	119/119~(100%)	114 (96%)	5(4%)	30	65
43	AS09	98/99~(99%)	86~(88%)	12 (12%)	5	22
43	BS09	98/99~(99%)	93~(95%)	5 (5%)	24	60
44	AS10	88/91~(97%)	86~(98%)	2 (2%)	50	78
44	BS10	88/91~(97%)	82~(93%)	6 (7%)	16	49
45	AS11	86/98~(88%)	81 (94%)	5 (6%)	20	55
45	BS11	86/98~(88%)	82 (95%)	4 (5%)	26	62
46	AS12	103/108~(95%)	101 (98%)	2 (2%)	57	81
46	BS12	103/108~(95%)	96~(93%)	7 (7%)	16	49
47	AS13	94/100~(94%)	91~(97%)	3 (3%)	39	71
47	BS13	94/100~(94%)	89~(95%)	5(5%)	22	58
48	AS14	49/49~(100%)	44 (90%)	5 (10%)	7	29
48	BS14	49/49~(100%)	47 (96%)	2 (4%)	30	66
49	AS15	79/79~(100%)	71 (90%)	8 (10%)	7	29
49	BS15	79/79~(100%)	77~(98%)	2(2%)	47	77
50	AS16	72/74~(97%)	68~(94%)	4 (6%)	21	57
50	BS16	72/74~(97%)	71~(99%)	1 (1%)	67	86
51	AS17	94/96~(98%)	93~(99%)	1 (1%)	73	88
51	BS17	94/96~(98%)	89~(95%)	5 (5%)	22	58
52	AS18	61/76~(80%)	58~(95%)	3(5%)	25	61
52	BS18	61/76~(80%)	57~(93%)	4 (7%)	16	51
53	AS19	69/79~(87%)	64 (93%)	5 (7%)	14	47
53	BS19	69/79~(87%)	65~(94%)	4 (6%)	20	55
54	AS20	76/81~(94%)	74 (97%)	2 (3%)	46	76
54	BS20	76/81~(94%)	72~(95%)	4 (5%)	22	58
55	ATHX	19/21~(90%)	14 (74%)	5 (26%)	0	2
55	BTHX	19/21~(90%)	19 (100%)	0	100	100
All	All	9865/10378~(95%)	9372~(95%)	493 (5%)	24	60

 $5~{\rm of}~493$ residues with a non-rotameric side chain are listed below:



Mol	Chain	Res	Type
52	AS18	43	PHE
42	BS08	112	LEU
8	BL05	126	ASP
41	BS07	154	TYR
49	BS15	24	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A16S	1517/1518~(99%)	322 (21%)	22 (1%)
1	B16S	1517/1518~(99%)	321 (21%)	26 (1%)
2	A23S	$2874/2881 \ (99\%)$	618 (21%)	33 (1%)
2	B23S	2875/2881 (99%)	610 (21%)	32 (1%)
3	A5S	$118/119 \ (99\%)$	23 (19%)	3 (2%)
3	B5S	118/119~(99%)	12 (10%)	1 (0%)
34	AMRN	8/17~(47%)	5~(62%)	0
34	BMRN	17/17~(100%)	16 (94%)	8 (47%)
35	APTN	72/76~(94%)	38~(52%)	12 (16%)
35	BPTN	72/76~(94%)	54 (75%)	21 (29%)
56	BATN	82/85~(96%)	58 (70%)	10 (12%)
All	All	9270/9307 (99%)	2077 (22%)	168 (1%)

5.3.3 RNA (i)

5 of 2077 RNA backbone outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	A16S	4	U
1	A16S	6	G
1	A16S	9	G
1	A16S	14	U
1	A16S	32	А

5 of 168 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B23S	2119	А
34	BMRN	13	А
2	B23S	2171	А
56	BATN	6	G
35	BPTN	11	С



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

17 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).

Mal	Tuno	Chain	Dog	Link	Bond lengths		B	ond ang	gles	
	туре	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
56	PSU	BATN	55	56	18,21,22	1.31	1 (5%)	22,30,33	1.78	7 (31%)
35	PSU	BPTN	55	35	18,21,22	1.18	1 (5%)	22,30,33	1.86	4 (18%)
56	PSU	BATN	39	56	18,21,22	1.73	3 (16%)	22,30,33	1.84	4 (18%)
56	QUO	BATN	34	56	29,35,36	1.56	5 (17%)	31,52,55	1.74	7 (22%)
35	6MZ	BPTN	37	35	18,25,26	1.51	3 (16%)	16,36,39	1.73	4 (25%)
56	MIA	BATN	37	56	24,31,32	2.20	6 (25%)	26,44,47	4.00	12 (46%)
35	4SU	BPTN	8	35	18,21,22	<mark>3.78</mark>	9 (50%)	26,30,33	2.80	7 (26%)
35	5MU	BPTN	54	35	19,22,23	4.88	7 (36%)	28,32,35	<mark>3.54</mark>	11 (39%)
35	CM0	BPTN	34	35	22,26,27	2.25	7 (31%)	28,37,40	2.41	12 (42%)
35	4SU	APTN	8	35	18,21,22	<mark>3.59</mark>	7 (38%)	26,30,33	2.37	5 (19%)
35	G7M	APTN	46	35	20,26,27	2.47	7 (35%)	17,39,42	1.22	1 (5%)
35	5MU	APTN	54	35	19,22,23	4.88	7 (36%)	28,32,35	<mark>3.60</mark>	9 (32%)
35	CM0	APTN	34	35	22,26,27	4.02	7 (31%)	28,37,40	1.86	5 (17%)
35	PSU	APTN	55	35	18,21,22	1.00	1 (5%)	22,30,33	1.90	4 (18%)
35	G7M	BPTN	46	35	20,26,27	1.53	3 (15%)	17,39,42	1.43	2 (11%)
56	5MU	BATN	54	56	19,22,23	4.97	7 (36%)	28,32,35	<mark>3.32</mark>	10 (35%)
35	6MZ	APTN	37	35	18,25,26	2.46	3 (16%)	16,36,39	2.47	5 (31%)

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	PSU	BATN	55	56	-	3/7/25/26	0/2/2/2
35	PSU	BPTN	55	35	-	0/7/25/26	0/2/2/2
56	PSU	BATN	39	56	-	0/7/25/26	0/2/2/2



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	QUO	BATN	34	56	-	1/6/43/44	0/4/4/4
35	6MZ	BPTN	37	35	-	2/5/27/28	0/3/3/3
56	MIA	BATN	37	56	-	1/11/33/34	0/3/3/3
35	4SU	BPTN	8	35	-	0/7/25/26	0/2/2/2
35	5MU	BPTN	54	35	-	0/7/25/26	0/2/2/2
35	CM0	BPTN	34	35	-	6/12/30/31	0/2/2/2
35	4SU	APTN	8	35	-	0/7/25/26	0/2/2/2
35	G7M	APTN	46	35	-	1/3/25/26	0/3/3/3
35	5MU	APTN	54	35	-	4/7/25/26	0/2/2/2
35	CM0	APTN	34	35	-	9/12/30/31	0/2/2/2
35	PSU	APTN	55	35	-	0/7/25/26	0/2/2/2
35	G7M	BPTN	46	35	-	1/3/25/26	0/3/3/3
56	5MU	BATN	54	56	-	2/7/25/26	0/2/2/2
35	6MZ	APTN	37	35	-	2/5/27/28	0/3/3/3

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The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	APTN	34	CM0	C6-C5	13.63	1.49	1.34
56	BATN	54	5MU	C6-N1	11.65	1.57	1.38
35	APTN	54	5MU	C2-N1	11.47	1.56	1.38
35	BPTN	54	5MU	C2-N1	11.33	1.56	1.38
56	BATN	54	5MU	C2-N1	10.81	1.55	1.38

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
56	BATN	54	5MU	C5-C4-N3	11.90	125.47	115.31
35	APTN	54	5MU	C5-C4-N3	11.80	125.38	115.31
56	BATN	37	MIA	C12-N6-C6	-11.47	105.56	122.55
35	BPTN	54	5MU	C5-C4-N3	10.84	124.56	115.31
56	BATN	37	MIA	C12-C13-C14	-10.47	106.76	127.14

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	BATN	37	MIA	C12-C13-C14-C16
35	APTN	34	CM0	C3'-C4'-C5'-O5'
35	BPTN	34	CM0	O4'-C1'-N1-C2



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Mol	Chain	Res	Type	Atoms
35	BPTN	34	CM0	O4'-C1'-N1-C6
35	BPTN	34	CM0	C3'-C4'-C5'-O5'

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)

Of 361 ligands modelled in this entry, 359 are monoatomic - leaving 2 for Mogul analysis.

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

Mol Type Cha		Chain	Chain Res		Bond lengths			E	Bond angles
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ # Z > 2
58	SF4	BS04	501	38	0,12,12	-	-	-	
58	SF4	AS04	501	38	0,12,12	-	-	-	

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
58	SF4	BS04	501	38	-	-	0/6/5/5
58	SF4	AS04	501	38	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B23S	3
2	A23S	3
35	BPTN	1
35	APTN	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B23S	1141(A):C	O3'	1141:U	Р	9.81
1	A23S	1141(A):C	O3'	1141:U	Р	9.19
1	B23S	1140:C	O3'	1141(A):C	Р	7.44
1	A23S	1140:C	O3'	1141(A):C	Р	7.28
1	B23S	1141:U	O3'	1142:A	Р	6.83



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, 95^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A16S	1517/1518~(99%)	-0.01	44 (2%) 51 36	55, 88, 161, 216	0
1	B16S	1517/1518~(99%)	-0.00	39 (2%) 56 40	49,90,173,240	0
2	A23S	2879/2881~(99%)	-0.11	37 (1%) 77 65	36, 76, 173, 238	0
2	B23S	2879/2881~(99%)	0.04	35 (1%) 79 67	28,63,165,232	0
3	A5S	119/119~(100%)	0.49	9 (7%) 13 7	73, 99, 117, 126	0
3	B5S	119/119~(100%)	0.35	5 (4%) 36 23	46, 84, 106, 122	0
4	AL01	228/228~(100%)	1.77	69 (30%) 0 0	131, 167, 179, 191	0
4	BL01	228/228~(100%)	3.10	135 (59%) 0 0	126, 162, 178, 184	0
5	AL02	271/276~(98%)	0.82	31 (11%) 5 3	37, 56, 77, 85	0
5	BL02	271/276~(98%)	-0.05	2 (0%) 87 81	30,51,69,77	0
6	AL03	204/206~(99%)	0.01	9 (4%) 34 21	50, 76, 97, 107	0
6	BL03	204/206~(99%)	0.01	7 (3%) 45 29	39, 66, 92, 107	0
7	AL04	202/205~(98%)	-0.18	3 (1%) 73 61	51, 85, 108, 120	0
7	BL04	202/205~(98%)	0.08	5 (2%) 57 43	34,67,91,103	0
8	AL05	181/181~(100%)	3.17	111 (61%) 0 0	89, 121, 139, 147	0
8	BL05	181/181 (100%)	2.68	94 (51%) 0 0	82, 110, 138, 151	0
9	AL06	167/180~(92%)	0.04	7 (4%) 36 23	114, 151, 173, 182	0
9	BL06	167/180~(92%)	0.88	20 (11%) 4 2	116, 150, 172, 179	0
10	AL09	145/148~(97%)	0.06	13 (8%) 9 5	75, 112, 133, 140	0
10	BL09	145/148~(97%)	0.00	11 (7%) 13 7	78, 101, 118, 127	0
11	AL13	137/140~(97%)	-0.23	0 100 100	66, 87, 116, 122	0
11	BL13	137/140~(97%)	-0.15	0 100 100	48, 66, 91, 105	0
12	AL14	122/122~(100%)	-0.17	0 100 100	51, 63, 77, 85	0
12	BL14	$12\overline{2}/122~(100\%)$	0.05	2 (1%) 72 59	38, 58, 73, 81	0



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Mol	Chain	Analysed	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(A^2)$	Q<0.9
13	AL15	146/150~(97%)	0.02	9 (6%) 20 11	56, 88, 107, 125	0
13	BL15	146/150~(97%)	0.17	6 (4%) 37 24	45, 77, 98, 123	0
14	AL16	134/141~(95%)	0.19	6 (4%) 33 21	60, 82, 103, 109	0
14	BL16	134/141~(95%)	0.23	6 (4%) 33 21	52,69,83,95	0
15	AL17	117/118~(99%)	0.01	2 (1%) 70 57	50,69,83,92	0
15	BL17	117/118~(99%)	0.18	7 (5%) 21 12	43, 59, 76, 83	0
16	AL18	98/111~(88%)	2.56	59 (60%) 0 0	68, 83, 95, 102	0
16	BL18	98/111 (88%)	1.58	31 (31%) 0 0	47, 69, 94, 101	0
17	AL19	137/146~(93%)	-0.38	2 (1%) 73 61	54, 77, 113, 121	0
17	BL19	137/146~(93%)	-0.31	0 100 100	52, 68, 116, 134	0
18	AL20	117/118~(99%)	0.07	6 (5%) 28 16	50, 84, 101, 108	0
18	BL20	117/118~(99%)	-0.25	1 (0%) 84 75	42, 59, 74, 92	0
19	AL21	101/101~(100%)	-0.22	3 (2%) 50 34	65, 98, 111, 116	0
19	BL21	101/101~(100%)	-0.20	0 100 100	46, 72, 92, 98	0
20	AL22	112/113~(99%)	0.15	4 (3%) 42 27	54, 69, 98, 135	0
20	BL22	112/113~(99%)	-0.39	0 100 100	40, 56, 82, 113	0
21	AL23	92/96~(95%)	0.67	7 (7%) 13 7	48, 71, 96, 108	0
21	BL23	92/96~(95%)	0.19	7 (7%) 13 7	43, 58, 97, 115	0
22	AL24	100/110~(90%)	1.71	37~(37%) 0 0	83, 98, 123, 132	0
22	BL24	100/110~(90%)	0.40	10 (10%) 7 4	60, 80, 116, 141	0
23	AL25	187/206~(90%)	1.20	51 (27%) 0 0	86, 102, 123, 129	0
23	BL25	187/206~(90%)	-0.20	2 (1%) 80 69	65, 91, 108, 121	0
24	AL27	82/84~(97%)	2.84	51 (62%) 0 0	54, 66, 93, 105	0
24	BL27	82/84~(97%)	2.33	37~(45%) 0 0	51, 63, 95, 101	0
25	AL28	88/98~(89%)	0.16	2 (2%) 60 47	52, 78, 107, 121	0
25	BL28	88/98~(89%)	0.64	10 (11%) 5 3	44, 70, 95, 106	0
26	AL29	62/72~(86%)	0.16	3 (4%) 30 18	66, 86, 114, 125	0
26	BL29	62/72~(86%)	0.20	4 (6%) 18 11	40, 74, 102, 114	0
27	AL30	59/60~(98%)	0.79	12 (20%) 1 1	67, 89, 107, 124	0
27	BL30	59/60~(98%)	0.02	2 (3%) 45 29	46, 68, 90, 114	0
28	AL31	45/71 (63%)	2.20	21 (46%) 0 0	$1\overline{24}, 142, 151, 157$	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
28	BL31	45/71~(63%)	3.38	25~(55%) 0 0	123, 143, 150, 157	0
29	AL32	59/59~(100%)	0.22	2 (3%) 45 29	50,67,133,140	0
29	BL32	59/59~(100%)	0.33	8 (13%) 3 2	42, 63, 126, 135	0
30	AL33	44/54~(81%)	0.08	3 (6%) 17 10	61, 77, 87, 90	0
30	BL33	44/54~(81%)	0.99	8 (18%) 1 1	44, 72, 78, 88	0
31	AL34	48/49~(97%)	-0.06	1 (2%) 63 49	36, 52, 67, 85	0
31	BL34	48/49~(97%)	-0.14	1 (2%) 63 49	29, 39, 62, 69	0
32	AL35	63/64~(98%)	0.36	2 (3%) 47 31	54, 67, 76, 88	0
32	BL35	63/64~(98%)	0.11	3 (4%) 30 18	46, 57, 69, 81	0
33	AL36	37/37~(100%)	0.97	6 (16%) 1 1	70, 80, 95, 115	0
33	BL36	37/37~(100%)	0.96	8 (21%) 0 1	58, 72, 93, 95	0
34	AMRN	10/17~(58%)	1.50	2(20%) 1 1	108, 136, 165, 166	0
34	BMRN	17/17~(100%)	0.26	0 100 100	109, 144, 173, 178	0
35	APTN	70/76~(92%)	0.99	13 (18%) 1 1	77, 172, 208, 231	0
35	BPTN	70/76~(92%)	0.20	2 (2%) 51 36	70, 140, 172, 182	0
36	AS02	234/255~(91%)	-0.27	1 (0%) 92 89	82, 108, 131, 141	0
36	BS02	234/255~(91%)	-0.39	0 100 100	91, 110, 133, 146	0
37	AS03	206/238~(86%)	-0.19	5 (2%) 59 44	76, 98, 117, 123	0
37	BS03	206/238~(86%)	-0.26	3 (1%) 73 61	83, 106, 123, 132	0
38	AS04	208/208~(100%)	0.85	26 (12%) 3 2	53, 78, 93, 108	0
38	BS04	208/208~(100%)	0.71	29 (13%) 2 1	63, 85, 98, 105	0
39	AS05	151/161~(93%)	0.36	11 (7%) 15 9	59, 76, 96, 102	0
39	BS05	151/161~(93%)	0.44	12 (7%) 12 6	61, 80, 97, 112	0
40	AS06	101/101~(100%)	0.23	6 (5%) 22 13	68, 88, 99, 103	0
40	BS06	101/101~(100%)	-0.21	1 (0%) 82 72	74, 88, 101, 106	0
41	AS07	155/155~(100%)	-0.18	5 (3%) 47 31	101, 122, 141, 158	0
41	BS07	155/155~(100%)	0.41	21 (13%) 3 2	108, 125, 136, 142	0
42	AS08	138/138~(100%)	-0.39	0 100 100	65, 78, 86, 90	0
42	BS08	138/138~(100%)	0.33	10 (7%) 15 9	64, 82, 96, 108	0
43	AS09	127/128~(99%)	0.52	11 (8%) 10 5	97, 133, 144, 150	0
43	BS09	127/128~(99%)	2.06	48 (37%) 0 0	100, 134, 146, 152	0



Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(A^2)$	Q<0.9
44	AS10	98/104~(94%)	0.97	15 (15%) 2 1	99, 122, 143, 158	0
44	BS10	98/104 (94%)	-0.02	5 (5%) 28 16	98, 120, 137, 142	0
45	AS11	114/128 (89%)	1.48	34 (29%) 0 0	68, 97, 117, 120	0
45	BS11	114/128 (89%)	-0.01	5 (4%) 34 21	56, 98, 120, 129	0
46	AS12	122/131~(93%)	-0.01	1 (0%) 86 78	56, 74, 88, 98	0
46	BS12	122/131~(93%)	-0.15	4 (3%) 46 30	56, 78, 93, 98	0
47	AS13	117/125~(93%)	0.93	18 (15%) 2 1	115, 132, 144, 166	0
47	BS13	117/125~(93%)	2.31	55 (47%) 0 0	121, 139, 152, 156	0
48	AS14	60/60~(100%)	1.38	17 (28%) 0 0	93, 112, 144, 153	0
48	BS14	60/60~(100%)	0.61	7 (11%) 4 2	95, 112, 148, 156	0
49	AS15	88/88 (100%)	-0.10	3 (3%) 45 29	55, 75, 89, 94	0
49	BS15	88/88~(100%)	-0.01	1 (1%) 80 69	57, 74, 95, 104	0
50	AS16	83/88~(94%)	0.55	7 (8%) 11 6	70, 82, 105, 117	0
50	BS16	83/88~(94%)	1.11	19 (22%) 0 0	66, 78, 99, 124	0
51	AS17	99/104~(95%)	-0.57	0 100 100	56, 70, 83, 91	0
51	BS17	99/104~(95%)	0.29	3 (3%) 50 34	59, 71, 82, 87	0
52	AS18	70/87~(80%)	-0.02	1 (1%) 75 63	68, 82, 100, 108	0
52	BS18	70/87~(80%)	-0.15	1 (1%) 75 63	69, 93, 110, 120	0
53	AS19	78/92~(84%)	2.69	47 (60%) 0 0	124, 135, 144, 152	0
53	BS19	78/92~(84%)	1.95	35 (44%) 0 0	111, 130, 142, 145	0
54	AS20	99/105~(94%)	0.95	18 (18%) 1 1	75, 94, 112, 122	0
54	BS20	99/105~(94%)	0.06	3 (3%) 50 34	64, 84, 105, 112	0
55	ATHX	24/26~(92%)	4.24	16 (66%) 0 0	134, 153, 159, 163	0
55	BTHX	24/26~(92%)	9.19	21 (87%) 0 0	139, 155, 161, 170	0
56	BATN	80/85~(94%)	3.42	50 (62%) 0 0	104, 171, 217, 231	0
All	All	$21\overline{191/21839}\ (97\%)$	0.31	1745 (8%) 11 6	28, 83, 162, 240	0

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The worst 5 of 1745 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	AL01	3	LYS	27.8
55	BTHX	19	GLY	25.2
4	AL01	5	GLY	24.6



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Mol	Chain	Res	Type	RSRZ
22	AL24	59	GLY	19.6
56	BATN	47(E)	А	19.2

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, 95^{th} 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	PSU	BATN	39	20/21	0.52	0.29	140,150,156,157	0
56	PSU	BATN	55	20/21	0.58	0.41	138,155,160,163	0
56	QUO	BATN	34	32/33	0.60	0.24	125,131,141,145	0
56	5MU	BATN	54	21/22	0.70	0.61	126,150,160,164	0
35	G7M	APTN	46	24/25	0.70	0.37	175,184,204,220	0
35	5MU	BPTN	54	21/22	0.72	0.36	128,135,141,147	0
35	6MZ	BPTN	37	23/24	0.73	0.17	65,76,84,98	0
56	MIA	BATN	37	29/30	0.73	0.22	133,139,142,148	0
35	4SU	APTN	8	20/21	0.73	0.27	179,188,195,198	0
35	4SU	BPTN	8	20/21	0.74	0.16	145,150,159,163	0
35	5MU	APTN	54	21/22	0.75	0.18	155,167,169,170	0
35	6MZ	APTN	37	23/24	0.77	0.30	115,122,128,133	0
35	PSU	BPTN	55	20/21	0.79	0.21	132,146,156,160	0
35	PSU	APTN	55	20/21	0.81	0.16	163,176,182,183	0
35	CM0	APTN	34	25/26	0.83	0.35	119,126,131,132	0
35	G7M	BPTN	46	24/25	0.83	0.16	144,157,172,188	0
35	CM0	BPTN	34	25/26	0.87	0.18	96,104,116,117	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
57	MG	A5S	201	1/1	0.50	0.20	98,98,98,98	0
57	MG	B23S	2924	1/1	0.50	0.18	62,62,62,62	0
57	MG	A23S	2947	1/1	0.51	0.16	47,47,47,47	0
57	MG	B23S	2906	1/1	0.57	0.20	37,37,37,37	0
57	MG	A23S	2910	1/1	0.63	0.22	83,83,83,83	0
57	MG	B23S	2976	1/1	0.64	0.18	46,46,46,46	0
57	MG	AL02	302	1/1	0.65	0.85	50,50,50,50	0
57	MG	B23S	2949	1/1	0.66	0.20	31,31,31,31	0
57	MG	A23S	2940	1/1	0.66	0.21	63,63,63,63	0
57	MG	BL30	101	1/1	0.66	0.10	72,72,72,72	0
57	MG	B16S	1608	1/1	0.67	0.16	56, 56, 56, 56	0
57	MG	B23S	3025	1/1	0.67	0.33	45,45,45,45	0
57	MG	AL14	201	1/1	0.67	0.25	58,58,58,58	0
57	MG	BL01	302	1/1	0.68	0.15	90,90,90,90	0
57	MG	AL15	202	1/1	0.69	0.17	61,61,61,61	0
57	MG	A16S	1603	1/1	0.69	0.17	$57,\!57,\!57,\!57$	0
57	MG	BATN	101	1/1	0.69	0.22	80,80,80,80	0
57	MG	B16S	1624	1/1	0.69	0.16	56, 56, 56, 56	0
57	MG	B23S	2959	1/1	0.69	0.13	69,69,69,69	0
57	MG	AS06	202	1/1	0.71	0.13	68,68,68,68	0
57	MG	A23S	2936	1/1	0.72	0.15	40,40,40,40	0
57	MG	B5S	203	1/1	0.72	0.17	58, 58, 58, 58	0
57	MG	B23S	2990	1/1	0.72	0.37	$51,\!51,\!51,\!51$	0
57	MG	B23S	3011	1/1	0.72	0.14	52,52,52,52	0
57	MG	B23S	3015	1/1	0.72	0.10	$50,\!50,\!50,\!50$	0
57	MG	BL15	202	1/1	0.73	0.11	64,64,64,64	0
57	MG	B16S	1629	1/1	0.73	0.20	82,82,82,82	0
57	MG	B23S	2972	1/1	0.74	0.14	$62,\!62,\!62,\!62$	0
57	MG	B23S	2989	1/1	0.75	0.15	56, 56, 56, 56	0
57	MG	BL15	203	1/1	0.75	0.40	48,48,48,48	0
57	MG	A23S	2927	1/1	0.75	0.15	$37,\!37,\!37,\!37$	0
57	MG	AL04	301	1/1	0.76	0.10	$57,\!57,\!57,\!57$	0
57	MG	B23S	2953	1/1	0.76	0.17	44,44,44,44	0
57	MG	AL17	202	1/1	0.76	0.10	47,47,47,47	0
57	MG	B23S	3000	1/1	0.76	0.15	$35,\!35,\!35,\!35$	0
57	MG	B23S	3010	1/1	0.76	0.23	56, 56, 56, 56	0
57	MG	B23S	2932	1/1	0.76	0.14	43,43,43,43	0
57	MG	B23S	2974	1/1	0.76	0.17	45,45,45,45	0
57	MG	B16S	1603	1/1	0.77	0.27	57,57,57,57	0
57	MG	B23S	2936	1/1	0.77	0.10	54,54,54,54	0
57	MG	A23S	2959	1/1	0.77	0.12	57,57,57,57	0
57	MG	BL31	101	1/1	0.77	0.17	78, 78, 78, 78, 78	0
57	MG	A16S	1610	1/1	0.78	0.22	74,74,74,74	0


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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors (A^2)	Q < 0.9	
57	MG	BL01	301	1/1	0.78	0.14	$105,\!105,\!105,\!105$	0	
57	MG	A23S	2970	1/1	0.78	0.25	73,73,73,73	0	
57	MG	AL34	100	1/1	0.78	0.41	$55,\!55,\!55,\!55$	0	
57	MG	B23S	2963	1/1	0.78	0.18	$37,\!37,\!37,\!37$	0	
57	MG	BL23	101	1/1	0.78	0.65	46,46,46,46	0	
57	MG	B23S	3031	1/1	0.78	0.13	53,53,53,53	0	
57	MG	A23S	2911	1/1	0.78	0.65	40,40,40,40	0	
57	MG	B23S	2908	1/1	0.79	0.18	32,32,32,32	0	
57	MG	B23S	2960	1/1	0.79	0.25	59, 59, 59, 59, 59	0	
57	MG	A23S	2962	1/1	0.79	0.20	50, 50, 50, 50	0	
57	MG	B5S	204	1/1	0.79	0.10	$55,\!55,\!55,\!55$	0	
57	MG	BL33	102	1/1	0.79	0.10	51,51,51,51	0	
57	MG	AL23	101	1/1	0.80	0.09	57,57,57,57	0	
57	MG	AL23	102	1/1	0.80	0.33	73,73,73,73	0	
57	MG	BL22	201	1/1	0.80	0.14	34,34,34,34	0	
57	MG	B16S	1627	1/1	0.80	0.13	85,85,85,85	0	
57	MG	A23S	2953	1/1	0.80	0.09	62,62,62,62	0	
57	MG	A23S	2969	1/1	0.80	0.08	47,47,47,47	0	
57	MG	A16S	1601	1/1	0.80	0.11	47,47,47,47	0	
57	MG	A23S	2916	1/1	0.81	0.15	36,36,36,36	0	
57	MG	B23S	3009	1/1	0.81	0.36	46,46,46,46	0	
57	MG	AL06	201	1/1	0.81	0.12	67,67,67,67	0	
57	MG	B16S	1630	1/1	0.81	0.11	58,58,58,58	0	
57	MG	AL01	301	1/1	0.81	0.17	$105,\!105,\!105,\!105$	0	
57	MG	A16S	1625	1/1	0.81	0.19	62,62,62,62	0	
57	MG	B23S	3026	1/1	0.81	0.20	42,42,42,42	0	
57	MG	B23S	2986	1/1	0.81	0.09	$55,\!55,\!55,\!55$	0	
57	MG	B23S	2956	1/1	0.81	0.18	42,42,42,42	0	
57	MG	B23S	2918	1/1	0.81	0.44	34,34,34,34	0	
57	MG	B23S	2951	1/1	0.82	0.11	50,50,50,50	0	
57	MG	B16S	1610	1/1	0.82	0.16	70,70,70,70	0	
57	MG	A16S	1626	1/1	0.82	0.07	58, 58, 58, 58	0	
57	MG	B23S	2934	1/1	0.82	0.17	24,24,24,24	0	
57	MG	BL18	201	1/1	0.82	0.30	$57,\!57,\!57,\!57$	0	
57	MG	BL19	202	1/1	0.82	0.10	$63,\!63,\!63,\!63$	0	
57	MG	A16S	1619	1/1	0.82	0.14	42,42,42,42	0	
57	MG	B23S	2961	1/1	0.82	0.36	42,42,42,42	0	
57	MG	B23S	2996	1/1	0.82	0.13	40,40,40,40	0	
57	MG	B23S	2962	1/1	0.82	0.24	50,50,50,50	0	
57	MG	A16S	1613	1/1	0.82	0.18	78,78,78,78	0	
57	MG	B16S	1622	1/1	0.83	0.19	44,44,44,44	0	
57	MG	B16S	1604	1/1	0.83	0.07	58, 58, 58, 58	0	



Mol		Chain	Res	Atoms	BSCC	RSR	B-factors $(Å^2)$	Q<0.9
57	MG	BL16	201	1/1	0.83	0.46	52 52 52 52	0
57	MG	B23S	2984	1/1	0.83	0.15	41.41.41.41	0
57	MG	B23S	3021	1/1	0.83	0.12	63.63.63.63	0
57	MG	BL34	101	1/1	0.83	0.48	41.41.41.41	0
57	MG	A5S	202	1/1	0.84	0.69	70.70.70.70	0
57	MG	B23S	2955	1/1	0.84	0.36	45.45.45.45	0
57	MG	A23S	2925	1/1	0.84	0.10	44.44.44.44	0
57	MG	B23S	2958	1/1	0.84	0.15	40,40,40,40	0
57	MG	B23S	3002	1/1	0.84	0.22	43,43,43,43	0
57	MG	B23S	3003	1/1	0.84	0.11	46,46,46,46	0
57	MG	B23S	3007	1/1	0.84	0.23	34,34,34,34	0
57	MG	B23S	2910	1/1	0.84	0.36	59,59,59,59	0
57	MG	B16S	1626	1/1	0.84	0.14	61,61,61,61	0
57	MG	B16S	1631	1/1	0.84	0.13	40,40,40,40	0
57	MG	BL03	301	1/1	0.84	0.43	51,51,51,51	0
57	MG	BL02	303	1/1	0.85	0.69	60,60,60,60	0
57	MG	B23S	3016	1/1	0.85	0.32	47,47,47,47	0
57	MG	AS03	301	1/1	0.85	0.15	67,67,67,67	0
57	MG	B23S	3022	1/1	0.85	0.21	46,46,46,46	0
57	MG	A16S	1622	1/1	0.85	0.13	68,68,68,68	0
57	MG	A16S	1607	1/1	0.85	0.12	51,51,51,51	0
57	MG	AL04	302	1/1	0.85	0.16	73,73,73,73	0
57	MG	B23S	3032	1/1	0.85	0.19	47,47,47,47	0
57	MG	B16S	1628	1/1	0.85	0.15	78,78,78,78	0
57	MG	B16S	1605	1/1	0.85	0.13	30,30,30,30	0
57	MG	A23S	2941	1/1	0.85	0.13	46,46,46,46	0
57	MG	AL01	302	1/1	0.85	0.18	$93,\!93,\!93,\!93$	0
57	MG	B23S	2939	1/1	0.85	0.12	57,57,57,57	0
57	MG	B23S	2979	1/1	0.86	0.20	51,51,51,51	0
57	MG	BL02	301	1/1	0.86	0.13	31,31,31,31	0
57	MG	B23S	2937	1/1	0.86	0.14	52,52,52,52	0
57	MG	A16S	1611	1/1	0.86	0.10	52,52,52,52	0
57	MG	B23S	2915	1/1	0.86	0.10	34,34,34,34	0
57	MG	B16S	1613	1/1	0.86	0.14	61,61,61,61	0
57	MG	B23S	2994	1/1	0.86	0.11	53,53,53,53	0
57	MG	BL16	202	1/1	0.86	0.08	45,45,45,45	0
57	MG	AL28	101	1/1	0.86	0.26	44,44,44	0
57	MG	B23S	2998	1/1	0.86	0.19	51,51,51,51	0
57	MG	B23S	2964	1/1	0.86	0.25	62,62,62,62	0
57	MG	B23S	2967	1/1	0.86	0.12	64,64,64,64	0
57	MG	BL29	104	1/1	0.86	0.22	46,46,46,46	0
57	MG	BL29	105	1/1	0.86	0.22	58, 58, 58, 58	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	AL33	103	1/1	0.86	0.18	48,48,48,48	0
57	MG	A16S	1614	1/1	0.86	0.16	42,42,42,42	0
57	MG	B23S	3008	1/1	0.86	0.14	53,53,53,53	0
57	MG	A23S	2943	1/1	0.86	0.11	52,52,52,52	0
57	MG	B23S	3019	1/1	0.87	0.12	51,51,51,51	0
57	MG	A23S	2907	1/1	0.87	0.18	51,51,51,51	0
57	MG	A16S	1624	1/1	0.87	0.10	50,50,50,50	0
57	MG	B23S	2916	1/1	0.87	0.15	43,43,43,43	0
57	MG	A16S	1605	1/1	0.87	0.16	78,78,78,78	0
57	MG	B23S	3027	1/1	0.87	0.14	39,39,39,39	0
57	MG	B23S	3028	1/1	0.87	0.10	69,69,69,69	0
57	MG	B23S	2954	1/1	0.87	0.14	56, 56, 56, 56	0
57	MG	A16S	1612	1/1	0.87	0.53	54,54,54,54	0
57	MG	B23S	2926	1/1	0.87	0.22	41,41,41,41	0
57	MG	B16S	1618	1/1	0.87	0.28	61,61,61,61	0
57	MG	B5S	205	1/1	0.87	0.13	38,38,38,38	0
57	MG	B23S	2933	1/1	0.87	0.08	60,60,60,60	0
57	MG	AL04	303	1/1	0.87	0.11	78,78,78,78	0
57	MG	B16S	1623	1/1	0.87	0.18	46,46,46,46	0
57	MG	A23S	2921	1/1	0.87	0.11	35,35,35,35	0
57	MG	B16S	1611	1/1	0.88	0.06	63,63,63,63	0
57	MG	B23S	2944	1/1	0.88	0.08	41,41,41,41	0
57	MG	B23S	2948	1/1	0.88	0.12	32,32,32,32	0
57	MG	A23S	2971	1/1	0.88	0.09	102,102,102,102	0
57	MG	B23S	2928	1/1	0.88	0.18	35,35,35,35	0
57	MG	B23S	2931	1/1	0.88	0.09	33,33,33,33	0
57	MG	A16S	1608	1/1	0.88	0.17	79,79,79,79	0
57	MG	A23S	2964	1/1	0.88	0.10	52,52,52,52	0
57	MG	A23S	2951	1/1	0.88	0.12	50,50,50,50	0
57	MG	B23S	2917	1/1	0.88	0.16	50,50,50,50	0
57	MG	B23S	2983	1/1	0.88	0.13	46,46,46,46	0
57	MG	A23S	2961	1/1	0.88	0.16	61,61,61,61	0
57	MG	AL02	301	1/1	0.89	0.37	51,51,51,51	0
57	MG	A23S	2966	1/1	0.89	0.07	46,46,46,46	0
57	MG	BL15	201	1/1	0.89	0.17	46,46,46,46	0
57	MG	A23S	2912	1/1	0.89	0.19	39,39,39,39	0
57	MG	A23S	2938		0.89	0.17	35,35,35,35	0
57	MG	B23S	2999		0.89	0.10	35,35,35,35	0
57	MG	A23S	2901		0.89	0.21	33,33,33,33	
57	MG	A23S	2972		0.89	0.15	50,50,50,50	0
57	MG	BL19	201		0.89	0.13	68,68,68,68	
57	MG	A16S	1620	1/1	0.89	0.10	48,48,48,48	0



	Type	Chain	Bes	 Atoms	BSCC	BSB	B -factors($Å^2$)	Q<0.9
57	MG	B23S	3006	1/1	0.89	0.10		0
57	MG	B23S	2977	1/1	0.89	0.10	63 63 63 63	0
57	MG	BL28	101	1/1	0.89	0.15	55.55.55.55	0
57	MG	A16S	1630	1/1	0.89	0.08	55.55.55.55	0
57	MG	A23S	2963	1/1	0.89	0.15	58,58,58,58	0
57	MG	B23S	2938	1/1	0.89	0.10	45,45,45,45	0
57	MG	B23S	2985	1/1	0.89	0.08	42,42,42,42	0
57	MG	A16S	1633	1/1	0.89	0.10	48,48,48,48	0
57	MG	B23S	2942	1/1	0.89	0.09	41,41,41,41	0
57	MG	BTHX	101	1/1	0.89	0.08	117,117,117,117	0
57	MG	B23S	3017	1/1	0.90	0.07	46,46,46,46	0
57	MG	A23S	2919	1/1	0.90	0.58	44,44,44,44	0
57	MG	B23S	2919	1/1	0.90	0.17	33,33,33,33	0
57	MG	AL21	201	1/1	0.90	0.30	49,49,49,49	0
57	MG	B23S	3023	1/1	0.90	0.17	54,54,54,54	0
57	MG	B16S	1612	1/1	0.90	0.09	61,61,61,61	0
57	MG	B23S	2973	1/1	0.90	0.15	54,54,54,54	0
57	MG	A16S	1604	1/1	0.90	0.12	56, 56, 56, 56	0
57	MG	B23S	2930	1/1	0.90	0.09	54,54,54,54	0
57	MG	BL21	201	1/1	0.90	0.14	69,69,69,69	0
57	MG	B16S	1617	1/1	0.90	0.13	53,53,53,53	0
57	MG	B23S	2905	1/1	0.90	0.14	31,31,31,31	0
57	MG	B16S	1601	1/1	0.90	0.23	58, 58, 58, 58	0
57	MG	BL29	101	1/1	0.90	0.15	46,46,46,46	0
57	MG	B16S	1621	1/1	0.90	0.11	38,38,38,38	0
57	MG	A16S	1631	1/1	0.90	0.09	46,46,46,46	0
57	MG	AL24	201	1/1	0.90	0.08	63,63,63,63	0
57	MG	B23S	3013	1/1	0.90	0.15	77,77,77,77	0
57	MG	BL32	101	1/1	0.90	0.21	84,84,84,84	0
57	MG	B23S	3014	1/1	0.90	0.12	48,48,48,48	0
57	MG	A16S	1617	1/1	0.90	0.20	61,61,61,61	0
57	MG	A23S	2935	1/1	0.90	0.18	58,58,58,58	0
57	MG	B23S	2987	1/1	0.91	0.11	32,32,32,32	0
57	MG	A16S	1606	1/1	0.91	0.09	29,29,29,29	0
57	MG	BL18	202	1/1	0.91	0.39	45,45,45,45	0
57	MG	B23S	2952	1/1	0.91	0.07	42,42,42,42	0
57	MG	B23S	3033	1/1	0.91	0.18	67,67,67,67	0
57	MG	B23S	2993	1/1	0.91	0.20	43,43,43,43	0
57	MG	A16S	1618	1/1	0.91	0.14	65,65,65,65	0
57	MG	B23S	2995	1/1	0.91	0.20	57,57,57,57	0
57	MG	A23S	2926	1/1	0.91	0.12	64,64,64,64	0
57	MG	AL17	201	1/1	0.91	0.15	$51,\!51,\!51,\!51$	0



Mol		Chain	Bes	Atoms	BSCC	RSR	B-factors $(Å^2)$	Q<0.9
57	MG	B23S	3018	1/1	0.91	0.06	35 35 35 35	
57	MG	A16S	1616	1/1	0.91	0.07	62.62.62.62	0
57	MG	A23S	2973	1/1	0.91	0.08	46.46.46.46	0
57	MG	B23S	2943	1/1	0.91	0.13	50.50.50.50	0
57	MG	A23S	2933	1/1	0.91	0.32	58,58,58,58	0
57	MG	B23S	2946	1/1	0.91	0.11	46,46,46,46	0
57	MG	B16S	1614	1/1	0.91	0.10	46,46,46,46	0
57	MG	A23S	2967	1/1	0.91	0.08	60,60,60,60	0
57	MG	A16S	1615	1/1	0.92	0.23	51,51,51,51	0
57	MG	B23S	2997	1/1	0.92	0.23	49,49,49,49	0
57	MG	A23S	2942	1/1	0.92	0.17	38,38,38,38	0
57	MG	A23S	2965	1/1	0.92	0.11	62,62,62,62	0
57	MG	B23S	2929	1/1	0.92	0.13	38,38,38,38	0
57	MG	A23S	2928	1/1	0.92	0.26	32,32,32,32	0
57	MG	AS08	201	1/1	0.92	0.28	43,43,43,43	0
57	MG	B23S	3004	1/1	0.92	0.26	58,58,58,58	0
57	MG	A23S	2945	1/1	0.92	0.24	45,45,45,45	0
57	MG	BL02	304	1/1	0.92	0.11	45,45,45,45	0
57	MG	A23S	2908	1/1	0.92	0.12	52,52,52,52	0
57	MG	A23S	2948	1/1	0.92	0.10	60,60,60,60	0
57	MG	B23S	2968	1/1	0.92	0.13	38,38,38,38	0
57	MG	B23S	2971	1/1	0.92	0.13	45,45,45,45	0
57	MG	A23S	2950	1/1	0.92	0.16	34,34,34,34	0
57	MG	B23S	3012	1/1	0.92	0.07	54,54,54,54	0
57	MG	A23S	2934	1/1	0.92	0.09	39,39,39,39	0
57	MG	B16S	1632	1/1	0.92	0.09	50,50,50,50	0
57	MG	A23S	2920	1/1	0.92	0.16	56,56,56,56	0
57	MG	B23S	2941	1/1	0.92	0.14	35,35,35,35	0
57	MG	B23S	2978	1/1	0.92	0.09	39,39,39,39	0
57	MG	A16S	1632	1/1	0.92	0.10	65,65,65,65	0
57	MG	A23S	2960	1/1	0.92	0.08	56,56,56,56	0
57	MG	A5S	203	1/1	0.92	0.13	58,58,58,58	0
57	MG	B23S	2911	1/1	0.92	0.18	38,38,38,38	0
57	MG	BL29	103	1/1	0.92	0.16	30,30,30,30	0
57	MG	A16S	1627	1/1	0.92	0.13	47,47,47,47	0
57	MG	B23S	3024	1/1	0.92	0.12	47,47,47,47	0
57	MG	B16S	1616		0.92	0.17	44,44,44,44	
57	MG	AL27	101	1/1	0.92	0.20	40,40,40,40	
57	MG	A16S	1623		0.92	0.17	42,42,42,42	
57	MG	B16S	1619	1/1	0.92	0.09	50,50,50,50	
57	MG	B23S	2921	1/1	0.92	0.23	56,56,56,56	0
57	MG	BL35	101	1/1	0.92	0.23	58,58,58,58	0



	Type	Chain	Bes	 Atoms	BSCC	BSB	B-factors $(Å^2)$	Q<0.9
57	MG	B23S	2923	1/1	0.92	0.13	53 53 53 53	0
57	MG	A23S	2925	1/1	0.93	0.13	41.41.41.41	0
57	MG	A23S	2952	1/1	0.93	0.12	43.43.43.43	0
57	MG	B23S	2940	1/1	0.93	0.31	44,44,44,44	0
57	MG	B23S	2903	1/1	0.93	0.11	34.34.34.34	0
57	MG	A16S	1629	1/1	0.93	0.41	93,93,93,93	0
57	MG	AL28	102	1/1	0.93	0.09	50,50,50,50	0
57	MG	A23S	2955	1/1	0.93	0.49	58,58,58,58	0
57	MG	B23S	2966	1/1	0.93	0.14	51,51,51,51	0
57	MG	BL25	301	1/1	0.93	0.11	46,46,46,46	0
57	MG	A23S	2929	1/1	0.93	0.11	52,52,52,52	0
57	MG	B23S	2947	1/1	0.93	0.14	41,41,41,41	0
57	MG	AS02	301	1/1	0.93	0.12	90,90,90,90	0
57	MG	B23S	2912	1/1	0.93	0.22	27,27,27,27	0
57	MG	B23S	2913	1/1	0.93	0.12	28,28,28,28	0
57	MG	A23S	2930	1/1	0.93	0.08	44,44,44,44	0
57	MG	BL02	305	1/1	0.93	0.09	59,59,59,59	0
57	MG	A23S	2932	1/1	0.93	0.13	43,43,43,43	0
57	MG	B23S	2935	1/1	0.93	0.10	30,30,30,30	0
57	MG	A23S	2949	1/1	0.93	0.58	71,71,71,71	0
57	MG	A23S	2902	1/1	0.93	0.18	45,45,45,45	0
57	MG	B23S	2981	1/1	0.93	0.09	31,31,31,31	0
57	MG	B23S	3005	1/1	0.94	0.24	50,50,50,50	0
57	MG	AL20	201	1/1	0.94	0.12	75,75,75,75	0
57	MG	BL16	203	1/1	0.94	0.16	69,69,69,69	0
57	MG	B16S	1602	1/1	0.94	0.15	44,44,44,44	0
57	MG	B23S	3029	1/1	0.94	0.23	43,43,43,43	0
57	MG	B23S	2920	1/1	0.94	0.14	31,31,31,31	0
57	MG	A23S	2958	1/1	0.94	0.11	50,50,50,50	0
57	MG	B23S	2988	1/1	0.94	0.11	51,51,51,51	0
57	MG	B23S	2950	1/1	0.94	0.35	33,33,33,33	0
57	MG	B16S	1615	1/1	0.94	0.17	$65,\!65,\!65,\!65$	0
57	MG	BL24	201	1/1	0.94	0.21	89,89,89,89	0
57	MG	B23S	2991	1/1	0.94	0.04	63,63,63,63	0
57	MG	A23S	2903	1/1	0.94	0.19	41,41,41,41	0
57	MG	B23S	2925	1/1	0.94	0.18	46,46,46,46	0
57	MG	A16S	1602	1/1	0.94	0.08	37,37,37,37	0
57	MG	B23S	2927	1/1	0.94	0.14	58,58,58,58	0
57	MG	B16S	1606	1/1	0.94	0.27	65,65,65,65	0
57	MG	B23S	2957	1/1	0.94	0.22	23,23,23,23	0
57	MG	A23S	2924	1/1	0.94	0.05	46,46,46,46	0
57	MG	A23S	2954	1/1	0.94	0.09	40,40,40,40	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
57	MG	BL33	101	1/1	0.94	0.29	57,57,57,57	0
57	MG	BL04	301	1/1	0.94	0.25	55,55,55,55	0
57	MG	B23S	2980	1/1	0.94	0.38	47,47,47,47	0
57	MG	A16S	1609	1/1	0.94	0.15	71,71,71,71	0
57	MG	B23S	2945	1/1	0.94	0.18	35,35,35,35	0
57	MG	A23S	2968	1/1	0.95	0.19	51,51,51,51	0
57	MG	AL33	102	1/1	0.95	0.07	45,45,45,45	0
57	MG	BL24	202	1/1	0.95	0.09	53,53,53,53	0
57	MG	A23S	2956	1/1	0.95	0.22	66,66,66,66	0
57	MG	AL21	203	1/1	0.95	0.09	86,86,86,86	0
57	MG	BL28	102	1/1	0.95	0.17	41,41,41,41	0
57	MG	A23S	2957	1/1	0.95	0.12	53,53,53,53	0
57	MG	B23S	2914	1/1	0.95	0.24	31,31,31,31	0
57	MG	B23S	3001	1/1	0.95	0.14	32,32,32,32	0
57	MG	B5S	201	1/1	0.95	0.28	47,47,47,47	0
57	MG	B23S	2970	1/1	0.95	0.09	57,57,57,57	0
57	MG	A23S	2913	1/1	0.95	0.08	47,47,47,47	0
57	MG	AS06	201	1/1	0.95	0.12	82,82,82,82	0
57	MG	B23S	2902	1/1	0.95	0.16	24,24,24,24	0
57	MG	A23S	2944	1/1	0.95	0.18	46,46,46,46	0
57	MG	A23S	2917	1/1	0.95	0.16	52,52,52,52	0
57	MG	A23S	2914	1/1	0.95	0.12	$59,\!59,\!59,\!59$	0
57	MG	BS17	201	1/1	0.95	0.09	66,66,66,66	0
57	MG	B23S	2907	1/1	0.95	0.12	31,31,31,31	0
57	MG	A23S	2905	1/1	0.96	0.08	38,38,38,38	0
57	MG	B23S	2901	1/1	0.96	0.22	43,43,43,43	0
57	MG	BL29	102	1/1	0.96	0.15	23,23,23,23	0
57	MG	B16S	1625	1/1	0.96	0.08	$52,\!52,\!52,\!52$	0
57	MG	AL15	201	1/1	0.96	0.12	74,74,74,74	0
57	MG	B23S	2904	1/1	0.96	0.14	40,40,40,40	0
57	MG	BL02	302	1/1	0.96	0.07	$65,\!65,\!65,\!65$	0
57	MG	B23S	2992	1/1	0.96	0.18	32,32,32,32	0
57	MG	B23S	3030	1/1	0.96	0.07	61,61,61,61	0
57	MG	A23S	2922	1/1	0.96	0.13	58,58,58,58	0
57	MG	B23S	2969	1/1	0.96	0.23	67,67,67,67	0
57	MG	BL33	103	1/1	0.96	0.18	61,61,61,61	0
57	MG	A23S	2923	1/1	0.96	0.12	61,61,61,61	0
57	MG	A23S	2918	1/1	0.96	0.24	65,65,65,65	0
57	MG	A23S	2915	1/1	0.96	0.09	40,40,40,40	0
57	MG	A23S	2909	1/1	0.96	0.13	40,40,40,40	0
57	MG	A23S	2939	1/1	0.97	0.16	55,55,55,55	0
57	MG	B23S	2965	1/1	0.97	0.13	43,43,43,43	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	B16S	1620	1/1	0.97	0.16	76,76,76,76	0
57	MG	B16S	1607	1/1	0.97	0.15	60,60,60,60	0
57	MG	A16S	1628	1/1	0.97	0.06	38,38,38,38	0
57	MG	B5S	202	1/1	0.97	0.08	58, 58, 58, 58	0
57	MG	A23S	2937	1/1	0.97	0.12	78,78,78,78	0
57	MG	A23S	2931	1/1	0.97	0.10	40,40,40,40	0
57	MG	BL34	102	1/1	0.97	0.28	38,38,38,38	0
57	MG	B23S	2922	1/1	0.97	0.13	31,31,31,31	0
57	MG	BL36	101	1/1	0.97	0.19	62,62,62,62	0
57	MG	BS16	101	1/1	0.97	0.19	71,71,71,71	0
57	MG	BL20	201	1/1	0.97	0.06	44,44,44,44	0
57	MG	AL21	202	1/1	0.97	0.06	77,77,77,77	0
57	MG	B23S	2975	1/1	0.98	0.15	37,37,37,37	0
57	MG	A23S	2904	1/1	0.98	0.14	48,48,48,48	0
57	MG	B23S	3020	1/1	0.98	0.09	$53,\!53,\!53,\!53$	0
57	MG	AL33	101	1/1	0.98	0.11	60,60,60,60	0
58	SF4	BS04	501	8/8	0.98	0.23	76,98,101,103	0
57	MG	B23S	2982	1/1	0.99	0.21	74,74,74,74	0
57	MG	A23S	2946	1/1	0.99	0.03	63,63,63,63	0
57	MG	B16S	1609	1/1	0.99	0.18	$65,\!65,\!65,\!65$	0
57	MG	A16S	1621	1/1	0.99	0.09	63,63,63,63	0
57	MG	B23S	2909	1/1	0.99	0.14	32,32,32,32	0
58	SF4	AS04	501	8/8	0.99	0.21	60,86,91,92	0
57	MG	BL18	203	1/1	0.99	0.13	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.

