

wwPDB EM Validation Summary Report (i)

Apr 16, 2024 - 04:05 am BST

PDB ID	:	70YD
EMDB ID	:	EMD-13114
Title	:	Cryo-EM structure of a rabbit 80S ribosome with zebrafish Dap1b
Authors	:	Leesch, F.; Lorenzo-Orts, L.; Grishkovskaya, I.; Kandolf, S.; Belacic, K.; Mein-
		hart, A.; Haselbach, D.; Pauli, A.
Deposited on	:	2021-06-24
Resolution	:	2.30 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp 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:

EMDB validation analysis	:	0.0.1. dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
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: $ELECTRON\ MICROSCOPY$

The reported resolution of this entry is 2.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain	
1	х	217	74% .	25%
2	5	3740	74%	15% • 10%
3	8	156	83%	10% 8%
4	9	1786	67%	25% • 5%
5	А	257	95%	• •
6	AA	295	73% •	26%
7	Aa	115	87%	• 12%
8	В	403	97%	•••
9	BB	264	78%	• 19%



Mol	Chain	Length	Quality of chain	
10	Bb	84	99%	·
11	С	413	86%	• 13%
12	CC	293	75% .	25%
13	Cc	69	86%	• 10%
14	D	297	96%	• •
15	DD	243	92%	• 6%
16	Dd	56	95%	• •
17	Е	291	73% •	27%
18	EE	263	97%	•
19	Ee	133	· 59%	
20	F	249	90%	10%
21	\mathbf{FF}	204	87%	• 9%
22	G	266	80% •	19%
23	GG	249	91%	• 5%
24	Gg	317	97%	••
25	Н	192	96%	•••
26	HH	432	42% 57%	
27	Ι	214	93%	• 6%
28	II	208	96%	••
29	J	178	94%	• 6%
30	JJ	194	94%	• 5%
31	K	120	93%	6% •
32	KK	165	57% • 42%	
33	L	211	96%	•••
34	LL	158	89%	• 9%



Mol	Chain	Length	Quality of chain	
35	М	218	62% 38%	
36	Ν	204	99%	•
37	NN	151	98%	
38	0	203	97%	••
39	00	151	89%	• 10%
40	Р	187	80% .	19%
41	PP	145	81% 6%	6 14%
42	Q	188	99%	
43	QQ	146	95%	• •
44	R	196	84%	15%
45	RR	135	95%	•••
46	S	224	77% .	21%
47	SS	152	92%	• 5%
48	Т	160	98%	
49	TT	145	95%	• •
50	U	141	70% 30	0%
51	UU	119	83% •	16%
52	V	140	93%	7%
53	VV	83	98%	•
54	W	157	39% 61%	
55	WW	130	98%	•••
56	Х	156	76%	24%
57	XX	143	95%	
58	Y	145	88%	• 9%
59	YY	133	92%	• 7%



Mol	Chain	Length	Quality of chain		
60	Z	136	99%		
61	ZZ	124	60%	40%	
62	a	148	99%		
63	b	245	40% 60%		
64	с	115	82%	18	3%
65	d	125	85%		15%
66	е	157	82%	18	3%
67	f	110	99%		·
68	g	117	94%		• 5%
69	h	123	98%		•
70	i	105	96%		·
71	j	97	89%		11%
72	k	70	97%		·
73	1	51	98%		·
74	m	128	40% 60%		
75	n	25	100%		
76	0	106	95%		•••
77	р	92	99%		
78	r	137	89%	·	10%
79	S	318	61%	38%	
80	s1	109	16% • 83%		
81	t	154	79%	• 18	3%
82	v	858	83%	• 1	5%
83	W	407	8% 92%		



2 Entry composition (i)

There are 85 unique types of molecules in this entry. The entry contains 213014 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	x	163	Total 1291	C 832	N 225	O 228	S 6	0	0

• Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
2	5	3358	Total 72165	C 32204	N 13226	O 23377	Р 3358	0	0

• Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	144	Total 3072	C 1370	N 547	0 1011	Р 144	0	0

• Molecule 4 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	9	1698	Total 36291	C 16217	N 6509	O 11868	Р 1697	0	0

• Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms				AltConf	Trace	
5	А	247	Total 1891	C 1185	N 388	0 312	S 6	0	0

• Molecule 6 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues		At	AltConf	Trace			
6	AA	217	Total 1710	C 1086	N 300	O 316	S 8	0	0



There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	114	THR	ALA	conflict	UNP G1TLT8

• Molecule 7 is a protein called 40S ribosomal protein S26-like.

Mol	Chain	Residues		At	AltConf	Trace			
7	Aa	101	Total	С	Ν	Ο	S	0	0
'	110	101	814	507	170	132	5		

• Molecule 8 is a protein called Ribosomal protein L3.

Mol	Chain	Residues		At	AltConf	Trace			
8	В	394	Total 3172	C 2020	N 597	O 542	S 13	0	0

• Molecule 9 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BB	213	Total 1729	C 1098	N 309	O 308	S 14	0	0

• Molecule 10 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	Bb	83	Total 651	C 408	N 121	0 115	${ m S} 7$	0	0

• Molecule 11 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues		At	AltConf	Trace			
11	С	358	Total 2856	C 1797	N 572	0 473	S 14	0	0

• Molecule 12 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues		At	AltConf	Trace			
12	CC	221	Total 1716	C 1111	N 295	O 301	S 9	0	0

• Molecule 13 is a protein called 40S ribosomal protein S28.



Mol	Chain	Residues	Atoms					AltConf	Trace
13	Cc	62	Total 488	C 297	N 97	O 92	${ m S} { m 2}$	0	0

• Molecule 14 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues		At	AltConf	Trace			
14	D	289	Total 2361	C 1495	N 431	0 421	S 14	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

• Molecule 15 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DD	228	Total 1768	C 1126	N 318	0 316	S 8	0	0

• Molecule 16 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
16	Dd	55	Total 459	C 286	N 94	0 74	${ m S}{ m 5}$	0	0

• Molecule 17 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues		At	AltConf	Trace			
17	Е	213	Total 1710	C 1103	N 325	0 279	$\frac{S}{3}$	0	0

• Molecule 18 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	EE	262	Total 2076	C 1324	N 386	O 358	S 8	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	conflict	UNP G1TK17



0 0	J. J	Figure P			
Chain	Residue	Modelled	Actual	Comment	Reference
\mathbf{EE}	51	ARG	LYS	conflict	UNP G1TK17
\mathbf{EE}	78	THR	ALA	conflict	UNP G1TK17
EE	156	VAL	MET	conflict	UNP G1TK17

• Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues		Ato	AltConf	Trace			
19	Ee	55	Total 443	С 274	N 97	0 71	S 1	0	0

• Molecule 20 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues		Ate	AltConf	Trace			
20	F	225	Total 1875	C 1205	N 358	O 303	${f S}$ 9	0	0

• Molecule 21 is a protein called Ribosomal protein S5.

Mol	Chain	Residues		At	AltConf	Trace			
21	\mathbf{FF}	185	Total 1471	C 921	N 277	O 266	${ m S} 7$	0	0

• Molecule 22 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues		Ate	AltConf	Trace			
22	G	215	Total 1747	C 1115	N 337	0 291	$\frac{S}{4}$	0	0

• Molecule 23 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues		Ate	AltConf	Trace			
23	GG	237	Total 1923	C 1200	N 387	O 329	${f S}7$	0	0

• Molecule 24 is a protein called RACK1.

Mol	Chain	Residues		At	AltConf	Trace			
24	Gg	313	Total 2436	C 1535	N 424	O 465	S 12	0	0

• Molecule 25 is a protein called 60S ribosomal protein L9.



Mol	Chain	Residues		At	oms			AltConf	Trace
25	Н	186	Total 1484	C 933	N 277	O 268	S 6	0	0

• Molecule 26 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	HH	185	Total 1488	C 952	N 271	O 264	S 1	0	0

• Molecule 27 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ι	202	Total 1640	C 1041	N 317	O 269	S 13	0	0

• Molecule 28 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	II	206	Total 1686	C 1058	N 332	O 291	${ m S}{ m 5}$	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

• Molecule 29 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	J	168	Total 1344	C 850	N 251	0 237	S 6	0	0

• Molecule 30 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues		At	oms			AltConf	Trace
30	JJ	185	Total 1525	C 969	N 306	0 248	${ m S} { m 2}$	0	0

• Molecule 31 is a RNA chain called 5S rRNA.



Mol	Chain	Residues		A	AltConf	Trace			
31	K	119	Total 2538	C 1132	N 454	O 834	Р 118	0	0

 $\bullet\,$ Molecule 32 is a protein called S10_plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	KK	96	Total 810	C 530	N 143	0 131	S 6	0	0

• Molecule 33 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	205	Total 1658	C 1037	N 346	0 271	$\frac{S}{4}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3
L	190	ARG	HIS	conflict	UNP G1TKB3

• Molecule 34 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LL	143	Total 1175	C 749	N 222	0 198	${ m S}{ m 6}$	0	0

• Molecule 35 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	М	135	Total 1117	C 715	N 217	0 178	${f S}{7}$	0	0

• Molecule 36 is a protein called Ribosomal protein L15.

Mol	Chain	Residues		Ate	AltConf	Trace			
36	Ν	203	Total 1701	C 1072	N 359	O 266	${S \atop 4}$	0	0

• Molecule 37 is a protein called 40S ribosomal protein S13.



Mol	Chain	Residues		At	oms			AltConf	Trace
37	NN	149	Total 1202	C 770	N 228	O 203	S 1	0	0

• Molecule 38 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues		Ate	AltConf	Trace			
38	Ο	199	Total 1630	C 1051	N 319	O 255	${f S}{5}$	0	0

• Molecule 39 is a protein called 40S ribosomal protein S14-like.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	00	136	Total 1016	C 621	N 199	0 190	S 6	0	0

• Molecule 40 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
40	Р	152	Total 1233	C 772	N 240	0 212	S 9	0	0

• Molecule 41 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues		At	AltConf	Trace			
41	PP	125	Total 1025	C 652	N 192	0 174	${ m S} 7$	0	0

• Molecule 42 is a protein called Ribosomal protein L18.

Mol	Chain	Residues		At	oms			AltConf	Trace
42	Q	187	Total 1515	C 946	N 315	O 250	$\frac{S}{4}$	0	0

• Molecule 43 is a protein called Ribosomal protein S16.

Mol	Chain	Residues		At	oms	AltConf	Trace		
43	QQ	142	Total 1128	C 717	N 213	0 195	${ m S} { m 3}$	0	0

• Molecule 44 is a protein called Ribosomal protein L19.



Mol	Chain	Residues		At	oms	AltConf	Trace		
44	R	166	Total 1383	C 859	N 298	O 217	S 9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	38	ARG	HIS	conflict	UNP G1TYL6
R	151	ARG	HIS	conflict	UNP G1TYL6

• Molecule 45 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues		At	AltConf	Trace			
45	RR	132	Total 1068	C 670	N 199	0 195	$\begin{array}{c} \mathrm{S} \\ \mathrm{4} \end{array}$	0	0

• Molecule 46 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	AltConf	Trace			
46	S	176	Total 1456	C 927	N 282	O 236	S 11	0	0

• Molecule 47 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues		At	oms			AltConf	Trace
47	\mathbf{SS}	144	Total 1190	С 746	N 241	O 202	S 1	0	0

• Molecule 48 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues		At	oms			AltConf	Trace
48	Т	158	Total 1292	C 820	N 251	0 215	S 6	0	0

• Molecule 49 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
49	TT	141	Total 1097	C 688	N 211	0 195	${ m S} { m 3}$	0	0

There is a discrepancy between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

• Molecule 50 is a protein called 60S ribosomal protein L22-like.

Mol	Chain	Residues		At	oms			AltConf	Trace
50	U	98	Total 800	C 514	N 139	0 145	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 51 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues		At	oms	AltConf	Trace		
51	UU	100	Total 795	C 498	N 152	0 141	$\frac{S}{4}$	0	0

• Molecule 52 is a protein called Ribosomal protein L23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
52	V	130	Total 973	C 615	N 183	0 170	${f S}{5}$	0	0

• Molecule 53 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues		At	AltConf	Trace			
53	VV	83	Total 636	C 393	N 117	0 121	${ m S}{ m 5}$	0	0

• Molecule 54 is a protein called Ribosomal protein L24.

Mol	Chain	Residues		Ate	oms		AltConf	Trace	
54	W	62	Total 519	C 332	N 101	O 83	${ m S} { m 3}$	0	0

• Molecule 55 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues		At	oms			AltConf	Trace
55	WW	129	Total 1034	C 659	N 193	0 176	S 6	0	0

• Molecule 56 is a protein called 60S ribosomal protein L23a.



Mol	Chain	Residues		At	oms			AltConf	Trace
56	X	118	Total 967	C 618	N 181	O 167	S 1	0	0

• Molecule 57 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues		At	oms			AltConf	Trace
57	XX	141	Total 1098	C 693	N 219	0 183	${ m S} { m 3}$	0	0

• Molecule 58 is a protein called Ribosomal protein L26.

Mol	Chain	Residues		At	oms			AltConf	Trace
58	Y	132	Total 1102	C 692	N 223	0 184	${ m S} { m 3}$	0	0

• Molecule 59 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues		At	oms			AltConf	Trace
59	YY	124	Total 1011	C 640	N 198	O 168	${ m S}{ m 5}$	0	0

• Molecule 60 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues		At	oms			AltConf	Trace
60	Ζ	135	Total 1107	С 714	N 208	0 182	${ m S} { m 3}$	0	0

• Molecule 61 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues		At	oms			AltConf	Trace
61	ZZ	75	Total 598	C 382	N 111	0 104	S 1	0	0

• Molecule 62 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues		At	oms			AltConf	Trace
62	a	147	Total 1162	С 734	N 239	0 185	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 63 is a protein called 60S ribosomal protein L29.



Mol	Chain	Residues		At	oms			AltConf	Trace
63	b	98	Total 806	C 498	N 182	0 123	${ m S} { m 3}$	0	0

• Molecule 64 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues		At	oms		AltConf	Trace	
64	С	94	Total 732	C 464	N 130	0 132	S 6	0	0

• Molecule 65 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues		At	oms	AltConf	Trace		
65	d	106	Total 879	C 555	N 170	0 152	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 66 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues		At	oms			AltConf	Trace
66	е	128	Total 1053	C 667	N 216	0 165	${ m S}{ m 5}$	0	0

• Molecule 67 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues		At	oms		AltConf	Trace	
67	f	109	Total 876	$\begin{array}{c} \mathrm{C} \\ 555 \end{array}$	N 174	0 143	$\frac{S}{4}$	0	0

• Molecule 68 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues		At	oms			AltConf	Trace
68	g	111	Total 882	C 552	N 182	0 142	S 6	0	0

• Molecule 69 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues		At	oms			AltConf	Trace
69	h	121	Total 1008	C 637	N 203	0 167	S 1	0	0

• Molecule 70 is a protein called 60S ribosomal protein L36.



Mol	Chain	Residues		At	oms			AltConf	Trace
70	i	101	Total 821	C 514	N 174	0 128	${f S}{5}$	0	0

• Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues		At	oms			AltConf	Trace
71	j	86	Total	C	N	0	S	0	0
	5		705	434	155	111	\mathbf{b}		

• Molecule 72 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues		Ate	\mathbf{oms}	AltConf	Trace		
72	k	68	Total 559	C 360	N 101	O 97	S 1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	24	LYS	ASN	conflict	UNP G1U001

• Molecule 73 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
73	1	50	Total 447	C 286	N 96	O 64	S 1	0	0

• Molecule 74 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
74	m	51	Total 420	C 261	N 88	O 65	${f S}{6}$	0	0

• Molecule 75 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues		Ato	\mathbf{ms}			AltConf	Trace
75	n	25	Total	С	Ν	Ο	\mathbf{S}	0	0
10	11	20	239	145	64	27	3	0	0

• Molecule 76 is a protein called 60S ribosomal protein L36a-like.



Mol	Chain	Residues		At	oms			AltConf	Trace
76	0	102	Total 834	C 522	N 171	0 135	S 6	0	0

• Molecule 77 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
77	р	91	Total 708	С 445	N 136	O 120	${ m S} 7$	0	0

• Molecule 78 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues		At	oms	AltConf	Trace		
78	r	123	Total 986	C 611	N 204	0 166	${f S}{5}$	0	0

• Molecule 79 is a protein called 60S ribosomal protein L10E.

Mol	Chain	Residues		At	AltConf	Trace			
79	s	196	Total 1501	C 953	N 263	0 276	${ m S} 9$	0	0

• Molecule 80 is a protein called Dap1b.

Mol	Chain	Residues		Ate	\mathbf{oms}	AltConf	Trace		
80	s1	18	Total 150	C 96	N 30	O 23	S 1	0	0

• Molecule 81 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms				AltConf	Trace	
81	t	126	Total 961	C 603	N 168	0 182	S 8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	36	SER	GLY	conflict	UNP P10160

• Molecule 82 is a protein called Elongation factor 2.



Mol	Chain	Residues	Atoms				AltConf	Trace	
82	V	726	Total 5669	C 3611	N 072	0 1046	S 40	0	0
			0009	3011	912	1040	40		

• Molecule 83 is a protein called SERPINE1 mRNA binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	W	32	Total 252	C 148	N 55	O 49	0	0

• Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
84	5	195	Total Mg 195 195	0
84	8	2	Total Mg 2 2	0
84	Ι	1	Total Mg 1 1	0
84	Р	1	Total Mg 1 1	0
84	g	1	Total Mg 1 1	0
84	V	1	Total Mg 1 1	0

• Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
85	Aa	1	Total Zn 1 1	0
85	KK	1	Total Zn 1 1	0
85	g	1	Total Zn 1 1	0
85	j	1	Total Zn 1 1	0
85	m	1	Total Zn 1 1	0
85	О	1	Total Zn 1 1	0
85	р	1	Total Zn 1 1	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. 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. 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: Ribosomal protein uL1











• Molecule 3: 5.8S rRNA



 \bullet Molecule 4: 18S rRNA







• Molecule 9: 40S ribosomal protein S3a



Chain BB:	78%	• 19%	
MET VAL GLY GLY CYS CLYS ARG LYS THR THR THR CLY CLY	LYS GLY ALA ALA LYS LYS LYS K34 K34 K34 K36 K34 K34 K34 K34 K34 K34 K34 K34 K37 S K22 K22 S K222	CC233 CC233 CC233 CC233 CC233 CC20 CC10 CC17 CC17 CC17 CC17 CC17 CC17 CC1	ARG ALA ASP
GLY TYR GLU PRO PRO VAL GLN GLU SER VAL			
• Molecule 10: 40S	ribosomal protein S27		
Chain Bb:	99%		
MET P2 H84			
• Molecule 11: 60S	ribosomal protein L4		
Chain C:	86%	• 13%	
MET 42 4150 1150 1150 1150 125 125 125 125 125 125 125 125 125 125	LYR LYR GLU GLU GLU GLU LYS LYS LYS LYS LYS CLY CLYS CLY SYL LYS CLY SYL LYS CLY SYL CYS CLY SYL CYS CLY SYL CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	ALA ALA ALA ALA ALA LYS LYS PRO PRO ALA ASP ALA ASP ALA ASP ASP CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	GLU ASP LYS
LYS PRO ALA ALA			
• Molecule 12: 40S	ribosomal protein S2		
Chain CC:	75%	• 25%	
MET ALA ALA ASP ASP ASP ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY	GLY GLY PRO GLY PRO GLY GLY GLY GLY CLY CLY CLY CLY CLY CLY CLY CLY CLY C	ARG GLY GLY GLY GLY GLY GLY GLY GLY GLY GL	K58 R167
Y248 1278 ARG VAL SER VAL SER ARG ALA ALA ALA ALA	VAL VAL ALA THR THR		
• Molecule 13: 40S	ribosomal protein S28		
Chain Cc:	86%	• 10%	
MET ASP THR SER ARG VAL VAL R40 R40 R63 R63 R65 R67 R65	LL68 ARG		
• Molecule 14: 60S	ribosomal protein L5		
Chain D:	96%	•••	
MET GLY F3 M42 P26 D72 D72 D72 D72 C9 GLU	ARG ALA ALA GLU SER SER		
• Molecule 15: Rib	osomal protein S3		



Chain DD:	92%	• 6%
M1 R45 R64 R76 L113	V1553 G127 G127 G127 F120 F120 F120 F120 F120 F120 F120 F120	
• Molecule 16	: 40S ribosomal protein S29	
Chain Dd:	95%	
MET G2 N26 K48 K48 D56		
• Molecule 17	: 60S ribosomal protein L6	
Chain E:	73% · 27%	
MET ALA GLY GLV GLU CVS ALA ALA ALA ALA ALA CVS	PR0 ALA THR LLYS SER ALA ALA ALA ALA ALA ALA ALA ALA ALA AL	LYS LYS LYS LYS ARG GLU CYS VAL
G100 G100 GLY ASP ASN G105 G105	V197 LYS LEU ARG ARG ARG ARG ARG ALU CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV	
• Molecule 18	: 40S ribosomal protein S4	
Chain EE:	97%	·
MET A2 L20 D73 G132	n 148 X 259 C 263	
• Molecule 19	: 40S ribosomal protein S30	
Chain Ee:	39% · 59%	
MET GLN GLN LEU VAL ARG ALA GLU GLU	HIS HHIS CILU CILU CILU CILU CILU CILU CILU CILU	THR LEU GLY GLN CYS GLY VAL CLU
ALA LEU SER THR LEU GLU ALA GLY ARG	MET GLY GLY CITY CITY CITY CITY CITY CITY CITY CIT	
• Molecule 20	: 60S ribosomal protein L7	
Chain F:	90%	10%
LEU PHE ALA ASN ASN ASN TLE ASS GLU CYS	VAL VAL ALA ALA ALA CLU CLYS CLYS ARG ARG ARG ARG ARG ARG	
• Molecule 21	: Ribosomal protein S5	
Chain FF:	87% .	9%
	WORLDWIDE PROTEIN DATA BANK	







• Molecule 27: 6	0S ribosomal protein L10)	
Chain I:	93%		• 6%
MET G2 V96 N102 LEU CV8 A1A A1A A1A	ARG LEU GLN THR G114 V126 N202 S214		
• Molecule 28: 4	0S ribosomal protein S8		
Chain II:	96	5%	•••
MET G2 R47 R47 R47 R92 R92	q165 207 LVS		
• Molecule 29: 6	0S ribosomal protein L1	1	
Chain J:	94%	2	• 6%
MET ALA GLN GLN GLV GLV CLV CLV CLV CLV CLV CLV CLV	177 177		
• Molecule 30: 4	0S ribosomal protein S9		
Chain JJ:	94	1%	• 5%
MET P2 R70 R79 R169 G146 G17 ALA ALA	ASF ASF GLU GLU ASP		
• Molecule 31: 5	S rRNA		
Chain K:	93%	6	6% •
61 67 67 133 133 153 153 153 664 664 7100			
• Molecule 32: S	10_plectin domain-conta	aining protein	
Chain KK:	57%	• 42%	
M1 L35 PR0 SER ARG GLU CHX	ARC ARC PRO ARC ARC PRO PRO CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	CLY CLU ALA ASP ASP ASP ASP ASP ASP ASP ASP ALA ALA ASP ALA ASP ALA ASP ALA	GLU ALA ALA ALA GLY SER SER ALA ALA ALU
PHE GLN GLN ARG GLY GLY ARG GLY GLY GLY	PRO PRO GLN		
• Molecule 33: 6	0S ribosomal protein L13	3	
Chain L:	96	%	







Chain P:	80%	• 19%	6
PR0 ALA LYS MET V2 V2 C57	K163 GLN GLN CLN CLN CLN CLN VAL LYS CLU GLU CLN CLU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN		
• Molecule 4	1: 40S ribosomal protein uS19		
Chain PP:	81%	6%	14%
MET ALA ALA GLU CLU GLU CJN LYS LYS LYS	THG THG T13 T13 T13 T13 T13 T13 T13 T13 T13 T13		
• Molecule 4	2: Ribosomal protein L18		
Chain Q:	99%		·
MET G2 M188			
• Molecule 4	3: Ribosomal protein S16		
Chain QQ:	95%		
MET PRO SER LYS G5 M41 H1	M 100		
• Molecule 4	4: Ribosomal protein L19		
Chain R:	84%	• 1	5%
MET S2 L10 K167 GLU ALA ARG	LYES ARG GIUU GIUU GIUU CIPS CIUU CIPS GIUU CIPS GIUU CIUU GIUU GIUU CIUU CIVS CIUU CIUU		
• Molecule 4	5: 40S ribosomal protein $eS17$		
Chain RR:	95%		• •
MET G2 R5 T6 K7 R81	0115 G133 ALA VAL		
• Molecule 4	6: 60S ribosomal protein L18a		
Chain S:	77%	21%	
MET LYS LYS GLN TRP GLY ARG GLY	ALL ALL ALL ALL ALLA ALLA ALA ALA ALA A	GLY GLU SER ALA M1 L7	V39 R87 F176
• Molecule 4	7: 40S ribosomal protein uS13		



Chain SS:	92%		• 5%
MET S2 T60 K91 K94 L111	T145 VAL CIY LYS LYS LYS LYS		
• Molecule 48:	60S ribosomal protein L21		
Chain T:	98%		••
MET T2 D38 V72 M159 ALA			
• Molecule 49:	40S ribosomal protein S19		
Chain TT:	95%		• •
MET PRO G3 K43 M75 M75 K143	HIS		
• Molecule 50:	60S ribosomal protein L22-like		
Chain U:	70%	30%	
MET ARG PHE SER SER SER PHE LEU LYS	LEC LEC SER ALA ALA ALA ALA ALA ALA ALA CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY		
• Molecule 51:	40S ribosomal protein uS10		
Chain UU:	83%	·	16%
MET ALA ALA PHE LYS ASP ASP GLY CYS THR THR YAL	GLU CAL ALA ALA HIS HIS AIIT AIIT ALA		
• Molecule 52:	Ribosomal protein L23		
Chain V:	93%		7%
MET SER LIYS ARG GLY GLY GLY SER SER SER	- 1 4		
• Molecule 53:	40S ribosomal protein S21		
Chain VV:	98%		
M1 132 L70 F83			

• Molecule 54: Ribosomal protein L24



Chain W:	39%		61%	
M1 GCA GLU GLU GLU GLU CLU CLU CLN CLN CLN CLN CLN CLN CLN CLN CLN CLN	ARG ARG ARG ARG ALA VAL LYS PHE CLN ARG ARG ARG ALA	THR GLY ALA ALA LEU LEU LEU ALA ALA CLYS ALA ALA ALA CLYS CLN	PRO GLU VAL ARG LYS ALA GLN GLN GLN GLN ALA ALA ARG	ALA ALA LYS LYS GLU ALA LYS ALA LYS
GLN ALA SER LYS LYS LYS THR ALA ALA ALA	LYS PRO THR LYS LYS ALA ALA PRO CLN CVS CLN TLE	VAL LYS PRO LYS VAL VAL SER ALA ALA ALA ALA GLY CJY SARG ALY		
• Molecule 55:	Ribosomal prote	ein S15a		
Chain WW:		98%		•••
MET V2 L69 V103 F130				
• Molecule 56:	60S ribosomal p	rotein L23a		
Chain X:		76%	24%	
MET ALA PRO FRO ALA ALA CVS GLU ALA ALA	PRO PRO LYS ALA ALA GLU CYS ALA ALA ALA ALA ALA CUS	ALA LYS LYS LYS ALA ALA ALA LY CLS CLY LYS LYS LYS LYS LYS	K39 1156	
• Molecule 57:	40S ribosomal p	rotein S23		
Chain XX:		95%		• ••
MET G2 L7 P62 P62 P62 P62 P62 P86 R142	SER			
• Molecule 58:	Ribosomal prote	ein L26		
Chain Y:		88%		9%
M1 V55 Y74 V79 V104 K132	GLY LYS LYS CLYS GLU GLU GLU CLU GLU MET MET	diu a		
• Molecule 59:	40S ribosomal p	rotein S24		
Chain YY:		92%		• 7%
MET ASN ASP ASP X32 K32 K32 K113 A127 GLY	LYS PRO GLU GLU			
• Molecule 60:	60S ribosomal p	rotein L27		
Chain Z:		99%		
MET G2 F136				



• Molecule 61: 40	S ribosomal prot	ein S25			
Chain ZZ:	60%		40)%	
PRO PRO ASP ASP ASP LYS LYS LYS LYS LYS ASP ALA ALA GLY CYS	SER ALA LYS LYS ASP ASP PRO VAL ASN SER SER	GLY GLYS ALLA LYS LYS LYS LYS TRP SER	LYS GLY VAL VAL G115 G115 GLY ASP ALA ALA	ALA ALA GLV ASP ALA ALA	
• Molecule 62: 60	S ribosomal prot	ein L27a			
Chain a:		99%			
MET P2 A148					
• Molecule 63: 60	S ribosomal prote	ein L29			
Chain b:	40%		60%		
MET A2 E7 A1A A1A A1A A1A A1A A1A A1A LEU VAI VAI	PRO LYS GLU VAL LYS PRO THR THR TLE PRO CLY V39 V39	R117 LEU SER ARG PRO GLN CHR LYS ALA	LYS ALA LYS CHU GLU PRO GLN CLY CLYS CLYS	VAL LYS ALA GLN TLE CLN TLA ALA ALA ALA ALA ALA ALA ALA ALA	ILE LYS
SER LYS CLY CLYS CLYS GLY ALA GLN GLN THR THR TYS PRO	LYS LYS GLN ALA ALA GLU FYS FYC ALA ALA ALA	GLM LYS PRO LYS ALA GLN GLN GLN GLN	LYS PRO LYS ALA GLN GLN GLN GLY LYS LYS	ALA ALA GLN GLN ALA ALA ALA GLN GLN GLN	ALA LYS
PRO LYS ALA GLN ALA ALA CLN LYS LYS PRO PRO PRO ALA ALA	THR PRO PRO PRO VAL PRO PRO GLN ALA ALA PRO PRO	LTS GLY ALA GLN PRO PRO ALA ALA PRO			
• Molecule 64: 60	S ribosomal prote	ein L30			
Chain c:		82%		18%	
MET VAL VAL ALA ALA ALA LYS LYS LYS SER LEU GLU SER SER	114 8107 MET MET PRO GLN GLN GLN GLV GLV LYS				
• Molecule 65: 60	S ribosomal prot	ein L31			
Chain d:		85%		15%	
MET ALA ALA ALA LYS LYS GLY GLV CJY LYS LYS CJY GLY	ARG SER ALA ILE N18 GLU GLU ASN				
• Molecule 66: 60	S ribosomal prot	ein L32			
Chain e:		82%		18%	
MET CYS CYS CYS CYS LEU LEU LEU LEU LEU LEU LEU CLEU CLEU C	LYS LYS GLY CYS CYS PRO PRO LEU LEU LEU LEU LEU LIE THE THE	LIZS SER GLU GLU GLU GLU			
• Molecule 67: 60	S ribosomal prote	ein L35a			
Chain f:		99%			

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MET	S2	I110	

• Molecule 68: 60S ribosomal protein L34

Chain g:		94%		• 5%
MET V2 H73 H73 ER CLN CLN LYS ALLA LYS LYS				
• Molecule 69:	60S ribosomal protein	n L35		
Chain h:		98%		·
MET ALA K3 A123				
• Molecule 70:	60S ribosomal protein	n L36		
Chain i:		96%		·
MET A2 A102 LYS LYS ASP				
• Molecule 71:	Ribosomal protein L	37		
Chain j:		89%		1%
MET T2 K87 AR6 ALA ALA ALA ALA SER SER	出 S S S S S S S S S S S S S S S S S S S			
• Molecule 72:	60S ribosomal protein	n L38		
Chain k:		97%		·
MET P2 L69 LYS				
• Molecule 73:	60S ribosomal protein	n L39-like		
Chain l:		98%		·
MET S2 L51				
• Molecule 74:	Ubiquitin-60S riboso	mal protein L40		
Chain m:	40%		60%	_



ILE GLN CLN CLV GLU SER THR LEU HIS	LEU LEU ARG CLY ARG CLY CLY CLY LIYS	
• Molecule	75: 60s ribosomal protein l41	
Chain n:	100%	
There are n	no outlier residues recorded for this chain.	
• Molecule	76: 60S ribosomal protein L36a-like	
Chain o:	95% •••	
MET V2 R99 L103 LLR GLN GLN	법	
• Molecule	77: 60S ribosomal protein L37a	
Chain p:	99% .	
MET A2 Q92		
• Molecule	78: 60S ribosomal protein L28	
Chain r:	89% • 10%	
MET S2 H103 V124 MET VAL	LYS ARG LYS ARG ARG ARG THR ITR SER SER SER	
• Molecule	79: 60S ribosomal protein L10E	
Chain s:	61% 38%	
MET PRO ARG GLU D5 D5 P118 P118	N200 PR0 PR0 PR0 PR0 PR0 PR0 PR0 PR0 PR0 P	LEU ALA LEU
SER VAL GLU GLU ASP ASP TYR THR PHE	PR0 CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ASP GLU ASP
MET GLY PHE GLY LEU PHE ASP		
• Molecule	80: Dap1b	
Chain s1:	16% · 83%	
MET VAL GLN GLN LEU SER LYS CLY GLY VAL	VAL VAL THR THR ASP ASP ALA ALA ALA ALA ALA ALA ALA ALA ASP CLU VAL VAL VAL VAL VAL VAL VAL VAL VAL ALA ASP ASP ASP ASP ASP ASP ASP ASP ASP AS	MET GLN HIS



LEU SERR LEU LEU LEU LEU LEU LEU LEU LEU LEU LEU
• Molecule 81: Eukaryotic translation initiation factor 5A-1
Chain t: 79% • 18%
MET ASP ASP ASP ASP ASP ASP PHE TIO TIO TIO CUU TIS ASP ASP ASP ASP ASP ASP ASP ASP ASP AS
• Molecule 82: Elongation factor 2
Chain v: 83% • 15%
MET VAL ASS ASS ASS ALA ASS ALA ASS ALA ASS ALA ASS ALA ASS ALA ASS ALA ASS ALA ASS ALA ASS ALA ASS ALA ASS ASS
ASP ASP ASN ASN ASN ASN ASN ASN ALA ASN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
PR0 PR0 THR THR THR THR CLVS CLVS CLVS CLV CLVS CLV CLV CLV CLV CLV CLV CLV CLV CLV CLV
\bullet Molecule 83: SERPINE1 mRNA binding protein 1
Molecule 83: SERPINE1 mRNA binding protein 1 Chain w: 8% 92%
Molecule 83: SERPINE1 mRNA binding protein 1 Chain w: 8% 92% ERBERGERERERERERERERERERERERERERERERERER
Molecule 83: SERPINE1 mRNA binding protein 1 Chain w: 8% 92%
Molecule 83: SERPINE1 mRNA binding protein 1 Chain w: 8% 92% Boo a set boo
Molecule 83: SERPINE1 mRNA binding protein 1 Chain w: 8% 92%
Molecule 83: SERPINE1 mRNA binding protein 1 Chain w: 8% 92% get the second sec
Molecule 83: SERPINE1 mRNA binding protein 1 Chain w: 8% 92% Molecule 83: SERPINE1 mRNA binding protein 1 Molecule 83: SERPINE1 mR



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	479754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor



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: 4AC, OMG, B8T, OMU, 2MG, 7MG, 1MA, M7A, A2M, UR3, B8W, 6MZ, P4U, ZN, DDE, B9B, MA6, E3C, E7G, PSU, B9H, BGH, B8K, B8H, 5MC, B8N, B8Q, I4U, E6G, MHG, MG, 5MU, 5CT, MLZ, P7G, OMC

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	
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	Х	0.30	0/1311	0.44	0/1762
2	5	0.22	0/78172	0.71	7/121809~(0.0%)
3	8	0.21	0/3406	0.69	0/5301
4	9	0.64	0/39723	1.15	275/61870~(0.4%)
5	А	0.25	0/1929	0.44	0/2586
6	AA	0.40	0/1747	0.63	0/2374
7	Aa	0.37	0/828	0.56	0/1109
8	В	0.24	0/3240	0.43	0/4339
9	BB	0.37	0/1756	0.72	4/2350~(0.2%)
10	Bb	0.33	0/665	0.59	0/891
11	С	0.23	0/2899	0.40	0/3895
12	CC	0.47	0/1753	0.64	0/2369
13	Cc	0.32	0/490	0.61	0/656
14	D	0.25	0/2407	0.40	0/3224
15	DD	0.39	0/1796	0.65	0/2417
16	Dd	0.41	0/470	0.61	0/623
17	Е	0.24	0/1743	0.42	0/2337
18	EE	0.38	0/2118	0.70	5/2849~(0.2%)
19	Ee	0.36	0/447	0.55	0/587
20	F	0.24	0/1911	0.38	0/2549
21	\mathbf{FF}	0.35	0/1492	0.68	2/2005~(0.1%)
22	G	0.23	0/1778	0.39	0/2397
23	GG	0.32	0/1946	0.68	3/2590~(0.1%)
24	Gg	0.32	0/2493	0.64	2/3394~(0.1%)
25	Н	0.23	0/1502	0.42	0/2020
26	HH	0.37	0/1510	0.67	1/2022~(0.0%)
27	Ι	0.24	0/1678	0.40	0/2239
28	II	0.36	0/1715	0.65	0/2287
29	J	0.24	0/1367	0.40	0/1829
30	JJ	0.39	0/1550	0.63	0/2069



Mal	Chain	Bond	lengths	I	Bond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
31	K	0.19	0/2836	0.68	0/4421
32	KK	0.39	0/834	0.65	1/1125~(0.1%)
33	L	0.23	0/1689	0.41	0/2261
34	LL	0.44	0/1195	0.60	0/1597
35	М	0.24	0/1138	0.38	0/1521
36	Ν	0.30	0/1746	0.44	0/2338
37	NN	0.36	0/1226	0.58	0/1649
38	0	0.24	0/1662	0.38	0/2222
39	00	0.33	0/1029	0.63	0/1380
40	Р	0.23	0/1259	0.40	0/1688
41	PP	0.34	0/1045	0.66	2/1396~(0.1%)
42	Q	0.24	0/1539	0.42	0/2054
43	QQ	0.33	0/1146	0.66	1/1534~(0.1%)
44	R	0.22	0/1399	0.37	0/1851
45	RR	0.33	0/1082	0.62	0/1452
46	S	0.25	0/1495	0.42	0/2005
47	SS	0.32	0/1208	0.67	0/1618
48	Т	0.24	0/1320	0.40	0/1763
49	TT	0.30	0/1115	0.59	0/1493
50	U	0.24	0/814	0.40	0/1092
51	UU	0.33	0/805	0.61	0/1081
52	V	0.25	0/987	0.42	0/1324
53	VV	0.41	0/643	0.61	0/860
54	W	0.25	0/532	0.40	0/708
55	WW	0.48	0/1051	0.69	1/1406~(0.1%)
56	Х	0.23	0/984	0.40	0/1323
57	XX	0.46	0/1116	0.64	1/1490~(0.1%)
58	Y	0.23	0/1119	0.40	0/1488
59	YY	0.33	0/1028	0.56	0/1366
60	Ζ	0.25	0/1130	0.40	0/1507
61	ZZ	0.31	0/604	0.69	0/810
62	a	0.24	0/1191	0.43	0/1590
63	b	0.23	0/819	0.35	0/1081
64	с	0.24	0/742	0.39	0/995
65	d	0.23	0/894	0.41	0/1204
66	е	0.23	0/1071	0.40	0/1429
67	f	0.25	0/895	0.45	0/1198
68	g	0.24	0/892	0.41	0/1189
69	h	0.22	0/1016	0.38	0/1341
70	i	0.23	0/832	0.37	0/1101
71	j	0.24	0/720	0.44	0/952
72	k	0.24	0/565	0.39	0/750
73	1	0.21	0/459	0.41	0/608



Mal	Chain	Bond	lengths]	Bond angles
1VIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
74	m	0.23	0/415	0.41	0/550
75	n	0.20	0/240	0.32	0/305
76	0	0.28	0/847	0.44	0/1117
77	р	0.23	0/718	0.42	0/953
78	r	0.23	0/1002	0.41	0/1344
79	S	0.24	0/1523	0.42	0/2055
80	s1	0.21	0/154	0.37	0/205
81	t	0.34	0/958	0.60	0/1288
82	V	0.24	0/5758	0.41	0/7779
83	W	0.23	0/257	0.43	0/339
All	All	0.36	0/224586	0.75	305/327945~(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
6	AA	0	2
15	DD	0	1
18	EE	0	1
21	\mathbf{FF}	0	1
24	Gg	0	1
28	II	0	1
41	PP	0	1
47	SS	0	1
51	UU	0	1
53	VV	0	1
57	XX	0	1
All	All	0	12

There are no bond length outliers.

The worst 5 of 305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
4	9	1116	С	N1-C2-O2	12.77	126.56	118.90
4	9	1116	С	C2-N1-C1'	11.82	131.81	118.80
4	9	501	С	N1-C2-O2	11.01	125.50	118.90
4	9	501	С	C2-N1-C1'	10.28	130.11	118.80
4	9	1116	С	N3-C2-O2	-10.12	114.81	121.90

There are no chirality outliers.



Mol	Chain	Res	Type	Group
6	AA	42	LYS	Peptide
6	AA	43	SER	Peptide
15	DD	153	VAL	Peptide
18	EE	132	GLY	Peptide
21	\mathbf{FF}	41	VAL	Peptide

5 of 12 planarity outliers are listed below:

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 PDB entries followed by that with respect to all EM entries.

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	Perce	ntiles
1	х	159/217~(73%)	151 (95%)	8 (5%)	0	100	100
5	А	245/257~(95%)	233~(95%)	12 (5%)	0	100	100
6	AA	215/295~(73%)	206 (96%)	9 (4%)	0	100	100
7	Aa	99/115~(86%)	89 (90%)	10 (10%)	0	100	100
8	В	392/403~(97%)	382 (97%)	10 (3%)	0	100	100
9	BB	211/264~(80%)	203 (96%)	8 (4%)	0	100	100
10	Bb	81/84~(96%)	78~(96%)	3 (4%)	0	100	100
11	С	355/413~(86%)	344 (97%)	11 (3%)	0	100	100
12	CC	219/293~(75%)	205 (94%)	14 (6%)	0	100	100
13	Cc	60/69~(87%)	57~(95%)	3 (5%)	0	100	100
14	D	287/297~(97%)	281 (98%)	6 (2%)	0	100	100
15	DD	226/243~(93%)	216 (96%)	10 (4%)	0	100	100
16	Dd	53/56~(95%)	48 (91%)	5 (9%)	0	100	100
17	Е	205/291~(70%)	197 (96%)	8 (4%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
18	EE	260/263~(99%)	244 (94%)	16 (6%)	0	100	100
19	Ee	53/133~(40%)	50 (94%)	3 (6%)	0	100	100
20	F	223/249~(90%)	216 (97%)	7 (3%)	0	100	100
21	FF	181/204~(89%)	162 (90%)	19 (10%)	0	100	100
22	G	211/266~(79%)	208 (99%)	3 (1%)	0	100	100
23	GG	235/249~(94%)	224 (95%)	11 (5%)	0	100	100
24	Gg	311/317~(98%)	281 (90%)	30 (10%)	0	100	100
25	Н	182/192~(95%)	179 (98%)	3 (2%)	0	100	100
26	HH	181/432~(42%)	173 (96%)	8 (4%)	0	100	100
27	Ι	198/214~(92%)	192 (97%)	6 (3%)	0	100	100
28	II	204/208~(98%)	185 (91%)	19 (9%)	0	100	100
29	J	166/178~(93%)	165 (99%)	1 (1%)	0	100	100
30	JJ	183/194~(94%)	180 (98%)	3 (2%)	0	100	100
32	KK	94/165~(57%)	86 (92%)	8 (8%)	0	100	100
33	L	203/211~(96%)	198 (98%)	4 (2%)	1 (0%)	29	35
34	LL	139/158~(88%)	131 (94%)	8 (6%)	0	100	100
35	М	133/218~(61%)	130 (98%)	3 (2%)	0	100	100
36	Ν	201/204~(98%)	195 (97%)	6 (3%)	0	100	100
37	NN	147/151~(97%)	138 (94%)	9 (6%)	0	100	100
38	Ο	197/203~(97%)	193 (98%)	4 (2%)	0	100	100
39	00	134/151~(89%)	123~(92%)	11 (8%)	0	100	100
40	Р	150/187~(80%)	147 (98%)	3 (2%)	0	100	100
41	PP	123/145~(85%)	118 (96%)	5 (4%)	0	100	100
42	Q	185/188~(98%)	177 (96%)	8 (4%)	0	100	100
43	QQ	140/146~(96%)	132 (94%)	8 (6%)	0	100	100
44	R	164/196~(84%)	162 (99%)	2 (1%)	0	100	100
45	RR	130/135~(96%)	121 (93%)	9 (7%)	0	100	100
46	S	$174/22\overline{4\ (78\%)}$	168 (97%)	6 (3%)	0	100	100
47	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
48	Т	156/160 (98%)	151 (97%)	5 (3%)	0	100	100
49	TT	139/145~(96%)	133 (96%)	6 (4%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
50	U	96/141~(68%)	93~(97%)	3 (3%)	0	100	100
51	UU	98/119~(82%)	94 (96%)	4 (4%)	0	100	100
52	V	128/140~(91%)	127~(99%)	1 (1%)	0	100	100
53	VV	81/83~(98%)	76 (94%)	5 (6%)	0	100	100
54	W	60/157~(38%)	59 (98%)	1 (2%)	0	100	100
55	WW	127/130~(98%)	118 (93%)	9 (7%)	0	100	100
56	Х	116/156~(74%)	115 (99%)	1 (1%)	0	100	100
57	XX	139/143~(97%)	132 (95%)	4 (3%)	3 (2%)	6	5
58	Y	130/145~(90%)	128 (98%)	2 (2%)	0	100	100
59	YY	122/133~(92%)	120 (98%)	2 (2%)	0	100	100
60	Z	133/136~(98%)	125 (94%)	8 (6%)	0	100	100
61	ZZ	73/124~(59%)	70 (96%)	3 (4%)	0	100	100
62	a	145/148~(98%)	137 (94%)	8 (6%)	0	100	100
63	b	94/245~(38%)	92 (98%)	2 (2%)	0	100	100
64	с	92/115~(80%)	91 (99%)	1 (1%)	0	100	100
65	d	104/125~(83%)	101 (97%)	3 (3%)	0	100	100
66	е	126/157~(80%)	122 (97%)	4 (3%)	0	100	100
67	f	107/110~(97%)	106 (99%)	1 (1%)	0	100	100
68	g	109/117~(93%)	107 (98%)	2 (2%)	0	100	100
69	h	119/123~(97%)	119 (100%)	0	0	100	100
70	i	99/105~(94%)	98 (99%)	1 (1%)	0	100	100
71	j	84/97~(87%)	83 (99%)	1 (1%)	0	100	100
72	k	66/70~(94%)	66 (100%)	0	0	100	100
73	1	48/51~(94%)	44 (92%)	4 (8%)	0	100	100
74	m	48/128 (38%)	47 (98%)	1 (2%)	0	100	100
75	n	23/25~(92%)	23 (100%)	0	0	100	100
76	0	100/106~(94%)	98 (98%)	2 (2%)	0	100	100
77	р	89/92~(97%)	87 (98%)	2 (2%)	0	100	100
78	r	121/137~(88%)	118 (98%)	3 (2%)	0	100	100
79	s	194/318~(61%)	185 (95%)	8 (4%)	1 (0%)	29	35
80	s1	14/109~(13%)	13 (93%)	1 (7%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
81	t	121/154~(79%)	117~(97%)	4 (3%)	0	100	100
82	v	711/858~(83%)	684 (96%)	27 (4%)	0	100	100
83	W	30/407~(7%)	28~(93%)	2 (7%)	0	100	100
All	All	12093/14939~(81%)	11610 (96%)	478 (4%)	5~(0%)	100	100

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All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	XX	62	PRO
57	XX	61	GLN
57	XX	86	PRO
79	s	118	PRO
33	L	62	PRO

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	х	146/195~(75%)	143~(98%)	3~(2%)	53 70
5	А	189/199~(95%)	187~(99%)	2(1%)	73 86
6	AA	180/245~(74%)	179~(99%)	1 (1%)	86 94
7	Aa	88/98~(90%)	87~(99%)	1 (1%)	73 86
8	В	342/348~(98%)	338~(99%)	4 (1%)	71 84
9	BB	194/231~(84%)	190 (98%)	4 (2%)	53 70
10	Bb	75/76~(99%)	75~(100%)	0	100 100
11	\mathbf{C}	298/336~(89%)	295~(99%)	3 (1%)	76 87
12	CC	187/224~(84%)	185~(99%)	2(1%)	73 86
13	\mathbf{Cc}	55/62~(89%)	52 (94%)	3~(6%)	21 30
14	D	245/250~(98%)	241 (98%)	4 (2%)	62 78
15	DD	190/202~(94%)	186 (98%)	4 (2%)	53 70



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
16	Dd	48/49~(98%)	46 (96%)	2(4%)	30	42
17	Ε	189/251~(75%)	187 (99%)	2(1%)	73	86
18	\mathbf{EE}	224/225~(100%)	221 (99%)	3 (1%)	69	82
19	Ee	46/106~(43%)	43 (94%)	3 (6%)	17	23
20	F	196/218~(90%)	196 (100%)	0	100	100
21	\mathbf{FF}	158/170~(93%)	152 (96%)	6 (4%)	33	47
22	G	188/224~(84%)	186 (99%)	2 (1%)	73	86
23	GG	207/218~(95%)	199 (96%)	8 (4%)	32	46
24	Gg	272/275~(99%)	268~(98%)	4 (2%)	65	79
25	Н	166/171~(97%)	165 (99%)	1 (1%)	86	94
26	HH	165/360~(46%)	164 (99%)	1 (1%)	86	94
27	Ι	172/181~(95%)	169 (98%)	3 (2%)	60	76
28	II	178/180~(99%)	173 (97%)	5 (3%)	43	60
29	J	141/149~(95%)	140 (99%)	1 (1%)	84	92
30	JJ	161/168~(96%)	158 (98%)	3 (2%)	57	73
32	KK	87/136~(64%)	86 (99%)	1 (1%)	73	86
33	L	170/176~(97%)	168 (99%)	2(1%)	71	84
34	LL	130/142~(92%)	128 (98%)	2(2%)	65	79
35	М	115/160~(72%)	115 (100%)	0	100	100
36	Ν	171/172~(99%)	169 (99%)	2(1%)	71	84
37	NN	130/131~(99%)	129 (99%)	1 (1%)	81	91
38	О	171/174~(98%)	168 (98%)	3 (2%)	59	75
39	00	106/119~(89%)	105 (99%)	1 (1%)	78	89
40	Р	133/165~(81%)	131 (98%)	2 (2%)	65	79
41	PP	111/130~(85%)	106 (96%)	5 (4%)	27	39
42	Q	164/165~(99%)	164 (100%)	0	100	100
43	QQ	$117/121 \ (97\%)$	115 (98%)	2 (2%)	60	76
44	R	147/175~(84%)	146 (99%)	1 (1%)	84	92
45	RR	119/121 (98%)	115 (97%)	4 (3%)	37	51
46	S	156/192~(81%)	153 (98%)	3 (2%)	57	73
47	SS	125/132~(95%)	122 (98%)	3 (2%)	49	66



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
48	Т	139/140~(99%)	137~(99%)	2 (1%)	67	81
49	TT	111/115~(96%)	108 (97%)	3 (3%)	44	61
50	U	88/127~(69%)	88 (100%)	0	100	100
51	UU	92/107~(86%)	92 (100%)	0	100	100
52	V	100/107~(94%)	100 (100%)	0	100	100
53	VV	67/67~(100%)	66 (98%)	1 (2%)	65	79
54	W	54/126~(43%)	54 (100%)	0	100	100
55	WW	112/113~(99%)	111 (99%)	1 (1%)	78	89
56	Х	106/133~(80%)	106 (100%)	0	100	100
57	XX	113/115~(98%)	112 (99%)	1 (1%)	78	89
58	Y	123/135~(91%)	119 (97%)	4 (3%)	38	53
59	YY	107/115~(93%)	105 (98%)	2 (2%)	57	73
60	Ζ	117/118~(99%)	117 (100%)	0	100	100
61	ZZ	66/102~(65%)	66 (100%)	0	100	100
62	a	119/120~(99%)	119 (100%)	0	100	100
63	b	80/184 (44%)	79~(99%)	1 (1%)	69	82
64	с	80/98~(82%)	80 (100%)	0	100	100
65	d	97/110~(88%)	97 (100%)	0	100	100
66	е	114/141 (81%)	114 (100%)	0	100	100
67	f	88/89~(99%)	88 (100%)	0	100	100
68	g	95/100~(95%)	94 (99%)	1 (1%)	73	86
69	h	109/110~(99%)	109 (100%)	0	100	100
70	i	85/89~(96%)	85 (100%)	0	100	100
71	j	73/80~(91%)	73 (100%)	0	100	100
72	k	63/65~(97%)	63 (100%)	0	100	100
73	1	47/48 (98%)	47 (100%)	0	100	100
74	m	46/115 (40%)	46 (100%)	0	100	100
75	n	24/24~(100%)	24 (100%)	0	100	100
76	0	90/94~(96%)	89 (99%)	1 (1%)	73	86
77	р	74/75~(99%)	74 (100%)	0	100	100
78	r	107/121~(88%)	106 (99%)	1 (1%)	78	89



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
79	S	163/258~(63%)	163 (100%)	0	100 100
80	s1	18/97~(19%)	17 (94%)	1 (6%)	21 29
81	t	105/128~(82%)	101 (96%)	4 (4%)	33 47
82	v	619/729~(85%)	610~(98%)	9(2%)	65 79
83	W	26/327~(8%)	26 (100%)	0	100 100
All	All	10569/12644~(84%)	10430 (99%)	139 (1%)	70 82

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
58	Y	55	VAL
59	YY	32	LYS
82	V	4	PHE
22	G	249	ARG
22	G	162	GLU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 119 such side chains are listed below:

Mol	Chain	Res	Type
38	0	180	GLN
79	s	39	GLN
50	U	44	GLN
78	r	95	HIS
83	W	206	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	5	3290/3740~(87%)	480 (14%)	38~(1%)
3	8	140/156~(89%)	14 (10%)	0
31	Κ	118/120~(98%)	7 (5%)	0
4	9	1670/1786~(93%)	387 (23%)	18 (1%)
All	All	5218/5802~(89%)	888 (17%)	56 (1%)

5 of 888 RNA backbone outliers are listed below:

Mol	Chain	Res	Type						
2	5	17	А						
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Mol	Chain	Res	Type
2	5	25	А
2	5	39	А
2	5	42	А
2	5	56	А

5 of 56 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	5	2506	А
4	9	1664	А
2	5	4888	G
4	9	1637	А
4	9	1137	U

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

138 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	Bos	Link	B	ond leng	gths	Bond angles		
WIOI	туре	Ullalli	nes	LIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	6MZ	9	1832	4	18,25,26	2.24	3 (16%)	16,36,39	1.53	1 (6%)
4	A2M	9	27	4	18,25,26	4.68	9 (50%)	18,36,39	2.69	4 (22%)
2	OMC	5	3705	2,84	19,22,23	3.31	8 (42%)	26,31,34	0.75	0
4	M7A	9	1806	4	20,25,26	2.04	3 (15%)	28,37,40	3.72	8 (28%)
2	OMG	5	1887	2	18,26,27	2.58	8 (44%)	19,38,41	1.54	4 (21%)
2	A2M	5	4575	2	18,25,26	4.50	7 (38%)	18,36,39	2.83	3 (16%)
4	B8Q	9	1219	4	17,22,23	2.92	4 (23%)	22,32,35	2.34	7 (31%)
4	E3C	9	568	4	18,23,24	<mark>3.37</mark>	6 (33%)	21,33,36	2.23	5 (23%)
2	PSU	5	4535	2	18,21,22	4.93	7 (38%)	22,30,33	1.81	5 (22%)
4	4AC	9	1842	4	21,24,25	<mark>3.13</mark>	10 (47%)	29,34,37	1.18	4 (13%)
2	5MC	5	3786	2	18,22,23	3.91	7 (38%)	26,32,35	1.03	2(7%)
2	A2M	5	3829	2	18,25,26	4.49	7 (38%)	18,36,39	2.79	3 (16%)



Mal	Turne	Chain	Dec	Link	B	ond leng	gths	B	Bond angles		
	туре	Chan	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	OMC	9	1710	4	19,22,23	2.94	7 (36%)	26,31,34	0.92	1 (3%)	
2	A2M	5	2367	2,84	18,25,26	4.49	7 (38%)	18,36,39	2.86	3 (16%)	
2	OMG	5	4374	2	18,26,27	2.58	8 (44%)	19,38,41	1.50	4 (21%)	
2	$5 \mathrm{MC}$	5	4451	2	18,22,23	3.93	7 (38%)	26,32,35	1.05	1 (3%)	
2	OMG	5	4200	2	18,26,27	2.58	8 (44%)	19,38,41	1.51	4 (21%)	
2	OMG	5	2054	2	18,26,27	2.56	8 (44%)	19,38,41	1.54	4 (21%)	
2	A2M	5	1330	2	18,25,26	4.44	7 (38%)	18,36,39	2.80	3 (16%)	
2	A2M	5	3789	2	18,25,26	4.36	8 (44%)	18,36,39	2.83	3 (16%)	
2	A2M	5	3727	2,70	18,25,26	4.51	7 (38%)	18,36,39	2.84	3 (16%)	
2	B8Q	5	1460	2	17,22,23	2.93	5 (29%)	22,32,35	2.08	4 (18%)	
2	2MG	5	1521	2	18,26,27	2.76	7 (38%)	16,38,41	1.48	4 (25%)	
2	A2M	5	3871	2	18,25,26	4.46	7 (38%)	18,36,39	2.78	3 (16%)	
2	B8H	5	4300	2	19,22,23	6.53	6 (31%)	22,32,35	2.34	5 (22%)	
2	OMU	5	4310	2	19,22,23	3.03	8 (42%)	26,31,34	1.71	5 (19%)	
2	PSU	5	2512	2	18,21,22	4.95	7 (38%)	22,30,33	1.88	5 (22%)	
2	OMG	5	1320	2	18,26,27	2.60	8 (44%)	19,38,41	1.58	5 (26%)	
2	B9H	5	2790	2	20,25,26	2.95	5 (25%)	22,35,38	1.47	3 (13%)	
4	OMC	9	174	4	19,22,23	2.95	7 (36%)	26,31,34	0.81	1 (3%)	
2	E6G	5	4359	2	20,27,28	2.04	3 (15%)	22,39,42	2.16	7 (31%)	
2	PSU	5	4640	$2,\!65$	18,21,22	4.96	7 (38%)	22,30,33	1.89	5 (22%)	
2	1MA	5	1326	2,84	16,25,26	4.04	4 (25%)	18,37,40	1.77	3 (16%)	
2	PSU	5	4407	2	18,21,22	4.92	7 (38%)	22,30,33	1.76	<mark>5 (22%)</mark>	
4	PSU	9	1081	4	18,21,22	1.06	1 (5%)	22,30,33	1.77	5 (22%)	
2	OMG	5	2777	2	18,26,27	2.60	8 (44%)	19,38,41	1.57	4 (21%)	
2	PSU	5	4504	2	18,21,22	4.95	7 (38%)	22,30,33	1.88	5 (22%)	
4	B8N	9	1248	4	24,29,30	2.79	6 (25%)	29,42,45	1.75	5 (17%)	
2	PSU	5	4297	2	18,21,22	4.91	7 (38%)	22,30,33	1.86	5 (22%)	
4	PSU	9	822	4	18,21,22	1.03	2 (11%)	22,30,33	1.93	5 (22%)	
2	PSU	5	3768	2	18,21,22	4.97	7 (38%)	22,30,33	1.71	<mark>6 (27%)</mark>	
4	OMG	9	683	4	18,26,27	2.48	8 (44%)	19,38,41	1.55	4 (21%)	
2	PSU	5	4446	2	18,21,22	4.95	7 (38%)	22,30,33	1.86	5 (22%)	
2	5MC	5	4339	2	18,22,23	3.92	7 (38%)	26,32,35	1.04	2 (7%)	
2	B8W	5	2384	2	18,26,27	2.03	2 (11%)	21,38,41	2.23	5 (23%)	
2	OMG	5	1629	2	18,26,27	2.59	8 (44%)	19,38,41	1.50	4 (21%)	
2	PSU	5	1586	2	18,21,22	4.95	7 (38%)	22,30,33	1.85	5 (22%)	



Mal	Turne	Chain	Dec	Tiple	В	ond leng	gths	B	Bond angles		
	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
2	OMC	5	2865	2	19,22,23	<mark>-3.33</mark>	8 (42%)	26,31,34	0.69	0	
2	OMG	5	4498	2	18,26,27	2.57	8 (44%)	19,38,41	1.51	4 (21%)	
2	OMC	5	4540	2	19,22,23	3.34	8 (42%)	26,31,34	0.74	0	
2	UR3	5	4534	2	19,22,23	3.20	7 (36%)	26,32,35	1.31	3 (11%)	
2	E7G	5	1801	2	24,27,28	3.87	11 (45%)	30,40,43	2.22	10 (33%)	
2	OMG	5	4641	2	18,26,27	2.57	8 (44%)	19,38,41	1.55	4 (21%)	
4	5MC	9	1374	4	18,22,23	<mark>3.69</mark>	7 (38%)	26,32,35	1.34	4 (15%)	
2	PSU	5	1687	2	18,21,22	4.91	7 (38%)	22,30,33	1.84	5 (22%)	
2	B8W	5	4533	2,84	18,26,27	2.00	2 (11%)	21,38,41	2.55	7 (33%)	
2	OMG	5	3796	2	18,26,27	2.57	8 (44%)	19,38,41	1.51	4 (21%)	
2	PSU	5	4632	2	18,21,22	4.90	7 (38%)	22,30,33	1.93	5 (22%)	
4	OMC	9	1703	4	19,22,23	2.94	7 (36%)	26,31,34	0.83	1 (3%)	
4	PSU	9	1243	4	18,21,22	1.06	1 (5%)	22,30,33	1.83	4 (18%)	
2	P7G	5	1913	2	24,28,29	4.23	11 (45%)	27,41,44	1.56	3 (11%)	
2	B9B	5	237	2	21,28,29	1.99	3 (14%)	23,40,43	1.91	5 (21%)	
4	PSU	9	612	4	18,21,22	0.99	1 (5%)	22,30,33	1.74	4 (18%)	
2	2MG	5	729	2	18,26,27	2.75	6 (33%)	16,38,41	1.36	3 (18%)	
2	B8W	5	4476	2	18,26,27	2.03	2 (11%)	21,38,41	2.78	8 (38%)	
2	OMG	5	4627	2	18,26,27	2.58	8 (44%)	19,38,41	1.56	4 (21%)	
2	B8K	5	4694	2	24,28,29	<mark>3.38</mark>	11 (45%)	30,42,45	2.33	11 (36%)	
4	UR3	9	1830	4	19,22,23	2.69	<mark>6 (31%)</mark>	26,32,35	1.57	4 (15%)	
4	MA6	9	1850	4	18,26,27	1.02	1 (5%)	19,38,41	2.74	2 (10%)	
4	OMU	9	116	4	19,22,23	2.88	7 (36%)	26,31,34	1.75	5 (19%)	
4	MA6	9	1851	4	18,26,27	0.98	1 (5%)	19,38,41	2.62	2 (10%)	
4	PSU	9	119	4	18,21,22	0.94	1 (5%)	22,30,33	1.60	5 (22%)	
2	UR3	5	4601	2	19,22,23	3.21	7 (36%)	26,32,35	1.29	2 (7%)	
4	A2M	9	668	4	18,25,26	4.68	8 (44%)	18,36,39	2.70	5 (27%)	
2	5MU	5	4087	2	19,22,23	4.98	7 (36%)	28,32,35	3.62	9 (32%)	
2	A2M	5	1538	2,84	18,25,26	4.49	7 (38%)	18,36,39	2.89	3 (16%)	
2	B8T	5	4487	2	19,22,23	3.25	8 (42%)	26,31,34	0.85	1 (3%)	
2	A2M	5	2405	2,84	18,25,26	4.48	7 (38%)	18,36,39	2.84	3 (16%)	
4	A2M	9	1031	4	18,25,26	4.75	8 (44%)	18,36,39	2.78	4 (22%)	
2	OMC	5	3913	2	19,22,23	3.34	8 (42%)	26,31,34	0.71	0	
4	A2M	9	1678	4	18,25,26	4.81	9 (50%)	18,36,39	2.59	3 (16%)	
2	OMG	5	1526	2	18,26,27	2.58	8 (44%)	19,38,41	1.51	4 (21%)	



Mal	Tune	Chain	Dec	Link	B	ond leng	gths	Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	PSU	5	3733	2	18,21,22	4.95	7 (38%)	22,30,33	1.82	5 (22%)
2	OMC	5	2808	2	19,22,23	<mark>3.33</mark>	8 (42%)	26,31,34	0.71	0
2	6MZ	5	4224	2	18,25,26	2.19	3 (16%)	16,36,39	2.05	4 (25%)
4	4AC	9	1337	4	21,24,25	<mark>3.19</mark>	9 (42%)	29,34,37	1.23	3 (10%)
2	P7G	5	3884	2	24,28,29	4.14	11 (45%)	27,41,44	1.60	3 (11%)
2	2MG	5	4876	2	18,26,27	2.72	7 (38%)	16,38,41	1.55	4 (25%)
2	A2M	5	3722	2	18,25,26	4.49	7 (38%)	18,36,39	2.85	3 (16%)
2	A2M	5	1875	2,84	18,25,26	4.51	7 (38%)	18,36,39	2.87	3 (16%)
2	B8K	5	3901	2	24,28,29	3.30	11 (45%)	30,42,45	2.28	11 (36%)
2	PSU	5	1681	2	18,21,22	4.95	8 (44%)	22,30,33	1.88	5 (22%)
2	PSU	5	3719	2	18,21,22	4.94	7 (38%)	22,30,33	1.86	5 (22%)
82	DDE	v	715	82	14,20,21	1.02	1 (7%)	14,28,30	1.09	1 (7%)
2	OMG	5	373	2	18,26,27	2.55	8 (44%)	19,38,41	1.56	4 (21%)
2	7MG	5	1609	2	22,26,27	<mark>3.92</mark>	10 (45%)	29,39,42	2.03	9 (31%)
4	PSU	9	823	4	18,21,22	1.09	1 (5%)	22,30,33	1.83	4 (18%)
2	1MA	5	4419	2	16,25,26	4.01	4 (25%)	18,37,40	1.71	3 (16%)
2	7MG	5	2526	2	22,26,27	3.92	10 (45%)	29,39,42	2.04	9 (31%)
2	B8H	5	1864	2	19,22,23	6.50	6 (31%)	22,32,35	2.35	5 (22%)
4	A2M	9	159	4	18,25,26	4.83	9 (50%)	18,36,39	2.75	4 (22%)
4	A2M	9	484	4	18,25,26	4.71	9 (50%)	18,36,39	2.71	3 (16%)
2	A2M	5	398	2	18,25,26	4.49	7 (38%)	18,36,39	2.86	3 (16%)
2	MHG	5	4375	2	29,32,33	3.95	11 (37%)	34,46,49	2.29	10 (29%)
2	M7A	5	4568	2	20,25,26	2.02	3 (15%)	28,37,40	3.67	8 (28%)
2	OMC	5	2369	2	19,22,23	3.34	8 (42%)	26,31,34	0.75	0
11	MLZ	С	333	11	8,9,10	0.77	0	4,9,11	0.67	0
4	OMU	9	121	4	19,22,23	2.96	8 (42%)	26,31,34	1.77	5 (19%)
2	OMG	5	4874	2	18,26,27	2.59	8 (44%)	19,38,41	1.53	4 (21%)
2	P4U	5	1352	2	21,24,25	4.09	7 (33%)	27,33,36	0.98	1 (3%)
2	OMC	5	2426	2,40,84	19,22,23	<mark>3.35</mark>	8 (42%)	26,31,34	0.76	0
2	7MG	5	4554	2	22,26,27	3.95	10 (45%)	29,39,42	1.99	9 (31%)
74	MLZ	m	72	74	8,9,10	0.76	0	4,9,11	0.64	0
4	5MU	9	814	4	19,22,23	4.87	7 (36%)	28,32,35	<mark>3.59</mark>	12 (42%)
4	OMG	9	509	4	18,26,27	2.46	8 (44%)	19,38,41	1.46	4 (21%)
2	B8T	5	4675	2	19,22,23	3.25	8 (42%)	26,31,34	0.91	1 (3%)
2	OMC	5	3891	2	19,22,23	3.34	8 (42%)	26,31,34	0.72	0



Mal	Trune	Chain	Dec	Tinle	B	ond leng	gths	E	Bond ang	gles
IVIOI	Type	Chain	Res	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
81	5CT	t	51	81	13,14,15	0.66	0	9,15,17	1.20	1 (11%)
2	OMC	5	3873	2	19,22,23	<mark>3.34</mark>	8 (42%)	26,31,34	0.74	0
2	BGH	5	3903	2,84	25,29,30	4.62	18 (72%)	31,43,46	2.35	12 (38%)
2	OMU	5	4624	2,52	19,22,23	3.00	8 (42%)	26,31,34	1.69	5 (19%)
4	A2M	9	166	4	18,25,26	4.79	9 (50%)	18,36,39	2.78	4 (22%)
2	B8W	5	4133	2	18,26,27	2.06	2 (11%)	21,38,41	2.34	6 (28%)
4	OMC	9	517	4	19,22,23	2.84	7 (36%)	26,31,34	0.64	0
2	B8W	5	4189	2	18,26,27	2.04	2 (11%)	21,38,41	2.43	6 (28%)
2	OMG	5	2428	2	18,26,27	2.58	8 (44%)	19,38,41	1.48	4 (21%)
2	PSU	5	4454	2,84	18,21,22	4.95	7 (38%)	22,30,33	1.84	5 (22%)
2	B9B	5	2758	2,84	21,28,29	1.98	3 (14%)	23,40,43	1.87	4 (17%)
2	I4U	5	4198	2	21,24,25	3.61	8 (38%)	27,34,37	1.00	1 (3%)
4	OMG	9	644	4	18,26,27	2.47	8 (44%)	19,38,41	1.52	4 (21%)
3	OMU	8	14	2,3	19,22,23	3.00	8 (42%)	26,31,34	1.69	4 (15%)
2	B9B	5	1578	2	21,28,29	1.98	3 (14%)	23,40,43	1.85	5 (21%)
2	UR3	5	1870	2	19,22,23	3.20	7 (36%)	26,32,35	1.27	3 (11%)
2	A2M	5	4527	2,84	18,25,26	4.50	7 (38%)	18,36,39	2.81	3 (16%)
2	E7G	5	2301	2	24,27,28	<mark>3.86</mark>	11 (45%)	30,40,43	2.24	10 (33%)
2	I4U	5	1663	2	21,24,25	<mark>3.63</mark>	9 (42%)	27,34,37	0.95	1 (3%)
2	OMG	5	2368	2	18,26,27	2.57	8 (44%)	19,38,41	1.55	4 (21%)
2	A2M	5	1528	2	18,25,26	4.47	7 (38%)	18,36,39	2.87	3 (16%)

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
4	6MZ	9	1832	4	-	2/5/27/28	0/3/3/3
4	A2M	9	27	4	-	0/5/27/28	0/3/3/3
2	OMC	5	3705	2,84	-	4/9/27/28	0/2/2/2
4	M7A	9	1806	4	-	0/7/37/38	0/3/3/3
2	OMG	5	1887	2	-	0/5/27/28	0/3/3/3
2	A2M	5	4575	2	-	0/5/27/28	0/3/3/3
4	B8Q	9	1219	4	-	0/7/42/43	0/2/2/2
4	E3C	9	568	4	-	4/9/44/45	0/2/2/2
2	PSU	5	4535	2	-	2/7/25/26	0/2/2/2



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10101	$\frac{1}{4AC}$		18/12		Cimais	0/11/20/30	0/2/2/2
4 2	5MC	5	3786	4 2	_	$\frac{0/11/23/30}{0/7/25/26}$	0/2/2/2
2	A2M	5	3829	2	_	$\frac{0/1/20/20}{0/5/27/28}$	0/2/2/2 0/3/3/3
4	OMC	9	1710	4	_	$\frac{0/9/27/28}{0/9/27/28}$	0/2/2/2
2	A2M	5	2367	2.84	-	$\frac{3}{1/5/27/28}$	0/3/3/3
2	OMG	5	4374	2	-	0/5/27/28	0/3/3/3
2	5MC	5	4451	2	_	4/7/25/26	0/2/2/2
2	OMG	5	4200	2	-	0/5/27/28	0/3/3/3
2	OMG	5	2054	2	-	0/5/27/28	0/3/3/3
2	A2M	5	1330	2	-	1/5/27/28	0/3/3/3
2	A2M	5	3789	2	-	2/5/27/28	0/3/3/3
2	A2M	5	3727	2,70	-	1/5/27/28	0/3/3/3
2	B8Q	5	1460	2	-	0/7/42/43	0/2/2/2
2	2MG	5	1521	2	-	0/5/27/28	0/3/3/3
2	A2M	5	3871	2	-	3/5/27/28	0/3/3/3
2	B8H	5	4300	2	-	0/7/25/26	0/2/2/2
2	OMU	5	4310	2	-	0/9/27/28	0/2/2/2
2	PSU	5	2512	2	-	0/7/25/26	0/2/2/2
2	OMG	5	1320	2	-	0/5/27/28	0/3/3/3
2	B9H	5	2790	2	-	1/12/47/48	0/2/2/2
4	OMC	9	174	4	-	0/9/27/28	0/2/2/2
2	E6G	5	4359	2	-	2/6/28/29	0/3/3/3
2	PSU	5	4640	$2,\!65$	-	3/7/25/26	0/2/2/2
2	1MA	5	1326	2,84	-	0/3/25/26	0/3/3/3
2	PSU	5	4407	2	-	2/7/25/26	0/2/2/2
4	PSU	9	1081	4	-	3/7/25/26	0/2/2/2
2	OMG	5	2777	2	-	1/5/27/28	0/3/3/3
2	PSU	5	4504	2	-	3/7/25/26	0/2/2/2
4	B8N	9	1248	4	-	3/16/34/35	0/2/2/2
2	PSU	5	4297	2	-	2/7/25/26	0/2/2/2
4	PSU	9	822	4	-	2/7/25/26	0/2/2/2
2	PSU	5	3768	2	-	4/7/25/26	0/2/2/2
4	OMG	9	683	4	-	2/5/27/28	0/3/3/3
2	PSU	5	4446	2	-	0/7/25/26	0/2/2/2
2	5MC	5	4339	2	-	0/7/25/26	0/2/2/2
2	B8W	5	2384	2	-	4/5/27/28	0/3/3/3
2	OMG	5	1629	2	-	0/5/27/28	0/3/3/3
2	PSU	5	1586	2	-	0/7/25/26	0/2/2/2
2	OMC	5	2865	2	-	0/9/27/28	0/2/2/2



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	5	4498	2	-	0/5/27/28	0/3/3/3
2	OMC	5	4540	2	-	0/9/27/28	0/2/2/2
2	UR3	5	4534	2	-	2/7/25/26	0/2/2/2
2	E7G	5	1801	2	-	2/9/39/40	0/3/3/3
2	OMG	5	4641	2	-	3/5/27/28	0/3/3/3
4	5MC	9	1374	4	-	0/7/25/26	0/2/2/2
2	PSU	5	1687	2	-	0/7/25/26	0/2/2/2
2	B8W	5	4533	2,84	-	2/5/27/28	0/3/3/3
2	OMG	5	3796	2	-	2/5/27/28	0/3/3/3
2	PSU	5	4632	2	-	0/7/25/26	0/2/2/2
4	OMC	9	1703	4	-	2/9/27/28	0/2/2/2
4	PSU	9	1243	4	-	2/7/25/26	0/2/2/2
2	P7G	5	1913	2	-	2/10/40/41	0/3/3/3
2	B9B	5	237	2	-	2/7/29/30	0/3/3/3
4	PSU	9	612	4	-	0/7/25/26	0/2/2/2
2	2MG	5	729	2	-	1/5/27/28	0/3/3/3
2	B8W	5	4476	2	-	2/5/27/28	0/3/3/3
2	OMG	5	4627	2	-	0/5/27/28	0/3/3/3
2	B8K	5	4694	2	-	0/11/41/42	0/3/3/3
4	UR3	9	1830	4	-	4/7/25/26	0/2/2/2
4	MA6	9	1850	4	-	1/7/29/30	0/3/3/3
4	OMU	9	116	4	-	3/9/27/28	0/2/2/2
4	MA6	9	1851	4	-	3/7/29/30	0/3/3/3
4	PSU	9	119	4	-	2/7/25/26	0/2/2/2
2	UR3	5	4601	2	-	0/7/25/26	0/2/2/2
4	A2M	9	668	4	-	4/5/27/28	0/3/3/3
2	5MU	5	4087	2	-	0/7/25/26	0/2/2/2
2	A2M	5	1538	2,84	-	2/5/27/28	0/3/3/3
2	B8T	5	4487	2	-	0/7/27/28	0/2/2/2
2	A2M	5	2405	2,84	-	2/5/27/28	0/3/3/3
4	A2M	9	1031	4	-	0/5/27/28	0/3/3/3
2	OMC	5	3913	2	-	0/9/27/28	0/2/2/2
4	A2M	9	1678	4	-	0/5/27/28	0/3/3/3
2^{-}	OMG	5	1526	2	-	$0/5/27\overline{/28}$	0/3/3/3
2	PSU	5	3733	2	-	2/7/25/26	0/2/2/2
2	OMC	5	2808	2	-	$0/\overline{9/27/28}$	0/2/2/2
2	6MZ	5	4224	2	-	0/5/27/28	0/3/3/3
4	4AC	9	1337	4	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P7G	5	3884	2	-	2/10/40/41	0/3/3/3
2	2MG	5	4876	2	-	0/5/27/28	0/3/3/3
2	A2M	5	3722	2	-	0/5/27/28	0/3/3/3
2	A2M	5	1875	2,84	-	0/5/27/28	0/3/3/3
2	B8K	5	3901	2	-	3/11/41/42	0/3/3/3
2	PSU	5	1681	2	-	2/7/25/26	0/2/2/2
2	PSU	5	3719	2	-	0/7/25/26	0/2/2/2
82	DDE	V	715	82	-	16/20/21/23	0/1/1/1
2	OMG	5	373	2	-	1/5/27/28	0/3/3/3
2	7MG	5	1609	2	-	0/7/37/38	0/3/3/3
4	PSU	9	823	4	-	0/7/25/26	0/2/2/2
2	1MA	5	4419	2	-	2/3/25/26	0/3/3/3
2	7MG	5	2526	2	-	0/7/37/38	0/3/3/3
2	B8H	5	1864	2	-	0/7/25/26	0/2/2/2
4	A2M	9	159	4	-	3/5/27/28	0/3/3/3
4	A2M	9	484	4	-	0/5/27/28	0/3/3/3
2	A2M	5	398	2	-	2/5/27/28	0/3/3/3
2	MHG	5	4375	2	-	7/16/46/47	0/3/3/3
2	M7A	5	4568	2	-	0/7/37/38	0/3/3/3
2	OMC	5	2369	2	-	0/9/27/28	0/2/2/2
11	MLZ	С	333	11	-	0/7/8/10	-
4	OMU	9	121	4	-	2/9/27/28	0/2/2/2
2	OMG	5	4874	2	-	4/5/27/28	0/3/3/3
2	P4U	5	1352	2	-	3/10/29/30	0/2/2/2
2	OMC	5	2426	2,40,84	-	1/9/27/28	0/2/2/2
2	7MG	5	4554	2	-	0/7/37/38	0/3/3/3
74	MLZ	m	72	74	-	0/7/8/10	-
4	$5 \mathrm{MU}$	9	814	4	-	0/7/25/26	0/2/2/2
4	OMG	9	509	4	-	0/5/27/28	0/3/3/3
2	B8T	5	4675	2	-	1/7/27/28	0/2/2/2
2	OMC	5	3891	2	-	0/9/27/28	0/2/2/2
81	$5\mathrm{CT}$	\mathbf{t}	51	81	-	5/13/14/16	-
2	OMC	5	3873	2	-	0/9/27/28	0/2/2/2
2	BGH	5	3903	2,84	-	2/13/43/44	0/3/3/3
2	OMU	5	4624	2,52	-	1/9/27/28	0/2/2/2
4	A2M	9	166	4	-	2/5/27/28	0/3/3/3
2	B8W	5	4133	2	-	2/5/27/28	0/3/3/3
4	OMC	9	517	4	-	2/9/27/28	0/2/2/2



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8W	5	4189	2	-	2/5/27/28	0/3/3/3
2	OMG	5	2428	2	-	2/5/27/28	0/3/3/3
2	PSU	5	4454	2,84	-	3/7/25/26	0/2/2/2
2	B9B	5	2758	2,84	-	2/7/29/30	0/3/3/3
2	I4U	5	4198	2	-	2/9/29/30	0/2/2/2
4	OMG	9	644	4	-	1/5/27/28	0/3/3/3
3	OMU	8	14	2,3	-	1/9/27/28	0/2/2/2
2	B9B	5	1578	2	-	2/7/29/30	0/3/3/3
2	UR3	5	1870	2	-	0/7/25/26	0/2/2/2
2	A2M	5	4527	2,84	-	3/5/27/28	0/3/3/3
2	E7G	5	2301	2	-	1/9/39/40	0/3/3/3
2	I4U	5	1663	2	-	1/9/29/30	0/2/2/2
2	OMG	5	2368	2	-	2/5/27/28	0/3/3/3
2	A2M	5	1528	2	-	1/5/27/28	0/3/3/3

The worst 5 of 920 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
4	9	166	A2M	O4'-C1'	16.42	1.64	1.41
4	9	159	A2M	O4'-C1'	16.40	1.64	1.41
4	9	1678	A2M	O4'-C1'	16.34	1.63	1.41
2	5	1875	A2M	O4'-C1'	16.24	1.63	1.41
2	5	4527	A2M	O4'-C1'	16.22	1.63	1.41

The worst 5 of 558 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	9	1806	M7A	C5-C6-N6	12.77	145.55	123.74
2	5	4568	M7A	C5-C6-N6	12.30	144.75	123.74
2	5	4087	5MU	C5-C4-N3	12.06	125.61	115.31
4	9	814	5MU	C5-C4-N3	11.64	125.25	115.31
4	9	1806	M7A	N6-C6-N1	-10.95	94.37	118.35

There are no chirality outliers.

5 of 187 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	8	14	OMU	C1'-C2'-O2'-CM2
81	t	51	5CT	NZ-C1-C2-C3
2	5	237	B9B	C5-C6-O6-C61



Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	5	237	B9B	N1-C6-O6-C61
2	5	1352	P4U	N3-C4-O4-C41

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 208 ligands modelled in this entry, 208 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
4	9	12
2	5	11

The worst 5 of 23 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1223:G	O3'	1237:G	Р	24.58



	• -					
Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	9	834:C	O3'	841:G	Р	17.65
1	9	697:G	O3'	729:C	Р	17.13
1	9	756:C	O3'	788:G	Р	17.02
1	5	994:U	O3'	1068:G	Р	16.68



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13114. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

This section was not generated.

6.2 Central slices (i)

This section was not generated.

6.3 Largest variance slices (i)

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

6.5 Orthogonal surface views (i)

This section was not generated.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)

This section was not generated.

7.2 Volume estimate versus contour level (i)

This section was not generated.

7.3 Rotationally averaged power spectrum (i)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section was not generated.

