



Full wwPDB EM Validation Report ⓘ

Feb 27, 2023 – 05:28 pm GMT

PDB ID : 8AGU
EMDB ID : EMD-15424
Title : Yeast RQC complex in state E
Authors : Tesina, P.; Buschauer, R.; Beckmann, R.
Deposited on : 2022-07-20
Resolution : 2.70 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

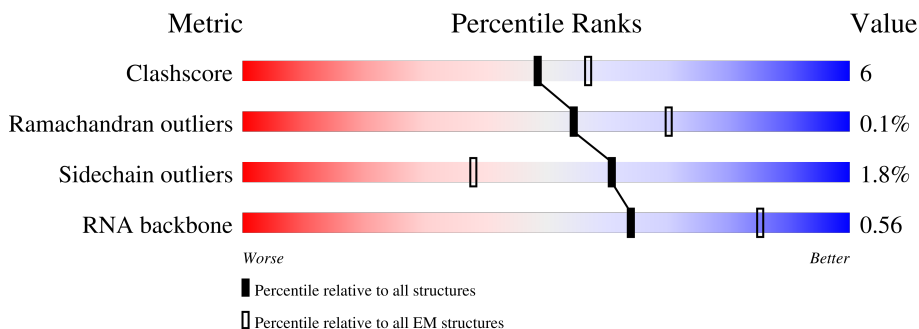
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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






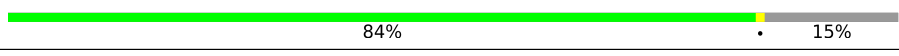
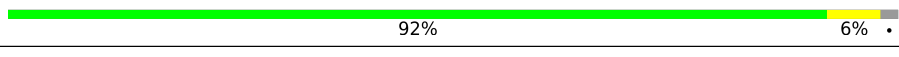
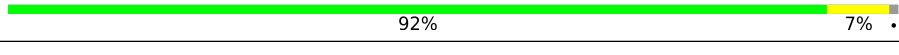
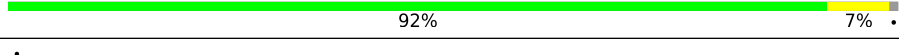

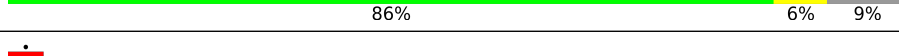
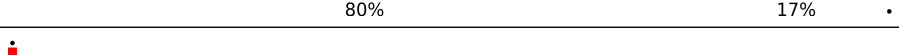
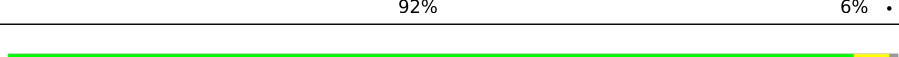
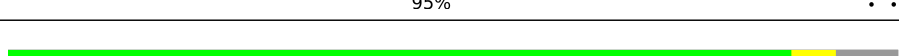

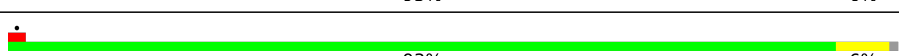
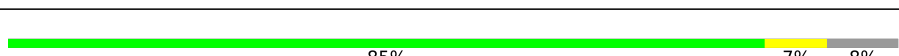
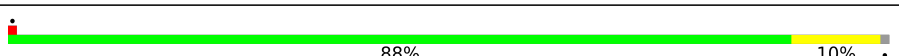
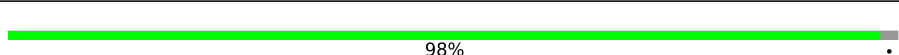

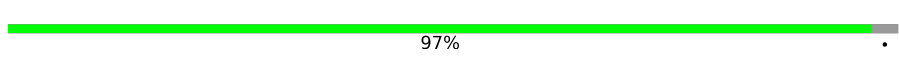
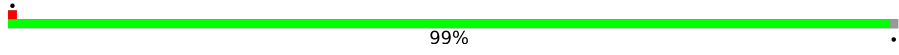

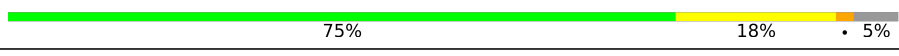

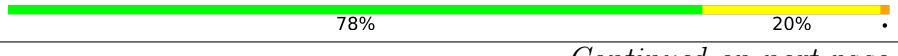

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	204	91% 8%
2	B	199	87% 12% ..
3	C	184	88% 12% .
4	D	186	92% 8% .
5	E	189	76% 6% 17%
6	F	172	87% 12% .
7	G	160	90% 9% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	121	 74% 9% 17%
9	I	137	 88% 11%
10	J	155	 37% 59%
11	K	142	 84% 15%
12	L	127	 92% 6%
13	M	136	 92% 7%
14	N	149	 92% 7%
15	O	59	 83% 12%
16	P	105	 86% 6% 9%
17	Q	113	 80% 17%
18	R	130	 92% 6%
19	S	107	 95%
20	T	121	 88% 5% 7%
21	U	120	 93% 6%
22	V	100	 93% 6%
23	W	88	 85% 7% 8%
24	X	78	 88% 10%
25	Y	51	 98%
26	Z	128	 41% 59%
27	b	106	 97%
28	c	92	 99%
29	d	25	 16% 88% 12%
30	f	3395	 75% 18% 5%
31	h	121	 85% 15%
32	i	158	 78% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	j	254	96%
34	k	387	99%
35	l	362	99%
36	m	297	98%
37	n	176	94% 5%
38	o	244	91% 9%
39	p	256	89% 9%
40	q	191	98%
41	r	221	98%
42	s	174	95%
43	t	199	96%
44	u	138	97%
45	a	1038	14% 78% 18%
46	e	1562	68% 93% 5%
47	g	245	51% 91% 8%
48	v	157	87% 10%
49	w	217	99%
50	y	76	61% 36%
51	z	165	89% 10%
52	0	312	31% 7% 61%
53	1	18	94% 6%

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 149748 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 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	203	1720	1077	361	281	1	0	0

- Molecule 2 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	197	1555	1003	289	262	1	197	0

- Molecule 3 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	183	1416	879	284	253	0	0

- Molecule 4 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	185	1441	908	290	241	2	0	0

- Molecule 5 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	156	1258	781	265	212	0	0

- Molecule 6 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	171	1437	925	266	243	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	159	1272	802	245	221	4	0	0

- Molecule 8 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	100	796	516	131	149	0	0

- Molecule 9 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	136	1003	628	189	179	7	0	0

- Molecule 10 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	63	518	333	102	82	1	0	0

- Molecule 11 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	121	964	620	169	173	2	0	0

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	L	125	984	620	191	173	0	0

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	M	135	1080	701	199	180	0	0

- Molecule 14 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	148	1169	747	231	188	3	0	0

- Molecule 15 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	58	462	289	100	73		0	0

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	P	96	737	476	123	137	1	0	0

- Molecule 17 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Q	109	876	556	167	152	1	0	0

- Molecule 18 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	R	127	1013	642	205	165	1	0	0

- Molecule 19 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	S	106	850	540	165	144	1	0	0

- Molecule 20 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	T	112	880	545	179	152	4	0	0

- Molecule 21 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 23 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 24 is a protein called BJ4_G0032190.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 25 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 26 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 27 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	91	694	429	138	121	6	0	0

- Molecule 29 is a protein called RPL41A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	22	207	127	56	23	1	0	0

- Molecule 30 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	f	3216	68782	30723	12389	22454	3216	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	h	121	2579	1152	461	845	121	0	0

- Molecule 32 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
32	i	158	3353	1500	586	1109	158	0	0

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	j	246	1874	1168	380	325	1	0	0

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	386	3075	1950	584	533	8	0	0

- Molecule 35 is a protein called BJ4_G0008850.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 37 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	n	167	Total	C	N	O	0	0
			1307	843	234	230		

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 42 is a protein called BJ4_G0027750.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	s	169	1346	843	252	247	4	0	0

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	t	193	1543	962	315	266		0	0

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	u	136	1053	675	199	177	2	0	0

- Molecule 45 is a protein called RQC2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	a	848	6569	4188	1138	1226	17	0	0

- Molecule 46 is a protein called E3 ubiquitin-protein ligase listerin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	e	1527	11509	7353	1937	2181	38	0	0

- Molecule 47 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	g	225	1651	1030	282	332	7	0	0

- Molecule 48 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	v	142	1085	676	183	217	9	0	0

- Molecule 49 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	w	216	1709	1092	298	310	9	0	0

- Molecule 50 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
50	y	73	1556	692	273	518	73	0	0

- Molecule 51 is a protein called 60S ribosomal protein L12-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	z	148	728	432	148	148	0	0

- Molecule 52 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	0	121	961	618	167	173	3	0	0

- Molecule 53 is a protein called CAT-tailed nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	1	17	85	51	17	17	0	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	1	Total	Mg	0
			1	1	
54	C	1	Total	Mg	0
			1	1	
54	E	1	Total	Mg	0
			1	1	
54	I	1	Total	Mg	0
			1	1	
54	R	1	Total	Mg	0
			1	1	
54	T	1	Total	Mg	0
			1	1	

Continued on next page...

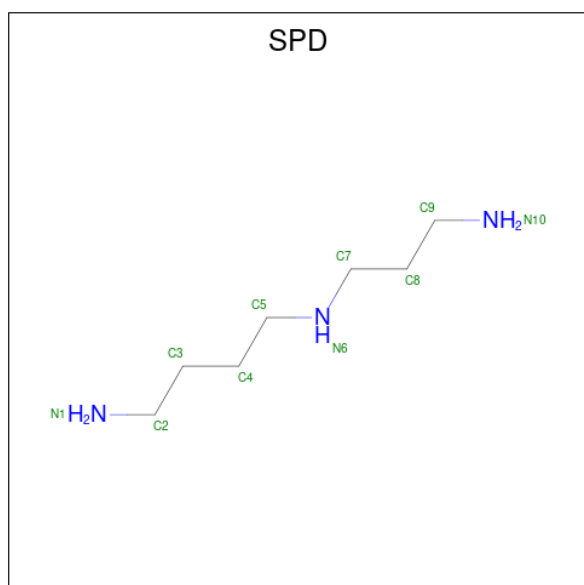
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
54	f	3	Total 3	Mg 3	0
54	h	1	Total 1	Mg 1	0
54	j	2	Total 2	Mg 2	0
54	k	1	Total 1	Mg 1	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total 1	Zn 1	0
55	W	1	Total 1	Zn 1	0
55	Z	1	Total 1	Zn 1	0
55	b	1	Total 1	Zn 1	0
55	c	1	Total 1	Zn 1	0
55	e	2	Total 2	Zn 2	0

- Molecule 56 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).

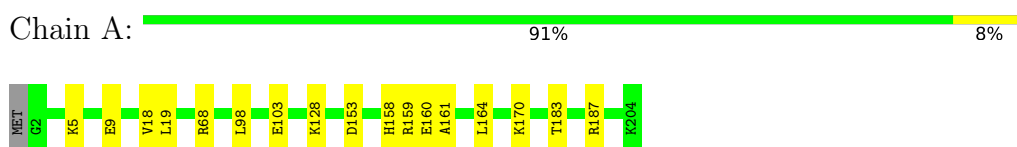


Mol	Chain	Residues	Atoms			AltConf
56	f	1	Total	C	N	0
			10	7	3	

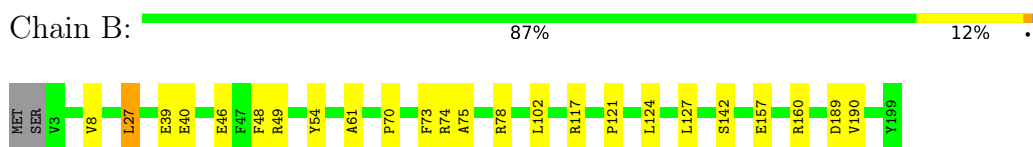
3 Residue-property plots [i](#)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

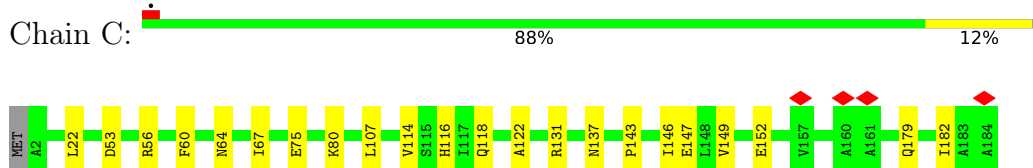
- Molecule 1: 60S ribosomal protein L15-A



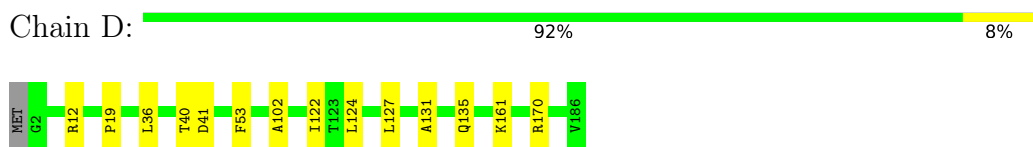
- Molecule 2: 60S ribosomal protein L16-A



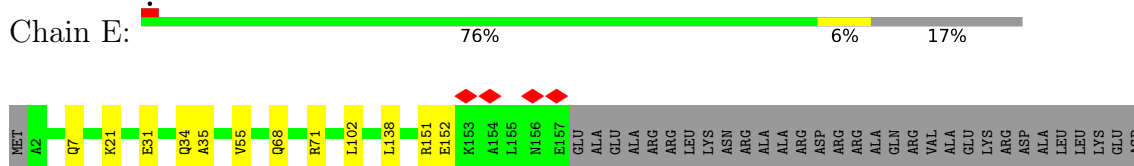
- Molecule 3: 60S ribosomal protein L17-A



- Molecule 4: 60S ribosomal protein L18-A

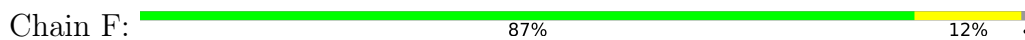


- Molecule 5: 60S ribosomal protein L19-A

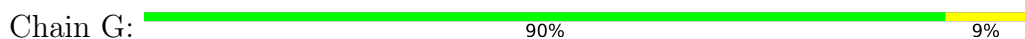


ALA

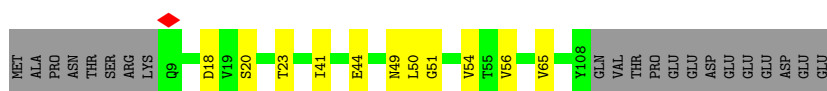
• Molecule 6: 60S ribosomal protein L20-A



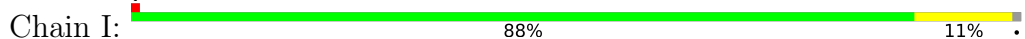
• Molecule 7: 60S ribosomal protein L21-A



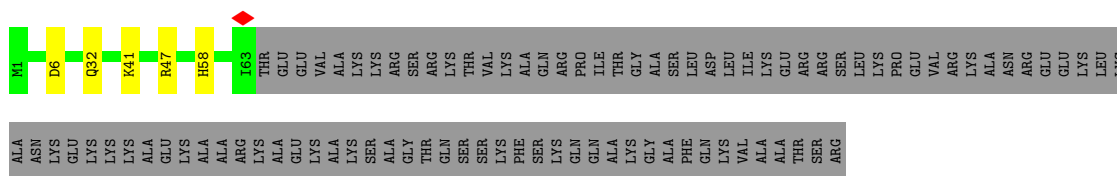
• Molecule 8: 60S ribosomal protein L22-A



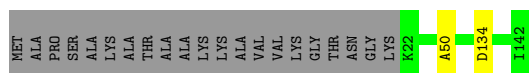
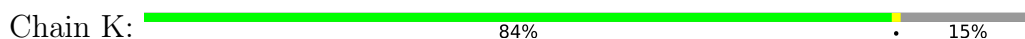
• Molecule 9: 60S ribosomal protein L23-A



• Molecule 10: 60S ribosomal protein L24-A



• Molecule 11: 60S ribosomal protein L25



• Molecule 12: 60S ribosomal protein L26-A

Chain L:  92% 6%



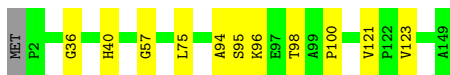
- Molecule 13: 60S ribosomal protein L27-A

Chain M:  92% 7%




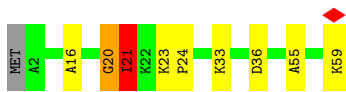
- Molecule 14: 60S ribosomal protein L28

Chain N:  92% 7%




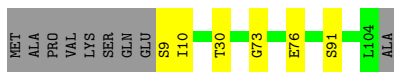
- Molecule 15: 60S ribosomal protein L29

Chain O:  83% 12%




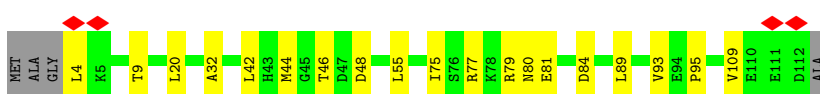
- Molecule 16: 60S ribosomal protein L30

Chain P:  86% 6% 9%



- Molecule 17: 60S ribosomal protein L31-A

Chain Q:  80% 17%



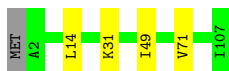
- Molecule 18: 60S ribosomal protein L32

Chain R:  92% 6%




- Molecule 19: 60S ribosomal protein L33-A

Chain S:  95%



- Molecule 20: 60S ribosomal protein L34-A

Chain T:  88% 5% 7%



- Molecule 21: 60S ribosomal protein L35-A

Chain U:  93% 6%




- Molecule 22: 60S ribosomal protein L36-A

Chain V:  93% 6%




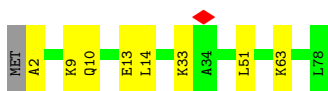
- Molecule 23: 60S ribosomal protein L37-A

Chain W:  85% 7% 8%



- Molecule 24: BJ4_G0032190.mRNA.1.CDS.1

Chain X:  88% 10%

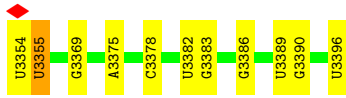
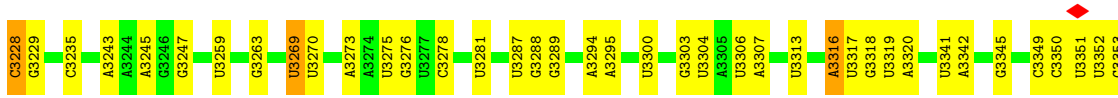


- Molecule 25: 60S ribosomal protein L39

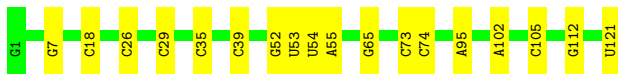
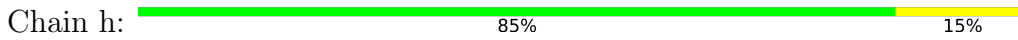
Chain Y:  98%



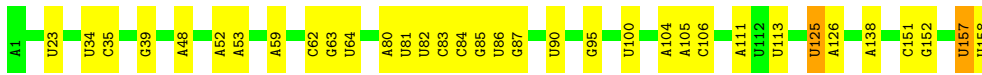
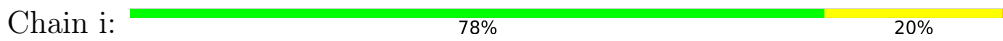
- Molecule 26: Ubiquitin-60S ribosomal protein L40



• Molecule 31: 5S rRNA



• Molecule 32: 5.8S rRNA



• Molecule 33: 60S ribosomal protein L2-A



• Molecule 34: 60S ribosomal protein L3



• Molecule 35: BJ4_G0008850.mRNA.1.CDS.1

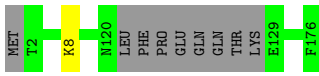


• Molecule 36: 60S ribosomal protein L5




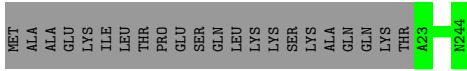
- Molecule 37: 60S ribosomal protein L6-B

Chain n:  94% 5%




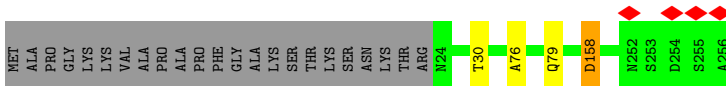
- Molecule 38: 60S ribosomal protein L7-A

Chain o:  91% 9%



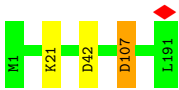
- Molecule 39: 60S ribosomal protein L8-A

Chain p:  89% 9%



- Molecule 40: 60S ribosomal protein L9-A

Chain q:  98% ..



- Molecule 41: 60S ribosomal protein L10

Chain r:  98% ..



- Molecule 42: BJ4_G0027750.mRNA.1.CDS.1

Chain s:  95% ..

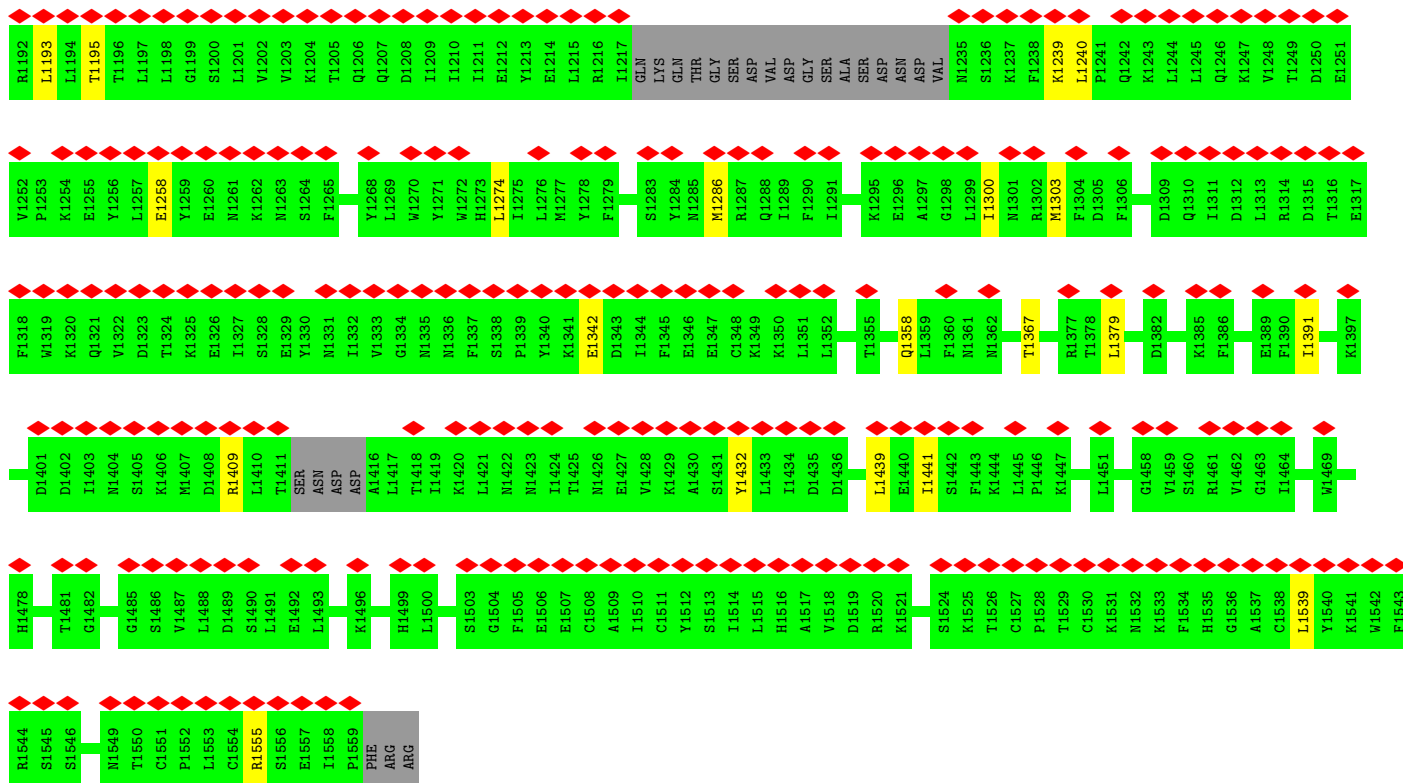


- Molecule 43: 60S ribosomal protein L13-A

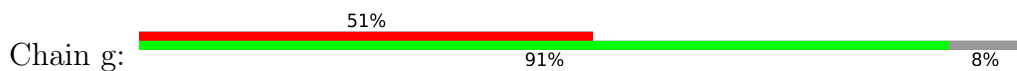
Chain t:  96% ..



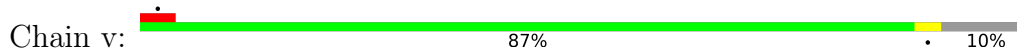
I1132	E1133	A1072	F1073	E1074	L1075	S1076	E1077	R1078	L1079	L1080	A1081	D1082	S1083	L1084	S1085	M1086	C1087	Q1088	I1089	D1090	D1091	I1092	T1093	K1094	Y1095	L1096	L1097	E1098	L1099	S1100	S1101	C1102	L1103	N1104	L1105	Y1106	E1107	L1108	L1109	S1110	Q1111	GLY	R1172	SER	L1173	L1174	F1175	E1176	V1177	V1178	L1179	N1180	D1181	K1182	D1183	I1184	G1185	S1186	N1187	I1188	N1189	Q1190	S1191																																																							
K952	D953	Y954	L955	L956	C957	A958	I959	L960	L961	L962	M963	F964	N965	R966	S967	N968	K970	D971	I972	E973	T974	K975	L976	R977	T978	L979	N980	L981	S982	F983	H984	S985	F986	T987	R988	L989	L990	S991	C992	L993	A994	S995	F996	F997	K998	S999	L1000	A1001	L1002	L1003	N1004	M1005	L1006	L1007	D1008	I1009	P1010	Q1011																																																												
H833	H834	W835	A836	F837	T838	R839	W840	V841	S842	E843	L844	W845	T846	D847	W848	N849	C850	L851	S852	T853	E854	P855	H856	D857	L858	Y859	S860	D861	F862	G863	H864	S865	F866	F867	K868	N869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951
V772	L713	Q714	L715	A716	G717	N718	W719	S720	I721	I722	A723	M724	K725	L726	A727	Q728	W729	I730	L731	H732	H733	A734	Q735	L736	F737	F738	S739	P740	G741	A742	K743	E744	L745	Y746	V747	T748	W749	Q750	V751	E752	L753	I754	N755	G756	C757	L758	Y759	T760	A761	E762	L763	F764	W765	P766	A767	N768	F769	I770	E771																																																											
S532	D533	M534	I535	F536	L537	N538	G539	K540	E541	G542	K543	F544	I545	N546	E547	I548	P549	T550	L551	V552	Q553	E554	S555	T556	Y557	Q558	N559	F560	A561	G562	I563	M564	A565	Q566	Y567	S568	N569	S570	K571	D572	F573	K574	M575	N576	T577	D578	A579	I580	T581	S582	L583	E584	D585	F586	N587	Y588	G589	L590	L591																																																											
L402	M403	W406	L410	K411	F412	A413	E414	D415	S416	S417	E418	E419	R420	V421	E428	I429	F430	M431	S434	C435	G436	K437	S438	L439	S440	E441	Y442	T443	K444	L445	M446	Q447	T448	L449	S450	G451	W452	F453	P454	P455	D456	K457	W458	E459	R460	E461	I462	E463	D464	Y465	F466	T467	S468	D469	F529	L530	L531																																																													
D471	I472	R473	K474	I475	K476	V477	S478	F479	E480	K481	M482	L483	F484	A485	L486	L487	V488	T489	S490	P491	M492	M493	E494	S495	K496	I497	S498	R499	L500	F501	D502	F503	F504	V505	Q506	L507	I508	E509	T510	D511	P512	S513	N514	N515	V516	L517	D520	G521	V522	Y523	D524	A525	L526	Y527	F529	L530	L531																																																													



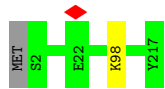
• Molecule 47: Eukaryotic translation initiation factor 6



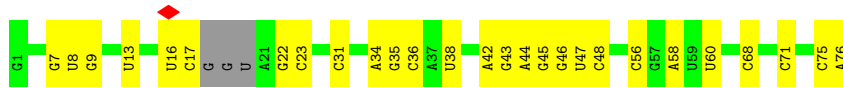
• Molecule 48: Eukaryotic translation initiation factor 5A-1



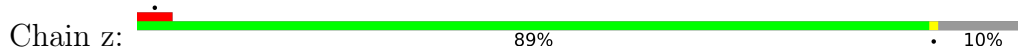
• Molecule 49: 60S ribosomal protein L1-A



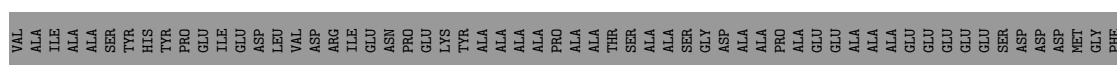
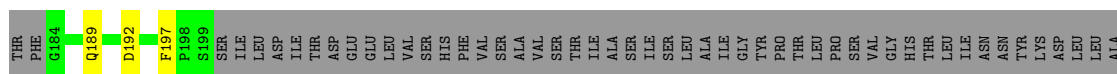
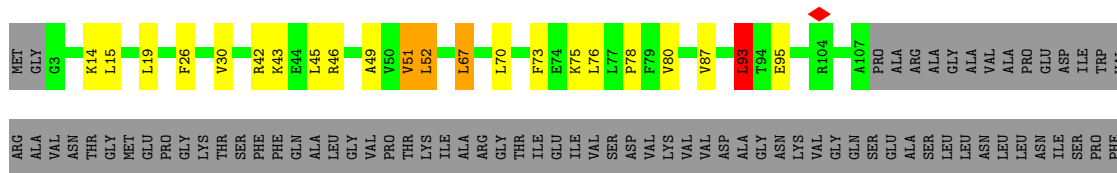
- Molecule 50: P-site tRNA



- Molecule 51: 60S ribosomal protein L12-B



- Molecule 52: 60S acidic ribosomal protein P0



- Molecule 53: CAT-tailed nascent peptide



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	44241	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.554	Depositor
Minimum map value	-0.671	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.128	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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: MG, 5CT, ZN, SPD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/1757	0.70	1/2354 (0.0%)
2	B	0.39	0/1585	0.64	1/2128 (0.0%)
3	C	0.38	0/1439	0.71	2/1938 (0.1%)
4	D	0.34	0/1465	0.67	1/1965 (0.1%)
5	E	0.37	0/1275	0.67	0/1702
6	F	0.38	0/1473	0.65	0/1980
7	G	0.36	0/1296	0.62	0/1739
8	H	0.37	0/812	0.73	3/1099 (0.3%)
9	I	0.35	0/1018	0.64	0/1369
10	J	0.36	0/530	0.62	0/703
11	K	0.41	0/979	0.69	1/1321 (0.1%)
12	L	0.35	0/995	0.68	1/1329 (0.1%)
13	M	0.36	0/1106	0.61	0/1485
14	N	0.40	0/1200	0.62	0/1607
15	O	0.32	0/473	0.72	2/629 (0.3%)
16	P	0.35	0/745	0.67	0/1001
17	Q	0.39	0/890	0.77	2/1196 (0.2%)
18	R	0.32	0/1034	0.59	0/1385
19	S	0.38	0/868	0.61	0/1168
20	T	0.35	0/890	0.67	0/1189
21	U	0.34	0/978	0.65	1/1301 (0.1%)
22	V	0.34	0/772	0.66	0/1026
23	W	0.39	0/660	0.69	0/875
24	X	0.33	0/618	0.78	1/826 (0.1%)
25	Y	0.33	0/443	0.65	0/588
26	Z	0.33	0/416	0.70	0/553
27	b	0.36	0/836	0.66	0/1104
28	c	0.36	0/701	0.67	0/934
29	d	0.26	0/208	0.84	0/267
30	f	0.61	0/76989	1.03	289/120031 (0.2%)
31	h	0.53	0/2883	0.98	9/4491 (0.2%)
32	i	0.60	0/3746	0.96	7/5832 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.38	0/1908	0.68	0/2564
34	k	0.36	0/3146	0.64	1/4228 (0.0%)
35	l	0.36	0/2800	0.64	2/3790 (0.1%)
36	m	0.34	0/2400	0.67	4/3239 (0.1%)
37	n	0.36	0/1329	0.67	0/1794
38	o	0.37	0/1821	0.61	0/2451
39	p	0.34	0/1836	0.62	2/2481 (0.1%)
40	q	0.37	0/1529	0.68	2/2060 (0.1%)
41	r	0.33	0/1801	0.64	0/2416
42	s	0.33	0/1367	0.70	3/1834 (0.2%)
43	t	0.36	0/1568	0.69	1/2106 (0.0%)
44	u	0.34	0/1068	0.66	1/1438 (0.1%)
45	a	0.28	0/6679	0.48	0/9012
46	e	0.28	0/11708	0.48	0/15899
47	g	0.32	0/1672	0.63	0/2281
48	v	0.33	0/1084	0.63	1/1456 (0.1%)
49	w	0.33	0/1736	0.65	0/2332
50	y	0.23	0/1735	0.66	0/2701
51	z	0.38	0/726	0.61	0/1006
52	0	0.33	0/976	0.55	0/1313
All	All	0.50	0/159969	0.87	338/233516 (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
15	O	0	1
21	U	0	1
34	k	0	1
35	l	0	2
39	p	0	3
40	q	0	1
44	u	0	1
46	e	0	1
47	g	0	1
All	All	0	12

There are no bond length outliers.

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	3217	C	N1-C2-O2	12.15	126.19	118.90
30	f	3217	C	C2-N1-C1'	11.32	131.25	118.80
30	f	3217	C	N3-C2-O2	-9.76	115.07	121.90
11	K	134	ASP	CB-CG-OD1	9.69	127.02	118.30
17	Q	84	ASP	CB-CG-OD1	9.31	126.68	118.30
30	f	922	U	C2-N1-C1'	9.28	128.84	117.70
30	f	2531	C	N1-C2-O2	8.91	124.25	118.90
30	f	922	U	N1-C2-O2	8.83	128.98	122.80
30	f	3181	C	N1-C2-O2	8.69	124.11	118.90
30	f	3278	C	N1-C2-O2	8.66	124.10	118.90
30	f	3181	C	C2-N1-C1'	8.46	128.11	118.80
30	f	2836	C	N3-C2-O2	-8.33	116.07	121.90
30	f	1279	C	C5-C6-N1	8.30	125.15	121.00
30	f	2836	C	C2-N1-C1'	8.21	127.83	118.80
36	m	230	ASP	CB-CG-OD1	8.11	125.60	118.30
30	f	1496	C	C2-N1-C1'	8.10	127.71	118.80
30	f	922	U	N3-C2-O2	-7.96	116.63	122.20
30	f	406	G	O4'-C1'-N9	7.95	114.56	108.20
30	f	1645	U	N3-C2-O2	-7.93	116.65	122.20
30	f	2205	U	N1-C2-O2	7.85	128.30	122.80
30	f	3217	C	C6-N1-C2	-7.84	117.16	120.30
30	f	2444	C	C2-N1-C1'	7.80	127.38	118.80
30	f	1208	U	N1-C2-O2	7.78	128.25	122.80
30	f	3217	C	C6-N1-C1'	-7.75	111.50	120.80
4	D	41	ASP	CB-CG-OD1	7.74	125.27	118.30
30	f	2983	C	C2-N1-C1'	7.72	127.29	118.80
30	f	3306	U	N3-C2-O2	-7.67	116.83	122.20
30	f	2652	U	N3-C2-O2	-7.64	116.85	122.20
30	f	3278	C	N3-C2-O2	-7.57	116.60	121.90
30	f	3306	U	C2-N1-C1'	7.56	126.77	117.70
30	f	2541	U	P-O3'-C3'	7.55	128.76	119.70
30	f	2205	U	N3-C2-O2	-7.55	116.92	122.20
30	f	3278	C	C2-N1-C1'	7.54	127.10	118.80
30	f	758	C	C2-N1-C1'	7.49	127.03	118.80
30	f	1645	U	N1-C2-O2	7.49	128.04	122.80
30	f	2836	C	N1-C2-O2	7.45	123.37	118.90
30	f	1277	C	C2-N1-C1'	7.42	126.96	118.80
30	f	2502	A	OP2-P-O3'	7.38	121.44	105.20
30	f	2235	C	C2-N1-C1'	7.31	126.84	118.80
30	f	3181	C	N3-C2-O2	-7.25	116.82	121.90
30	f	1556	C	N1-C2-O2	7.25	123.25	118.90
15	O	36	ASP	CB-CG-OD1	7.24	124.81	118.30
30	f	2923	U	N1-C2-O2	7.22	127.86	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1239	C	C2-N1-C1'	7.21	126.73	118.80
42	s	170	ASP	CB-CG-OD1	7.21	124.79	118.30
30	f	2531	C	C2-N1-C1'	7.20	126.72	118.80
30	f	1349	G	N3-C4-C5	-7.18	125.01	128.60
30	f	2502	A	P-O3'-C3'	7.15	128.28	119.70
30	f	1227	C	C2-N1-C1'	7.14	126.66	118.80
30	f	78	U	N3-C2-O2	-7.14	117.20	122.20
30	f	2205	U	C2-N1-C1'	7.11	126.23	117.70
39	p	158	ASP	CB-CG-OD1	7.11	124.70	118.30
30	f	1277	C	N1-C2-O2	7.09	123.16	118.90
30	f	14	U	O5'-P-OP2	-7.06	99.34	105.70
30	f	982	C	C2-N1-C1'	7.05	126.56	118.80
30	f	36	C	N1-C2-O2	7.05	123.13	118.90
30	f	1307	G	P-O3'-C3'	7.05	128.16	119.70
30	f	1815	U	P-O3'-C3'	7.04	128.15	119.70
30	f	1604	G	C4-N9-C1'	7.04	135.65	126.50
30	f	1227	C	N1-C2-O2	7.03	123.12	118.90
30	f	1645	U	C2-N1-C1'	7.00	126.10	117.70
30	f	3217	C	C5-C6-N1	7.00	124.50	121.00
30	f	1872	C	N1-C2-O2	6.97	123.08	118.90
30	f	1349	G	C4-N9-C1'	6.96	135.56	126.50
30	f	1272	C	N1-C2-O2	6.91	123.05	118.90
30	f	1208	U	C2-N1-C1'	6.90	125.98	117.70
30	f	3275	U	OP1-P-O3'	6.88	120.34	105.20
30	f	3235	C	C2-N1-C1'	6.87	126.36	118.80
30	f	3306	U	N1-C2-O2	6.87	127.61	122.80
30	f	2923	U	N3-C2-O2	-6.83	117.42	122.20
30	f	2846	U	C2-N1-C1'	6.78	125.83	117.70
12	L	11	ASP	CB-CG-OD1	6.75	124.38	118.30
30	f	270	U	N1-C2-O2	6.74	127.52	122.80
30	f	1227	C	C5-C6-N1	6.73	124.36	121.00
30	f	2846	U	N3-C2-O2	-6.72	117.49	122.20
30	f	1227	C	C6-N1-C2	-6.71	117.62	120.30
30	f	2983	C	N3-C2-O2	-6.71	117.21	121.90
30	f	2531	C	N3-C2-O2	-6.69	117.22	121.90
30	f	2537	U	P-O3'-C3'	6.67	127.70	119.70
31	h	26	C	N1-C2-O2	6.66	122.90	118.90
30	f	2836	C	C6-N1-C2	-6.65	117.64	120.30
30	f	270	U	N3-C2-O2	-6.64	117.55	122.20
30	f	1239	C	N1-C2-O2	6.64	122.88	118.90
30	f	2112	U	OP2-P-O3'	6.60	119.73	105.20
30	f	3058	U	C2-N1-C1'	6.58	125.60	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2189	U	N1-C2-O2	6.58	127.41	122.80
30	f	3214	U	C2-N1-C1'	6.54	125.54	117.70
2	B	27[A]	LEU	CB-CG-CD2	-6.52	99.91	111.00
32	i	64	U	N3-C2-O2	-6.52	117.64	122.20
30	f	3034	C	N1-C2-O2	6.51	122.80	118.90
30	f	2101	C	P-O3'-C3'	6.49	127.49	119.70
30	f	2235	C	C6-N1-C2	-6.49	117.70	120.30
30	f	1208	U	N3-C2-O2	-6.47	117.67	122.20
30	f	524	U	N1-C2-O2	6.46	127.33	122.80
30	f	2189	U	N3-C2-O2	-6.46	117.68	122.20
30	f	2112	U	P-O3'-C3'	6.44	127.43	119.70
31	h	105	C	N1-C2-O2	6.44	122.76	118.90
30	f	2550	U	N3-C2-O2	-6.43	117.70	122.20
30	f	2983	C	N1-C2-O2	6.42	122.75	118.90
35	l	155	ASP	CB-CG-OD1	6.41	124.07	118.30
30	f	524	U	N3-C2-O2	-6.38	117.73	122.20
30	f	1269	U	C2-N1-C1'	6.38	125.35	117.70
30	f	986	U	N3-C2-O2	-6.36	117.75	122.20
30	f	2274	U	N1-C2-O2	6.36	127.25	122.80
21	U	79	ASP	CB-CG-OD1	6.34	124.01	118.30
36	m	137	ASP	CB-CG-OD1	6.34	124.00	118.30
30	f	3058	U	N1-C2-O2	6.33	127.23	122.80
44	u	47	ASP	CB-CG-OD1	6.33	123.99	118.30
30	f	1269	U	N1-C2-O2	6.32	127.22	122.80
30	f	1556	C	N3-C2-O2	-6.31	117.48	121.90
30	f	2464	U	C2-N1-C1'	6.30	125.27	117.70
30	f	1496	C	C6-N1-C2	-6.29	117.78	120.30
1	A	153	ASP	CB-CG-OD1	6.28	123.95	118.30
30	f	2617	U	N3-C2-O2	-6.27	117.81	122.20
30	f	2726	C	N3-C2-O2	-6.26	117.52	121.90
30	f	36	C	N3-C2-O2	-6.26	117.52	121.90
30	f	922	U	C6-N1-C1'	-6.25	112.45	121.20
30	f	865	U	N3-C2-O2	-6.25	117.83	122.20
30	f	1716	U	P-O3'-C3'	6.23	127.18	119.70
30	f	2726	C	C2-N1-C1'	6.23	125.66	118.80
40	q	42	ASP	CB-CG-OD1	6.22	123.90	118.30
30	f	192	C	C2-N1-C1'	6.21	125.64	118.80
30	f	1269	U	N3-C2-O2	-6.21	117.85	122.20
30	f	1097	G	P-O3'-C3'	6.17	127.11	119.70
30	f	1878	G	C4-N9-C1'	6.16	134.51	126.50
30	f	2444	C	C6-N1-C2	-6.15	117.84	120.30
30	f	2132	C	C6-N1-C2	-6.15	117.84	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	2846	U	N1-C2-O2	6.14	127.10	122.80
30	f	1349	G	N3-C4-N9	6.13	129.68	126.00
30	f	2550	U	C2-N1-C1'	6.13	125.05	117.70
30	f	637	C	P-O3'-C3'	6.12	127.05	119.70
30	f	1115	G	C4-N9-C1'	6.11	134.45	126.50
30	f	3104	U	N1-C2-O2	6.11	127.08	122.80
30	f	995	U	N1-C2-O2	6.11	127.08	122.80
30	f	2842	U	N1-C2-O2	6.11	127.08	122.80
30	f	3104	U	N3-C2-O2	-6.11	117.92	122.20
30	f	2388	U	N3-C2-O2	-6.09	117.94	122.20
30	f	915	A	C2-N3-C4	6.05	113.63	110.60
30	f	2553	U	C2-N1-C1'	6.05	124.96	117.70
30	f	1064	A	P-O3'-C3'	6.04	126.95	119.70
30	f	3131	U	C2-N1-C1'	6.03	124.93	117.70
30	f	2274	U	C2-N1-C1'	6.02	124.92	117.70
30	f	2923	U	C2-N1-C1'	6.02	124.92	117.70
30	f	1872	C	N3-C2-O2	-6.01	117.69	121.90
30	f	1604	G	C8-N9-C1'	-6.00	119.19	127.00
30	f	1604	G	N3-C4-N9	6.00	129.60	126.00
30	f	1907	C	N1-C2-O2	6.00	122.50	118.90
30	f	3300	U	N3-C2-O2	-5.99	118.00	122.20
30	f	1279	C	C6-N1-C2	-5.99	117.90	120.30
30	f	3181	C	C6-N1-C1'	-5.99	113.61	120.80
30	f	2132	C	N3-C2-O2	-5.99	117.71	121.90
30	f	1556	C	C2-N1-C1'	5.98	125.38	118.80
8	H	51	GLY	C-N-CA	5.97	136.62	121.70
34	k	87	VAL	CG1-CB-CG2	-5.95	101.38	110.90
30	f	985	U	N3-C2-O2	-5.95	118.03	122.20
8	H	18	ASP	CB-CG-OD1	5.94	123.64	118.30
30	f	2652	U	N1-C2-O2	5.94	126.96	122.80
30	f	969	C	C6-N1-C2	-5.93	117.93	120.30
30	f	1355	A	P-O3'-C3'	5.91	126.79	119.70
30	f	1425	U	N3-C2-O2	-5.91	118.06	122.20
30	f	1604	G	N3-C4-C5	-5.89	125.65	128.60
32	i	100	U	C2-N1-C1'	5.89	124.77	117.70
30	f	2585	G	N3-C4-C5	-5.89	125.66	128.60
30	f	3048	A	O4'-C1'-N9	5.89	112.91	108.20
30	f	1820	U	P-O3'-C3'	5.87	126.74	119.70
30	f	2531	C	C6-N1-C2	-5.87	117.95	120.30
30	f	1562	C	P-O3'-C3'	5.86	126.73	119.70
30	f	1437	C	C2-N1-C1'	5.85	125.24	118.80
30	f	2274	U	N3-C2-O2	-5.85	118.11	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	142	C	N1-C2-O2	5.85	122.41	118.90
30	f	2638	C	N1-C2-O2	5.84	122.41	118.90
30	f	865	U	N1-C2-O2	5.84	126.89	122.80
30	f	2622	C	N1-C2-O2	5.84	122.40	118.90
30	f	3350	C	C6-N1-C2	-5.83	117.97	120.30
31	h	26	C	C6-N1-C2	-5.83	117.97	120.30
30	f	1525	G	C4-N9-C1'	5.83	134.07	126.50
30	f	1577	G	N1-C6-O6	-5.83	116.41	119.90
30	f	3214	U	N3-C2-O2	-5.82	118.12	122.20
30	f	3316	A	P-O3'-C3'	5.82	126.68	119.70
30	f	835	G	O4'-C1'-N9	5.80	112.84	108.20
30	f	1272	C	N3-C2-O2	-5.80	117.84	121.90
30	f	2204	C	C6-N1-C2	-5.80	117.98	120.30
42	s	9	MET	CA-CB-CG	5.76	123.10	113.30
30	f	270	U	C2-N1-C1'	5.74	124.58	117.70
30	f	758	C	C6-N1-C2	-5.74	118.01	120.30
30	f	3228	C	P-O3'-C3'	5.73	126.58	119.70
30	f	2992	U	N3-C2-O2	-5.72	118.19	122.20
30	f	3218	A	P-O3'-C3'	5.71	126.55	119.70
30	f	1190	A	C4-N9-C1'	5.71	136.57	126.30
30	f	142	C	C6-N1-C2	-5.70	118.02	120.30
30	f	282	G	P-O3'-C3'	5.69	126.53	119.70
30	f	1448	U	N3-C2-O2	-5.69	118.22	122.20
30	f	2531	C	C5-C6-N1	5.69	123.84	121.00
30	f	3034	C	N3-C2-O2	-5.68	117.92	121.90
30	f	97	U	N3-C2-O2	-5.68	118.22	122.20
30	f	1277	C	N3-C2-O2	-5.68	117.92	121.90
30	f	2899	C	N3-C2-O2	-5.68	117.93	121.90
30	f	354	U	N1-C2-O2	5.67	126.77	122.80
30	f	1496	C	C5-C6-N1	5.67	123.84	121.00
30	f	2366	C	C2-N1-C1'	5.67	125.03	118.80
32	i	64	U	N1-C2-O2	5.66	126.77	122.80
8	H	50	LEU	CA-CB-CG	5.65	128.29	115.30
30	f	916	G	P-O3'-C3'	5.65	126.48	119.70
30	f	2553	U	C6-N1-C1'	-5.64	113.30	121.20
30	f	2899	C	C2-N1-C1'	5.63	124.99	118.80
30	f	2204	C	C5-C6-N1	5.62	123.81	121.00
30	f	1349	G	C8-N9-C1'	-5.62	119.70	127.00
30	f	2378	C	C2-N1-C1'	5.62	124.98	118.80
30	f	1496	C	N1-C2-O2	5.61	122.26	118.90
30	f	2137	U	C2-N1-C1'	5.60	124.42	117.70
30	f	777	U	N3-C2-O2	-5.60	118.28	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	113	C	C2-N1-C1'	5.60	124.96	118.80
30	f	3058	U	N3-C2-O2	-5.60	118.28	122.20
30	f	2764	C	N1-C2-O2	5.59	122.25	118.90
30	f	2842	U	N3-C2-O2	-5.58	118.29	122.20
30	f	3057	U	N3-C2-O2	-5.58	118.30	122.20
30	f	2132	C	N1-C2-O2	5.58	122.25	118.90
30	f	3269	U	P-O3'-C3'	5.58	126.39	119.70
30	f	2983	C	C6-N1-C2	-5.57	118.07	120.30
31	h	26	C	N3-C2-O2	-5.57	118.00	121.90
40	q	107	ASP	CB-CG-OD1	5.55	123.30	118.30
30	f	2366	C	C5-C6-N1	5.55	123.78	121.00
32	i	125	U	C2-N1-C1'	5.54	124.34	117.70
31	h	35	C	N1-C2-O2	5.53	122.22	118.90
30	f	1554	U	P-O3'-C3'	5.53	126.33	119.70
3	C	53	ASP	CB-CG-OD1	5.52	123.27	118.30
30	f	995	U	N3-C2-O2	-5.51	118.34	122.20
30	f	283	G	N3-C4-N9	5.50	129.30	126.00
30	f	315	C	C2-N1-C1'	5.50	124.85	118.80
30	f	986	U	N1-C2-O2	5.50	126.65	122.80
30	f	982	C	N1-C2-O2	5.50	122.20	118.90
30	f	2726	C	N1-C2-O2	5.49	122.19	118.90
30	f	411	U	N3-C2-O2	-5.49	118.36	122.20
30	f	2552	C	N1-C2-O2	5.48	122.19	118.90
30	f	2585	G	N3-C4-N9	5.48	129.29	126.00
31	h	52	G	P-O3'-C3'	5.47	126.27	119.70
24	X	14	LEU	CA-CB-CG	5.46	127.86	115.30
30	f	2444	C	N1-C2-O2	5.46	122.18	118.90
30	f	2210	G	N3-C4-C5	-5.46	125.87	128.60
30	f	3214	U	N1-C2-O2	5.45	126.62	122.80
30	f	3355	U	C2-N1-C1'	5.45	124.24	117.70
30	f	283	G	C4-N9-C1'	5.44	133.57	126.50
30	f	2783	U	N3-C2-O2	-5.44	118.39	122.20
30	f	3153	U	C2-N1-C1'	5.42	124.21	117.70
30	f	3057	U	N1-C2-O2	5.42	126.59	122.80
30	f	78	U	N1-C2-O2	5.42	126.59	122.80
30	f	1878	G	C8-N9-C1'	-5.42	119.96	127.00
30	f	1688	U	N3-C2-O2	-5.42	118.41	122.20
30	f	3350	C	P-O3'-C3'	5.41	126.19	119.70
30	f	1437	C	C6-N1-C2	-5.41	118.14	120.30
30	f	2726	C	C6-N1-C2	-5.40	118.14	120.30
30	f	2552	C	C2-N1-C1'	5.39	124.73	118.80
30	f	1277	C	C6-N1-C2	-5.39	118.14	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	114	VAL	CG1-CB-CG2	-5.39	102.28	110.90
30	f	2622	C	N3-C2-O2	-5.37	118.14	121.90
30	f	142	C	N3-C2-O2	-5.36	118.15	121.90
30	f	1425	U	N1-C2-O2	5.36	126.55	122.80
30	f	1349	G	C2-N3-C4	5.35	114.58	111.90
30	f	3278	C	C6-N1-C1'	-5.35	114.38	120.80
30	f	1496	C	C6-N1-C1'	-5.35	114.38	120.80
30	f	1732	U	N1-C2-O2	5.34	126.54	122.80
30	f	2500	A	P-O3'-C3'	5.34	126.11	119.70
30	f	915	A	C4-N9-C1'	5.33	135.90	126.30
30	f	2497	U	N3-C2-O2	-5.33	118.47	122.20
30	f	2366	C	C6-N1-C2	-5.33	118.17	120.30
30	f	2336	U	N3-C2-O2	-5.33	118.47	122.20
30	f	2568	C	O4'-C1'-N1	5.33	112.46	108.20
30	f	2836	C	C6-N1-C1'	-5.33	114.41	120.80
30	f	1732	U	N3-C2-O2	-5.30	118.49	122.20
30	f	982	C	C6-N1-C2	-5.29	118.18	120.30
30	f	1115	G	C8-N9-C1'	-5.29	120.12	127.00
30	f	890	C	N1-C2-O2	5.29	122.07	118.90
43	t	136	GLU	CA-CB-CG	5.29	125.03	113.40
30	f	1608	C	C2-N1-C1'	5.28	124.61	118.80
30	f	2114	C	C6-N1-C2	-5.28	118.19	120.30
30	f	954	U	N3-C2-O2	-5.27	118.51	122.20
30	f	1525	G	C8-N9-C1'	-5.27	120.15	127.00
30	f	982	C	C5-C6-N1	5.25	123.63	121.00
30	f	2235	C	N1-C2-O2	5.25	122.05	118.90
31	h	105	C	N3-C2-O2	-5.24	118.23	121.90
48	v	50	GLY	N-CA-C	-5.24	100.00	113.10
30	f	1907	C	N3-C2-O2	-5.24	118.23	121.90
30	f	1560	G	N3-C4-N9	-5.24	122.86	126.00
30	f	1190	A	C2-N3-C4	5.24	113.22	110.60
30	f	2446	U	O4'-C1'-N1	5.24	112.39	108.20
42	s	108	GLU	CA-CB-CG	5.24	124.92	113.40
32	i	125	U	N1-C2-O2	5.23	126.46	122.80
30	f	3349	C	C6-N1-C2	-5.22	118.21	120.30
30	f	192	C	C6-N1-C2	-5.21	118.21	120.30
30	f	2235	C	C5-C6-N1	5.21	123.61	121.00
30	f	2899	C	N1-C2-O2	5.21	122.03	118.90
30	f	1608	C	C5-C6-N1	5.21	123.60	121.00
30	f	3235	C	N1-C2-O2	5.20	122.02	118.90
30	f	2444	C	C5-C6-N1	5.20	123.60	121.00
30	f	2772	C	N1-C2-O2	5.20	122.02	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	i	100	U	N1-C2-O2	5.20	126.44	122.80
30	f	2496	C	C2-N1-C1'	5.19	124.51	118.80
30	f	2585	G	C4-N9-C1'	5.19	133.25	126.50
30	f	915	A	C8-N9-C4	-5.18	103.73	105.80
30	f	1237	G	N3-C4-N9	5.18	129.11	126.00
30	f	3148	U	N3-C2-O2	-5.17	118.58	122.20
30	f	969	C	N3-C2-O2	-5.17	118.28	121.90
30	f	1239	C	C6-N1-C1'	-5.17	114.59	120.80
30	f	890	C	N3-C2-O2	-5.17	118.28	121.90
30	f	87	U	N1-C2-O2	5.16	126.41	122.80
30	f	2622	C	C6-N1-C2	-5.16	118.24	120.30
30	f	637	C	OP1-P-O3'	5.16	116.55	105.20
30	f	849	C	P-O3'-C3'	5.16	125.89	119.70
30	f	1563	C	C6-N1-C1'	5.16	126.99	120.80
31	h	18	C	C2-N1-C1'	5.15	124.47	118.80
30	f	2983	C	C6-N1-C1'	-5.15	114.62	120.80
30	f	149	U	N3-C2-O2	-5.14	118.60	122.20
30	f	166	C	C2-N1-C1'	5.14	124.46	118.80
30	f	3181	C	C6-N1-C2	-5.13	118.25	120.30
30	f	2638	C	N3-C2-O2	-5.13	118.31	121.90
30	f	1951	C	C2-N1-C1'	5.12	124.43	118.80
30	f	758	C	N1-C2-O2	5.10	121.96	118.90
36	m	222	LEU	CA-CB-CG	5.08	126.99	115.30
17	Q	42	LEU	CA-CB-CG	5.08	126.98	115.30
30	f	2873	U	C2-N1-C1'	5.08	123.79	117.70
30	f	1097	G	OP2-P-O3'	5.07	116.36	105.20
30	f	1608	C	C6-N1-C2	-5.07	118.27	120.30
30	f	2444	C	C6-N1-C1'	-5.07	114.71	120.80
35	l	4	PRO	C-N-CA	5.07	134.38	121.70
30	f	2550	U	N1-C2-O2	5.06	126.34	122.80
30	f	3355	U	N1-C2-O2	5.06	126.34	122.80
30	f	969	C	N1-C2-O2	5.05	121.93	118.90
15	O	21	ILE	CG1-CB-CG2	-5.04	100.30	111.40
30	f	1820	U	OP2-P-O3'	5.04	116.30	105.20
30	f	1597	C	C5-C6-N1	5.04	123.52	121.00
30	f	1272	C	C6-N1-C2	-5.04	118.28	120.30
36	m	146	LEU	CB-CG-CD1	-5.04	102.44	111.00
32	i	157	U	N1-C2-O2	5.02	126.32	122.80
31	h	39	C	N1-C2-O2	5.02	121.91	118.90
39	p	79	GLN	CA-CB-CG	5.02	124.45	113.40
30	f	777	U	N1-C2-O2	5.02	126.31	122.80
30	f	1562	C	N3-C2-O2	-5.01	118.39	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	f	1277	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	O	20	GLY	Peptide
21	U	83	LYS	Peptide
46	e	392	GLY	Peptide
47	g	8	GLU	Peptide
34	k	141	GLY	Peptide
35	l	13	GLY	Peptide
35	l	318	LEU	Peptide
39	p	158	ASP	Peptide
39	p	30	THR	Peptide
39	p	76	ALA	Peptide
40	q	21	LYS	Peptide
44	u	12	TRP	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	A	1720	0	1779	10	0
2	B	1555	0	1659	13	0
3	C	1416	0	1433	11	0
4	D	1441	0	1543	7	0
5	E	1258	0	1342	6	0
6	F	1437	0	1475	15	0
7	G	1272	0	1312	9	0
8	H	796	0	812	4	0
9	I	1003	0	1048	8	0
10	J	518	0	542	3	0
11	K	964	0	1025	1	0
12	L	984	0	1075	4	0
13	M	1080	0	1122	5	0
14	N	1169	0	1211	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	462	0	491	6	0
16	P	737	0	792	3	0
17	Q	876	0	912	9	0
18	R	1013	0	1077	5	0
19	S	850	0	880	2	0
20	T	880	0	942	3	0
21	U	969	0	1078	3	0
22	V	766	0	844	4	0
23	W	645	0	645	3	0
24	X	612	0	682	3	0
25	Y	436	0	475	0	0
26	Z	410	0	442	0	0
27	b	824	0	888	0	0
28	c	694	0	734	0	0
29	d	207	0	250	0	0
30	f	68782	0	34563	0	0
31	h	2579	0	1304	0	0
32	i	3353	0	1695	0	0
33	j	1874	0	1943	0	0
34	k	3075	0	3142	0	0
35	l	2748	0	2859	0	0
36	m	2351	0	2294	0	0
37	n	1307	0	1377	0	0
38	o	1784	0	1862	0	0
39	p	1804	0	1877	0	0
40	q	1508	0	1572	0	0
41	r	1764	0	1804	0	0
42	s	1346	0	1370	0	0
43	t	1543	0	1608	0	0
44	u	1053	0	1149	0	0
45	a	6569	0	6459	0	0
46	e	11509	0	10765	0	0
47	g	1651	0	1613	0	0
48	v	1085	0	1086	0	0
49	w	1709	0	1799	0	0
50	y	1556	0	788	0	0
51	z	728	0	337	0	0
52	0	961	0	979	11	0
53	1	85	0	19	0	0
54	A	1	0	0	0	0
54	C	1	0	0	0	0
54	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	I	1	0	0	0	0
54	R	1	0	0	0	0
54	T	1	0	0	0	0
54	f	3	0	0	0	0
54	h	1	0	0	0	0
54	j	2	0	0	0	0
54	k	1	0	0	0	0
55	T	1	0	0	0	0
55	W	1	0	0	0	0
55	Z	1	0	0	0	0
55	b	1	0	0	0	0
55	c	1	0	0	0	0
55	e	2	0	0	0	0
56	f	10	0	19	0	0
All	All	149748	0	112793	146	0

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 6.

All (146) 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)
15:O:16:ALA:O	15:O:20:GLY:HA3	1.69	0.90
15:O:16:ALA:O	15:O:20:GLY:CA	2.36	0.73
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.58	0.69
2:B:46[A]:GLU:HB3	2:B:49[A]:ARG:HG3	1.75	0.68
52:0:26:PHE:HB2	52:0:87:VAL:HB	1.73	0.68
7:G:84:TYR:HB2	15:O:24:PRO:HD3	1.78	0.64
2:B:27[A]:LEU:HD21	2:B:102[A]:LEU:HB2	1.80	0.63
13:M:27:LYS:HB3	13:M:42:LEU:HB2	1.81	0.62
9:I:14:SER:O	9:I:81:GLN:NE2	2.33	0.62
6:F:80:ARG:HH21	6:F:87:THR:HG21	1.66	0.60
52:0:192:ASP:HB2	52:0:197:PHE:HE2	1.67	0.59
6:F:8:GLN:HB3	6:F:64:ILE:HD11	1.85	0.59
1:A:183:THR:HG22	1:A:187:ARG:HB2	1.85	0.59
21:U:5:LYS:HB2	21:U:8:GLU:HG2	1.84	0.58
6:F:77:VAL:HG22	6:F:126:VAL:HG23	1.85	0.58
52:0:43:LYS:HA	52:0:46:ARG:HG2	1.87	0.57
11:K:50:ALA:HB1	21:U:66:VAL:HG11	1.86	0.57
17:Q:4:LEU:O	17:Q:79:ARG:NH2	2.38	0.56
17:Q:55:LEU:HB2	17:Q:95:PRO:HD3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:87:GLU:OE2	20:T:91:ARG:NH1	2.39	0.55
52:O:42:ARG:HG2	52:O:51:VAL:HG11	1.88	0.55
18:R:19:ARG:HD3	18:R:33:ARG:HB2	1.89	0.55
2:B:157[A]:GLU:OE2	2:B:160[A]:ARG:NH2	2.40	0.54
17:Q:9:THR:HG23	17:Q:109:VAL:HG23	1.88	0.54
14:N:95:SER:OG	14:N:98:THR:OG1	2.25	0.54
7:G:17:ARG:HG2	7:G:22:HIS:HA	1.90	0.53
8:H:56:VAL:HG12	8:H:65:VAL:HG22	1.88	0.53
2:B:75[A]:ALA:HB3	2:B:78[A]:ARG:HG2	1.90	0.53
10:J:6:ASP:OD1	10:J:32:GLN:N	2.40	0.53
8:H:44:GLU:OE2	8:H:49:ASN:ND2	2.41	0.52
10:J:47:ARG:HH21	10:J:58:HIS:HB2	1.73	0.52
2:B:61[A]:ALA:HA	2:B:70[A]:PRO:HD2	1.90	0.52
6:F:96:ASP:OD1	6:F:97:VAL:N	2.38	0.52
6:F:77:VAL:HG11	6:F:106:LEU:HD22	1.92	0.52
3:C:118:GLN:NE2	3:C:147:GLU:OE2	2.39	0.52
4:D:36:LEU:O	4:D:40:THR:OG1	2.27	0.52
6:F:80:ARG:HB2	6:F:122:HIS:HB2	1.91	0.52
7:G:136:ARG:HD2	7:G:139:ARG:HH12	1.74	0.52
9:I:94:TYR:OH	10:J:41:LYS:NZ	2.39	0.52
14:N:100:PRO:HG2	14:N:123:VAL:HG23	1.93	0.51
1:A:103:GLU:HG3	1:A:160:GLU:HB2	1.93	0.51
7:G:99:SER:HG	7:G:101:CYS:HG	1.59	0.50
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50
3:C:107:LEU:HD12	3:C:152:GLU:HG3	1.92	0.50
2:B:74[A]:ARG:O	2:B:142[A]:SER:OG	2.23	0.50
3:C:60:PHE:HB3	3:C:64:ASN:HB3	1.93	0.49
17:Q:77:ARG:HD2	17:Q:89:LEU:HD13	1.94	0.49
2:B:46[A]:GLU:HG3	2:B:48[A]:PHE:H	1.77	0.49
16:P:30:THR:HG23	16:P:91:SER:HB2	1.95	0.49
16:P:9:SER:OG	16:P:10:ILE:N	2.39	0.49
6:F:155:ARG:HB2	6:F:172:TYR:HD1	1.77	0.49
7:G:108:ARG:O	7:G:112:ASN:HB2	2.12	0.49
14:N:94:ALA:HA	14:N:121:VAL:HG23	1.95	0.48
4:D:131:ALA:HB1	4:D:135:GLN:H	1.79	0.48
17:Q:80:ASN:OD1	17:Q:81:GLU:N	2.45	0.48
19:S:49:ILE:HD11	19:S:71:VAL:HG22	1.96	0.48
4:D:102:ALA:HA	4:D:122:ILE:O	2.14	0.48
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.95	0.48
6:F:93:GLU:HG3	6:F:140:VAL:HG11	1.95	0.48
4:D:19:PRO:HB3	4:D:53:PHE:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	0.47
17:Q:75:ILE:HG12	17:Q:93:VAL:HG22	1.96	0.47
3:C:22:LEU:HD12	3:C:146:ILE:HD12	1.97	0.47
52:O:26:PHE:HZ	52:O:93:LEU:HA	1.80	0.47
5:E:151:ARG:NH2	5:E:152:GLU:OE2	2.45	0.47
4:D:170:ARG:HD2	14:N:57:GLY:HA3	1.97	0.47
5:E:21:LYS:HE3	5:E:55:VAL:HA	1.97	0.47
9:I:18:PRO:HA	9:I:51:ALA:HA	1.97	0.47
1:A:5:LYS:HE2	22:V:40:VAL:HG21	1.97	0.47
5:E:68:GLN:OE1	5:E:71:ARG:NH2	2.43	0.46
3:C:67:ILE:HD11	3:C:80:LYS:HB3	1.98	0.46
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.46
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
12:L:74:TYR:HB3	12:L:77:LYS:HB2	1.98	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
2:B:39[A]:GLU:HG2	2:B:40[A]:GLU:HG2	1.97	0.46
14:N:96:LYS:HB2	14:N:96:LYS:HE2	1.70	0.46
18:R:60:ASN:HB3	18:R:63:THR:HB	1.97	0.46
13:M:22:LYS:NZ	13:M:132:SER:O	2.47	0.45
1:A:159:ARG:HB3	1:A:164:LEU:HB2	1.98	0.45
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.45
9:I:10:LYS:NZ	9:I:56:ASP:OD1	2.41	0.45
17:Q:44:MET:O	17:Q:77:ARG:NH1	2.49	0.45
6:F:22:PRO:O	7:G:146:ASN:ND2	2.38	0.45
22:V:53:TYR:HA	22:V:56:ARG:HG2	1.99	0.45
1:A:170:LYS:HB3	1:A:170:LYS:HE3	4.56	0.45
9:I:38:ALA:HB3	9:I:59:MET:HB2	1.99	0.44
6:F:80:ARG:HG3	6:F:124:LEU:HD21	1.99	0.44
15:O:21:ILE:HD12	15:O:21:ILE:HG23	1.83	0.44
24:X:10:GLN:HA	24:X:13:GLU:HG2	1.99	0.44
2:B:127[A]:LEU:HD22	6:F:156:VAL:HG13	2.00	0.44
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.44
9:I:129:VAL:O	9:I:133:SER:HB3	2.17	0.44
14:N:36:GLY:HA3	14:N:40:HIS:CE1	2.53	0.44
4:D:161:LYS:HD3	4:D:161:LYS:HA	1.82	0.43
6:F:80:ARG:HD2	7:G:155:PRO:HA	2.00	0.43
52:O:45:LEU:HB3	52:O:49:ALA:HB3	1.99	0.43
8:H:20:SER:HA	8:H:23:THR:HG22	2.00	0.43
9:I:117:PRO:HA	9:I:135:VAL:HG13	2.00	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.43
52:0:15:LEU:O	52:0:19:LEU:HG	2.18	0.43
4:D:124:LEU:HD13	4:D:127:LEU:HD23	2.01	0.43
52:0:75:LYS:O	52:0:78:PRO:HD2	2.19	0.43
1:A:158:HIS:HB3	1:A:161:ALA:HB3	2.00	0.43
3:C:56:ARG:NH2	3:C:75:GLU:OE2	2.51	0.43
5:E:102:LEU:HD22	5:E:138:LEU:HD22	2.01	0.43
24:X:2:ALA:N	24:X:51:LEU:O	2.52	0.43
1:A:68:ARG:HA	1:A:98:LEU:HD21	2.01	0.43
2:B:54[A]:TYR:OH	2:B:73[A]:PHE:O	2.37	0.43
18:R:3:SER:OG	18:R:4:LEU:N	2.51	0.43
12:L:86:THR:OG1	12:L:94:SER:OG	2.36	0.42
3:C:179:GLN:HA	3:C:182:ILE:HG22	2.00	0.42
9:I:80:ARG:HB2	9:I:99:ALA:HB3	2.00	0.42
6:F:95:ARG:HB2	6:F:140:VAL:HG23	2.00	0.42
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.42
52:0:14:LYS:HE3	52:0:52:LEU:HD11	2.00	0.42
52:0:70:LEU:HB3	52:0:73:PHE:CD1	2.55	0.42
6:F:32:SER:HB2	6:F:36:ILE:HD12	2.01	0.42
8:H:41:ILE:HG21	8:H:54:VAL:HG21	2.02	0.42
24:X:33:LYS:HA	24:X:33:LYS:HD3	1.84	0.42
3:C:182:ILE:HD12	3:C:182:ILE:HA	1.85	0.42
16:P:73:GLY:N	16:P:76:GLU:OE1	2.42	0.42
52:0:67:LEU:HD22	52:0:67:LEU:HA	1.85	0.42
20:T:95:ILE:HD13	20:T:95:ILE:HG21	1.81	0.42
1:A:98:LEU:HD22	1:A:128:LYS:HD2	2.02	0.41
3:C:116:HIS:HB3	3:C:149:VAL:HB	2.02	0.41
2:B:8[A]:VAL:HG12	2:B:117[A]:ARG:HG3	2.03	0.41
12:L:63:LYS:HA	12:L:63:LYS:HD3	1.92	0.41
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
3:C:122:ALA:HB3	3:C:143:PRO:HB2	2.02	0.41
3:C:131:ARG:HG3	3:C:137:ASN:ND2	2.36	0.41
5:E:7:GLN:NE2	5:E:35:ALA:O	2.53	0.41
7:G:102:ARG:HD2	7:G:102:ARG:HA	1.77	0.41
1:A:9:GLU:HG3	22:V:44:VAL:HG21	2.03	0.41
14:N:75:LEU:HD23	14:N:75:LEU:HA	1.92	0.41
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.01	0.41
1:A:18:VAL:HG13	1:A:19:LEU:HD12	2.02	0.40
2:B:189[A]:ASP:OD1	2:B:190[A]:VAL:N	2.53	0.40
2:B:121[A]:PRO:HA	2:B:124[A]:LEU:HD12	2.03	0.40
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:93:PHE:HD2	20:T:94:LEU:HD22	1.86	0.40
5:E:31:GLU:HA	5:E:34:GLN:HB2	2.03	0.40
6:F:40:ARG:HA	6:F:40:ARG:HD2	1.84	0.40
7:G:73:GLY:HA2	7:G:89:LEU:O	2.21	0.40

There are no symmetry-related clashes.

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	Percentiles	
1	A	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
2	B	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
3	C	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
4	D	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
5	E	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
6	F	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
7	G	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
8	H	98/121 (81%)	93 (95%)	5 (5%)	0	100	100
9	I	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
10	J	61/155 (39%)	61 (100%)	0	0	100	100
11	K	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
12	L	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	8	21
16	P	94/105 (90%)	93 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	107/113 (95%)	98 (92%)	9 (8%)	0	100	100
18	R	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
19	S	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
20	T	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
21	U	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
22	V	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
23	W	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
24	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	Y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
26	Z	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
27	b	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
28	c	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
29	d	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
33	j	244/254 (96%)	225 (92%)	19 (8%)	0	100	100
34	k	384/387 (99%)	364 (95%)	20 (5%)	0	100	100
35	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	41	66
36	m	292/297 (98%)	278 (95%)	14 (5%)	0	100	100
37	n	163/176 (93%)	154 (94%)	9 (6%)	0	100	100
38	o	220/244 (90%)	207 (94%)	13 (6%)	0	100	100
39	p	231/256 (90%)	220 (95%)	11 (5%)	0	100	100
40	q	189/191 (99%)	174 (92%)	14 (7%)	1 (0%)	29	54
41	r	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
42	s	167/174 (96%)	161 (96%)	5 (3%)	1 (1%)	25	50
43	t	191/199 (96%)	174 (91%)	16 (8%)	1 (0%)	29	54
44	u	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
45	a	842/1038 (81%)	831 (99%)	11 (1%)	0	100	100
46	e	1519/1562 (97%)	1505 (99%)	11 (1%)	3 (0%)	47	73
47	g	223/245 (91%)	215 (96%)	8 (4%)	0	100	100
48	v	139/157 (88%)	139 (100%)	0	0	100	100
49	w	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
51	z	144/165 (87%)	137 (95%)	6 (4%)	1 (1%)	22	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	0	117/312 (38%)	116 (99%)	0	1 (1%)	17	40
All	All	9314/10279 (91%)	8970 (96%)	334 (4%)	10 (0%)	54	78

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	e	393	PHE
51	z	88	PRO
46	e	396	ARG
35	l	4	PRO
40	q	107	ASP
42	s	108	GLU
52	0	93	LEU
46	e	855	PRO
15	O	21	ILE
43	t	47	ALA

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/176 (99%)	175 (100%)	0	100	100
2	B	160/162 (99%)	160 (100%)	0	100	100
3	C	138/146 (94%)	138 (100%)	0	100	100
4	D	150/151 (99%)	149 (99%)	1 (1%)	84	94
5	E	129/154 (84%)	129 (100%)	0	100	100
6	F	155/156 (99%)	155 (100%)	0	100	100
7	G	135/137 (98%)	134 (99%)	1 (1%)	84	94
8	H	87/107 (81%)	87 (100%)	0	100	100
9	I	104/105 (99%)	104 (100%)	0	100	100
10	J	54/129 (42%)	54 (100%)	0	100	100
11	K	104/118 (88%)	104 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	108/110 (98%)	108 (100%)	0	100	100
13	M	112/116 (97%)	112 (100%)	0	100	100
14	N	117/119 (98%)	117 (100%)	0	100	100
15	O	46/47 (98%)	45 (98%)	1 (2%)	52	79
16	P	81/88 (92%)	81 (100%)	0	100	100
17	Q	92/97 (95%)	92 (100%)	0	100	100
18	R	107/111 (96%)	107 (100%)	0	100	100
19	S	90/91 (99%)	90 (100%)	0	100	100
20	T	95/103 (92%)	94 (99%)	1 (1%)	73	90
21	U	104/105 (99%)	104 (100%)	0	100	100
22	V	80/82 (98%)	80 (100%)	0	100	100
23	W	67/71 (94%)	67 (100%)	0	100	100
24	X	68/69 (99%)	66 (97%)	2 (3%)	42	71
25	Y	45/46 (98%)	45 (100%)	0	100	100
26	Z	45/116 (39%)	45 (100%)	0	100	100
27	b	87/91 (96%)	87 (100%)	0	100	100
28	c	71/72 (99%)	71 (100%)	0	100	100
29	d	20/23 (87%)	20 (100%)	0	100	100
33	j	189/196 (96%)	188 (100%)	1 (0%)	88	96
34	k	320/323 (99%)	318 (99%)	2 (1%)	86	95
35	l	288/289 (100%)	288 (100%)	0	100	100
36	m	241/245 (98%)	241 (100%)	0	100	100
37	n	139/155 (90%)	138 (99%)	1 (1%)	84	94
38	o	186/205 (91%)	186 (100%)	0	100	100
39	p	187/208 (90%)	187 (100%)	0	100	100
40	q	168/171 (98%)	168 (100%)	0	100	100
41	r	185/187 (99%)	183 (99%)	2 (1%)	73	90
42	s	145/150 (97%)	145 (100%)	0	100	100
43	t	154/159 (97%)	154 (100%)	0	100	100
44	u	107/109 (98%)	107 (100%)	0	100	100
45	a	676/949 (71%)	639 (94%)	37 (6%)	21	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	e	1150/1451 (79%)	1073 (93%)	77 (7%)	16	37
47	g	180/211 (85%)	180 (100%)	0	100	100
48	v	119/132 (90%)	116 (98%)	3 (2%)	47	76
49	w	197/198 (100%)	196 (100%)	1 (0%)	88	96
52	0	104/254 (41%)	95 (91%)	9 (9%)	10	23
All	All	7561/8690 (87%)	7422 (98%)	139 (2%)	61	83

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
7	G	83	ARG
15	O	33	LYS
20	T	106	LYS
24	X	9	LYS
24	X	63	LYS
33	j	221	LYS
34	k	332	ARG
34	k	369	ARG
37	n	8	LYS
41	r	112	GLN
41	r	144	ASN
45	a	3	GLN
45	a	9	ASP
45	a	10	LEU
45	a	25	ARG
45	a	27	SER
45	a	28	ASN
45	a	32	ILE
45	a	63	THR
45	a	89	LEU
45	a	121	ASN
45	a	139	LEU
45	a	156	LEU
45	a	285	ILE
45	a	293	TYR
45	a	316	ILE
45	a	368	ARG
45	a	453	ASP
45	a	589	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	a	605	ILE
45	a	609	ASP
45	a	627	LYS
45	a	630	VAL
45	a	649	TRP
45	a	665	VAL
45	a	682	ARG
45	a	696	GLN
45	a	697	LEU
45	a	837	VAL
45	a	868	THR
45	a	881	GLU
45	a	896	ARG
45	a	917	TYR
45	a	928	LEU
45	a	934	VAL
45	a	947	LEU
45	a	1003	GLN
45	a	1014	LEU
46	e	28	ASN
46	e	102	ASP
46	e	105	VAL
46	e	125	ILE
46	e	143	LEU
46	e	175	GLU
46	e	178	LEU
46	e	190	GLU
46	e	251	ASN
46	e	264	VAL
46	e	299	THR
46	e	310	LEU
46	e	328	ILE
46	e	358	VAL
46	e	394	SER
46	e	401	VAL
46	e	403	ASN
46	e	412	PHE
46	e	698	TYR
46	e	704	THR
46	e	707	LYS
46	e	710	LYS
46	e	731	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	e	733	HIS
46	e	754	ILE
46	e	759	ASP
46	e	770	ILE
46	e	782	TYR
46	e	807	LYS
46	e	819	LEU
46	e	820	ASP
46	e	823	LEU
46	e	826	LEU
46	e	842	SER
46	e	862	PHE
46	e	866	PHE
46	e	893	MET
46	e	895	THR
46	e	904	VAL
46	e	921	ILE
46	e	933	LEU
46	e	987	ILE
46	e	990	VAL
46	e	997	PHE
46	e	1019	ILE
46	e	1047	THR
46	e	1050	LEU
46	e	1061	ARG
46	e	1079	LEU
46	e	1084	LEU
46	e	1086	MET
46	e	1094	TYR
46	e	1102	CYS
46	e	1171	TYR
46	e	1179	LEU
46	e	1189	ASN
46	e	1190	GLN
46	e	1193	LEU
46	e	1195	THR
46	e	1239	LYS
46	e	1240	LEU
46	e	1258	GLU
46	e	1274	LEU
46	e	1286	MET
46	e	1300	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	e	1303	MET
46	e	1342	GLU
46	e	1358	GLN
46	e	1367	THR
46	e	1379	LEU
46	e	1391	ILE
46	e	1409	ARG
46	e	1432	TYR
46	e	1439	LEU
46	e	1441	ILE
46	e	1539	LEU
46	e	1555	ARG
48	v	54	HIS
48	v	71	GLU
48	v	73	LEU
49	w	98	LYS
52	0	30	VAL
52	0	51	VAL
52	0	52	LEU
52	0	67	LEU
52	0	76	LEU
52	0	80	VAL
52	0	93	LEU
52	0	95	GLU
52	0	189	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
45	a	3	GLN
45	a	382	GLN
45	a	413	GLN
45	a	445	GLN
45	a	532	GLN
45	a	599	GLN
45	a	664	ASN
45	a	696	GLN
45	a	957	GLN
45	a	1003	GLN
46	e	160	ASN
46	e	174	GLN
46	e	226	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
46	e	233	ASN
46	e	254	ASN
46	e	1111	GLN
46	e	1138	ASN
46	e	1141	GLN
46	e	1206	GLN
46	e	1293	GLN
46	e	1354	HIS
46	e	1455	GLN
46	e	1484	ASN
46	e	1532	ASN
47	g	9	ASN
48	v	52	HIS
52	0	36	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	f	3212/3395 (94%)	594 (18%)	0
31	h	120/121 (99%)	12 (10%)	0
32	i	157/158 (99%)	32 (20%)	0
50	y	71/76 (93%)	27 (38%)	0
All	All	3560/3750 (94%)	665 (18%)	0

All (665) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	f	6	A
30	f	13	A
30	f	14	U
30	f	26	A
30	f	40	A
30	f	43	A
30	f	49	A
30	f	59	G
30	f	60	A
30	f	65	A
30	f	66	A
30	f	92	G
30	f	99	A
30	f	109	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	110	G
30	f	111	C
30	f	116	A
30	f	120	G
30	f	121	A
30	f	122	A
30	f	133	U
30	f	134	U
30	f	135	C
30	f	136	G
30	f	156	G
30	f	157	A
30	f	165	A
30	f	166	C
30	f	172	G
30	f	173	G
30	f	187	A
30	f	190	U
30	f	191	U
30	f	200	C
30	f	206	G
30	f	210	U
30	f	211	A
30	f	213	A
30	f	218	G
30	f	219	A
30	f	234	G
30	f	240	U
30	f	241	G
30	f	242	C
30	f	243	G
30	f	245	U
30	f	249	U
30	f	252	U
30	f	269	G
30	f	283	G
30	f	286	U
30	f	295	A
30	f	305	U
30	f	323	A
30	f	329	U
30	f	339	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	350	C
30	f	374	A
30	f	376	G
30	f	398	A
30	f	399	A
30	f	401	U
30	f	402	A
30	f	403	C
30	f	421	G
30	f	422	A
30	f	439	C
30	f	440	A
30	f	441	U
30	f	442	G
30	f	443	G
30	f	445	G
30	f	446	U
30	f	447	U
30	f	448	U
30	f	450	G
30	f	487	U
30	f	488	U
30	f	489	U
30	f	490	C
30	f	494	G
30	f	518	G
30	f	520	U
30	f	521	A
30	f	523	A
30	f	535	G
30	f	536	U
30	f	543	C
30	f	544	C
30	f	546	C
30	f	547	G
30	f	548	G
30	f	551	A
30	f	552	G
30	f	555	U
30	f	557	A
30	f	559	A
30	f	578	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	579	G
30	f	589	A
30	f	597	G
30	f	604	G
30	f	608	A
30	f	609	G
30	f	611	A
30	f	620	U
30	f	621	A
30	f	622	A
30	f	637	C
30	f	638	C
30	f	649	A
30	f	660	A
30	f	667	C
30	f	677	A
30	f	681	U
30	f	684	G
30	f	690	A
30	f	691	A
30	f	705	A
30	f	712	G
30	f	715	A
30	f	716	A
30	f	719	U
30	f	720	A
30	f	758	C
30	f	763	G
30	f	764	U
30	f	765	C
30	f	766	U
30	f	767	U
30	f	776	U
30	f	777	U
30	f	780	A
30	f	781	G
30	f	785	G
30	f	786	A
30	f	806	A
30	f	817	A
30	f	830	A
30	f	846	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	849	C
30	f	850	U
30	f	861	C
30	f	874	U
30	f	879	U
30	f	896	A
30	f	907	G
30	f	908	G
30	f	914	A
30	f	916	G
30	f	917	A
30	f	920	A
30	f	921	A
30	f	924	G
30	f	925	A
30	f	937	G
30	f	944	C
30	f	959	C
30	f	960	U
30	f	981	U
30	f	982	C
30	f	991	G
30	f	994	G
30	f	1001	G
30	f	1002	A
30	f	1010	G
30	f	1015	U
30	f	1016	C
30	f	1017	C
30	f	1018	G
30	f	1021	G
30	f	1024	G
30	f	1025	A
30	f	1028	U
30	f	1036	A
30	f	1041	U
30	f	1047	A
30	f	1049	C
30	f	1063	G
30	f	1064	A
30	f	1065	A
30	f	1072	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	1081	U
30	f	1087	G
30	f	1093	A
30	f	1094	U
30	f	1095	U
30	f	1097	G
30	f	1098	A
30	f	1103	A
30	f	1104	G
30	f	1117	G
30	f	1131	G
30	f	1144	U
30	f	1153	A
30	f	1159	A
30	f	1160	C
30	f	1177	G
30	f	1180	A
30	f	1181	U
30	f	1192	C
30	f	1193	A
30	f	1196	C
30	f	1197	A
30	f	1201	C
30	f	1202	A
30	f	1208	U
30	f	1217	A
30	f	1218	U
30	f	1219	C
30	f	1222	G
30	f	1225	A
30	f	1227	C
30	f	1235	U
30	f	1236	G
30	f	1238	C
30	f	1241	U
30	f	1242	G
30	f	1244	A
30	f	1245	A
30	f	1251	A
30	f	1252	A
30	f	1254	C
30	f	1258	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	1259	A
30	f	1263	A
30	f	1264	G
30	f	1265	U
30	f	1269	U
30	f	1272	C
30	f	1277	C
30	f	1278	A
30	f	1279	C
30	f	1282	G
30	f	1285	G
30	f	1286	A
30	f	1287	A
30	f	1295	G
30	f	1307	G
30	f	1308	A
30	f	1309	U
30	f	1313	G
30	f	1330	A
30	f	1348	U
30	f	1349	G
30	f	1351	U
30	f	1352	A
30	f	1354	G
30	f	1355	A
30	f	1356	U
30	f	1357	G
30	f	1386	A
30	f	1392	G
30	f	1399	A
30	f	1400	G
30	f	1419	A
30	f	1434	G
30	f	1437	C
30	f	1446	A
30	f	1450	G
30	f	1481	A
30	f	1482	A
30	f	1483	G
30	f	1487	G
30	f	1488	G
30	f	1502	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	1508	C
30	f	1536	G
30	f	1539	A
30	f	1555	U
30	f	1556	C
30	f	1557	A
30	f	1560	G
30	f	1562	C
30	f	1563	C
30	f	1566	A
30	f	1568	U
30	f	1569	U
30	f	1572	U
30	f	1573	G
30	f	1575	A
30	f	1576	G
30	f	1580	A
30	f	1581	C
30	f	1582	C
30	f	1583	A
30	f	1589	A
30	f	1590	G
30	f	1605	A
30	f	1607	U
30	f	1620	U
30	f	1629	U
30	f	1639	C
30	f	1642	A
30	f	1643	A
30	f	1645	U
30	f	1657	C
30	f	1683	A
30	f	1716	U
30	f	1717	U
30	f	1724	U
30	f	1725	C
30	f	1736	G
30	f	1741	A
30	f	1750	A
30	f	1751	G
30	f	1760	A
30	f	1761	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	1764	U
30	f	1765	U
30	f	1766	G
30	f	1770	G
30	f	1775	G
30	f	1780	G
30	f	1797	A
30	f	1814	A
30	f	1816	A
30	f	1819	U
30	f	1820	U
30	f	1821	U
30	f	1835	A
30	f	1839	A
30	f	1840	U
30	f	1841	A
30	f	1842	A
30	f	1846	C
30	f	1849	C
30	f	1850	A
30	f	1866	C
30	f	1867	A
30	f	1880	U
30	f	1881	A
30	f	1893	A
30	f	1906	G
30	f	1943	C
30	f	1952	G
30	f	1953	G
30	f	1954	G
30	f	2094	C
30	f	2101	C
30	f	2102	U
30	f	2111	G
30	f	2112	U
30	f	2113	A
30	f	2114	C
30	f	2121	G
30	f	2122	G
30	f	2131	A
30	f	2134	G
30	f	2140	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	2144	A
30	f	2158	A
30	f	2160	G
30	f	2169	G
30	f	2176	U
30	f	2201	G
30	f	2206	G
30	f	2207	A
30	f	2208	A
30	f	2209	U
30	f	2222	A
30	f	2223	A
30	f	2225	U
30	f	2228	A
30	f	2249	G
30	f	2270	A
30	f	2272	G
30	f	2273	G
30	f	2274	U
30	f	2281	A
30	f	2282	U
30	f	2288	G
30	f	2307	G
30	f	2308	C
30	f	2310	U
30	f	2313	A
30	f	2314	U
30	f	2315	G
30	f	2334	U
30	f	2335	G
30	f	2336	U
30	f	2373	A
30	f	2374	C
30	f	2375	G
30	f	2385	G
30	f	2388	U
30	f	2393	G
30	f	2397	A
30	f	2402	A
30	f	2403	G
30	f	2404	A
30	f	2411	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	2419	A
30	f	2437	G
30	f	2446	U
30	f	2447	A
30	f	2450	G
30	f	2461	A
30	f	2463	G
30	f	2464	U
30	f	2468	A
30	f	2469	G
30	f	2470	C
30	f	2471	U
30	f	2472	U
30	f	2474	G
30	f	2479	C
30	f	2480	A
30	f	2484	A
30	f	2486	A
30	f	2487	U
30	f	2488	A
30	f	2494	A
30	f	2495	C
30	f	2496	C
30	f	2499	U
30	f	2501	U
30	f	2502	A
30	f	2503	G
30	f	2505	U
30	f	2514	U
30	f	2515	A
30	f	2522	G
30	f	2526	C
30	f	2531	C
30	f	2537	U
30	f	2538	U
30	f	2539	C
30	f	2540	A
30	f	2541	U
30	f	2542	U
30	f	2544	U
30	f	2547	A
30	f	2548	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	2549	G
30	f	2552	C
30	f	2554	A
30	f	2555	G
30	f	2561	A
30	f	2569	A
30	f	2570	U
30	f	2571	U
30	f	2572	C
30	f	2573	G
30	f	2581	U
30	f	2585	G
30	f	2593	A
30	f	2594	C
30	f	2606	G
30	f	2607	G
30	f	2614	G
30	f	2648	G
30	f	2651	G
30	f	2652	U
30	f	2656	A
30	f	2674	A
30	f	2677	G
30	f	2678	A
30	f	2689	A
30	f	2691	A
30	f	2694	A
30	f	2696	A
30	f	2704	A
30	f	2714	G
30	f	2719	U
30	f	2728	G
30	f	2729	U
30	f	2740	A
30	f	2752	U
30	f	2753	G
30	f	2755	C
30	f	2772	C
30	f	2773	C
30	f	2777	G
30	f	2778	G
30	f	2788	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	2796	G
30	f	2800	G
30	f	2801	A
30	f	2803	A
30	f	2810	C
30	f	2814	G
30	f	2817	A
30	f	2818	U
30	f	2821	C
30	f	2834	G
30	f	2842	U
30	f	2844	C
30	f	2845	A
30	f	2849	C
30	f	2860	U
30	f	2867	C
30	f	2871	G
30	f	2872	A
30	f	2875	U
30	f	2887	A
30	f	2898	G
30	f	2899	C
30	f	2911	A
30	f	2914	G
30	f	2923	U
30	f	2935	U
30	f	2936	A
30	f	2938	G
30	f	2941	A
30	f	2942	C
30	f	2947	G
30	f	2955	U
30	f	2971	A
30	f	2983	C
30	f	2990	G
30	f	2992	U
30	f	2996	U
30	f	2997	G
30	f	3006	A
30	f	3012	A
30	f	3056	U
30	f	3059	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	3078	U
30	f	3079	U
30	f	3080	G
30	f	3086	A
30	f	3092	C
30	f	3104	U
30	f	3113	A
30	f	3122	A
30	f	3130	A
30	f	3131	U
30	f	3142	A
30	f	3143	C
30	f	3151	U
30	f	3154	C
30	f	3155	U
30	f	3156	U
30	f	3157	U
30	f	3165	A
30	f	3170	A
30	f	3173	G
30	f	3174	A
30	f	3175	U
30	f	3176	G
30	f	3179	U
30	f	3181	C
30	f	3186	A
30	f	3187	A
30	f	3196	U
30	f	3207	U
30	f	3209	A
30	f	3217	C
30	f	3218	A
30	f	3219	G
30	f	3228	C
30	f	3229	G
30	f	3243	A
30	f	3245	A
30	f	3247	G
30	f	3259	U
30	f	3263	G
30	f	3269	U
30	f	3270	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	f	3273	A
30	f	3276	G
30	f	3281	U
30	f	3287	U
30	f	3288	G
30	f	3289	G
30	f	3294	A
30	f	3295	A
30	f	3303	G
30	f	3304	U
30	f	3307	A
30	f	3313	U
30	f	3316	A
30	f	3317	U
30	f	3318	G
30	f	3319	U
30	f	3320	A
30	f	3341	U
30	f	3342	A
30	f	3345	G
30	f	3351	U
30	f	3352	U
30	f	3353	G
30	f	3354	U
30	f	3355	U
30	f	3369	G
30	f	3375	A
30	f	3378	C
30	f	3382	U
30	f	3383	G
30	f	3386	G
30	f	3389	U
30	f	3390	G
30	f	3396	U
31	h	7	G
31	h	29	C
31	h	53	U
31	h	54	U
31	h	55	A
31	h	65	G
31	h	73	C
31	h	74	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	h	95	A
31	h	102	A
31	h	112	G
31	h	121	U
32	i	23	U
32	i	34	U
32	i	35	C
32	i	39	G
32	i	48	A
32	i	52	A
32	i	53	A
32	i	59	A
32	i	62	C
32	i	63	G
32	i	80	A
32	i	81	U
32	i	82	U
32	i	83	C
32	i	84	C
32	i	85	G
32	i	86	U
32	i	87	G
32	i	90	U
32	i	95	G
32	i	104	A
32	i	105	A
32	i	106	C
32	i	111	A
32	i	113	U
32	i	125	U
32	i	126	A
32	i	138	A
32	i	151	C
32	i	152	G
32	i	157	U
32	i	158	U
50	y	7	G
50	y	8	U
50	y	9	G
50	y	13	U
50	y	16	U
50	y	17	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
50	y	22	G
50	y	23	C
50	y	31	C
50	y	34	A
50	y	35	G
50	y	36	C
50	y	38	U
50	y	42	A
50	y	43	G
50	y	44	A
50	y	45	G
50	y	46	G
50	y	47	U
50	y	48	C
50	y	56	C
50	y	58	A
50	y	60	U
50	y	68	C
50	y	71	C
50	y	75	C
50	y	76	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
48	5CT	v	51	48	13,14,15	0.76	0	9,15,17	1.29	1 (11%)

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
48	5CT	v	51	48	-	9/13/14/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	v	51	5CT	C4-C3-C2	-2.19	108.85	113.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	v	51	5CT	NZ-C1-C2-C3
48	v	51	5CT	O1-C2-C3-C4
48	v	51	5CT	C2-C3-C4-N1
48	v	51	5CT	C-CA-CB-CG
48	v	51	5CT	N-CA-CB-CG
48	v	51	5CT	NZ-C1-C2-O1
48	v	51	5CT	C1-C2-C3-C4
48	v	51	5CT	CE-CD-CG-CB
48	v	51	5CT	C2-C1-NZ-CE

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 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	SPD	f	3401	-	9,9,9	0.32	0	8,8,8	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	SPD	f	3401	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	f	3401	SPD	C3-C4-C5-N6
56	f	3401	SPD	N6-C7-C8-C9
56	f	3401	SPD	C2-C3-C4-C5
56	f	3401	SPD	C8-C7-N6-C5
56	f	3401	SPD	C4-C5-N6-C7

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](#)

There are no chain breaks in this entry.

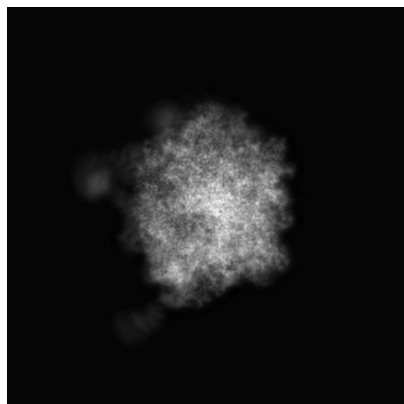
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15424. These allow visual inspection of the internal detail of the map and identification of artifacts.

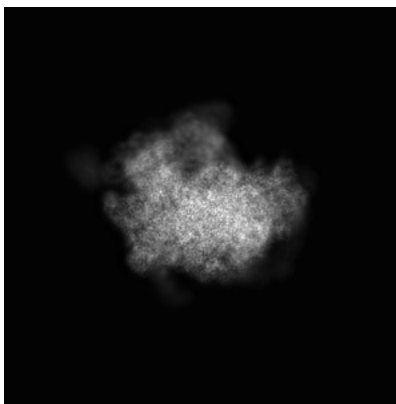
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

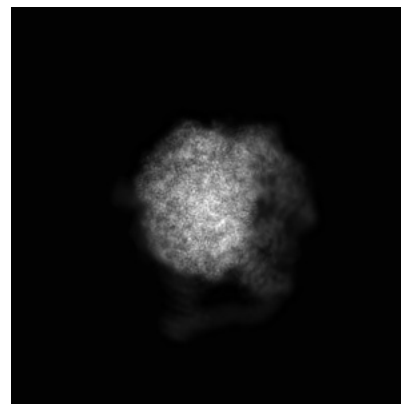
6.1.1 Primary map



X

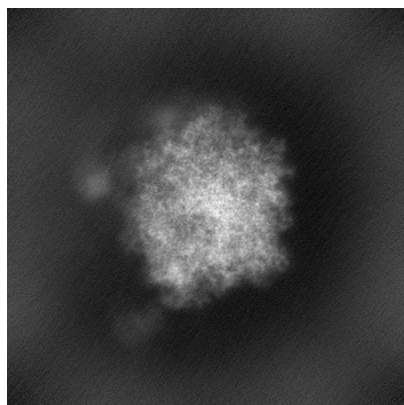


Y

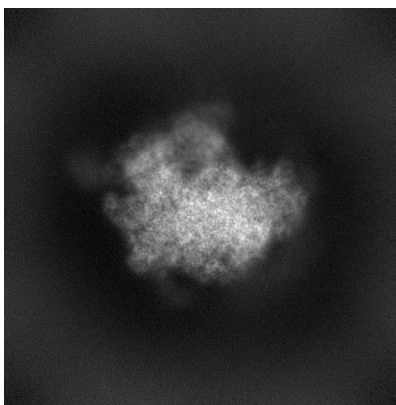


Z

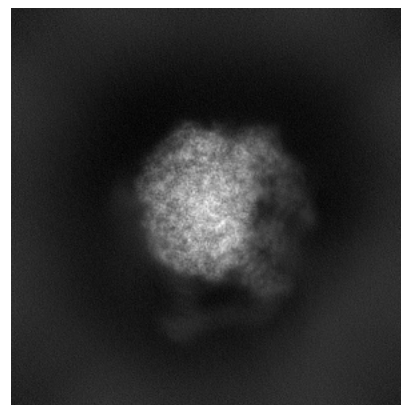
6.1.2 Raw map



X



Y

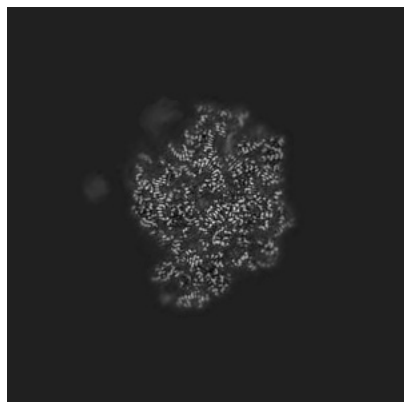


Z

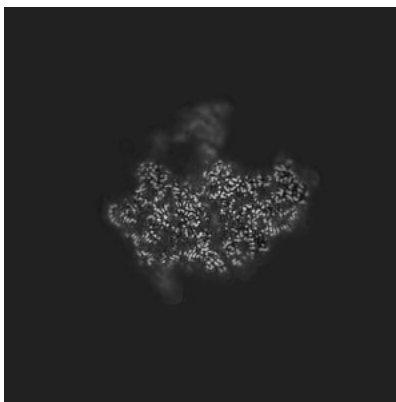
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

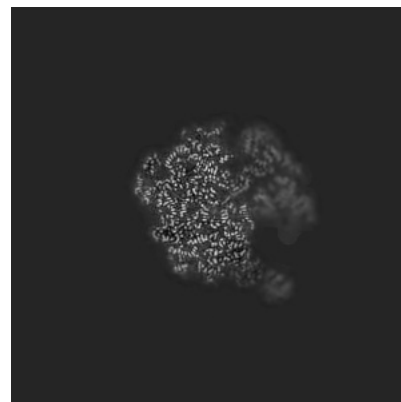
6.2.1 Primary map



X Index: 225

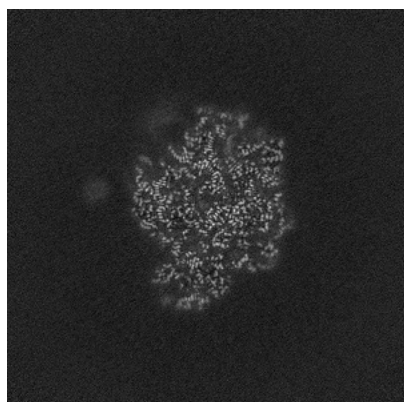


Y Index: 225

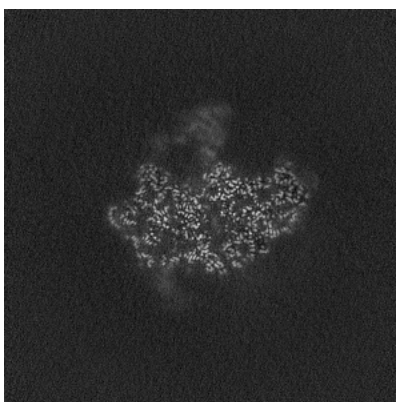


Z Index: 225

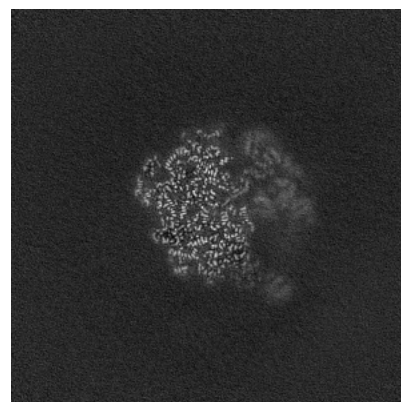
6.2.2 Raw map



X Index: 225



Y Index: 225

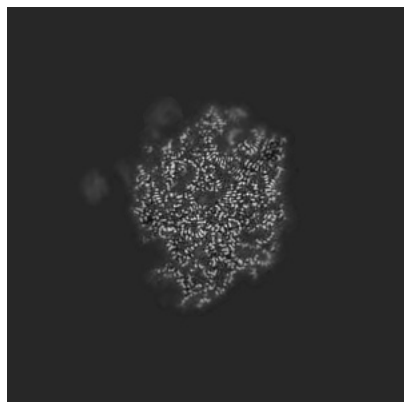


Z Index: 225

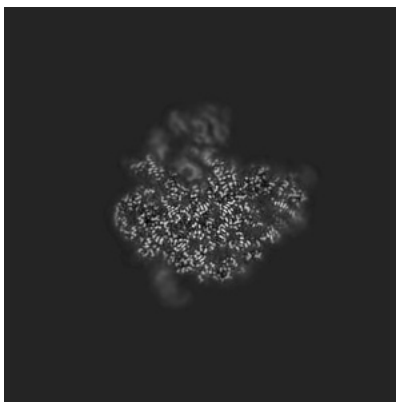
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

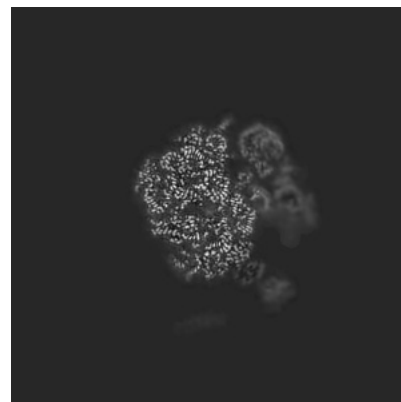
6.3.1 Primary map



X Index: 219

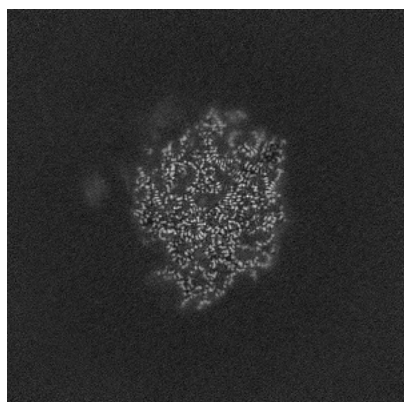


Y Index: 237

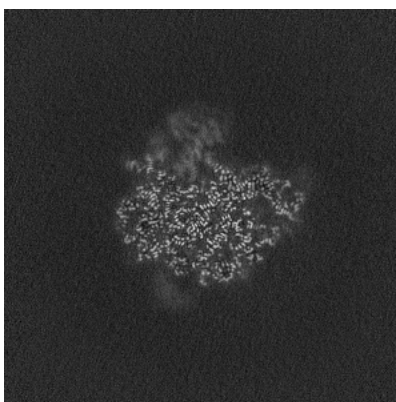


Z Index: 231

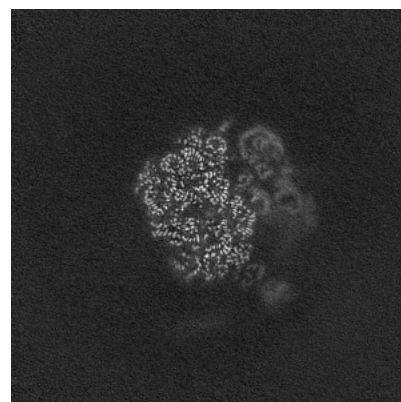
6.3.2 Raw map



X Index: 219



Y Index: 241

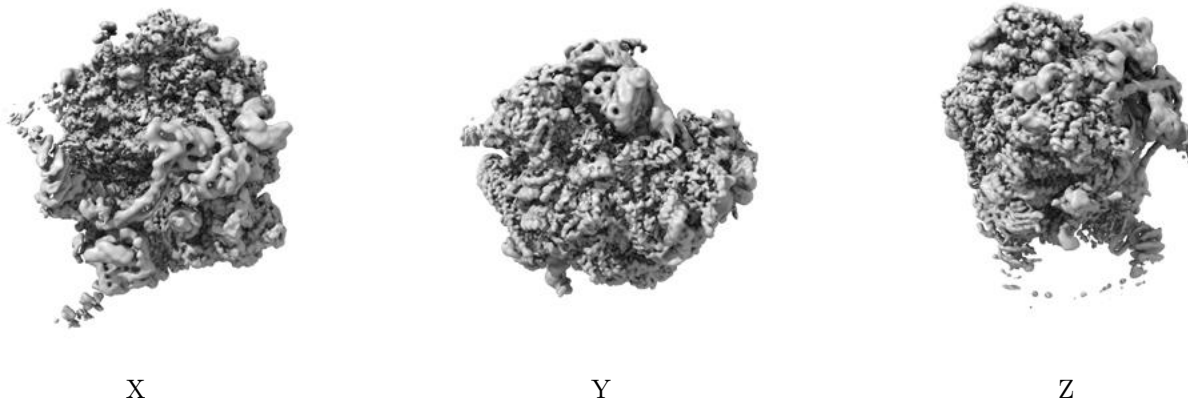


Z Index: 231

The images above show the largest variance slices of the map in three orthogonal directions.

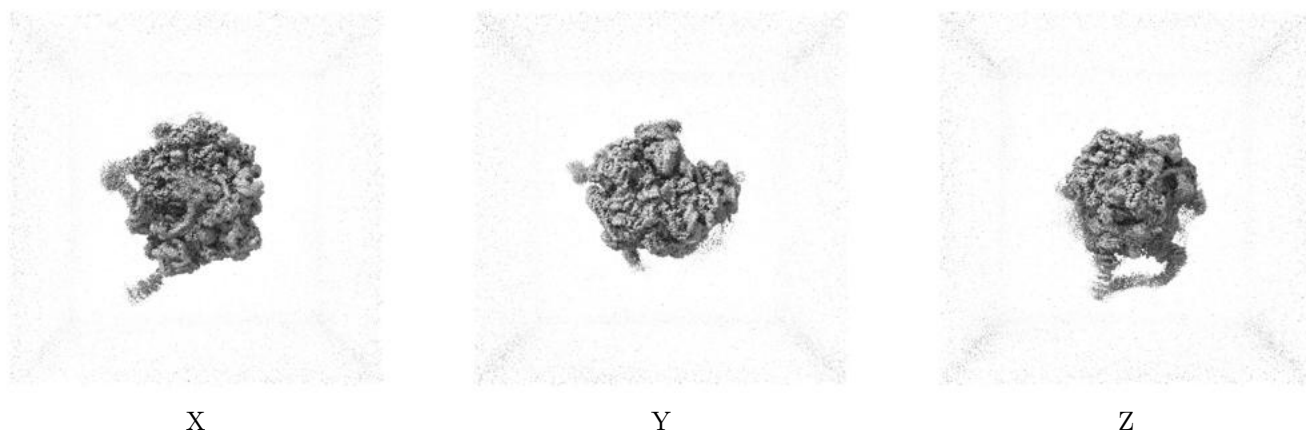
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

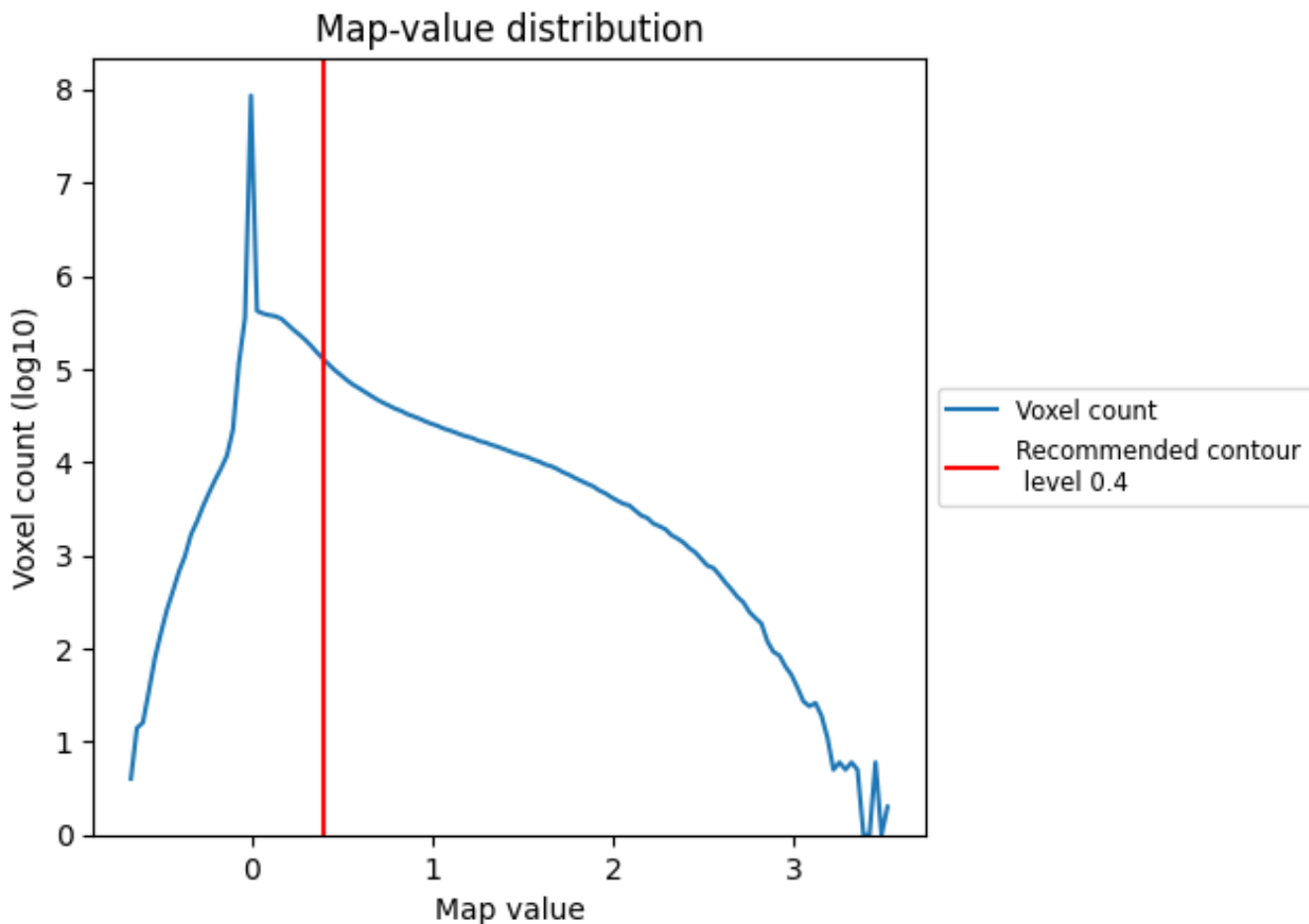
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

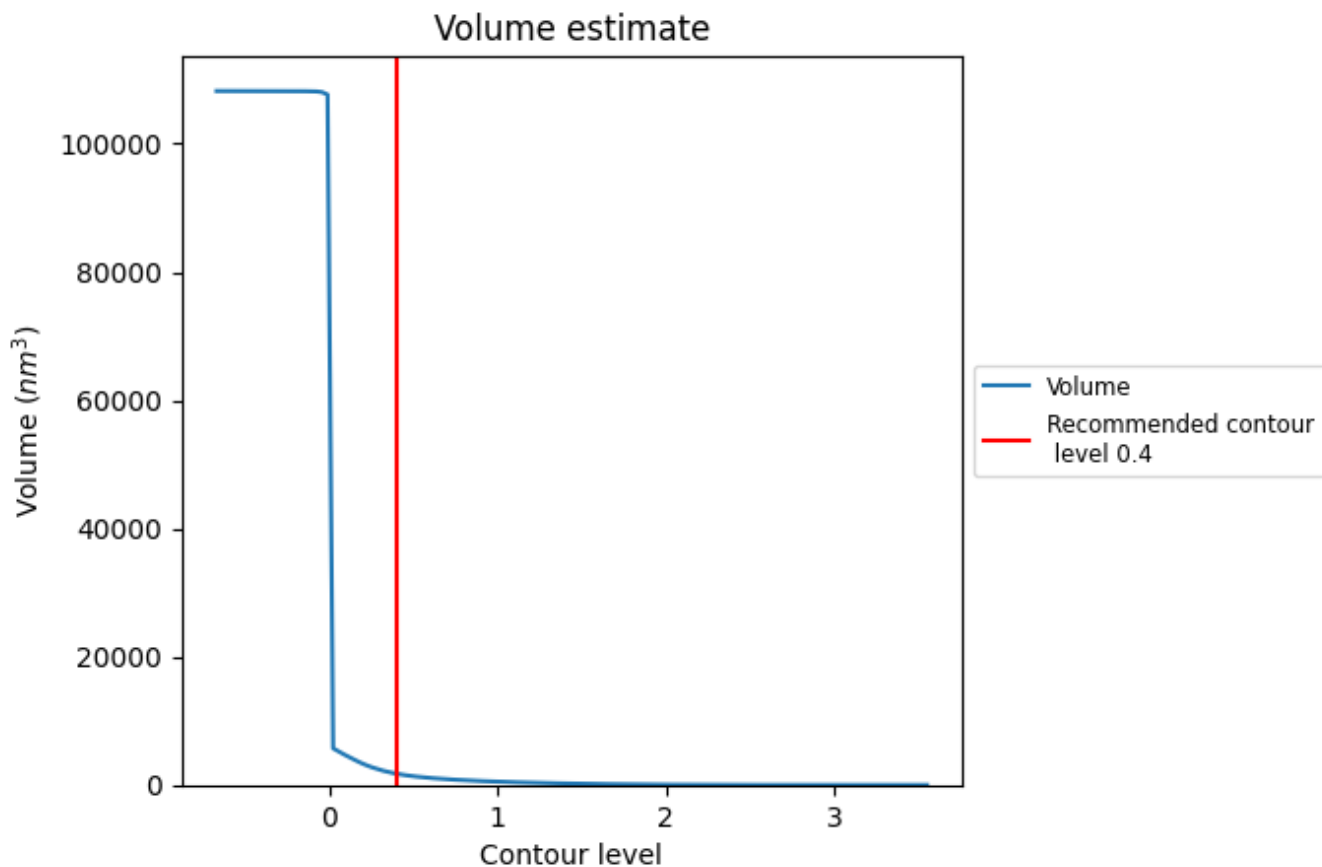
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

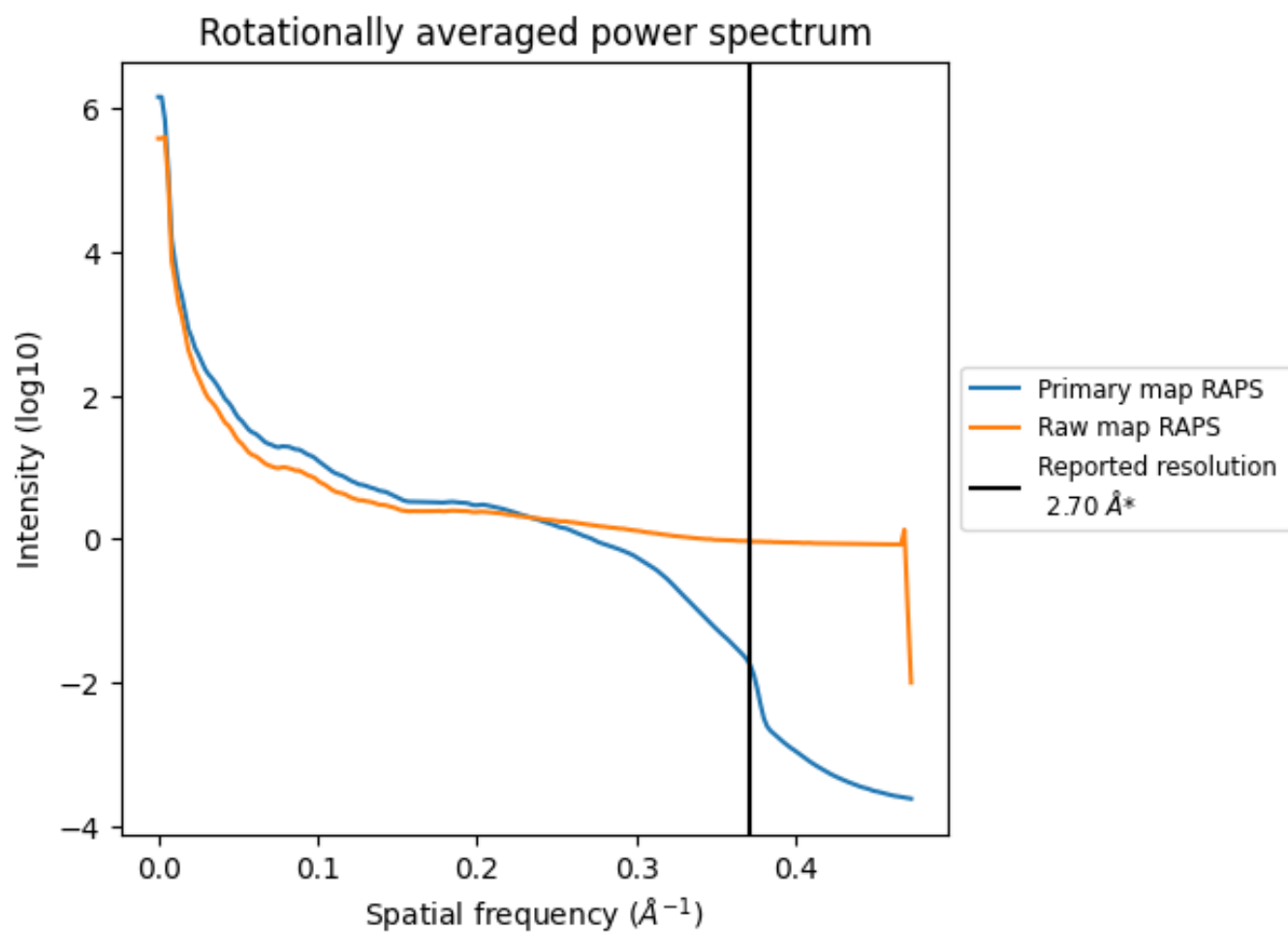
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1749 nm³; this corresponds to an approximate mass of 1580 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

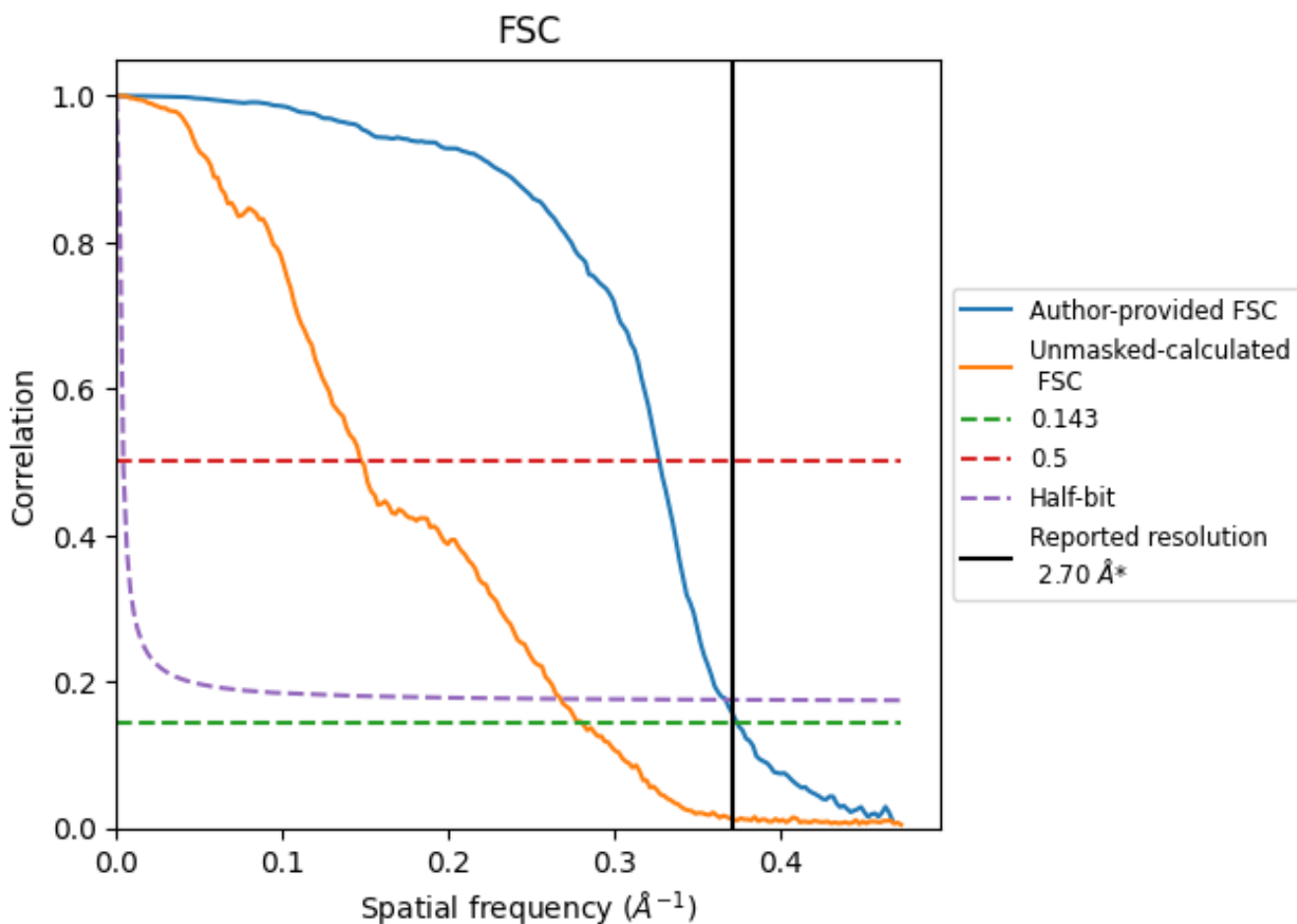


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

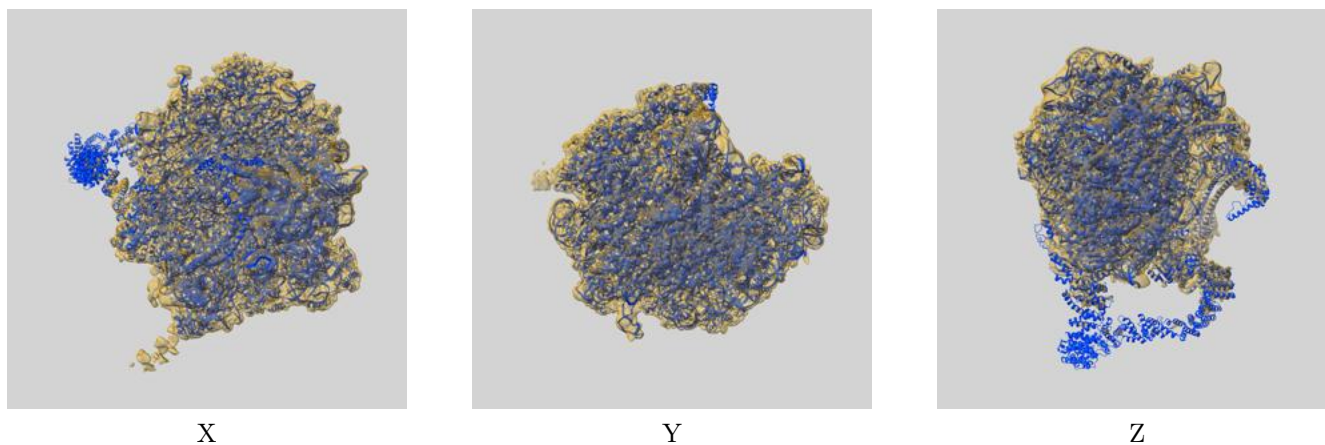
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.06	2.73
Unmasked-calculated*	3.57	6.78	3.74

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.57 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

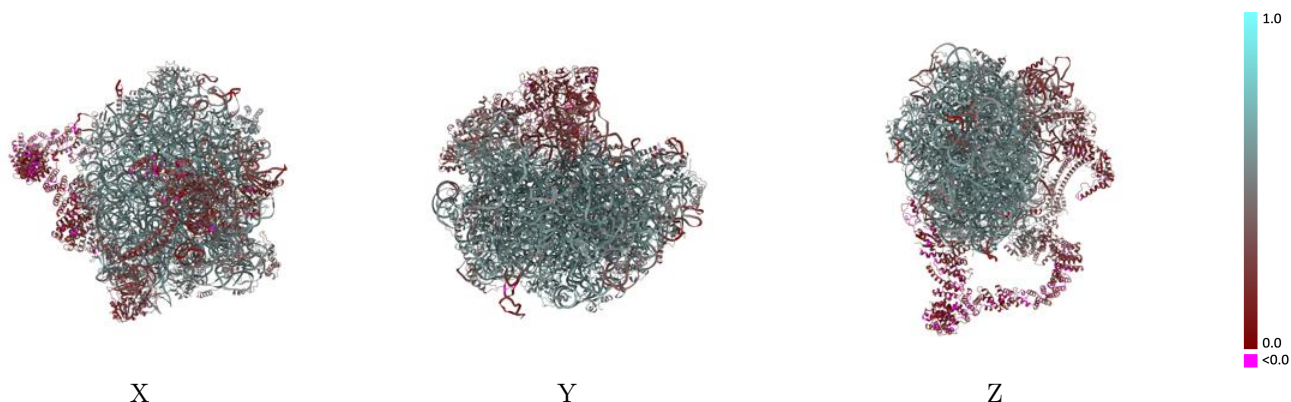
This section contains information regarding the fit between EMDB map EMD-15424 and PDB model 8AGU. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



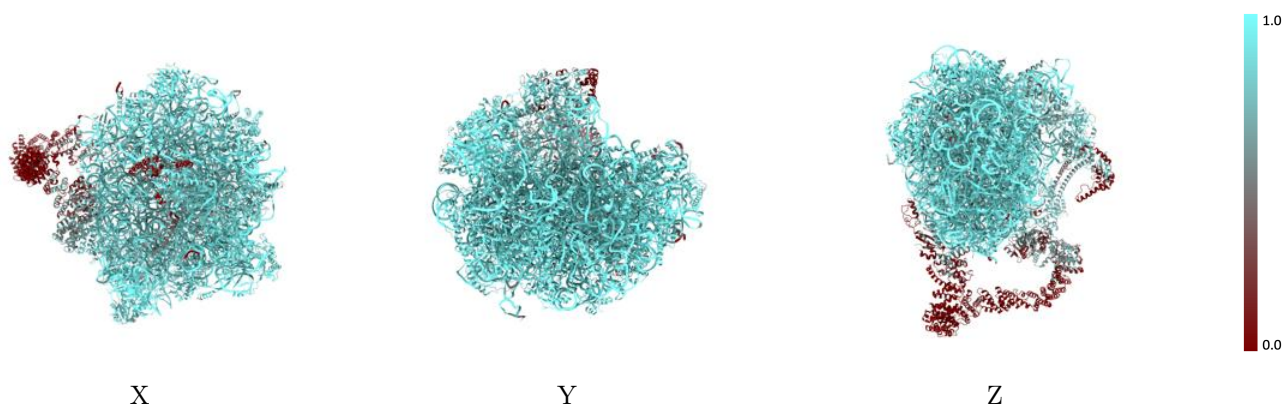
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



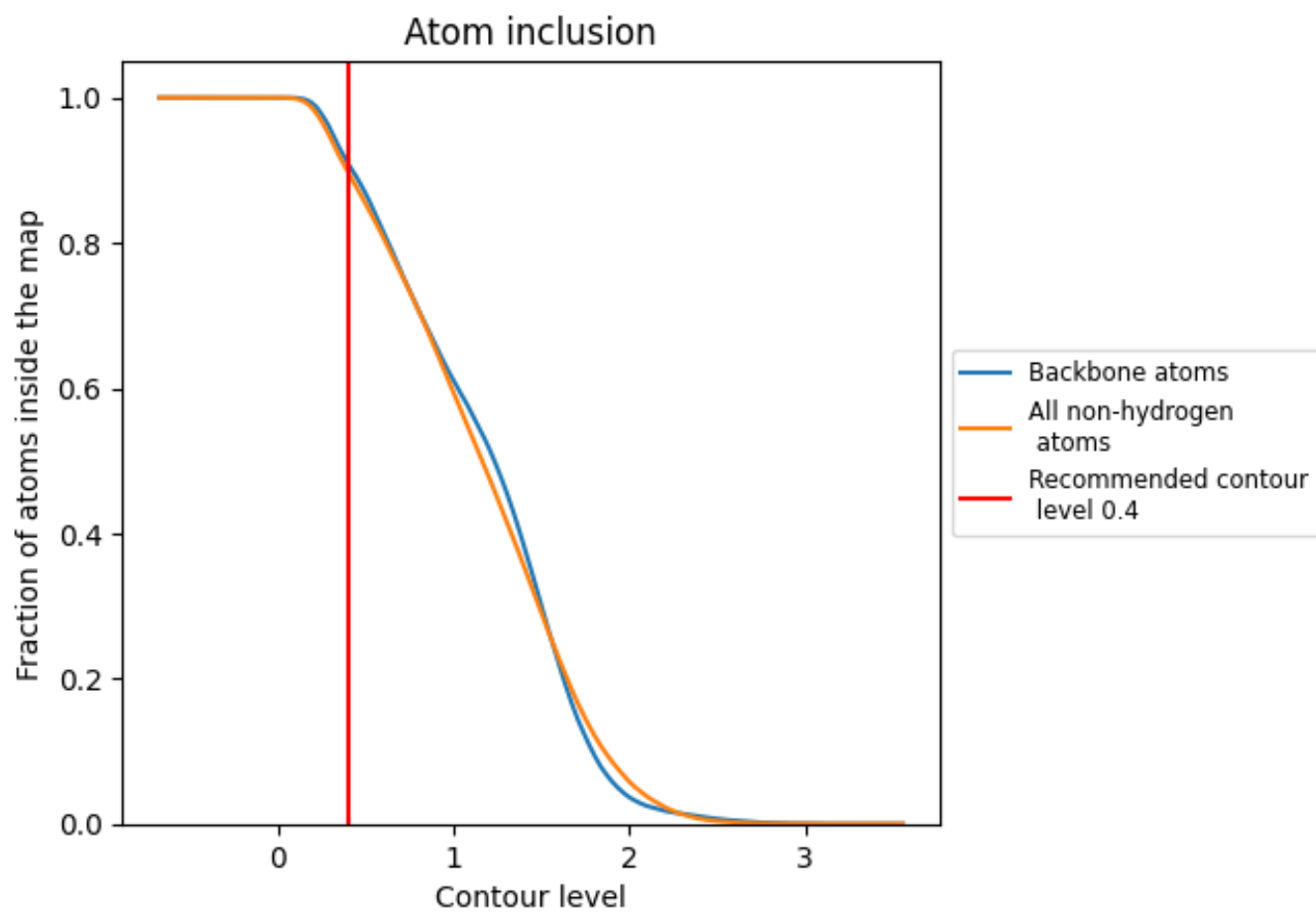
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary







































The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8977	 0.4960
0	 0.8066	 0.2580
1	 0.9882	 0.4550
A	 0.9921	 0.5990
B	 0.9789	 0.5770
C	 0.9679	 0.5790
D	 0.9756	 0.5700
E	 0.9340	 0.5360
F	 0.9720	 0.5680
G	 0.9652	 0.5510
H	 0.9130	 0.4540
I	 0.9561	 0.5630
J	 0.9582	 0.5570
K	 0.9692	 0.5560
L	 0.9676	 0.5530
M	 0.9396	 0.5040
N	 0.9745	 0.5820
O	 0.9447	 0.5240
P	 0.9366	 0.5070
Q	 0.9200	 0.5350
R	 0.9767	 0.5880
S	 0.9903	 0.6100
T	 0.9695	 0.5620
U	 0.9618	 0.5400
V	 0.9541	 0.5170
W	 1.0000	 0.6140
X	 0.9082	 0.4740
Y	 0.9976	 0.5930
Z	 0.9647	 0.5610
a	 0.6672	 0.2240
b	 0.9628	 0.5560
c	 0.9672	 0.5530
d	 0.7181	 0.3780
e	 0.2490	 0.1560
f	 0.9895	 0.5600



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.3759	 0.3870
h	 0.9992	 0.5570
i	 0.9943	 0.5870
j	 0.9824	 0.5950
k	 0.9716	 0.5730
l	 0.9717	 0.5620
m	 0.9384	 0.4740
n	 0.9508	 0.5130
o	 0.9701	 0.5580
p	 0.9374	 0.5060
q	 0.9561	 0.5330
r	 0.9508	 0.5240
s	 0.9213	 0.4230
t	 0.9650	 0.5490
u	 0.9678	 0.5350
v	 0.8409	 0.3850
w	 0.8053	 0.2370
y	 0.9704	 0.2580
z	 0.9080	 0.2700