



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 10:19 PM EDT

PDB ID : 9BLN / pdb_00009bln
EMDB ID : EMD-44671
Title : The structure of human Pdcd4 bound to the 40S-eIF4A-eIF3-eIF1 complex
Authors : Brito Querido, J.; Sokabe, M.; Diaz-Lopez, I.; Gordiyenko, Y.; Zuber, P.; Yifei, D.; Albacete-Albacete, L.; Ramakrishnan, V.; S Fraser, C.
Deposited on : 2024-04-30
Resolution : 3.90 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:

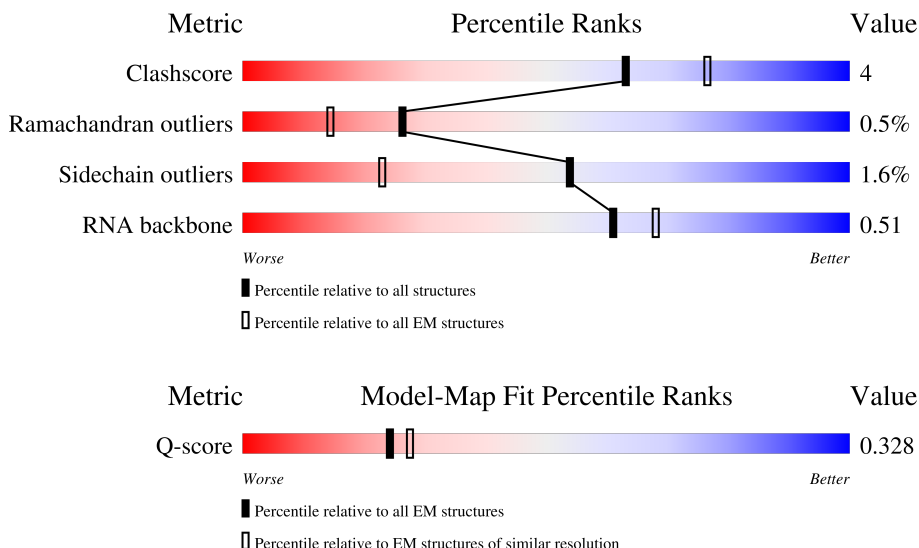
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	X	325	100% 99%
2	U	661	85% 80% 15%
3	3	218	98% 97%

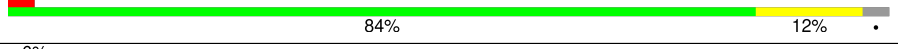
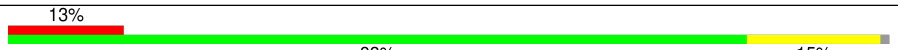
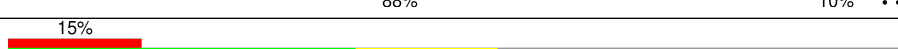
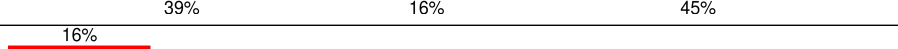
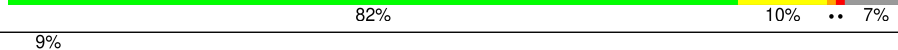
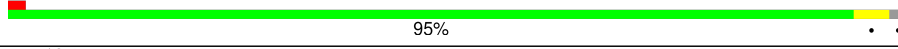
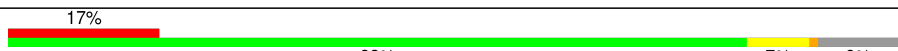
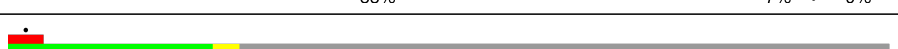
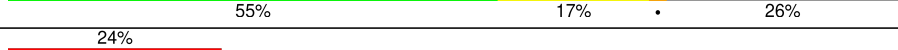
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Mol	Chain	Length	Quality of chain
4	4	357	
5	5	564	
6	6	374	
7	8	352	
8	9	25	
9	A	1719	
10	B	158	
11	C	263	
12	D	194	
13	E	143	
14	F	59	
15	G	194	
16	H	84	
17	I	151	
18	J	130	
19	K	83	
20	L	293	
21	M	135	
22	N	295	
23	O	264	
24	P	151	
25	Q	115	
26	R	208	
27	S	249	
28	T	133	

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Mol	Chain	Length	Quality of chain
29	V	204	
30	W	113	
31	Y	146	
32	Z	243	
33	a	165	
34	b	145	
35	c	317	
36	d	145	
37	e	125	
38	f	152	
39	h	119	
40	i	56	
41	k	156	
42	l	388	
43	m	132	
44	n	69	
45	o	320	
46	p	469	
47	u	1382	
48	v	445	
49	x	548	
50	y	913	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 104352 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 Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	X	325	Total	C	N	O	0	0
			1598	947	325	326		

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	U	560	Total	C	N	O	0	0
			2770	1650	560	560		

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	3	213	Total	C	N	O	0	0
			1057	631	213	213		

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	4	257	Total	C	N	O	0	0
			1272	757	257	258		

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	5	319	Total	C	N	O	0	0
			1581	943	319	319		

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	350	Total	C	N	O	S	0	0
			1917	1159	376	380	2		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	8	317	Total	C	N	O	0	0
			1571	936	317	318		

- Molecule 8 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 9 is a RNA chain called rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	1672	Total	C	N	O	P	0	0
			35720	15962	6403	11683	1672		

- Molecule 10 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	143	Total	C	N	O	S	0	0
			1177	749	222	200	6		

- Molecule 11 is a protein called Small ribosomal subunit protein eS4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	256	Total	C	N	O	S	0	0
			2035	1302	378	347	8		

- Molecule 12 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	177	Total	C	N	O	S	0	0
			1477	941	295	239	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	140	Total	C	N	O	S	0	0
			1087	687	215	182	3		

- Molecule 14 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	54	Total	C	N	O	S	0	0
			424	262	92	69	1		

- Molecule 15 is a protein called Small ribosomal subunit protein eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	173	Total	C	N	O	S	0	0
			1399	895	255	248	1		

- Molecule 16 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	81	Total	C	N	O	S	0	0
			631	397	116	111	7		

- Molecule 17 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 19 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	81	Total	C	N	O	S	0	0
			617	380	114	118	5		

- Molecule 20 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	220	Total	C	N	O	S	0	0
			1707	1104	292	301	10		

- Molecule 21 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	131	Total	C	N	O	S	0	0
			1064	668	198	194	4		

- Molecule 22 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	207	Total	C	N	O	S	0	0
			1633	1040	288	297	8		

- Molecule 23 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	211	Total	C	N	O	S	0	0
			1715	1088	307	306	14		

- Molecule 24 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	131	Total	C	N	O	S	0	0
			981	600	193	182	6		

- Molecule 25 is a protein called Small ribosomal subunit protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	99	Total	C	N	O	S	0	0
			792	492	165	130	5		

- Molecule 26 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	198	Total	C	N	O	S	0	0
			1627	1021	322	279	5		

- Molecule 27 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 28 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 29 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

- Molecule 30 is a protein called Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	84	Total	C	N	O	S	0	0
			683	434	124	123	2		

- Molecule 31 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 32 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	231	Total	C	N	O	S	0	0
			1783	1135	321	319	8		

- Molecule 33 is a protein called Small ribosomal subunit protein eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	99	Total	C	N	O	S	0	0
			834	544	149	135	6		

- Molecule 34 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	118	Total	C	N	O	S	0	0
			972	617	182	166	7		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 36 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	142	Total	C	N	O	S	0	0
			1105	692	213	197	3		

- Molecule 37 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	69	Total	C	N	O	S	0	0
			551	356	100	94	1		

- Molecule 38 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	142	Total	C	N	O	S	0	0
			1176	737	239	199	1		

- Molecule 39 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	103	Total	C	N	O	S	0	0
			817	511	155	147	4		

- Molecule 40 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 41 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	52	Total	C	N	O	S	0	0
			429	271	82	69	7		

- Molecule 42 is a protein called Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	l	345	Total	C	N	O	0	0
			1706	1016	345	345		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	19	MET	-	initiating methionine	UNP P60842

- Molecule 43 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	122	Total	C	N	O	S	0	0
			950	596	168	177	9		

- Molecule 44 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	63	Total	C	N	O	S	0	0
			498	302	101	93	2		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	o	85	Total	C	N	O	0	0
			420	249	85	86		

- Molecule 46 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	p	346	Total	C	N	O	0	0
			1839	1100	367	372		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	u	572	Total	C	N	O	S	1	0
			4708	2975	847	863	23		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	v	384	Total	C	N	O	S	0	0
			2635	1657	477	489	12		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	x	428	Total	C	N	O	0	0
			2121	1265	428	428		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	535	Total	C	N	O	S	0	0
			4325	2723	768	801	33		

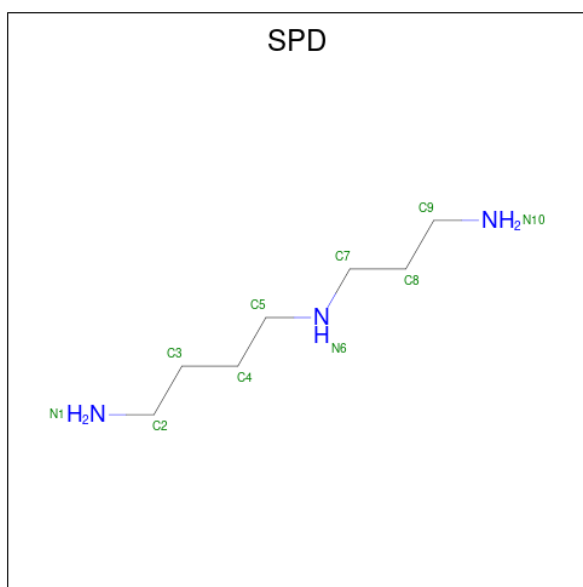
- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
51	A	87	Total	Mg	0
			87	87	
51	f	1	Total	Mg	0
			1	1	

- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
52	A	18	Total	K	0
			18	18	
52	i	1	Total	K	0
			1	1	

- Molecule 53 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).

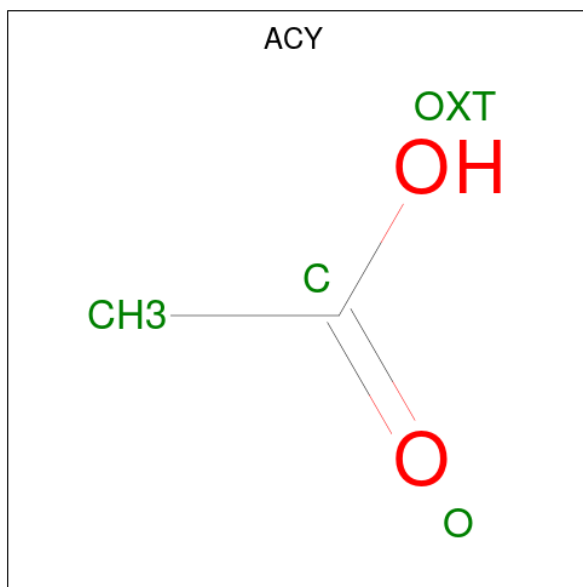


Mol	Chain	Residues	Atoms			AltConf
53	A	1	Total	C	N	0
			10	7	3	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
54	Q	1	Total	Zn	0
			1	1	
54	i	1	Total	Zn	0
			1	1	
54	k	1	Total	Zn	0
			1	1	

- Molecule 55 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂) (labeled as "Ligand of Interest" by depositor).

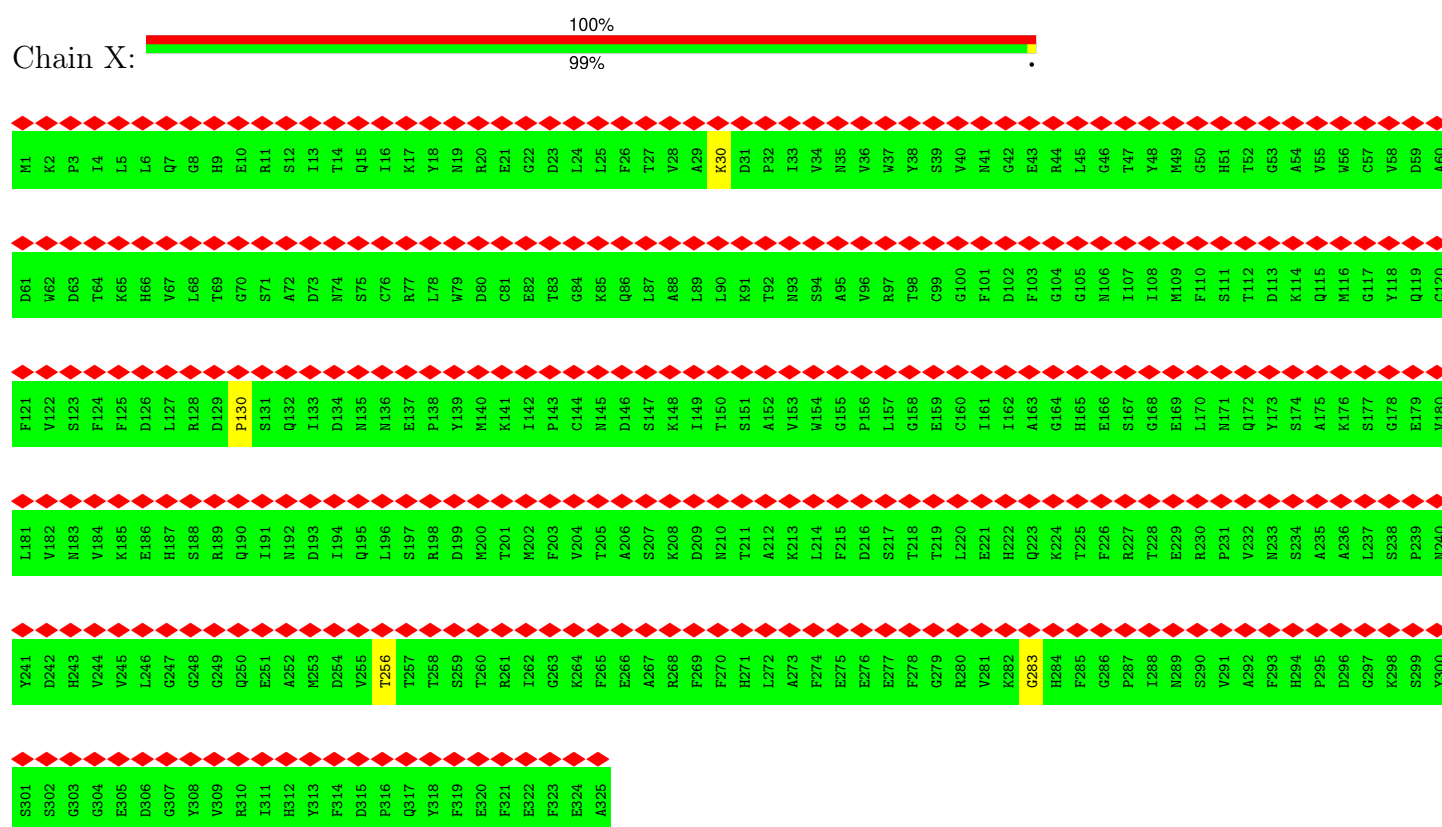


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
55	1	1	3	1	2	0

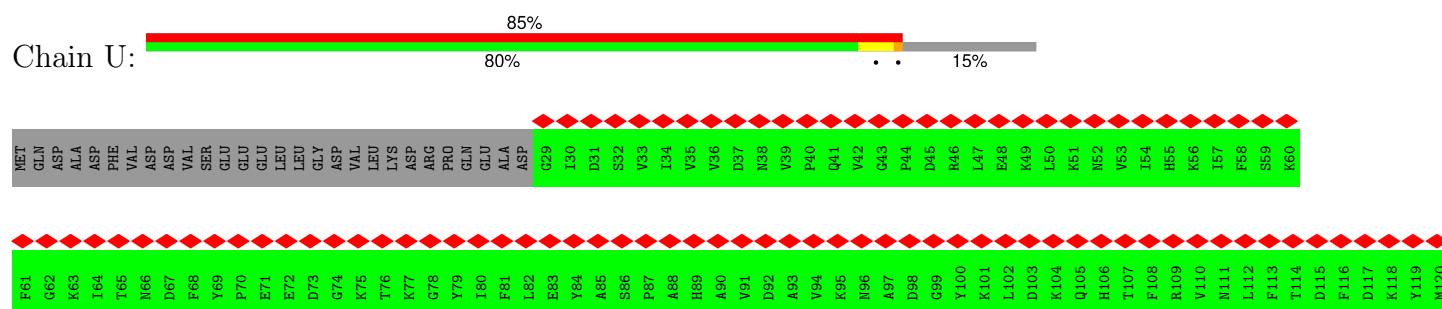
3 Residue-property plots

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: Eukaryotic translation initiation factor 3 subunit I



• Molecule 2: Eukaryotic translation initiation factor 3 subunit B



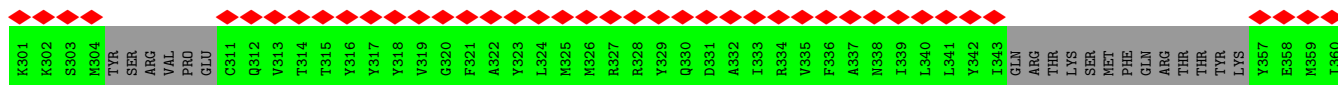
T121	R181	L241	M301	D361	G421	A481	N541	MET
I122	W182	M242	G302	C362	S422	L482	N542	GLU
S123	T183	D243	L303	K363	K423	A483	K543	ASP
D124	E184	T244	L304	L364	F424	F484	D544	ARG
E125	T185	D245	K306	H365	A425	V485	R545	LYS
W126	Y186	Q246	K307	V366	V426	D486	F546	TYR
D127	V187	D247	S308	Q367	L427	T487	C547	ARG
I128	R188	Q248	S309	K368	H428	S488	Q548	LYS
P129	W189	Q249	L309	N369	G429	L489	Q549	MET
E130	S190	A250	K310	G370	E430	C490	L550	GLN
K131	P191	I251	I311	D371	A431	T491	W551	LEU
Q132	K192	I252	S312	Y372	P432	V492	R552	TYR
P133	G193	I253	G313	L373	R433	M493	P553	MET
F134	T194	W254	I314	C374	I434	N494	R554	GLU
K135	Y195	D255	K315	V375	S435	I495	P555	LYS
D136	L196	I256	D316	K376	V436	A496	P556	ASN
L137	T197	I257	F317	V377	S437	E497	T557	GLU
G138	A198	T258	S318	D378	F438	H498	L558	ARG
N139	F199	G259	W319	R379	Y439	Y499	L559	GLU
L140	H200	H260	S320	T380	H440	M500	S560	ARG
R141	Q201	K261	P321	P381	V441	A501	Q561	GLY
Y142	R202	K262	G322	LYS	K442	S502	E562	GLY
W143	G203	R263	G323	GLY	M443	D503	Q563	VAL
L144	I204	G264	N324	THR	N444	V504	T564	ASP
E145	A205	F265	I325	GLN	G445	E505	K565	THR
E146	L206	H266	I326	G386	K446	W506	Q566	ASP
A147	W207	C267	A327	V387	I447	D507	L567	GLU
E148	G208	E268	F328	V388	E448	P508	K568	LEU
C149	G209	S269	W329	T389	L449	T509	K569	SER
R150	E210	S270	V330	F391	I450	G510	D570	ASN
D151	K211	A271	P331	E392	K451	R511	L571	VAL
Q152	F212	H272	E332	I393	M452	V512	K572	ASP
Y153	K213	W273	D333	F394	F453	V513	K573	TRP
S154	Q214	P274	K334	R395	D454	V514	Y574	GLU
V155	I215	I275	D335	K396	K455	T515	S575	GLU
I156	Q216	F276	I336	R397	Q456	S516	K576	THR
F157	R217	K277	P337	E398	A457	V517	L577	ILE
E158	F218	W278	A338	K399	M458	S518	F578	GLU
S159	S219	S279	R339	Q400	M459	W519	E579	PHE
G160	H220	H280	V340	V401	T460	W520	Q580	VAL
D161	Q221	D281	T341	P402	I461	S521	K581	THR
T163	G222	G282	L342	V403	F462	H522	D582	GLU
S164	V223	K283	M343	D404	W463	K523	R583	ILE
I165	Q224	F284	Q344	V405	S464	V524	L584	PRO
F166	L225	F285	L345	V406	P465	D525	S585	LEU
W167	I226	A286	P346	E407	Q466	W526	Q586	GLY
N168	D227	R287	T347	M408	G467	A527	S587	ASN
D169	F228	M288	R348	K409	Q468	Y528	K588	GLN
V170	S229	T289	Q349	E410	F469	W529	A589	
K171	C231	D291	E350	T411	V470	L530	S590	
D172	E232	T292	I351	I412	V471	W531	K591	
P173	R233	L293	R353	I413	A473	F533	E592	LEU
V174	Y234	S294	V354	A414	G474	Q534	VAL	VAL
S175	L235	I295	N355	F415	L475	G535	GLU	GLU
I176	V236	Y296	L356	A416	R476	R536	ARG	ARG
E177	T237	E297	F357	W417	S477	L537	THR	THR
E178	F238	T298	N358	P419	M478	L538	MET	MET
R179	S239	P299	V359	M420	M479	Q539		
A180	P240	S300	V360		G480	K540		

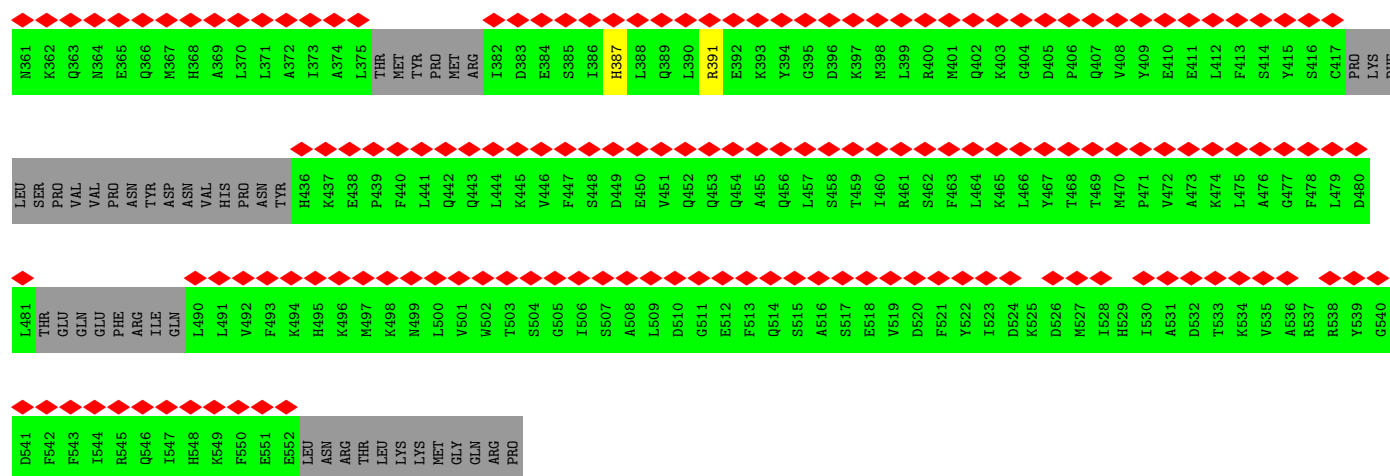
GLU

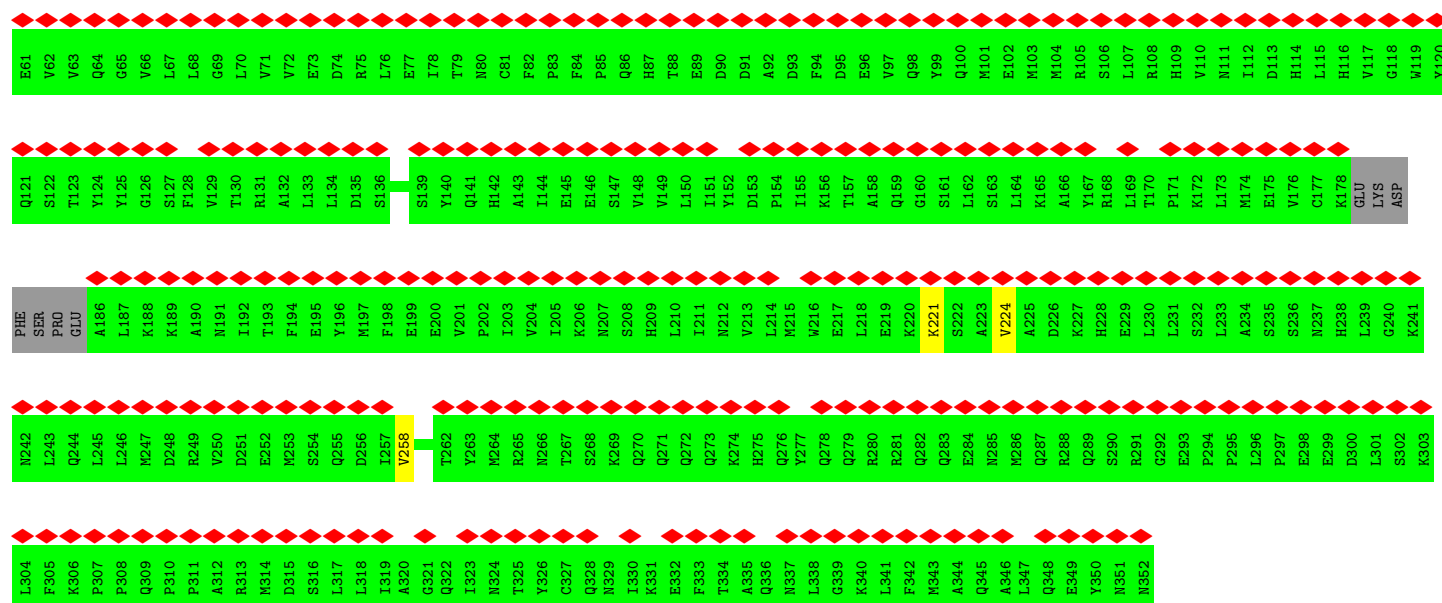
- Molecule 3: Eukaryotic translation initiation factor 3 subunit K



MET	F61	L121	MET
A2	Q62	D122	A2
K3	T63	E123	K3
F4	T64	N124	F4
E5	V65	M125	E5
Q6	T66	D126	Q6
W7	A67	L127	W7
R8	Q68	L128	R8
A9	L69	E129	A9
N10	L70	G130	N10
V11	L71	I131	V11
G12	K72	T132	G12
K13	A73	G133	K13
L14	L74	F134	L14
L15	T75	E135	L15
K16	W76	D136	K16
G17	L77	S137	G17
I18	P78	V138	I18
D19	H79	R139	D19
R20	T80	K140	R20
Y21	D81	F141	Y21
N22	F82	I142	N22
P23	T83	C143	P23
E24	L84	H144	E24
N25	C85	V145	N25
L26	K86	W146	L26
A27	C87	G147	A27
T28	H88	I148	T28
L29	R89	T149	L29
E30	D90	Y150	E30
R31	Q91	Q151	R31
Y32	A92	H152	Y32
V33	H93	I153	V33
E34	Q94	D154	E34
T35	E95	R155	T35
Q36	E96	W156	Q36
A37	R97	L157	A37
K38	P98	L158	K38
E39	I99	A159	E39
N40	Q100	E160	N40
A41	Q101	M161	A41
Y42	I102	L162	Y42
D43	L103	G163	D43
L44	Y104	D164	L44
E45	L105	L165	E45
A46	G106	S166	A46
W47	D107	D167	W47
L48	L108	S168	L48
A49	L109	Q169	A49
V50	E110	L170	V50
L51	T111	K171	L51
K52	C112	V172	K52
H113	F113	W173	H113
Y54	M174	M175	Y54
Q55	Q115	S175	Q55
F56	A116	K176	F56
N57	F117	Y177	N57
P58	W118	G178	P58
A59	Q119	W179	A59
F60	A120	S180	F60

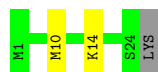






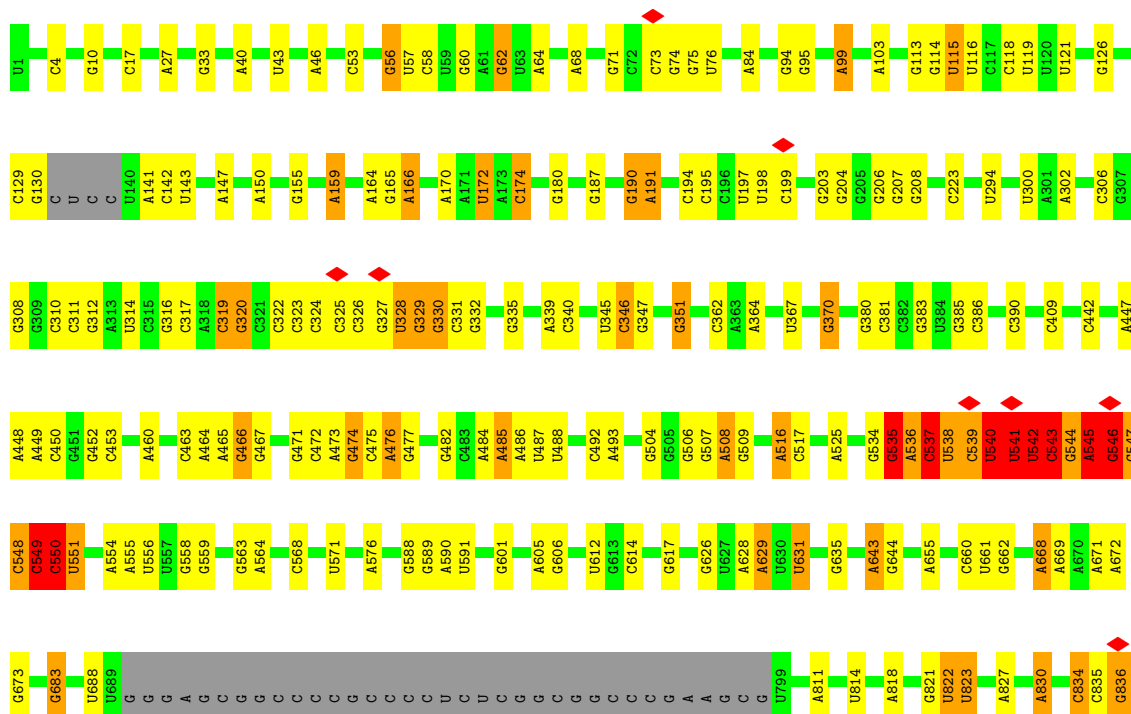
• Molecule 8: Small ribosomal subunit protein eS32

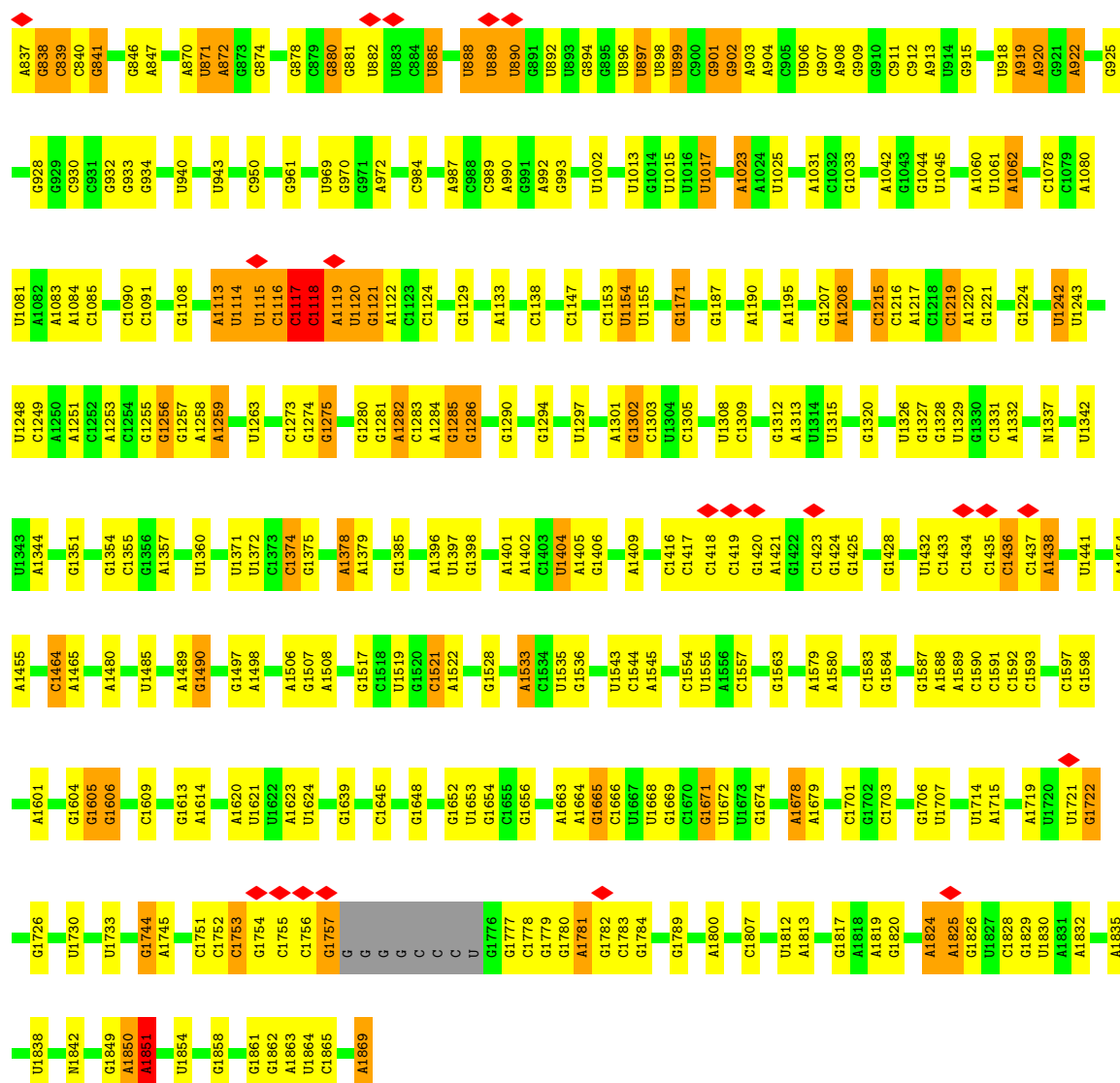
Chain 9: 88% 8% .



• Molecule 9: rRNA

Chain A: 66% 24% 6% . .





- Molecule 10: Small ribosomal subunit protein uS17

Chain B: 81% 9% 9%

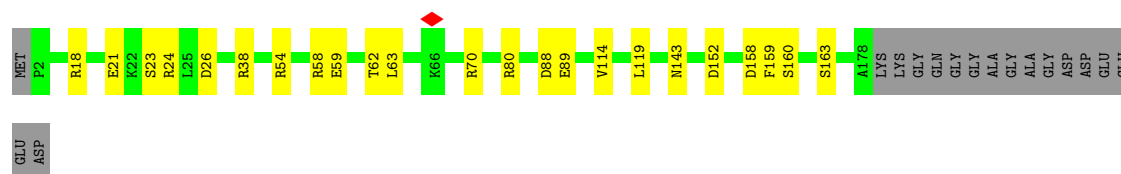
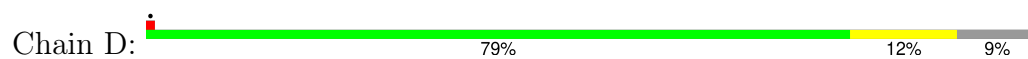


- Molecule 11: Small ribosomal subunit protein eS4, X isoform

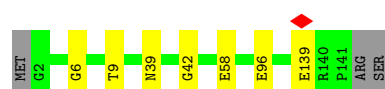
Chain C: 90% 7%



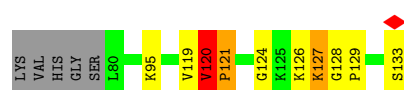
- Molecule 12: Small ribosomal subunit protein uS4



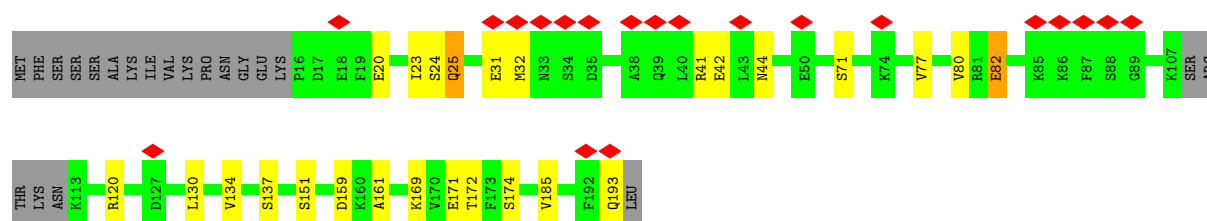
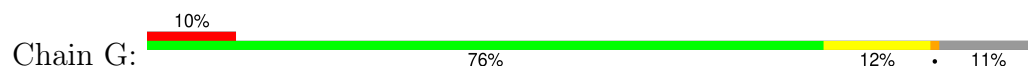
- Molecule 13: Small ribosomal subunit protein uS12



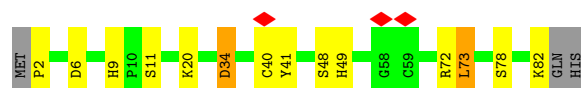
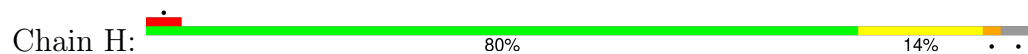
- Molecule 14: Small ribosomal subunit protein eS30



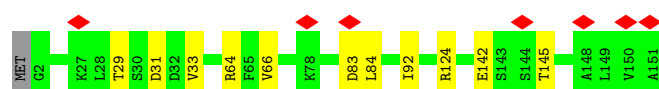
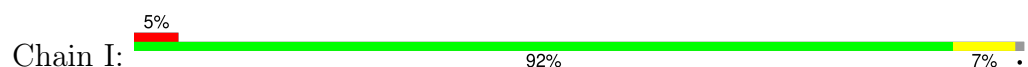
- Molecule 15: Small ribosomal subunit protein eS7



- Molecule 16: Small ribosomal subunit protein eS27



- Molecule 17: Small ribosomal subunit protein uS15



- Molecule 18: Small ribosomal subunit protein uS8

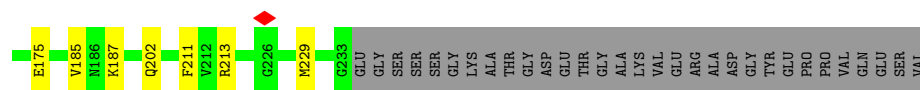
-
- | Amino Acid Type | Relative Frequency (approx.) |
|-----------------|------------------------------|
| M1 | 0.15 |
| Q2 | 0.10 |
| G6 | 0.10 |
| A37 | 0.10 |
| D40 | 0.10 |
| K41 | 0.10 |
| V42 | 0.10 |
| T43 | 0.10 |
| F46 | 0.10 |
| E64 | 0.10 |
| I78 | 0.10 |
| K81 | 0.10 |
| ASN | 0.10 |
| PHE | 0.10 |

-
- Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows amino acids: MET, ASP, ASP, ALA, GLY, ALA, GLY, PRO, GLY, PRO, GLY, MET, GLY, ASN, ARG, GLY, PHE, ARG, PHE, GLY, SER, GLY, ILE, ARG, GLY, ARG, GLY, ARG, GLY, ARG, GLY, ALA, ARG, GLY, LYS, ALA, GLU, D57, K58. The bars are colored by amino acid: MET (grey), ASP (yellow), ALA (green), GLY (blue), PRO (red), PHE (purple), ARG (brown), ILE (pink), SER (orange), LYS (light blue), and others. MET is the most frequent residue at this position.

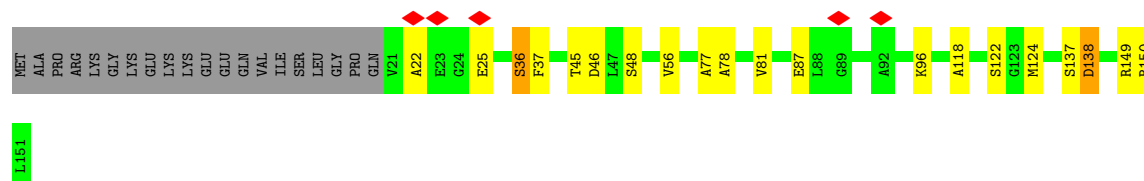
- [illegible]

- | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|
| GLN | PRO | GLU | VAL | ALA | ASP | TRP | SER | GLY | GLY | VAL | GLN | VAL | PRO | SER | VAL | PRO | PRO | ILE | GLN | PHE | PRO | PRO | THR | GLY | ASP | TRP | SER | ALA | GLN | GLN | ALA | ALA | ALA | PRO | THR | ALA | GLN | THR | THR | GLU | TRP | VAL | GLY | ALA | THR | THR | ASP | TRP | SER |
| MET | S2 | G3 | D6 | E12 | E69 | K69 | R128 | L134 | T144 | D151 | D158 | S190 | R191 | E192 | F208 | GLU | ILE | GLU | LYS | GLU | GLU | GLN | ALA | ALA | ALA | GLU | LYS | ALA | VAL | THR | LYS | GLU | GLU | PHE | GLN | GLY | GLY | THR | THR | THR | ALA | ALA | PRO | GLU | GLY | PHE | THR | ALA | |

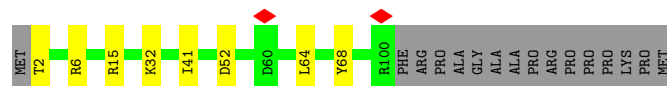
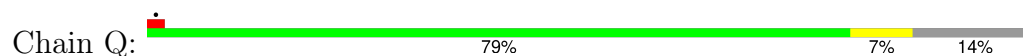
- [illegible]



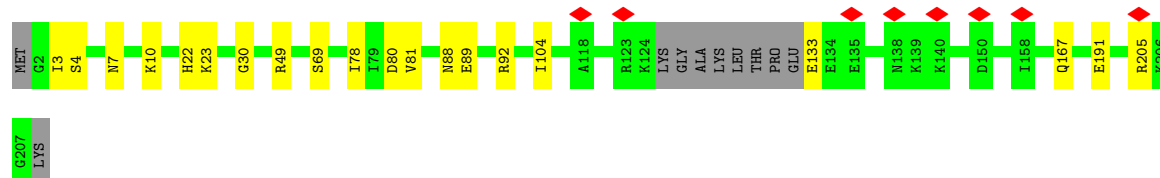
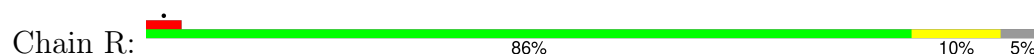
- Molecule 24: 40S ribosomal protein S14



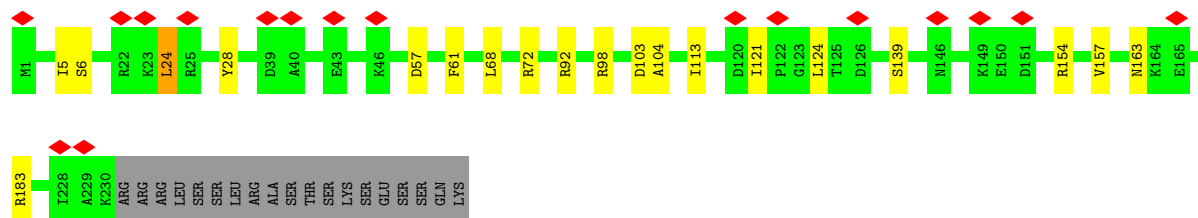
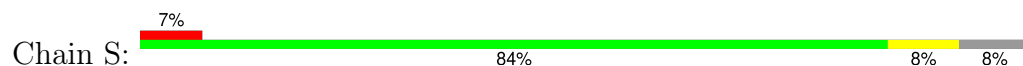
- Molecule 25: Small ribosomal subunit protein eS26



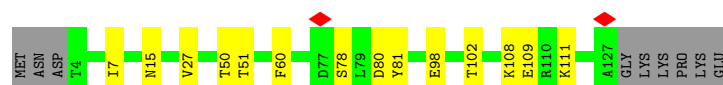
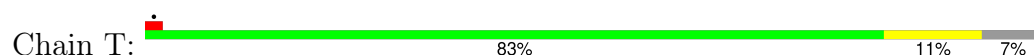
- Molecule 26: Small ribosomal subunit protein eS8



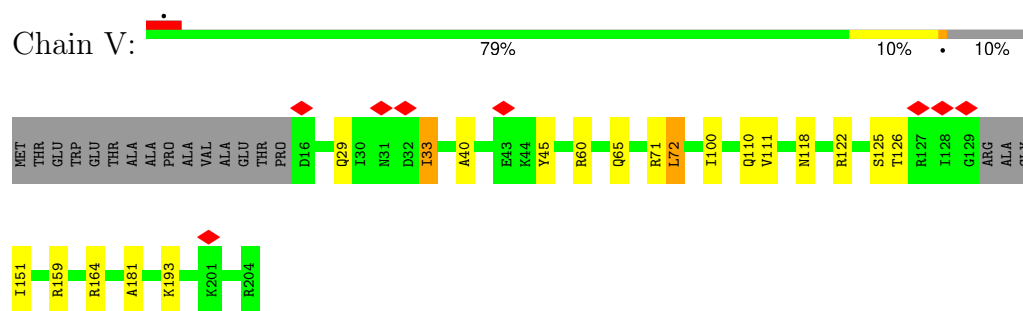
- Molecule 27: Small ribosomal subunit protein eS6



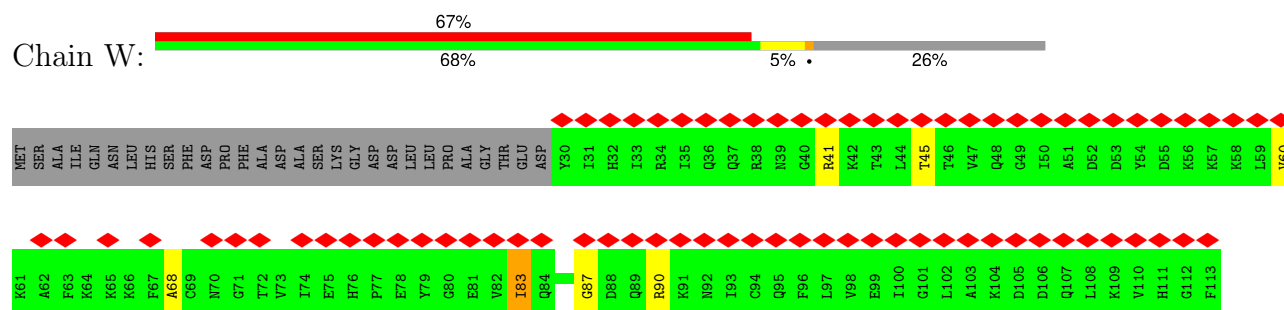
- Molecule 28: Small ribosomal subunit protein eS24



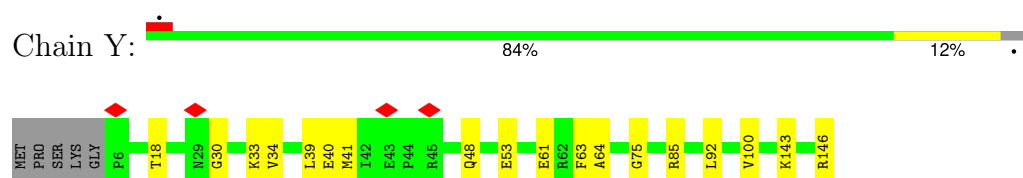
- Molecule 29: Small ribosomal subunit protein uS7



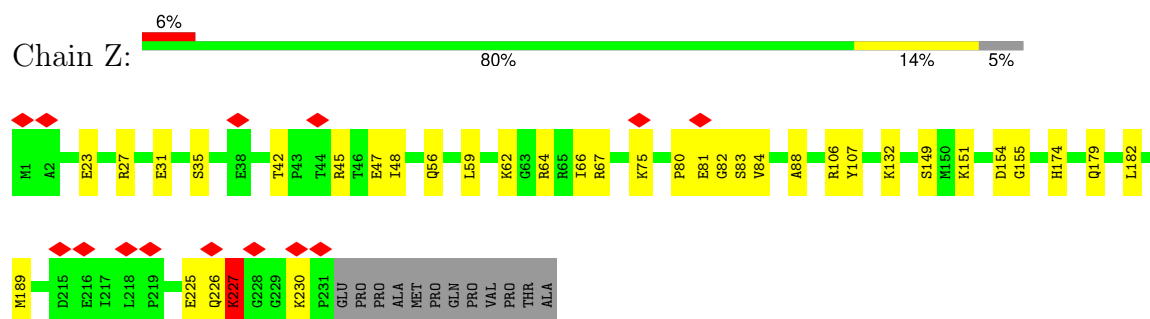
- Molecule 30: Eukaryotic translation initiation factor 1



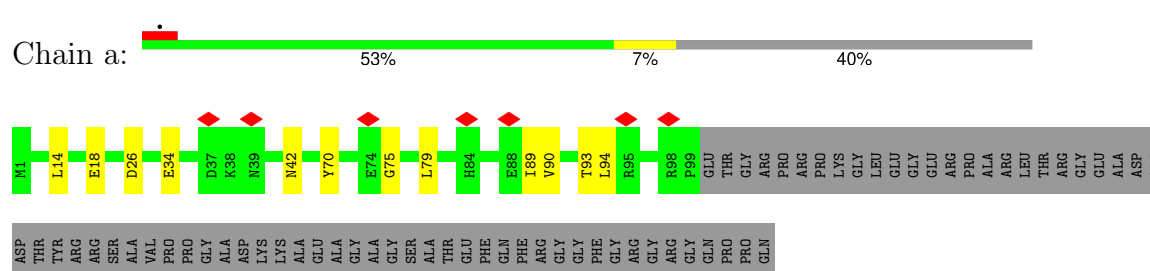
- Molecule 31: Small ribosomal subunit protein uS9

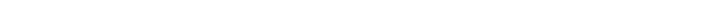


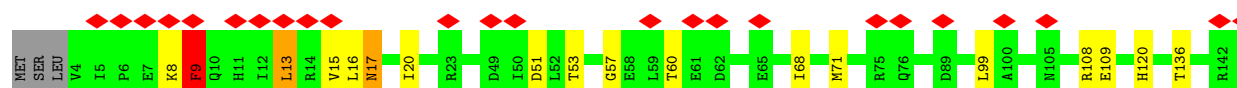
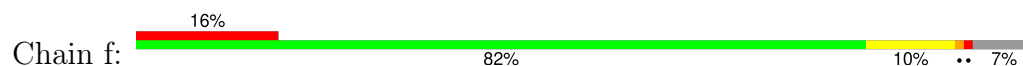
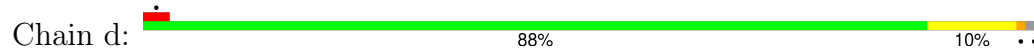
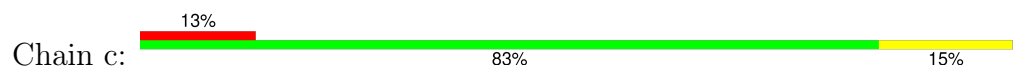
- Molecule 32: Small ribosomal subunit protein uS3

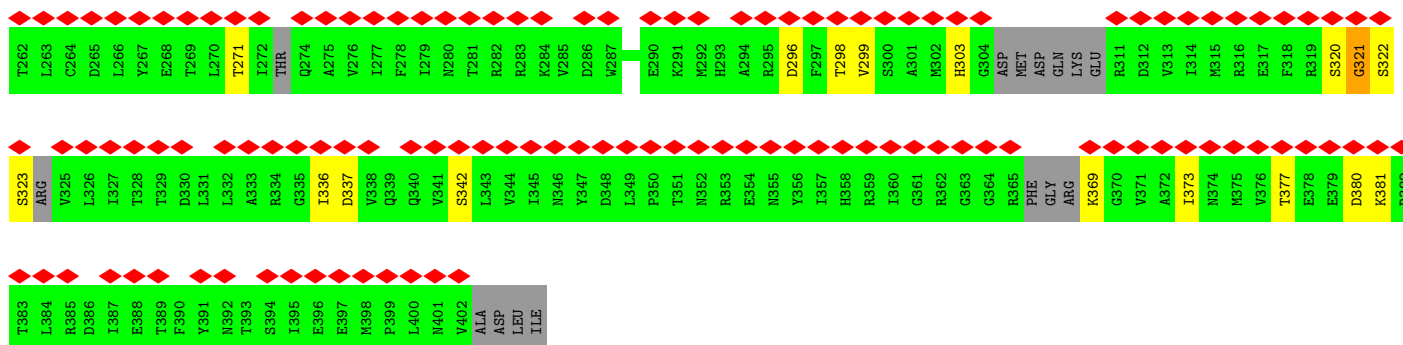


- Molecule 33: Small ribosomal subunit protein eS10

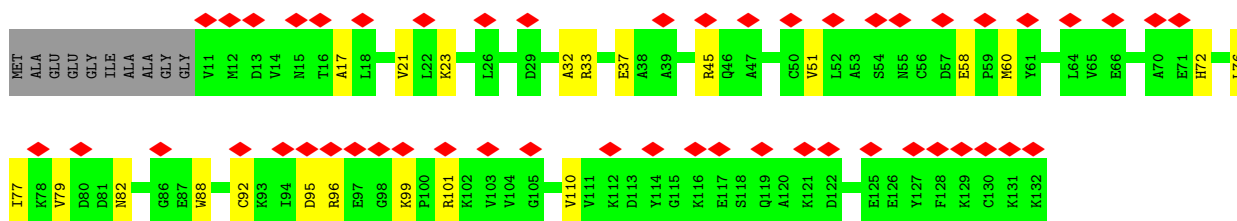
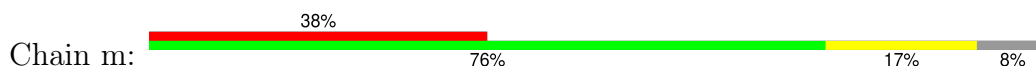


- Chain b: 

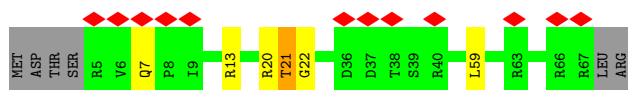
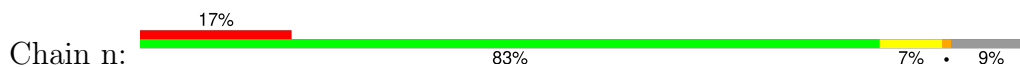




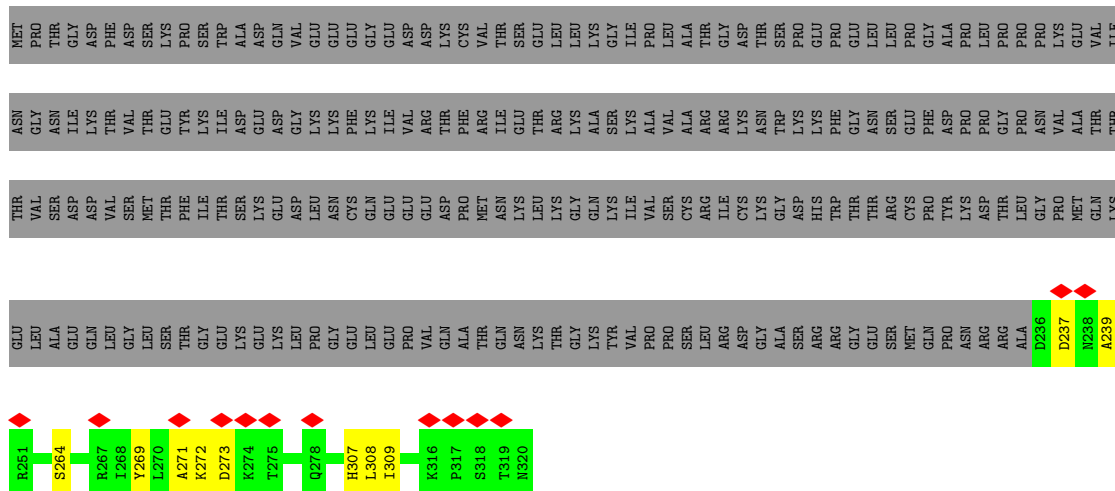
• Molecule 43: Small ribosomal subunit protein eS12



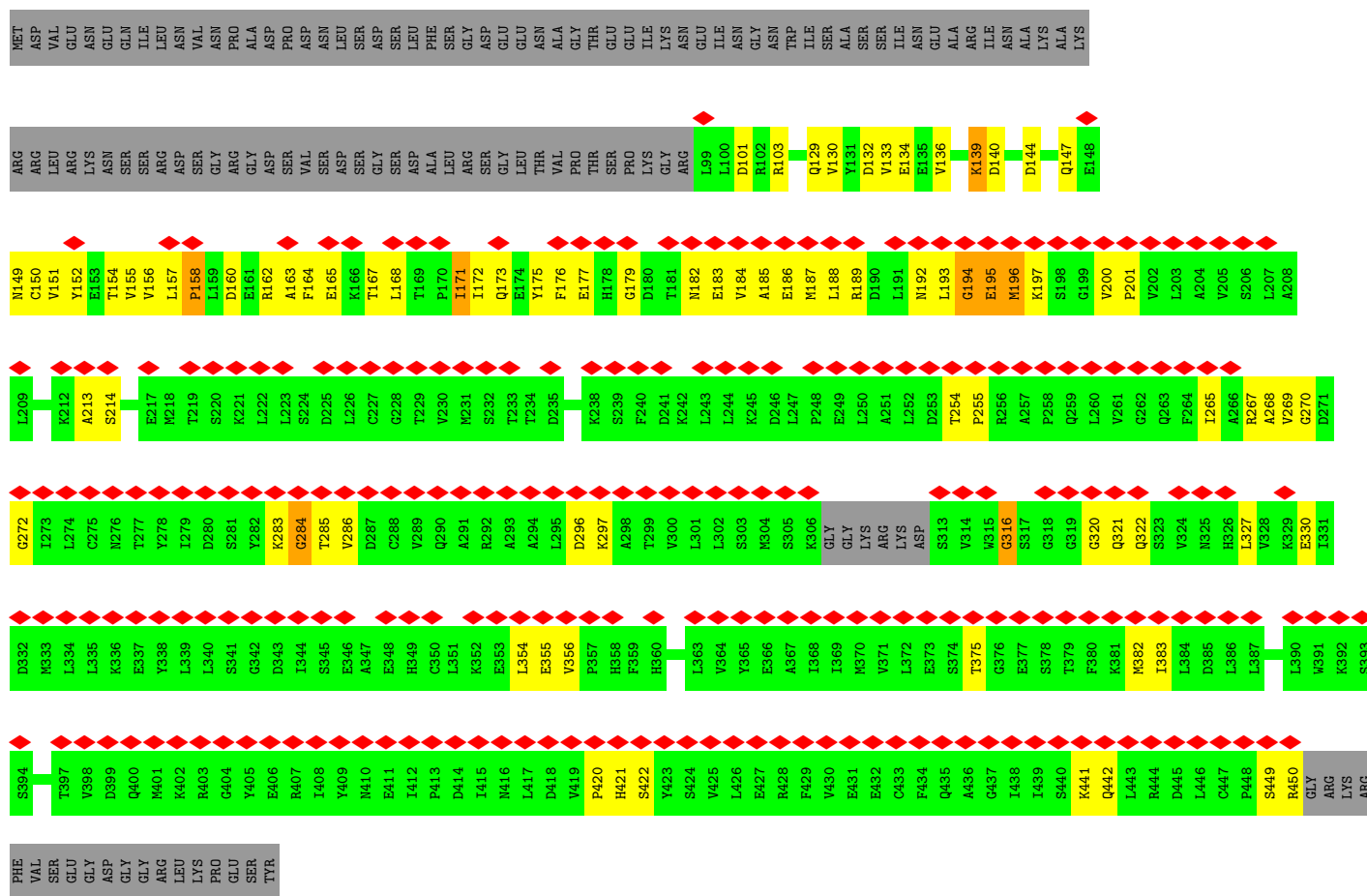
• Molecule 44: Small ribosomal subunit protein eS28



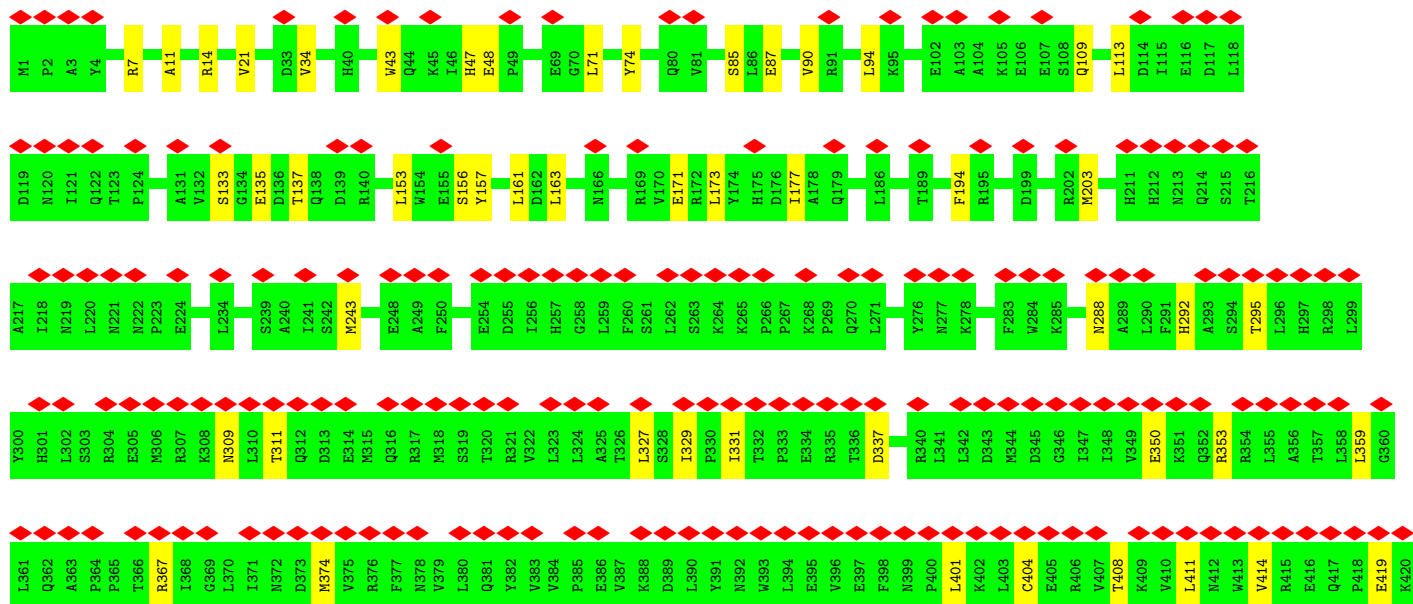
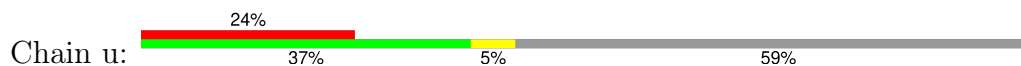
• Molecule 45: Eukaryotic translation initiation factor 3 subunit G

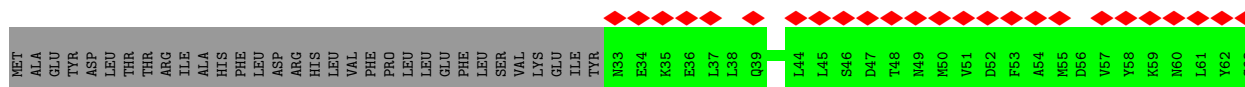


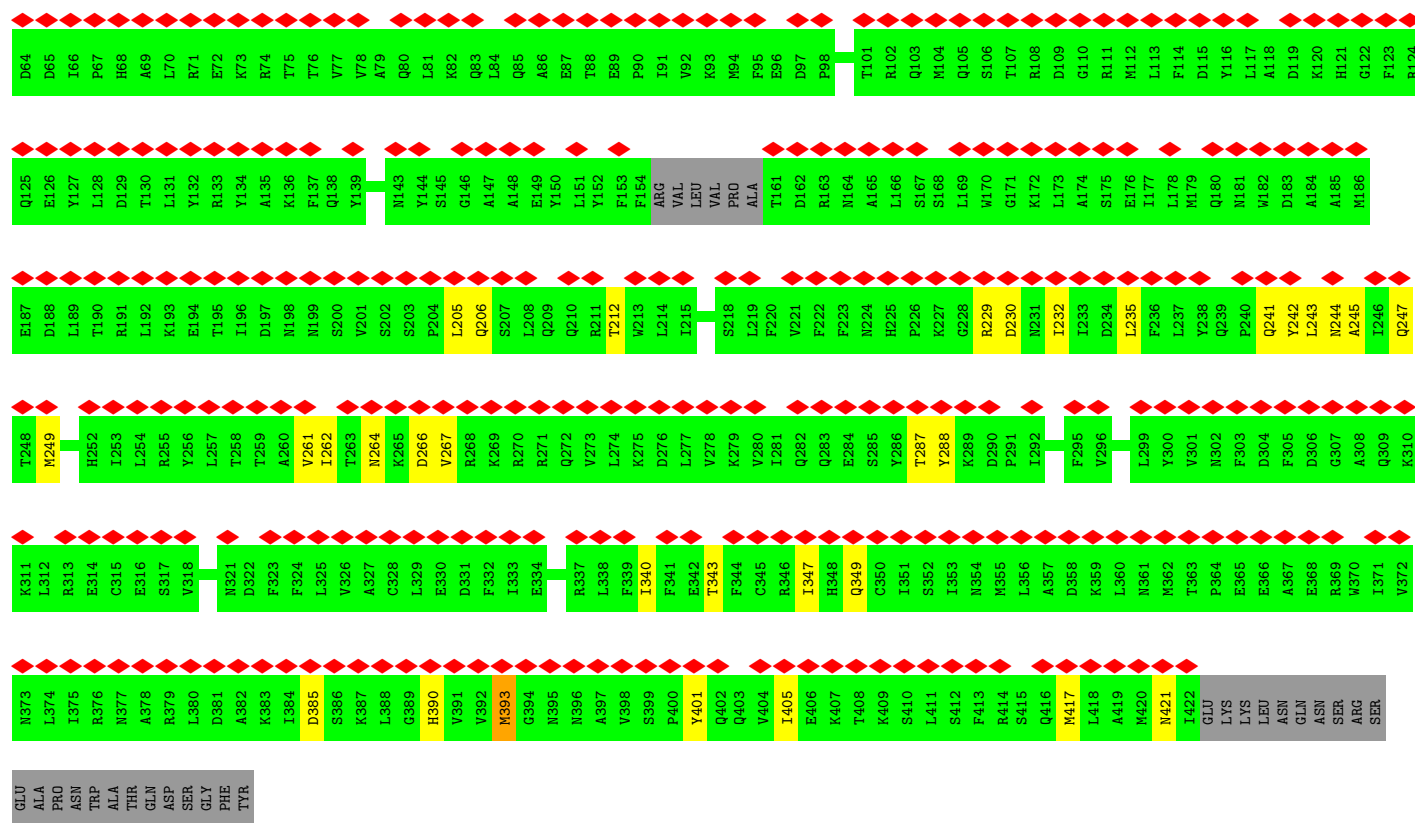
• Molecule 46: Programmed cell death protein 4



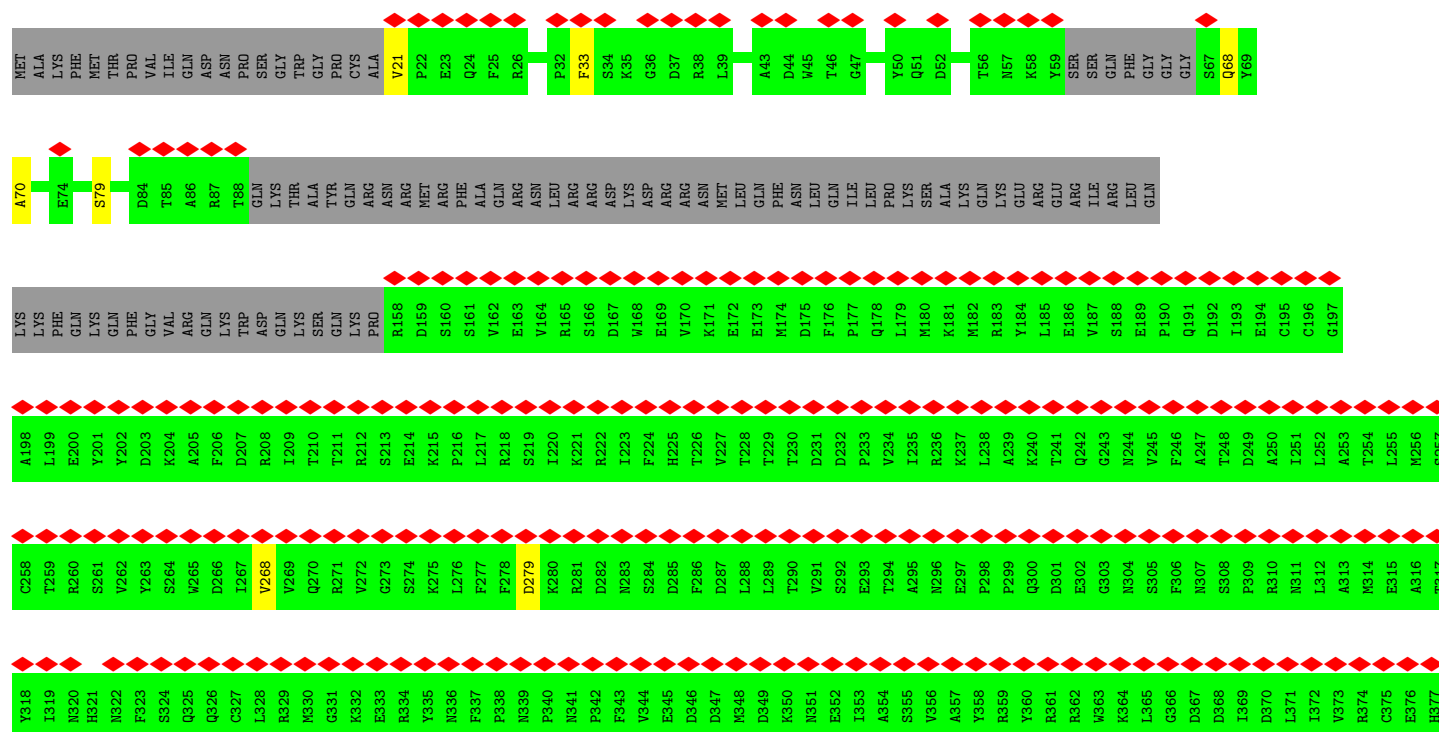
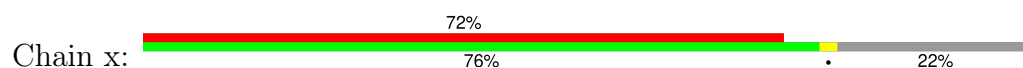
• Molecule 47: Eukaryotic translation initiation factor 3 subunit A

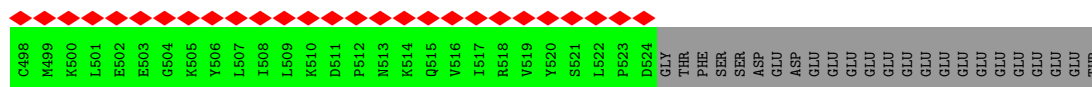
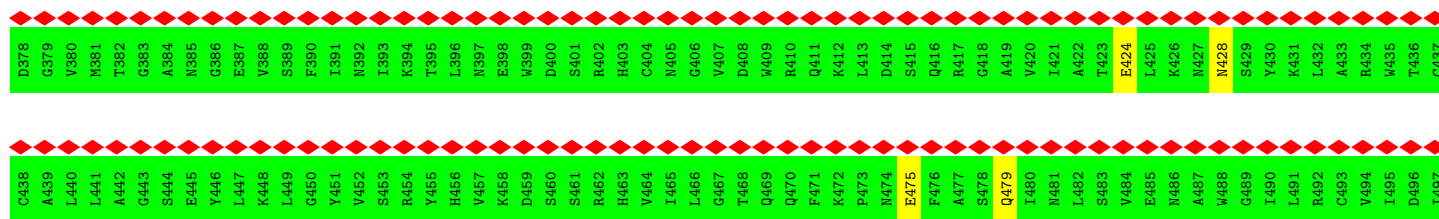




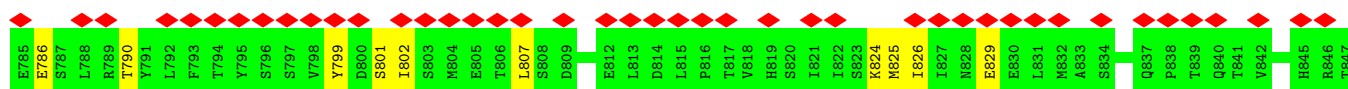
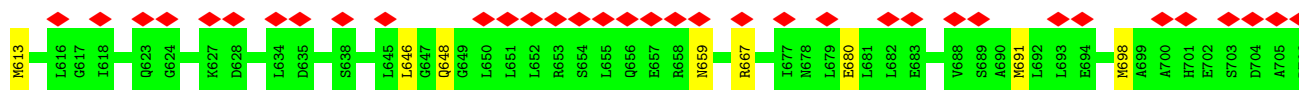
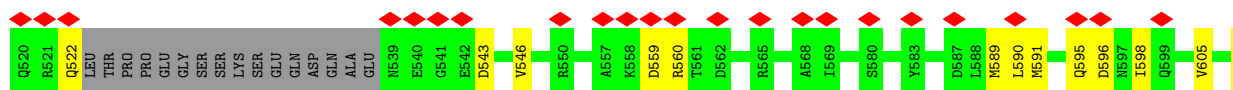
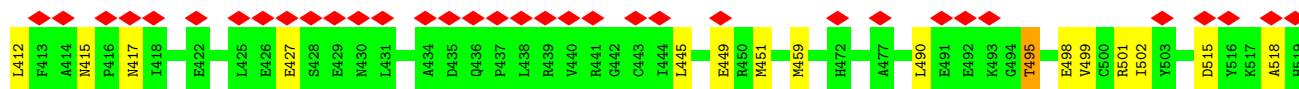
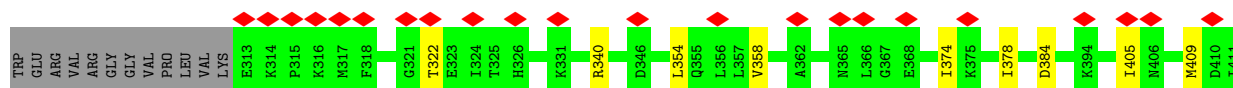
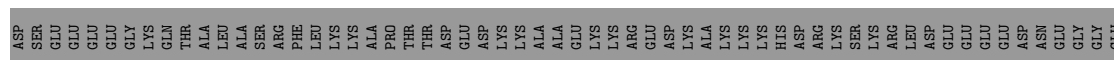
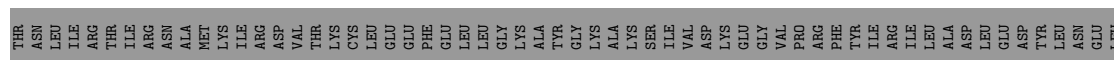


• Molecule 49: Eukaryotic translation initiation factor 3 subunit D





• Molecule 50: Eukaryotic translation initiation factor 3 subunit C



SER	GLN	THR	ALA	TYR	E348	A851	Q852	Q853	N854	L855	A856	L857	Q858	L859	A860	E861	K862	L863	GLY	SER	LEU	VAL	GLU	ASN	ASN	GLU	ARG	VAL	PHE	ASP	HIS	HIS	LYS	GLN	GLY	THR	THR	GLY	GLY	TYR	PHE	ARG	ASP	GLN	LYS	LYS	ASP	GLY	TYR	ARG	LYS	ASN	GLU	GLY	TYR	MET	ARG	ARG	GLY	GLY	TYR	ARG	GLN	GLN	GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	8515	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	410.0, 410.0, 410.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.025, 1.025, 1.025	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, SPD, PSU, A2M, ZN, 5MU, OMG, MG, ACY, JMH, OMC, 6MZ, OMU, 5MC, K, UR3, 4AC

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	X	0.68	0/1597	1.20	0/2216
2	U	0.68	0/2768	1.12	0/3854
3	3	0.15	0/1055	0.35	0/1469
4	4	0.18	0/1269	0.44	0/1762
5	5	0.13	0/1575	0.30	0/2187
6	6	0.21	0/1926	0.53	0/2669
7	8	0.17	0/1569	0.40	0/2183
8	9	0.29	0/231	0.69	0/294
9	A	0.28	0/39097	0.41	22/60929 (0.0%)
10	B	0.25	0/1197	0.44	1/1599 (0.1%)
11	C	0.25	0/2077	0.45	0/2796
12	D	0.27	0/1502	0.52	0/2008
13	E	0.24	0/1105	0.46	0/1476
14	F	0.52	0/429	0.76	0/566
15	G	0.25	0/1420	0.55	0/1901
16	H	0.26	0/644	0.49	0/864
17	I	0.25	0/1232	0.44	0/1656
18	J	0.25	0/1051	0.42	0/1406
19	K	0.27	0/623	0.52	0/833
20	L	0.28	0/1743	0.51	0/2354
21	M	0.26	0/1078	0.58	0/1447
22	N	0.23	0/1670	0.43	0/2271
23	O	0.25	0/1742	0.54	0/2330
24	P	0.27	0/993	0.56	0/1330
25	Q	0.24	0/805	0.42	0/1079
26	R	0.23	0/1654	0.44	0/2203
27	S	0.24	0/1885	0.50	0/2510
28	T	0.25	0/1028	0.53	0/1366
29	V	0.26	0/1481	0.55	0/1988
30	W	0.28	0/693	0.58	0/925
31	Y	0.23	0/1142	0.50	0/1528

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.27	0/1811	0.45	0/2438
33	a	0.35	0/859	0.71	0/1159
34	b	0.30	0/991	0.70	1/1325 (0.1%)
35	c	0.24	0/2493	0.55	1/3394 (0.0%)
36	d	0.22	0/1123	0.44	0/1504
37	e	0.33	0/557	0.73	0/748
38	f	0.30	0/1194	0.58	0/1599
39	h	0.25	0/827	0.52	0/1110
40	i	0.28	0/470	0.47	0/623
41	k	0.28	0/438	0.57	0/580
42	l	1.04	1/1700 (0.1%)	1.35	13/2359 (0.6%)
43	m	0.31	0/960	0.71	0/1286
44	n	0.28	0/500	0.60	0/669
45	o	0.65	0/419	1.15	0/580
46	p	0.92	0/1834	1.18	4/2517 (0.2%)
47	u	0.27	0/4800	0.61	0/6488
48	v	0.28	0/2672	0.59	0/3647
49	x	0.27	0/2118	0.50	0/2949
50	y	0.26	0/4400	0.58	0/5939
All	All	0.34	1/108447 (0.0%)	0.57	42/154913 (0.0%)

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
16	H	0	1
24	P	0	1
46	p	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	l	107	ALA	CA-CB	-5.88	1.46	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	550	C	O3'-P-O5'	-25.25	66.12	104.00
9	A	1118	C	C4'-C3'-O3'	13.38	129.47	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	549	C	P-O3'-C3'	-9.48	105.98	120.20
9	A	545	A	P-O3'-C3'	-8.56	107.36	120.20
9	A	536	A	P-O3'-C3'	-8.41	107.59	120.20
42	l	336	ILE	N-CA-C	8.12	119.08	107.88
9	A	550	C	OP1-P-O3'	7.93	131.80	108.00
9	A	541	U	P-O3'-C3'	-7.83	108.45	120.20
9	A	1117	C	P-O3'-C3'	-7.80	108.50	120.20
42	l	107	ALA	CA-C-N	-7.78	111.70	119.56
42	l	107	ALA	C-N-CA	-7.78	111.70	119.56
9	A	546	G	P-O3'-C3'	-7.65	108.72	120.20
9	A	540	U	P-O3'-C3'	-7.59	108.81	120.20
42	l	192	PHE	N-CA-C	7.58	126.95	110.80
9	A	538	U	P-O3'-C3'	-7.43	109.06	120.20
9	A	543	C	P-O3'-C3'	-7.21	109.39	120.20
42	l	139	ASN	N-CA-C	7.20	120.92	112.72
9	A	535	G	P-O3'-C3'	-6.73	110.11	120.20
46	p	285	THR	N-CA-C	-6.67	107.02	114.62
9	A	1120	U	P-O3'-C3'	-6.44	110.54	120.20
9	A	547	G	P-O3'-C3'	-6.18	110.93	120.20
9	A	1118	C	P-O3'-C3'	-6.15	110.98	120.20
42	l	299	VAL	N-CA-C	6.13	116.94	107.99
42	l	81	GLY	N-CA-C	-6.13	104.93	112.77
42	l	303	HIS	N-CA-C	6.11	117.52	108.60
9	A	537	C	P-O3'-C3'	-6.07	111.10	120.20
46	p	267	ARG	N-CA-C	-6.03	104.78	111.36
42	l	140	VAL	CB-CA-C	-6.03	104.17	111.88
9	A	542	U	P-O3'-C3'	-5.94	111.30	120.20
42	l	342	SER	N-CA-C	5.50	120.12	113.41
9	A	550	C	P-O3'-C3'	5.50	128.44	120.20
34	b	93	MET	CB-CG-SD	5.37	128.81	112.70
46	p	356	VAL	CA-C-N	5.26	124.71	119.24
46	p	356	VAL	C-N-CA	5.26	124.71	119.24
35	c	223	GLU	CB-CG-CD	5.22	121.48	112.60
9	A	1113	A	P-O3'-C3'	-5.16	112.47	120.20
42	l	205	SER	N-CA-C	5.15	119.04	112.34
9	A	1121	G	P-O3'-C3'	-5.13	112.50	120.20
42	l	193	LYS	N-CA-C	-5.12	104.97	111.11
10	B	49	GLU	CB-CG-CD	5.07	121.22	112.60
42	l	160	GLY	N-CA-C	5.07	118.38	112.50
9	A	1118	C	C2'-C3'-O3'	5.05	117.08	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	H	72	ARG	Sidechain
24	P	137	SER	Peptide
46	p	286	VAL	Peptide
46	p	316	GLY	Peptide

5.2 Too-close contacts

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	X	1598	0	723	1	0
2	U	2770	0	1200	20	0
3	3	1057	0	475	1	0
4	4	1272	0	564	2	0
5	5	1581	0	689	1	0
6	6	1917	0	1096	9	0
7	8	1571	0	683	3	0
8	9	230	0	276	2	0
9	A	35720	0	18064	226	0
10	B	1177	0	1246	7	0
11	C	2035	0	2138	11	0
12	D	1477	0	1589	15	0
13	E	1087	0	1154	5	0
14	F	424	0	457	5	0
15	G	1399	0	1481	15	0
16	H	631	0	657	9	0
17	I	1208	0	1293	8	0
18	J	1034	0	1080	6	0
19	K	617	0	622	6	0
20	L	1707	0	1794	13	0
21	M	1064	0	1118	13	0
22	N	1633	0	1640	7	0
23	O	1715	0	1785	16	0
24	P	981	0	1005	15	0
25	Q	792	0	841	6	0
26	R	1627	0	1706	11	0
27	S	1862	0	2018	11	0
28	T	1011	0	1083	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	V	1461	0	1511	16	0
30	W	683	0	702	4	0
31	Y	1124	0	1193	14	0
32	Z	1783	0	1874	31	0
33	a	834	0	861	8	0
34	b	972	0	1014	13	0
35	c	2436	0	2393	27	0
36	d	1105	0	1138	13	0
37	e	551	0	610	13	0
38	f	1176	0	1233	14	0
39	h	817	0	882	6	0
40	i	459	0	448	2	0
41	k	429	0	424	3	0
42	l	1706	0	757	22	0
43	m	950	0	987	16	0
44	n	498	0	525	6	0
45	o	420	0	197	17	0
46	p	1839	0	1003	62	0
47	u	4708	0	4785	44	0
48	v	2635	0	2207	24	0
49	x	2121	0	925	8	0
50	y	4325	0	4328	51	0
51	A	87	0	0	0	0
51	f	1	0	0	0	0
52	A	18	0	0	0	0
52	i	1	0	0	0	0
53	A	10	0	19	2	0
54	Q	1	0	0	0	0
54	i	1	0	0	0	0
54	k	1	0	0	0	0
55	l	3	0	0	0	0
All	All	104352	0	78493	753	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 4.

All (753) 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)
1:X:130:PRO:CB	46:p:375:THR:CB	2.02	1.37
46:p:195:GLU:C	46:p:196:MSE:N	1.86	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:p:184:VAL:O	46:p:188:LEU:N	1.65	1.30
46:p:185:ALA:O	46:p:189:ARG:N	1.69	1.25
46:p:185:ALA:C	46:p:186:GLU:C	2.11	1.17
32:Z:59:LEU:CD2	45:o:307:HIS:CB	2.25	1.15
46:p:195:GLU:CB	46:p:196:MSE:N	2.12	1.13
46:p:185:ALA:C	46:p:186:GLU:N	2.09	1.10
46:p:183:GLU:O	46:p:187:MSE:N	1.84	1.09
46:p:182:ASN:O	46:p:186:GLU:N	1.88	1.07
2:U:394:PHE:HA	2:U:403:VAL:HA	1.37	1.06
46:p:185:ALA:HB3	46:p:186:GLU:N	1.72	1.04
2:U:140:LEU:HA	2:U:209:GLY:HA2	1.36	1.03
46:p:195:GLU:CA	46:p:196:MSE:N	2.21	1.02
32:Z:59:LEU:HD21	45:o:307:HIS:CB	1.92	0.97
9:A:1033:G:H1	9:A:1080:A:HO2'	0.97	0.95
32:Z:88:ALA:N	45:o:307:HIS:O	1.99	0.93
9:A:925:G:H1	9:A:1017:U:H3	0.99	0.93
46:p:185:ALA:C	46:p:186:GLU:CA	2.41	0.93
9:A:550:C:H5''	9:A:550:C:H6	1.34	0.91
46:p:195:GLU:C	46:p:196:MSE:CA	2.42	0.91
46:p:195:GLU:C	46:p:197:LYS:N	2.27	0.91
46:p:185:ALA:CA	46:p:186:GLU:N	2.34	0.90
46:p:185:ALA:CB	46:p:186:GLU:N	2.33	0.90
2:U:374:CYS:HA	2:U:393:ILE:HA	1.58	0.85
50:y:358:VAL:HG21	50:y:378:ILE:HD11	1.61	0.81
9:A:1652:G:H1	9:A:1672:U:H3	1.28	0.80
2:U:372:TYR:HA	2:U:395:ARG:HA	1.64	0.79
32:Z:59:LEU:HD23	45:o:307:HIS:CB	2.13	0.79
9:A:94:G:HO2'	9:A:508:A:HO2'	1.24	0.78
45:o:271:ALA:HA	46:p:150:CYS:HA	1.65	0.78
46:p:195:GLU:C	46:p:197:LYS:H	1.91	0.78
9:A:1396:A:O2'	9:A:1398:G:N7	2.18	0.76
9:A:1286:G:N2	9:A:1312:G:O2'	2.18	0.76
14:F:120:VAL:H	14:F:121:PRO:HD2	1.51	0.76
9:A:1604:G:O2'	9:A:1605:G:O5'	2.04	0.75
9:A:506:G:OP1	28:T:108:LYS:NZ	2.21	0.74
9:A:1744:G:O2'	9:A:1789:G:N2	2.19	0.74
32:Z:88:ALA:O	45:o:308:LEU:HA	1.88	0.73
9:A:1828:C:OP2	30:W:41:ARG:NH1	2.22	0.73
9:A:830:A:OP2	9:A:846:G:N2	2.22	0.73
50:y:731:GLU:N	50:y:731:GLU:OE1	2.22	0.73
9:A:1554:C:OP2	9:A:1555:U:O2'	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:69:VAL:HG21	23:O:74:LEU:HD13	1.71	0.72
9:A:878:G:O6	9:A:908:A:N1	2.23	0.72
47:u:43:TRP:O	47:u:47:HIS:ND1	2.23	0.72
35:c:84:ASP:OD1	35:c:86:THR:OG1	2.08	0.72
27:S:98:ARG:NH2	27:S:103:ASP:OD1	2.22	0.71
9:A:1521:C:OP2	38:f:136:THR:OG1	2.07	0.71
35:c:159:ASN:OD1	35:c:161:SER:OG	2.07	0.71
2:U:394:PHE:CA	2:U:403:VAL:HA	2.18	0.71
9:A:987:A:OP1	25:Q:32:LYS:NZ	2.24	0.71
9:A:839:C:O2'	9:A:841:G:O4'	2.09	0.71
35:c:67:SER:OG	35:c:108:VAL:O	2.08	0.71
2:U:394:PHE:HA	2:U:403:VAL:CA	2.18	0.70
37:e:60:LYS:NZ	37:e:61:GLU:OE1	2.25	0.70
9:A:115:U:O2'	9:A:381:C:O2	2.07	0.70
9:A:629:A:O2'	9:A:631:U:OP1	2.10	0.70
15:G:82:GLU:N	15:G:82:GLU:OE2	2.24	0.70
9:A:885:U:N3	9:A:901:G:N1	2.40	0.69
38:f:16:LEU:O	38:f:17:ASN:ND2	2.25	0.69
9:A:928:G:H1	9:A:1013:U:H3	1.39	0.69
35:c:153:CYS:SG	35:c:155:ARG:NH1	2.65	0.69
23:O:29:ASP:OD1	23:O:29:ASP:N	2.26	0.69
9:A:1528:G:O2'	9:A:1666:C:OP1	2.10	0.69
12:D:54:ARG:NH2	20:L:200:ARG:O	2.25	0.69
39:h:45:GLU:OE2	39:h:46:LYS:NZ	2.25	0.69
36:d:8:ASP:OD1	36:d:8:ASP:N	2.23	0.69
9:A:547:G:H2'	9:A:548:C:H4'	1.75	0.68
9:A:1255:G:OP1	9:A:1256:G:O2'	2.07	0.68
9:A:1091:C:HO2'	18:J:2:VAL:N	1.91	0.68
9:A:317:C:OP2	27:S:183:ARG:NH1	2.27	0.68
9:A:1605:G:O2'	9:A:1606:G:O5'	2.11	0.68
9:A:40:A:O2'	9:A:485:A:O2'	2.09	0.68
28:T:78:SER:OG	28:T:80:ASP:OD1	2.09	0.68
9:A:319:C:O2'	9:A:320:G:O5'	2.10	0.68
48:v:241:GLN:NE2	49:x:33:PHE:O	2.27	0.68
9:A:919:A:OP2	17:I:64:ARG:NH2	2.27	0.68
9:A:1593:C:OP2	37:e:104:ARG:NH1	2.26	0.68
26:R:133:GLU:OE2	26:R:133:GLU:N	2.27	0.67
9:A:1249:C:O2'	31:Y:143:LYS:NZ	2.27	0.67
9:A:549:C:H2'	9:A:550:C:C6	2.30	0.67
12:D:21:GLU:OE2	12:D:23:SER:OG	2.12	0.67
27:S:121:ILE:HG21	27:S:124:LEU:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:p:195:GLU:C	46:p:196:MSE:C	2.63	0.67
50:y:824:LYS:O	50:y:824:LYS:NZ	2.26	0.67
47:u:171:GLU:N	47:u:171:GLU:OE1	2.28	0.66
9:A:1589:A:N3	9:A:1653:U:O2'	2.26	0.66
47:u:133:SER:OG	47:u:135:GLU:OE1	2.13	0.66
24:P:118:ALA:O	24:P:122:SER:OG	2.13	0.66
50:y:786:GLU:OE2	50:y:790:THR:OG1	2.13	0.66
9:A:890:U:O4	9:A:897:U:O2'	2.11	0.66
9:A:823:PSU:N1	12:D:143:ASN:OD1	2.28	0.66
9:A:1480:A:O2'	40:i:56:ASP:O	2.14	0.66
26:R:80:ASP:OD1	26:R:81:VAL:N	2.29	0.66
50:y:495:THR:OG1	50:y:498:GLU:OE1	2.14	0.66
27:S:57:ASP:OD1	27:S:61:PHE:N	2.29	0.65
36:d:114:GLU:N	36:d:114:GLU:OE1	2.29	0.65
38:f:9:PHE:CD1	38:f:57:GLY:HA3	2.31	0.65
47:u:485:ASP:OD1	50:y:801:SER:OG	2.13	0.65
9:A:1597:C:OP2	37:e:85:ARG:NH2	2.29	0.65
9:A:880:G:H1	9:A:906:U:H3	1.45	0.65
46:p:449:SER:O	46:p:450:ARG:C	2.39	0.64
15:G:134:VAL:O	15:G:137:SER:OG	2.11	0.64
37:e:67:LEU:HD21	37:e:108:ILE:HD11	1.80	0.64
9:A:922:A:OP2	18:J:3:ARG:NH2	2.31	0.64
11:C:117:GLU:OE1	11:C:117:GLU:N	2.30	0.64
12:D:59:GLU:O	12:D:62:THR:OG1	2.14	0.64
9:A:1824:A:O2'	9:A:1825:A:OP2	2.16	0.64
9:A:885:U:O4	9:A:901:G:O6	2.15	0.64
9:A:545:A:H4'	9:A:546:G:H8	1.63	0.64
29:V:29:GLN:O	29:V:110:GLN:NE2	2.31	0.64
9:A:1604:G:HO2'	9:A:1605:G:P	2.21	0.63
15:G:41:ARG:NH2	15:G:44:ASN:OD1	2.30	0.63
35:c:282:GLU:OE1	35:c:282:GLU:N	2.31	0.63
9:A:1432:U:O2'	9:A:1436:C:O2	2.15	0.63
46:p:184:VAL:O	46:p:187:MSE:CB	2.46	0.63
11:C:21:ASP:OD2	11:C:24:THR:OG1	2.13	0.63
21:M:94:GLU:N	21:M:94:GLU:OE1	2.30	0.63
47:u:309:ASN:OD1	47:u:311:THR:OG1	2.09	0.63
9:A:919:A:O3'	53:A:2005:SPD:N10	2.32	0.63
9:A:190:G:O2'	9:A:191:A:OP1	2.16	0.63
9:A:1114:U:H3	9:A:1119:A:H61	1.46	0.63
24:P:56:VAL:HG12	24:P:81:VAL:HG13	1.80	0.63
46:p:184:VAL:O	46:p:187:MSE:C	2.40	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:27:TRP:HA	42:l:237:LYS:O	1.99	0.63
46:p:185:ALA:C	46:p:187:MSE:N	2.55	0.63
9:A:538:U:H2'	9:A:539:C:H2'	1.81	0.63
9:A:1669:G:OP1	39:h:79:ARG:NH1	2.32	0.63
9:A:1679:A:OP1	44:n:20:ARG:NH2	2.31	0.63
45:o:269:TYR:HA	46:p:152:TYR:HA	1.79	0.63
9:A:915:G:OP1	15:G:120:ARG:NH2	2.32	0.63
29:V:33:ILE:HD12	49:x:475:GLU:HA	1.80	0.63
9:A:1114:U:H3	9:A:1119:A:N6	1.97	0.63
9:A:1613:G:OP1	34:b:42:ARG:NH2	2.32	0.63
31:Y:48:GLN:OE1	31:Y:48:GLN:N	2.31	0.63
50:y:708:ARG:O	50:y:708:ARG:NH1	2.32	0.63
47:u:11:ALA:HB2	47:u:34:VAL:HG21	1.81	0.62
13:E:139:GLU:N	13:E:139:GLU:OE2	2.31	0.62
9:A:588:G:OP2	9:A:588:G:N2	2.25	0.62
9:A:888:U:O2'	9:A:889:U:O5'	2.18	0.62
47:u:414:VAL:O	47:u:425:GLN:NE2	2.31	0.62
28:T:98:GLU:OE1	28:T:98:GLU:N	2.32	0.62
47:u:48:GLU:OE2	47:u:48:GLU:N	2.32	0.62
9:A:880:G:O6	9:A:906:U:O4	2.16	0.62
9:A:1672:U:OP1	31:Y:18:THR:OG1	2.10	0.62
47:u:337:ASP:OD1	50:y:742:LYS:NZ	2.32	0.62
9:A:1485:U:OP1	32:Z:151:LYS:NZ	2.33	0.62
22:N:69:GLU:OE2	22:N:69:GLU:N	2.33	0.62
22:N:144:THR:N	22:N:158:ASP:OD2	2.33	0.62
46:p:327:LEU:O	46:p:330:GLU:N	2.32	0.62
50:y:358:VAL:HG22	50:y:374:ILE:HG13	1.81	0.62
26:R:69:SER:OG	26:R:191:GLU:OE2	2.10	0.62
34:b:110:GLU:OE2	34:b:110:GLU:N	2.33	0.62
35:c:18:VAL:O	35:c:287:THR:OG1	2.15	0.62
9:A:453:C:O2'	27:S:92:ARG:O	2.15	0.62
9:A:1116:C:C4	9:A:1117:C:C5	2.88	0.61
47:u:157:TYR:O	47:u:161:LEU:HD23	2.00	0.61
9:A:1535:U:O4	29:V:159:ARG:NH1	2.34	0.61
31:Y:61:GLU:N	31:Y:61:GLU:OE1	2.32	0.61
9:A:1117:C:C5	9:A:1118:C:C5	2.89	0.61
10:B:114:SER:OG	10:B:116:CYS:SG	2.54	0.61
43:m:17:ALA:O	43:m:21:VAL:HG23	1.99	0.61
9:A:57:U:OP1	9:A:504:G:O2'	2.18	0.61
21:M:77:GLU:OE2	21:M:81:ARG:NH2	2.33	0.61
21:M:87:GLU:N	21:M:87:GLU:OE1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:463:C:O2'	9:A:466:G:O6	2.18	0.60
36:d:59:SER:OG	36:d:79:TYR:OH	2.13	0.60
44:n:13:ARG:NH2	49:x:479:GLN:O	2.34	0.60
31:Y:40:GLU:N	31:Y:40:GLU:OE1	2.33	0.60
47:u:411:LEU:HD11	47:u:431:LEU:HD22	1.83	0.60
35:c:145:GLU:O	35:c:175:LYS:NZ	2.35	0.60
47:u:295:THR:HG22	47:u:359:LEU:HD11	1.82	0.60
9:A:643:A:OP1	12:D:38:ARG:NH1	2.33	0.60
15:G:159:ASP:OD1	15:G:161:ALA:N	2.35	0.60
32:Z:31:GLU:OE2	32:Z:31:GLU:N	2.33	0.60
38:f:108:ARG:NH2	38:f:109:GLU:OE1	2.34	0.60
47:u:350:GLU:O	47:u:353:ARG:NH1	2.34	0.60
2:U:140:LEU:HA	2:U:209:GLY:CA	2.22	0.60
9:A:84:A:N3	9:A:150:A:O2'	2.33	0.60
13:E:6:GLY:O	13:E:9:THR:OG1	2.12	0.60
2:U:140:LEU:CA	2:U:209:GLY:HA2	2.23	0.59
32:Z:23:GLU:OE2	32:Z:27:ARG:NE	2.30	0.59
13:E:58:GLU:N	13:E:58:GLU:OE1	2.34	0.59
9:A:1436:C:O2'	9:A:1438:A:O5'	2.19	0.59
18:J:30:CYS:SG	18:J:31:SER:N	2.75	0.59
46:p:175:TYR:O	46:p:179:GLY:N	2.35	0.59
48:v:205:LEU:HD12	48:v:206:GLN:N	2.18	0.59
9:A:549:C:H2'	9:A:550:C:N1	2.18	0.59
45:o:273:ASP:HA	46:p:149:ASN:CB	2.33	0.59
9:A:550:C:H5''	9:A:550:C:C6	2.26	0.59
49:x:424:GLU:O	49:x:428:ASN:N	2.35	0.59
6:6:350:LEU:O	6:6:353:THR:OG1	2.19	0.58
9:A:1113:A:C2	9:A:1121:G:C5	2.90	0.58
9:A:989:C:OP2	23:O:155:TYR:OH	2.21	0.58
47:u:515:PRO:O	47:u:520:ARG:NH2	2.36	0.58
9:A:1285:G:N2	43:m:82:ASN:OD1	2.37	0.58
43:m:45:ARG:NH1	43:m:72:HIS:O	2.36	0.58
32:Z:56:GLN:OE1	32:Z:56:GLN:N	2.35	0.58
32:Z:226:GLN:HG3	35:c:186:THR:HG22	1.85	0.58
47:u:71:LEU:HD13	47:u:163:LEU:HD22	1.86	0.58
9:A:62:G:O2'	9:A:172:U:OP1	2.21	0.58
9:A:1425:G:O3'	31:Y:33:LYS:NZ	2.37	0.58
20:L:61:MET:HE3	20:L:61:MET:HA	1.86	0.58
46:p:320:GLY:C	46:p:322:GLN:H	2.12	0.58
9:A:984:C:O2'	24:P:138:ASP:OD2	2.20	0.57
36:d:13:GLU:OE2	36:d:13:GLU:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:R:22:HIS:ND1	26:R:23:LYS:O	2.31	0.57
39:h:35:VAL:O	39:h:39:LEU:HD23	2.04	0.57
9:A:1155:U:OP1	20:L:185:THR:OG1	2.11	0.57
9:A:1544:C:O2'	31:Y:75:GLY:O	2.19	0.57
15:G:24:SER:OG	15:G:25:GLN:OE1	2.17	0.57
21:M:115:SER:OG	21:M:116:ASN:N	2.36	0.57
37:e:75:GLU:O	37:e:78:LYS:NZ	2.27	0.57
48:v:385:ASP:OD2	48:v:390:HIS:N	2.36	0.57
21:M:14:ARG:HG2	21:M:69:ILE:HD11	1.86	0.57
34:b:23:ASP:OD1	34:b:24:GLN:N	2.38	0.57
47:u:94:LEU:HD11	47:u:177:ILE:HD12	1.85	0.57
48:v:212:THR:HG23	48:v:242:TYR:OH	2.04	0.57
50:y:680:GLU:N	50:y:680:GLU:OE2	2.37	0.57
9:A:1593:C:O2	36:d:12:GLN:NE2	2.36	0.57
20:L:77:SER:OG	20:L:80:GLU:OE2	2.15	0.57
50:y:714:PHE:CZ	50:y:718:LEU:HD11	2.39	0.57
20:L:174:ILE:O	20:L:200:ARG:NH2	2.38	0.57
46:p:194:GLY:O	46:p:197:LYS:CB	2.53	0.56
9:A:534:G:N1	9:A:550:C:C4	2.74	0.56
9:A:1115:U:H2'	9:A:1116:C:H3'	1.86	0.56
9:A:1707:U:O2	30:W:68:ALA:HB1	2.05	0.56
43:m:95:ASP:O	43:m:96:ARG:NH1	2.37	0.56
9:A:1614:A:OP2	34:b:42:ARG:NH1	2.39	0.56
9:A:1722:G:H1	9:A:1812:U:H3	1.53	0.56
14:F:120:VAL:O	14:F:121:PRO:C	2.48	0.56
15:G:171:GLU:N	15:G:171:GLU:OE1	2.37	0.56
50:y:646:LEU:O	50:y:646:LEU:HD23	2.06	0.56
12:D:158:ASP:OD1	12:D:159:PHE:N	2.38	0.56
25:Q:41:ILE:HD12	25:Q:41:ILE:O	2.04	0.56
46:p:184:VAL:O	46:p:187:MSE:CA	2.53	0.56
9:A:60:G:H22	9:A:316:G:H21	1.54	0.56
21:M:27:ASP:OD2	21:M:30:THR:HG23	2.06	0.56
35:c:72:SER:OG	35:c:74:ASP:OD1	2.18	0.56
47:u:331:ILE:HD11	47:u:438:ARG:NH2	2.20	0.56
9:A:383:G:O2'	10:B:133:PRO:O	2.22	0.56
32:Z:106:ARG:NE	32:Z:174:HIS:O	2.37	0.56
34:b:29:SER:OG	34:b:30:TYR:N	2.35	0.56
42:l:320:SER:O	42:l:321:GLY:C	2.47	0.56
43:m:99:LYS:O	43:m:101:ARG:NH1	2.39	0.56
48:v:347:ILE:HG23	50:y:826:ILE:HD12	1.86	0.56
8:9:10:MET:HE1	8:9:14:LYS:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:542:U:H2'	9:A:543:C:H6	1.71	0.56
9:A:1665:G:C5	36:d:88:MET:HE1	2.40	0.56
12:D:160:SER:O	12:D:163:SER:OG	2.23	0.56
32:Z:81:GLU:OE1	32:Z:82:GLY:N	2.39	0.55
9:A:549:C:H3'	9:A:549:C:H6	1.70	0.55
9:A:1545:A:N3	9:A:1671:G:O2'	2.30	0.55
34:b:123:TYR:OH	38:f:120:HIS:NE2	2.28	0.55
7:8:221:LYS:O	7:8:224:VAL:C	2.49	0.55
31:Y:63:PHE:CZ	31:Y:92:LEU:HD22	2.42	0.55
43:m:32:ALA:HB3	43:m:110:VAL:HG13	1.87	0.55
13:E:39:ASN:ND2	13:E:42:GLY:O	2.40	0.55
24:P:36:SER:OG	24:P:37:PHE:N	2.39	0.55
28:T:50:THR:OG1	28:T:51:THR:N	2.40	0.55
47:u:401:LEU:HD12	47:u:458:LEU:HD21	1.88	0.55
17:I:29:THR:OG1	17:I:31:ASP:OD1	2.12	0.55
9:A:925:G:O6	9:A:1017:U:O4	2.25	0.55
9:A:1455:A:OP1	21:M:5:ARG:NH2	2.39	0.55
50:y:340:ARG:NH1	50:y:384:ASP:OD2	2.40	0.55
2:U:398:GLU:O	2:U:399:LYS:C	2.49	0.55
26:R:88:ASN:OD1	26:R:205:ARG:NH1	2.40	0.55
9:A:1273:C:O2'	9:A:1506:A:N1	2.25	0.55
46:p:283:LYS:O	46:p:284:GLY:C	2.50	0.55
47:u:14[B]:ARG:NE	47:u:14[B]:ARG:HA	2.22	0.55
13:E:96:GLU:OE2	13:E:96:GLU:N	2.39	0.54
15:G:193:GLN:OE1	15:G:193:GLN:N	2.40	0.54
4:4:122:GLY:N	4:4:168:LEU:O	2.40	0.54
29:V:72:LEU:HA	29:V:151:ILE:HD11	1.89	0.54
9:A:548:C:H5'	9:A:549:C:C5	2.42	0.54
9:A:1354:G:N2	9:A:1357:A:OP2	2.32	0.54
50:y:405:ILE:HD12	50:y:451:MET:CE	2.38	0.54
6:6:351:TYR:O	6:6:355:ASN:ND2	2.40	0.54
9:A:940:U:H3	9:A:1002:U:H3	1.54	0.54
9:A:1329:U:O2'	9:A:1332:A:OP2	2.12	0.54
9:A:1351:G:O2'	9:A:1378:A:N1	2.34	0.54
7:8:221:LYS:O	7:8:224:VAL:O	2.25	0.54
9:A:818:A:OP1	12:D:80:ARG:NH2	2.39	0.54
15:G:42:GLU:OE1	15:G:42:GLU:N	2.41	0.54
35:c:10:THR:O	35:c:10:THR:OG1	2.25	0.54
44:n:7:GLN:NE2	44:n:59:LEU:O	2.41	0.54
47:u:481:GLN:O	47:u:494:GLY:N	2.41	0.54
50:y:748:ASP:OD1	50:y:749:TRP:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1533:A:N3	9:A:1536:G:O2'	2.38	0.54
32:Z:42:THR:OG1	32:Z:45:ARG:O	2.20	0.54
37:e:48:VAL:O	37:e:83:LEU:HD22	2.07	0.54
39:h:46:LYS:HE2	39:h:101:ILE:HD11	1.89	0.54
47:u:113:LEU:HD11	47:u:137:THR:HG23	1.90	0.54
17:I:83:ASP:OD2	17:I:84:LEU:N	2.41	0.53
34:b:34:MET:HA	34:b:34:MET:HE3	1.90	0.53
2:U:373:LEU:N	2:U:396:MET:H	2.05	0.53
23:O:68:GLU:OE2	24:P:96:LYS:NZ	2.42	0.53
23:O:104:ASP:OD1	23:O:105:LEU:N	2.41	0.53
29:V:40:ALA:HB1	29:V:45:TYR:CD2	2.44	0.53
46:p:162:ARG:O	46:p:163:ALA:C	2.51	0.53
48:v:393:MET:SD	48:v:393:MET:N	2.80	0.53
9:A:1119:A:H3'	9:A:1120:U:C6	2.44	0.53
9:A:540:U:H4'	9:A:541:U:H2'	1.91	0.53
9:A:834:C:O2'	9:A:836:G:N2	2.41	0.53
9:A:918:U:O2'	9:A:919:A:O5'	2.26	0.53
9:A:1121:G:C2	9:A:1122:A:C8	2.97	0.53
18:J:10:ALA:HA	18:J:27:ILE:HD12	1.89	0.53
35:c:32:LEU:HD12	35:c:40:ILE:HG22	1.91	0.53
9:A:534:G:H2'	9:A:535:G:C8	2.43	0.53
34:b:92:SER:O	34:b:107:ILE:HD12	2.09	0.53
46:p:163:ALA:O	46:p:164:PHE:C	2.52	0.53
50:y:499:VAL:HA	50:y:502:ILE:HG22	1.91	0.53
9:A:1119:A:H2'	9:A:1120:U:C2	2.44	0.53
9:A:1620:A:OP1	34:b:115:TYR:OH	2.27	0.53
9:A:370:G:O2'	26:R:10:LYS:NZ	2.41	0.53
9:A:535:G:C8	9:A:535:G:H5''	2.43	0.53
9:A:1665:G:C6	36:d:88:MET:HE1	2.44	0.53
3:3:159:ALA:O	3:3:164:ASP:N	2.41	0.52
9:A:547:G:C2'	9:A:548:C:H4'	2.38	0.52
9:A:1587:G:N2	9:A:1587:G:OP1	2.41	0.52
9:A:1757:G:OP2	9:A:1757:G:N2	2.40	0.52
20:L:79:GLU:OE2	20:L:79:GLU:N	2.40	0.52
38:f:8:LYS:O	38:f:9:PHE:C	2.52	0.52
45:o:271:ALA:CA	46:p:150:CYS:HA	2.38	0.52
47:u:329:ILE:O	47:u:367:ARG:NH1	2.42	0.52
50:y:802:ILE:HD11	50:y:807:LEU:HD11	1.91	0.52
9:A:1360:U:O2'	9:A:1379:A:OP2	2.25	0.52
12:D:58:ARG:O	12:D:62:THR:HG23	2.08	0.52
29:V:118:ASN:O	29:V:193:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:11:LEU:HD12	35:c:43:TRP:CE3	2.44	0.52
44:n:21:THR:OG1	44:n:22:GLY:N	2.42	0.52
46:p:183:GLU:O	46:p:187:MSE:CB	2.57	0.52
9:A:920:A:O2'	9:A:922:A:OP1	2.22	0.52
20:L:201:GLY:N	20:L:221:ASP:OD1	2.42	0.52
37:e:90:GLU:O	37:e:93:SER:OG	2.26	0.52
9:A:1060:A:O2'	9:A:1062:A:N7	2.36	0.52
30:W:45:THR:OG1	30:W:87:GLY:O	2.23	0.52
42:l:146:LYS:O	42:l:147:LEU:C	2.53	0.52
46:p:176:PHE:O	46:p:177:GLU:C	2.53	0.52
6:6:168:LEU:O	6:6:172:LEU:N	2.42	0.52
9:A:543:C:H3'	9:A:544:G:C5'	2.40	0.52
50:y:354:LEU:O	50:y:358:VAL:HG23	2.10	0.52
9:A:535:G:N2	9:A:550:C:N3	2.57	0.52
9:A:1113:A:C4	9:A:1119:A:N6	2.77	0.52
50:y:646:LEU:HD22	50:y:648:GLN:HG2	1.92	0.52
38:f:13:LEU:HD23	38:f:13:LEU:H	1.75	0.51
2:U:400:GLN:O	2:U:401:VAL:C	2.53	0.51
42:l:88:ILE:O	42:l:89:SER:C	2.52	0.51
35:c:35:SER:OG	35:c:36:ARG:N	2.44	0.51
48:v:229:ARG:HD3	48:v:232:ILE:HD12	1.92	0.51
9:A:1013:U:OP1	9:A:1129:G:O2'	2.23	0.51
21:M:58:MET:HE3	21:M:58:MET:HA	1.91	0.51
9:A:537:C:H3'	9:A:538:U:H6	1.76	0.51
9:A:1242:U:O2	9:A:1517:G:O2'	2.19	0.51
34:b:31:GLU:OE2	34:b:31:GLU:N	2.41	0.51
43:m:32:ALA:HB3	43:m:110:VAL:CG1	2.41	0.51
9:A:540:U:O2	9:A:543:C:H2'	2.11	0.51
29:V:122:ARG:HB2	44:n:59:LEU:HD21	1.92	0.51
32:Z:88:ALA:O	45:o:309:ILE:N	2.44	0.51
4:4:203:ASP:N	4:4:212:SER:O	2.44	0.51
9:A:542:U:H2'	9:A:543:C:C6	2.46	0.51
22:N:12:GLU:N	22:N:12:GLU:OE1	2.43	0.51
32:Z:75:LYS:NZ	33:a:34:GLU:OE2	2.34	0.51
9:A:1374:5MC:O2'	9:A:1464:C:O2	2.28	0.51
9:A:1753:C:N3	9:A:1781:A:N6	2.58	0.51
19:K:78:ILE:O	22:N:3:GLY:N	2.44	0.51
10:B:128:VAL:HG12	10:B:142:VAL:HA	1.93	0.50
42:l:27:TRP:O	42:l:28:ASN:C	2.54	0.50
46:p:420:PRO:C	46:p:422:SER:H	2.19	0.50
47:u:87:GLU:HG2	47:u:173:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:440:LEU:HD21	47:u:471:ILE:HD13	1.92	0.50
9:A:351:G:OP1	26:R:7:ASN:ND2	2.44	0.50
15:G:169:LYS:O	15:G:172:THR:OG1	2.23	0.50
32:Z:225:GLU:HB3	35:c:187:ASN:OD1	2.11	0.50
11:C:87:MET:HE1	11:C:236:ILE:HD13	1.93	0.50
35:c:244:ASN:OD1	35:c:245:ARG:N	2.42	0.50
12:D:63:LEU:O	12:D:70:ARG:NH1	2.43	0.50
47:u:203:MET:HE3	47:u:203:MET:O	2.12	0.50
50:y:559:ASP:OD1	50:y:560:ARG:N	2.45	0.50
50:y:799:TYR:CE2	50:y:802:ILE:HD12	2.47	0.50
9:A:1171:G:O2'	9:A:1187:G:O6	2.25	0.50
16:H:40:CYS:SG	16:H:41:TYR:N	2.84	0.50
33:a:89:ILE:O	33:a:89:ILE:HD12	2.12	0.50
9:A:1701:C:O2'	46:p:103:ARG:NH2	2.44	0.50
16:H:34:ASP:N	16:H:34:ASP:OD1	2.44	0.50
23:O:138:PHE:O	23:O:213:ARG:N	2.45	0.50
23:O:147:ASN:OD1	23:O:148:ASN:N	2.44	0.50
47:u:331:ILE:HG23	47:u:437:LEU:HD23	1.93	0.50
43:m:60:MET:HE3	43:m:60:MET:H	1.77	0.50
50:y:752:CYS:HB2	50:y:783:ILE:HD11	1.93	0.50
42:l:377:THR:H	42:l:380:ASP:CB	2.25	0.49
9:A:1124:C:O2'	21:M:126:MET:O	2.29	0.49
9:A:1215:C:O2'	9:A:1645:C:OP2	2.24	0.49
9:A:1850:MA6:N6	9:A:1851:MA6:H93	2.27	0.49
24:P:46:ASP:OD1	24:P:48:SER:N	2.43	0.49
42:l:245:GLY:O	42:l:369:LYS:N	2.45	0.49
2:U:373:LEU:H	2:U:396:MET:H	1.60	0.49
9:A:1120:U:C2	9:A:1121:G:C8	3.00	0.49
48:v:206:GLN:NE2	49:x:21:VAL:O	2.46	0.49
9:A:571:U:O2'	28:T:60:PHE:O	2.28	0.49
9:A:1248:U:O4'	31:Y:146:ARG:NH1	2.45	0.49
9:A:1620:A:O2'	34:b:40:ARG:NH1	2.45	0.49
12:D:152:ASP:OD2	12:D:152:ASP:N	2.44	0.49
15:G:31:GLU:OE2	15:G:41:ARG:NH1	2.45	0.49
20:L:80:GLU:OE2	20:L:80:GLU:N	2.43	0.49
41:k:125:GLU:N	41:k:125:GLU:OE1	2.45	0.49
9:A:1679:A:OP1	29:V:60:ARG:NH2	2.46	0.49
24:P:124:MET:HE3	24:P:124:MET:HA	1.94	0.49
32:Z:59:LEU:HD22	45:o:307:HIS:CB	2.35	0.49
46:p:158:PRO:HA	46:p:193:LEU:HA	1.94	0.49
48:v:401:TYR:O	48:v:405:ILE:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:304:GLY:N	6:6:307:ASP:OD2	2.44	0.49
9:A:1282:A:O2'	9:A:1283:C:O4'	2.29	0.49
27:S:5:ILE:CG2	27:S:113:ILE:HD11	2.43	0.49
46:p:185:ALA:N	46:p:186:GLU:N	2.60	0.49
36:d:87:VAL:HG23	36:d:88:MET:CE	2.43	0.49
23:O:113:MET:HE1	23:O:211:PHE:HD2	1.78	0.49
21:M:120:THR:OG1	21:M:121:GLN:N	2.46	0.48
9:A:836:G:O2'	9:A:838:G:O6	2.31	0.48
9:A:95:G:N2	9:A:474:G:O5'	2.46	0.48
9:A:1115:U:C2'	9:A:1116:C:H3'	2.44	0.48
12:D:88:ASP:OD1	12:D:89:GLU:N	2.46	0.48
23:O:77:ASP:OD1	47:u:7:ARG:NH2	2.44	0.48
26:R:3:ILE:O	26:R:30:GLY:N	2.45	0.48
15:G:77:VAL:O	15:G:80:VAL:HG22	2.13	0.48
21:M:114:LEU:O	21:M:117:LEU:HD22	2.13	0.48
27:S:24:LEU:HD13	27:S:24:LEU:O	2.13	0.48
28:T:80:ASP:OD1	28:T:81:TYR:N	2.46	0.48
38:f:51:ASP:OD1	38:f:53:THR:OG1	2.26	0.48
9:A:919:A:O2'	53:A:2005:SPD:N10	2.46	0.48
11:C:40:GLU:N	11:C:40:GLU:OE2	2.46	0.48
31:Y:53:GLU:OE1	31:Y:85:ARG:NH1	2.42	0.48
35:c:244:ASN:ND2	35:c:294:ASP:O	2.46	0.48
43:m:33:ARG:N	43:m:37:GLU:OE1	2.46	0.48
46:p:185:ALA:O	46:p:188:LEU:N	2.47	0.48
47:u:74:TYR:OH	47:u:85:SER:OG	2.14	0.48
33:a:18:GLU:OE1	33:a:18:GLU:N	2.47	0.48
45:o:264:SER:CB	46:p:163:ALA:HB2	2.44	0.48
46:p:269:VAL:O	46:p:272:GLY:N	2.42	0.48
9:A:1678:A2M:HM'2	9:A:1679:A:O4'	2.13	0.48
15:G:20:GLU:HA	15:G:23:ILE:HD12	1.94	0.48
9:A:466:G:O2'	27:S:72:ARG:NH2	2.45	0.48
43:m:51:VAL:CG2	43:m:79:VAL:HG23	2.44	0.48
48:v:243:LEU:O	48:v:249:MET:N	2.41	0.48
48:v:340:ILE:O	48:v:343:THR:OG1	2.27	0.48
31:Y:100:VAL:HG12	31:Y:100:VAL:O	2.14	0.48
2:U:372:TYR:HA	2:U:395:ARG:CA	2.39	0.47
35:c:260:ASP:O	35:c:264:LYS:N	2.44	0.47
49:x:268:VAL:N	49:x:279:ASP:O	2.42	0.47
9:A:43:U:OP2	9:A:485:A:N6	2.46	0.47
9:A:605:A:H4'	14:F:129:PRO:HG2	1.94	0.47
9:A:1656:G:H1	9:A:1668:U:H3	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:L:271:ASP:OD2	20:L:271:ASP:N	2.46	0.47
9:A:899:U:O2'	9:A:902:G:O6	2.14	0.47
29:V:65:GLN:N	29:V:65:GLN:OE1	2.47	0.47
43:m:76:LEU:C	43:m:77:ILE:HD12	2.39	0.47
46:p:441:LYS:O	46:p:442:GLN:C	2.57	0.47
50:y:415:ASN:ND2	50:y:417:ASN:OD1	2.47	0.47
7:8:258:VAL:HA	50:y:857:LEU:HD13	1.97	0.47
32:Z:47:GLU:C	32:Z:48:ILE:HD12	2.40	0.47
37:e:79:ILE:HD12	37:e:80:ARG:O	2.14	0.47
43:m:51:VAL:HG21	43:m:79:VAL:HG23	1.95	0.47
9:A:1331:C:N4	46:p:101:ASP:O	2.46	0.47
9:A:1302:G:H21	41:k:95:ARG:HE	1.61	0.47
31:Y:41:MET:HE3	31:Y:41:MET:HA	1.96	0.47
48:v:264:ASN:ND2	48:v:266:ASP:OD1	2.48	0.47
49:x:68:GLN:O	49:x:70:ALA:N	2.48	0.47
9:A:993:G:N7	25:Q:15:ARG:NH1	2.63	0.47
9:A:1116:C:H2'	9:A:1117:C:O4'	2.15	0.47
47:u:292:HIS:HE2	47:u:427:TYR:HH	1.61	0.47
47:u:419:GLU:OE2	47:u:419:GLU:N	2.46	0.47
50:y:515:ASP:OD1	50:y:518:ALA:N	2.42	0.47
8:9:10:MET:HE3	8:9:10:MET:C	2.39	0.47
34:b:16:THR:OG1	34:b:20:VAL:N	2.48	0.47
47:u:11:ALA:CB	47:u:34:VAL:HG21	2.45	0.47
9:A:535:G:N1	9:A:550:C:N4	2.54	0.47
9:A:661:U:OP2	9:A:662:G:O2'	2.31	0.47
9:A:1023:A:OP2	17:I:124:ARG:NH1	2.48	0.47
9:A:1147:C:OP1	25:Q:6:ARG:NH1	2.44	0.47
32:Z:66:ILE:HD13	45:o:307:HIS:CB	2.45	0.47
35:c:30:MET:HE3	35:c:30:MET:C	2.40	0.47
42:l:140:VAL:O	42:l:141:ARG:C	2.56	0.47
9:A:1116:C:C2	9:A:1117:C:C6	3.03	0.46
9:A:1282:A:HO2'	9:A:1283:C:C4'	2.28	0.46
25:Q:52:ASP:OD1	25:Q:52:ASP:N	2.48	0.46
36:d:118:ASP:OD1	36:d:119:GLY:N	2.48	0.46
47:u:153:LEU:O	47:u:156:SER:OG	2.30	0.46
16:H:2:PRO:HA	19:K:64:GLU:OE2	2.15	0.46
27:S:28:TYR:OH	27:S:104:ALA:HB2	2.15	0.46
29:V:100:ILE:HG21	29:V:111:VAL:HG11	1.97	0.46
47:u:94:LEU:CD1	47:u:177:ILE:HD12	2.46	0.46
11:C:44:LEU:HD13	11:C:72:ILE:HD11	1.98	0.46
16:H:6:ASP:OD1	16:H:9:HIS:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:u:404:CYS:O	47:u:408:THR:HG23	2.16	0.46
48:v:243:LEU:CD1	48:v:247:GLN:HE22	2.28	0.46
9:A:56:G:OP1	28:T:111:LYS:NZ	2.41	0.46
9:A:540:U:H5''	9:A:541:U:C5	2.50	0.46
16:H:78:SER:OG	49:x:79:SER:O	2.16	0.46
32:Z:132:LYS:HD3	32:Z:189:MET:HE2	1.97	0.46
9:A:885:U:N3	9:A:901:G:C6	2.80	0.46
32:Z:154:ASP:OD1	32:Z:155:GLY:N	2.48	0.46
50:y:445:LEU:HD12	50:y:498:GLU:HB2	1.98	0.46
50:y:659:ASN:OD1	50:y:667:ARG:NH2	2.49	0.46
12:D:26:ASP:OD1	12:D:26:ASP:N	2.48	0.46
18:J:14:ILE:CD1	18:J:27:ILE:HD11	2.45	0.46
35:c:162:ASN:O	35:c:162:ASN:ND2	2.49	0.46
46:p:382:MSE:O	46:p:383:ILE:C	2.57	0.46
9:A:550:C:H3'	9:A:551:U:H6	1.81	0.46
50:y:752:CYS:CB	50:y:783:ILE:HD11	2.45	0.46
9:A:550:C:H3'	9:A:551:U:C5'	2.46	0.46
9:A:1869:A:N6	23:O:114:VAL:O	2.49	0.46
43:m:23:LYS:NZ	43:m:88:TRP:O	2.37	0.46
42:l:249:PHE:O	42:l:373:ILE:HA	2.16	0.46
50:y:756:ILE:O	50:y:766:TRP:NE1	2.44	0.46
9:A:191:A:N6	9:A:208:G:O2'	2.44	0.46
9:A:1282:A:O2'	9:A:1283:C:O5'	2.31	0.46
29:V:125:SER:OG	29:V:136:ARG:NE	2.48	0.46
35:c:226:HIS:NE2	35:c:229:THR:OG1	2.45	0.46
40:i:49:ASP:N	40:i:49:ASP:OD2	2.49	0.46
46:p:171:ILE:O	46:p:172:ILE:C	2.58	0.46
47:u:331:ILE:CG2	47:u:437:LEU:HD23	2.46	0.46
2:U:134:PHE:O	2:U:135:LYS:C	2.59	0.45
9:A:1648:G:O2'	9:A:1674:G:O6	2.31	0.45
9:A:1121:G:C6	9:A:1122:A:C5	3.04	0.45
9:A:1344:A:N1	9:A:1385:G:O2'	2.38	0.45
23:O:38:MET:SD	23:O:185:VAL:HG11	2.57	0.45
38:f:71:MET:SD	38:f:99:LEU:HD21	2.56	0.45
9:A:1285:G:H22	43:m:82:ASN:CG	2.24	0.45
38:f:15:VAL:CG1	38:f:20:ILE:HD13	2.47	0.45
9:A:537:C:H3'	9:A:538:U:C6	2.51	0.45
9:A:1121:G:C6	9:A:1122:A:N7	2.84	0.45
37:e:47:LEU:HB2	37:e:79:ILE:HG22	1.99	0.45
6:6:252:TYR:O	6:6:257:GLN:N	2.45	0.45
28:T:7:ILE:HD12	28:T:7:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:391:PHE:O	2:U:392:GLU:C	2.59	0.45
6:6:330:ARG:HD3	6:6:332:VAL:HG13	1.97	0.45
9:A:329:G:O2'	9:A:330:G:OP1	2.32	0.45
27:S:6:SER:O	27:S:113:ILE:HD12	2.17	0.45
42:l:150:GLU:O	42:l:151:ALA:C	2.59	0.45
48:v:243:LEU:HA	48:v:247:GLN:HB3	1.98	0.45
32:Z:227:LYS:HD3	35:c:184:LEU:HB3	1.98	0.45
9:A:549:C:H3'	9:A:549:C:C6	2.50	0.45
9:A:1117:C:N4	9:A:1118:C:C2	2.85	0.45
9:A:1355:C:O3'	20:L:238:LYS:NZ	2.50	0.45
37:e:94:LYS:HE3	37:e:94:LYS:HA	1.99	0.45
19:K:2:GLN:NE2	19:K:6:GLY:O	2.46	0.45
37:e:67:LEU:CD2	37:e:108:ILE:HD11	2.46	0.45
37:e:100:VAL:HG13	37:e:108:ILE:HG23	2.00	0.45
42:l:121:MET:C	42:l:124:GLY:H	2.24	0.45
46:p:320:GLY:C	46:p:322:GLN:N	2.75	0.45
9:A:548:C:H2'	9:A:549:C:N3	2.32	0.44
9:A:871:U:O2'	9:A:872:A:OP1	2.30	0.44
9:A:1117:C:C4	9:A:1118:C:C2	3.05	0.44
16:H:48:SER:OG	16:H:49:HIS:ND1	2.50	0.44
39:h:26:SER:OG	39:h:27:ARG:N	2.50	0.44
46:p:354:LEU:O	46:p:355:GLU:C	2.61	0.44
9:A:516:A:N1	9:A:643:A:O2'	2.50	0.44
12:D:114:VAL:HG23	12:D:119:LEU:HD13	1.99	0.44
15:G:174:SER:OG	15:G:185:VAL:O	2.30	0.44
22:N:134:LEU:HD11	22:N:144:THR:HG21	2.00	0.44
28:T:7:ILE:HG22	28:T:27:VAL:HG22	1.99	0.44
29:V:111:VAL:HG23	29:V:181:ALA:CB	2.47	0.44
46:p:144:ASP:OD1	46:p:144:ASP:N	2.50	0.44
9:A:164:A:H3'	9:A:165:G:H21	1.81	0.44
9:A:346:C:OP1	11:C:38:LEU:N	2.50	0.44
9:A:549:C:C6	9:A:549:C:C3'	3.01	0.44
9:A:1275:G:O4'	9:A:1506:A:N6	2.51	0.44
23:O:229:MET:HE3	23:O:229:MET:HA	1.98	0.44
25:Q:41:ILE:HG22	25:Q:68:TYR:CD2	2.51	0.44
50:y:596:ASP:OD1	50:y:596:ASP:N	2.47	0.44
9:A:390:C:O2'	10:B:8:ARG:NH2	2.51	0.44
21:M:82:ASP:O	22:N:89:LYS:NZ	2.42	0.44
32:Z:227:LYS:N	35:c:185:LYS:O	2.50	0.44
33:a:75:GLY:O	33:a:79:LEU:HD23	2.17	0.44
42:l:126:TYR:O	42:l:127:MET:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:v:349:GLN:OE1	48:v:393:MET:N	2.51	0.44
50:y:774:LYS:O	50:y:777:THR:OG1	2.30	0.44
9:A:543:C:H3'	9:A:544:G:H5''	2.00	0.44
46:p:185:ALA:C	46:p:186:GLU:O	2.54	0.44
11:C:176:ASP:OD1	11:C:177:THR:N	2.50	0.44
34:b:104:GLN:N	34:b:104:GLN:OE1	2.50	0.44
36:d:5:THR:HG22	36:d:6:VAL:H	1.83	0.44
48:v:241:GLN:O	48:v:245:ALA:HB2	2.18	0.44
9:A:172:U:OP1	9:A:314:U:O2'	2.36	0.44
9:A:1207:G:O2'	9:A:1208:A:OP1	2.29	0.44
12:D:18:ARG:O	12:D:24:ARG:NH2	2.48	0.44
32:Z:179:GLN:OE1	32:Z:179:GLN:N	2.48	0.44
33:a:26:ASP:O	33:a:42:ASN:ND2	2.49	0.44
42:l:29:GLU:C	42:l:31:VAL:H	2.25	0.44
46:p:185:ALA:O	46:p:186:GLU:C	2.55	0.44
46:p:213:ALA:O	46:p:214:SER:C	2.59	0.44
47:u:90:VAL:CG2	47:u:173:LEU:HD21	2.48	0.44
48:v:287:THR:OG1	48:v:288:TYR:N	2.50	0.44
2:U:373:LEU:H	2:U:395:ARG:HA	1.83	0.43
9:A:537:C:N4	9:A:544:G:N1	2.66	0.43
9:A:888:U:HO2'	9:A:889:U:P	2.41	0.43
9:A:1015:U:OP2	16:H:20:LYS:NZ	2.48	0.43
10:B:111:VAL:HG12	10:B:140:PHE:HB2	1.99	0.43
32:Z:48:ILE:HD13	32:Z:84:VAL:HG23	2.00	0.43
43:m:32:ALA:HB1	43:m:37:GLU:HB3	2.00	0.43
50:y:691:MET:HE3	50:y:741:SER:CB	2.48	0.43
9:A:475:C:O2'	9:A:507:G:N3	2.44	0.43
20:L:120:GLN:N	20:L:120:GLN:OE1	2.52	0.43
32:Z:67:ARG:NE	33:a:93:THR:O	2.41	0.43
42:l:322:SER:O	42:l:323:SER:CB	2.66	0.43
50:y:427:GLU:N	50:y:427:GLU:OE1	2.52	0.43
50:y:495:THR:HG1	50:y:498:GLU:CD	2.16	0.43
6:6:333:VAL:HG13	6:6:334:VAL:HG23	2.01	0.43
9:A:1583:C:OP2	9:A:1584:G:O2'	2.31	0.43
11:C:54:TYR:O	28:T:15:ASN:ND2	2.51	0.43
17:I:142:GLU:OE2	17:I:142:GLU:N	2.51	0.43
45:o:237:ASP:C	45:o:239:ALA:N	2.73	0.43
24:P:78:ALA:HB3	24:P:118:ALA:HB3	2.00	0.43
42:l:95:GLU:O	42:l:97:ASP:N	2.51	0.43
46:p:254:THR:O	46:p:255:PRO:C	2.60	0.43
48:v:267:VAL:HG22	48:v:267:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:404:ASP:O	2:U:405:VAL:C	2.62	0.43
29:V:122:ARG:CB	44:n:59:LEU:HD21	2.49	0.43
30:W:60:VAL:HG23	30:W:83:ILE:HD12	2.01	0.43
42:l:112:LEU:O	42:l:113:ALA:C	2.62	0.43
32:Z:107:TYR:CD2	46:p:140:ASP:HA	2.54	0.43
46:p:167:THR:O	46:p:168:LEU:C	2.62	0.43
48:v:229:ARG:CD	48:v:232:ILE:HD12	2.49	0.43
50:y:613:MET:HE3	50:y:613:MET:O	2.19	0.43
9:A:114:G:OP2	10:B:67:SER:OG	2.37	0.43
35:c:197:THR:HG21	35:c:238:ALA:HA	2.01	0.43
47:u:331:ILE:HG23	47:u:331:ILE:O	2.19	0.43
50:y:744:MET:HE2	50:y:744:MET:HA	2.01	0.43
6:6:313:ILE:HA	6:6:316:VAL:HG12	2.01	0.42
9:A:969:U:OP1	9:A:970:G:O2'	2.25	0.42
9:A:1154:U:OP1	9:A:1155:U:O2'	2.30	0.42
17:I:145:THR:O	17:I:145:THR:HG22	2.19	0.42
38:f:9:PHE:C	38:f:9:PHE:CD2	2.97	0.42
50:y:560:ARG:H	50:y:560:ARG:HD3	1.83	0.42
9:A:380:G:N1	9:A:383:G:OP2	2.47	0.42
9:A:1025:U:OP1	9:A:1090:C:O2'	2.37	0.42
46:p:296:ASP:O	46:p:297:LYS:C	2.60	0.42
17:I:33:VAL:HG21	17:I:66:VAL:HG11	2.01	0.42
21:M:105:MET:O	21:M:109:LEU:HD22	2.19	0.42
42:l:139:ASN:O	42:l:140:VAL:C	2.62	0.42
45:o:272:LYS:H	46:p:151:VAL:H	1.67	0.42
9:A:1598:G:OP2	37:e:82:SER:OG	2.15	0.42
11:C:20:LEU:HD21	11:C:46:ILE:HD12	2.00	0.42
19:K:37:ALA:HB1	19:K:46:PHE:CD1	2.54	0.42
23:O:187:LYS:HG2	47:u:21:VAL:HG21	2.02	0.42
29:V:71:ARG:NH2	29:V:148:ASN:OD1	2.53	0.42
47:u:288:ASN:ND2	47:u:288:ASN:O	2.52	0.42
48:v:417:MET:O	48:v:421:ASN:ND2	2.50	0.42
50:y:543:ASP:OD1	50:y:546:VAL:HG22	2.20	0.42
9:A:328:U:O2	9:A:328:U:O2'	2.37	0.42
9:A:539:C:H1'	9:A:540:U:H5'	2.01	0.42
9:A:1113:A:C2	9:A:1121:G:C6	3.08	0.42
27:S:154:ARG:O	27:S:157:VAL:HG12	2.20	0.42
50:y:405:ILE:HD12	50:y:451:MET:HE2	2.00	0.42
35:c:50:THR:OG1	35:c:51:ASN:N	2.52	0.42
6:6:310:ALA:O	6:6:313:ILE:HG22	2.20	0.42
9:A:550:C:H3'	9:A:551:U:H5''	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Z:64:ARG:CD	33:a:94:LEU:HD13	2.50	0.42
48:v:247:GLN:C	48:v:249:MET:N	2.77	0.42
50:y:322:THR:O	50:y:322:THR:HG23	2.19	0.42
50:y:522:GLN:N	50:y:522:GLN:OE1	2.53	0.42
9:A:1543:U:OP2	36:d:62:ARG:NH2	2.47	0.42
29:V:72:LEU:CA	29:V:151:ILE:HD11	2.50	0.42
50:y:449:GLU:OE2	50:y:501:ARG:NH1	2.53	0.42
9:A:1084:A:OP1	9:A:1858:G:O2'	2.32	0.42
9:A:1854:U:OP1	24:P:150:ARG:NH1	2.52	0.42
24:P:87:GLU:OE2	24:P:87:GLU:N	2.49	0.42
41:k:141:CYS:SG	41:k:144:CYS:N	2.88	0.42
42:l:124:GLY:O	42:l:125:ASP:C	2.63	0.42
47:u:194:PHE:CG	47:u:243:MET:HE1	2.54	0.42
47:u:374:MET:N	47:u:374:MET:HE3	2.35	0.42
2:U:128:ILE:O	2:U:129:PRO:C	2.63	0.42
9:A:635:G:OP1	14:F:95:LYS:NZ	2.49	0.42
42:l:192:PHE:O	42:l:193:LYS:C	2.63	0.42
5:5:387:HIS:O	5:5:391:ARG:N	2.47	0.41
9:A:447:A:OP1	26:R:49:ARG:NH2	2.53	0.41
38:f:71:MET:CE	38:f:99:LEU:HD21	2.50	0.41
46:p:139:LYS:H	46:p:139:LYS:HG2	1.60	0.41
48:v:230:ASP:O	48:v:235:LEU:N	2.53	0.41
50:y:825:MET:HE1	50:y:829:GLU:HB2	2.02	0.41
48:v:244:ASN:HD21	48:v:249:MET:HE3	1.85	0.41
50:y:445:LEU:HD21	50:y:490:LEU:HD22	2.01	0.41
36:d:88:MET:N	36:d:88:MET:HE2	2.35	0.41
50:y:409:MET:HE1	50:y:412:LEU:HD23	2.02	0.41
50:y:598:ILE:HD11	50:y:605:VAL:HG12	2.02	0.41
32:Z:62:LYS:O	32:Z:67:ARG:NH2	2.49	0.41
46:p:200:VAL:O	46:p:201:PRO:C	2.63	0.41
9:A:476:A:N3	9:A:488:U:O2'	2.30	0.41
14:F:127:LYS:O	14:F:128:GLY:C	2.61	0.41
23:O:175:GLU:OE2	23:O:175:GLU:N	2.53	0.41
24:P:22:ALA:HB1	24:P:25:GLU:OE1	2.21	0.41
38:f:15:VAL:CG2	38:f:68:ILE:HD11	2.51	0.41
47:u:401:LEU:HD12	47:u:458:LEU:HD11	2.01	0.41
48:v:261:VAL:HG23	48:v:262:ILE:HG13	2.01	0.41
11:C:103:TYR:CD1	11:C:189:LEU:HD11	2.56	0.41
18:J:77:PRO:O	18:J:79:PHE:N	2.54	0.41
42:l:259:LYS:O	42:l:260:LEU:C	2.63	0.41
45:o:237:ASP:C	45:o:239:ALA:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:y:698:MET:HA	50:y:698:MET:HE2	2.01	0.41
2:U:395:ARG:O	2:U:401:VAL:HA	2.21	0.41
9:A:1114:U:H5'	23:O:202:GLN:NE2	2.36	0.41
9:A:1706:G:O2'	9:A:1850:MA6:O2'	2.35	0.41
22:N:128:ARG:NH2	22:N:151:ASP:O	2.53	0.41
24:P:56:VAL:HG13	24:P:77:ALA:HB1	2.02	0.41
32:Z:88:ALA:HB3	45:o:307:HIS:O	2.20	0.41
50:y:691:MET:HA	50:y:691:MET:HE2	2.02	0.41
9:A:539:C:O2'	9:A:545:A:N6	2.54	0.41
9:A:545:A:C4'	9:A:546:G:H8	2.33	0.41
9:A:878:G:C6	9:A:908:A:N1	2.89	0.41
32:Z:80:PRO:O	32:Z:83:SER:OG	2.13	0.41
9:A:885:U:C4	9:A:901:G:O6	2.74	0.41
17:I:31:ASP:OD1	17:I:31:ASP:N	2.54	0.41
23:O:35:ALA:HB2	23:O:44:ILE:HD11	2.03	0.41
24:P:56:VAL:CG1	24:P:81:VAL:HG13	2.48	0.41
33:a:14:LEU:HD12	33:a:18:GLU:OE1	2.20	0.41
35:c:91:ASP:OD2	35:c:93:THR:OG1	2.18	0.41
46:p:183:GLU:O	46:p:187:MSE:CA	2.65	0.41
46:p:265:ILE:O	46:p:268:ALA:N	2.53	0.41
47:u:553:ALA:HA	47:u:556:ALA:HB3	2.02	0.41
2:U:132:GLN:O	2:U:133:PRO:C	2.64	0.41
9:A:1850:MA6:C9	9:A:1851:MA6:H93	2.50	0.41
10:B:35:ARG:NH2	10:B:55:TYR:O	2.50	0.41
16:H:34:ASP:CG	16:H:82:LYS:HZ2	2.28	0.41
26:R:89:GLU:OE2	26:R:92:ARG:NH1	2.54	0.41
38:f:15:VAL:HG11	38:f:20:ILE:HD13	2.03	0.41
47:u:327:LEU:HD23	47:u:367:ARG:NH2	2.36	0.41
9:A:1190:A:N3	9:A:1714:U:O2'	2.54	0.40
26:R:78:ILE:HA	26:R:104:ILE:HG22	2.03	0.40
35:c:46:THR:O	35:c:46:THR:OG1	2.38	0.40
42:l:95:GLU:C	42:l:97:ASP:H	2.29	0.40
43:m:58:GLU:OE2	43:m:58:GLU:N	2.54	0.40
50:y:589:MET:SD	50:y:590:LEU:N	2.94	0.40
9:A:10:G:O2'	20:L:113:GLN:OE1	2.37	0.40
9:A:961:G:OP1	24:P:149:ARG:NH2	2.50	0.40
9:A:1404:U:OP2	39:h:21:ARG:NH2	2.55	0.40
11:C:162:ILE:C	11:C:162:ILE:HD12	2.46	0.40
19:K:41:LYS:HE2	19:K:41:LYS:H	1.86	0.40
24:P:45:THR:OG1	24:P:46:ASP:N	2.54	0.40
31:Y:30:GLY:N	31:Y:64:ALA:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:y:358:VAL:HG22	50:y:374:ILE:CG1	2.48	0.40
9:A:4:C:H4'	20:L:207:ALA:HB2	2.02	0.40
9:A:1563:G:OP1	36:d:121:ARG:NH1	2.53	0.40
35:c:30:MET:HE1	35:c:32:LEU:HD23	2.02	0.40
9:A:535:G:C2	9:A:550:C:N3	2.89	0.40
15:G:32:MET:N	15:G:32:MET:SD	2.95	0.40
16:H:73:LEU:HD22	16:H:73:LEU:H	1.87	0.40
19:K:40:ASP:OD2	19:K:43:THR:OG1	2.12	0.40
31:Y:34:VAL:HG23	31:Y:39:LEU:HD11	2.03	0.40
42:l:121:MET:HA	42:l:124:GLY:HA3	2.04	0.40
9:A:932:G:O2'	9:A:934:G:OP2	2.36	0.40
9:A:1259:A:N6	9:A:1519:U:O5'	2.54	0.40
29:V:33:ILE:HD13	29:V:33:ILE:N	2.37	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	X	323/325 (99%)	311 (96%)	9 (3%)	3 (1%)	14	47
2	U	556/661 (84%)	519 (93%)	25 (4%)	12 (2%)	5	31
3	3	209/218 (96%)	203 (97%)	6 (3%)	0	100	100
4	4	251/357 (70%)	231 (92%)	20 (8%)	0	100	100
5	5	307/564 (54%)	294 (96%)	13 (4%)	0	100	100
6	6	348/374 (93%)	303 (87%)	45 (13%)	0	100	100
7	8	313/352 (89%)	285 (91%)	28 (9%)	0	100	100
8	9	22/25 (88%)	22 (100%)	0	0	100	100
10	B	139/158 (88%)	136 (98%)	3 (2%)	0	100	100
11	C	254/263 (97%)	250 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	D	175/194 (90%)	172 (98%)	3 (2%)	0	100	100
13	E	138/143 (96%)	134 (97%)	4 (3%)	0	100	100
14	F	52/59 (88%)	45 (86%)	3 (6%)	4 (8%)	1	12
15	G	169/194 (87%)	166 (98%)	3 (2%)	0	100	100
16	H	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
17	I	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
18	J	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
19	K	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
20	L	218/293 (74%)	214 (98%)	4 (2%)	0	100	100
21	M	129/135 (96%)	124 (96%)	5 (4%)	0	100	100
22	N	205/295 (70%)	203 (99%)	2 (1%)	0	100	100
23	O	209/264 (79%)	205 (98%)	4 (2%)	0	100	100
24	P	129/151 (85%)	126 (98%)	3 (2%)	0	100	100
25	Q	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
26	R	194/208 (93%)	191 (98%)	3 (2%)	0	100	100
27	S	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
28	T	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
29	V	180/204 (88%)	169 (94%)	11 (6%)	0	100	100
30	W	82/113 (73%)	78 (95%)	4 (5%)	0	100	100
31	Y	139/146 (95%)	132 (95%)	7 (5%)	0	100	100
32	Z	229/243 (94%)	218 (95%)	9 (4%)	2 (1%)	14	47
33	a	97/165 (59%)	94 (97%)	3 (3%)	0	100	100
34	b	116/145 (80%)	113 (97%)	3 (3%)	0	100	100
35	c	311/317 (98%)	288 (93%)	23 (7%)	0	100	100
36	d	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
37	e	67/125 (54%)	65 (97%)	2 (3%)	0	100	100
38	f	140/152 (92%)	131 (94%)	8 (6%)	1 (1%)	18	53
39	h	101/119 (85%)	93 (92%)	8 (8%)	0	100	100
40	i	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
41	k	48/156 (31%)	43 (90%)	5 (10%)	0	100	100
42	l	333/388 (86%)	288 (86%)	32 (10%)	13 (4%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	m	120/132 (91%)	110 (92%)	10 (8%)	0	100	100
44	n	61/69 (88%)	60 (98%)	1 (2%)	0	100	100
45	o	83/320 (26%)	80 (96%)	3 (4%)	0	100	100
46	p	340/469 (72%)	258 (76%)	64 (19%)	18 (5%)	1	17
47	u	571/1382 (41%)	529 (93%)	42 (7%)	0	100	100
48	v	380/445 (85%)	338 (89%)	42 (11%)	0	100	100
49	x	422/548 (77%)	401 (95%)	21 (5%)	0	100	100
50	y	531/913 (58%)	507 (96%)	24 (4%)	0	100	100
All	All	9764/12930 (76%)	9174 (94%)	537 (6%)	53 (0%)	26	59

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	380	THR
42	l	27	TRP
46	p	155	VAL
46	p	158	PRO
2	U	395	ARG
2	U	405	VAL
32	Z	230	LYS
42	l	28	ASN
42	l	96	LEU
42	l	271	THR
42	l	321	GLY
42	l	381	LYS
46	p	192	ASN
46	p	196	MSE
46	p	284	GLY
46	p	321	GLN
1	X	256	THR
2	U	394	PHE
2	U	399	LYS
14	F	120	VAL
32	Z	227	LYS
38	f	9	PHE
42	l	89	SER
46	p	157	LEU
46	p	194	GLY
46	p	195	GLU

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Mol	Chain	Res	Type
1	X	30	LYS
2	U	135	LYS
2	U	388	VAL
2	U	476	ARG
14	F	124	GLY
14	F	126	LYS
42	l	126	TYR
46	p	156	VAL
46	p	421	HIS
2	U	396	MET
2	U	402	PRO
14	F	121	PRO
42	l	296	ASP
46	p	154	THR
46	p	160	ASP
46	p	165	GLU
46	p	173	GLN
46	p	270	GLY
42	l	298	THR
42	l	337	ASP
1	X	283	GLY
2	U	138	GLY
46	p	316	GLY
46	p	171	ILE
2	U	387	VAL
42	l	30	ILE
42	l	151	ALA

5.3.2 Protein sidechains ⓘ

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	
6	6	49/335 (15%)	48 (98%)	1 (2%)	48	65
8	9	23/24 (96%)	23 (100%)	0	100	100
10	B	130/142 (92%)	126 (97%)	4 (3%)	35	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	C	220/225 (98%)	219 (100%)	1 (0%)	81	82
12	D	158/168 (94%)	158 (100%)	0	100	100
13	E	112/115 (97%)	112 (100%)	0	100	100
14	F	42/48 (88%)	38 (90%)	4 (10%)	8	29
15	G	155/174 (89%)	150 (97%)	5 (3%)	34	56
16	H	73/76 (96%)	70 (96%)	3 (4%)	27	51
17	I	130/131 (99%)	129 (99%)	1 (1%)	73	77
18	J	112/113 (99%)	111 (99%)	1 (1%)	70	75
19	K	65/67 (97%)	65 (100%)	0	100	100
20	L	186/225 (83%)	186 (100%)	0	100	100
21	M	119/122 (98%)	116 (98%)	3 (2%)	42	62
22	N	173/243 (71%)	172 (99%)	1 (1%)	78	80
23	O	192/231 (83%)	190 (99%)	2 (1%)	68	75
24	P	102/119 (86%)	100 (98%)	2 (2%)	48	65
25	Q	86/98 (88%)	84 (98%)	2 (2%)	44	63
26	R	172/180 (96%)	170 (99%)	2 (1%)	63	72
27	S	200/218 (92%)	196 (98%)	4 (2%)	48	65
28	T	107/115 (93%)	105 (98%)	2 (2%)	50	66
29	V	156/170 (92%)	152 (97%)	4 (3%)	40	60
30	W	73/96 (76%)	71 (97%)	2 (3%)	39	60
31	Y	117/121 (97%)	117 (100%)	0	100	100
32	Z	190/202 (94%)	186 (98%)	4 (2%)	47	65
33	a	90/136 (66%)	88 (98%)	2 (2%)	45	64
34	b	106/130 (82%)	105 (99%)	1 (1%)	70	75
35	c	272/275 (99%)	265 (97%)	7 (3%)	40	60
36	d	112/115 (97%)	110 (98%)	2 (2%)	51	67
37	e	61/103 (59%)	59 (97%)	2 (3%)	33	56
38	f	123/132 (93%)	119 (97%)	4 (3%)	33	56
39	h	94/107 (88%)	94 (100%)	0	100	100
40	i	48/49 (98%)	48 (100%)	0	100	100
41	k	46/140 (33%)	42 (91%)	4 (9%)	9	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	m	104/108 (96%)	103 (99%)	1 (1%)	68	75
44	n	56/62 (90%)	55 (98%)	1 (2%)	51	67
46	p	38/395 (10%)	30 (79%)	8 (21%)	1	7
47	u	526/1259 (42%)	525 (100%)	1 (0%)	87	87
48	v	206/406 (51%)	205 (100%)	1 (0%)	81	82
50	y	473/811 (58%)	467 (99%)	6 (1%)	61	71
All	All	5497/7986 (69%)	5409 (98%)	88 (2%)	54	69

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	311	PHE
10	B	52	GLU
10	B	67	SER
10	B	74	SER
10	B	104	LYS
11	C	91	SER
14	F	119	VAL
14	F	120	VAL
14	F	127	LYS
14	F	133	SER
15	G	25	GLN
15	G	71	SER
15	G	82	GLU
15	G	130	LEU
15	G	151	SER
16	H	11	SER
16	H	34	ASP
16	H	73	LEU
17	I	92	ILE
18	J	30	CYS
21	M	43	SER
21	M	70	SER
21	M	76	GLU
22	N	190	SER
23	O	29	ASP
23	O	128	LYS
24	P	36	SER
24	P	138	ASP
25	Q	2	THR

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Mol	Chain	Res	Type
25	Q	64	LEU
26	R	4	SER
26	R	167	GLN
27	S	24	LEU
27	S	68	LEU
27	S	139	SER
27	S	163	ASN
28	T	102	THR
28	T	109	GLU
29	V	33	ILE
29	V	72	LEU
29	V	126	THR
29	V	164	ARG
30	W	83	ILE
30	W	90	ARG
32	Z	35	SER
32	Z	149	SER
32	Z	182	LEU
32	Z	227	LYS
33	a	70	TYR
33	a	90	VAL
34	b	55	SER
35	c	87	LEU
35	c	159	ASN
35	c	219	TRP
35	c	267	VAL
35	c	289	LEU
35	c	303	THR
35	c	314	ILE
36	d	8	ASP
36	d	90	SER
37	e	101	SER
37	e	102	LYS
38	f	9	PHE
38	f	13	LEU
38	f	17	ASN
38	f	60	THR
41	k	93	HIS
41	k	98	VAL
41	k	100	LEU
41	k	123	SER
43	m	92	CYS

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Mol	Chain	Res	Type
44	n	21	THR
46	p	129	GLN
46	p	130	VAL
46	p	132	ASP
46	p	133	VAL
46	p	134	GLU
46	p	136	VAL
46	p	139	LYS
46	p	147	GLN
47	u	109	GLN
48	v	393	MET
50	y	459	MET
50	y	495	THR
50	y	591	MET
50	y	595	GLN
50	y	612	THR
50	y	779	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
10	B	11	GLN
10	B	19	ASN
10	B	94	HIS
11	C	142	HIS
13	E	31	HIS
17	I	13	GLN
20	L	272	HIS
23	O	186	ASN
26	R	35	ASN
27	S	227	GLN
28	T	106	GLN
31	Y	24	HIS
31	Y	86	GLN
33	a	84	HIS
34	b	54	HIS
35	c	76	GLN
35	c	237	ASN
36	d	63	HIS
37	e	89	GLN
38	f	72	GLN
44	n	7	GLN

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Mol	Chain	Res	Type
46	p	129	GLN
46	p	142	ASN
47	u	221	ASN
47	u	257	HIS
47	u	277	ASN
47	u	288	ASN
47	u	417	GLN
47	u	512	GLN
47	u	518	GLN
48	v	241	GLN
48	v	244	ASN
48	v	402	GLN
50	y	406	ASN
50	y	606	GLN
50	y	854	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	A	1667/1719 (96%)	360 (21%)	19 (1%)

All (360) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	17	C
9	A	33	G
9	A	46	A
9	A	53	C
9	A	56	G
9	A	58	C
9	A	62	G
9	A	64	A
9	A	68	A
9	A	71	G
9	A	73	C
9	A	74	G
9	A	75	G
9	A	76	U
9	A	99	A2M
9	A	103	A
9	A	113	G

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Mol	Chain	Res	Type
9	A	115	U
9	A	118	C
9	A	126	G
9	A	129	C
9	A	130	G
9	A	141	A
9	A	142	C
9	A	143	U
9	A	147	A
9	A	155	G
9	A	159	A2M
9	A	166	A2M
9	A	170	A
9	A	172	U
9	A	174	OMC
9	A	180	G
9	A	187	G
9	A	190	G
9	A	191	A
9	A	194	C
9	A	195	C
9	A	197	U
9	A	198	U
9	A	199	C
9	A	204	G
9	A	206	G
9	A	207	G
9	A	223	C
9	A	294	U
9	A	300	U
9	A	302	A
9	A	306	C
9	A	308	G
9	A	311	C
9	A	312	G
9	A	319	C
9	A	320	G
9	A	322	C
9	A	323	C
9	A	324	C
9	A	325	C
9	A	326	C

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Mol	Chain	Res	Type
9	A	327	G
9	A	328	U
9	A	330	G
9	A	331	C
9	A	332	G
9	A	335	G
9	A	339	A
9	A	340	C
9	A	346	C
9	A	347	G
9	A	351	G
9	A	362	C
9	A	364	A
9	A	367	U
9	A	370	G
9	A	385	G
9	A	386	C
9	A	409	C
9	A	442	C
9	A	448	A
9	A	449	A
9	A	450	C
9	A	452	G
9	A	460	A
9	A	464	A
9	A	465	A
9	A	466	G
9	A	467	G
9	A	471	G
9	A	472	C
9	A	473	A
9	A	474	G
9	A	476	A
9	A	477	G
9	A	482	G
9	A	485	A
9	A	486	A
9	A	487	U
9	A	492	C
9	A	493	A
9	A	508	A
9	A	516	A

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Mol	Chain	Res	Type
9	A	525	A
9	A	535	G
9	A	536	A
9	A	537	C
9	A	539	C
9	A	540	U
9	A	541	U
9	A	542	U
9	A	543	C
9	A	544	G
9	A	545	A
9	A	546	G
9	A	548	C
9	A	549	C
9	A	550	C
9	A	551	U
9	A	554	A
9	A	555	A
9	A	556	U
9	A	558	G
9	A	559	G
9	A	563	G
9	A	564	A
9	A	568	C
9	A	576	A
9	A	589	G
9	A	590	A
9	A	591	U
9	A	606	G
9	A	614	C
9	A	617	G
9	A	626	G
9	A	628	A
9	A	629	A
9	A	631	U
9	A	643	A
9	A	655	A
9	A	660	C
9	A	668	A2M
9	A	669	A
9	A	671	A
9	A	672	A

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Mol	Chain	Res	Type
9	A	673	G
9	A	683	OMG
9	A	688	U
9	A	811	A
9	A	821	G
9	A	822	PSU
9	A	827	A
9	A	830	A
9	A	834	C
9	A	835	C
9	A	836	G
9	A	837	A
9	A	838	G
9	A	839	C
9	A	840	C
9	A	841	G
9	A	847	A
9	A	870	A
9	A	871	U
9	A	872	A
9	A	874	G
9	A	880	G
9	A	881	G
9	A	882	U
9	A	885	U
9	A	888	U
9	A	889	U
9	A	890	U
9	A	892	U
9	A	894	G
9	A	896	U
9	A	897	U
9	A	898	U
9	A	899	U
9	A	901	G
9	A	902	G
9	A	903	A
9	A	904	A
9	A	907	G
9	A	909	G
9	A	912	C
9	A	913	A

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Mol	Chain	Res	Type
9	A	919	A
9	A	920	A
9	A	922	A
9	A	930	C
9	A	933	G
9	A	943	U
9	A	950	C
9	A	972	A
9	A	990	A
9	A	992	A
9	A	1017	U
9	A	1023	A
9	A	1042	A
9	A	1044	G
9	A	1045	U
9	A	1061	U
9	A	1062	A
9	A	1078	C
9	A	1083	A
9	A	1085	C
9	A	1108	G
9	A	1114	U
9	A	1115	U
9	A	1116	C
9	A	1117	C
9	A	1118	C
9	A	1119	A
9	A	1133	A
9	A	1138	C
9	A	1153	C
9	A	1154	U
9	A	1171	G
9	A	1195	A
9	A	1208	A
9	A	1215	C
9	A	1216	C
9	A	1217	A
9	A	1219	JMH
9	A	1220	A
9	A	1221	G
9	A	1224	G
9	A	1242	U

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Mol	Chain	Res	Type
9	A	1251	A
9	A	1253	A
9	A	1256	G
9	A	1257	G
9	A	1258	A
9	A	1259	A
9	A	1263	U
9	A	1274	G
9	A	1275	G
9	A	1280	G
9	A	1281	G
9	A	1282	A
9	A	1284	A
9	A	1285	G
9	A	1286	G
9	A	1290	G
9	A	1294	G
9	A	1297	U
9	A	1301	A
9	A	1302	G
9	A	1303	C
9	A	1305	C
9	A	1308	U
9	A	1309	C
9	A	1313	A
9	A	1315	U
9	A	1320	G
9	A	1326	U
9	A	1327	G
9	A	1342	U
9	A	1371	U
9	A	1372	U
9	A	1375	G
9	A	1378	A
9	A	1397	U
9	A	1401	A
9	A	1402	A
9	A	1404	U
9	A	1405	A
9	A	1406	G
9	A	1409	A
9	A	1416	C

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Mol	Chain	Res	Type
9	A	1417	C
9	A	1418	C
9	A	1419	C
9	A	1420	G
9	A	1421	A
9	A	1423	C
9	A	1424	G
9	A	1428	G
9	A	1433	C
9	A	1434	C
9	A	1435	C
9	A	1436	C
9	A	1437	C
9	A	1438	A
9	A	1441	U
9	A	1454	A
9	A	1464	C
9	A	1465	A
9	A	1489	A
9	A	1490	OMG
9	A	1497	G
9	A	1498	A
9	A	1507	G
9	A	1508	A
9	A	1521	C
9	A	1522	A
9	A	1533	A
9	A	1557	C
9	A	1579	A
9	A	1580	A
9	A	1588	A
9	A	1590	C
9	A	1591	C
9	A	1592	C
9	A	1601	A
9	A	1605	G
9	A	1606	G
9	A	1609	C
9	A	1621	U
9	A	1623	A
9	A	1624	U
9	A	1639	G

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Mol	Chain	Res	Type
9	A	1654	G
9	A	1663	A
9	A	1664	A
9	A	1665	G
9	A	1671	G
9	A	1715	A
9	A	1719	A
9	A	1721	U
9	A	1722	G
9	A	1726	G
9	A	1730	U
9	A	1733	U
9	A	1744	G
9	A	1745	A
9	A	1751	C
9	A	1752	C
9	A	1753	C
9	A	1754	G
9	A	1755	C
9	A	1756	C
9	A	1757	G
9	A	1777	G
9	A	1778	C
9	A	1779	G
9	A	1780	G
9	A	1781	A
9	A	1782	G
9	A	1783	C
9	A	1784	G
9	A	1800	A
9	A	1807	C
9	A	1813	A
9	A	1817	G
9	A	1819	A
9	A	1820	G
9	A	1824	A
9	A	1825	A
9	A	1826	G
9	A	1829	G
9	A	1835	A
9	A	1838	U
9	A	1849	G

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Mol	Chain	Res	Type
9	A	1851	MA6
9	A	1861	G
9	A	1862	G
9	A	1863	A
9	A	1864	U
9	A	1865	C
9	A	1869	A

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	74	G
9	A	190	G
9	A	198	U
9	A	203	G
9	A	310	C
9	A	329	G
9	A	345	U
9	A	476	A
9	A	535	G
9	A	539	C
9	A	544	G
9	A	548	C
9	A	871	U
9	A	911	C
9	A	1114	U
9	A	1118	C
9	A	1605	G
9	A	1751	C
9	A	1781	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	OMC	A	1703	9	19,22,23	3.06	8 (42%)	25,31,34	0.73	0
9	A2M	A	27	51,9	22,25,26	3.53	9 (40%)	30,36,39	2.50	12 (40%)
9	OMG	A	1490	51,9	23,26,27	2.40	9 (39%)	32,38,41	2.16	10 (31%)
9	OMG	A	1328	52,9	23,26,27	2.40	9 (39%)	32,38,41	2.27	13 (40%)
9	MA6	A	1851	9	23,26,27	1.41	4 (17%)	33,38,41	3.74	14 (42%)
9	A2M	A	1031	9	22,25,26	3.52	9 (40%)	30,36,39	2.54	13 (43%)
9	OMC	A	174	51,9	19,22,23	3.10	8 (42%)	25,31,34	0.78	0
9	4AC	A	1337	9	21,24,25	3.15	10 (47%)	28,34,37	1.92	6 (21%)
9	PSU	A	822	9	18,21,22	4.48	8 (44%)	21,30,33	2.04	6 (28%)
9	A2M	A	484	9	22,25,26	3.50	9 (40%)	30,36,39	2.55	13 (43%)
9	OMC	A	517	9	19,22,23	3.03	8 (42%)	25,31,34	0.78	0
9	A2M	A	166	9	22,25,26	3.54	9 (40%)	30,36,39	2.62	16 (53%)
9	5MU	A	814	9	19,22,23	0.51	0	27,32,35	0.82	1 (3%)
9	5MC	A	1374	9	19,22,23	3.91	8 (42%)	26,32,35	1.02	2 (7%)
9	MA6	A	1850	9	23,26,27	1.41	4 (17%)	33,38,41	3.77	13 (39%)
9	PSU	A	119	9	18,21,22	4.53	7 (38%)	21,30,33	1.90	4 (19%)
9	OMU	A	121	9	19,22,23	3.23	8 (42%)	25,31,34	1.81	5 (20%)
9	JMH	A	1219	51,9	18,22,23	2.71	6 (33%)	23,32,35	0.95	2 (8%)
9	A2M	A	159	9	22,25,26	3.53	9 (40%)	30,36,39	2.61	14 (46%)
9	A2M	A	1678	9	22,25,26	3.55	9 (40%)	30,36,39	2.55	12 (40%)
9	OMG	A	509	51,9	23,26,27	2.40	9 (39%)	32,38,41	2.26	10 (31%)
9	UR3	A	1830	9	19,22,23	3.05	8 (42%)	26,32,35	1.69	3 (11%)
9	4AC	A	1842	9	21,24,25	3.11	10 (47%)	28,34,37	1.14	4 (14%)
9	OMG	A	601	9	23,26,27	2.41	9 (39%)	32,38,41	2.29	13 (40%)
9	6MZ	A	1832	51,52,9	22,25,26	3.00	4 (18%)	29,36,39	2.50	11 (37%)
9	OMG	A	683	9	23,26,27	2.41	9 (39%)	32,38,41	2.19	10 (31%)
9	PSU	A	823	9	18,21,22	4.46	7 (38%)	21,30,33	1.92	5 (23%)
9	A2M	A	99	51,9	22,25,26	3.50	9 (40%)	30,36,39	2.52	14 (46%)
9	OMU	A	116	9	19,22,23	3.22	8 (42%)	25,31,34	1.74	5 (20%)
9	PSU	A	1243	9	18,21,22	4.44	7 (38%)	21,30,33	2.00	5 (23%)
9	PSU	A	612	51,9	18,21,22	4.46	8 (44%)	21,30,33	2.04	6 (28%)
9	PSU	A	1081	9	18,21,22	4.49	8 (44%)	21,30,33	2.12	5 (23%)
9	OMG	A	644	9	23,26,27	2.37	9 (39%)	32,38,41	2.29	13 (40%)
9	A2M	A	668	51,9	22,25,26	3.44	10 (45%)	30,36,39	2.43	14 (46%)

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
9	OMC	A	1703	9	-	1/9/27/28	0/2/2/2
9	A2M	A	27	51,9	-	0/9/27/28	0/3/3/3
9	OMG	A	1490	51,9	-	1/9/27/28	0/3/3/3
9	OMG	A	1328	52,9	-	0/9/27/28	0/3/3/3
9	MA6	A	1851	9	-	4/11/29/30	0/3/3/3
9	A2M	A	1031	9	-	0/9/27/28	0/3/3/3
9	OMC	A	174	51,9	-	3/9/27/28	0/2/2/2
9	4AC	A	1337	9	-	2/11/29/30	0/2/2/2
9	PSU	A	822	9	-	2/7/25/26	0/2/2/2
9	A2M	A	484	9	-	0/9/27/28	0/3/3/3
9	OMC	A	517	9	-	0/9/27/28	0/2/2/2
9	A2M	A	166	9	-	2/9/27/28	0/3/3/3
9	5MU	A	814	9	-	0/7/25/26	0/2/2/2
9	5MC	A	1374	9	-	0/7/25/26	0/2/2/2
9	MA6	A	1850	9	-	0/11/29/30	0/3/3/3
9	PSU	A	119	9	-	0/7/25/26	0/2/2/2
9	OMU	A	121	9	-	0/9/27/28	0/2/2/2
9	JMH	A	1219	51,9	-	2/7/25/26	0/2/2/2
9	A2M	A	159	9	-	2/9/27/28	0/3/3/3
9	A2M	A	1678	9	-	0/9/27/28	0/3/3/3
9	OMG	A	509	51,9	-	0/9/27/28	0/3/3/3
9	UR3	A	1830	9	-	0/7/25/26	0/2/2/2
9	4AC	A	1842	9	-	0/11/29/30	0/2/2/2
9	OMG	A	601	9	-	0/9/27/28	0/3/3/3
9	6MZ	A	1832	51,52,9	-	2/9/27/28	0/3/3/3
9	OMG	A	683	9	-	2/9/27/28	0/3/3/3
9	PSU	A	823	9	-	2/7/25/26	0/2/2/2
9	A2M	A	99	51,9	-	2/9/27/28	0/3/3/3
9	OMU	A	116	9	-	0/9/27/28	0/2/2/2
9	PSU	A	1243	9	-	0/7/25/26	0/2/2/2
9	PSU	A	612	51,9	-	0/7/25/26	0/2/2/2
9	PSU	A	1081	9	-	1/7/25/26	0/2/2/2
9	OMG	A	644	9	-	1/9/27/28	0/3/3/3
9	A2M	A	668	51,9	-	2/9/27/28	0/3/3/3

All (266) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1832	6MZ	C6-N6	12.52	1.48	1.34
9	A	119	PSU	C6-C5	11.35	1.47	1.35
9	A	612	PSU	C6-C5	11.19	1.47	1.35
9	A	822	PSU	C6-C5	11.10	1.47	1.35
9	A	1081	PSU	C6-C5	10.95	1.47	1.35
9	A	823	PSU	C6-C5	10.89	1.47	1.35
9	A	1243	PSU	C6-C5	10.73	1.47	1.35
9	A	823	PSU	C2-N1	9.95	1.49	1.36
9	A	1243	PSU	C2-N1	9.89	1.49	1.36
9	A	119	PSU	C2-N1	9.87	1.49	1.36
9	A	1081	PSU	C2-N1	9.81	1.49	1.36
9	A	822	PSU	C2-N1	9.58	1.49	1.36
9	A	612	PSU	C2-N1	9.57	1.49	1.36
9	A	1678	A2M	C2'-C1'	-9.14	1.30	1.53
9	A	166	A2M	O4'-C1'	9.06	1.62	1.42
9	A	27	A2M	C2'-C1'	-9.06	1.30	1.53
9	A	159	A2M	C2'-C1'	-9.01	1.30	1.53
9	A	1031	A2M	C2'-C1'	-8.98	1.31	1.53
9	A	1374	5MC	C6-C5	8.96	1.49	1.34
9	A	99	A2M	C2'-C1'	-8.92	1.31	1.53
9	A	484	A2M	C2'-C1'	-8.92	1.31	1.53
9	A	166	A2M	C2'-C1'	-8.85	1.31	1.53
9	A	159	A2M	O4'-C1'	8.77	1.62	1.42
9	A	1031	A2M	O4'-C1'	8.74	1.62	1.42
9	A	99	A2M	O4'-C1'	8.74	1.62	1.42
9	A	1678	A2M	O4'-C1'	8.71	1.62	1.42
9	A	27	A2M	O4'-C1'	8.59	1.61	1.42
9	A	668	A2M	C2'-C1'	-8.47	1.32	1.53
9	A	484	A2M	O4'-C1'	8.33	1.61	1.42
9	A	668	A2M	O4'-C1'	8.31	1.61	1.42
9	A	1830	UR3	C2-N1	7.94	1.49	1.38
9	A	116	OMU	C2-N3	7.86	1.51	1.38
9	A	121	OMU	C2-N3	7.83	1.51	1.38
9	A	174	OMC	C2-N3	7.48	1.51	1.36
9	A	116	OMU	C2-N1	7.39	1.50	1.38
9	A	121	OMU	C2-N1	7.30	1.49	1.38
9	A	1703	OMC	C2-N3	7.27	1.50	1.36
9	A	612	PSU	C2-N3	7.18	1.49	1.37
9	A	517	OMC	C2-N3	7.18	1.50	1.36
9	A	1842	4AC	C4-N3	7.17	1.44	1.32
9	A	1243	PSU	C2-N3	7.13	1.49	1.37
9	A	822	PSU	C2-N3	7.13	1.49	1.37
9	A	1081	PSU	C2-N3	7.05	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	119	PSU	C2-N3	7.02	1.49	1.37
9	A	1374	5MC	C2-N3	7.00	1.50	1.36
9	A	1337	4AC	C4-N3	7.00	1.44	1.32
9	A	1219	JMH	C2-N1	6.96	1.48	1.38
9	A	668	A2M	O4'-C4'	-6.91	1.29	1.45
9	A	1830	UR3	C6-C5	6.82	1.50	1.35
9	A	823	PSU	C2-N3	6.82	1.48	1.37
9	A	484	A2M	O4'-C4'	-6.79	1.29	1.45
9	A	1678	A2M	O4'-C4'	-6.74	1.30	1.45
9	A	1374	5MC	C4-N4	6.67	1.51	1.34
9	A	27	A2M	O4'-C4'	-6.64	1.30	1.45
9	A	159	A2M	O4'-C4'	-6.59	1.30	1.45
9	A	174	OMC	C6-C5	6.52	1.50	1.35
9	A	1031	A2M	O4'-C4'	-6.50	1.30	1.45
9	A	1703	OMC	C6-C5	6.49	1.50	1.35
9	A	166	A2M	O4'-C4'	-6.48	1.30	1.45
9	A	517	OMC	C6-C5	6.43	1.50	1.35
9	A	99	A2M	O4'-C4'	-6.38	1.30	1.45
9	A	1490	OMG	C4-N3	6.35	1.48	1.34
9	A	509	OMG	C4-N3	6.35	1.48	1.34
9	A	683	OMG	C4-N3	6.28	1.48	1.34
9	A	1328	OMG	C4-N3	6.28	1.48	1.34
9	A	601	OMG	C4-N3	6.22	1.48	1.34
9	A	121	OMU	C6-C5	6.19	1.49	1.35
9	A	1374	5MC	C4-N3	6.13	1.44	1.34
9	A	644	OMG	C4-N3	6.13	1.48	1.34
9	A	1219	JMH	C6-C5	6.11	1.49	1.35
9	A	1842	4AC	C2-N3	6.09	1.48	1.36
9	A	1337	4AC	C6-C5	6.06	1.49	1.35
9	A	116	OMU	C6-C5	6.06	1.49	1.35
9	A	1374	5MC	C5-C4	6.03	1.48	1.44
9	A	1337	4AC	C2-N3	5.86	1.48	1.36
9	A	1842	4AC	C6-C5	5.84	1.48	1.35
9	A	823	PSU	O4-C4	-5.68	1.12	1.23
9	A	1830	UR3	C2-N3	5.61	1.50	1.39
9	A	822	PSU	O4-C4	-5.58	1.13	1.23
9	A	1081	PSU	O4-C4	-5.58	1.13	1.23
9	A	1243	PSU	O4-C4	-5.57	1.13	1.23
9	A	612	PSU	O4-C4	-5.55	1.13	1.23
9	A	119	PSU	O4-C4	-5.49	1.13	1.23
9	A	119	PSU	C6-N1	5.31	1.45	1.36
9	A	174	OMC	C4-N3	5.30	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	509	OMG	C2-N3	5.20	1.45	1.33
9	A	1490	OMG	C2-N3	5.17	1.45	1.33
9	A	601	OMG	C2-N3	5.17	1.45	1.33
9	A	823	PSU	C6-N1	5.16	1.44	1.36
9	A	1243	PSU	C6-N1	5.15	1.44	1.36
9	A	1081	PSU	C6-N1	5.15	1.44	1.36
9	A	644	OMG	C2-N3	5.13	1.45	1.33
9	A	1328	OMG	C2-N3	5.13	1.45	1.33
9	A	683	OMG	C2-N3	5.10	1.45	1.33
9	A	822	PSU	C6-N1	5.07	1.44	1.36
9	A	1703	OMC	C4-N3	5.05	1.44	1.34
9	A	517	OMC	C4-N3	4.90	1.44	1.34
9	A	1219	JMH	C2-N3	4.90	1.48	1.39
9	A	612	PSU	C6-N1	4.86	1.44	1.36
9	A	683	OMG	C2-N2	4.79	1.45	1.34
9	A	1328	OMG	C2-N2	4.75	1.45	1.34
9	A	1490	OMG	C2-N2	4.72	1.45	1.34
9	A	601	OMG	C2-N2	4.71	1.45	1.34
9	A	644	OMG	C2-N2	4.53	1.44	1.34
9	A	509	OMG	C2-N2	4.51	1.44	1.34
9	A	1374	5MC	C6-N1	4.42	1.45	1.38
9	A	1678	A2M	C6-N6	4.40	1.45	1.34
9	A	1337	4AC	C7-N4	4.40	1.46	1.37
9	A	159	A2M	C6-N6	4.38	1.45	1.34
9	A	166	A2M	C6-N6	4.34	1.45	1.34
9	A	517	OMC	C2-N1	4.32	1.49	1.40
9	A	99	A2M	C6-N6	4.32	1.45	1.34
9	A	668	A2M	C6-N6	4.29	1.45	1.34
9	A	27	A2M	C6-N6	4.29	1.45	1.34
9	A	484	A2M	C6-N6	4.25	1.45	1.34
9	A	174	OMC	C2-N1	4.24	1.49	1.40
9	A	1031	A2M	C6-N6	4.23	1.45	1.34
9	A	1703	OMC	C2-N1	4.21	1.48	1.40
9	A	1337	4AC	C4-N4	4.19	1.46	1.39
9	A	1842	4AC	C7-N4	4.15	1.45	1.37
9	A	822	PSU	C4-N3	4.06	1.46	1.38
9	A	612	PSU	C4-N3	4.03	1.46	1.38
9	A	121	OMU	C4-N3	3.98	1.45	1.38
9	A	119	PSU	C4-N3	3.98	1.46	1.38
9	A	1243	PSU	C4-N3	3.98	1.46	1.38
9	A	1842	4AC	C4-N4	3.94	1.45	1.39
9	A	1081	PSU	C4-N3	3.93	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	116	OMU	C4-N3	3.91	1.45	1.38
9	A	823	PSU	C4-N3	3.84	1.46	1.38
9	A	1374	5MC	C2-N1	3.82	1.48	1.40
9	A	1337	4AC	C5-C4	3.79	1.49	1.41
9	A	1842	4AC	C2-N1	3.75	1.47	1.40
9	A	1851	MA6	C5-N7	-3.68	1.32	1.39
9	A	174	OMC	C4-N4	3.68	1.42	1.33
9	A	517	OMC	C4-N4	3.65	1.42	1.33
9	A	1703	OMC	C4-N4	3.62	1.42	1.33
9	A	1337	4AC	C2-N1	3.59	1.47	1.40
9	A	1081	PSU	O2-C2	-3.57	1.15	1.23
9	A	509	OMG	C5-N7	-3.53	1.32	1.39
9	A	823	PSU	O2-C2	-3.53	1.15	1.23
9	A	119	PSU	O2-C2	-3.51	1.15	1.23
9	A	601	OMG	C5-N7	-3.50	1.32	1.39
9	A	822	PSU	O2-C2	-3.50	1.15	1.23
9	A	1243	PSU	O2-C2	-3.43	1.16	1.23
9	A	668	A2M	C5-C4	-3.41	1.33	1.39
9	A	1842	4AC	C5-C4	3.40	1.48	1.41
9	A	1850	MA6	C5-N7	-3.37	1.32	1.39
9	A	612	PSU	O2-C2	-3.36	1.16	1.23
9	A	1490	OMG	C5-N7	-3.36	1.32	1.39
9	A	1851	MA6	C5-C4	-3.33	1.33	1.39
9	A	1031	A2M	C5-C4	-3.32	1.33	1.39
9	A	644	OMG	C5-N7	-3.31	1.32	1.39
9	A	517	OMC	C6-N1	3.29	1.45	1.38
9	A	174	OMC	C6-N1	3.29	1.45	1.38
9	A	1703	OMC	C6-N1	3.28	1.45	1.38
9	A	683	OMG	C5-N7	-3.25	1.32	1.39
9	A	1830	UR3	O4-C4	-3.22	1.16	1.23
9	A	1328	OMG	C5-N7	-3.20	1.32	1.39
9	A	27	A2M	C5-C4	-3.20	1.33	1.39
9	A	166	A2M	O3'-C3'	-3.20	1.35	1.43
9	A	99	A2M	C5-C4	-3.19	1.33	1.39
9	A	1678	A2M	C5-C4	-3.18	1.33	1.39
9	A	166	A2M	C5-C4	-3.16	1.33	1.39
9	A	1850	MA6	C5-C4	-3.15	1.33	1.39
9	A	1832	6MZ	C5-C4	-3.14	1.33	1.39
9	A	484	A2M	C5-C4	-3.10	1.33	1.39
9	A	27	A2M	O3'-C3'	-3.06	1.35	1.43
9	A	1832	6MZ	C5-N7	-3.05	1.33	1.39
9	A	159	A2M	O3'-C3'	-3.05	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1031	A2M	O3'-C3'	-3.03	1.35	1.43
9	A	484	A2M	O3'-C3'	-3.00	1.35	1.43
9	A	159	A2M	C5-C4	-2.99	1.33	1.39
9	A	668	A2M	O3'-C3'	-2.98	1.35	1.43
9	A	1678	A2M	O3'-C3'	-2.94	1.35	1.43
9	A	116	OMU	O4-C4	-2.92	1.18	1.24
9	A	121	OMU	O4-C4	-2.92	1.18	1.24
9	A	1219	JMH	C6-N1	2.91	1.45	1.38
9	A	1703	OMC	O2-C2	-2.91	1.18	1.23
9	A	1031	A2M	C5-N7	-2.88	1.33	1.39
9	A	27	A2M	O2'-C2'	2.88	1.49	1.42
9	A	99	A2M	O3'-C3'	-2.88	1.35	1.43
9	A	1678	A2M	C5-N7	-2.87	1.33	1.39
9	A	1337	4AC	C6-N1	2.87	1.44	1.38
9	A	1337	4AC	O2-C2	-2.87	1.18	1.23
9	A	1678	A2M	O2'-C2'	2.86	1.49	1.42
9	A	166	A2M	C5-N7	-2.85	1.33	1.39
9	A	484	A2M	O2'-C2'	2.85	1.49	1.42
9	A	1031	A2M	O2'-C2'	2.84	1.49	1.42
9	A	27	A2M	C5-N7	-2.83	1.33	1.39
9	A	99	A2M	O2'-C2'	2.83	1.49	1.42
9	A	484	A2M	C5-N7	-2.83	1.33	1.39
9	A	1850	MA6	C6-N6	2.82	1.44	1.36
9	A	99	A2M	C5-N7	-2.82	1.33	1.39
9	A	116	OMU	C6-N1	2.80	1.44	1.38
9	A	517	OMC	O2-C2	-2.80	1.18	1.23
9	A	159	A2M	O2'-C2'	2.80	1.49	1.42
9	A	668	A2M	C5-N7	-2.78	1.34	1.39
9	A	509	OMG	O6-C6	-2.78	1.18	1.23
9	A	121	OMU	C6-N1	2.77	1.44	1.38
9	A	1842	4AC	O2-C2	-2.77	1.18	1.23
9	A	166	A2M	O2'-C2'	2.76	1.49	1.42
9	A	601	OMG	O6-C6	-2.75	1.18	1.23
9	A	159	A2M	C5-N7	-2.73	1.34	1.39
9	A	644	OMG	O6-C6	-2.73	1.18	1.23
9	A	1328	OMG	C2-N1	2.73	1.44	1.37
9	A	1490	OMG	O6-C6	-2.72	1.18	1.23
9	A	1842	4AC	C6-N1	2.71	1.44	1.38
9	A	683	OMG	O6-C6	-2.70	1.18	1.23
9	A	1830	UR3	C5-C4	2.69	1.50	1.43
9	A	174	OMC	O2-C2	-2.68	1.18	1.23
9	A	1081	PSU	O4'-C1'	-2.68	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1219	JMH	C5-C4	2.66	1.49	1.42
9	A	509	OMG	C2-N1	2.65	1.44	1.37
9	A	668	A2M	O2'-C2'	2.65	1.49	1.42
9	A	1328	OMG	O6-C6	-2.64	1.18	1.23
9	A	683	OMG	C2-N1	2.64	1.44	1.37
9	A	484	A2M	C8-N9	-2.62	1.33	1.37
9	A	644	OMG	C2-N1	2.62	1.44	1.37
9	A	601	OMG	C2-N1	2.61	1.44	1.37
9	A	121	OMU	C5-C4	2.59	1.49	1.43
9	A	1490	OMG	C2-N1	2.52	1.43	1.37
9	A	1830	UR3	O2-C2	-2.50	1.17	1.22
9	A	683	OMG	C4-N9	-2.45	1.31	1.38
9	A	1832	6MZ	C6-N1	-2.43	1.31	1.35
9	A	822	PSU	O4'-C1'	-2.43	1.40	1.43
9	A	1851	MA6	C6-N6	2.43	1.43	1.36
9	A	1328	OMG	C5-C6	2.41	1.53	1.44
9	A	174	OMC	C5-C4	2.41	1.48	1.42
9	A	1703	OMC	C5-C4	2.40	1.48	1.42
9	A	644	OMG	C4-N9	-2.40	1.32	1.38
9	A	644	OMG	C5-C6	2.40	1.53	1.44
9	A	159	A2M	C8-N9	-2.38	1.33	1.37
9	A	1328	OMG	C6-N1	2.38	1.43	1.38
9	A	116	OMU	C5-C4	2.37	1.48	1.43
9	A	517	OMC	C5-C4	2.36	1.48	1.42
9	A	1830	UR3	C6-N1	2.34	1.43	1.38
9	A	1490	OMG	C4-N9	-2.32	1.32	1.38
9	A	601	OMG	C6-N1	2.30	1.43	1.38
9	A	99	A2M	C8-N9	-2.28	1.33	1.37
9	A	509	OMG	C5-C6	2.27	1.52	1.44
9	A	683	OMG	C5-C6	2.27	1.52	1.44
9	A	1374	5MC	O2-C2	-2.26	1.19	1.23
9	A	601	OMG	C5-C6	2.26	1.52	1.44
9	A	27	A2M	C8-N9	-2.25	1.33	1.37
9	A	1830	UR3	C4-N3	2.24	1.45	1.40
9	A	601	OMG	C4-N9	-2.24	1.32	1.38
9	A	1031	A2M	C8-N9	-2.24	1.33	1.37
9	A	612	PSU	O4'-C1'	-2.23	1.40	1.43
9	A	1328	OMG	C4-N9	-2.23	1.32	1.38
9	A	1490	OMG	C5-C6	2.23	1.52	1.44
9	A	668	A2M	C8-N9	-2.23	1.33	1.37
9	A	683	OMG	C6-N1	2.22	1.43	1.38
9	A	1337	4AC	O7-C7	-2.19	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	166	A2M	C8-N9	-2.19	1.33	1.37
9	A	1842	4AC	O7-C7	-2.18	1.18	1.23
9	A	644	OMG	C6-N1	2.17	1.42	1.38
9	A	121	OMU	O2-C2	-2.16	1.19	1.23
9	A	509	OMG	C4-N9	-2.14	1.32	1.38
9	A	1678	A2M	C8-N9	-2.14	1.33	1.37
9	A	116	OMU	O2-C2	-2.13	1.19	1.23
9	A	1219	JMH	O2-C2	-2.13	1.18	1.22
9	A	1490	OMG	C6-N1	2.13	1.42	1.38
9	A	1850	MA6	C4-N9	-2.08	1.33	1.37
9	A	509	OMG	C6-N1	2.07	1.42	1.38
9	A	668	A2M	C4-N9	-2.02	1.33	1.37
9	A	1851	MA6	C5-C6	-2.00	1.36	1.41

All (274) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1851	MA6	N1-C6-N6	-11.31	103.08	116.86
9	A	1850	MA6	N1-C6-N6	-10.67	103.86	116.86
9	A	1850	MA6	C1'-N9-C8	-8.81	107.55	127.09
9	A	1850	MA6	C4-N9-C1'	8.14	145.66	126.63
9	A	1851	MA6	C1'-N9-C8	-7.73	109.94	127.09
9	A	1850	MA6	C5-C6-N6	7.65	137.44	125.33
9	A	1851	MA6	C4-N9-C1'	7.58	144.35	126.63
9	A	1851	MA6	C5-C6-N6	7.30	136.89	125.33
9	A	1337	4AC	CM7-C7-N4	6.93	126.46	115.27
9	A	1830	UR3	C4-N3-C2	-6.02	119.74	124.58
9	A	1832	6MZ	N1-C2-N3	-5.92	119.62	128.58
9	A	1850	MA6	N1-C2-N3	-5.73	119.91	128.58
9	A	1851	MA6	N1-C2-N3	-5.73	119.91	128.58
9	A	99	A2M	N3-C2-N1	-5.68	119.98	128.58
9	A	27	A2M	N3-C2-N1	-5.65	120.02	128.58
9	A	166	A2M	N3-C2-N1	-5.57	120.15	128.58
9	A	121	OMU	C4-N3-C2	-5.56	119.71	126.61
9	A	668	A2M	N3-C2-N1	-5.53	120.22	128.58
9	A	1678	A2M	N3-C2-N1	-5.44	120.34	128.58
9	A	1851	MA6	C5-C4-N3	-5.44	119.23	126.72
9	A	484	A2M	N3-C2-N1	-5.37	120.45	128.58
9	A	1031	A2M	N3-C2-N1	-5.32	120.53	128.58
9	A	509	OMG	C5-C4-N3	-5.30	119.95	128.39
9	A	159	A2M	C1'-N9-C8	-5.27	115.41	127.09
9	A	601	OMG	C5-C4-N3	-5.26	120.01	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	159	A2M	N3-C2-N1	-5.21	120.70	128.58
9	A	509	OMG	C1'-N9-C8	-5.16	112.07	126.73
9	A	1081	PSU	C4-N3-C2	-5.13	119.30	126.37
9	A	1328	OMG	C1'-N9-C8	-5.12	112.17	126.73
9	A	644	OMG	C5-C4-N3	-5.12	120.25	128.39
9	A	116	OMU	C4-N3-C2	-5.08	120.31	126.61
9	A	484	A2M	C1'-N9-C8	-5.06	115.85	127.09
9	A	1328	OMG	C5-C4-N3	-5.04	120.36	128.39
9	A	601	OMG	C1'-N9-C8	-5.04	112.42	126.73
9	A	822	PSU	C4-N3-C2	-5.04	119.43	126.37
9	A	509	OMG	C1'-N9-C4	5.03	141.35	126.49
9	A	1243	PSU	C4-N3-C2	-5.01	119.48	126.37
9	A	644	OMG	C1'-N9-C8	-4.99	112.56	126.73
9	A	159	A2M	C5-C4-N3	-4.99	119.85	126.72
9	A	1031	A2M	C5-C4-N3	-4.99	119.85	126.72
9	A	601	OMG	C1'-N9-C4	4.96	141.14	126.49
9	A	1490	OMG	C1'-N9-C8	-4.95	112.66	126.73
9	A	1832	6MZ	C1'-N9-C8	-4.94	116.13	127.09
9	A	823	PSU	C4-N3-C2	-4.89	119.64	126.37
9	A	119	PSU	C4-N3-C2	-4.87	119.67	126.37
9	A	1678	A2M	C5-C4-N3	-4.85	120.04	126.72
9	A	484	A2M	C5-C4-N3	-4.83	120.07	126.72
9	A	1328	OMG	C1'-N9-C4	4.82	140.72	126.49
9	A	1678	A2M	C1'-N9-C8	-4.82	116.41	127.09
9	A	683	OMG	C1'-N9-C8	-4.80	113.08	126.73
9	A	612	PSU	C4-N3-C2	-4.80	119.76	126.37
9	A	1490	OMG	C5-C4-N3	-4.76	120.82	128.39
9	A	1081	PSU	N1-C2-N3	4.73	120.16	115.17
9	A	27	A2M	C5-C4-N3	-4.71	120.23	126.72
9	A	1031	A2M	C1'-N9-C8	-4.70	116.66	127.09
9	A	683	OMG	C5-C4-N3	-4.68	120.94	128.39
9	A	644	OMG	C1'-N9-C4	4.67	140.29	126.49
9	A	1832	6MZ	C5-C4-N3	-4.65	120.31	126.72
9	A	1678	A2M	N9-C8-N7	-4.64	107.36	113.94
9	A	1490	OMG	C1'-N9-C4	4.64	140.18	126.49
9	A	1851	MA6	C4-C5-C6	4.63	120.70	115.91
9	A	166	A2M	C1'-N9-C8	-4.62	116.85	127.09
9	A	601	OMG	C2-N3-C4	4.58	120.19	112.30
9	A	668	A2M	C5-C4-N3	-4.58	120.42	126.72
9	A	1328	OMG	C2-N3-C4	4.58	120.18	112.30
9	A	99	A2M	N9-C8-N7	-4.54	107.50	113.94
9	A	27	A2M	C1'-N9-C8	-4.54	117.02	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	166	A2M	C5-C4-N3	-4.52	120.49	126.72
9	A	644	OMG	C2-N3-C4	4.51	120.07	112.30
9	A	166	A2M	N9-C8-N7	-4.50	107.55	113.94
9	A	99	A2M	C1'-N9-C8	-4.50	117.11	127.09
9	A	99	A2M	C5-C4-N3	-4.45	120.59	126.72
9	A	822	PSU	N1-C2-N3	4.44	119.85	115.17
9	A	1850	MA6	C5-C4-N3	-4.44	120.61	126.72
9	A	668	A2M	N9-C8-N7	-4.44	107.64	113.94
9	A	1031	A2M	N9-C8-N7	-4.43	107.65	113.94
9	A	612	PSU	N1-C2-N3	4.39	119.80	115.17
9	A	1832	6MZ	N9-C8-N7	-4.38	107.72	113.94
9	A	823	PSU	N1-C2-N3	4.38	119.79	115.17
9	A	683	OMG	C2-N3-C4	4.36	119.81	112.30
9	A	1490	OMG	C2-N3-C4	4.35	119.80	112.30
9	A	1243	PSU	N1-C2-N3	4.34	119.74	115.17
9	A	683	OMG	C1'-N9-C4	4.34	139.30	126.49
9	A	509	OMG	C2-N3-C4	4.32	119.74	112.30
9	A	119	PSU	N1-C2-N3	4.32	119.72	115.17
9	A	27	A2M	N9-C8-N7	-4.30	107.83	113.94
9	A	159	A2M	N9-C8-N7	-4.26	107.89	113.94
9	A	484	A2M	N9-C8-N7	-4.22	107.95	113.94
9	A	1850	MA6	N9-C8-N7	-4.16	108.04	113.94
9	A	159	A2M	C4-N9-C1'	4.13	136.28	126.63
9	A	1832	6MZ	C4-N9-C1'	4.07	136.16	126.63
9	A	1850	MA6	C4-C5-C6	4.06	120.11	115.91
9	A	484	A2M	C4-N9-C1'	3.93	135.83	126.63
9	A	121	OMU	N3-C2-N1	3.92	119.99	114.89
9	A	116	OMU	N3-C2-N1	3.90	119.97	114.89
9	A	1850	MA6	C2-N1-C6	3.83	121.18	111.83
9	A	1830	UR3	C5-C4-N3	3.79	120.03	115.04
9	A	1851	MA6	N9-C8-N7	-3.75	108.61	113.94
9	A	1031	A2M	C5-C6-N6	-3.74	114.02	123.29
9	A	1678	A2M	C5-C6-N6	-3.74	114.03	123.29
9	A	166	A2M	C5-C6-N6	-3.71	114.10	123.29
9	A	668	A2M	C1'-N9-C8	-3.66	118.98	127.09
9	A	159	A2M	C5-C6-N6	-3.64	114.28	123.29
9	A	27	A2M	C5-C6-N6	-3.61	114.34	123.29
9	A	1031	A2M	C4-N9-C1'	3.61	135.08	126.63
9	A	121	OMU	C5-C4-N3	3.60	119.84	114.80
9	A	1678	A2M	C4-N9-C1'	3.58	135.01	126.63
9	A	99	A2M	C5-C6-N6	-3.56	114.48	123.29
9	A	1337	4AC	O7-C7-N4	-3.51	116.37	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	644	OMG	C2-N1-C6	-3.49	118.78	125.11
9	A	1832	6MZ	C4-C5-C6	3.48	119.67	116.78
9	A	27	A2M	C4-N9-C1'	3.48	134.77	126.63
9	A	1851	MA6	C2-N3-C4	3.46	120.29	111.83
9	A	166	A2M	C4-N9-C1'	3.45	134.70	126.63
9	A	484	A2M	C5-C6-N6	-3.44	114.77	123.29
9	A	612	PSU	C6-N1-C2	-3.44	119.50	122.69
9	A	601	OMG	C2-N1-C6	-3.43	118.88	125.11
9	A	509	OMG	C2-N1-C6	-3.41	118.93	125.11
9	A	166	A2M	N6-C6-N1	3.38	125.90	118.38
9	A	1081	PSU	C6-C5-C4	3.37	120.45	118.17
9	A	683	OMG	N9-C8-N7	-3.36	107.17	113.40
9	A	1832	6MZ	C2-N3-C4	3.36	120.03	111.83
9	A	99	A2M	N6-C6-N1	3.35	125.84	118.38
9	A	1031	A2M	N6-C6-N1	3.33	125.80	118.38
9	A	644	OMG	N9-C8-N7	-3.32	107.24	113.40
9	A	1678	A2M	N6-C6-N1	3.32	125.77	118.38
9	A	668	A2M	C5-C6-N6	-3.31	115.08	123.29
9	A	1081	PSU	C6-N1-C2	-3.30	119.63	122.69
9	A	1678	A2M	C2-N3-C4	3.30	119.88	111.83
9	A	99	A2M	C4-N9-C1'	3.29	134.33	126.63
9	A	1328	OMG	C2-N1-C6	-3.29	119.15	125.11
9	A	1851	MA6	C2-N1-C6	3.29	119.86	111.83
9	A	612	PSU	O2-C2-N1	-3.28	119.41	122.79
9	A	119	PSU	C6-N1-C2	-3.27	119.65	122.69
9	A	116	OMU	C5-C4-N3	3.27	119.38	114.80
9	A	1031	A2M	C2-N3-C4	3.27	119.81	111.83
9	A	484	A2M	C2-N3-C4	3.26	119.80	111.83
9	A	27	A2M	N6-C6-N1	3.26	125.64	118.38
9	A	1850	MA6	C5-N7-C8	3.26	108.57	103.45
9	A	1851	MA6	C5-C4-N9	3.25	109.36	105.81
9	A	27	A2M	C2-N3-C4	3.25	119.78	111.83
9	A	159	A2M	C2-N3-C4	3.24	119.74	111.83
9	A	1850	MA6	C5-C4-N9	3.20	109.30	105.81
9	A	159	A2M	N6-C6-N1	3.20	125.49	118.38
9	A	99	A2M	C2-N3-C4	3.18	119.60	111.83
9	A	822	PSU	C6-N1-C2	-3.18	119.74	122.69
9	A	1678	A2M	C5-N7-C8	3.17	108.44	103.45
9	A	668	A2M	C2-N3-C4	3.17	119.58	111.83
9	A	166	A2M	C2-N3-C4	3.17	119.57	111.83
9	A	1490	OMG	N9-C8-N7	-3.16	107.54	113.40
9	A	1328	OMG	N9-C8-N7	-3.15	107.56	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1850	MA6	C2-N3-C4	3.14	119.49	111.83
9	A	1243	PSU	C6-N1-C2	-3.14	119.78	122.69
9	A	1337	4AC	C5-C4-N3	-3.10	117.75	122.60
9	A	822	PSU	O2-C2-N1	-3.10	119.59	122.79
9	A	1851	MA6	C5-N7-C8	3.10	108.31	103.45
9	A	1832	6MZ	C5-N7-C8	3.08	108.29	103.45
9	A	823	PSU	C6-N1-C2	-3.07	119.84	122.69
9	A	1374	5MC	C5-C6-N1	-3.06	119.99	123.31
9	A	683	OMG	C2-N1-C6	-3.05	119.59	125.11
9	A	159	A2M	N3-C4-N9	3.04	132.34	127.17
9	A	484	A2M	N6-C6-N1	3.02	125.11	118.38
9	A	1678	A2M	N3-C4-N9	3.01	132.29	127.17
9	A	166	A2M	C5-N7-C8	2.99	108.15	103.45
9	A	1031	A2M	N3-C4-N9	2.99	132.25	127.17
9	A	668	A2M	N6-C6-N1	2.98	125.02	118.38
9	A	99	A2M	C5-N7-C8	2.97	108.11	103.45
9	A	668	A2M	C5-N7-C8	2.96	108.10	103.45
9	A	1031	A2M	C5-N7-C8	2.96	108.10	103.45
9	A	1243	PSU	C6-C5-C4	2.93	120.15	118.17
9	A	159	A2M	C5-N7-C8	2.90	108.02	103.45
9	A	601	OMG	N9-C8-N7	-2.88	108.05	113.40
9	A	27	A2M	C5-N7-C8	2.88	107.98	103.45
9	A	1850	MA6	C4-C5-N7	-2.87	107.30	110.58
9	A	484	A2M	N3-C4-N9	2.87	132.04	127.17
9	A	1337	4AC	C5-C4-N4	2.86	127.77	122.94
9	A	668	A2M	C2'-C1'-N9	2.85	118.45	113.75
9	A	121	OMU	O4-C4-C5	-2.84	120.26	125.16
9	A	116	OMU	O4-C4-C5	-2.83	120.29	125.16
9	A	484	A2M	C5-N7-C8	2.82	107.89	103.45
9	A	509	OMG	N9-C8-N7	-2.80	108.22	113.40
9	A	99	A2M	C2'-C1'-N9	-2.78	109.17	113.75
9	A	27	A2M	N3-C4-N9	2.76	131.86	127.17
9	A	1842	4AC	C5-C4-N3	-2.76	118.28	122.60
9	A	1081	PSU	O2-C2-N1	-2.75	119.95	122.79
9	A	1337	4AC	O7-C7-CM7	-2.74	117.17	122.05
9	A	601	OMG	C5-C6-N1	2.74	120.22	113.25
9	A	644	OMG	C5-C6-N1	2.74	120.22	113.25
9	A	166	A2M	N3-C4-N9	2.72	131.79	127.17
9	A	1490	OMG	C2-N1-C6	-2.69	120.22	125.11
9	A	99	A2M	C4-N9-C8	2.68	108.56	105.74
9	A	1328	OMG	C5-C6-N1	2.68	120.08	113.25
9	A	683	OMG	C5-C6-N1	2.66	120.04	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	99	A2M	N3-C4-N9	2.65	131.67	127.17
9	A	509	OMG	C5-C6-N1	2.64	119.98	113.25
9	A	668	A2M	C4-N9-C1'	2.64	132.81	126.63
9	A	1678	A2M	C4-N9-C8	2.64	108.50	105.74
9	A	644	OMG	C8-N7-C5	2.63	108.95	104.26
9	A	1337	4AC	C6-C5-C4	2.61	120.14	117.00
9	A	601	OMG	O6-C6-C5	-2.60	119.66	126.53
9	A	166	A2M	C2'-C1'-N9	-2.60	109.48	113.75
9	A	166	A2M	C4-N9-C8	2.58	108.44	105.74
9	A	823	PSU	O2-C2-N1	-2.57	120.14	122.79
9	A	683	OMG	O6-C6-C5	-2.57	119.75	126.53
9	A	612	PSU	C6-C5-C4	2.55	119.89	118.17
9	A	1243	PSU	O2-C2-N1	-2.55	120.16	122.79
9	A	509	OMG	O6-C6-C5	-2.54	119.82	126.53
9	A	159	A2M	C2'-C1'-N9	-2.54	109.57	113.75
9	A	1374	5MC	CM5-C5-C6	-2.54	119.42	122.85
9	A	1328	OMG	O6-C6-C5	-2.53	119.85	126.53
9	A	644	OMG	O6-C6-C5	-2.52	119.87	126.53
9	A	1490	OMG	C5-C6-N1	2.50	119.62	113.25
9	A	1851	MA6	N3-C4-N9	2.50	131.41	127.17
9	A	668	A2M	N3-C4-N9	2.49	131.40	127.17
9	A	1832	6MZ	N3-C4-N9	2.47	131.38	127.17
9	A	1328	OMG	C8-N7-C5	2.46	108.64	104.26
9	A	484	A2M	C4-N9-C8	2.45	108.31	105.74
9	A	159	A2M	C4-N9-C8	2.45	108.31	105.74
9	A	1842	4AC	C6-C5-C4	2.45	119.95	117.00
9	A	814	5MU	C6-N1-C2	-2.44	118.87	121.30
9	A	683	OMG	C8-N7-C5	2.43	108.60	104.26
9	A	509	OMG	N9-C4-N3	2.43	130.82	125.95
9	A	119	PSU	O2-C2-N1	-2.42	120.29	122.79
9	A	601	OMG	C8-N7-C5	2.41	108.55	104.26
9	A	1219	JMH	C6-N1-C2	-2.41	119.83	121.80
9	A	484	A2M	C3'-C2'-C1'	2.40	107.40	102.81
9	A	1031	A2M	C4-N9-C8	2.39	108.24	105.74
9	A	1490	OMG	C8-N7-C5	2.38	108.50	104.26
9	A	612	PSU	O4'-C1'-C2'	2.37	108.43	105.15
9	A	1490	OMG	O6-C6-C5	-2.37	120.29	126.53
9	A	1842	4AC	N4-C4-N3	2.35	117.68	113.87
9	A	668	A2M	C4-C5-N7	-2.35	107.90	110.58
9	A	27	A2M	C4-N9-C8	2.34	108.19	105.74
9	A	823	PSU	C6-C5-C4	2.31	119.74	118.17
9	A	644	OMG	C4-C5-N7	-2.30	107.03	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	668	A2M	C4-N9-C8	2.29	108.14	105.74
9	A	484	A2M	C4-C5-N7	-2.29	107.96	110.58
9	A	1832	6MZ	C5-C4-N9	2.29	108.31	105.81
9	A	159	A2M	C4-C5-N7	-2.29	107.97	110.58
9	A	1832	6MZ	C4-C5-N7	-2.28	107.97	110.58
9	A	822	PSU	C6-C5-C4	2.28	119.71	118.17
9	A	601	OMG	C5-C4-N9	2.27	109.72	105.66
9	A	509	OMG	C8-N7-C5	2.26	108.29	104.26
9	A	1830	UR3	C1'-N1-C2	2.24	120.71	117.04
9	A	1678	A2M	C4-C5-N7	-2.24	108.03	110.58
9	A	644	OMG	C5-C4-N9	2.23	109.65	105.66
9	A	1851	MA6	C4-C5-N7	-2.23	108.03	110.58
9	A	644	OMG	N2-C2-N1	2.21	121.42	116.76
9	A	1328	OMG	N2-C2-N1	2.21	121.42	116.76
9	A	822	PSU	O4'-C1'-C2'	2.19	108.18	105.15
9	A	27	A2M	C4-C5-N7	-2.18	108.09	110.58
9	A	99	A2M	C4-C5-N7	-2.17	108.10	110.58
9	A	668	A2M	C5-C4-N9	2.17	108.18	105.81
9	A	1031	A2M	C4-C5-N7	-2.17	108.10	110.58
9	A	1031	A2M	C6-C5-C4	2.16	120.13	117.18
9	A	601	OMG	N9-C4-N3	2.16	130.27	125.95
9	A	166	A2M	C4'-O4'-C1'	-2.15	104.71	109.47
9	A	166	A2M	C5'-C4'-C3'	-2.15	107.48	115.21
9	A	601	OMG	N2-C2-N1	2.15	121.29	116.76
9	A	166	A2M	C4-C5-N7	-2.14	108.13	110.58
9	A	1328	OMG	N9-C4-N3	2.14	130.23	125.95
9	A	601	OMG	C4-C5-N7	-2.14	107.28	110.67
9	A	1328	OMG	C4-C5-N7	-2.13	107.29	110.67
9	A	159	A2M	C6-C5-C4	2.12	120.07	117.18
9	A	166	A2M	O4'-C1'-N9	2.12	112.16	108.09
9	A	1842	4AC	O7-C7-CM7	-2.11	118.30	122.05
9	A	99	A2M	O4'-C1'-N9	2.11	112.14	108.09
9	A	121	OMU	O2-C2-N1	-2.11	120.06	122.80
9	A	1328	OMG	C5-C4-N9	2.10	109.41	105.66
9	A	644	OMG	N9-C4-N3	2.08	130.11	125.95
9	A	116	OMU	C6-N1-C2	-2.06	118.49	121.00
9	A	683	OMG	C4-C5-N7	-2.03	107.46	110.67
9	A	1219	JMH	C5-C4-N3	2.02	119.75	116.07
9	A	1490	OMG	N9-C4-N3	2.01	129.98	125.95

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	166	A2M	O4'-C4'-C5'-O5'
9	A	683	OMG	O4'-C4'-C5'-O5'
9	A	823	PSU	O4'-C1'-C5-C4
9	A	823	PSU	O4'-C1'-C5-C6
9	A	1219	JMH	O4'-C4'-C5'-O5'
9	A	1832	6MZ	N1-C6-N6-C9
9	A	1851	MA6	C5-C6-N6-C10
9	A	159	A2M	O4'-C4'-C5'-O5'
9	A	159	A2M	C3'-C4'-C5'-O5'
9	A	166	A2M	C3'-C4'-C5'-O5'
9	A	99	A2M	O4'-C4'-C5'-O5'
9	A	822	PSU	O4'-C4'-C5'-O5'
9	A	1219	JMH	C3'-C4'-C5'-O5'
9	A	1851	MA6	N1-C6-N6-C10
9	A	822	PSU	C3'-C4'-C5'-O5'
9	A	668	A2M	C3'-C4'-C5'-O5'
9	A	683	OMG	C3'-C4'-C5'-O5'
9	A	174	OMC	C3'-C4'-C5'-O5'
9	A	174	OMC	O4'-C4'-C5'-O5'
9	A	668	A2M	O4'-C4'-C5'-O5'
9	A	1851	MA6	C5-C6-N6-C9
9	A	1337	4AC	O7-C7-N4-C4
9	A	1337	4AC	CM7-C7-N4-C4
9	A	1832	6MZ	C5-C6-N6-C9
9	A	644	OMG	C4'-C5'-O5'-P
9	A	1851	MA6	C4'-C5'-O5'-P
9	A	1703	OMC	O4'-C4'-C5'-O5'
9	A	174	OMC	C4'-C5'-O5'-P
9	A	1081	PSU	C4'-C5'-O5'-P
9	A	1490	OMG	C4'-C5'-O5'-P
9	A	99	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1851	MA6	2	0
9	A	1374	5MC	1	0
9	A	1850	MA6	3	0
9	A	1678	A2M	1	0
9	A	823	PSU	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 112 ligands modelled in this entry, 110 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
53	SPD	A	2005	-	9,9,9	0.33	0	8,8,8	0.52	0
55	ACY	1	501	-	2,2,3	0.67	0	1,1,3	0.14	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
53	SPD	A	2005	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

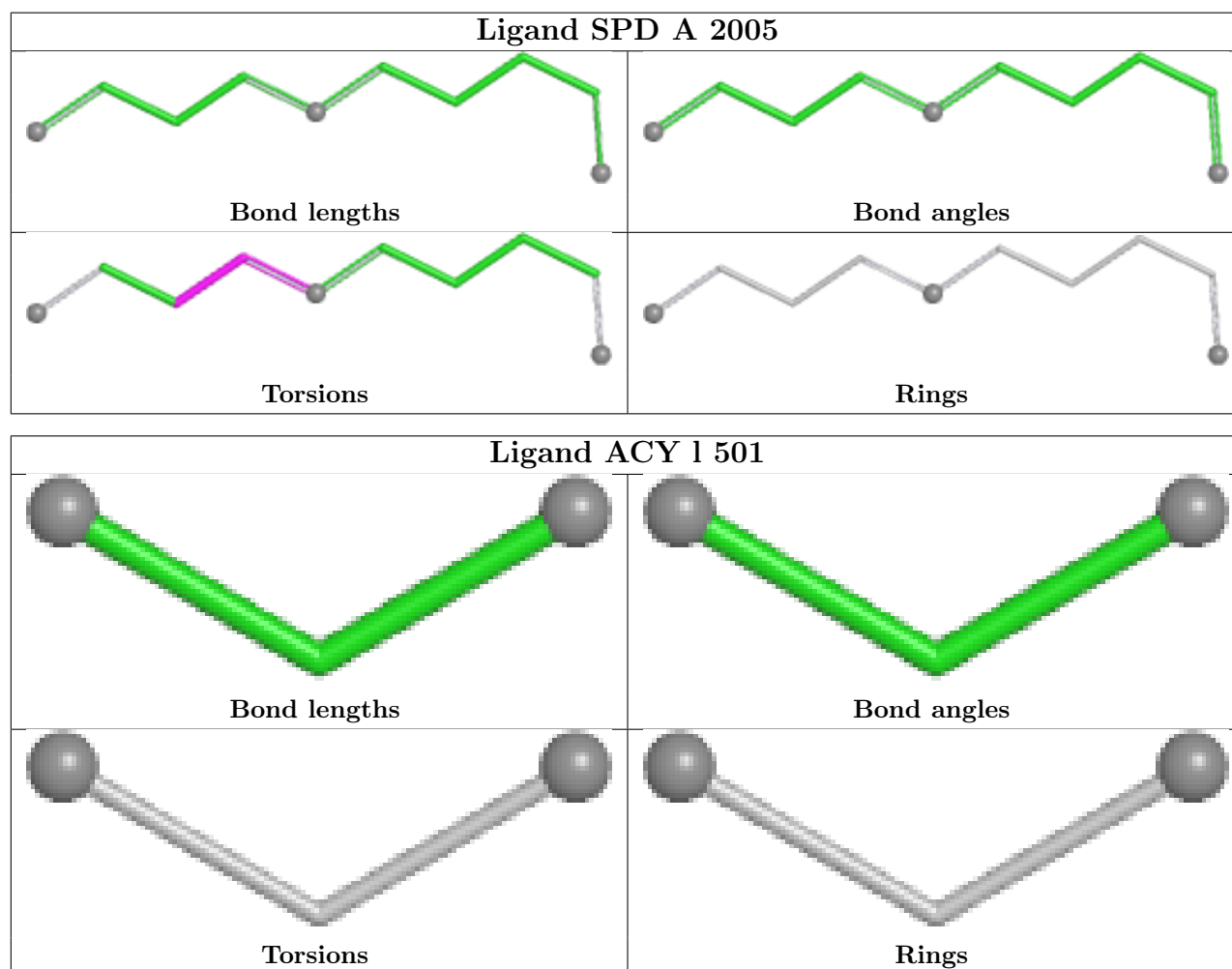
Mol	Chain	Res	Type	Atoms
53	A	2005	SPD	N6-C7-C8-C9
53	A	2005	SPD	C8-C7-N6-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	A	2005	SPD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	A	2
46	p	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	225:G	O3'	287:U	P	8.10
1	A	1219:JMH	O3'	1220:A	P	3.00
1	p	185:ALA	C	186:GLU	N	2.09
1	p	195:GLU	C	196:MSE	N	1.86

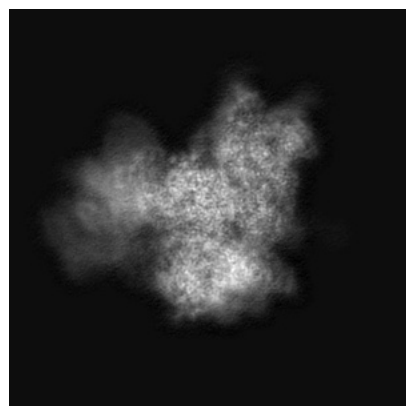
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44671. These allow visual inspection of the internal detail of the map and identification of artifacts.

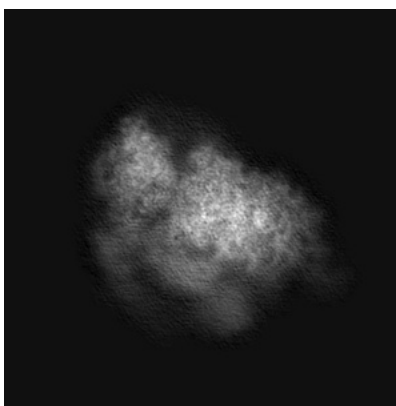
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

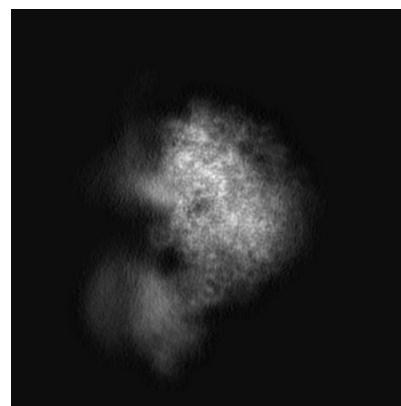
6.1.1 Primary map



X

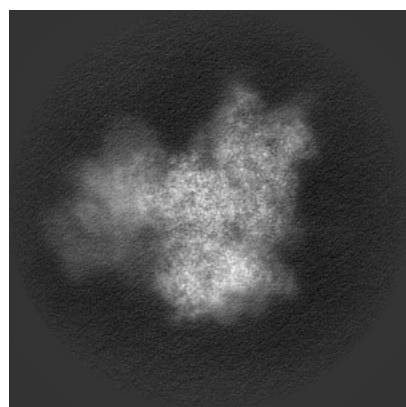


Y

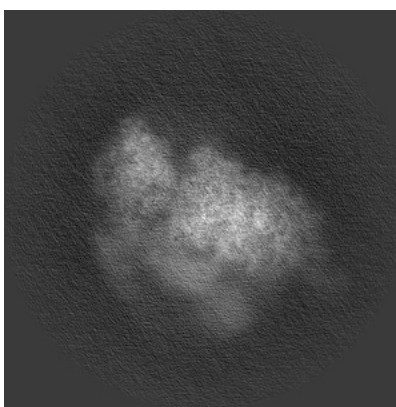


Z

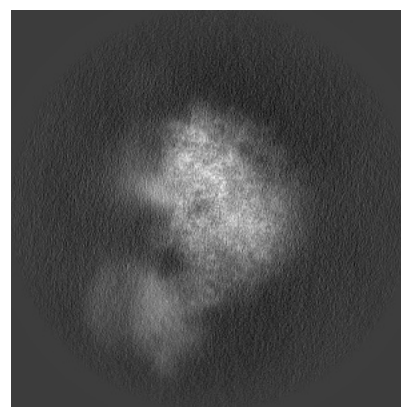
6.1.2 Raw map



X



Y

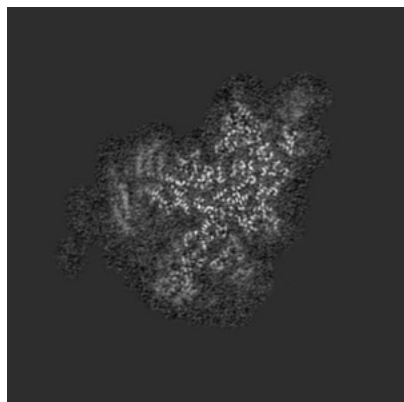


Z

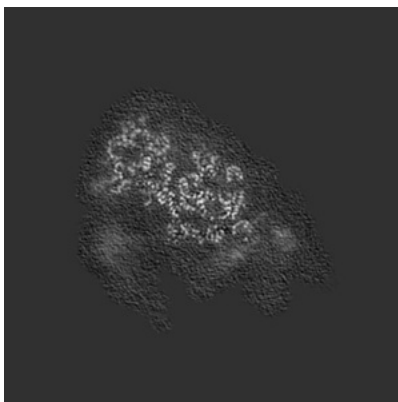
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

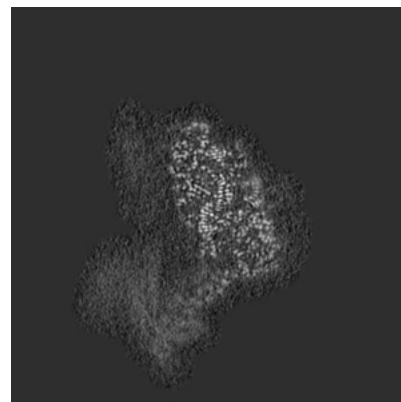
6.2.1 Primary map



X Index: 200

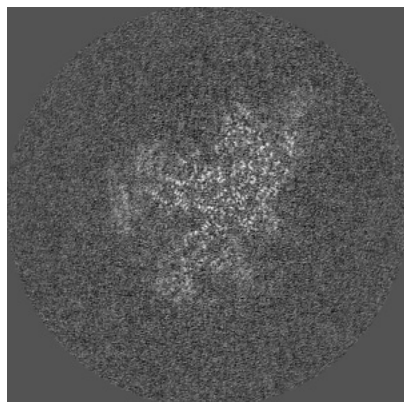


Y Index: 200

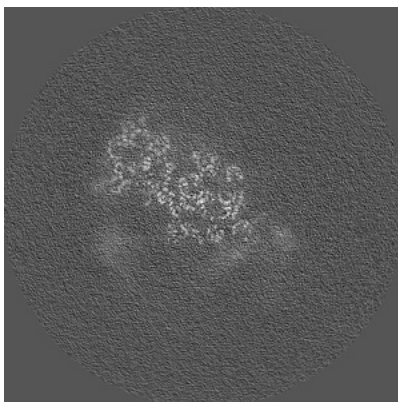


Z Index: 200

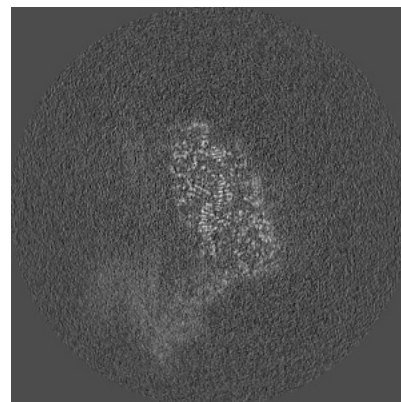
6.2.2 Raw map



X Index: 200



Y Index: 200

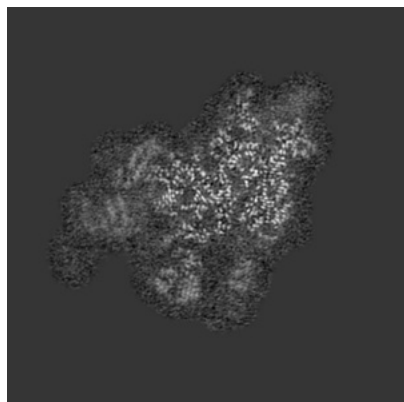


Z Index: 200

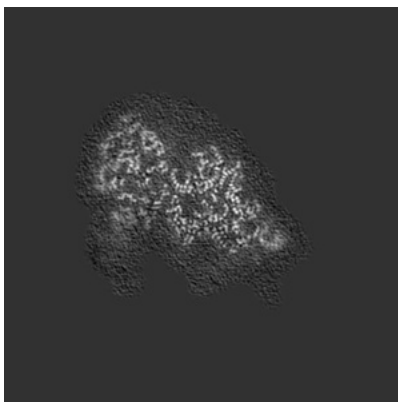
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

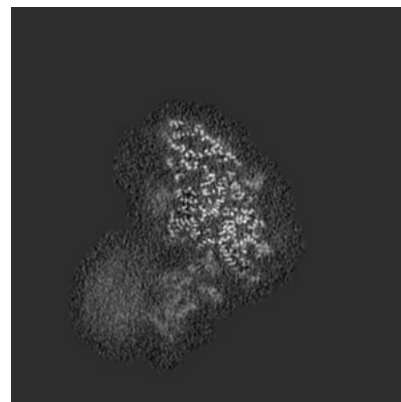
6.3.1 Primary map



X Index: 190

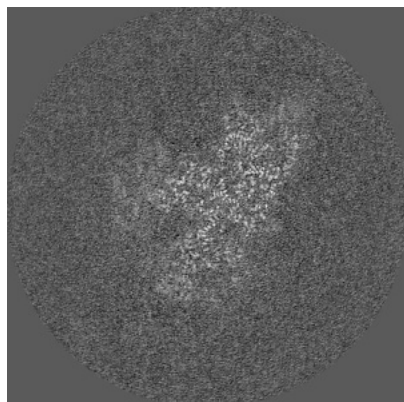


Y Index: 189

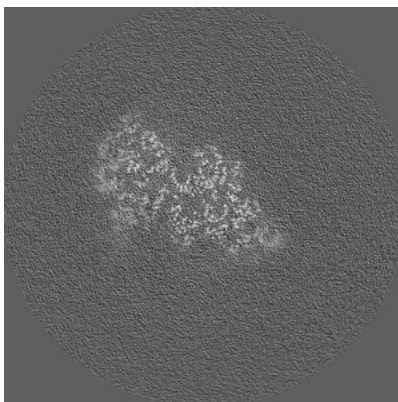


Z Index: 219

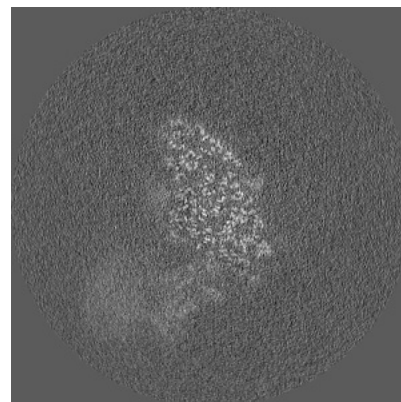
6.3.2 Raw map



X Index: 203



Y Index: 188

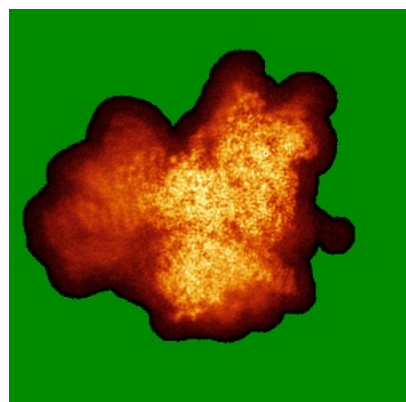


Z Index: 218

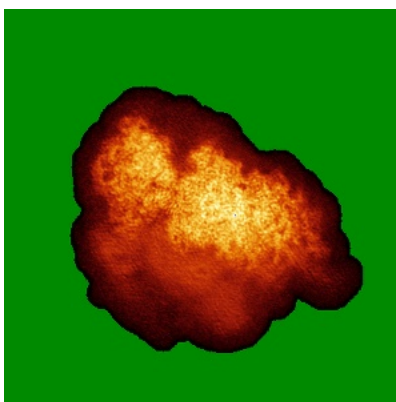
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

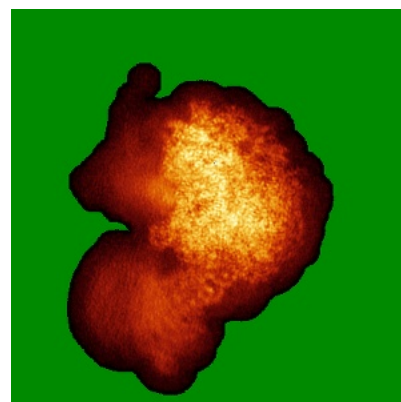
6.4.1 Primary map



X

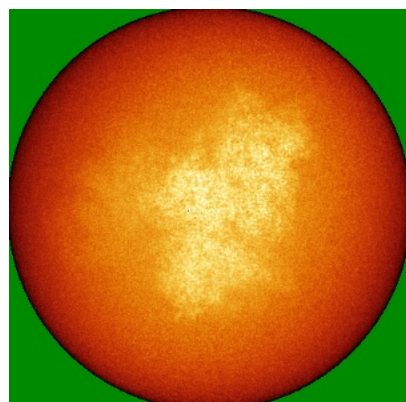


Y

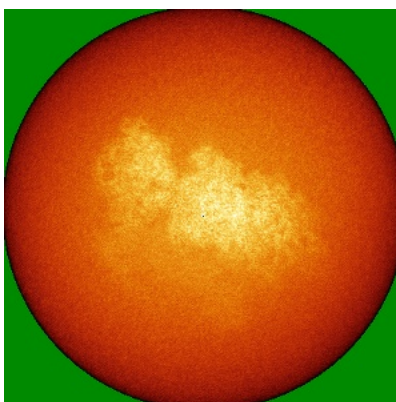


Z

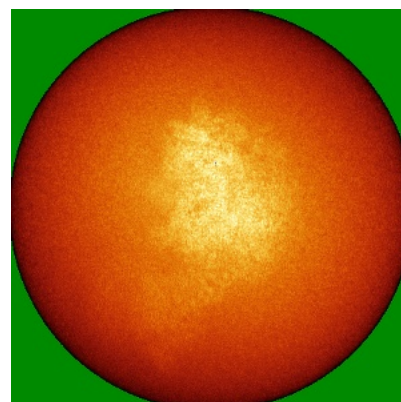
6.4.2 Raw map



X



Y

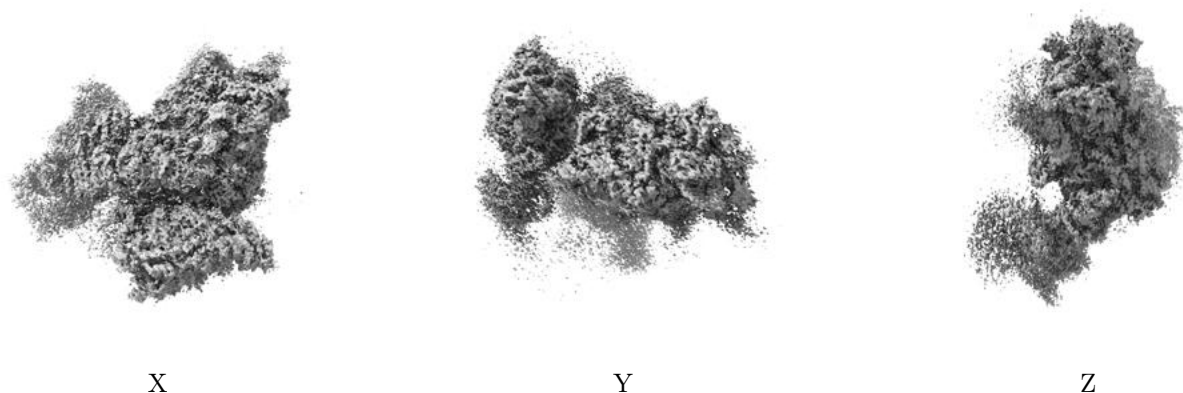


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

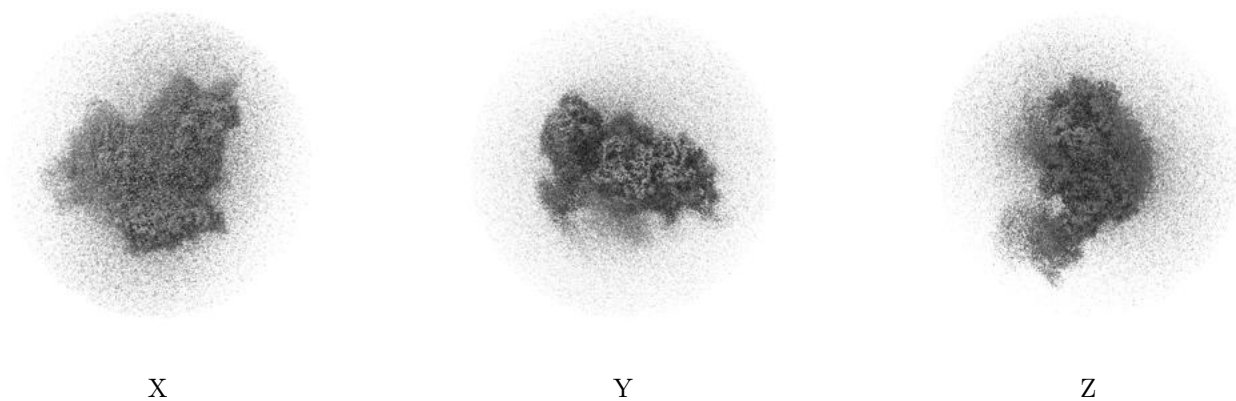
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

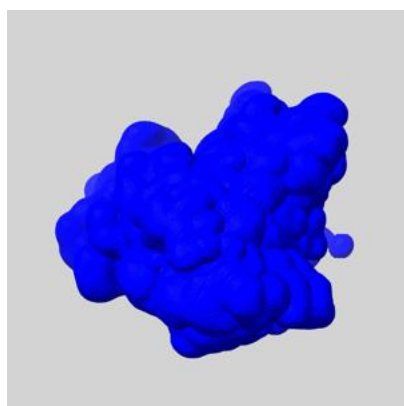
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

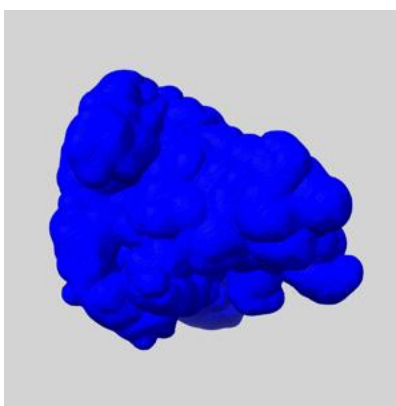
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

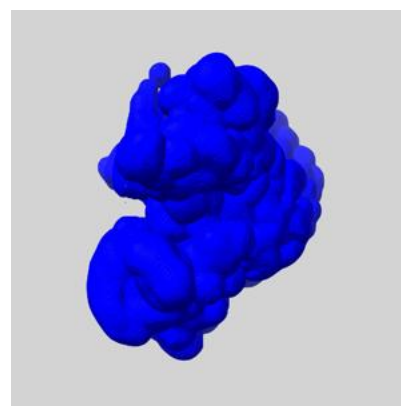
6.6.1 emd_44671_msk_1.map [i](#)



X



Y

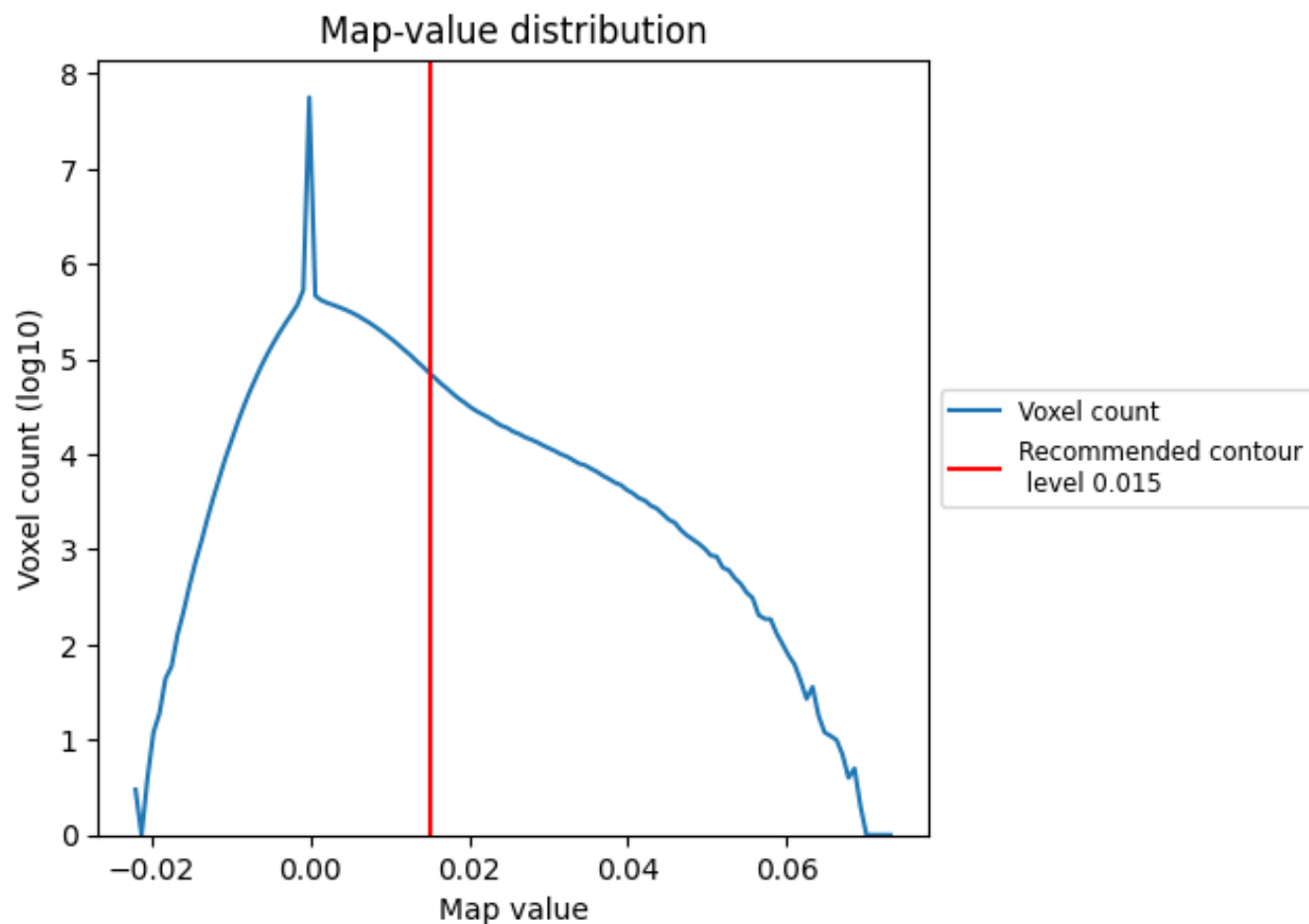


Z

7 Map analysis [i](#)

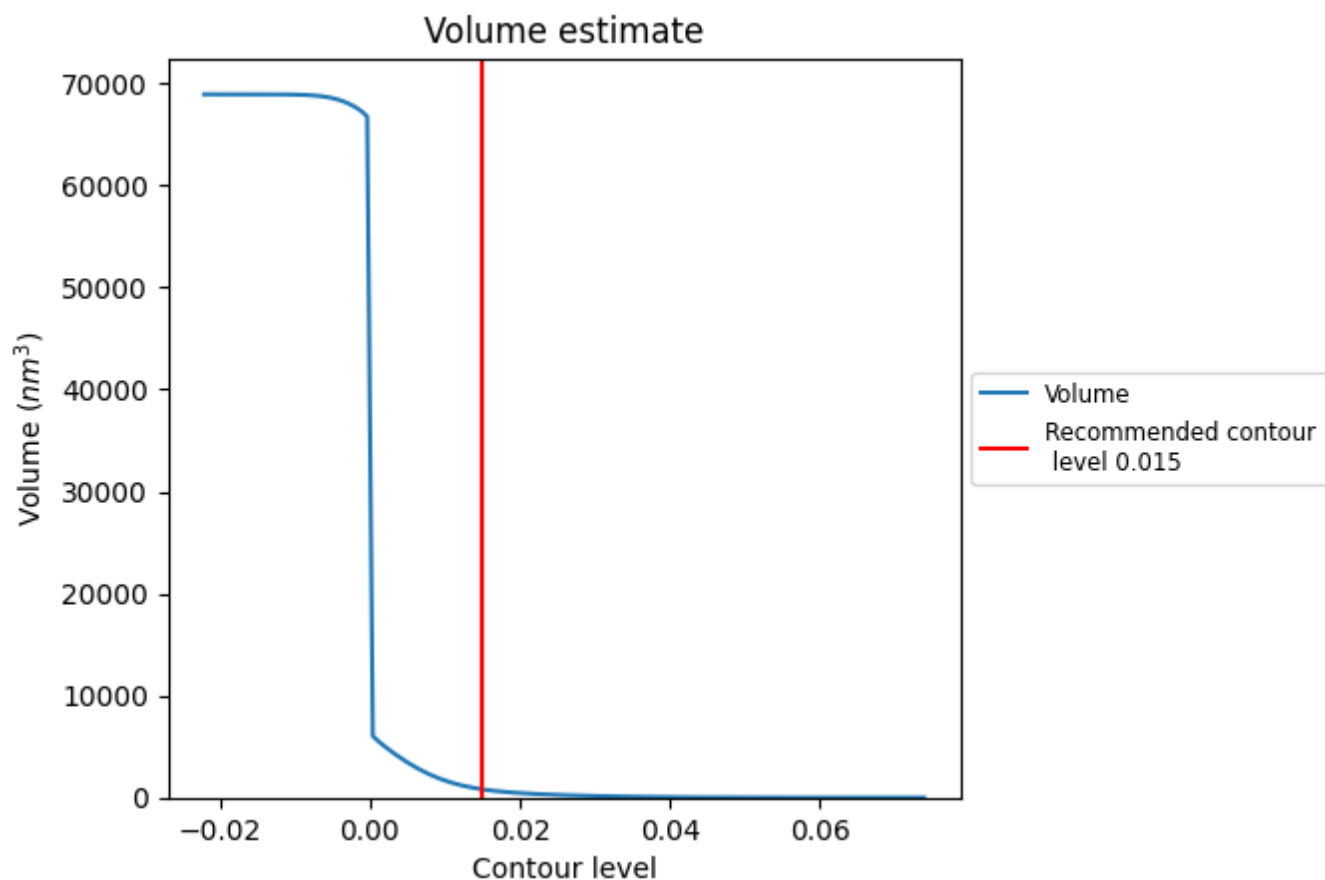
This section contains the results of statistical analysis of the map.

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.

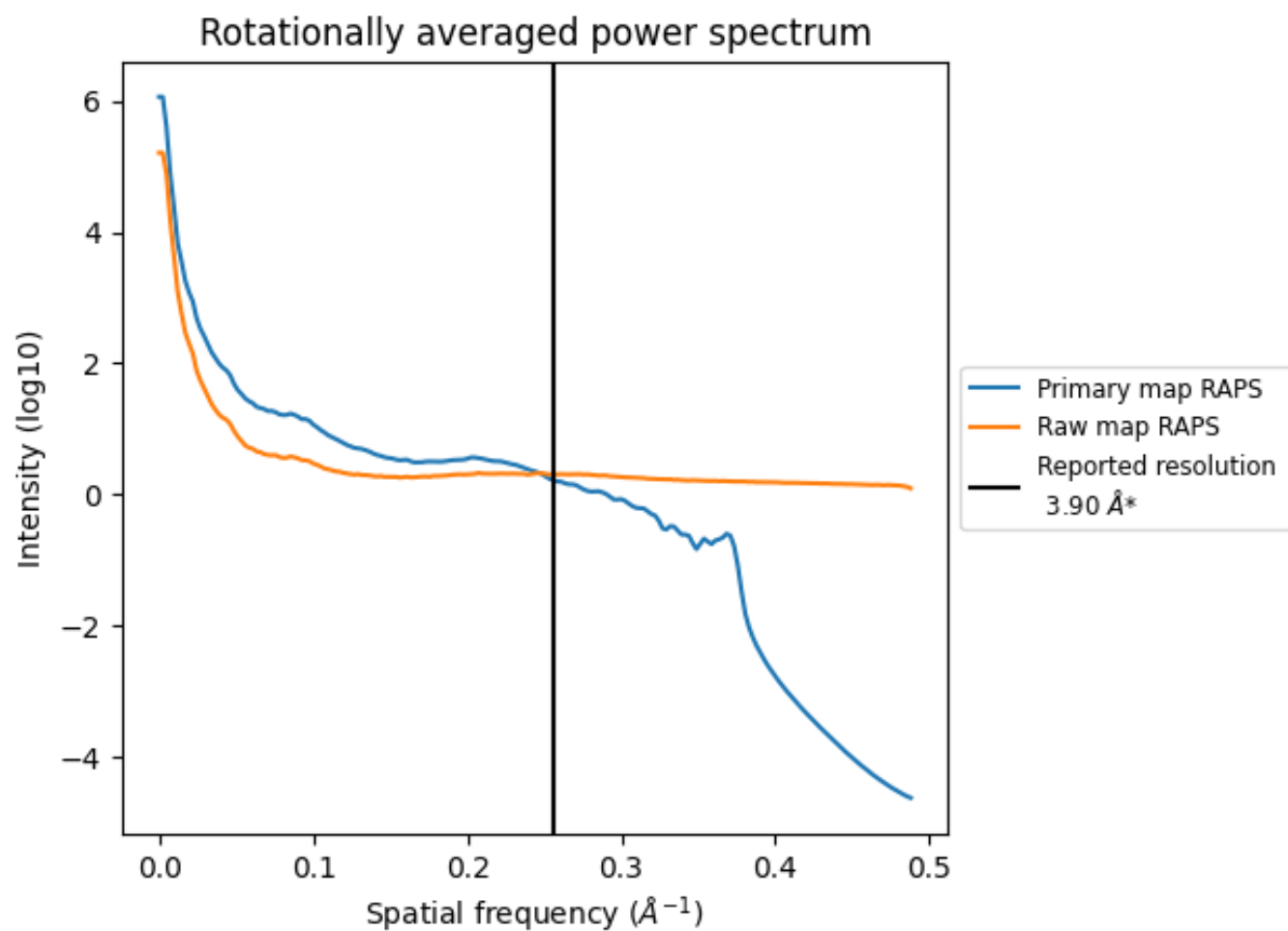
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 809 nm³; this corresponds to an approximate mass of 730 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 ⓘ

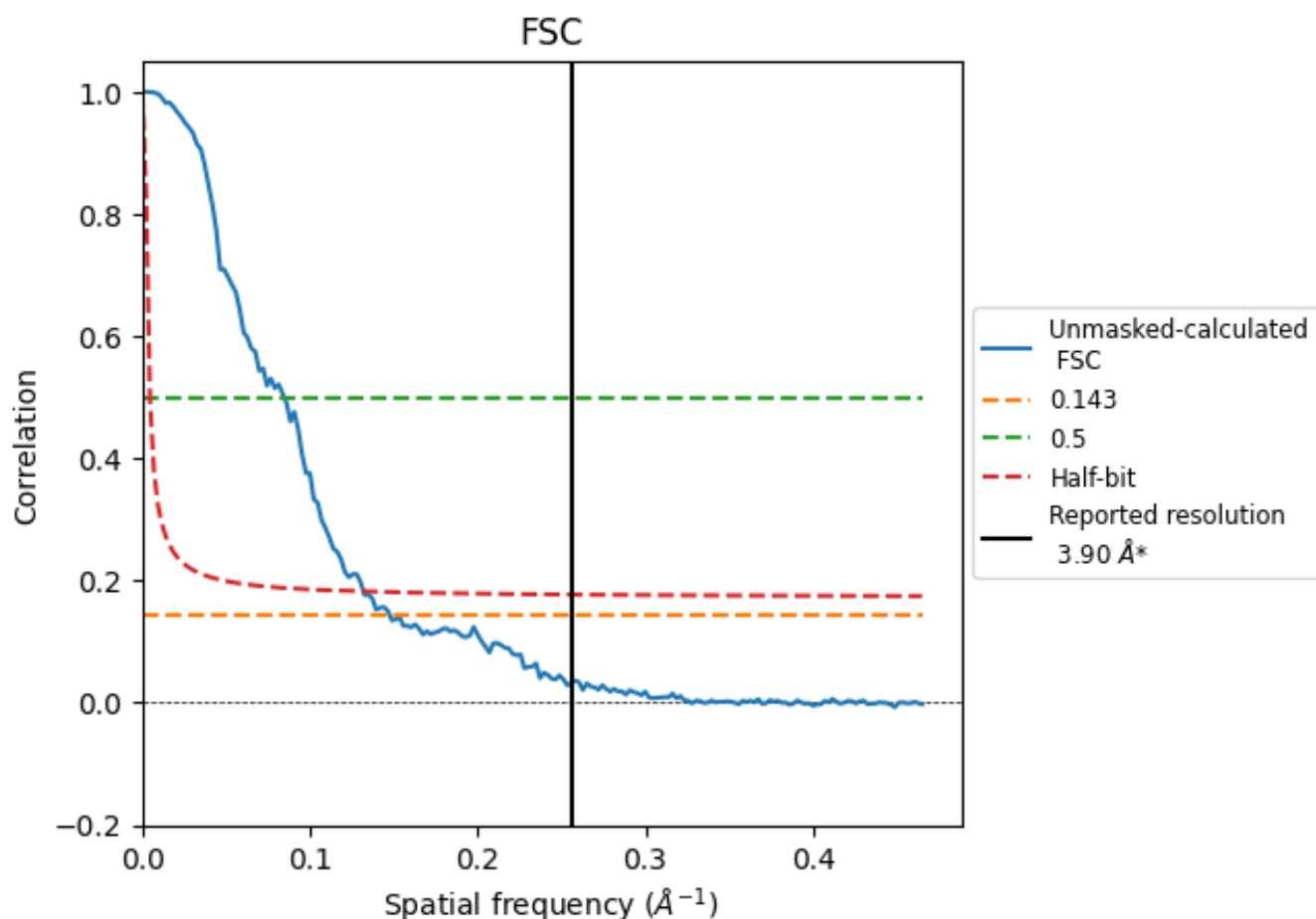


*Reported resolution corresponds to spatial frequency of 0.256 $\text{\AA}^{-1}$

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 0.256 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

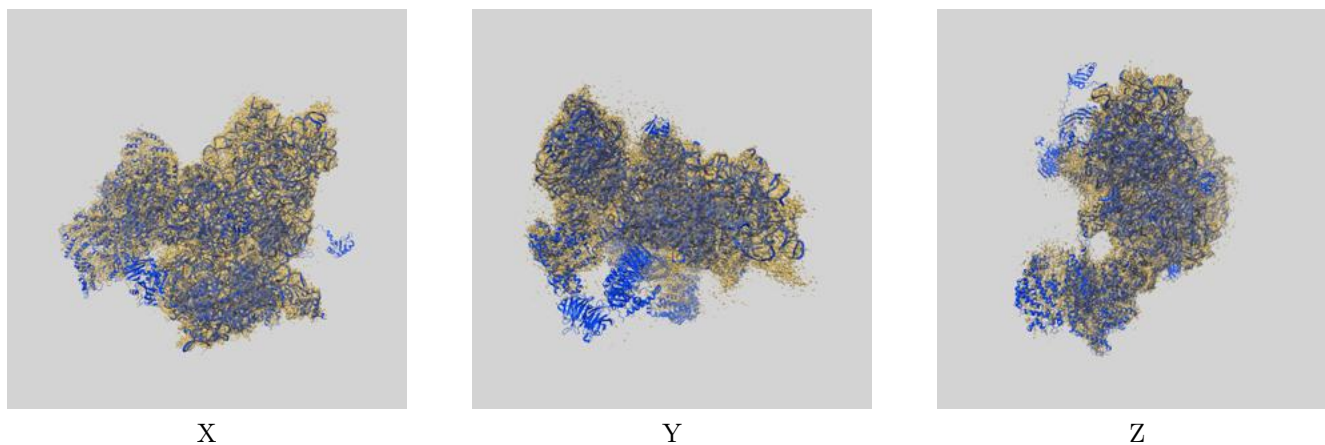
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.78	11.82	7.58

*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 6.78 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

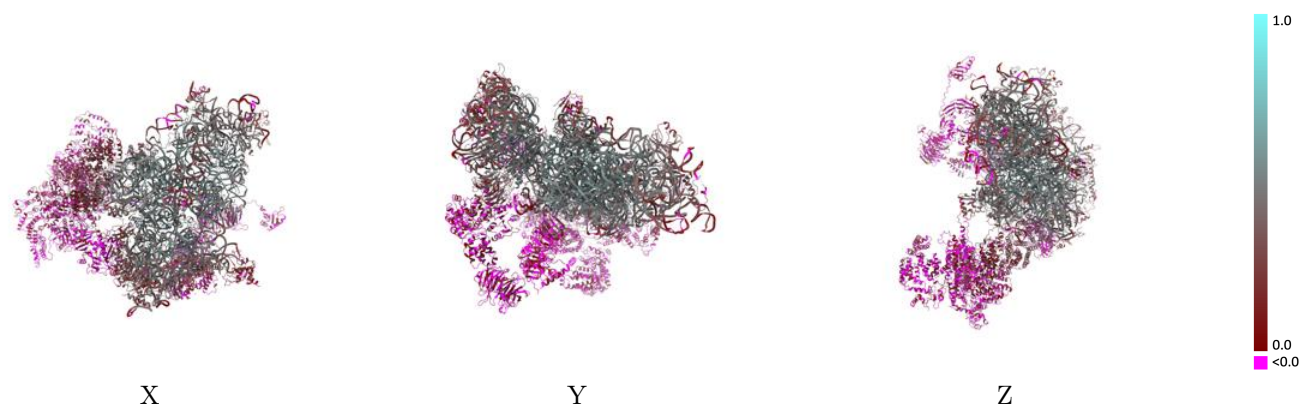
This section contains information regarding the fit between EMDB map EMD-44671 and PDB model 9BLN. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



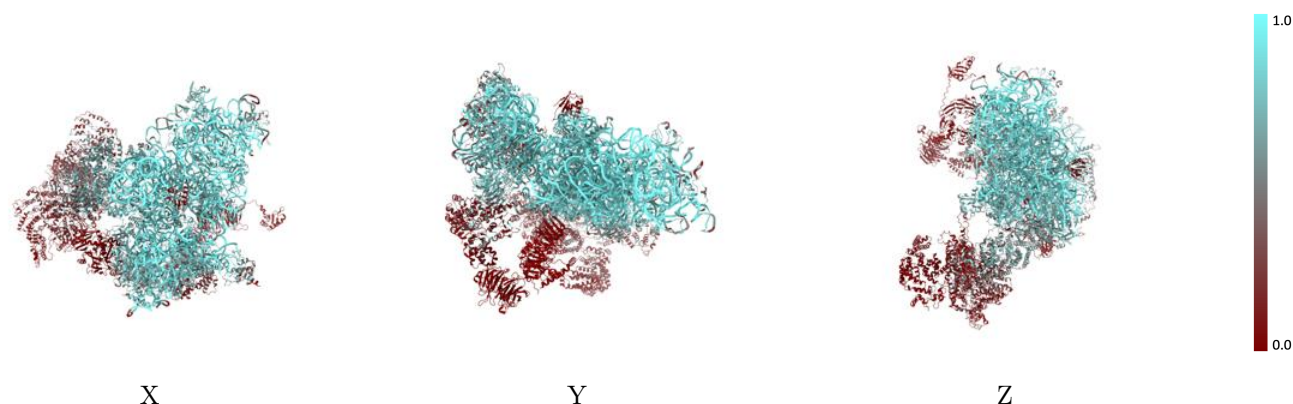
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



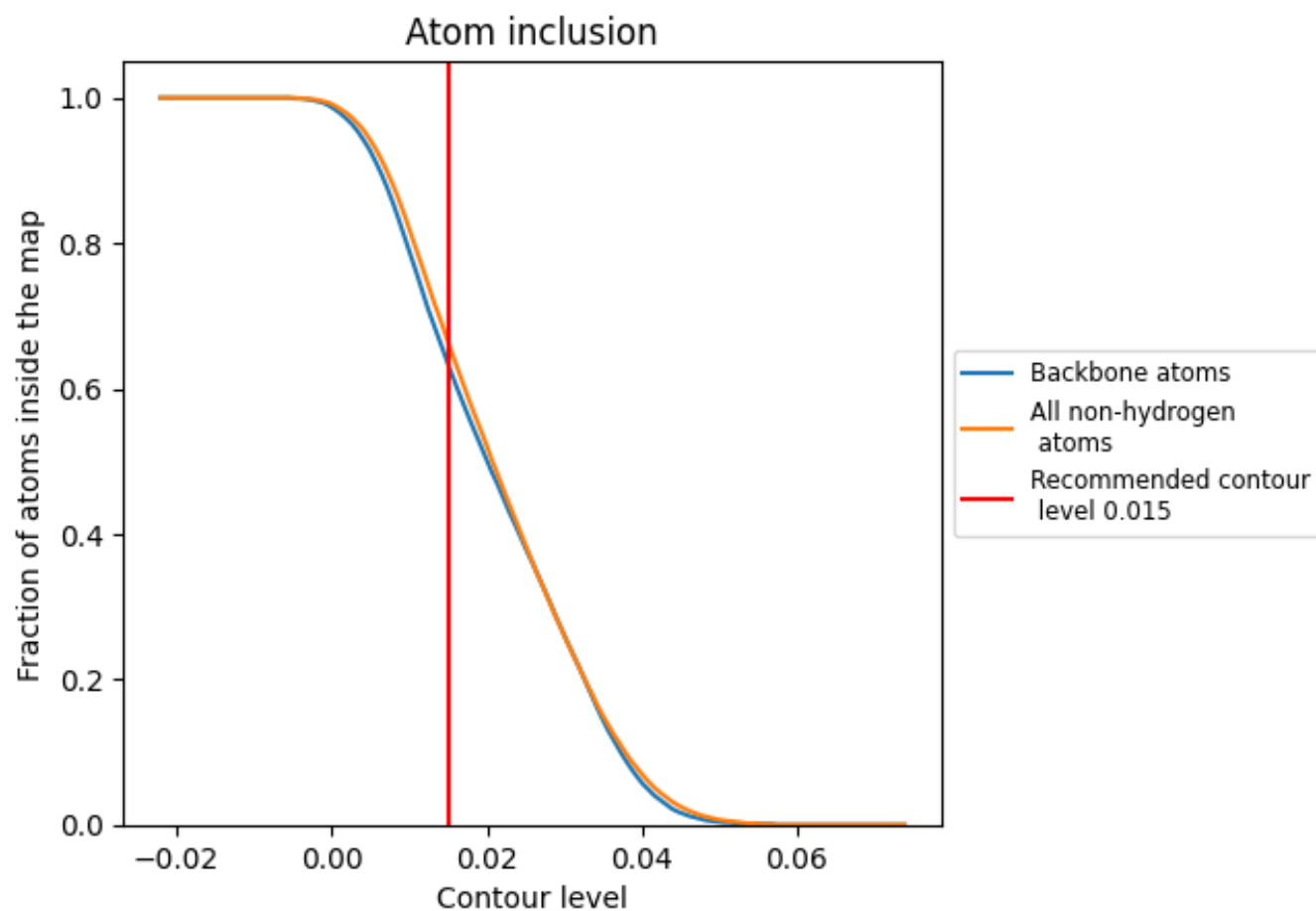
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 66% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.3280
3	 0.0170	 0.0040
4	 0.1080	 0.0320
5	 0.0510	 0.0200
6	 0.0770	 0.0210
8	 0.1150	 0.0260
9	 0.7890	 0.4180
A	 0.9350	 0.4560
B	 0.8560	 0.4670
C	 0.8700	 0.4920
D	 0.8550	 0.4980
E	 0.8740	 0.4990
F	 0.7800	 0.4310
G	 0.6990	 0.3600
H	 0.7880	 0.4350
I	 0.8200	 0.4460
J	 0.8770	 0.5070
K	 0.8560	 0.4770
L	 0.8500	 0.4980
M	 0.7580	 0.4070
N	 0.8510	 0.4890
O	 0.7610	 0.4050
P	 0.7870	 0.4320
Q	 0.8620	 0.4760
R	 0.7950	 0.3880
S	 0.7460	 0.3510
T	 0.8400	 0.4630
U	 0.0170	 0.0290
V	 0.7400	 0.3540
W	 0.1070	 0.1470
X	 0.0020	 -0.0050
Y	 0.8060	 0.4210
Z	 0.7900	 0.4320
a	 0.7720	 0.3970
b	 0.6680	 0.3400



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.6590	 0.2950
d	 0.7930	 0.3910
e	 0.5540	 0.2740
f	 0.6440	 0.3040
h	 0.7310	 0.3730
i	 0.8870	 0.4900
k	 0.5380	 0.2230
l	 0.1420	 0.0080
m	 0.4130	 0.1710
n	 0.6380	 0.3120
o	 0.7290	 0.2790
p	 0.3250	 0.1470
u	 0.3650	 0.1420
v	 0.1870	 0.0450
x	 0.0710	 0.0040
y	 0.4950	 0.1860